Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Mechanistic Study on the Formation of the Alkyl Acrylates from CO_2, Ethylene and Alkyl Iodides over Nickel-based Catalyst

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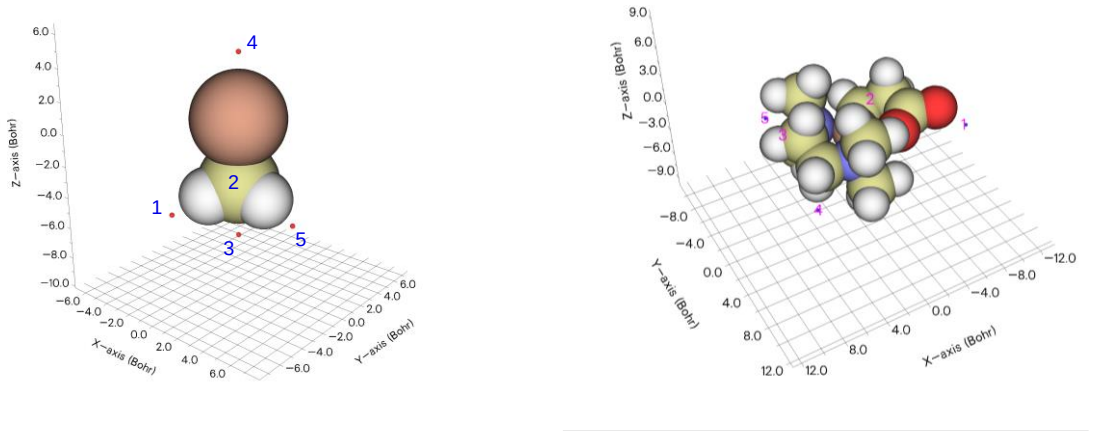

Fig. S1 Molecular electrostatic potential on the 0.001 a.u. electron density isosurface for the isolated monomers. Maxima and minima critical point are shown in blue and pink dots.

Table S1. Maxima value of the molecular electrostatic potential (in a.u.) on the 0.001 a.u. electron density isosurface for the electrophile CH_3I.

	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
1	0.0296	0.805	18.568	-1.143110	-1.973406	-2.678815
2	0.0296	0.805	18.568	-1.123386	1.940165	-2.767811
3	0.0210	0.571	13.168	0.055031	-0.065939	-3.704153
4	0.0255	0.695	16.021	0.061755	-0.063511	2.524135
5	0.0300	0.805	18.574	2.250611	-0.028197	-2.748466

Table S2. Minima value of the molecular electrostatic potential (in a.u.) on the 0.001 a.u. electron density isosurface for the nickelacycle.

	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
1	-0.119	-3.226	-74.397	-4.623217	2.234365	0.088548
2	-0.025	-0.693	-15.992	-2.667759	-3.022518	-1.235356
3	0.0336	0.915	21.090	1.981217	-3.577681	-2.020507
4	0.040	1.088	25.099	3.346576	2.713042	-1.076352
5	0.0449	1.222	28.190	4.000950	-0.741090	1.871607

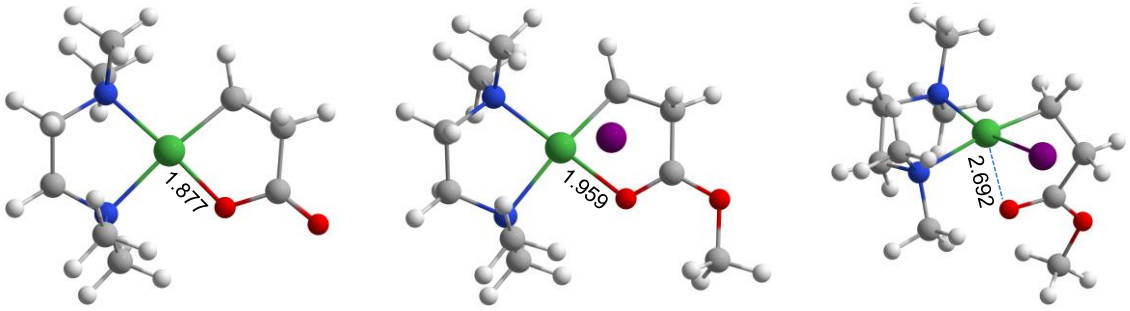

Fig. S2 Structures of intermediates for the interaction of the nickellacycle with CH_3I and its cleavage using the TMEDA ligand. Bond lengths are in Å.

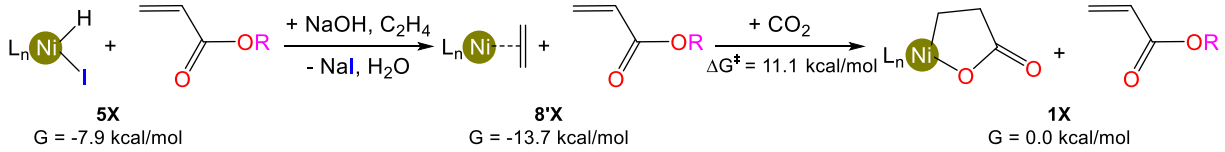

Fig. S3 Regenerate the catalyst from **5X**.

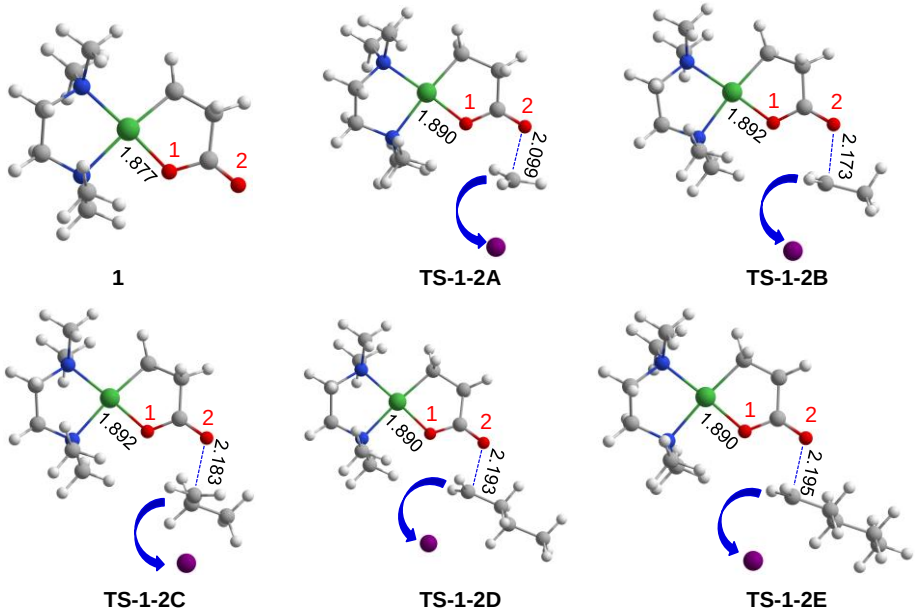

Fig. S4 Geometrical features of **1** and the transition state **TS-1-2A**. Bond distances are in Å.

Table S3. NPA charges of **1A** and the transition state **TS-1-2'X**.

			NPA charge	
	Ni	O1	O2	$CH_3(CH_2)_nI$
1A	0.655	-0.735	-0.651	—
TS-1-2'A	0.695	-0.690	-0.619	-0.216
TS-1-2'B	0.709	-0.706	-0.618	-0.196
TS-1-2'C	0.697	-0.704	-0.627	-0.189
TS-1-2'D	0.696	-0.704	-0.628	-0.188
TS-1-2'E	0.714	-0.707	-0.619	-0.180

Table S4. The HOMO and LUMO compositions of intermediate **2G**.

Atom	Ni	I	C_α	Others
HOMO composition (%)	0.5	98.1	0.0	1.4
HOMO composition (%)	58.8	0.4	20.3	20.5

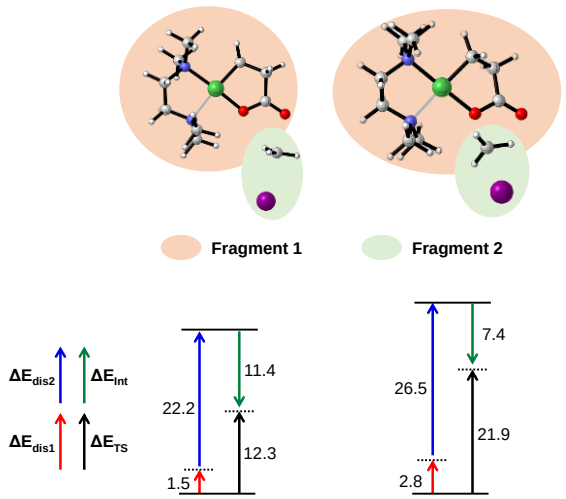

Fig. S5 Distortion/interaction analysis of competitive methylation of nickelalactone with MeI.

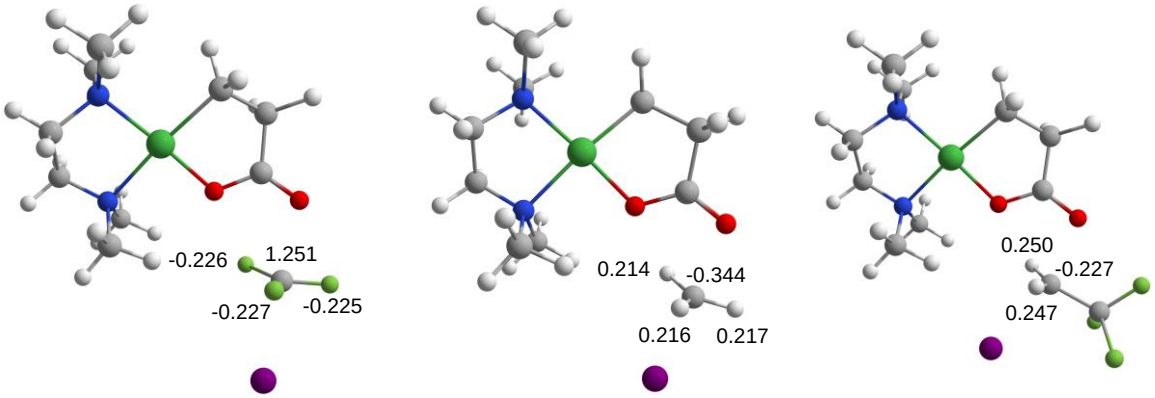

Fig. S6 NPA charges of the transition state **TS-1-2X**.

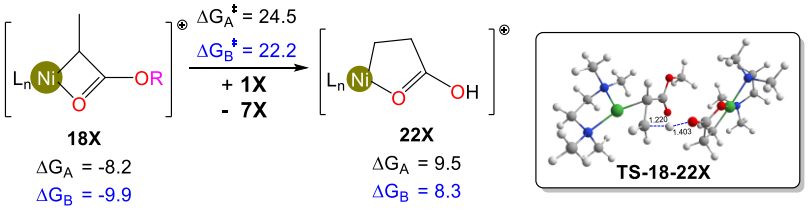

Fig. S7 Formation of intermediate **22X** originated from four-membered nickellacycle **18X**. The A and B denote an electrophilic reagent using CH_3I and C_2H_5I, respectively.

List of Cartesian coordinates

1A
Geometry with 34 atoms:
Thermal correction to Gibbs Free Energy: 0.254553
Total energy: -2123.436211

C	-2.892058	0.069600	0.031799
C	2.292599	1.275442	-0.197137
H	2.965770	2.062243	0.191166
H	2.466796	1.206300	-1.280070
C	2.598017	-0.054294	0.466358
H	2.503115	0.038974	1.556872
H	3.634425	-0.371995	0.252706
Ni	-0.160811	-0.197630	-0.060052
O	-4.007105	0.571647	-0.035107
O	-1.779510	0.751471	-0.079133
C	1.695355	-2.227207	0.983660
H	1.064820	-3.051538	0.634068
H	2.733313	-2.593315	1.084696
H	1.330631	-1.895608	1.965364
C	1.952005	-1.590071	-1.331406
H	2.958612	-2.046836	-1.360549
H	1.206683	-2.338187	-1.628898
H	1.914205	-0.762185	-2.050767
C	0.381729	2.538662	-1.028445
H	-0.694154	2.690658	-0.881890
H	0.911132	3.509810	-0.992085
H	0.533976	2.085068	-2.018404
C	0.612984	2.182475	1.346998
H	1.114195	3.160659	1.479371
H	-0.471338	2.303653	1.467958
H	0.967558	1.494841	2.126691
C	-1.263734	-1.779243	-0.281071
H	-0.874891	-2.714054	0.157501
H	-1.343375	-1.945401	-1.375896
C	-2.634766	-1.411395	0.290617
H	-3.486089	-2.010765	-0.081615
H	-2.631368	-1.528378	1.390808
N	1.633124	-1.103696	0.027143
N	0.872422	1.622402	0.011445

2A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.287183
Total energy: -2461.241960

C	-1.028976	2.082994	-0.800098
C	2.938696	-0.503222	1.545851
H	3.160727	-0.925520	2.542387
H	3.813039	0.088877	1.241091
C	2.679575	-1.611297	0.545596
H	1.839278	-2.233947	0.880763
H	3.560842	-2.267833	0.442498
Ni	1.101418	0.481095	-0.381069
O	-2.043420	2.886888	-0.624159
O	-0.204785	1.857572	0.105220
C	1.640257	-2.108083	-1.574389
H	1.451234	-1.756381	-2.593833
H	2.285470	-3.003244	-1.620767
H	0.681331	-2.366481	-1.105639
C	3.490939	-0.543696	-1.511665
H	4.206032	-1.364677	-1.699869
H	3.173245	-0.114811	-2.469935
H	3.990900	0.240976	-0.929643
C	2.148584	1.749591	2.041976
H	1.264750	2.399433	2.021633
H	2.560648	1.728379	3.068034
H	2.904198	2.166966	1.360890
C	0.681395	-0.132329	2.432238
H	0.993608	-0.192946	3.491633
H	-0.193999	0.523100	2.344034
H	0.381071	-1.127708	2.082627
C	-2.238999	3.456475	0.687751
H	-2.394139	2.654788	1.424195
H	-3.134930	4.083398	0.609794
H	-1.368503	4.064172	0.974507
I	-2.441736	-1.544830	0.251856
C	0.552528	0.876205	-2.207874
H	0.621846	0.057588	-2.938804
H	1.228469	1.686301	-2.549426
C	-0.886236	1.398353	-2.116298
H	-1.226482	2.059377	-2.932812
H	-1.601807	0.556717	-2.068653
N	2.302857	-1.043811	-0.785897
N	1.767790	0.401408	1.591589

2A'
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.287904
Total energy: -2461.222360

C	1.527741	2.764462	-0.471825
C	2.035224	2.017755	-1.669045
C	1.124520	0.822551	-1.949668
H	2.124950	2.747879	-2.492070
H	3.062984	1.683576	-1.433613
H	0.116023	1.161312	-2.251057
H	1.536486	0.215258	-2.768430
C	1.639498	-2.268686	1.387753
H	1.473067	-2.918984	2.264237
H	2.715356	-2.287827	1.168105

C	0.851841	-2.762607	0.195474
H	-0.224643	-2.736914	0.410744
H	1.119031	-3.802312	-0.060524
O	0.889450	1.865533	0.380154
O	1.586155	3.933187	-0.217672
C	0.038556	-2.103675	-1.983364
H	0.229673	-1.496064	-2.874263
H	0.023996	-3.169564	-2.271438
H	-0.935458	-1.820138	-1.564082
C	2.426462	-2.134724	-1.562962
H	2.493838	-3.187252	-1.890219
H	2.583565	-1.481340	-2.427711
H	3.219852	-1.935754	-0.831936
C	2.346420	-0.167987	2.378030
H	2.056198	0.869127	2.584005
H	2.593359	-0.663013	3.335167
H	3.242228	-0.156670	1.740798
C	0.023843	-0.842472	2.502963
H	-0.235635	0.189225	2.758149
H	-0.817350	-1.271767	1.945540
H	0.171631	-1.407886	3.441484
C	0.017136	2.415267	1.399147
H	-0.314722	3.411998	1.085681
H	0.555031	2.488076	2.353820
H	-0.842690	1.740395	1.465904
I	-3.073002	0.029735	-0.091444
Ni	1.018153	-0.051407	-0.231207
N	1.095039	-1.866428	-0.972260
N	1.250928	-0.867426	1.682712

3A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.286432
Total energy: -2461.256133

Ni	0.213279	0.392671	-0.370947
I	1.840798	-1.704123	-0.198070
C	-0.800638	-0.535325	-1.751411
C	-1.682904	-1.619948	-1.122281
H	-0.150442	-1.008396	-2.507927
H	-1.454652	0.160087	-2.304345
C	-2.436333	-1.170119	0.103764
H	-1.056787	-2.459003	-0.767374
H	-2.407323	-2.057265	-1.831893
O	-3.610472	-1.797176	0.251340
O	-2.030219	-0.356579	0.914383
C	-4.361196	-1.494716	1.433148
H	-3.793307	-1.761215	2.338343
H	-5.278585	-2.094531	1.375523
H	-4.613520	-0.423600	1.475292
H	-0.660398	1.864354	-2.980054
C	-0.148764	2.542015	-2.287606
H	-0.428134	3.582586	-2.536673
H	0.935329	2.419099	-2.413788
C	0.141102	3.185910	0.020143
C	-1.988978	2.307985	-0.733813
C	0.248527	2.588327	1.403774
H	1.141386	3.397936	-0.379603
H	-0.411139	4.141911	0.040420
H	-2.344458	3.324267	-0.983674
H	-2.480273	1.586915	-1.396115
H	-2.270301	2.060758	0.295521
H	0.720456	3.302311	2.103926
H	-0.751036	2.359174	1.797060
C	0.734665	0.514562	2.538015
C	2.458305	1.593262	1.233546
H	1.321115	-0.411396	2.500667
H	0.997002	1.071497	3.457433
H	-0.330169	0.250108	2.557404
H	2.813889	2.176807	2.103762
H	3.004614	0.644083	1.188772
H	2.679656	2.152011	0.314820
N	-0.523079	2.220028	-0.895779
N	1.012476	1.323341	1.336813

4A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.286316
Total energy: -2461.236536

Ni	-0.078874	-0.174476	-0.233816
C	2.774027	-1.190637	-0.240500
C	1.445909	-1.465609	-0.828545
C	0.421839	-2.129736	-0.133680
H	1.461347	-1.479419	-1.920840
H	-0.397367	-0.351548	-1.604868
H	0.589118	-2.449246	0.898164
H	-0.311324	-2.715288	-0.694007
O	3.621643	-0.708680	-1.172989
O	3.122048	-1.369938	0.912769
C	4.950319	-0.407458	-0.738525
H	5.487918	-0.046699	-1.624830
H	4.944095	0.371574	0.040336
H	5.445828	-1.304540	-0.335680
I	-2.795786	-0.583074	-0.365010
N	0.329939	1.822423	-0.713044
H	0.000347	-1.391222	2.863522
C	0.719677	-0.568092	2.754895
N	0.185004	0.421880	1.801371
H	0.872984	-0.105263	3.747915
H	1.671128	-0.967143	2.390430
C	1.167841	1.513998	1.598241
C	-1.076958	0.946427	2.363404
C	0.666174	2.507217	0.565131
H	2.110217	1.054852	1.267819
H	1.371262	2.039159	2.551662

H	-0.881936	1.496902	3.303197
H	-1.752683	0.108842	2.572595
H	-1.588005	1.607487	1.655930
H	1.422743	3.292914	0.397699
H	-0.234767	3.012248	0.934491
C	-0.809721	2.481080	-1.374758
C	1.497938	1.832309	-1.615891
H	-1.031231	1.966074	-2.318447
H	-0.585097	3.543265	-1.586065
H	-1.698709	2.415092	-0.735141
H	1.752953	2.867109	-1.912648
H	1.276852	1.243758	-2.515037
H	2.363087	1.381174	-1.118998

5A

Geometry with 27 atoms:

Thermal correction to Gibbs Free Energy: 0.195959

Total energy: -2154.665589

C	-2.872182	0.419476	-0.413420
H	-3.950200	0.397561	-0.173262
H	-2.778703	0.504590	-1.504707
C	-2.188425	1.589337	0.262911
H	-2.334417	1.535199	1.350344
H	-2.625313	2.545676	-0.077913
Ni	-0.286403	-0.484188	0.031861
C	-0.017793	2.338957	1.017249
H	1.057687	2.335496	0.802866
H	-0.380519	3.383932	1.027874
H	-0.175238	1.892520	2.009253
C	-0.407716	2.042743	-1.348337
H	-0.699781	3.103996	-1.461824
H	0.671476	1.942514	-1.521114
H	-0.930458	1.446984	-2.108611
C	-2.568596	-1.917755	-0.971139
H	-2.124064	-2.866071	-0.648629
H	-3.666354	-2.032114	-1.038306
H	-2.168680	-1.662749	-1.961507
C	-2.619733	-1.260615	1.355415
H	-3.709781	-1.440599	1.404050
H	-2.083692	-2.178479	1.625297
H	-2.352731	-0.482617	2.081504
I	2.283238	-0.321771	-0.002598
H	-0.058586	-1.933370	0.070240
N	-0.729466	1.545155	0.001398
N	-2.218578	-0.852898	-0.007980

6A

Geometry with 39 atoms:

Thermal correction to Gibbs Free Energy: 0.279761

Total energy: -2461.233607

C	0.573048	-0.364573	-2.167812
H	-0.363073	-0.650393	-2.661255
H	1.269983	0.197861	-2.805312
C	1.120276	-1.237826	-1.171414
H	0.590569	-2.136020	-0.841119
C	2.552635	-1.190271	-0.854497
O	3.361988	-0.384243	-1.286683
O	2.901703	-2.138172	0.050123
C	4.272268	-2.161663	0.450931
H	4.933078	-2.349453	-0.410246
H	4.571468	-1.209221	0.916883
H	4.366654	-2.978231	1.178878
Ni	0.423047	0.437340	-0.419286
C	-0.193154	1.798005	1.903581
H	-1.203575	1.364480	1.906263
H	0.001591	2.209730	2.911984
C	-0.104269	2.902254	0.857951
H	0.885541	3.376340	0.891949
H	-0.844684	3.691836	1.071760
C	-1.732264	2.356382	-0.880059
C	0.488274	3.069800	-1.513290
C	0.489028	-0.496611	2.390470
C	2.158339	1.115080	1.746106
H	-0.890747	-0.261882	-0.209171
H	1.559911	2.967584	-1.289035
H	0.226460	4.144436	-1.533094
H	0.299308	2.638001	-2.504676
H	-2.095502	3.393787	-1.004296
H	-1.870987	1.805580	-1.819348
H	-2.327804	1.858385	-0.106003
H	1.142382	-1.308907	2.043278
H	0.680708	-0.306079	3.463350
H	-0.554371	-0.809525	2.260802
H	2.349736	1.482455	2.771822
H	2.425547	1.904399	1.031264
H	2.808649	0.252755	1.555372
I	-2.656194	-1.272029	0.051291
N	-0.306775	2.343026	-0.507116
N	0.752134	0.704111	1.581717

7A

Geometry with 37 atoms:

Thermal correction to Gibbs Free Energy: 0.277989

Total energy: -2162.729122

C	-0.294733	-2.239997	-0.610583
H	0.109639	-2.828499	-1.451251
H	-0.477996	-2.872395	0.274755
C	-1.310055	-1.242331	-0.927271
H	-1.552730	-0.981869	-1.966359
C	-2.330292	-0.879870	0.044087
O	-2.483494	-1.316940	1.176829
O	-3.154237	0.113704	-0.433837

C	-4.166634	0.571154	0.453188
H	-4.857208	-0.241991	0.732227
H	-3.740879	0.988212	1.381164
H	-4.719577	1.356201	-0.081860
Ni	0.362944	-0.480034	-0.284989
C	1.748816	1.964324	-0.067218
H	2.120874	1.977871	-1.101570
H	1.880642	2.985615	0.339337
C	2.548235	0.963759	0.759693
H	2.220452	1.000295	1.807900
H	3.622881	1.226861	0.745760
C	3.126221	-0.704831	-0.934796
C	2.623408	-1.407128	1.317888
C	-0.375349	2.182772	-1.255266
C	-0.381680	1.912768	1.137875
H	1.972711	-1.229580	2.185333
H	3.681606	-1.353312	1.642234
H	2.415608	-2.414473	0.934016
H	4.212104	-0.653108	-0.720037
H	2.877423	-1.709477	-1.301214
H	2.887695	0.013195	-1.730362
H	-1.409681	1.813563	-1.272124
H	-0.380649	3.289442	-1.195476
H	0.118606	1.878323	-2.188706
H	-0.379536	3.005115	1.324136
H	0.086189	1.405652	1.991657
H	-1.420240	1.565975	1.067837
N	0.320708	1.579472	-0.110359
N	2.328414	-0.419257	0.269326

8A
Geometry with 31 atoms:
Thermal correction to Gibbs Free Energy: 0.238967
Total energy: -1934.768468

Ni	-0.000521	0.770359	-0.000107
C	-0.684574	-1.941325	0.331896
H	-0.570139	-1.978610	1.424322
H	-1.252807	-2.844092	0.034518
C	0.687254	-1.940681	-0.330813
H	0.572850	-1.979081	-1.423203
H	1.256697	-2.842427	-0.032693
C	2.000442	-0.742468	1.350071
C	2.476026	-0.430302	-0.990666
C	-2.475750	-0.433017	0.990099
C	-1.998706	-0.745903	-1.350223
H	2.972450	0.516298	-0.739733
H	3.232723	-1.240351	-1.018402
H	2.026317	-0.326602	-1.988093
H	-2.759568	-1.547451	-1.443637
H	-1.211992	-0.917121	-2.096700
H	-2.466132	0.222756	-1.571625
H	-3.231521	-1.243935	1.017824
H	-2.026612	-0.328410	1.987693
H	-2.973108	0.512914	0.738524
H	2.466194	0.227119	1.570929
H	1.214304	-0.914841	2.096894
H	2.762750	-1.542634	1.443415
N	-1.423876	-0.702766	0.001836
N	1.424928	-0.700830	-0.001783
C	-0.732388	2.530428	0.020830
C	0.728372	2.531755	-0.020807
H	-1.235427	2.874178	0.944301
H	-1.288270	2.878936	-0.870152
H	1.230808	2.876636	-0.944173
H	1.283642	2.880923	0.870290

C_2H_4
Geometry with 6 atoms:
Thermal correction to Gibbs Free Energy: 0.028389
Total energy: -78.601490

C	-0.667009	-0.000000	0.000003
C	0.667009	0.000000	-0.000004
H	-1.243421	-0.932069	-0.000010
H	-1.243419	0.932071	0.000025
H	1.243421	0.932069	0.000012
H	1.243419	-0.932071	-0.000022

CH_3I
Geometry with 5 atoms:
Thermal correction to Gibbs Free Energy: 0.011361
Total energy: -337.795173

C	-0.000000	0.000000	-1.842880
H	0.000000	1.046171	-2.172275
H	-0.906011	-0.523086	-2.172275
H	0.906011	-0.523086	-2.172275
I	0.000000	-0.000000	0.331587

HI
Geometry with 2 atoms:
Thermal correction to Gibbs Free Energy: -0.014892
Total energy: -298.476669

I	0.000000	0.000000	0.030095
H	0.000000	0.000000	-1.595058

I^-
Geometry with 1 atoms:
Thermal correction to Gibbs Free Energy: -0.016848
Total energy: -297.960620

```
 I   0.000000   0.000000   0.000000
```

MA

```
Geometry with 12 atoms:
Thermal correction to Gibbs Free Energy:
0.064733
Total energy: -306.545074
 C  -1.317732  -0.645412   0.000034
 C  -2.498370  -0.017008  -0.000098
 H  -3.441203  -0.571020  -0.000310
 H  -2.545170   1.076788  -0.000164
 H  -1.237960  -1.735980   0.000001
 C  -0.042013   0.118783   0.000174
 O   0.058555   1.327510   0.000053
 O   1.015275  -0.710160   0.000141
 C   2.308624  -0.097846  -0.000176
 H   3.037866  -0.918155  -0.002508
 H   2.445396   0.530982  -0.894145
 H   2.447375   0.527481   0.895975
```

ts-1-2A

```
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.282246
Total energy: -2461.211766
Ni  -2.027780   0.335175  -0.012925
 O  -0.254779   0.971750   0.138330
 C  -0.086420   2.244682   0.175481
 O   1.038719   2.785816   0.169497
 C  -2.501953   2.194841  -0.331465
 H  -3.482352   2.517402   0.054354
 H  -2.528024   2.318289  -1.433478
 C  -1.370242   3.042586   0.262378
 H  -1.230262   4.040838  -0.188246
 H  -1.537853   3.209146   1.342525
 C  -4.218792  -0.469114  -1.591601
 H  -5.192040  -0.969345  -1.747601
 H  -4.279414   0.563067  -1.958258
 H  -3.449179  -0.994544  -2.170933
 C  -4.907734   0.267622   0.602930
 H  -4.578482   0.407783   1.641242
 H  -5.089901   1.249468   0.153389
 H  -5.851619  -0.306402   0.593464
 C  -0.196543  -1.880956  -0.718648
 H  -0.528257  -1.709832  -1.752840
 H   0.622354  -1.186322  -0.497699
 H   0.168243  -2.920729  -0.624118
 C  -0.855304  -1.739840   1.600538
 H  -1.689948  -1.558024   2.291033
 H  -0.438128  -2.744433   1.802161
 H  -0.084250  -0.980753   1.785223
 C  -3.744495  -1.831819   0.394801
 H  -3.738626  -1.743417   1.490200
 H  -4.629398  -2.431007   0.115188
 C  -2.467779  -2.498025  -0.081633
 H  -2.350836  -3.489384   0.392518
 H  -2.507210  -2.662096  -1.167122
 C   2.579636   1.366133   0.051714
 H   3.281292   2.195387   0.060735
 H   2.156293   1.022516  -0.885171
 H   2.228451   0.940951   0.984477
 I   4.491917  -0.450799  -0.092758
 N  -1.312022  -1.621463   0.205694
 N  -3.862035  -0.449726  -0.156061
```

ts-1-2A'

```
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.285129
Total energy: -2461.196546
 C   0.195461   2.503468   0.687260
 C   1.519438   3.012922   0.155100
 C   2.011377   2.022640  -0.900566
 H   1.385907   4.053486  -0.190611
 H   2.222484   3.049634   1.007536
 H   1.389871   2.096614  -1.815201
 H   3.053000   2.232467  -1.192442
 C   2.682182  -2.155563   0.939383
 H   2.586285  -3.223984   1.205616
 H   3.350682  -1.694071   1.679309
 C   3.253829  -2.002519  -0.454199
 H   2.598286  -2.489527  -1.188144
 H   4.246298  -2.478696  -0.532851
Ni   1.709320   0.299813  -0.071231
 O   0.138747   1.171488   0.646958
 O  -0.725022   3.196500   1.077472
 C   3.418080  -0.431337  -2.287146
 H   3.534512   0.621223  -2.567113
 H   4.276992  -1.005101  -2.678855
 H   2.491524  -0.815251  -2.734807
 C   4.540075   0.050754  -0.194161
 H   5.456123  -0.455495  -0.547777
 H   4.593082   1.113113  -0.455143
 H   4.484471  -0.032209   0.898417
 C   1.022810  -1.153452   2.404798
 H   0.081310  -0.592927   2.427531
 H   0.918924  -2.073966   3.008824
 H   1.805575  -0.520672   2.846651
 C   0.318797  -2.280845   0.381422
 H  -0.645801  -1.772145   0.461637
 H   0.535268  -2.433587  -0.684128
 H   0.234975  -3.267805   0.873727
 C  -1.746401   0.534667   0.282577
 H  -1.785886  -0.028774   1.208648
 H  -1.364288   0.079575  -0.623871
```

```
 H  -2.120772   1.553653   0.276778
 I  -4.203801  -0.409374  -0.376131
 N   3.341402  -0.557260  -0.815400
 N   1.374029  -1.465858   1.010175
```

ts-1-3A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.282890
Total energy: -2461.167760

```
Ni  -0.967439   0.486540  -0.205248
 O   0.483652   1.535393   0.489641
 C   0.915667   2.512934  -0.291121
 O   1.874507   3.218908  -0.024278
 C  -0.472544   1.263157  -1.909608
 H  -1.286285   1.337484  -2.647497
 H   0.326477   0.632613  -2.343559
 C   0.074598   2.641571  -1.550128
 H   0.680300   3.134012  -2.331959
 H  -0.752322   3.334649  -1.307471
 C  -2.319453   0.966094   2.253874
 H  -1.667071   1.847507   2.319661
 H  -3.154484   1.212426   1.584787
 H  -2.724046   0.733914   3.257596
 C  -0.430423  -0.476266   2.631471
 H   0.253805  -1.189566   2.153171
 H   0.118820   0.441241   2.861837
 H  -0.811137  -0.906717   3.576934
 C  -3.318793  -0.161776  -1.932269
 H  -3.740772   0.781045  -1.558476
 H  -2.776459   0.035423  -2.862568
 H  -4.139523  -0.868739  -2.148540
 C  -1.669282  -1.876150  -1.510144
 H  -0.988620  -2.316754  -0.770868
 H  -2.374414  -2.649377  -1.866545
 H  -1.064461  -1.517382  -2.351679
 C  -2.355198  -1.362386   1.474310
 H  -1.666054  -2.204739   1.321847
 H  -2.983765  -1.604894   2.351899
 C  -3.221558  -1.165643   0.248435
 H  -3.772089  -2.092183   0.007053
 H  -3.969197  -0.382446   0.434137
 C   2.447747   1.027547   1.745931
 H   2.503018   0.073257   2.264903
 H   3.258802   1.324254   1.083979
 H   1.840471   1.818731   2.169940
 I   2.392180  -1.256696  -0.296450
 N  -1.535081  -0.159218   1.717168
 N  -2.404640  -0.732335  -0.921054
```

ts-2-3A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.288181
Total energy: -2461.241428

```
 C  -1.649236   1.955623  -0.081089
 C   2.709606   0.030176   1.604007
 H   3.340837  -0.451617   2.373766
 H   2.566674   1.077359   1.906070
 C   3.377777  -0.039812   0.246644
 H   3.520163  -1.085660  -0.054118
 H   4.375800   0.431677   0.269992
Ni   0.611601   0.191692  -0.244208
 O  -2.663431   2.758937   0.212139
 O  -0.886917   1.524395   0.777307
 C   2.861942   0.106772  -2.116243
 H   2.646455  -0.968951  -2.163026
 H   3.932420   0.276438  -2.335428
 H   2.260685   0.618908  -2.875826
 C   2.718464   2.080739  -0.721226
 H   3.774351   2.334104  -0.928676
 H   2.083581   2.574192  -1.464242
 H   2.446012   2.463695   0.270386
 C   0.545581  -0.241366   2.680255
 H  -0.461998  -0.651884   2.534907
 H   0.974504  -0.634715   3.620754
 H   0.463056   0.849884   2.743947
 C   1.519334  -2.079413   1.472657
 H   2.117090  -2.442053   2.329982
 H   0.526573  -2.539701   1.501213
 H   2.001604  -2.391452   0.538027
 C  -2.869110   3.077340   1.597481
 H  -3.042674   2.161932   2.183224
 H  -3.755010   3.723615   1.632606
 H  -1.996474   3.608090   2.008072
 I  -1.604372  -1.863982  -0.369682
 C  -0.150841   1.002520  -1.842125
 H  -0.223650   0.260800  -2.656575
 H   0.492457   1.818461  -2.212932
 C  -1.537902   1.577402  -1.528027
 H  -1.829310   2.443360  -2.148192
 H  -2.324116   0.816210  -1.674703
 N   2.516212   0.616402  -0.774950
 N   1.379067  -0.610055   1.523831
```

ts-2A'-3A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.289090
Total energy: -2461.233068

```
 C   1.524911  -2.652074  -0.059613
 C   0.417636  -2.662624  -1.080665
 C   0.148649  -1.273285  -1.670620
 H   0.698415  -3.414372  -1.838742
 H  -0.482703  -3.059516  -0.574354
```

H	1.079990	-0.868791	-2.101334
H	-0.569583	-1.367649	-2.499935
C	-2.615969	0.103064	1.618188
H	-3.194188	0.599684	2.418841
H	-2.714984	-0.980859	1.771398
C	-3.145988	0.488877	0.256576
H	-3.009959	1.566226	0.092919
H	-4.225823	0.276123	0.170456
O	1.444412	-1.541835	0.715919
O	2.390108	-3.482677	0.081433
C	-2.509506	0.523661	-2.071899
H	-2.009639	-0.018805	-2.881670
H	-3.572896	0.664037	-2.338786
H	-2.028287	1.504049	-1.958218
C	-2.930600	-1.594474	-0.977874
H	-3.995301	-1.554239	-1.271211
H	-2.372524	-2.121572	-1.759007
H	-2.839070	-2.158601	-0.041373
C	-0.534499	-0.338258	2.764043
H	0.511583	-0.029565	2.861430
H	-1.038621	-0.185357	3.736692
H	-0.564822	-1.404913	2.504783
C	-1.012730	1.887890	1.997534
H	0.055360	2.123357	2.062443
H	-1.437877	2.496986	1.190420
H	-1.506475	2.150953	2.951955
C	2.516958	-1.299116	1.635263
H	3.482462	-1.539404	1.168706
H	2.389952	-1.909159	2.542941
H	2.480871	-0.230712	1.876880
I	1.533249	1.783137	-0.564510
Ni	-0.473033	-0.196494	-0.189095
N	-2.389423	-0.231360	-0.805693
N	-1.179506	0.453049	1.703410

ts-3-4A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.284040
Total energy: -2461.216992

Ni	-0.246456	0.002900	-0.127025
C	-2.629833	-1.259498	-0.710203
C	-1.197934	-1.621845	-0.919382
C	-0.432097	-0.969561	-1.893180
H	-0.914266	-2.601400	-0.528846
H	-0.089673	-1.225651	0.573284
H	-0.932276	-0.305455	-2.598844
H	0.510365	-1.416319	-2.219469
O	-3.172025	-1.997015	0.272034
O	-3.249972	-0.413037	-1.324169
C	-4.536802	-1.720061	0.604659
H	-4.798707	-2.407411	1.418889
H	-4.654139	-0.677295	0.938472
H	-5.194025	-1.891897	-0.261610
I	2.921376	-0.847780	-0.020711
N	-0.478338	0.806327	1.705625
H	-0.817037	1.689418	-2.955734
C	-1.214148	2.164002	-2.050266
N	-0.297046	1.929058	-0.915647
H	-1.313647	3.246595	-2.248046
H	-2.198109	1.731272	-1.829330
C	-0.743424	2.762071	0.233298
C	1.080988	2.274898	-1.324983
C	-0.163337	2.247264	1.533660
H	-1.841058	2.722366	0.264408
H	-0.462028	3.819099	0.078247
H	1.126616	3.313418	-1.701455
H	1.406498	1.584087	-2.113040
H	1.772250	2.163008	-0.482207
H	-0.545506	2.834534	2.388023
H	0.930994	2.341468	1.529248
C	0.381439	0.234599	2.761764
C	-1.899289	0.591449	2.060049
H	0.129109	-0.823244	2.907531
H	0.233553	0.777040	3.713051
H	1.432511	0.301637	2.455819
H	-2.142915	1.087469	3.017177
H	-2.084620	-0.485771	2.148465
H	-2.555781	0.986970	1.275104

ts-4-5A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.284406
Total energy: -2461.221310

Ni	-0.328966	0.229799	-0.398359
C	2.760693	-1.465642	-0.137258
C	1.567741	-1.535953	-1.003703
C	0.420638	-2.134823	-0.605961
H	1.692704	-1.186689	-2.029105
H	-0.513417	0.145819	-1.842700
H	0.327470	-2.566738	0.392253
H	-0.377317	-2.335649	-1.319026
O	3.823600	-0.984929	-0.810862
O	2.824517	-1.798806	1.032235
C	5.054862	-0.887459	-0.087955
H	5.797632	-0.505109	-0.799644
H	4.957307	-0.195166	0.763210
H	5.366341	-1.873135	0.290926
I	-2.806938	-0.713507	-0.290393
N	0.695221	1.969038	-0.713598
H	-0.814953	-1.261618	2.343983
C	0.083622	-0.640360	2.458615
N	-0.060561	0.569013	1.629389
H	0.202428	-0.372955	3.525401
H	0.962883	-1.210701	2.138415

C	1.200787	1.346819	1.616800
C	-1.177473	1.379313	2.157629
C	1.092410	2.490487	0.626899
H	2.011472	0.665265	1.327245
H	1.437310	1.733325	2.626624
H	-0.911180	1.816503	3.138227
H	-2.059663	0.740992	2.278438
H	-1.445619	2.184493	1.462863
H	2.045887	3.040773	0.564557
H	0.333651	3.208706	0.961558
C	-0.213126	2.917818	-1.390778
C	1.891700	1.749783	-1.547570
H	-0.466765	2.532126	-2.385661
H	0.262875	3.910881	-1.497033
H	-1.140730	3.020244	-0.812306
H	2.395879	2.710112	-1.765622
H	1.600575	1.272463	-2.491019
H	2.595353	1.091183	-1.028495

ts-4-6A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.279510
Total energy: -2461.221407

Ni	-0.306373	0.198740	-0.268011
C	-2.471603	-1.357590	-0.777516
C	-1.030115	-1.448745	-1.106716
C	-0.483303	-0.568876	-2.073390
H	-0.546860	-2.390801	-0.835525
H	0.623908	-0.823145	0.118934
H	-1.167947	0.032540	-2.679903
H	0.472311	-0.823370	-2.543081
O	-2.856499	-2.349326	0.048884
O	-3.237813	-0.491545	-1.162993
C	-4.225817	-2.342283	0.463362
H	-4.353542	-3.217153	1.113730
H	-4.465194	-1.422195	1.019573
H	-4.899886	-2.415366	-0.404279
I	2.919967	-0.915468	-0.046868
N	-0.579722	0.648864	1.701864
H	-0.899049	2.262558	-2.712089
C	-1.282967	2.637788	-1.755288
N	-0.369459	2.247453	-0.667319
H	-1.373026	3.738290	-1.821866
H	-2.274038	2.196988	-1.581105
C	-0.809438	2.857530	0.611145
C	1.016354	2.627701	-1.005076
C	-0.248771	2.092868	1.797575
H	-1.907845	2.833488	0.631397
H	-0.506822	3.919373	0.665740
H	1.097294	3.718331	-1.174064
H	1.325821	2.094652	-1.913564
H	1.700584	2.335280	-0.198760
H	-0.632147	2.519105	2.742940
H	0.846765	2.175125	1.819265
C	0.223567	-0.118157	2.671270
C	-2.015083	0.397160	1.948822
H	-0.004116	-1.187073	2.568216
H	0.000202	0.203321	3.705176
H	1.290471	0.028753	2.465028
H	-2.319248	0.781744	2.939918
H	-2.192269	-0.684621	1.914205
H	-2.633362	0.867638	1.174319

1B
Geometry with 34 atoms:
Thermal correction to Gibbs Free Energy: 0.254553
Total energy: -2123.436211

C	-2.892058	0.069600	0.031799
C	2.292599	1.275442	-0.197137
H	2.965770	2.062243	0.191166
H	2.466796	1.206300	-1.280070
C	2.598017	-0.054294	0.466358
H	2.503115	0.038974	1.556872
H	3.634425	-0.371995	0.252706
Ni	-0.160811	-0.197630	-0.060052
O	-4.007105	0.571647	-0.035107
O	-1.779510	0.751471	-0.079133
C	1.695355	-2.227207	0.983660
H	1.064820	-3.051538	0.634068
H	2.733313	-2.593315	1.084696
H	1.330631	-1.895608	1.965364
C	1.952005	-1.590071	-1.331406
H	2.958612	-2.046836	-1.360549
H	1.206683	-2.338187	-1.628898
H	1.914205	-0.762185	-2.050767
C	0.381729	2.538662	-1.028445
H	-0.694154	2.690658	-0.881890
H	0.911132	3.509810	-0.992085
H	0.533976	2.085068	-2.018404
C	0.612984	2.182475	1.346998
H	1.114195	3.160659	1.479371
H	-0.471338	2.303653	1.467958
H	0.967558	1.494841	2.126691
C	-1.263734	-1.779243	-0.281071
H	-0.874891	-2.714054	0.157501
H	-1.343375	-1.945401	-1.375896
C	-2.634766	-1.411395	0.290617
H	-3.486089	-2.010765	-0.081615
H	-2.631368	-1.528378	1.390808
N	1.633124	-1.103696	0.027143
N	0.872422	1.622402	0.011445

2B

Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy:
0.313699
Total energy: -2500.569529

C	1.618389	-1.337231	-0.926783
C	-2.995151	-0.742254	1.586970
H	-3.333079	-0.491660	2.608475
H	-3.569732	-1.620181	1.260962
C	-3.235442	0.423155	0.648263
H	-2.699211	1.311848	1.007053
H	-4.308480	0.677588	0.594553
Ni	-0.974036	-0.786092	-0.411783
O	2.871754	-1.679890	-0.810760
O	0.794319	-1.531969	-0.012989
C	-2.586733	1.392468	-1.462688
H	-2.318479	1.190765	-2.504684
H	-3.546511	1.938344	-1.442896
H	-1.800508	2.008548	-1.006382
C	-3.608739	-0.802740	-1.448762
H	-4.607203	-0.348808	-1.582007
H	-3.175412	-1.018796	-2.433014
H	-3.715022	-1.748650	-0.902723
C	-1.349652	-2.512500	1.919955
H	-0.279032	-2.744188	1.857120
H	-1.708867	-2.726124	2.943783
H	-1.887557	-3.156444	1.209505
C	-0.754800	-0.228818	2.441897
H	-1.007468	-0.397188	3.505503
H	0.309315	-0.440557	2.277729
H	-0.923580	0.825652	2.192077
C	3.327124	-2.239998	0.455771
H	3.120438	-1.501325	1.245528
H	2.735699	-3.144945	0.664982
I	1.262831	2.575412	0.300385
C	-0.348828	-0.793034	-2.256580
H	-0.768878	-0.031465	-2.929417
H	-0.623251	-1.787127	-2.664773
C	1.177105	-0.661898	-2.180040
H	1.751707	-1.036562	-3.045180
H	1.465168	0.396790	-2.036227
N	-2.710980	0.118491	-0.718328
N	-1.558849	-1.099704	1.565568
C	4.800896	-2.536365	0.317876
H	5.367072	-1.618234	0.096880
H	5.177866	-2.958025	1.262697
H	4.983168	-3.266856	-0.485968

2B'
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy:
0.314947
Total energy: -2500.549999

C	1.936841	2.160313	-1.169620
C	2.344322	1.061742	-2.102968
C	1.221825	0.024202	-2.153830
H	2.599752	1.529786	-3.068937
H	3.275762	0.614054	-1.709480
H	0.302385	0.464160	-2.583036
H	1.518273	-0.825738	-2.786051
C	1.082261	-2.311856	1.800225
H	0.748600	-2.671715	2.788261
H	2.104423	-2.683812	1.651988
C	0.168573	-2.821625	0.709448
H	-0.855443	-2.456437	0.869399
H	0.137884	-3.925037	0.691972
O	1.208341	1.616605	-0.114626
O	2.113805	3.342140	-1.263627
C	-0.447106	-2.538093	-1.606844
H	-0.120098	-2.205680	-2.597528
H	-0.687386	-3.614995	-1.650468
H	-1.341811	-1.971910	-1.319057
C	1.867618	-2.978826	-1.044195
H	1.708861	-4.070286	-1.099630
H	2.160203	-2.610411	-2.033308
H	2.685878	-2.769140	-0.344848
C	2.408214	-0.311415	2.211033
H	2.426717	0.779567	2.108815
H	2.601315	-0.579099	3.266248
H	3.209858	-0.727874	1.584481
C	0.010194	-0.286257	2.578670
H	0.036352	0.806945	2.571882
H	-0.959705	-0.605260	2.176243
H	0.105622	-0.628185	3.625557
C	0.351268	2.555877	0.624527
H	-0.477995	1.937323	0.982507
H	-0.051698	3.262122	-0.113398
I	-3.066125	0.354860	-0.138440
Ni	0.953601	-0.394276	-0.290354
N	0.624206	-2.300392	-0.611865
N	1.106181	-0.827617	1.752699
C	1.089302	3.277409	1.729453
H	1.932965	3.854400	1.325437
H	0.390859	3.978613	2.214104
H	1.462463	2.588048	2.500866

3B
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy:
0.312994
Total energy: -2500.582123

Ni	0.597606	0.345374	-0.365699
I	1.568526	-2.118438	-0.149980
C	-0.489993	-0.231156	-1.875786
C	-1.697778	-1.030209	-1.372198
H	0.070789	-0.856174	-2.592441
H	-0.863639	0.632868	-2.451053

C	-2.404709	-0.404143	-0.196235
H	-1.370368	-2.018964	-1.001781
H	-2.446528	-1.230897	-2.158878
O	-3.713667	-0.675063	-0.170176
O	-1.858181	0.249905	0.675464
C	-4.470085	-0.190929	0.959786
H	-4.036155	-0.607084	1.883907
H	-4.369092	0.905572	1.013551
H	0.469070	2.054725	-2.970759
C	1.061676	2.551580	-2.194383
H	1.106925	3.633511	-2.418751
H	2.078584	2.136955	-2.210607
C	1.248323	3.039995	0.163046
C	-0.937772	2.811471	-0.856731
C	1.027497	2.400584	1.514097
H	2.307761	2.976133	-0.117278
H	0.980010	4.111018	0.179640
H	-0.967375	3.891085	-1.091432
H	-1.530182	2.269990	-1.602433
H	-1.392005	2.634597	0.124245
H	1.583827	2.942351	2.301441
H	-0.037711	2.439875	1.779763
C	0.824200	0.247231	2.585857
C	2.899407	0.850875	1.507210
H	1.144039	-0.801524	2.558610
H	1.127672	0.692019	3.552460
H	-0.268483	0.279642	2.491538
H	3.304381	1.303614	2.432335
H	3.175810	-0.209265	1.474161
H	3.356817	1.343812	0.639624
N	0.454986	2.319051	-0.868088
N	1.431279	0.978222	1.458309
C	-5.908444	-0.616577	0.769201
H	-6.517207	-0.263337	1.616483
H	-6.324808	-0.191846	-0.158188
H	-5.989963	-1.713929	0.717285

4B
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.311045
Total energy: -2500.561877

Ni	-0.281142	-0.171890	-0.149642
C	2.631280	-0.877958	0.100104
C	1.353019	-1.438332	-0.388801
C	0.373690	-1.984226	0.456430
H	1.400635	-1.746978	-1.435531
H	-0.504411	-0.696207	-1.448031
H	0.540402	-2.003299	1.536377
H	-0.292682	-2.758761	0.068682
O	3.454037	-0.607001	-0.933223
O	2.950116	-0.681126	1.259729
C	4.761617	-0.075559	-0.637984
H	5.068553	0.432996	-1.563367
H	4.677147	0.672377	0.165568
I	-2.956049	-0.871943	-0.300178
N	-0.030121	1.684965	-1.079852
H	-0.211100	-0.609057	3.164596
C	0.412598	0.245204	2.868602
N	-0.190344	0.907170	1.696398
H	0.469432	0.946995	3.721997
H	1.418138	-0.110428	2.623010
C	0.663223	2.042043	1.268048
C	-1.535036	1.376077	2.087863
C	0.114179	2.688279	0.009097
H	1.672665	1.645056	1.089380
H	0.740512	2.798527	2.072854
H	-1.461934	2.138316	2.886648
H	-2.118846	0.524264	2.455983
H	-2.075333	1.796424	1.233515
H	0.770634	3.516101	-0.310573
H	-0.871868	3.126407	0.207893
C	-1.158742	2.031789	-1.960826
C	1.213027	1.620426	-1.873094
H	-1.232845	1.292085	-2.768605
H	-1.020884	3.036205	-2.402882
H	-2.095894	2.007716	-1.390860
H	1.380947	2.572079	-2.411808
H	1.149294	0.800777	-2.599413
H	2.069499	1.430049	-1.218040
C	5.738844	-1.174517	-0.262965
H	6.744292	-0.746448	-0.120438
H	5.434848	-1.664129	0.674312
H	5.795180	-1.934469	-1.058597

5B
Geometry with 27 atoms:
Thermal correction to Gibbs Free Energy: 0.195959
Total energy: -2154.665589

C	-2.872182	0.419476	-0.413420
H	-3.950200	0.397561	-0.173262
H	-2.778703	0.504590	-1.504707
C	-2.188425	1.589337	0.262911
H	-2.334417	1.535199	1.350344
H	-2.625313	2.545676	-0.077913
Ni	-0.286403	-0.484188	0.031861
C	-0.017793	2.338957	1.017249
H	1.057687	2.335496	0.802866
H	-0.380519	3.383932	1.027874
H	-0.175238	1.892520	2.009253
C	-0.407716	2.042743	-1.348337
H	-0.699781	3.103996	-1.461824
H	0.671476	1.942514	-1.521114
H	-0.930458	1.446984	-2.108611
C	-2.568596	-1.917755	-0.971139

H	-2.124064	-2.866071	-0.648629
H	-3.666354	-2.032114	-1.038306
H	-2.168680	-1.662749	-1.961507
C	-2.619733	-1.260615	1.355415
H	-3.709781	-1.440599	1.404050
H	-2.083692	-2.178479	1.625297
H	-2.352731	-0.482617	2.081504
I	2.283238	-0.321771	-0.002598
H	-0.058586	-1.933370	0.070240
N	-0.729466	1.545155	0.001398
N	-2.218578	-0.852898	-0.007980

6B

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.306808

Total energy: -2500.559896

C	0.475665	-0.167991	-2.146591
H	-0.350644	-0.666493	-2.666740
H	1.046279	0.535442	-2.769394
C	1.172065	-0.885250	-1.119581
H	0.849131	-1.878448	-0.795080
C	2.535829	-0.503024	-0.736724
O	3.141530	0.483999	-1.128548
O	3.054818	-1.355012	0.181683
C	4.382379	-1.088051	0.669939
H	4.501695	-0.005980	0.835552
H	4.432337	-1.601013	1.641633
Ni	0.087827	0.595170	-0.418087
C	-0.891396	1.804372	1.864694
H	-1.764349	1.135824	1.861508
H	-0.822169	2.268226	2.866865
C	-1.054246	2.878836	0.798234
H	-0.215316	3.586186	0.841438
H	-1.973266	3.461488	0.981255
C	-2.451493	1.929693	-0.967286
C	-0.455620	3.158032	-1.556910
C	0.326548	-0.240968	2.413799
C	1.558650	1.719727	1.746773
H	-1.021255	-0.399130	-0.213935
H	0.603148	3.319109	-1.308244
H	-0.968935	4.137257	-1.594913
H	-0.511471	2.688477	-2.547761
H	-3.052043	2.846288	-1.118704
H	-2.426930	1.351731	-1.900267
H	-2.929607	1.310615	-0.199351
H	1.163919	-0.875215	2.092003
H	0.449321	0.012571	3.483727
H	-0.606203	-0.802567	2.280253
H	1.637736	2.145136	2.764865
H	1.632496	2.535408	1.015523
H	2.405710	1.042713	1.581631
I	-2.491721	-1.797360	0.046631
N	-1.076537	2.267590	-0.559341
N	0.299613	0.970595	1.579874
C	5.442501	-1.610106	-0.283264
H	5.398015	-1.074876	-1.243782
H	6.444772	-1.461568	0.150652
H	5.302068	-2.686656	-0.471067

7B

Geometry with 40 atoms:

Thermal correction to Gibbs Free Energy: 0.304333

Total energy: -2202.055062

C	-0.029085	-2.223429	-0.638684
H	0.379204	-2.818433	-1.472808
H	-0.240432	-2.853265	0.242256
C	-1.017714	-1.205368	-0.973416
H	-1.235079	-0.937751	-2.016103
C	-2.041293	-0.811689	-0.018571
O	-2.217032	-1.244270	1.113746
O	-2.826471	0.205435	-0.514701
C	-3.863176	0.713451	0.332050
H	-3.495587	0.786566	1.368056
H	-4.065907	1.730262	-0.038949
Ni	0.656830	-0.477387	-0.294282
C	2.088339	1.936977	-0.035601
H	2.481264	1.947148	-1.062252
H	2.232960	2.953546	0.378248
C	2.850561	0.916601	0.802136
H	2.502469	0.955289	1.843657
H	3.930419	1.157607	0.811021
C	3.428576	-0.755629	-0.888546
C	2.864582	-1.457998	1.350070
C	-0.006314	2.204673	-1.264780
C	-0.066068	1.924516	1.127038
H	2.197394	-1.272588	2.203236
H	3.915888	-1.426167	1.698710
H	2.646798	-2.459293	0.955952
H	4.510685	-0.728698	-0.651430
H	3.165705	-1.752577	-1.265998
H	3.221920	-0.028094	-1.684445
H	-1.046762	1.855345	-1.305695
H	0.008789	3.310926	-1.199154
H	0.501336	1.895213	-2.189213
H	-0.044893	3.015815	1.317970
H	0.375542	1.404423	1.987141
H	-1.110118	1.599286	1.036376
N	0.653652	1.582002	-0.108896
N	2.612477	-0.459290	0.300573
C	-5.114824	-0.146591	0.270989
H	-4.908558	-1.151672	0.668681
H	-5.920274	0.307084	0.872085
H	-5.470380	-0.244528	-0.767651

C_2H_5I
Geometry with 8 atoms:
Thermal correction to Gibbs Free Energy: 0.036545
Total energy: -377.117245

C	-2.443032	-0.430890	0.000000
C	-1.432920	0.695288	0.000000
H	-2.347390	-1.066454	0.893765
H	-3.457559	0.007143	0.000005
H	-2.347393	-1.066443	-0.893772
H	-1.490738	1.325095	-0.897095
H	-1.490734	1.325099	0.897094
I	0.648859	-0.039827	-0.000000

EA
Geometry with 15 atoms:
Thermal correction to Gibbs Free Energy: 0.090484
Total energy: -345.870895

O	-0.721117	1.426270	0.000256
C	-0.605410	0.218108	0.000009
O	0.579004	-0.412590	-0.000372
C	-3.001137	-0.343975	0.000032
H	-3.833229	-1.053612	0.000014
H	-3.237530	0.724990	-0.000009
C	-1.729044	-0.756881	0.000066
H	-1.460580	-1.816948	0.000071
C	1.763063	0.410242	-0.000385
C	2.964979	-0.507380	0.000377
H	1.743276	1.064261	0.887220
H	1.743793	1.063395	-0.888656
H	2.968443	-1.151799	-0.893140
H	3.890014	0.090458	0.000286
H	2.968009	-1.150877	0.894560

ts-1-2B
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.308446
Total energy: -2500.538674

Ni	2.073197	0.332009	0.035680
O	0.312979	1.017698	-0.075753
C	0.184388	2.296049	-0.139614
O	-0.922390	2.869251	-0.151330
C	2.596156	2.175046	0.368563
H	3.590923	2.478460	0.004218
H	2.605177	2.287767	1.472192
C	1.493633	3.052086	-0.234973
H	1.384197	4.059060	0.205290
H	1.667246	3.202594	-1.316553
C	0.811328	-1.728841	-1.533711
H	1.628395	-1.565609	-2.249404
H	0.371093	-2.727377	-1.715110
H	0.047543	-0.958593	-1.701207
C	0.212211	-1.834411	0.802312
H	0.574542	-1.659900	1.825648
H	-0.599849	-1.128592	0.594236
H	-0.176227	-2.867075	0.727116
C	4.897336	0.199077	-0.756394
H	4.499579	0.321248	-1.772804
H	5.120350	1.188089	-0.342524
H	5.833592	-0.385964	-0.798113
C	4.351984	-0.484945	1.495467
H	3.621858	-0.997866	2.134065
H	5.331688	-0.987410	1.592679
H	4.440961	0.552850	1.839956
C	2.452881	-2.502108	0.116892
H	2.528104	-2.634167	1.205052
H	2.295559	-3.503837	-0.322990
C	3.725964	-1.880694	-0.424264
H	4.606867	-2.494637	-0.165373
H	3.678693	-1.819052	-1.520285
C	-2.578909	1.467600	-0.042681
H	-2.078364	1.110537	0.850631
H	-2.199104	1.110166	-0.994222
I	-4.028204	-0.869337	0.066683
N	3.897818	-0.488655	0.087791
N	1.308249	-1.606630	-0.153255
C	-3.665101	2.486226	0.025686
H	-4.358770	2.398055	-0.822188
H	-4.228260	2.416044	0.966769
H	-3.198925	3.484716	-0.019066

ts-1-2B'
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.310407
Total energy: -2500.521498

C	0.584279	2.768436	-0.524821
C	1.322760	2.429454	-1.806652
C	1.234688	0.918366	-2.042685
H	0.936231	3.066391	-2.622559
H	2.374613	2.731963	-1.648159
H	0.230160	0.640458	-2.417855
H	1.969351	0.584962	-2.794445
C	2.877923	-1.509487	1.574459
H	2.902527	-2.122292	2.493441
H	3.891730	-1.115554	1.421003
C	2.456461	-2.350797	0.385761
H	1.455737	-2.771126	0.557244
H	3.150041	-3.195732	0.229847
Ni	1.503052	0.175121	-0.275359
O	0.523071	1.723605	0.310374
O	0.084521	3.844812	-0.258482

C	-1.475216	1.056292	0.350628
I	-3.633202	-0.826835	-0.158974
C	2.603674	0.786674	2.367422
H	1.903046	1.631233	2.374448
H	2.905383	0.545349	3.403909
H	3.494825	1.080791	1.794757
C	0.732366	-0.732338	2.447204
H	0.969108	-1.068238	3.474222
H	0.071356	0.140602	2.508304
H	0.199823	-1.538848	1.925297
C	3.734826	-1.222414	-1.370696
H	4.262216	-2.160515	-1.621189
H	3.650979	-0.604691	-2.272341
H	4.321869	-0.667414	-0.628270
C	1.587955	-2.224826	-1.869782
H	1.564038	-1.640982	-2.796666
H	2.031002	-3.214780	-2.079961
H	0.558970	-2.356567	-1.509086
N	2.382023	-1.510441	-0.846174
N	1.953798	-0.361094	1.715096
H	-1.571655	1.273015	-0.711435
H	-1.037072	0.103355	0.617160
C	-2.054407	1.982005	1.351966
H	-1.956832	1.601975	2.377991
H	-3.114955	2.172696	1.128990
H	-1.531600	2.948075	1.256645

ts-2-3B
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.314794
Total energy: -2500.567728

C	2.068057	-0.969676	-0.484589
C	-2.450381	-1.272165	1.734812
H	-3.121720	-1.194610	2.610489
H	-1.838827	-2.175852	1.869100
C	-3.253876	-1.365607	0.454468
H	-3.860954	-0.461092	0.320474
H	-3.947970	-2.223676	0.482189
Ni	-0.722247	-0.338436	-0.258264
O	3.355774	-1.255632	-0.363471
O	1.294735	-1.002160	0.467813
C	-3.020416	-1.032146	-1.935943
H	-3.272485	0.032726	-1.844634
H	-3.945019	-1.615326	-2.102687
H	-2.360182	-1.162822	-2.800658
C	-1.902723	-2.887922	-0.853536
H	-2.775399	-3.542459	-1.032672
H	-1.208239	-2.985236	-1.694162
H	-1.387899	-3.219316	0.057143
C	-0.505244	-0.182608	2.699345
H	0.200742	0.646491	2.560646
H	-0.956345	-0.117609	3.707162
H	0.049326	-1.123716	2.606661
C	-2.296382	1.148775	1.799892
H	-2.914968	1.126019	2.716834
H	-1.596164	1.988050	1.857056
H	-2.943425	1.317401	0.930172
C	3.859222	-1.561703	0.959282
H	3.623873	-0.718432	1.628098
H	3.330018	-2.449774	1.341033
I	0.386251	2.463905	-0.269188
C	0.111551	-0.593998	-2.001225
H	-0.223946	0.183246	-2.709899
H	-0.176206	-1.565651	-2.437799
C	1.639093	-0.554487	-1.861425
H	2.184422	-1.165355	-2.602547
H	2.024850	0.474172	-1.972261
N	-2.332434	-1.479588	-0.709566
N	-1.539053	-0.110936	1.653096
C	5.347831	-1.794738	0.841508
H	5.765196	-2.030531	1.833045
H	5.562896	-2.636903	0.164795
H	5.855959	-0.896832	0.455832

ts-2-3B'
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.315441
Total energy: -2500.559133

C	1.613110	-2.463160	-0.278449
C	0.505994	-2.505720	-1.301403
C	0.070621	-1.116850	-1.775020
H	0.865002	-3.160400	-2.115967
H	-0.331367	-3.053672	-0.830566
H	0.938156	-0.572886	-2.184493
H	-0.660355	-1.218759	-2.592441
C	-2.604530	-0.404438	1.753782
H	-3.192743	-0.091939	2.636397
H	-2.495618	-1.497058	1.804961
C	-3.303333	-0.010004	0.473997
H	-3.368208	1.083416	0.402484
H	-4.334310	-0.401952	0.442341
O	1.559813	-1.310990	0.433148
O	2.448028	-3.315292	-0.086821
C	-2.836322	0.338301	-1.872723
H	-2.314071	-0.045060	-2.756133
H	-3.923774	0.337353	-2.071202
H	-2.499347	1.366324	-1.685046
C	-2.883131	-1.908320	-0.976059
H	-3.959877	-1.992670	-1.210264
H	-2.309634	-2.279125	-1.831973
H	-2.659944	-2.537243	-0.104884
C	-0.407083	-0.524009	2.747772
H	0.566326	-0.026925	2.817602
H	-0.870508	-0.528332	3.752063

H	-0.252848	-1.559628	2.416316
C	-1.319593	1.617776	2.154865
H	-0.307715	2.037043	2.187423
H	-1.888977	2.185945	1.409169
H	-1.796958	1.737289	3.145840
C	2.673919	-0.987998	1.300443
H	2.827370	-1.822773	2.001838
H	2.333493	-0.106495	1.855689
I	1.039466	2.100341	-0.564786
Ni	-0.590071	-0.231396	-0.192037
N	-2.524550	-0.502587	-0.696772
N	-1.250392	0.193300	1.778039
C	3.934075	-0.666169	0.519681
H	4.718367	-0.337609	1.220880
H	4.304372	-1.544982	-0.026615
H	3.742934	0.149944	-0.193528

ts-3-4B
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.310841
Total energy: -2500.546024

Ni	0.041204	0.086776	-0.134100
I	2.902878	-1.217118	-0.031239
C	-0.379399	-0.841502	-1.875267
C	-1.217601	-1.349600	-0.870633
H	0.446392	-1.457694	-2.240182
H	-0.783248	-0.106328	-2.572659
C	-2.561004	-0.749684	-0.622913
H	-0.062015	-1.151901	0.562413
H	-1.103817	-2.369424	-0.496183
O	-3.198837	-1.405156	0.360189
O	-3.033502	0.205680	-1.209919
C	-4.511455	-0.939562	0.742835
H	-4.645052	-1.304999	1.770948
H	-4.514292	0.161108	0.753905
H	1.922109	1.390519	-2.144470
C	1.713421	2.131184	-1.362312
H	1.905958	3.147112	-1.753853
H	2.391820	1.930413	-0.525528
C	0.018200	2.895945	0.220575
C	-0.580477	2.371037	-2.051251
C	0.510053	2.288025	1.517281
H	0.477409	3.888016	0.061474
H	-1.069163	3.046705	0.260927
H	-0.510218	3.454923	-2.255211
H	-0.278121	1.834562	-2.958810
H	-1.616685	2.101549	-1.811000
H	1.603258	2.178586	1.497579
H	0.253594	2.940011	2.372316
C	-1.503051	0.985593	2.040604
C	0.662650	0.228330	2.776912
H	-1.878031	-0.038043	2.157990
H	-1.664599	1.545579	2.979940
H	-2.072217	1.465074	1.235094
H	0.584099	0.789735	3.725678
H	0.235182	-0.772900	2.914832
H	1.717970	0.119774	2.499315
C	-5.584839	-1.482986	-0.181438
H	-6.578369	-1.172428	0.180302
H	-5.452781	-1.097427	-1.203513
H	-5.554818	-2.583818	-0.209850
N	0.306622	1.998434	-0.930168
N	-0.063891	0.932131	1.701665

ts-4-5B
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.309927
Total energy: -2500.546996

Ni	-0.592072	0.256312	-0.399723
C	2.662545	-1.079122	-0.125515
C	1.493406	-1.264622	-1.009604
C	0.428176	-2.016335	-0.645792
H	1.584174	-0.867229	-2.020970
H	-0.772383	0.160566	-1.843702
H	0.381649	-2.486037	0.338620
H	-0.336459	-2.288221	-1.371767
O	3.644253	-0.403950	-0.754669
O	2.761494	-1.475673	1.021874
C	4.874939	-0.171934	-0.035576
H	5.328908	0.693693	-0.538895
H	4.639230	0.104042	1.003690
I	-2.938233	-0.984475	-0.287296
N	0.201731	2.112075	-0.706777
H	-0.889368	-1.299652	2.315361
C	-0.069768	-0.578756	2.439851
N	-0.358214	0.615214	1.626589
H	0.017571	-0.313715	3.510225
H	0.869553	-1.037595	2.111697
C	0.800432	1.539292	1.615893
C	-1.561468	1.281910	2.165770
C	0.553087	2.667534	0.633092
H	1.685766	0.961253	1.319677
H	0.992639	1.945552	2.627266
H	-1.346281	1.737385	3.150485
H	-2.361399	0.542342	2.281152
H	-1.924102	2.056906	1.479862
H	1.438768	3.320540	0.563986
H	-0.276525	3.297288	0.978200
C	-0.832156	2.942056	-1.359483
C	1.401661	2.051992	-1.563612
H	-1.048132	2.536923	-2.355553
H	-0.491475	3.989828	-1.460182
H	-1.757093	2.915946	-0.768083
H	1.775819	3.070061	-1.781321

```
 H   1.154621   1.548662  -2.506010
 H   2.192067   1.483759  -1.062251
 C   5.786881  -1.383302  -0.087787
 H   6.744351  -1.148012   0.404426
 H   5.331234  -2.238289   0.433758
 H   5.994223  -1.671825  -1.130487
```

ts-4-6B
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.306149
Total energy: -2500.548329

```
Ni  -0.048667   0.305852  -0.247829
 C  -2.495909  -0.785286  -0.618952
 C  -1.117236  -1.201010  -0.967092
 C  -0.426908  -0.513301  -1.996674
 H  -0.834718  -2.206319  -0.644302
 H   0.697457  -0.850176   0.166410
 H  -0.988249   0.177594  -2.633998
 H   0.442919  -0.988654  -2.461668
 O  -3.062607  -1.634896   0.258575
 O  -3.056916   0.215755  -1.033561
 C  -4.401064  -1.342521   0.711342
 H  -4.494696  -1.881139   1.665377
 H  -4.489950  -0.262326   0.904192
 I   2.912316  -1.392141  -0.056407
 N  -0.144452   0.910315   1.700586
 H  -0.340675   2.312980  -2.784118
 C  -0.586305   2.809371  -1.837034
 N   0.293887   2.302339  -0.769993
 H  -0.460378   3.900232  -1.970551
 H  -1.632661   2.585107  -1.589046
 C   0.061558   3.056223   0.485986
 C   1.705286   2.377554  -1.195480
 C   0.501749   2.246812   1.693416
 H  -1.013235   3.275543   0.548879
 H   0.589431   4.027230   0.465880
 H   1.987688   3.418216  -1.444309
 H   1.851964   1.739965  -2.077019
 H   2.364458   2.004746  -0.401673
 H   0.272321   2.795645   2.625547
 H   1.587844   2.081528   1.666123
 C   0.513355   0.037401   2.689681
 C  -1.586471   0.999803   2.010230
 H   0.057057  -0.960600   2.656042
 H   0.406174   0.451656   3.709145
 H   1.577930  -0.060295   2.445077
 H  -1.751403   1.487766   2.988687
 H  -2.004498  -0.013845   2.040725
 H  -2.117672   1.562694   1.233037
 C  -5.443156  -1.808207  -0.288886
 H  -6.452868  -1.640805   0.119827
 H  -5.354862  -1.250213  -1.233104
 H  -5.328705  -2.883412  -0.499877
```

2C
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.339808
Total energy: -2539.890322

```
 C   1.801332  -0.656649  -0.794922
 C  -2.847200  -1.609283   1.544775
 H  -3.292929  -1.453862   2.543644
 H  -3.073653  -2.641504   1.243924
 C  -3.430540  -0.629684   0.545621
 H  -3.252154   0.401324   0.880094
 H  -4.521494  -0.765911   0.445755
Ni  -0.844412  -1.015642  -0.386120
 O   3.089405  -0.543575  -0.622790
 O   1.051867  -1.085375   0.102955
 C  -3.060672   0.433191  -1.588805
 H  -2.688994   0.303945  -2.610610
 H  -4.150005   0.610864  -1.626827
 H  -2.558852   1.298940  -1.136389
 C  -3.260657  -1.978800  -1.501346
 H  -4.347634  -1.905899  -1.685577
 H  -2.736239  -2.064060  -2.461128
 H  -3.055896  -2.882917  -0.914042
 C  -0.713576  -2.699407   2.005526
 H   0.373851  -2.556088   1.976297
 H  -1.014998  -2.985052   3.030630
 H  -0.977783  -3.513043   1.314787
 C  -0.954289  -0.332532   2.437799
 H  -1.202587  -0.527413   3.497908
 H   0.128666  -0.189638   2.334083
 H  -1.441803   0.594840   2.113998
 C   3.651323  -0.860114   0.684709
 H   3.215700  -0.160671   1.414655
 H   3.344650  -1.883326   0.953792
 I   0.012894   2.961171   0.245502
 C  -0.173647  -0.864980  -2.206968
 H  -0.799392  -0.312109  -2.922016
 H  -0.079958  -1.905452  -2.579483
 C   1.214495  -0.222689  -2.094809
 H   1.919204  -0.418332  -2.921964
 H   1.125100   0.876271  -2.002982
 N  -2.771105  -0.778798  -0.788186
 N  -1.375108  -1.455428   1.581528
 C   5.157016  -0.725948   0.588166
 H   5.401472   0.308007   0.290371
 H   5.556118  -0.861985   1.607794
 C   5.798276  -1.726445  -0.372377
 H   5.408432  -1.598920  -1.395031
 H   6.891453  -1.596137  -0.409863
 H   5.592044  -2.764735  -0.060999
```

2C'
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.341491
Total energy: -2539.869795

C	-2.439866	-0.766025	-1.578539
C	-2.207050	0.491159	-2.355344
C	-0.729452	0.860734	-2.222308
H	-2.557872	0.312898	-3.385753
H	-2.850212	1.282350	-1.927480
H	-0.087870	0.071085	-2.656223
H	-0.522887	1.797177	-2.760404
C	0.102067	2.509368	1.969495
H	0.459766	2.604333	3.009087
H	-0.624667	3.315513	1.804127
C	1.250625	2.622471	0.994112
H	1.980631	1.819708	1.166215
H	1.777311	3.586567	1.100970
O	-1.709383	-0.713902	-0.391186
O	-3.077430	-1.732629	-1.886161
C	1.892816	2.225723	-1.298045
H	1.553098	2.168468	-2.337356
H	2.621645	3.049984	-1.204451
H	2.372140	1.276322	-1.026653
C	0.022070	3.690556	-0.827286
H	0.689382	4.567880	-0.761709
H	-0.313860	3.575488	-1.863003
H	-0.859242	3.862259	-0.197773
C	-2.003044	1.302767	2.136009
H	-2.509607	0.359811	1.905672
H	-2.120206	1.522556	3.213233
H	-2.486994	2.100282	1.554589
C	0.102344	0.158532	2.534855
H	-0.389393	-0.805617	2.387400
H	1.141638	0.057273	2.199581
H	0.084899	0.397972	3.613931
C	-1.432864	-2.008947	0.258011
H	-0.398965	-1.915081	0.609729
H	-1.455194	-2.768543	-0.534002
I	2.692736	-1.698731	-0.094307
Ni	-0.488710	0.940105	-0.311395
N	0.740266	2.468357	-0.398831
N	-0.581924	1.209020	1.756935
C	-2.396947	-2.359011	1.378451
H	-2.048355	-3.333408	1.764132
H	-2.276297	-1.648657	2.210949
C	-3.870866	-2.446986	0.989027
H	-4.033543	-3.176790	0.182090
H	-4.479252	-2.746304	1.857709
H	-4.250109	-1.475186	0.634165

3C
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.339256
Total energy: -2539.903315

Ni	0.829345	0.349709	-0.366487
I	1.861701	-2.089817	-0.178775
C	-0.281747	-0.251198	-1.849395
C	-1.461893	-1.070324	-1.313327
H	0.272569	-0.867827	-2.578110
H	-0.685405	0.604045	-2.417255
C	-2.138804	-0.460914	-0.111416
H	-1.109277	-2.056203	-0.958690
H	-2.232149	-1.278086	-2.077076
O	-3.439425	-0.760532	-0.037168
O	-1.574364	0.202973	0.741270
C	-4.166760	-0.298526	1.120771
H	-3.729488	-0.760105	2.021370
H	-4.039405	0.793383	1.210426
H	0.613700	2.052980	-2.969959
C	1.208086	2.564992	-2.204768
H	1.224430	3.647194	-2.431911
H	2.233939	2.174097	-2.238584
C	1.424006	3.061912	0.149083
C	-0.772541	2.782486	-0.832413
C	1.250628	2.412641	1.502496
H	2.478584	3.029984	-0.154009
H	1.124840	4.124467	0.175282
H	-0.830172	3.860078	-1.071227
H	-1.367232	2.225027	-1.564434
H	-1.203539	2.600878	0.158134
H	1.806751	2.969344	2.279679
H	0.190334	2.418092	1.790172
C	1.145203	0.255482	2.579473
C	3.167914	0.918630	1.439778
H	1.493454	-0.783854	2.541361
H	1.466174	0.708450	3.536583
H	0.049688	0.257348	2.519790
H	3.586859	1.382936	2.352884
H	3.473164	-0.133349	1.397986
H	3.585037	1.424391	0.559580
N	0.630375	2.321028	-0.867658
N	1.695980	1.003271	1.434403
C	-5.625164	-0.677851	0.944270
H	-6.149505	-0.405638	1.876483
H	-5.696820	-1.775562	0.852203
C	-6.289296	-0.000896	-0.254078
H	-5.777488	-0.269491	-1.191936
H	-7.345539	-0.300308	-0.347420
H	-6.257249	1.097954	-0.157459

4C
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy:

0.337694
Total energy: -2539.883019

Ni	-0.496386	-0.123750	-0.151158
C	2.477729	-0.525006	0.175152
C	1.276189	-1.196422	-0.367384
C	0.338306	-1.865978	0.435967
H	1.383830	-1.468610	-1.419790
H	-0.640024	-0.652114	-1.459479
H	0.477581	-1.894924	1.519725
H	-0.228881	-2.698800	0.012591
O	3.294595	-0.143873	-0.829016
O	2.738822	-0.336301	1.349715
C	4.562965	0.467160	-0.518715
H	4.654701	1.323403	-1.204131
H	4.546535	0.838677	0.516410
I	-3.068717	-1.086995	-0.337365
N	-0.413211	1.761296	-1.059734
H	-0.481386	-0.592433	3.146981
C	0.079238	0.313819	2.880453
N	-0.545591	0.942488	1.701894
H	0.058332	1.004071	3.744723
H	1.115541	0.043792	2.655246
C	0.225495	2.145171	1.301599
C	-1.931217	1.302021	2.066826
C	-0.350947	2.762418	0.040200
H	1.265522	1.830069	1.135722
H	0.230404	2.895380	2.115904
H	-1.933830	2.065897	2.867253
H	-2.452155	0.405842	2.423884
H	-2.487191	1.680405	1.202791
H	0.251777	3.635655	-0.263366
H	-1.366182	3.132324	0.229836
C	-1.574308	2.015306	-1.930040
C	0.825041	1.813889	-1.861494
H	-1.591093	1.276425	-2.741693
H	-1.526742	3.030366	-2.366769
H	-2.501703	1.908224	-1.353715
H	0.909315	2.784429	-2.385844
H	0.823288	1.003040	-2.600536
H	1.699518	1.683272	-1.215438
C	5.699173	-0.523463	-0.734168
H	6.643586	0.025735	-0.573458
H	5.696151	-0.841265	-1.791506
C	5.636056	-1.746571	0.179909
H	5.639757	-1.455106	1.242859
H	4.720667	-2.333459	-0.001319
H	6.495483	-2.413685	0.005335

6C
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy:
0.333585
Total energy: -2539.880873

C	0.167002	-0.109738	-2.167462
H	-0.631695	-0.671925	-2.665062
H	0.663875	0.635422	-2.804698
C	0.945836	-0.767583	-1.160107
H	0.713478	-1.782080	-0.823943
C	2.283613	-0.271850	-0.816022
O	2.807287	0.743296	-1.251194
O	2.879674	-1.051301	0.121438
C	4.187611	-0.669250	0.577905
H	4.239191	0.426673	0.676880
H	4.284411	-1.118100	1.578236
Ni	-0.232293	0.619655	-0.424707
C	-1.232096	1.739030	1.893855
H	-2.061777	1.017700	1.899110
H	-1.170897	2.193737	2.900712
C	-1.484782	2.813734	0.844858
H	-0.688946	3.569779	0.878545
H	-2.432626	3.338159	1.055158
C	-2.863382	1.801268	-0.900883
C	-0.958360	3.151566	-1.521122
C	0.113725	-0.237231	2.387021
C	1.217652	1.801673	1.735804
H	-1.273463	-0.446310	-0.212677
H	0.094802	3.372316	-1.295281
H	-1.528894	4.099219	-1.536152
H	-1.010403	2.689756	-2.515774
H	-3.518931	2.682249	-1.033773
H	-2.824030	1.230529	-1.837779
H	-3.288778	1.151183	-0.127513
H	0.981014	-0.815828	2.040796
H	0.240103	0.006262	3.458906
H	-0.786772	-0.850470	2.259798
H	1.281946	2.222168	2.756961
H	1.242698	2.626192	1.011311
H	2.098988	1.173007	1.560136
I	-2.651781	-1.929143	0.058930
N	-1.501958	2.216090	-0.519089
N	0.001277	0.983966	1.573762
C	5.281217	-1.174439	-0.354399
H	5.126392	-0.725537	-1.349336
H	5.167094	-2.265958	-0.470954
C	6.677143	-0.836637	0.166156
H	7.456985	-1.210987	-0.515997
H	6.815737	0.253546	0.264784
H	6.857119	-1.286070	1.157800

7C
Geometry with 43 atoms:
Thermal correction to Gibbs Free Energy:
0.330573
Total energy: -2241.375933

C	0.397122	-2.252562	-0.645282
H	0.868095	-2.848834	-1.444707

H	0.152713	-2.874375	0.232855
C	-0.597685	-1.267562	-1.053155
H	-0.764715	-1.023790	-2.110789
C	-1.680297	-0.885433	-0.161467
O	-1.902161	-1.300636	0.969195
O	-2.468553	0.097678	-0.718756
C	-3.559913	0.589165	0.063171
H	-3.253311	0.684183	1.117726
H	-3.772320	1.596326	-0.330362
Ni	1.016537	-0.482932	-0.294064
C	2.368379	1.974255	0.002207
H	2.824397	1.974112	-0.997971
H	2.461796	3.001818	0.403280
C	3.101808	0.989628	0.905217
H	2.686882	1.036369	1.921603
H	4.172449	1.259324	0.977393
C	3.821136	-0.691479	-0.721010
C	3.151579	-1.373604	1.494853
C	0.348568	2.163573	-1.359221
C	0.146600	1.927478	1.029506
H	2.431549	-1.194615	2.305347
H	4.179950	-1.304120	1.901459
H	2.986444	-2.387278	1.106803
H	4.887008	-0.626901	-0.424946
H	3.609990	-1.702566	-1.093217
H	3.637060	0.015587	-1.540773
H	-0.677317	1.784174	-1.458370
H	0.329630	3.270832	-1.315152
H	0.921754	1.851553	-2.243531
H	0.136698	3.021592	1.204929
H	0.539902	1.427711	1.924558
H	-0.883693	1.582789	0.876178
N	0.950459	1.580812	-0.152203
N	2.930804	-0.400116	0.415054
C	-4.792386	-0.301467	-0.047437
H	-4.530393	-1.301351	0.335207
H	-5.045304	-0.420287	-1.115548
C	-5.984093	0.264461	0.722733
H	-6.865660	-0.390612	0.634010
H	-5.753896	0.368746	1.796916
H	-6.270787	1.261797	0.346723

C_3H_7I
Geometry with 11 atoms:
Thermal correction to Gibbs Free Energy: 0.062809
Total energy: -416.438123

C	3.460499	0.021030	0.000076
C	2.021250	-0.505142	0.000057
H	4.179778	-0.814147	0.000120
H	3.662692	0.638946	-0.890848
H	3.662648	0.638999	0.890973
C	1.029828	0.645694	-0.000001
H	1.852628	-1.140089	-0.885499
H	1.852586	-1.140036	0.885644
H	1.110644	1.274641	0.896758
H	1.110682	1.274582	-0.896799
I	-1.066059	-0.032121	-0.000021

$CH_2CHCOOC_3H_7$
Geometry with 18 atoms:
Thermal correction to Gibbs Free Energy: 0.117184
Total energy: -385.191521

C	-1.033704	0.045907	-0.183042
C	-2.346293	-0.514774	0.236101
C	-3.426807	0.265906	0.344686
H	-2.377791	-1.586851	0.449093
H	-3.362063	1.336413	0.124823
H	-4.395649	-0.137256	0.652395
O	-0.094956	-0.915013	-0.220981
O	-0.823635	1.208828	-0.459510
C	1.245026	-0.534004	-0.589860
H	1.707917	-1.457844	-0.967843
H	1.202891	0.201703	-1.408506
C	2.020143	0.019701	0.598540
H	1.505929	0.923937	0.963407
H	1.989766	-0.722361	1.414840
C	3.465853	0.348385	0.229502
H	3.512734	1.106046	-0.570971
H	4.015559	0.745574	1.097544
H	4.004127	-0.546604	-0.126418

ts-1-2C
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.334317
Total energy: -2539.856895

Ni	2.365444	0.296763	-0.076118
O	0.538174	0.779645	-0.163349
C	0.266521	1.983493	-0.531568
O	-0.891722	2.440688	-0.564962
C	2.711493	2.199927	-0.270434
H	3.634979	2.480047	-0.802464
H	2.797117	2.595640	0.762508
C	1.475191	2.792863	-0.954221
H	1.294247	3.867612	-0.775951
H	1.541817	2.665596	-2.050570
C	1.201796	-2.198294	-0.930801
H	0.349104	-1.564245	-1.206264
H	1.935098	-2.161095	-1.747662
H	0.858822	-3.242651	-0.806085
C	0.816816	-1.734096	1.408081
H	1.246012	-1.272988	2.309097
H	-0.074679	-1.164929	1.119656

H	0.531108	-2.777494	1.638104
C	5.100757	0.184423	-1.136268
H	4.601212	-0.003684	-2.096216
H	5.247308	1.263275	-1.018644
H	6.089047	-0.309538	-1.136304
C	4.848518	0.073744	1.263706
H	4.239486	-0.307471	2.093092
H	5.880098	-0.309157	1.368186
H	4.861635	1.169303	1.321149
C	3.049468	-2.375956	0.671733
H	3.234298	-2.207006	1.741461
H	2.961905	-3.467820	0.524049
C	4.194946	-1.821240	-0.152459
H	5.155122	-2.275597	0.149668
H	4.039651	-2.054276	-1.214998
C	-2.419346	0.966516	-0.058063
H	-1.804016	0.237615	-0.576747
H	-3.014831	1.652501	-0.652095
I	-4.541115	-0.772357	-0.370482
N	4.265865	-0.334935	-0.032790
N	1.796561	-1.679033	0.311734
C	-2.334747	1.089563	1.431528
H	-2.471828	0.093197	1.880913
H	-1.290786	1.360657	1.659886
C	-3.302927	2.104595	2.028098
H	-4.346867	1.820526	1.817768
H	-3.180639	2.173221	3.120629
H	-3.127292	3.106223	1.602542

ts-1-2C'
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.338044
Total energy: -2539.845923

C	0.737777	2.668832	-0.968497
C	1.565011	2.142930	-2.126532
C	1.457440	0.615871	-2.157907
H	1.259919	2.665177	-3.051168
H	2.608525	2.449965	-1.926683
H	0.479895	0.302016	-2.573531
H	2.239485	0.172322	-2.796282
C	2.781128	-1.305436	1.858123
H	2.743299	-1.785505	2.852214
H	3.806228	-0.937885	1.714752
C	2.423923	-2.300521	0.771802
H	1.406056	-2.682937	0.929794
H	3.109134	-3.166445	0.781786
Ni	1.564258	0.120931	-0.288168
O	0.577798	1.755694	-0.005417
O	0.252265	3.783105	-0.897676
C	-1.414896	1.037264	-0.079893
H	-1.025435	0.276053	0.582146
H	-1.302306	0.869096	-1.148682
I	-3.378735	-1.133179	-0.250776
C	-2.204218	2.187443	0.416235
H	-1.687488	3.092300	0.044876
H	-3.172021	2.180057	-0.113070
C	-2.387342	2.238633	1.928078
C	0.598452	-0.423088	2.489071
H	0.778033	-0.619703	3.562563
H	-0.062392	0.446618	2.400830
H	0.091018	-1.292464	2.049713
C	2.479173	1.076874	2.312709
H	1.786952	1.915412	2.164593
H	2.716819	0.976600	3.388298
H	3.405090	1.291695	1.760284
C	1.705485	-2.472432	-1.533604
H	1.748067	-2.014979	-2.528142
H	2.143177	-3.485502	-1.584321
H	0.654353	-2.546906	-1.223889
C	3.838085	-1.441302	-1.029772
H	4.358171	-2.411912	-1.119953
H	3.828989	-0.946382	-2.007309
H	4.388524	-0.802870	-0.327443
N	2.447742	-1.636766	-0.564636
N	1.859879	-0.148562	1.782274
H	-3.011923	3.098367	2.216108
H	-2.874598	1.322084	2.298261
H	-1.415805	2.344629	2.436483

ts-2-3C
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.341315
Total energy: -2539.888864

C	2.012931	-0.299084	-0.469484
C	-2.265043	-1.811859	1.727873
H	-2.944901	-1.909703	2.594718
H	-1.433063	-2.512729	1.883257
C	-2.995141	-2.133592	0.440630
H	-3.825123	-1.431640	0.290557
H	-3.427428	-3.148981	0.471919
Ni	-0.840604	-0.450548	-0.261520
O	3.329688	-0.244633	-0.339209
O	1.268814	-0.536219	0.477607
C	-2.839249	-1.776976	-1.951847
H	-3.380378	-0.824405	-1.877724
H	-3.562265	-2.597732	-2.114175
H	-2.160689	-1.729830	-2.811262
C	-1.257050	-3.231119	-0.839319
H	-1.909397	-4.107374	-1.009078
H	-0.562216	-3.139167	-1.680453
H	-0.669074	-3.394864	0.072397
C	-0.694864	-0.226485	2.690314
H	-0.232788	0.757805	2.540179
H	-1.153726	-0.269347	3.695697

H	0.090670	-0.987166	2.613181
C	-2.777904	0.558210	1.775167
H	-3.360386	0.381053	2.698715
H	-2.337186	1.559438	1.811284
H	-3.452657	0.525493	0.910566
C	3.886193	-0.423587	0.986217
H	3.497333	0.375225	1.637523
H	3.536355	-1.388892	1.387976
I	-0.541157	2.565064	-0.265888
C	0.042292	-0.471102	-1.996659
H	-0.492836	0.171998	-2.717051
H	0.045495	-1.490033	-2.419597
C	1.493896	0.000985	-1.844553
H	2.195107	-0.410256	-2.591972
H	1.561534	1.099882	-1.928786
N	-2.065907	-1.998870	-0.714343
N	-1.703135	-0.446716	1.639730
C	5.397473	-0.377373	0.872212
H	5.801689	-0.409192	1.898579
H	5.690199	0.599136	0.449182
C	5.980932	-1.516075	0.036853
H	5.585230	-1.493811	-0.991120
H	7.078861	-1.445757	-0.021826
H	5.728343	-2.497908	0.472625

ts-2-3C'
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.341130
Total energy: -2539.880141

C	-1.411073	2.440099	-0.468792
C	-0.204347	2.493272	-1.372192
C	0.286698	1.110281	-1.809558
H	-0.480936	3.151420	-2.215655
H	0.577430	3.042733	-0.815374
H	-0.534119	0.561015	-2.300686
H	1.089205	1.226369	-2.554885
C	2.645230	0.418280	1.946788
H	3.152570	0.100645	2.876134
H	2.542580	1.511877	1.988344
C	3.448326	0.018902	0.730740
H	3.503448	-1.075240	0.659948
H	4.483526	0.397473	0.790115
O	-1.427888	1.282028	0.232367
O	-2.262382	3.290377	-0.355755
C	3.208927	-0.296882	-1.653236
H	2.771616	0.097140	-2.577149
H	4.310249	-0.287872	-1.746905
H	2.861968	-1.329414	-1.514431
C	3.146549	1.937577	-0.725688
H	4.239141	2.037121	-0.858123
H	2.649568	2.314997	-1.625674
H	2.835917	2.549178	0.130866
C	0.358531	0.578864	2.713064
H	-0.625868	0.099113	2.686662
H	0.711905	0.596783	3.761013
H	0.258432	1.609850	2.347989
C	1.306385	-1.583597	2.265149
H	0.294744	-1.997821	2.189600
H	1.955187	-2.170716	1.603235
H	1.665978	-1.682066	3.306809
C	-2.618227	0.943163	0.976868
H	-2.866939	1.776241	1.653590
H	-2.325422	0.068672	1.571626
I	-0.748934	-2.107380	-0.683397
Ni	0.813393	0.224110	-0.177756
N	2.780362	0.524437	-0.500598
N	1.289302	-0.168469	1.851467
C	-3.789028	0.592909	0.068389
H	-4.064979	1.477720	-0.525874
H	-3.456816	-0.187382	-0.635731
C	-4.990772	0.103016	0.875083
H	-5.342362	0.871392	1.584778
H	-5.833934	-0.148232	0.212148
H	-4.742287	-0.801284	1.456148

ts-3-4C
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.336533
Total energy: -2539.862670

Ni	0.205667	0.198834	-0.093694
I	3.104464	-1.474752	0.021051
C	-0.311668	-0.907407	-1.710987
C	-1.156609	-1.218317	-0.640033
H	0.477100	-1.609462	-1.992395
H	-0.672993	-0.233573	-2.488336
C	-2.440296	-0.480077	-0.446142
H	0.119828	-0.933821	0.763141
H	-1.101037	-2.178905	-0.124086
O	-3.087308	-0.941990	0.635271
O	-2.849207	0.419279	-1.154913
C	-4.361241	-0.366276	0.998094
H	-4.315931	-0.214882	2.086872
H	-4.471415	0.610611	0.505089
H	2.089726	1.040352	-2.291815
C	1.986653	1.882753	-1.595887
H	2.280989	2.819990	-2.103132
H	2.662117	1.698779	-0.752489
C	0.412461	3.015018	-0.100936
C	-0.290724	2.276094	-2.279773
C	0.929322	2.548542	1.243230
H	0.926222	3.943708	-0.408205
H	-0.660214	3.244646	-0.037823
H	-0.125119	3.316434	-2.613221
H	-0.060808	1.610821	-3.120773

H	-1.341057	2.136254	-1.995167
H	2.014990	2.386683	1.201809
H	0.736602	3.311407	2.018780
C	-1.101010	1.431278	2.049896
C	1.079283	0.623976	2.704084
H	-1.529734	0.448708	2.280818
H	-1.154829	2.077616	2.944867
H	-1.696962	1.882471	1.246810
H	1.131712	1.298118	3.578041
H	0.597973	-0.316085	3.001484
H	2.092101	0.397576	2.348657
C	-5.497878	-1.307962	0.626517
H	-6.428445	-0.860324	1.017455
H	-5.357459	-2.261537	1.164708
N	0.584556	1.958107	-1.132539
N	0.302816	1.253963	1.616268
C	-5.624586	-1.566366	-0.874178
H	-5.769289	-0.627830	-1.433633
H	-4.721386	-2.056320	-1.273264
H	-6.479673	-2.227275	-1.088758

ts-4-5C
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.337101
Total energy: -2539.867674

Ni	-0.902731	0.276838	-0.396387
C	2.429758	-0.923821	-0.263905
C	1.246629	-1.097387	-1.131475
C	0.227708	-1.924105	-0.799537
H	1.289711	-0.622964	-2.112142
H	-1.131323	0.232398	-1.836594
H	0.229726	-2.464942	0.149192
H	-0.543992	-2.177566	-1.524668
O	3.354346	-0.138711	-0.850804
O	2.584752	-1.416164	0.839019
C	4.585254	0.099886	-0.138892
H	4.977069	1.036475	-0.562429
H	4.363614	0.257997	0.928371
I	-3.177694	-1.090772	-0.250199
N	-0.214105	2.179769	-0.655122
H	-1.000853	-1.415999	2.243865
C	-0.214911	-0.658647	2.368363
N	-0.603484	0.556195	1.630987
H	-0.090192	-0.441811	3.445891
H	0.729327	-1.051592	1.975927
C	0.502657	1.543204	1.617271
C	-1.814791	1.124302	2.257953
C	0.155492	2.696524	0.695188
H	1.405419	1.029597	1.260507
H	0.714066	1.915690	2.637749
H	-1.579814	1.531809	3.258997
H	-2.569062	0.336370	2.360069
H	-2.248584	1.917280	1.637286
H	0.999841	3.402125	0.624705
H	-0.695079	3.260654	1.097285
C	-1.310050	2.983644	-1.235755
C	0.955443	2.219281	-1.553890
H	-1.542942	2.609551	-2.240098
H	-1.023115	4.050008	-1.303568
H	-2.210206	2.888909	-0.613940
H	1.273577	3.263610	-1.732425
H	0.697559	1.751757	-2.511954
H	1.788543	1.664556	-1.109537
C	5.575565	-1.041810	-0.323758
H	5.126508	-1.965501	0.075906
H	5.734392	-1.199054	-1.404369
C	6.903885	-0.756632	0.375491
H	6.764267	-0.621858	1.461543
H	7.613035	-1.587045	0.231297
H	7.377277	0.159600	-0.016579

ts-4-6C
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.332012
Total energy: -2539.868382

Ni	0.234682	0.418419	-0.244753
C	-2.371826	-0.267650	-0.501778
C	-1.091800	-0.920356	-0.864260
C	-0.333967	-0.400414	-1.942765
H	-0.967856	-1.943878	-0.501701
H	0.768943	-0.832415	0.219400
H	-0.798024	0.345630	-2.595549
H	0.430137	-1.031279	-2.408334
O	-3.042256	-0.975723	0.426479
O	-2.774583	0.794082	-0.947788
C	-4.305780	-0.454165	0.889699
H	-4.469930	-0.952686	1.856746
H	-4.210464	0.629466	1.057687
I	2.822590	-1.825486	-0.033728
N	0.308821	1.120021	1.671578
H	0.260161	2.302503	-2.900026
C	0.093675	2.882523	-1.983790
N	0.876317	2.300109	-0.880140
H	0.393737	3.930241	-2.172978
H	-0.976005	2.843771	-1.736655
C	0.758338	3.149971	0.328837
C	2.283452	2.121926	-1.289932
C	1.113075	2.365482	1.579501
H	-0.280380	3.504305	0.385368
H	1.402605	4.044787	0.246729
H	2.736964	3.088485	-1.580951
H	2.327475	1.429501	-2.140834
H	2.867290	1.681095	-0.472166
H	0.965973	2.991451	2.478751

H	2.170933	2.069337	1.553700
C	0.893459	0.216840	2.679529
C	-1.098048	1.402728	2.025902
H	0.311136	-0.712952	2.717940
H	0.888298	0.690615	3.678371
H	1.924023	-0.032837	2.399126
H	-1.161937	1.939392	2.990571
H	-1.640326	0.452609	2.106320
H	-1.580772	2.004798	1.246268
C	-5.440350	-0.757041	-0.081062
H	-6.363415	-0.339642	0.358366
H	-5.259128	-0.203545	-1.016839
C	-5.615272	-2.247221	-0.368145
H	-4.701985	-2.674833	-0.812236
H	-5.831928	-2.810688	0.555587
H	-6.444893	-2.421740	-1.071989

H	-1.046254	-0.357332	-2.932639
H	-0.253456	-1.909773	-2.565959
C	0.951594	-0.160629	-2.084893
H	1.676893	-0.335032	-2.899130
H	0.808925	0.933876	-2.013463
N	-3.015511	-0.885074	-0.806579
N	-1.609511	-1.502702	1.574486
C	4.852816	-0.293051	0.698295
H	4.988614	0.761125	0.399328
H	5.234098	-0.377157	1.731060
C	5.649395	-1.213492	-0.230369
H	5.230184	-1.145800	-1.249088
H	5.506457	-2.260956	0.092664
C	7.139802	-0.879791	-0.262225
H	7.590914	-0.964384	0.741462
H	7.691078	-1.557300	-0.934646
H	7.309720	0.151927	-0.614559

2D

Geometry with 48 atoms:

Thermal correction to Gibbs Free Energy:
0.366494

Total energy: -2579.211703

C	1.542541	-0.543979	-0.770711
C	-3.071865	-1.726923	1.522988
H	-3.534347	-1.598559	2.518142
H	-3.245566	-2.767452	1.215457
C	-3.692132	-0.771525	0.522448
H	-3.564263	0.265065	0.862322
H	-4.774855	-0.957114	0.413352
Ni	-1.083607	-1.041251	-0.389350
O	2.816418	-0.341549	-0.577314
O	0.808383	-1.015475	0.118464
C	-3.344237	0.320032	-1.602524
H	-2.956713	0.212081	-2.620942
H	-4.439213	0.455313	-1.651481
H	-2.881367	1.202041	-1.139872
C	-3.452434	-2.098711	-1.530866
H	-4.539446	-2.065253	-1.725818
H	-2.915647	-2.159121	-2.485588
H	-3.220378	-2.997765	-0.945960
C	-0.893806	-2.714725	2.003195
H	0.185888	-2.519954	1.985896
H	-1.192302	-3.017017	3.024340
H	-1.111693	-3.538341	1.308101
C	-1.250541	-0.362909	2.436679
H	-1.499828	-0.571620	3.493910
H	-0.174518	-0.169658	2.344007
H	-1.777568	0.541580	2.110187
C	3.371111	-0.598733	0.746637
H	2.837658	0.043329	1.463701
H	3.172879	-1.651159	1.004304
I	-0.373407	2.954264	0.241648
C	-0.401844	-0.871552	-2.205181

2D'

Geometry with 48 atoms:

Thermal correction to Gibbs Free Energy:
0.368890

Total energy: -2579.191525

C	2.048999	-0.011849	-2.003817
C	1.354120	-1.169309	-2.647363
C	-0.125828	-1.101242	-2.273988
H	1.570060	-1.124889	-3.728104
H	1.813948	-2.099066	-2.263883
H	-0.585247	-0.173972	-2.664091
H	-0.665257	-1.954980	-2.708401
C	-0.731182	-2.321321	2.108774
H	-0.949490	-2.253417	3.188113
H	-0.299571	-3.315236	1.931912
C	-1.991439	-2.135953	1.296628
H	-2.433066	-1.149660	1.494959
H	-2.747135	-2.901024	1.546294
O	1.532449	0.179935	-0.722680
O	2.877365	0.718758	-2.468683
C	-2.831479	-1.691848	-0.919839
H	-2.645285	-1.779882	-1.995149
H	-3.729444	-2.280601	-0.662430
H	-2.998221	-0.635685	-0.672700
C	-1.350806	-3.580422	-0.570367
H	-2.198776	-4.249507	-0.340569
H	-1.157719	-3.606477	-1.648090
H	-0.454789	-3.943416	-0.052518
C	1.633711	-1.799875	1.871294
H	2.347891	-1.059747	1.496121
H	1.856934	-2.013110	2.932845
H	1.760451	-2.722683	1.287444
C	0.046746	-0.063434	2.485162
H	0.769705	0.703137	2.196965
H	-0.957143	0.334818	2.293910

H	0.164504	-0.264589	3.565751
C	1.798849	1.493169	-0.108716
H	0.861066	1.750984	0.397417
H	1.945883	2.199748	-0.935018
I	-2.305283	2.340978	0.062817
Ni	-0.072857	-1.059343	-0.348582
N	-1.664382	-2.192729	-0.157268
N	0.260502	-1.293914	1.699486
C	2.988696	1.500704	0.836262
H	3.100156	2.550786	1.161272
H	2.750600	0.931594	1.749063
C	4.313531	0.993587	0.261714
H	4.566507	1.567142	-0.644141
H	4.187046	-0.051691	-0.071211
C	5.453031	1.068247	1.276837
H	6.397227	0.691917	0.850321
H	5.626416	2.106033	1.609225
H	5.229701	0.467465	2.175546
C	3.492336	0.868803	1.407854
H	1.794333	-0.797916	2.530572
H	1.814294	0.695921	3.523964
H	0.374371	0.275552	2.526960
H	3.930700	1.331281	2.312752
H	3.776708	-0.189103	1.371034
H	3.909595	1.359566	0.519246
N	0.956308	2.314164	-0.876059
N	2.022442	0.982412	1.418316
C	-5.326374	-0.552561	1.045632
H	-5.828086	-0.285743	1.992590
H	-5.425486	-1.647220	0.936052
C	-6.014105	0.154971	-0.125301
H	-5.478605	-0.093443	-1.057637
H	-5.911920	1.247954	0.005841
C	-7.490270	-0.214152	-0.262006
H	-8.055321	0.048405	0.649017
H	-7.961778	0.309421	-1.109869
H	-7.616511	-1.297874	-0.427358

3D
Geometry with 48 atoms:
Thermal correction to Gibbs Free Energy:
0.365791
Total energy: -2579.224079

Ni	1.122386	0.340513	-0.370692
I	2.114072	-2.116977	-0.191608
C	-0.020329	-0.242329	-1.836710
C	-1.209001	-1.035642	-1.280755
H	0.510901	-0.872790	-2.570694
H	-0.414469	0.618893	-2.402216
C	-1.855252	-0.409543	-0.070639
H	-0.871096	-2.027436	-0.928044
H	-1.994464	-1.230099	-2.032426
O	-3.160239	-0.682415	0.024973
O	-1.264011	0.244624	0.771426
C	-3.857918	-0.205828	1.195708
H	-3.415052	-0.678443	2.087699
H	-3.704313	0.882487	1.284689
H	0.907589	2.040284	-2.977164
C	1.522132	2.541937	-2.221074
H	1.558446	3.622878	-2.451906
H	2.538935	2.129227	-2.266693
C	1.777882	3.041237	0.128338
C	-0.436344	2.804201	-0.824800
C	1.606211	2.400510	1.486039
H	2.828049	2.985375	-0.186650
H	1.502342	4.110177	0.154013
H	-0.475124	3.882192	-1.065727
H	-1.051419	2.257221	-1.547808
H	-0.858585	2.634014	0.171493
H	2.181634	2.948706	2.255163
H	0.549409	2.428083	1.784946
C	1.470209	0.249090	2.572004

4D
Geometry with 48 atoms:
Thermal correction to Gibbs Free Energy:
0.364514
Total energy: -2579.203616

Ni	-0.734766	-0.094977	-0.135497
C	2.251439	-0.207229	0.146786
C	1.118370	-1.010847	-0.361949
C	0.258378	-1.745701	0.470204
H	1.239428	-1.296752	-1.409202
H	-0.833652	-0.642866	-1.438915
H	0.415443	-1.737703	1.551610
H	-0.236397	-2.635392	0.072630
O	3.010892	0.230142	-0.878599
O	2.507504	0.035812	1.312550
C	4.208905	0.983369	-0.602017
H	4.214464	1.804211	-1.334895
H	4.147112	1.409687	0.409940
I	-3.221621	-1.308658	-0.341757
N	-0.855126	1.775941	-1.057841
H	-0.610284	-0.532630	3.176298
C	-0.167061	0.430184	2.888489
N	-0.885574	0.965339	1.716898
H	-0.254084	1.123966	3.745752
H	0.889344	0.281753	2.644646
C	-0.279873	2.254162	1.300960
C	-2.299716	1.143952	2.103362
C	-0.936433	2.779529	0.036880
H	0.791653	2.074194	1.132188
H	-0.368699	3.006405	2.108519
H	-2.387894	1.893284	2.912790
H	-2.698538	0.185252	2.456010
H	-2.911342	1.456422	1.251185

H	-0.462334	3.728073	-0.269709
H	-1.994845	3.001281	0.223270
C	-2.013305	1.893845	-1.960541
C	0.389319	1.968086	-1.828546
H	-1.919940	1.158992	-2.770610
H	-2.070935	2.908147	-2.397695
H	-2.938081	1.679173	-1.410624
H	0.369944	2.935974	-2.363948
H	0.505616	1.155244	-2.555927
H	1.255676	1.952757	-1.159319
C	5.444906	0.109444	-0.762414
H	6.326501	0.765635	-0.647250
H	5.475972	-0.277492	-1.796753
C	5.531101	-1.055505	0.226903
H	5.466338	-0.664653	1.257347
H	4.651732	-1.709628	0.094698
C	6.805808	-1.881563	0.058901
H	6.842117	-2.718582	0.775317
H	6.874699	-2.308400	-0.956533
H	7.707065	-1.265048	0.219123
H	-3.113425	1.066932	-1.927225
H	-3.628990	0.986106	-0.231676
H	0.678295	-0.689257	2.098015
H	-0.153089	0.108396	3.479877
H	-1.089941	-0.825367	2.264809
H	0.776753	2.371919	2.772695
H	0.765520	2.747651	1.019986
H	1.690755	1.356772	1.617584
I	-2.838496	-2.042628	0.042459
N	-1.898127	2.150932	-0.586243
N	-0.390696	1.042285	1.572412
C	5.051420	-0.824952	-0.151031
H	4.901512	-0.383743	-1.150796
H	5.021807	-1.921925	-0.274583
C	6.409947	-0.395337	0.408188
H	6.418547	0.702227	0.538651
H	6.541422	-0.823116	1.419029
C	7.580421	-0.813767	-0.480959
H	7.492025	-0.374135	-1.489108
H	8.545655	-0.490158	-0.057993
H	7.618197	-1.909962	-0.601111

6D
Geometry with 48 atoms:
Thermal correction to Gibbs Free Energy:
0.359064
Total energy: -2579.201256

C	-0.053690	-0.105920	-2.141009
H	-0.806351	-0.717102	-2.652191
H	0.422980	0.654305	-2.775810
C	0.726205	-0.706603	-1.099470
H	0.536955	-1.726743	-0.753651
C	2.019940	-0.131114	-0.715283
O	2.494165	0.913358	-1.138053
O	2.631756	-0.869298	0.244407
C	3.895743	-0.401505	0.744997
H	3.868134	0.694611	0.848631
H	3.988448	-0.847608	1.746668
Ni	-0.541681	0.632789	-0.424842
C	-1.676458	1.726787	1.841518
H	-2.461529	0.957185	1.833424
H	-1.674510	2.199045	2.842129
C	-1.958053	2.768877	0.767495
H	-1.208286	3.570088	0.813772
H	-2.940708	3.240290	0.939966
C	-3.219098	1.648873	-1.002553
C	-1.378986	3.101991	-1.586482
C	-0.231574	-0.157864	2.408856
C	0.768770	1.933850	1.756982
H	-1.530720	-0.481160	-0.225471
H	-0.347556	3.386102	-1.332395
H	-2.002151	4.014769	-1.633396
H	-1.373771	2.623873	-2.574797
H	-3.921746	2.486292	-1.171278

7D
Geometry with 46 atoms:
Thermal correction to Gibbs Free Energy:
0.356332
Total energy: -2280.696592

C	0.714529	-2.238028	-0.670500
H	1.183901	-2.840712	-1.466064
H	0.440802	-2.859107	0.199410
C	-0.247174	-1.224980	-1.088631
H	-0.386185	-0.968669	-2.147417
C	-1.337231	-0.819262	-0.216748
O	-1.596260	-1.236653	0.905143
O	-2.082771	0.191760	-0.782747
C	-3.174515	0.713724	-0.020887
H	-2.892212	0.778976	1.042340
H	-3.335604	1.734829	-0.402229
Ni	1.371764	-0.487133	-0.294440
C	2.776946	1.933724	0.057127
H	3.248806	1.939414	-0.935607
H	2.887002	2.952251	0.476560
C	3.473072	0.918246	0.955418
H	3.042893	0.958343	1.965767
H	4.548334	1.161889	1.048675
C	4.177386	-0.753535	-0.687313
C	3.461717	-1.454202	1.507791
C	0.785429	2.190703	-1.333671
C	0.538868	1.923917	1.047967
H	2.733802	-1.272680	2.310691
H	4.485347	-1.413415	1.930034
H	3.280921	-2.457865	1.101128
H	5.240048	-0.720422	-0.374958

H	3.946792	-1.752662	-1.079730
H	4.023180	-0.028585	-1.497494
H	-0.247439	1.838081	-1.455559
H	0.792502	3.297305	-1.272708
H	1.365510	1.878300	-2.213380
H	0.549252	3.015675	1.237413
H	0.908729	1.404737	1.941971
H	-0.496003	1.602883	0.875417
N	1.353130	1.575437	-0.126202
N	3.277955	-0.459296	0.440763
C	-4.436079	-0.125772	-0.181007
H	-4.228412	-1.141553	0.195319
H	-4.663015	-0.221654	-1.257943
C	-5.638028	0.467863	0.557071
H	-5.392585	0.567395	1.630273
H	-5.821636	1.494851	0.190802
C	-6.909255	-0.365875	0.399016
H	-6.764764	-1.389645	0.784515
H	-7.757592	0.080183	0.944002
H	-7.201107	-0.451399	-0.661807

C_4H_9I

Geometry with 14 atoms:

Thermal correction to Gibbs Free Energy: 0.089115

Total energy: -455.759615

C	3.698142	-0.654314	-0.146713
C	2.324957	-0.293071	0.417940
H	4.154090	-1.490729	0.407802
H	3.626627	-0.956033	-1.205785
H	4.393712	0.200850	-0.093051
C	1.661105	0.863730	-0.331164
H	1.664495	-1.176645	0.378825
H	2.416730	-0.025279	1.486285
C	0.318591	1.312125	0.214550
H	2.318561	1.753877	-0.276079
H	1.568263	0.619937	-1.403733
H	-0.076087	2.190223	-0.311103
H	0.340698	1.506430	1.295491
I	-1.291016	-0.188556	-0.022761

$CH_2CHCOOC_4H_9$

Geometry with 21 atoms:

Thermal correction to Gibbs Free Energy: 0.143475

Total energy: -424.512239

C	-1.563689	0.038446	0.184607
C	-2.859800	0.192482	-0.529132
C	-3.859175	-0.675901	-0.339507
H	-2.948435	1.043960	-1.209409
H	-3.738742	-1.518513	0.348996
H	-4.815343	-0.570518	-0.859611
O	-0.712035	1.020570	-0.155500
O	-1.297522	-0.845763	0.972255
C	0.601597	1.008974	0.437861
H	0.946805	2.051690	0.377923
H	0.519525	0.723093	1.498188
C	1.546719	0.075538	-0.305788
H	1.151349	-0.952280	-0.244750
H	1.554804	0.356096	-1.373816
C	2.968893	0.118718	0.259206
H	2.942054	-0.145918	1.331831
H	3.350403	1.154920	0.209859
C	3.928719	-0.816898	-0.474953
H	4.944485	-0.768629	-0.049447
H	3.588917	-1.864817	-0.412960
H	4.001059	-0.555688	-1.544602

ts-1-2D

Geometry with 48 atoms:

Thermal correction to Gibbs Free Energy: 0.361442

Total energy: -2579.184215

Ni	2.366352	0.444532	-0.072213
O	0.527818	0.874098	-0.149008
C	0.220007	2.117208	-0.275992
O	-0.951792	2.517285	-0.413406
C	2.665722	2.290721	-0.602918
H	2.788172	2.304479	-1.704381
H	3.571913	2.750310	-0.170293
C	1.402912	3.062049	-0.199657
H	1.459863	3.368034	0.861311
H	1.194622	3.979881	-0.777266
C	1.234906	-2.125813	-0.713229
H	0.350787	-1.534016	-0.981724
H	1.929362	-2.117986	-1.564198
H	0.926715	-3.168862	-0.511656
C	0.940017	-1.531425	1.608432
H	1.391771	-1.000772	2.458902
H	0.018888	-1.010670	1.320873
H	0.693824	-2.564800	1.915885
C	5.091102	0.394428	-1.134930
H	4.611399	0.122329	-2.084357
H	5.163292	1.485850	-1.076370
H	6.109559	-0.032900	-1.104992
C	4.850809	0.361532	1.269302
H	4.255049	-0.005910	2.114272
H	5.894355	0.016720	1.387419
H	4.826809	1.458067	1.284657
C	3.155979	-2.167210	0.809850
H	3.370823	-1.958855	1.866917
H	3.097064	-3.265308	0.700815
C	4.258605	-1.607902	-0.070013
H	5.241888	-2.018578	0.221001
H	4.082694	-1.886044	-1.118449

C	-2.379050	0.852172	-0.407064
H	-1.856995	0.581658	0.503604
H	-1.916792	0.563401	-1.346124
I	-3.397870	-1.697347	-0.269564
N	4.282087	-0.116989	-0.009285
N	1.870808	-1.520000	0.469397
C	-3.597927	1.712495	-0.390530
H	-3.302155	2.670648	-0.854021
H	-4.358120	1.284724	-1.064291
C	-4.173835	1.960625	1.003275
H	-3.385182	2.407765	1.634198
H	-4.428445	0.989002	1.461236
C	-5.403010	2.866404	0.984082
H	-6.215131	2.422926	0.382879
H	-5.794590	3.035232	2.000490
H	-5.168094	3.852335	0.547426
H	2.249384	2.067366	3.104415
H	3.019976	2.182418	1.486412
C	4.329771	-1.025604	-0.555422
H	5.056962	-1.836750	-0.371213
H	4.285084	-0.819757	-1.630724
H	4.669513	-0.115265	-0.045721
C	2.522733	-2.622489	-0.784842
H	2.549223	-2.449798	-1.866337
H	3.170261	-3.484276	-0.542857
H	1.489562	-2.849747	-0.489195
H	-4.547368	2.957722	1.016834
H	-3.211635	4.131545	0.949976
H	-3.719637	3.448469	2.514776
C	0.643685	0.000295	2.458933
H	0.756805	0.060198	3.557528
H	-0.187412	0.649233	2.162640
H	0.391611	-1.032271	2.182716

ts-1-2D'

Geometry with 48 atoms:

Thermal correction to Gibbs Free Energy: 0.363559

Total energy: -2579.166319

C	0.574180	2.204951	-1.678896
C	1.542704	1.529781	-2.631745
C	1.674565	0.056455	-2.240235
H	1.216573	1.724277	-3.669543
H	2.511646	2.048721	-2.510114
H	0.780671	-0.514598	-2.559918
H	2.549211	-0.410372	-2.722069
C	3.031957	-0.392932	2.175993
H	3.025523	-0.593819	3.262575
H	3.947669	0.172907	1.956034
C	3.015099	-1.691504	1.394693
H	2.112195	-2.267374	1.639518
H	3.886450	-2.320405	1.647332
Ni	1.735360	0.113092	-0.305055
O	0.473329	1.555150	-0.514506
O	-0.059786	3.216054	-1.918842
C	-1.407943	0.595859	-0.445140
H	-0.949670	0.031577	0.356989
H	-1.253973	0.226576	-1.457053
I	-3.184073	-1.712464	-0.170127
C	-2.325844	1.732528	-0.199716
H	-1.892359	2.597355	-0.736165
H	-3.273021	1.523807	-0.725842
C	-2.570252	2.068491	1.269726
H	-1.607315	2.335141	1.738269
H	-2.935140	1.164695	1.787764
C	-3.564980	3.213185	1.449219
N	2.985840	-1.411959	-0.071493
N	1.872522	0.434732	1.774193
C	2.116326	1.863765	2.025436
H	1.266130	2.440727	1.641102

ts-2-3D

Geometry with 48 atoms:

Thermal correction to Gibbs Free Energy: 0.367740

Total energy: -2579.209893

C	1.728319	-0.229047	-0.470921
C	-2.508602	-1.854363	1.742741
H	-3.184220	-1.963046	2.611608
H	-1.659655	-2.533911	1.901196
C	-3.233164	-2.202276	0.459178
H	-4.080360	-1.521815	0.306587
H	-3.640327	-3.227725	0.497829
Ni	-1.121715	-0.471999	-0.258722
O	3.039273	-0.094379	-0.338266
O	0.997512	-0.500415	0.476973
C	-3.090998	-1.852955	-1.935255
H	-3.650910	-0.911040	-1.864695
H	-3.797830	-2.688935	-2.091090
H	-2.416142	-1.796854	-2.797006
C	-1.474637	-3.267363	-0.819957
H	-2.108223	-4.158615	-0.982305
H	-0.784950	-3.165257	-1.664156
H	-0.879937	-3.412754	0.090562
C	-0.973997	-0.225311	2.689865
H	-0.536771	0.769060	2.531863
H	-1.428006	-0.273302	3.697225
H	-0.170246	-0.966868	2.614348
C	-3.078274	0.503076	1.776631
H	-3.654601	0.317359	2.702386
H	-2.661207	1.514625	1.806276
H	-3.753620	0.449753	0.913494
C	3.600214	-0.222797	0.991319
H	3.112976	0.514933	1.647926
H	3.362528	-1.227953	1.377092
I	-0.892028	2.540991	-0.284869

C	-0.239478	-0.485791	-1.994310
H	-0.792904	0.135266	-2.720262
H	-0.210543	-1.508483	-2.407075
C	1.199505	0.026189	-1.851973
H	1.911223	-0.387465	-2.588376
H	1.243460	1.123323	-1.965749
N	-2.309754	-2.052306	-0.698787
N	-1.980272	-0.476682	1.644373
C	5.095338	0.005171	0.896438
H	5.491972	0.015840	1.926990
H	5.275588	1.012711	0.481376
C	5.834827	-1.045661	0.063971
H	5.401651	-1.068161	-0.950715
H	5.649480	-2.044634	0.499723
C	7.338304	-0.788371	-0.020557
H	7.801269	-0.785311	0.981354
H	7.847741	-1.559361	-0.621601
H	7.549816	0.190324	-0.484334
H	2.134771	-2.251142	1.525883
H	1.915238	-1.785056	3.245993
C	-2.333120	1.063468	1.052249
H	-2.583242	1.904338	1.718154
H	-2.060998	0.191487	1.659815
I	-0.623722	-2.052544	-0.670643
Ni	1.039810	0.217641	-0.176535
N	3.010161	0.424947	-0.552949
N	1.554197	-0.230060	1.831003
C	-3.487892	0.718865	0.121995
H	-3.775446	1.612801	-0.454047
H	-3.134855	-0.036953	-0.599094
C	-4.699761	0.178784	0.885323
H	-5.039616	0.931224	1.620450
H	-4.394830	-0.707261	1.471143
C	-5.857466	-0.195238	-0.039945
H	-6.720784	-0.581275	0.526625
H	-6.201033	0.676877	-0.622147
H	-5.553119	-0.973973	-0.759707

ts-2-3D'

Geometry with 48 atoms:

Thermal correction to Gibbs Free Energy: 0.368323

Total energy: -2579.201240

C	-1.097134	2.530269	-0.396908
C	0.098808	2.545992	-1.314542
C	0.510143	1.146498	-1.782661
H	-0.156189	3.232357	-2.141828
H	0.916321	3.042709	-0.759481
H	-0.350235	0.642834	-2.255139
H	1.294266	1.233043	-2.551145
C	2.933541	0.303987	1.896280
H	3.451278	-0.040145	2.810431
H	2.874204	1.400441	1.947902
C	3.689874	-0.115654	0.657379
H	3.703389	-1.210294	0.577051
H	4.739466	0.223970	0.693253
O	-1.125530	1.383701	0.323827
O	-1.935775	3.393807	-0.291301
C	3.363270	-0.411451	-1.719951
H	2.914931	0.005246	-2.628521
H	4.460300	-0.453056	-1.848949
H	2.973123	-1.427048	-1.571711
C	3.438845	1.819283	-0.784092
H	4.530256	1.865193	-0.950688
H	2.933281	2.226947	-1.665835
H	3.186167	2.440268	0.084891
C	0.676271	0.532794	2.733234
H	-0.325802	0.090241	2.721687
H	1.056932	0.512674	3.771566
H	0.605758	1.574908	2.393759
C	1.529385	-1.652512	2.217624
H	0.500421	-2.025227	2.164258

ts-3-4D

Geometry with 48 atoms:

Thermal correction to Gibbs Free Energy: 0.363090

Total energy: -2579.183562

Ni	0.485257	0.226917	-0.092293
I	3.209539	-1.692612	0.079280
C	-0.190776	-0.962521	-1.585319
C	-1.019453	-1.098991	-0.465710
H	0.516924	-1.758892	-1.829196
H	-0.519257	-0.325730	-2.407185
C	-2.219336	-0.223532	-0.303888
H	0.294251	-0.807342	0.867183
H	-1.037887	-2.014811	0.128783
O	-2.852448	-0.501061	0.846365
O	-2.577096	0.628938	-1.093596
C	-4.032364	0.252855	1.203450
H	-3.913231	0.491116	2.270751
H	-4.051118	1.189341	0.627542
H	2.368004	0.699092	-2.429167
C	2.368259	1.598073	-1.799720
H	2.725148	2.462220	-2.390032
H	3.056429	1.418524	-0.965674
C	0.962477	2.991150	-0.359399
C	0.107331	2.135309	-2.439461
C	1.490893	2.593172	1.002017
H	1.540495	3.841156	-0.764264
H	-0.083447	3.317815	-0.278922
H	0.355821	3.118846	-2.877404
H	0.234022	1.374162	-3.218777
H	-0.937858	2.127297	-2.105449
H	2.550043	2.310132	0.933948
H	1.415388	3.437331	1.710800

C	-0.607591	1.774291	1.976177
C	1.503379	0.799117	2.628606
H	-1.127866	0.865289	2.300731
H	-0.556366	2.491460	2.815536
H	-1.184660	2.223457	1.158211
H	1.662100	1.536871	3.435867
H	0.939878	-0.054533	3.025646
H	2.471215	0.434719	2.262586
C	-5.290797	-0.568951	0.969482
H	-6.138691	0.013079	1.373476
H	-5.230454	-1.492847	1.572093
N	0.998602	1.839174	-1.298931
N	0.751291	1.411787	1.514409
C	-5.555161	-0.922551	-0.496382
H	-5.584569	0.004823	-1.094864
H	-4.705787	-1.509572	-0.887424
C	-6.849381	-1.711212	-0.690683
H	-7.724641	-1.136971	-0.341136
H	-7.015118	-1.959654	-1.751762
H	-6.829313	-2.658642	-0.125048
H	-2.655147	1.792677	1.665147
H	0.465524	3.508283	0.645628
H	-1.210844	3.241501	1.130824
C	-1.826147	2.946283	-1.199081
C	0.484057	2.345802	-1.545791
H	-2.042349	2.566428	-2.204984
H	-1.615483	4.030804	-1.258365
H	-2.710978	2.782248	-0.569854
H	0.727471	3.411637	-1.715213
H	0.249420	1.872279	-2.506951
H	1.358219	1.844958	-1.116990
C	5.327789	-0.567143	-0.368690
H	4.956252	-1.536921	0.002541
H	5.498499	-0.679758	-1.453730
C	6.638880	-0.210145	0.336187
H	6.448664	-0.090845	1.418283
H	6.991426	0.774249	-0.022385
C	7.732387	-1.255893	0.121049
H	8.664074	-0.978685	0.640865
H	7.418858	-2.243822	0.499314
H	7.968343	-1.371997	-0.950556

ts-4-5D
Geometry with 48 atoms:
Thermal correction to Gibbs Free Energy: 0.363528
Total energy: -2579.188523

Ni	-1.217712	0.264277	-0.393716
C	2.181089	-0.702485	-0.291427
C	1.012277	-0.950049	-1.160465
C	0.054152	-1.849127	-0.835430
H	1.020718	-0.462699	-2.135746
H	-1.457870	0.218955	-1.831406
H	0.096227	-2.398342	0.107432
H	-0.699622	-2.147872	-1.562092
O	3.039683	0.163987	-0.863713
O	2.376912	-1.203292	0.801157
C	4.250514	0.485083	-0.149345
H	4.560843	1.461520	-0.549329
H	4.021792	0.596778	0.921945
I	-3.393385	-1.252427	-0.246403
N	-0.671088	2.215990	-0.637210
H	-1.180841	-1.452963	2.230506
C	-0.446549	-0.645744	2.357103
N	-0.922718	0.546518	1.634753
H	-0.327697	-0.431292	3.435758
H	0.518400	-0.970858	1.953253
C	0.110844	1.608688	1.623292
C	-2.165010	1.024862	2.275362
C	-0.325766	2.743547	0.715800
H	1.046334	1.165753	1.256456
H	0.302678	1.986091	2.645883
H	-1.950637	1.438234	3.278572
H	-2.864155	0.187321	2.374846

ts-4-6D
Geometry with 48 atoms:
Thermal correction to Gibbs Free Energy: 0.358254
Total energy: -2579.190904

Ni	0.531079	0.402017	-0.251665
C	-2.156146	0.048706	-0.357908
C	-0.987078	-0.781196	-0.730937
C	-0.219896	-0.426926	-1.869755
H	-0.976159	-1.790212	-0.310725
H	0.948954	-0.876163	0.256747
H	-0.615023	0.334769	-2.549998
H	0.429117	-1.180397	-2.327821
O	-2.858433	-0.509514	0.646974
O	-2.449909	1.123113	-0.856176
C	-4.015682	0.201321	1.135657
H	-4.185358	-0.210504	2.141606
H	-3.771358	1.270814	1.224113
I	2.884199	-2.031311	-0.008004
N	0.754304	1.192084	1.618731
H	0.615106	2.159486	-2.978558
C	0.598945	2.792585	-2.082635
N	1.383933	2.154869	-1.011597
H	1.016936	3.782487	-2.345510
H	-0.444139	2.906608	-1.757383
C	1.475801	3.057061	0.162527
C	2.720541	1.780307	-1.513331
C	1.757423	2.269958	1.431042
H	0.517996	3.587695	0.253127
H	2.256795	3.824279	0.009762
H	3.262810	2.667232	-1.892736

H	2.611878	1.047182	-2.323398
H	3.310552	1.310708	-0.716519
H	1.771013	2.946955	2.305300
H	2.743363	1.788157	1.370329
C	1.200354	0.264630	2.674068
C	-0.574138	1.733949	1.973503
H	0.473147	-0.552003	2.773156
H	1.291287	0.789225	3.643054
H	2.170740	-0.167074	2.400787
H	-0.517954	2.352297	2.888339
H	-1.259229	0.895837	2.148431
H	-0.980730	2.338319	1.153515
C	-5.234565	-0.005849	0.247016
H	-6.066377	0.570272	0.691128
H	-5.034000	0.443500	-0.739981
C	-5.642769	-1.471978	0.084470
H	-4.788335	-2.039330	-0.323087
H	-5.848934	-1.903889	1.080938
C	-6.860380	-1.652573	-0.820662
H	-6.667026	-1.255453	-1.832020
H	-7.133035	-2.715503	-0.926041
H	-7.740191	-1.119724	-0.420385

2E
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.391739
Total energy: -2618.531537

C	1.282287	-0.364210	-0.676870
C	-3.283071	-1.855456	1.534299
H	-3.803862	-1.720651	2.499409
H	-3.325827	-2.925630	1.287899
C	-3.955481	-1.037898	0.449623
H	-3.953517	0.025440	0.724699
H	-5.006643	-1.345344	0.311641
Ni	-1.293395	-1.094175	-0.345860
O	2.516162	-0.006619	-0.452505
O	0.560171	-0.838777	0.220418
C	-3.612549	-0.036603	-1.719964
H	-3.161479	-0.157766	-2.710298
H	-4.711338	-0.014050	-1.828971
H	-3.263606	0.910269	-1.286284
C	-3.496123	-2.448078	-1.509057
H	-4.572099	-2.534490	-1.744556
H	-2.916162	-2.506943	-2.438066
H	-3.201143	-3.285368	-0.863900
C	-1.037185	-2.552833	2.181514
H	0.013165	-2.236321	2.200150
H	-1.355718	-2.815212	3.207570
H	-1.122945	-3.442269	1.541012
C	-1.669829	-0.231695	2.414777
H	-1.943186	-0.391222	3.474706
H	-0.619411	0.078185	2.348125
H	-2.279647	0.580283	2.000923
C	3.028363	-0.079857	0.911274
H	2.449148	0.630579	1.520779
H	2.850656	-1.096904	1.293841
I	-0.790670	2.988696	0.111488
C	-0.553001	-1.011870	-2.145491
H	-1.211470	-0.631989	-2.940056
H	-0.290497	-2.058378	-2.402341
C	0.719376	-0.162271	-2.043262
H	1.495322	-0.338766	-2.809016
H	0.471655	0.914424	-2.083923
N	-3.210450	-1.159338	-0.841450
N	-1.858608	-1.464151	1.629682
C	4.502240	0.262730	0.875025
H	4.623967	1.272255	0.445291
H	4.844418	0.325156	1.922743
C	5.353736	-0.749279	0.105002
H	4.980243	-0.822925	-0.931807
H	5.216654	-1.751787	0.552073
C	6.843629	-0.400317	0.085029
H	7.210828	-0.317607	1.124517
H	6.974611	0.601594	-0.362907
C	7.689755	-1.418532	-0.678470
H	7.365563	-1.498165	-1.730413
H	8.756960	-1.141771	-0.678293
H	7.605815	-2.423973	-0.230845

2E'
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.394459
Total energy: -2618.512254

C	1.732890	-0.078912	-2.085735
C	0.994582	-1.224816	-2.701431
C	-0.471306	-1.125446	-2.281703
H	1.176913	-1.188666	-3.788665
H	1.448113	-2.162105	-2.329028
H	-0.923000	-0.189522	-2.660109
H	-1.042398	-1.968257	-2.696598
C	-0.952262	-2.317309	2.116985
H	-1.122576	-2.256533	3.205519
H	-0.552590	-3.318497	1.909553
C	-2.240855	-2.093312	1.359687
H	-2.642677	-1.094368	1.576705
H	-3.008404	-2.835188	1.640744
O	1.260904	0.129444	-0.789971
O	2.561109	0.631936	-2.580497
C	-3.149375	-1.604911	-0.822397
H	-3.010185	-1.701029	-1.904056
H	-4.061704	-2.153500	-0.529195
H	-3.259825	-0.542459	-0.570732
C	-1.746122	-3.558021	-0.531626
H	-2.624350	-4.180571	-0.285681

H	-1.576740	-3.591900	-1.612994
H	-0.862141	-3.972191	-0.032394
C	1.412949	-1.840296	1.804622
H	2.128710	-1.114985	1.404474
H	1.665700	-2.054671	2.859275
H	1.502945	-2.766962	1.220088
C	-0.122533	-0.072913	2.462083
H	0.601981	0.680458	2.144776
H	-1.125392	0.341994	2.303769
H	0.029040	-0.271777	3.538884
C	1.574512	1.439599	-0.191015
H	0.657958	1.721632	0.340756
H	1.712944	2.137281	-1.026192
I	-2.476948	2.407405	0.115759
Ni	-0.353596	-1.078847	-0.359390
N	-1.976183	-2.158127	-0.106458
N	0.044339	-1.309534	1.674940
C	2.793219	1.425212	0.717434
H	2.954262	2.477767	1.011431
H	2.563688	0.888547	1.651563
C	4.076435	0.852640	0.112928
H	4.326305	1.395688	-0.813005
H	3.897800	-0.193934	-0.193854
C	5.260676	0.892436	1.081620
H	5.442332	1.937732	1.391512
H	4.994799	0.345209	2.005023
C	6.539464	0.303505	0.486788
H	6.846463	0.852435	-0.419867
H	7.377587	0.343969	1.201903
H	6.396518	-0.752490	0.199020

3E
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.392480
Total energy: -2618.544176

Ni	1.415594	0.348004	-0.365960
I	2.492219	-2.070429	-0.152019
C	0.312768	-0.291811	-1.838122
C	-0.853349	-1.122487	-1.288729
H	0.876186	-0.909659	-2.558801
H	-0.106591	0.547828	-2.417753
C	-1.540049	-0.504017	-0.096946
H	-0.482527	-2.095345	-0.917411
H	-1.619075	-1.355880	-2.049391
O	-2.842727	-0.796725	-0.035078
O	-0.980631	0.162424	0.757140
C	-3.583077	-0.325500	1.111411
H	-3.186450	-0.819307	2.013737
H	-3.416592	0.758547	1.224102
H	1.152790	2.020457	-2.987886
C	1.739577	2.551391	-2.229763
H	1.732721	3.631512	-2.467078
H	2.773078	2.181228	-2.264012
C	1.952713	3.078493	0.117382
C	-0.240272	2.739346	-0.851665
C	1.803035	2.439530	1.478395
H	3.005910	3.069441	-0.191653
H	1.627417	4.133502	0.134686
H	-0.322553	3.812264	-1.103907
H	-0.826182	2.159673	-1.573430
H	-0.661621	2.560944	0.143566
H	2.352068	3.016739	2.245657
H	0.744894	2.424152	1.774020
C	1.753719	0.293883	2.580220
C	3.752643	0.987228	1.416756
H	2.127283	-0.736964	2.554182
H	2.069086	0.767603	3.529139
H	0.658164	0.268188	2.527201
H	4.168118	1.468229	2.322725
H	4.079867	-0.058431	1.381185
H	4.152032	1.494529	0.529260
N	1.172293	2.308518	-0.887893
N	2.279215	1.039706	1.422070
C	-5.049525	-0.645100	0.892731
H	-5.579871	-0.388772	1.825132
H	-5.161344	-1.735602	0.756248
C	-5.663918	0.096962	-0.298636
H	-5.054273	-0.114513	-1.193327
H	-5.584958	1.186491	-0.122353
C	-7.125287	-0.267154	-0.590074
H	-7.431926	0.234118	-1.525032
H	-7.193549	-1.352267	-0.791045
C	-8.106941	0.107760	0.522101
H	-9.145939	-0.118932	0.230912
H	-7.902667	-0.441526	1.455821
H	-8.053630	1.186060	0.753315

4E
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.390515
Total energy: -2618.523807

Ni	-1.031870	-0.098530	-0.135898
C	1.955653	-0.139769	0.153037
C	0.844991	-0.970816	-0.361454
C	0.000793	-1.727989	0.466147
H	0.973659	-1.247793	-1.410230
H	-1.119085	-0.647401	-1.439898
H	0.155805	-1.719723	1.547856
H	-0.473775	-2.626987	0.064991
O	2.696375	0.334991	-0.869353
O	2.207883	0.096496	1.321070
C	3.850662	1.152980	-0.591329
H	3.785975	1.999976	-1.291283
H	3.787165	1.535994	0.437561

I	-3.488581	-1.371263	-0.336817
N	-1.194118	1.771359	-1.055254
H	-0.899531	-0.537400	3.175141
C	-0.477734	0.435905	2.890404
N	-1.204813	0.957014	1.717830
H	-0.583107	1.125784	3.748766
H	0.582630	0.312354	2.649879
C	-0.624474	2.257766	1.303306
C	-2.622996	1.106492	2.101643
C	-1.292490	2.772209	0.040658
H	0.450162	2.098567	1.132866
H	-0.726598	3.007071	2.112035
H	-2.728179	1.853705	2.911035
H	-3.002626	0.139624	2.453073
H	-3.239254	1.406462	1.248345
H	-0.836569	3.729632	-0.265752
H	-2.354503	2.974275	0.228738
C	-2.357728	1.864776	-1.953728
C	0.043612	1.990634	-1.829503
H	-2.250130	1.134268	-2.765982
H	-2.440574	2.878506	-2.388113
H	-3.275070	1.626593	-1.401063
H	0.002692	2.959029	-2.362787
H	0.174633	1.181884	-2.558966
H	0.911491	1.991019	-1.162421
C	5.136211	0.369381	-0.812524
H	5.968327	1.086159	-0.705005
H	5.161749	0.012664	-1.857907
C	5.318948	-0.814950	0.141144
H	5.292539	-0.450357	1.184152
H	4.454774	-1.493059	0.033938
C	6.605529	-1.618575	-0.090285
H	6.578614	-2.515558	0.553196
H	6.616595	-1.992224	-1.130965
C	7.896509	-0.845608	0.187883
H	8.782188	-1.490942	0.066283
H	8.020881	0.011083	-0.494611
H	7.909810	-0.452551	1.219434

6E
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.385376
Total energy: -2618.521373

C	-0.261631	-0.130406	-2.099181
H	-0.954089	-0.809036	-2.610427
H	0.182558	0.639369	-2.745826
C	0.523207	-0.637470	-1.012864
H	0.395377	-1.656104	-0.635687
C	1.766275	0.037771	-0.621108
O	2.172224	1.102892	-1.063074
O	2.412403	-0.631379	0.364907
C	3.629740	-0.059524	0.874576
H	3.512287	1.031539	0.970100
H	3.746477	-0.490322	1.880396
Ni	-0.858394	0.632411	-0.428887
C	-2.125973	1.761110	1.752324
H	-2.875461	0.956725	1.763856
H	-2.174768	2.283051	2.726711
C	-2.423315	2.733138	0.619121
H	-1.708818	3.567063	0.638336
H	-3.429055	3.169966	0.743779
C	-3.584264	1.440519	-1.099532
C	-1.835132	2.977057	-1.742788
C	-0.614424	-0.026512	2.448427
C	0.306348	2.081449	1.730360
H	-1.776268	-0.533928	-0.215402
H	-0.828033	3.342557	-1.494936
H	-2.516941	3.842235	-1.844325
H	-1.786066	2.448115	-2.703544
H	-4.339176	2.220531	-1.311965
H	-3.431403	0.825562	-1.995889
H	-3.956295	0.787226	-0.302010
H	0.333244	-0.521966	2.196207
H	-0.591435	0.289328	3.508486
H	-1.430693	-0.744758	2.302770
H	0.259035	2.568412	2.722396
H	0.287458	2.856050	0.952565
H	1.258676	1.544470	1.648743
I	-2.990424	-2.177935	0.067845
N	-2.303958	2.048560	-0.697562
N	-0.802502	1.126287	1.553499
C	4.826726	-0.394290	-0.004885
H	4.662599	0.042119	-1.004449
H	4.869369	-1.488786	-0.132122
C	6.137328	0.135900	0.583931
H	6.028663	1.218680	0.776419
H	6.311440	-0.333496	1.570573
C	7.367815	-0.086421	-0.305837
H	7.201812	0.409361	-1.279914
H	8.230402	0.427337	0.154165
C	7.727246	-1.555440	-0.536546
H	7.888265	-2.081051	0.420849
H	6.934127	-2.093805	-1.080704
H	8.652716	-1.650699	-1.128300

7E
Geometry with 49 atoms:
Thermal correction to Gibbs Free Energy:
0.383508
Total energy: -2320.016818

C	0.940055	-2.161585	-0.838789
H	1.402528	-2.736522	-1.658547
H	0.603468	-2.822456	-0.021883
C	0.050058	-1.070726	-1.217569
H	-0.036859	-0.738638	-2.260784

C	-1.044188	-0.656827	-0.354850
O	-1.361579	-1.123921	0.732253
O	-1.715833	0.424756	-0.880530
C	-2.794500	0.968901	-0.115256
H	-2.532867	0.967184	0.955348
H	-2.889733	2.014692	-0.448856
Ni	1.677583	-0.478609	-0.324460
C	3.202591	1.829945	0.214616
H	3.693428	1.868244	-0.768274
H	3.359840	2.814187	0.696536
C	3.823557	0.725854	1.062425
H	3.377688	0.733239	2.066716
H	4.908857	0.901503	1.186300
C	4.472467	-0.891513	-0.655532
C	3.652665	-1.669871	1.476217
C	1.252946	2.291857	-1.182126
C	0.950598	1.872849	1.171803
H	2.916240	-1.488235	2.271283
H	4.664952	-1.719145	1.924294
H	3.419921	-2.635047	1.007608
H	5.525628	-0.943323	-0.314707
H	4.192240	-1.849828	-1.112093
H	4.386878	-0.113048	-1.425089
H	0.205056	2.006069	-1.344727
H	1.318722	3.389318	-1.042450
H	1.831476	2.010189	-2.073174
H	1.013910	2.947174	1.435947
H	1.279312	1.274853	2.031814
H	-0.096688	1.618551	0.965769
N	1.764984	1.563280	-0.013118
N	3.560582	-0.606448	0.464949
C	-4.096303	0.209358	-0.339668
H	-3.942378	-0.832029	-0.016267
H	-4.310010	0.184452	-1.423382
C	-5.273234	0.837009	0.411940
H	-5.055968	0.831926	1.496736
H	-5.356890	1.900830	0.123290
C	-6.623396	0.149724	0.166316
H	-7.413918	0.738642	0.664454
H	-6.854291	0.183521	-0.914508
C	-6.695545	-1.297628	0.657190
H	-7.704512	-1.718355	0.512803
H	-5.987936	-1.950617	0.120841
H	-6.456711	-1.364868	1.732985

$C_5H_{11}I$
Geometry with 17 atoms:
Thermal correction to Gibbs Free Energy:
0.115235
Total energy: -495.079066

C	4.775082	-0.440975	-0.029414
C	3.283512	-0.456329	0.304458
H	5.280618	-1.351861	0.331446
H	4.939686	-0.377569	-1.118851
H	5.279770	0.425861	0.431053
C	2.549559	0.796654	-0.185526
H	2.822677	-1.357853	-0.135834
H	3.148047	-0.548012	1.397861
C	1.061868	0.871292	0.201829
H	3.052224	1.689242	0.228246
H	2.647433	0.874836	-1.284266
H	0.665254	1.861807	-0.074444
H	0.960808	0.781368	1.296858
C	0.234304	-0.206114	-0.478945
H	0.511482	-1.224005	-0.179523
H	0.256550	-0.126964	-1.574291
I	-1.905481	-0.076113	0.034101

$CH_2CHCOOC_5H_{11}$
Geometry with 24 atoms:
Thermal correction to Gibbs Free Energy:
0.169433
Total energy: -463.832508

C	1.963252	-0.049011	0.178082
C	3.255973	0.050300	-0.551152
C	4.131552	1.022644	-0.274021
H	3.447592	-0.705883	-1.317381
H	3.909422	1.765135	0.499165
H	5.084055	1.103533	-0.805099
O	1.247047	-1.097528	-0.260680
O	1.592643	0.704577	1.054584
C	-0.046543	-1.324874	0.334277
H	-0.254956	-2.390078	0.155527
H	0.017964	-1.153727	1.420338
C	-1.117336	-0.441898	-0.291467
H	-0.841356	0.610642	-0.121997
H	-1.120599	-0.606413	-1.383508
C	-2.506173	-0.729964	0.286433
H	-2.492495	-0.541927	1.376313
H	-2.729046	-1.805389	0.164410
C	-3.636875	0.087963	-0.352375
H	-4.600133	-0.272447	0.049699
H	-3.663390	-0.119508	-1.438051
C	-3.534437	1.597326	-0.123904
H	-3.497189	1.834817	0.953553
H	-2.630722	2.025111	-0.587993
H	-4.403148	2.124823	-0.551443

ts-1-2E
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.385489
Total energy: -2618.504902

Ni	2.548995	0.518764	-0.093122
O	0.693654	0.769420	-0.346221

C	0.295658	1.956850	-0.642969
O	-0.890385	2.231076	-0.907344
C	2.737223	2.313288	-0.814548
H	2.946695	2.213961	-1.898307
H	3.564576	2.899002	-0.377163
C	1.387021	3.007769	-0.597869
H	1.331709	3.436827	0.419741
H	1.152112	3.830939	-1.295407
C	1.682208	-2.191089	-0.524740
H	0.774933	-1.712231	-0.914405
H	2.436204	-2.205349	-1.323494
H	1.449127	-3.232382	-0.233666
C	1.157737	-1.393063	1.692219
H	1.494070	-0.738610	2.509024
H	0.221052	-0.992756	1.286623
H	0.976032	-2.407725	2.092697
C	5.344461	0.594778	-0.957288
H	4.960208	0.184294	-1.900460
H	5.328185	1.688420	-1.015518
H	6.387526	0.260694	-0.812289
C	4.925701	0.796506	1.414362
H	4.297503	0.472232	2.253474
H	5.980545	0.555621	1.640638
H	4.818572	1.882741	1.304716
C	3.474024	-1.904881	1.125258
H	3.587999	-1.566940	2.164312
H	3.511525	-3.009321	1.136001
C	4.594554	-1.347683	0.267134
H	5.581314	-1.637721	0.670189
H	4.523522	-1.748991	-0.753215
C	-2.199653	0.477798	-0.737289
H	-1.653992	0.329825	0.187354
H	-1.726789	0.129060	-1.651076
I	-3.066208	-2.095801	-0.318035
N	4.494941	0.137832	0.162077
N	2.171704	-1.412862	0.626640
C	-3.469172	1.260535	-0.790397
H	-3.241968	2.174447	-1.367295
H	-4.212857	0.712465	-1.391308
C	-4.032135	1.631128	0.580266
H	-3.261113	2.193003	1.138137
H	-4.221190	0.705876	1.153315
C	-5.316130	2.459127	0.503689
H	-6.079036	1.891043	-0.059472
H	-5.123810	3.375196	-0.084540
C	-5.868870	2.836802	1.877524
H	-6.795080	3.429134	1.794617
H	-6.099184	1.938050	2.475049
H	-5.139638	3.435299	2.450410

ts-1-2E'
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy: 0.390869
Total energy: -2618.487884

C	0.307131	2.210920	-1.666896
C	1.412141	1.747438	-2.597350
C	1.792435	0.308811	-2.236177
H	1.094274	1.912905	-3.642498
H	2.268557	2.424809	-2.421980
H	1.029596	-0.402465	-2.608961
H	2.754585	0.022640	-2.692214
C	3.092691	-0.053910	2.208574
H	3.072516	-0.267345	3.292222
H	3.963616	0.588427	2.021075
C	3.209693	-1.340439	1.414603
H	2.348817	-1.990905	1.621033
H	4.121281	-1.899169	1.690315
Ni	1.790920	0.325067	-0.298657
O	0.309282	1.544338	-0.508208
O	-0.508919	3.079036	-1.918186
C	-1.325929	0.201158	-0.485986
H	-0.822948	-0.200553	0.383464
H	-1.015508	-0.179496	-1.456495
I	-2.489581	-2.477610	-0.151181
C	-2.491529	1.104124	-0.376360
H	-2.219206	2.012694	-0.944249
H	-3.325300	0.657525	-0.945471
C	-2.910524	1.447097	1.052404
H	-2.062267	1.939505	1.560467
H	-3.106124	0.507511	1.597083
C	-4.144030	2.353801	1.132676
N	3.204945	-1.046710	-0.048924
N	1.877842	0.675913	1.779658
C	2.012379	2.127221	1.985285
H	1.121540	2.624747	1.581378
H	2.122603	2.375206	3.057574
H	2.892290	2.497451	1.440029
C	4.517529	-0.521463	-0.484781
H	5.317012	-1.256169	-0.280465
H	4.487436	-0.313868	-1.560456
H	4.748251	0.414572	0.038761
C	2.889228	-2.286833	-0.791309
H	2.923045	-2.092671	-1.868967
H	3.617645	-3.080239	-0.545434
H	1.879241	-2.626441	-0.525052
H	-4.992743	1.854305	0.630235
H	-4.435498	2.454534	2.192805
C	0.679630	0.177818	2.473594
H	0.768691	0.311507	3.567888
H	-0.197232	0.735557	2.125787
H	0.522733	-0.887717	2.258779
C	-3.940610	3.747124	0.533413
H	-3.737530	3.706324	-0.549149
H	-4.833954	4.377272	0.676020
H	-3.087193	4.262417	1.007362

ts-2-3E
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.393433
Total energy: -2618.529945

C	1.467862	0.164162	-0.368475
C	-2.492103	-2.121335	1.727662
H	-3.171746	-2.337490	2.573068
H	-1.537066	-2.623119	1.938050
C	-3.081840	-2.629451	0.428448
H	-4.036915	-2.128790	0.224258
H	-3.285700	-3.713213	0.481573
Ni	-1.303449	-0.550450	-0.257005
O	2.750668	0.445177	-0.199590
O	0.737769	-0.161692	0.563001
C	-2.908264	-2.310751	-1.968560
H	-3.648263	-1.500025	-1.941247
H	-3.425579	-3.274233	-2.131842
H	-2.221970	-2.131934	-2.804065
C	-1.098943	-3.363509	-0.752653
H	-1.543234	-4.362788	-0.914178
H	-0.405264	-3.147187	-1.571577
H	-0.528460	-3.372411	0.184733
C	-1.343160	-0.207595	2.689038
H	-1.101543	0.850262	2.522258
H	-1.828097	-0.324091	3.676248
H	-0.407971	-0.779121	2.671303
C	-3.497459	0.086260	1.659546
H	-4.071874	-0.179518	2.566859
H	-3.279436	1.158827	1.669581
H	-4.109137	-0.117740	0.772045
C	3.285300	0.398848	1.145948
H	2.760011	1.152013	1.754566
H	3.071746	-0.593316	1.576088
I	-1.616301	2.474250	-0.349499
C	-0.367114	-0.424640	-1.961245
H	-0.991809	0.094934	-2.708721
H	-0.153066	-1.427425	-2.367999
C	0.960482	0.320792	-1.771229
H	1.757769	0.029602	-2.477276
H	0.824295	1.409866	-1.892973
N	-2.156270	-2.329636	-0.698843
N	-2.229894	-0.670990	1.608274
C	4.774626	0.668789	1.068772
H	5.150292	0.735729	2.104824
H	4.933968	1.661865	0.612895
C	5.556587	-0.396196	0.296328
H	5.146373	-0.474518	-0.725910
H	5.389868	-1.382282	0.769325
C	7.059021	-0.114965	0.221154
H	7.465284	-0.032810	1.246123
H	7.218787	0.873254	-0.247638
C	7.832673	-1.180812	-0.554297
H	7.468887	-1.260389	-1.593212
H	8.910540	-0.952505	-0.594761
H	7.719501	-2.175167	-0.088773

ts-2-3E'
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.394260
Total energy: -2618.521999

C	-0.714323	2.601844	-0.437751
C	0.520687	2.585478	-1.301708
C	0.906761	1.178409	-1.766736
H	0.324541	3.287176	-2.132249
H	1.328378	3.051167	-0.706847
H	0.055171	0.712322	-2.290509
H	1.731957	1.247753	-2.492998
C	3.110484	0.144838	2.011059
H	3.567307	-0.252459	2.936091
H	3.097989	1.240524	2.098401
C	3.906320	-0.271000	0.795714
H	3.878302	-1.362421	0.682903
H	4.966327	0.022604	0.888623
O	-0.820172	1.445832	0.260672
O	-1.521436	3.497104	-0.352394
C	3.687147	-0.486098	-1.601203
H	3.308747	-0.023202	-2.519057
H	4.786701	-0.573724	-1.672123
H	3.245194	-1.486874	-1.507214
C	3.796611	1.713770	-0.595188
H	4.896283	1.725648	-0.703072
H	3.352782	2.162018	-1.489919
H	3.517457	2.319624	0.276199
C	0.830643	0.452987	2.750285
H	-0.185125	0.046439	2.696447
H	1.173537	0.398432	3.800415
H	0.808954	1.503588	2.430822
C	1.607945	-1.753049	2.206090
H	0.570058	-2.080105	2.079944
H	2.229802	-2.357200	1.534126
H	1.926803	-1.928566	3.250813
C	-2.061659	1.180045	0.954018
H	-2.294011	2.033864	1.609692
H	-1.847234	0.300349	1.572982
I	-0.425123	-1.992627	-0.776571
Ni	1.315917	0.200942	-0.152698
N	3.307247	0.330304	-0.428320
N	1.713182	-0.323058	1.863648
C	-3.202748	0.881416	-0.007942
H	-3.436543	1.784928	-0.593007
H	-2.860332	0.109727	-0.716835
C	-4.454660	0.392784	0.723421
H	-4.787761	1.159715	1.447703
H	-4.202923	-0.503409	1.320455

```
 C  -5.609118   0.055816  -0.224427
 H  -5.861917   0.951920  -0.820241
 H  -5.266661  -0.704110  -0.949952
 C  -6.856903  -0.451075   0.497572
 H  -7.242482   0.300230   1.208409
 H  -7.668179  -0.686132  -0.211160
 H  -6.640553  -1.368193   1.072201
```

ts-3-4E
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.389206
Total energy: -2618.505392

```
Ni  -0.768375   0.220133   0.107359
 I  -3.304678  -1.833754  -0.232237
 C   0.110234  -1.107492   1.352483
 C   0.870464  -0.994129   0.180168
 H  -0.498282  -2.002139   1.507802
 H   0.440718  -0.576766   2.245996
 C   1.978207   0.005114   0.092161
 H  -0.513642  -0.632615  -1.005876
 H   0.936128  -1.810773  -0.542215
 O   2.567627  -0.053103  -1.112180
 O   2.304085   0.773507   0.976484
 C   3.657811   0.846168  -1.411811
 H   3.444432   1.240709  -2.416391
 H   3.650258   1.677292  -0.692045
 H  -2.585407   0.176512   2.550925
 C  -2.676265   1.161848   2.076758
 H  -3.058056   1.893274   2.812763
 H  -3.392613   1.066384   1.252815
 C  -1.442461   2.859931   0.819764
 C  -0.430608   1.764107   2.707608
 C  -2.005558   2.636046  -0.567422
 H  -2.061235   3.588807   1.373507
 H  -0.428323   3.277894   0.756034
 H  -0.721820   2.651606   3.298180
 H  -0.472415   0.889021   3.367322
 H   0.596397   1.880690   2.338781
 H  -3.037897   2.266033  -0.505334
 H  -2.025002   3.582889  -1.136527
 C   0.090724   2.145280  -1.742891
 C  -1.973469   1.112277  -2.448983
 H   0.652154   1.344285  -2.238138
 H  -0.057046   2.983477  -2.448151
 H   0.682338   2.496821  -0.888596
 H  -2.225514   1.947017  -3.127980
 H  -1.372417   0.373239  -2.993781
 H  -2.893218   0.624658  -2.103756
 C   4.985621   0.104551  -1.390368
 H   5.760346   0.814649  -1.730996
 H   4.953592  -0.706793  -2.139059
 N  -1.352287   1.578103   1.567862
 N  -1.210305   1.608518  -1.285979
 C   5.365577  -0.466150  -0.022581
 H   5.364999   0.345337   0.727285
 H   4.588241  -1.180396   0.303508
 C   6.724495  -1.170815  -0.017684
 H   7.504294  -0.457869  -0.343117
 H   6.717227  -1.977209  -0.773757
 C   7.096290  -1.749794   1.346906
 H   6.351437  -2.492010   1.682029
 H   8.078477  -2.250105   1.322737
 H   7.142375  -0.959888   2.116295
```

ts-4-5E
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.389707
Total energy: -2618.508467

```
Ni  -1.508569   0.260714  -0.392237
 C   1.936091  -0.525724  -0.273609
 C   0.783213  -0.811680  -1.153172
 C  -0.117786  -1.778487  -0.861758
 H   0.764175  -0.292019  -2.111404
 H  -1.741550   0.221440  -1.831230
 H  -0.046365  -2.351080   0.065245
 H  -0.852079  -2.098916  -1.599030
 O   2.708092   0.452269  -0.787316
 O   2.187654  -1.085511   0.777785
 C   3.901516   0.825095  -0.069226
 H   4.095336   1.865775  -0.368143
 H   3.699921   0.797637   1.012717
 I  -3.588996  -1.392899  -0.269611
 N  -1.079004   2.243790  -0.606524
 H  -1.373467  -1.488019   2.213859
 C  -0.685478  -0.642088   2.346680
 N  -1.230575   0.529493   1.639660
 H  -0.573945  -0.433557   3.427218
 H   0.294587  -0.908472   1.936149
 C  -0.260371   1.649832   1.644597
 C  -2.499334   0.926709   2.284334
 C  -0.760722   2.771366   0.753549
 H   0.699421   1.268676   1.271591
 H  -0.090264   2.022391   2.672710
 H  -2.309664   1.346262   3.289914
 H  -3.145497   0.047084   2.379994
 H  -3.035809   1.666156   1.678239
 H  -0.012279   3.578740   0.692752
 H  -1.670723   3.215181   1.176914
 C  -2.279177   2.910184  -1.153879
 C   0.061892   2.456902  -1.518185
 H  -2.473751   2.534230  -2.165610
 H  -2.136799   4.006491  -1.195111
 H  -3.150216   2.680260  -0.526105
 H   0.239742   3.538026  -1.671457
```

H	-0.150435	1.985969	-2.485747
H	0.967134	2.002603	-1.101861
C	5.071298	-0.078557	-0.430389
H	4.808808	-1.113091	-0.157802
H	5.210289	-0.056354	-1.525671
C	6.364005	0.348669	0.271385
H	6.224482	0.275178	1.366066
H	6.551824	1.416592	0.058074
C	7.600660	-0.463218	-0.137059
H	8.487422	-0.017121	0.346708
H	7.760282	-0.353763	-1.225589
C	7.530072	-1.948975	0.220594
H	7.357724	-2.090391	1.301793
H	6.715165	-2.463599	-0.314271
H	8.469042	-2.465856	-0.037778

ts-4-6E
Geometry with 51 atoms:
Thermal correction to Gibbs Free Energy:
0.386824
Total energy: -2618.510379

Ni	-0.812702	0.425936	0.255883
C	1.887438	0.385196	0.242283
C	0.844616	-0.601884	0.608447
C	0.092907	-0.405751	1.793569
H	0.933422	-1.579206	0.127428
H	-1.085906	-0.856335	-0.322512
H	0.424517	0.358715	2.503721
H	-0.449297	-1.253795	2.224188
O	2.608200	-0.028058	-0.816821
O	2.068230	1.458230	0.793741
C	3.667667	0.831073	-1.289219
H	3.859377	0.487997	-2.316619
H	3.303650	1.869333	-1.320861
I	-2.899649	-2.289179	-0.064727
N	-1.233193	1.291105	-1.536314
H	-0.947560	2.019520	3.081030
C	-1.084368	2.691033	2.224299
N	-1.845815	1.998376	1.169737
H	-1.619230	3.595209	2.570470
H	-0.093244	2.971246	1.841888
C	-2.158046	2.935946	0.061959
C	-3.071964	1.400890	1.735245
C	-2.382248	2.181973	-1.237683
H	-1.308478	3.624188	-0.043981
H	-3.043722	3.550857	0.303988
H	-3.704248	2.174371	2.211038
H	-2.795023	0.645762	2.482423
H	-3.648266	0.897021	0.949340
H	-2.550716	2.893326	-2.067550
H	-3.273961	1.544079	-1.160752
C	-1.574449	0.379110	-2.643432
C	-0.017286	2.054990	-1.888765
H	-0.733489	-0.302962	-2.825355
H	-1.787328	0.948091	-3.567120
H	-2.452761	-0.218950	-2.371949
H	-0.206373	2.722523	-2.749706
H	0.778072	1.347165	-2.152755
H	0.330637	2.653020	-1.037519
C	4.921090	0.720214	-0.431486
H	5.679092	1.393353	-0.870678
H	4.697315	1.113550	0.573920
C	5.478595	-0.700684	-0.327601
H	4.695338	-1.368150	0.073368
H	5.711435	-1.079207	-1.340600
C	6.726433	-0.798831	0.553427
H	6.487574	-0.410729	1.560607
H	7.510096	-0.131084	0.150300
C	7.273536	-2.221170	0.668791
H	8.169074	-2.261710	1.310749
H	6.521646	-2.903696	1.100984
H	7.553491	-2.623596	-0.320029

2F
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.260350
Total energy: -2759.062762

C	-1.546819	-0.742062	1.153691
C	2.875352	-1.463441	-1.602257
H	3.175173	-1.398882	-2.663311
H	3.275746	-2.407190	-1.207073
C	3.428732	-0.287230	-0.822633
H	3.072809	0.655708	-1.258425
H	4.532129	-0.274278	-0.850712
Ni	1.054244	-0.844174	0.482863
O	-2.892816	-0.764959	1.098917
O	-0.869487	-1.224165	0.249607
C	3.166684	1.022974	1.185407
H	2.937180	1.001932	2.255658
H	4.219144	1.329541	1.054012
H	2.504269	1.747501	0.693439
C	3.682665	-1.336030	1.388730
H	4.763151	-1.107901	1.411588
H	3.291552	-1.338956	2.413665
H	3.535408	-2.334574	0.958530
C	0.875177	-2.861739	-1.634030
H	-0.212875	-2.851447	-1.491178
H	1.103494	-3.250836	-2.643312
H	1.320891	-3.529065	-0.882758
C	0.727064	-0.567519	-2.385786
H	0.883980	-0.874730	-3.436314
H	-0.348212	-0.557953	-2.165755
H	1.104809	0.452498	-2.244652
I	-0.426210	2.892339	-0.380259
C	0.556990	-0.494997	2.338895

```
 H   1.153071   0.252819   2.879800
 H   0.667785  -1.462146   2.868709
 C  -0.921312  -0.078119   2.319259
 H  -1.509984  -0.264071   3.234707
 H  -1.017466   1.001565   2.091412
 N   2.954272  -0.319585   0.596354
 N   1.401313  -1.497236  -1.459803
 C  -3.535738  -1.240043  -0.035475
 F  -4.831035  -1.096085   0.182896
 F  -3.268557  -2.526119  -0.242150
 F  -3.192093  -0.547429  -1.114451
```

3F

```
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.260297
Total energy: -2759.083550
Ni   1.049031   0.303740  -0.370403
 I   1.383056  -2.316364  -0.182853
 C   0.037314   0.035626  -2.018159
 C  -1.339924  -0.574289  -1.744728
 H   0.566336  -0.625276  -2.726402
 H  -0.115329   0.990177  -2.548010
 C  -2.077003   0.024632  -0.587761
 H  -1.251921  -1.643349  -1.475590
 H  -2.015834  -0.547263  -2.618924
 O  -3.429116  -0.330081  -0.640817
 O  -1.645967   0.683304   0.318371
 H   1.522891   2.112014  -2.869678
 C   2.134172   2.424836  -2.015965
 H   2.433007   3.479192  -2.161078
 H   3.034041   1.796303  -1.978423
 C   2.207394   2.754299   0.372192
 C   0.118373   3.049915  -0.827763
 C   1.708649   2.153108   1.664880
 H   3.243443   2.442393   0.183923
 H   2.199303   3.857706   0.413491
 H   0.339758   4.120816  -0.985916
 H  -0.500200   2.689259  -1.656293
 H  -0.455222   2.924539   0.096875
 H   2.299150   2.519286   2.524561
 H   0.664073   2.444882   1.838644
 C   0.848084   0.084054   2.565004
 C   3.137004   0.192214   1.793704
 H   0.914179  -1.009643   2.521142
 H   1.105976   0.420665   3.586788
 H  -0.183801   0.379500   2.333137
 H   3.503014   0.492076   2.793718
 H   3.156905  -0.900700   1.714189
 H   3.812873   0.598503   1.029944
 N   1.371639   2.269594  -0.759683
 N   1.762253   0.676492   1.570602
 C  -4.262221   0.015792   0.381523
 F  -5.466436  -0.467702   0.086795
 F  -3.874033  -0.503670   1.548294
 F  -4.365652   1.339370   0.526241
```

4F

```
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.259305
Total energy: -2759.066891
Ni  -0.647414  -0.191902  -0.171816
 C   2.153097  -1.202351   0.069300
 C   0.905024  -1.524972  -0.611153
 C  -0.181125  -2.137791   0.045354
 H   1.002206  -1.590823  -1.696699
 H  -0.863973  -0.414169  -1.554878
 H  -0.093420  -2.407400   1.101139
 H  -0.864611  -2.757911  -0.539495
 O   3.093013  -0.737024  -0.877662
 O   2.451790  -1.289327   1.233131
 C   4.282478  -0.237900  -0.452676
 I  -3.296484  -0.606326  -0.535401
 N  -0.190947   1.787137  -0.685819
 H  -0.795136  -1.294740   2.970990
 C  -0.083324  -0.461528   2.893971
 N  -0.550101   0.484170   1.863023
 H  -0.021794   0.037482   3.879015
 H   0.902246  -0.855098   2.629786
 C   0.428610   1.587906   1.703150
 C  -1.863049   1.003832   2.299418
 C   0.000854   2.528954   0.590786
 H   1.406614   1.139158   1.476171
 H   0.536722   2.153226   2.648770
 H  -1.756699   1.584777   3.234740
 H  -2.541486   0.160815   2.475351
 H  -2.318508   1.635527   1.530296
 H   0.748699   3.330417   0.463844
 H  -0.945330   3.019066   0.851173
 C  -1.251615   2.409778  -1.497442
 C   1.071214   1.776361  -1.451662
 H  -1.357076   1.861980  -2.442870
 H  -1.010811   3.466376  -1.717112
 H  -2.208472   2.355667  -0.963908
 H   1.324071   2.795581  -1.798676
 H   0.977880   1.111797  -2.319403
 H   1.886161   1.414424  -0.818464
 F   5.031024  -1.144031   0.177065
 F   4.947220   0.179579  -1.528422
 F   4.120633   0.811158   0.369013
```

6F

```
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
```

0.254850
Total energy: -2759.065798

C	-0.070141	0.119874	-2.248809
H	-0.885297	-0.428058	-2.735829
H	0.358970	0.924314	-2.863163
C	0.814393	-0.612374	-1.382048
H	0.627467	-1.654359	-1.111037
C	2.150793	-0.122768	-1.126733
O	2.690613	0.896448	-1.484932
O	2.837924	-1.040651	-0.274063
C	4.099350	-0.776069	0.126362
Ni	-0.349387	0.684854	-0.434410
C	-1.280988	1.621416	1.985440
H	-2.061155	0.846511	2.000456
H	-1.189981	2.031328	3.008904
C	-1.662023	2.724326	1.008469
H	-0.922312	3.534980	1.044110
H	-2.633441	3.165211	1.288469
C	-3.059222	1.715339	-0.723136
C	-1.268625	3.208581	-1.360070
C	0.224859	-0.270170	2.313503
C	1.143277	1.867161	1.686088
H	-1.347459	-0.471685	-0.209523
H	-0.219173	3.478292	-1.174380
H	-1.891848	4.119707	-1.293824
H	-1.347864	2.795857	-2.373827
H	-3.769567	2.561092	-0.775027
H	-3.034919	1.198352	-1.691020
H	-3.405004	1.002396	0.034014
H	1.117054	-0.766464	1.908051
H	0.384339	-0.058446	3.387459
H	-0.631107	-0.947091	2.202425
H	1.243788	2.242825	2.721621
H	1.059831	2.724653	1.005517
H	2.055019	1.318966	1.422086
I	-2.551433	-1.993558	0.052716
N	-1.706185	2.192244	-0.383850
N	-0.020550	0.968944	1.558711
F	4.495068	-1.784578	0.906410
F	4.190322	0.355202	0.846847
F	4.960195	-0.677546	-0.892415

7F
Geometry with 37 atoms:
Thermal correction to Gibbs Free Energy:
0.250923
Total energy: -2460.563437

C	0.650891	-2.341677	-0.510020
H	1.153562	-2.915777	-1.304614
H	0.539316	-2.936046	0.412336
C	-0.490969	-1.532341	-0.920494
H	-0.721388	-1.349142	-1.975795
C	-1.523792	-1.193625	0.008514
O	-1.698641	-1.467668	1.174011
O	-2.489162	-0.319299	-0.661884
C	-3.543785	0.149154	0.011400
Ni	1.068104	-0.502499	-0.258559
C	2.238880	2.057607	-0.130949
H	2.566549	2.076167	-1.179949
H	2.297556	3.095752	0.248040
C	3.152994	1.150242	0.682550
H	2.872873	1.189154	1.744230
H	4.200810	1.495923	0.610027
C	3.807987	-0.512102	-0.989559
C	3.439437	-1.190646	1.298011
C	0.055611	2.094448	-1.219238
C	0.181504	1.838735	1.177569
H	2.801594	-1.048440	2.181175
H	4.496979	-1.030564	1.585003
H	3.315052	-2.222255	0.944423
H	4.889966	-0.358744	-0.810360
H	3.639420	-1.545376	-1.319645
H	3.482695	0.158865	-1.795448
H	-0.948029	1.649564	-1.196537
H	-0.033627	3.196901	-1.159726
H	0.531512	1.825718	-2.172844
H	0.110150	2.929072	1.358670
H	0.731376	1.376503	2.007667
H	-0.829418	1.413816	1.168359
N	0.846765	1.553106	-0.104840
N	3.025634	-0.260504	0.234717
F	-4.261309	0.918310	-0.821543
F	-3.205981	0.918763	1.066683
F	-4.357240	-0.815114	0.470613

CF_3I
Geometry with 5 atoms:
Thermal correction to Gibbs Free Energy:
-0.016534
Total energy: -635.600902

C	-1.195733	-0.000081	0.000018
I	0.983208	-0.000303	0.000027
F	-1.665527	-0.703391	-1.028032
F	-1.665586	-0.537925	1.123418
F	-1.661732	1.243154	-0.095558

$CH_2CHCOOCF_3$
Geometry with 12 atoms:
Thermal correction to Gibbs Free Energy:
0.037639
Total energy: -604.370182

C	1.016195	0.130210	-0.000099
C	2.222706	-0.717614	0.000025
C	3.439828	-0.159204	-0.000100
H	2.072389	-1.799724	0.000198

```
 H   3.558429   0.928953  -0.000198
 H   4.344288  -0.773372   0.000011
 O  -0.121902  -0.681057  -0.000588
 O   0.949636   1.327432   0.000156
 C  -1.362366  -0.110595   0.000069
 F  -1.570393   0.641713  -1.081596
 F  -2.248233  -1.102798  -0.000208
 F  -1.569725   0.640681   1.082256
```

ts-1-2F
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.257635
Total energy: -2758.997187

```
Ni  -2.459352   0.277644   0.024580
 O  -0.648624   0.802345  -0.120964
 C  -0.409584   2.064241  -0.185675
 O   0.746857   2.531851  -0.189271
 C  -2.827825   2.164127   0.312467
 H  -2.867189   2.331650   1.407158
 H  -3.789823   2.511087  -0.103836
 C  -1.646015   2.930336  -0.296470
 H  -1.799571   3.080008  -1.381273
 H  -1.450618   3.929842   0.130229
 C  -1.105675  -2.098492   0.917220
 H  -0.250038  -1.417859   1.013980
 H  -1.723795  -2.004845   1.820452
 H  -0.741913  -3.140398   0.840334
 C  -1.055663  -1.844758  -1.484278
 H  -1.621059  -1.486105  -2.356360
 H  -0.160150  -1.221869  -1.372322
 H  -0.755556  -2.895395  -1.656175
 C  -5.075951   0.241539   1.336560
 H  -4.502587   0.138387   2.267326
 H  -5.224712   1.306772   1.129355
 H  -6.062656  -0.239627   1.461838
 C  -5.039601  -0.142115  -1.049151
 H  -4.491144  -0.596503  -1.883704
 H  -6.061334  -0.562443  -1.017330
 H  -5.097971   0.939034  -1.224801
 C  -3.145795  -2.474849  -0.392206
 H  -3.467335  -2.437737  -1.442191
 H  -3.004598  -3.539809  -0.132969
 C  -4.201254  -1.849347   0.500869
 H  -5.176096  -2.352127   0.370634
 H  -3.913197  -1.956421   1.555931
 I   4.584775  -0.763077   0.125869
 N  -4.331671  -0.387847   0.225959
 N  -1.882103  -1.715554  -0.274281
 C   2.389694   1.072860  -0.055074
 F   1.980046   0.550266  -1.141920
 F   3.152292   2.090825  -0.097500
 F   1.917298   0.686952   1.062644
```

ts-2-3F
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.261575
Total energy: -2759.066614

```
 C   1.872237  -0.464973  -0.847759
 C  -2.418959  -1.777046   1.648027
 H  -3.000047  -1.895752   2.580926
 H  -1.800558  -2.678010   1.531294
 C  -3.340447  -1.614475   0.458815
 H  -3.936123  -0.698368   0.563093
 H  -4.046399  -2.459810   0.381998
Ni  -0.945287  -0.369251  -0.280166
 O   3.246066  -0.506461  -0.898060
 O   1.268578  -0.751941   0.160484
 C  -3.343315  -0.847816  -1.839949
 H  -3.571547   0.183527  -1.539890
 H  -4.285916  -1.401346  -2.004672
 H  -2.779758  -0.823968  -2.779319
 C  -2.116971  -2.843764  -1.234693
 H  -3.001576  -3.475042  -1.435635
 H  -1.523383  -2.765896  -2.151362
 H  -1.501290  -3.324558  -0.464261
 C  -0.347813  -0.903974   2.572084
 H   0.346778  -0.055194   2.537971
 H  -0.654976  -1.088464   3.618116
 H   0.175623  -1.787377   2.187040
 C  -2.235841   0.553546   2.290021
 H  -2.679317   0.291999   3.269030
 H  -1.539603   1.388154   2.421365
 H  -3.029787   0.886687   1.610683
 I  -0.351420   2.527620  -0.059823
 C  -0.259858  -0.298940  -2.107690
 H  -0.789269   0.460033  -2.706568
 H  -0.416529  -1.272835  -2.602185
 C   1.243275   0.006981  -2.110852
 H   1.803820  -0.404290  -2.968894
 H   1.433095   1.096144  -2.114364
 N  -2.534778  -1.496993  -0.788125
 N  -1.516050  -0.606186   1.724923
 C   3.962042  -0.820529   0.230608
 F   5.246220  -0.754323  -0.098465
 F   3.729439   0.036159   1.222625
 F   3.695739  -2.053511   0.661646
```

ts-3-4F
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.257525
Total energy: -2759.049028

```
Ni   0.429699   0.123743  -0.193292
```

I	3.061919	-1.297560	-0.057447
C	0.148943	-0.493976	-2.075195
C	-0.820900	-1.107048	-1.248769
H	0.959666	-1.109327	-2.471640
H	-0.155124	0.353371	-2.691797
C	-2.135393	-0.451797	-1.083911
H	0.055618	-1.198365	0.224557
H	-0.826851	-2.185741	-1.070090
O	-2.917031	-1.195227	-0.189688
O	-2.549317	0.551054	-1.602631
H	2.521732	1.631317	-1.842730
C	2.299344	2.246341	-0.961519
H	2.554250	3.301112	-1.172762
H	2.918901	1.881663	-0.134490
C	0.554731	2.827509	0.645501
C	0.062567	2.720257	-1.709827
C	0.886839	1.963113	1.843031
H	1.101970	3.785195	0.696214
H	-0.516457	3.069658	0.640159
H	0.198679	3.816647	-1.726380
H	0.386291	2.324090	-2.679834
H	-0.999192	2.482263	-1.567319
H	1.964006	1.748475	1.873600
H	0.620778	2.484171	2.781003
C	-1.271905	0.799464	1.971760
C	0.735744	-0.273699	2.751014
H	-1.732880	-0.193861	1.922131
H	-1.478803	1.242211	2.963299
H	-1.727249	1.429227	1.198923
H	0.583852	0.123647	3.770953
H	0.232651	-1.245309	2.664255
H	1.806946	-0.419479	2.569006
N	0.866168	2.117256	-0.625932
N	0.183628	0.660242	1.749505
C	-4.167472	-0.763193	0.140416
F	-4.981541	-0.714195	-0.913949
F	-4.661846	-1.632205	1.017498
F	-4.151598	0.445732	0.712930

ts-4-5F
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.258225
Total energy: -2759.050782

Ni	-0.947475	0.235452	-0.395650
C	2.207217	-1.324139	-0.118491
C	1.072962	-1.461325	-1.019723
C	-0.087206	-2.048792	-0.623149
H	1.219175	-1.138106	-2.050265
H	-1.113214	0.134479	-1.836926
H	-0.198323	-2.457248	0.383075
H	-0.846993	-2.310610	-1.357311
O	3.302938	-0.782674	-0.819605
O	2.293709	-1.604919	1.050347
C	4.424879	-0.420500	-0.142196
I	-3.339334	-0.834928	-0.312548
N	0.016198	2.011807	-0.721386
H	-1.377748	-1.252563	2.355191
C	-0.516229	-0.581741	2.476174
N	-0.714439	0.609869	1.632880
H	-0.427082	-0.299310	3.541653
H	0.396679	-1.107600	2.175978
C	0.499550	1.462038	1.631139
C	-1.883408	1.360090	2.138509
C	0.339910	2.581297	0.619964
H	1.359047	0.830914	1.367664
H	0.691374	1.877277	2.638612
H	-1.654937	1.822900	3.116574
H	-2.728853	0.673691	2.256884
H	-2.188014	2.141059	1.431261
H	1.255239	3.194271	0.572155
H	-0.475396	3.251249	0.920085
C	-0.917382	2.896727	-1.450136
C	1.251067	1.842919	-1.509911
H	-1.103004	2.485862	-2.449940
H	-0.496362	3.914700	-1.549196
H	-1.874292	2.950125	-0.914661
H	1.686379	2.826567	-1.766795
H	1.030422	1.290561	-2.430870
H	1.986881	1.279701	-0.928285
F	5.020982	-1.449112	0.460190
F	5.272350	0.096278	-1.028636
F	4.166599	0.515073	0.782770

ts-4-6F
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.254571
Total energy: -2759.056060

Ni	0.402581	0.276173	-0.275856
C	-2.145272	-0.361210	-1.031523
C	-0.827318	-0.948190	-1.262090
C	0.081090	-0.280130	-2.129174
H	-0.736922	-2.010196	-1.021671
H	0.979814	-1.009019	0.065243
H	-0.293646	0.547827	-2.739470
H	0.898032	-0.856288	-2.574810
O	-2.926074	-1.234356	-0.241671
O	-2.585081	0.699707	-1.398954
C	-4.192149	-0.883632	0.102345
I	3.070881	-1.468069	-0.065833
N	0.144092	0.678620	1.715538
H	0.455245	2.596610	-2.562268
C	0.170453	2.990496	-1.578638
N	0.936113	2.296922	-0.527372
H	0.375472	4.077402	-1.566253

H	-0.904072	2.815644	-1.433186
C	0.661653	2.913968	0.794506
C	2.376386	2.336492	-0.847434
C	0.921490	1.926446	1.917759
H	-0.389375	3.232858	0.805691
H	1.274194	3.822266	0.938438
H	2.725967	3.379961	-0.963598
H	2.557732	1.787272	-1.780787
H	2.956016	1.848320	-0.054483
H	0.676187	2.385362	2.893666
H	1.984296	1.646825	1.940900
C	0.595810	-0.355637	2.663326
C	-1.305497	0.900610	1.892929
H	0.051308	-1.289729	2.471815
H	0.413349	-0.037326	3.706209
H	1.667139	-0.543883	2.523748
H	-1.521742	1.345101	2.882183
H	-1.821963	-0.062908	1.820074
H	-1.701589	1.559357	1.110564
F	-4.981182	-0.706076	-0.959893
F	-4.693532	-1.877756	0.834110
F	-4.232675	0.234105	0.839887

ts-1-9F
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.261217
Total energy: -2759.005317

Ni	0.482388	0.046348	-0.103107
O	1.775920	1.429099	0.499876
C	1.953730	2.447883	-0.291010
O	2.792178	3.322857	-0.106565
C	0.545187	1.031214	-1.782949
H	-0.423161	0.983942	-2.299302
H	1.294463	0.530691	-2.412635
C	0.971021	2.454686	-1.458801
H	1.407949	2.989935	-2.319738
H	0.102093	3.049119	-1.123671
C	-0.415288	-1.811957	2.268072
H	-1.380712	-1.289952	2.271164
H	-0.487119	-2.661184	1.583508
H	-0.216924	-2.196427	3.285482
C	0.786500	0.154933	2.896869
H	1.541293	0.884778	2.588212
H	-0.175101	0.672974	3.015579
H	1.064615	-0.301564	3.864912
C	1.429315	-2.229006	-1.968175
H	0.471979	-2.726379	-1.778638
H	1.307667	-1.544433	-2.817768
H	2.184177	-2.991730	-2.237170
C	3.151322	-0.828572	-1.034386
H	3.451830	-0.218770	-0.176170
H	3.924535	-1.589967	-1.245196
H	3.070957	-0.163599	-1.902713
C	1.935570	-1.607734	1.696695
H	2.742988	-0.863862	1.711267
H	2.104268	-2.294230	2.547344
C	1.957968	-2.383616	0.392893
H	2.881680	-2.987446	0.326067
H	1.112947	-3.083204	0.353094
C	-1.920431	-1.087201	-0.909253
F	-1.398191	-2.233034	-0.444106
F	-1.592522	-0.965004	-2.194477
F	-3.247736	-1.243050	-0.854597
I	-1.882728	1.058832	0.406060
N	1.849848	-1.475264	-0.774355
N	0.654320	-0.882473	1.855009

2G
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy:
0.287064
Total energy: -2798.382112

C	1.327334	-0.603749	-1.000740
C	-3.148218	-1.641565	1.616374
H	-3.512455	-1.528508	2.652821
H	-3.424757	-2.650844	1.282387
C	-3.776891	-0.597172	0.715830
H	-3.543134	0.410560	1.084874
H	-4.875786	-0.699859	0.692804
Ni	-1.281699	-0.972647	-0.421708
O	2.634788	-0.491879	-0.908896
O	0.655377	-1.076981	-0.071988
C	-3.555908	0.561277	-1.386757
H	-3.265967	0.479504	-2.439200
H	-4.642377	0.750691	-1.332532
H	-3.010930	1.399232	-0.932145
C	-3.784288	-1.849913	-1.402115
H	-4.880940	-1.756030	-1.496981
H	-3.336729	-1.890823	-2.402966
H	-3.547517	-2.784817	-0.878468
C	-1.014914	-2.806774	1.837743
H	0.071209	-2.685604	1.737622
H	-1.247811	-3.153490	2.861631
H	-1.350514	-3.566444	1.117235
C	-1.159457	-0.470287	2.442644
H	-1.315785	-0.742096	3.503208
H	-0.087987	-0.329627	2.252480
H	-1.659471	0.483068	2.234382
C	3.245026	-0.858298	0.332348
H	2.916286	-0.186664	1.138837
H	3.012773	-1.899158	0.598446
I	-0.300138	2.910619	0.327274
C	-0.738697	-0.736478	-2.277116
H	-1.403796	-0.145241	-2.922122
H	-0.681537	-1.759059	-2.702205

```
 C   0.660990  -0.110290  -2.234410
 H   1.306902  -0.270416  -3.115232
 H   0.591112   0.983572  -2.080919
 N  -3.223966  -0.692052  -0.670597
 N  -1.673375  -1.522692   1.547664
 C   4.739920  -0.719980   0.144102
 F   5.196564  -1.529476  -0.824834
 F   5.094605   0.532427  -0.174431
 F   5.361585  -1.051082   1.286881
```

3G
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy:
0.286099
Total energy: -2798.398195

```
Ni   1.340191   0.330811  -0.359149
 I   2.164513  -2.176992  -0.119414
 C   0.242750  -0.191568  -1.883165
 C  -1.016105  -0.933474  -1.416821
 H   0.785805  -0.845901  -2.586928
 H  -0.076800   0.686707  -2.469195
 C  -1.760088  -0.254539  -0.299412
 H  -0.741917  -1.920825  -1.001728
 H  -1.729837  -1.131090  -2.235500
 O  -3.095483  -0.443756  -0.377202
 O  -1.264109   0.370007   0.615438
 C  -3.869272   0.097316   0.683548
 H  -3.643884  -0.396438   1.641593
 H  -3.705733   1.179878   0.795457
 H   1.304567   2.050483  -2.962229
 C   1.920992   2.506258  -2.179474
 H   2.029309   3.585267  -2.395006
 H   2.912103   2.033275  -2.193319
 C   2.123015   2.977921   0.177962
 C  -0.070579   2.864809  -0.852097
 C   1.846677   2.366327   1.531148
 H   3.178417   2.840729  -0.091128
 H   1.925699   4.064400   0.181601
 H  -0.043112   3.944691  -1.084974
 H  -0.685193   2.354890  -1.601886
 H  -0.539278   2.710140   0.125814
 H   2.429488   2.875860   2.320294
 H   0.784291   2.478939   1.786212
 C   1.454371   0.230719   2.588492
 C   3.609523   0.697036   1.600663
 H   1.708875  -0.835961   2.575554
 H   1.740890   0.658488   3.567816
 H   0.370883   0.330665   2.445030
 H   4.001111   1.120675   2.544887
 H   3.819307  -0.378471   1.574991
 H   4.135531   1.162279   0.756667
 N   1.295257   2.301585  -0.856733
 N   2.155768   0.919548   1.489082
 C  -5.322477  -0.141797   0.343233
 F  -5.678939   0.468920  -0.799098
 F  -5.602222  -1.447669   0.205453
 F  -6.100877   0.342883   1.326342
```

4G
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy:
0.285018
Total energy: -2798.379085

```
Ni  -0.921121  -0.151264  -0.076857
 C   2.012079  -0.405491   0.468445
 C   0.857063  -1.225618   0.071584
 C  -0.121897  -1.671381   0.977615
 H   1.018949  -1.762852  -0.865489
 H  -0.996264  -0.994119  -1.214182
 H  -0.038677  -1.415068   2.036724
 H  -0.660723  -2.597064   0.760451
 O   2.873485  -0.268706  -0.586544
 O   2.233985   0.102621   1.547895
 I  -3.468259  -1.170027  -0.179692
 N  -0.813449   1.446279  -1.423149
 H  -1.020685   0.220230   3.239068
 C  -0.485363   1.058493   2.772980
 N  -1.081482   1.344348   1.454305
 H  -0.572011   1.939311   3.436561
 H   0.569963   0.792705   2.661113
 C  -0.340354   2.445640   0.792711
 C  -2.493395   1.717095   1.677747
 C  -0.870675   2.690249  -0.609088
 H   0.720036   2.157199   0.758138
 H  -0.412051   3.377242   1.386527
 H  -2.557657   2.641677   2.282003
 H  -2.998646   0.903012   2.210965
 H  -3.023954   1.865909   0.731957
 H  -0.298119   3.498782  -1.095738
 H  -1.914473   3.025581  -0.566022
 C  -1.901246   1.424522  -2.416578
 C   0.486326   1.356067  -2.116589
 H  -1.829438   0.508175  -3.016710
 H  -1.840591   2.301372  -3.087834
 H  -2.871678   1.421746  -1.905155
 H   0.584354   2.161545  -2.868456
 H   0.575904   0.383170  -2.615215
 H   1.304599   1.447051  -1.395171
 C   4.059895   0.478125  -0.390011
 H   4.254311   1.060678  -1.301255
 H   3.987114   1.145914   0.479385
 C   5.229305  -0.462652  -0.169529
 F   5.438209  -1.261870  -1.228976
 F   5.035512  -1.256412   0.897334
 F   6.353299   0.243686   0.038238
```

6G
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.279390
Total energy: -2798.378104

C	-0.133959	0.047010	-2.137459
H	-0.816483	-0.627278	-2.667481
H	0.256570	0.870477	-2.752102
C	0.714784	-0.504856	-1.120527
H	0.639830	-1.549919	-0.808160
C	1.925705	0.198183	-0.713480
O	2.287791	1.305262	-1.069999
O	2.624922	-0.524132	0.228576
C	3.816819	0.036695	0.740625
H	3.850273	1.126703	0.605359
H	3.889180	-0.214561	1.807946
Ni	-0.683578	0.684413	-0.403586
C	-1.914917	1.666023	1.860465
H	-2.628650	0.829680	1.853331
H	-1.955505	2.137547	2.860533
C	-2.287730	2.677189	0.785545
H	-1.611483	3.541643	0.827166
H	-3.308045	3.060181	0.958048
C	-3.444116	1.432972	-0.972160
C	-1.758555	3.056489	-1.573892
C	-0.306033	-0.077777	2.435430
C	0.498689	2.096078	1.777707
H	-1.560760	-0.540544	-0.207649
H	-0.758346	3.441484	-1.328201
H	-2.469233	3.902889	-1.618908
H	-1.713185	2.577164	-2.560313
H	-4.228129	2.196953	-1.129926
H	-3.291145	0.867783	-1.900597
H	-3.777415	0.730465	-0.199713
H	0.651540	-0.523588	2.133439
H	-0.259341	0.198615	3.505612
H	-1.096752	-0.823764	2.289362
H	0.468594	2.529207	2.794943
H	0.414094	2.906662	1.042837
H	1.471850	1.612111	1.631898
I	-2.678005	-2.188353	0.041708
N	-2.175412	2.062700	-0.566868
N	-0.572028	1.099201	1.592940
C	5.017743	-0.561186	0.031848
F	6.150594	-0.007113	0.498954
F	5.106920	-1.888815	0.219936
F	4.972128	-0.350077	-1.294809

7G
Geometry with 40 atoms:
Thermal correction to Gibbs Free Energy: 0.276849
Total energy: -2499.874859

C	0.780204	-2.238794	-0.554572
H	1.166214	-2.837800	-1.395720
H	0.625201	-2.857101	0.345711
C	-0.251085	-1.256517	-0.867153
H	-0.512795	-1.005002	-1.902676
C	-1.220557	-0.850680	0.123939
O	-1.350199	-1.231265	1.276003
O	-2.044884	0.164784	-0.381990
C	-3.059458	0.660841	0.455724
H	-2.888896	0.393764	1.508736
H	-3.113878	1.754749	0.350334
Ni	1.439655	-0.473897	-0.262053
C	2.841958	1.968753	-0.067353
H	3.179878	1.998653	-1.112898
H	2.990058	2.982502	0.351592
C	3.664619	0.952436	0.716256
H	3.373102	0.973310	1.775567
H	4.739389	1.210528	0.668686
C	4.168280	-0.690038	-1.028513
C	3.762409	-1.426462	1.233335
C	0.682897	2.205632	-1.187519
C	0.750121	1.913152	1.203746
H	3.149678	-1.263264	2.130636
H	4.833394	-1.374902	1.512051
H	3.540065	-2.428134	0.843032
H	5.261847	-0.640126	-0.858397
H	3.904291	-1.689650	-1.397846
H	3.895972	0.038963	-1.802792
H	-0.353071	1.841158	-1.177894
H	0.684708	3.311500	-1.117449
H	1.146922	1.907617	-2.138192
H	0.745737	3.005223	1.389998
H	1.256690	1.413092	2.039409
H	-0.286145	1.552334	1.175725
N	1.411064	1.588886	-0.069774
N	3.422006	-0.422736	0.213281
C	-4.399403	0.086134	0.040118
F	-5.377786	0.557400	0.836702
F	-4.417597	-1.255970	0.121172
F	-4.720110	0.410097	-1.226189

CF_3CH_2I
Geometry with 8 atoms:
Thermal correction to Gibbs Free Energy: 0.009995
Total energy: -674.934853

C	-1.734185	0.002665	-0.000001
C	-0.564857	0.958465	0.000005
H	-0.614953	1.582485	-0.900278
H	-0.614952	1.582480	0.900291
I	1.370036	-0.019870	-0.000000
F	-1.757573	-0.792095	1.083014

F	-2.883490	0.708768	0.000005
F	-1.757573	-0.792080	-1.083023

$CH_2CHCOOCH_2CF_3$
Geometry with 15 atoms:
Thermal correction to Gibbs Free Energy: 0.064156
Total energy: -643.686902

C	1.471134	-0.204406	-0.271525
C	2.627436	0.682675	-0.000378
C	3.773552	0.187622	0.480555
H	2.492106	1.747004	-0.209331
H	3.878036	-0.883322	0.681537
H	4.631444	0.833863	0.685527
O	0.425881	0.520892	-0.756216
O	1.432970	-1.400644	-0.106690
C	-0.788913	-0.157030	-1.031167
H	-1.229436	0.282333	-1.936555
H	-0.634894	-1.236330	-1.168398
C	-1.757665	0.047743	0.118358
F	-2.908551	-0.598711	-0.129218
F	-1.260631	-0.418860	1.277069
F	-2.048743	1.345887	0.304974

ts-1-2G
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.284012
Total energy: -2798.345624

Ni	2.395454	0.422341	-0.010728
O	0.548022	0.833279	0.087147
C	0.233357	2.069476	0.191649
O	-0.951143	2.479922	0.183762
C	2.654536	2.339357	-0.211121
H	2.731303	2.549947	-1.296080
H	3.572208	2.730338	0.261809
C	1.403510	3.011870	0.370840
H	1.502957	3.138981	1.464569
H	1.158237	4.007642	-0.037270
C	1.238542	-1.992480	-1.066701
H	0.331740	-1.382144	-1.164105
H	1.880579	-1.801876	-1.937303
H	0.956671	-3.061826	-1.055911
C	1.067491	-1.857485	1.338410
H	1.560791	-1.489074	2.249301
H	0.124945	-1.313342	1.204076
H	0.849542	-2.935211	1.455573
C	5.056214	0.611567	-1.211973
H	4.527196	0.512172	-2.168951
H	5.126838	1.674230	-0.955857
H	6.076123	0.199833	-1.314773
C	4.950013	0.124516	1.153266
H	4.399925	-0.397781	1.946130
H	5.997220	-0.228436	1.148194
H	4.930768	1.198928	1.373008
C	3.239675	-2.295010	0.318708
H	3.512638	-2.284214	1.382871
H	3.177980	-3.354012	0.009468
C	4.289798	-1.566116	-0.498719
H	5.289130	-2.009736	-0.342352
H	4.057758	-1.646171	-1.569759
C	-2.243909	0.860270	0.052305
H	-1.880978	0.597825	1.036362
H	-1.707833	0.595242	-0.847808
I	-3.169856	-1.693205	-0.038341
N	4.311602	-0.112074	-0.160082
N	1.934970	-1.612863	0.175300
C	-3.554718	1.627109	-0.069186
F	-3.407857	2.958664	-0.033625
F	-4.169867	1.346185	-1.231624
F	-4.394960	1.315537	0.933316

ts-2-3G
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.287625
Total energy: -2798.381846

C	1.532964	-0.329709	-0.709705
C	-2.610899	-1.841195	1.770304
H	-3.219765	-1.949955	2.686941
H	-1.820044	-2.603726	1.809560
C	-3.466493	-2.031903	0.535795
H	-4.254313	-1.268807	0.496644
H	-3.964918	-3.016795	0.545247
Ni	-1.279740	-0.449134	-0.258677
O	2.867070	-0.302015	-0.682393
O	0.875557	-0.583006	0.290723
C	-3.488185	-1.549075	-1.838759
H	-3.958907	-0.571925	-1.667702
H	-4.272960	-2.315313	-1.977196
H	-2.883908	-1.494003	-2.751401
C	-1.913987	-3.156420	-0.945580
H	-2.634355	-3.981127	-1.096607
H	-1.293158	-3.060318	-1.842157
H	-1.259868	-3.403506	-0.099874
C	-0.849318	-0.427871	2.670545
H	-0.329959	0.528700	2.527796
H	-1.215820	-0.498548	3.711473
H	-0.134677	-1.237240	2.480667
C	-2.945425	0.549112	2.012683
H	-3.446880	0.350038	2.978292
H	-2.432479	1.514565	2.062740
H	-3.701107	0.618223	1.220515
C	3.489853	-0.529486	0.578182
H	3.256382	0.278083	1.288187

H	3.182616	-1.492253	1.012397
I	-0.876311	2.593564	-0.173016
C	-0.552912	-0.412658	-2.065953
H	-1.132712	0.276035	-2.704033
H	-0.614495	-1.411423	-2.529485
C	0.918156	0.019746	-2.026762
H	1.546466	-0.387858	-2.837960
H	1.012420	1.118692	-2.085445
N	-2.628575	-1.886462	-0.686533
N	-1.963354	-0.512985	1.710992
C	4.982014	-0.557375	0.334748
F	5.332314	-1.538364	-0.513213
F	5.432312	0.598066	-0.177516
F	5.621765	-0.770525	1.496656

ts-3-4G
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.284207
Total energy: -2798.359051

Ni	0.694992	0.264695	-0.125670
I	3.235903	-1.711769	-0.028885
C	0.134320	-0.562207	-1.876729
C	-0.779747	-0.929993	-0.875863
H	0.844495	-1.305749	-2.246870
H	-0.139096	0.237817	-2.565401
C	-1.987123	-0.095166	-0.632267
H	0.333901	-0.929083	0.569721
H	-0.857138	-1.958552	-0.516534
O	-2.736187	-0.633855	0.367644
O	-2.288612	0.925851	-1.209755
C	-3.940598	0.022179	0.729260
H	-4.054334	-0.046610	1.819501
H	-3.946076	1.073188	0.410301
H	2.808968	1.096290	-2.121885
C	2.771294	1.864711	-1.339520
H	3.195945	2.809478	-1.725796
H	3.377012	1.510652	-0.497626
C	1.279803	3.002814	0.229059
C	0.592331	2.615979	-2.045282
C	1.628608	2.308220	1.527536
H	1.942964	3.870937	0.066339
H	0.250925	3.385306	0.266720
H	0.895590	3.660032	-2.241937
H	0.781638	2.031233	-2.953426
H	-0.480436	2.577383	-1.815971
H	2.675259	1.974567	1.513979
H	1.509465	2.999875	2.381232
C	-0.610690	1.452946	2.057405
C	1.354888	0.249631	2.770748
H	-1.192197	0.529375	2.168586
H	-0.646474	2.022982	3.003762
H	-1.069778	2.051986	1.261027
H	1.414130	0.809516	3.721569
H	0.722178	-0.635761	2.911774
H	2.356494	-0.084295	2.474291
C	-5.118452	-0.680963	0.080299
F	-5.018543	-0.681246	-1.260067
F	-5.219058	-1.960931	0.473304
F	-6.261950	-0.058915	0.411135
N	1.367889	2.058493	-0.917417
N	0.783610	1.101034	1.708273

ts-4-5G
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.282945
Total energy: -2798.363038

Ni	-1.290157	0.248578	-0.402774
C	2.077524	-0.696211	0.129488
C	1.014035	-1.045430	-0.823121
C	-0.002749	-1.877249	-0.490545
H	1.140489	-0.688821	-1.845488
H	-1.376726	0.059268	-1.845327
H	-0.078854	-2.303443	0.511672
H	-0.673071	-2.264906	-1.255735
O	3.025255	0.081247	-0.475835
O	2.152219	-1.024377	1.294850
C	4.170591	0.448681	0.274282
H	4.438133	1.480576	0.008890
H	3.996216	0.367706	1.355846
I	-3.470069	-1.245351	-0.328323
N	-0.673171	2.158503	-0.777164
H	-1.574170	-1.182702	2.397410
C	-0.836156	-0.376474	2.505808
N	-1.204091	0.733312	1.609913
H	-0.820936	-0.042039	3.559933
H	0.156266	-0.757996	2.242530
C	-0.150922	1.775934	1.602748
C	-2.499708	1.290759	2.050358
C	-0.460144	2.817950	0.545180
H	0.805960	1.283278	1.383332
H	-0.058090	2.252666	2.597228
H	-2.393053	1.797880	3.027383
H	-3.227689	0.477189	2.144030
H	-2.894719	2.001576	1.314871
H	0.354120	3.558842	0.484119
H	-1.369616	3.371322	0.809610
C	-1.752288	2.836256	-1.526906
C	0.571599	2.193768	-1.568440
H	-1.864223	2.363837	-2.510315
H	-1.521777	3.909461	-1.664335
H	-2.702247	2.735102	-0.985796
H	0.841438	3.236160	-1.821572
H	0.435567	1.621195	-2.493867
H	1.391292	1.744557	-0.998997

```
 C   5.329238  -0.457854  -0.097193
 F   6.415744  -0.138207   0.624431
 F   5.040750  -1.749806   0.135366
 F   5.653359  -0.349291  -1.396235
```

ts-4-6G

```
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy:
0.280969
Total energy: -2798.367202
Ni   0.710166   0.373796  -0.238953
 C  -1.960701   0.012198  -0.599066
 C  -0.757646  -0.761112  -0.953438
 C   0.095791  -0.292876  -1.985325
 H  -0.766100  -1.805696  -0.632321
 H   1.094252  -0.946385   0.189103
 H  -0.249110   0.531477  -2.617428
 H   0.781662  -0.999660  -2.463289
 O  -2.709173  -0.659142   0.329109
 O  -2.271102   1.110718  -1.014572
 C  -3.914855  -0.063101   0.770811
 H  -4.030420  -0.270630   1.843581
 H  -3.928278   1.020446   0.589759
 I   3.094358  -1.876100  -0.062338
 N   0.748127   0.996249   1.708480
 H   0.908296   2.421703  -2.770233
 C   0.793735   2.945659  -1.813131
 N   1.539827   2.229414  -0.763287
 H   1.172240   3.977943  -1.934235
 H  -0.274158   2.970525  -1.556469
 C   1.521211   3.010177   0.498920
 C   2.921639   1.968173  -1.212023
 C   1.735656   2.103700   1.698211
 H   0.545096   3.508886   0.571277
 H   2.288712   3.805049   0.481086
 H   3.434776   2.911886  -1.477875
 H   2.900847   1.306138  -2.087685
 H   3.488601   1.459586  -0.422374
 H   1.676794   2.688640   2.634969
 H   2.733988   1.645919   1.654626
 C   1.132333  -0.011368   2.713720
 C  -0.616996   1.479306   2.002819
 H   0.424921  -0.850440   2.678195
 H   1.125531   0.426644   3.728850
 H   2.135338  -0.393933   2.489493
 H  -0.644464   2.027574   2.962714
 H  -1.289664   0.615369   2.066864
 H  -0.983368   2.134959   1.203418
 C  -5.090508  -0.682455   0.038164
 F  -5.193562  -2.000991   0.273711
 F  -4.987837  -0.522497  -1.292332
 F  -6.236661  -0.105519   0.437729
```

2H

```
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy:
0.314695
Total energy: -2837.711202
 C   1.157367  -0.277999  -0.780636
 C  -3.288234  -1.921771   1.546774
 H  -3.765227  -1.852000   2.541023
 H  -3.330728  -2.975282   1.236825
 C  -4.017557  -1.050008   0.544331
 H  -4.013879  -0.004914   0.881763
 H  -5.070816  -1.361322   0.435629
Ni  -1.392678  -1.049602  -0.374545
 O   2.391308   0.108417  -0.585437
 O   0.486968  -0.809135   0.122743
 C  -3.770555   0.090492  -1.568579
 H  -3.365237   0.035374  -2.584138
 H  -4.873134   0.117789  -1.625840
 H  -3.402116   1.007567  -1.089483
 C  -3.650796  -2.329607  -1.519610
 H  -4.736155  -2.397134  -1.714623
 H  -3.111013  -2.331289  -2.474411
 H  -3.334720  -3.207003  -0.941108
 C  -1.011624  -2.623521   2.066381
 H   0.036251  -2.298739   2.054836
 H  -1.284147  -2.934856   3.091954
 H  -1.117482  -3.484263   1.390725
 C  -1.652051  -0.320627   2.431112
 H  -1.875653  -0.530131   3.493894
 H  -0.608537   0.003411   2.330955
 H  -2.286449   0.502858   2.082047
 C   2.940910   0.001416   0.751591
 H   2.393852   0.697304   1.404283
 H   2.792890  -1.022372   1.124171
 I  -0.815409   3.013910   0.229869
 C  -0.735546  -0.871971  -2.199952
 H  -1.428894  -0.449529  -2.941691
 H  -0.491180  -1.904457  -2.522258
 C   0.544662  -0.031898  -2.116542
 H   1.293314  -0.188574  -2.913360
 H   0.306244   1.047417  -2.115081
 N  -3.330841  -1.086600  -0.784216
 N  -1.864876  -1.519057   1.600258
 C   4.408087   0.369520   0.693736
 H   4.552370   1.333633   0.184223
 H   4.785800   0.467603   1.722105
 C   5.274598  -0.658089   0.004468
 F   4.977354  -0.799856  -1.301156
 F   5.145685  -1.879590   0.567581
 F   6.576360  -0.323859   0.080526
```

3H

Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy:
0.313493
Total energy: -2837.725122

Ni	1.484769	0.356626	-0.371176
I	2.577699	-2.055016	-0.184704
C	0.346732	-0.289828	-1.813553
C	-0.788600	-1.147603	-1.243588
H	0.899486	-0.889225	-2.557695
H	-0.104527	0.548136	-2.370847
C	-1.446310	-0.569616	-0.017441
H	-0.396336	-2.124961	-0.907792
H	-1.579149	-1.373677	-1.980971
O	-2.724721	-0.954378	0.110591
O	-0.897969	0.135641	0.809764
C	-3.430477	-0.519617	1.282835
H	-3.004553	-1.012125	2.171091
H	-3.308609	0.566927	1.409744
H	1.115959	2.039044	-2.979729
C	1.726607	2.566966	-2.238597
H	1.707537	3.648477	-2.468579
H	2.759500	2.200622	-2.310719
C	2.014427	3.087282	0.101401
C	-0.207766	2.732821	-0.793791
C	1.906894	2.448861	1.466443
H	3.058059	3.080457	-0.238715
H	1.686881	4.141412	0.127124
H	-0.307778	3.804987	-1.042679
H	-0.813404	2.147764	-1.494455
H	-0.592152	2.550792	0.215601
H	2.474350	3.029103	2.217694
H	0.857753	2.427984	1.792250
C	1.892970	0.301343	2.565614
C	3.861457	1.006586	1.358616
H	2.272594	-0.727012	2.530606
H	2.225825	0.776413	3.507860
H	0.796590	0.268624	2.536831
H	4.294372	1.488543	2.255828
H	4.193521	-0.037219	1.314562
H	4.238431	1.517340	0.463304
N	1.206483	2.314283	-0.879335
N	2.388200	1.051402	1.396924
C	-4.891544	-0.894845	1.128131
H	-5.410576	-0.714481	2.081191
H	-5.000363	-1.960184	0.876115
C	-5.623488	-0.094244	0.077181
F	-5.164351	-0.316864	-1.168362
F	-5.519444	1.234903	0.298610
F	-6.938610	-0.389812	0.070770

4H
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy:
0.312296
Total energy: -2837.706248

Ni	-1.315855	-0.144878	-0.208654
C	1.632947	-0.777560	-0.090402
C	0.373691	-1.270633	-0.679284
C	-0.578204	-2.004419	0.049397
H	0.421727	-1.364070	-1.766659
H	-1.567192	-0.459513	-1.568565
H	-0.398214	-2.220636	1.105692
H	-1.217227	-2.719250	-0.474931
O	2.437340	-0.252884	-1.047116
O	1.969856	-0.819815	1.078895
I	-3.949609	-0.899342	-0.369111
N	-1.145191	1.849498	-0.829447
H	-1.166932	-1.116731	2.967220
C	-0.558935	-0.214796	2.813905
N	-1.193484	0.627809	1.782919
H	-0.493866	0.330175	3.774275
H	0.445365	-0.508868	2.494780
C	-0.360995	1.826862	1.520466
C	-2.528872	1.014153	2.283626
C	-0.957101	2.664231	0.402439
H	0.645576	1.479655	1.246753
H	-0.262799	2.442309	2.435661
H	-2.434017	1.645478	3.187200
H	-3.093824	0.108967	2.535374
H	-3.102014	1.553660	1.522935
H	-0.311177	3.535038	0.196779
H	-1.933225	3.061789	0.707079
C	-2.327933	2.304791	-1.580914
C	0.050668	1.948744	-1.689017
H	-2.434688	1.702380	-2.492303
H	-2.232455	3.370380	-1.861216
H	-3.231607	2.165858	-0.974163
H	0.177633	2.982082	-2.063037
H	-0.047821	1.265621	-2.541838
H	0.944942	1.663297	-1.125705
C	3.696226	0.285018	-0.630325
H	4.003604	0.968869	-1.432662
H	3.574124	0.855035	0.302486
C	4.725548	-0.826053	-0.444520
H	4.847564	-1.396918	-1.376786
H	4.406713	-1.512953	0.351665
C	6.077809	-0.287287	-0.057707
F	6.988263	-1.270274	0.064661
F	6.556916	0.585352	-0.970855
F	6.041165	0.368500	1.121819

6H
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy:
0.307713
Total energy: -2837.704796

C	-0.585124	-0.063688	-2.178670
H	-1.367235	-0.650923	-2.673679
H	-0.125828	0.707180	-2.813569
C	0.233881	-0.706829	-1.192178
H	0.045860	-1.733875	-0.866778
C	1.551882	-0.164403	-0.859054
O	2.038489	0.875260	-1.277332
O	2.197910	-0.939846	0.058121
C	3.471423	-0.485567	0.518074
H	3.446284	0.599095	0.699919
H	3.646202	-1.005338	1.469871
Ni	-0.987801	0.627294	-0.422810
C	-2.013078	1.690176	1.908505
H	-2.814780	0.937748	1.912930
H	-1.962830	2.138987	2.918532
C	-2.313246	2.762184	0.869438
H	-1.547722	3.548762	0.905918
H	-3.280078	3.246829	1.087911
C	-3.660222	1.713644	-0.880176
C	-1.804475	3.134677	-1.495842
C	-0.591508	-0.236092	2.381836
C	0.432483	1.845378	1.735935
H	-1.994001	-0.481564	-0.211581
H	-0.758867	3.389131	-1.270328
H	-2.406903	4.062382	-1.502795
H	-1.843161	2.678178	-2.493431
H	-4.347211	2.571356	-1.005240
H	-3.602471	1.150814	-1.820807
H	-4.059303	1.043915	-0.109627
H	0.296232	-0.779886	2.030907
H	-0.470775	0.006655	3.454478
H	-1.468043	-0.883070	2.254717
H	0.489996	2.257899	2.760671
H	0.421650	2.676989	1.019357
H	1.335017	1.251998	1.546893
I	-3.306015	-2.000245	0.055946
N	-2.313516	2.174150	-0.499066
N	-0.753798	0.984274	1.575419
C	4.567083	-0.821518	-0.490694
H	4.380742	-0.298248	-1.438914
H	4.595125	-1.903981	-0.684508
C	5.932497	-0.407917	-0.010614
F	6.008461	0.921849	0.215793
F	6.888356	-0.709389	-0.908963
F	6.272043	-1.016329	1.146784

7H
Geometry with 43 atoms:
Thermal correction to Gibbs Free Energy: 0.303856
Total energy: -2539.201003

C	1.353076	-2.288658	-0.631106
H	1.904589	-2.891143	-1.371864
H	1.061687	-2.891355	0.245901
C	0.361602	-1.353318	-1.148207
H	0.276804	-1.139901	-2.221678
C	-0.790586	-0.971032	-0.356848
O	-1.095864	-1.341195	0.769786
O	-1.566602	-0.033004	-1.017087
C	-2.696247	0.474884	-0.319542
H	-2.443561	0.674655	0.733092
H	-2.953869	1.424423	-0.810373
Ni	1.886865	-0.490982	-0.283481
C	3.147420	2.010508	0.051033
H	3.663892	2.007339	-0.919075
H	3.185944	3.046287	0.439277
C	3.851239	1.061520	1.013430
H	3.371801	1.107834	2.001000
H	4.906952	1.364061	1.147800
C	4.711842	-0.614006	-0.549408
C	3.945815	-1.291837	1.636809
C	1.213104	2.118218	-1.437250
C	0.867983	1.917381	0.939225
H	3.179349	-1.126011	2.406450
H	4.948654	-1.184178	2.095274
H	3.832924	-2.314779	1.254594
H	5.757167	-0.509367	-0.197214
H	4.554686	-1.636255	-0.917678
H	4.548955	0.076264	-1.387886
H	0.207589	1.705873	-1.595881
H	1.158362	3.224817	-1.414070
H	1.850777	1.810236	-2.277774
H	0.816723	3.013602	1.091859
H	1.219309	1.445732	1.866332
H	-0.141412	1.540443	0.731876
N	1.753213	1.573307	-0.184070
N	3.752166	-0.338891	0.533536
C	-3.870924	-0.499602	-0.393119
H	-3.607637	-1.439968	0.110499
H	-4.124227	-0.718494	-1.441193
C	-5.108405	0.036805	0.272550
F	-4.907755	0.296347	1.583210
F	-5.530992	1.192353	-0.287970
F	-6.134711	-0.832602	0.197531

$CF_3CH_2CH_2I$
Geometry with 11 atoms:
Thermal correction to Gibbs Free Energy: 0.036212
Total energy: -714.260585

C	-2.507068	0.068894	0.000048
C	-1.070866	0.542891	0.000032
C	-0.098661	-0.625069	-0.000017
H	-0.941153	1.174476	-0.891013
H	-0.941116	1.174428	0.891106
H	-0.202258	-1.247563	0.897120

H	-0.202292	-1.247517	-0.897182
I	1.979465	0.048068	-0.000035
F	-3.363211	1.107232	0.000124
F	-2.794273	-0.682544	-1.083139
F	-2.794213	-0.682656	1.083173

$CH_2CHCOOCH_2CH_2CF_3$
Geometry with 18 atoms:
Thermal correction to Gibbs Free Energy: 0.090718
Total energy: -683.013997

C	2.120173	-0.004278	-0.164221
C	3.456844	0.422876	0.321587
C	4.479686	-0.438060	0.366489
H	3.556409	1.465161	0.636201
H	4.347517	-1.475918	0.044296
H	5.467663	-0.132870	0.722206
O	1.244256	1.021020	-0.120200
O	1.828382	-1.115058	-0.552886
C	-0.093950	0.766828	-0.563996
H	-0.519841	1.753048	-0.791824
H	-0.077622	0.159710	-1.481158
C	-0.900254	0.067624	0.527162
H	-0.483459	-0.928423	0.731688
H	-0.879799	0.656466	1.456053
C	-2.343902	-0.119847	0.140334
F	-3.038368	-0.742155	1.110678
F	-2.963060	1.056704	-0.096907
F	-2.476744	-0.860742	-0.980093

ts-1-2H
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.312400
Total energy: -2837.684427

Ni	2.420370	0.093771	-0.392414
O	0.635767	0.526576	-0.857649
C	0.423870	1.718338	-1.285158
O	-0.712172	2.153164	-1.570574
C	2.896338	1.684555	-1.401111
H	3.110501	1.370451	-2.442111
H	3.790494	2.215625	-1.031211
C	1.659613	2.589798	-1.361455
H	1.640728	3.184577	-0.429478
H	1.562817	3.312900	-2.190693
C	1.233324	-2.532079	-0.355263
H	0.432092	-2.047308	-0.927816
H	2.038737	-2.801843	-1.051615
H	0.841539	-3.453796	0.114437
C	0.651475	-1.224061	1.590277
H	0.991998	-0.420226	2.257800
H	-0.209029	-0.857354	1.022300
H	0.339163	-2.093662	2.198032
C	5.240454	-0.364859	-1.001527
H	4.859712	-0.923278	-1.867052
H	5.376420	0.683031	-1.289884
H	6.217715	-0.782354	-0.699170
C	4.715128	0.398104	1.231704
H	3.997812	0.344129	2.060263
H	5.710068	0.082060	1.595041
H	4.768393	1.439238	0.890596
C	2.915983	-2.102185	1.376042
H	2.999878	-1.555900	2.325713
H	2.802679	-3.172938	1.625857
C	4.158932	-1.886131	0.533249
H	5.066563	-2.195759	1.081278
H	4.104406	-2.492107	-0.381802
C	-2.293531	0.874323	-0.888568
H	-1.501426	0.155960	-0.713995
H	-2.701673	0.974687	-1.889054
I	-3.979137	-1.256201	-0.538208
N	4.271716	-0.458935	0.110415
N	1.730737	-1.586237	0.658198
C	-2.743877	1.841755	0.164029
H	-2.555884	2.865184	-0.194144
H	-3.824002	1.756860	0.345147
C	-2.045496	1.703708	1.497239
F	-2.577697	2.552730	2.397177
F	-2.141740	0.464026	2.015823
F	-0.726670	1.987200	1.426213

ts-2-3H
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.314125
Total energy: -2837.709720

C	1.368763	0.237166	-0.456296
C	-2.487211	-2.208524	1.679120
H	-3.130422	-2.469389	2.540083
H	-1.528537	-2.728547	1.816394
C	-3.137830	-2.634098	0.379604
H	-4.097059	-2.117266	0.247021
H	-3.347555	-3.717949	0.376171
Ni	-1.385264	-0.523351	-0.264726
O	2.656997	0.534123	-0.329648
O	0.693094	-0.152106	0.489844
C	-3.064599	-2.179718	-2.000637
H	-3.797322	-1.368528	-1.896762
H	-3.594863	-3.130550	-2.194180
H	-2.413493	-1.958070	-2.853796
C	-1.209870	-3.304159	-0.924360
H	-1.665221	-4.292458	-1.118794
H	-0.553433	-3.045166	-1.761281
H	-0.598315	-3.363300	-0.015246
C	-1.269979	-0.361967	2.689244

H	-1.011491	0.696844	2.558259
H	-1.707943	-0.515358	3.693089
H	-0.350066	-0.951024	2.598051
C	-3.475443	0.003442	1.798951
H	-4.007542	-0.323386	2.712050
H	-3.249441	1.071694	1.874386
H	-4.130845	-0.134089	0.930017
C	3.239276	0.418972	0.982989
H	2.746844	1.132861	1.660376
H	3.066971	-0.595610	1.373365
I	-1.762693	2.494944	-0.206174
C	-0.520504	-0.302290	-1.997033
H	-1.182390	0.238152	-2.695838
H	-0.301502	-1.280714	-2.457237
C	0.796957	0.463370	-1.821908
H	1.569323	0.239126	-2.578146
H	0.626698	1.553752	-1.865383
N	-2.259162	-2.272656	-0.767277
N	-2.218077	-0.754875	1.633185
C	4.718995	0.728657	0.879612
H	5.137900	0.797797	1.894347
H	4.885262	1.692030	0.375120
C	5.522636	-0.320442	0.148213
F	5.195924	-0.419532	-1.153819
F	5.352179	-1.547703	0.687165
F	6.840494	-0.045534	0.204388

ts-3-4H
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.310617
Total energy: -2837.683728

Ni	0.847103	0.255593	-0.078771
I	3.510942	-1.723764	0.031159
C	0.088870	-0.903098	-1.547610
C	-0.681125	-1.053678	-0.385571
H	0.767725	-1.706060	-1.845940
H	-0.279621	-0.251262	-2.340238
C	-1.852675	-0.161129	-0.144633
H	0.642226	-0.780717	0.879319
H	-0.690695	-1.986406	0.182406
O	-2.453234	-0.476199	1.019858
O	-2.221685	0.736277	-0.874146
C	-3.603564	0.276452	1.436995
H	-3.458286	0.488764	2.505072
H	-3.653036	1.224949	0.884918
H	2.647789	0.672731	-2.478826
C	2.702996	1.571271	-1.851241
H	3.061297	2.423819	-2.457123
H	3.419530	1.369992	-1.046372
C	1.410445	3.005031	-0.347835
C	0.434828	2.186149	-2.391505
C	1.960117	2.577167	0.996096
H	2.015607	3.828095	-0.767957
H	0.384491	3.381438	-0.235244
H	0.694243	3.164571	-2.834271
H	0.505495	1.426793	-3.179569
H	-0.594997	2.207849	-2.012855
H	3.003418	2.248141	0.896320
H	1.941660	3.420770	1.709500
C	-0.152088	1.839173	2.007326
C	1.931566	0.789344	2.628627
H	-0.690297	0.951508	2.361028
H	-0.062870	2.569287	2.832282
H	-0.733707	2.288414	1.192696
H	2.125332	1.520978	3.433761
H	1.346135	-0.045919	3.033173
H	2.881542	0.394081	2.248847
C	-4.880825	-0.531408	1.258877
H	-5.705468	-0.012384	1.770279
H	-4.774983	-1.529601	1.708982
C	-5.308693	-0.722988	-0.175721
F	-4.410439	-1.433447	-0.891379
F	-6.477700	-1.389365	-0.247044
F	-5.482942	0.449860	-0.815907
N	1.364754	1.855753	-1.291482
N	1.185046	1.426435	1.524968

ts-4-5H
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.311615
Total energy: -2837.690591

Ni	-1.671003	0.272937	-0.383716
C	1.701410	-0.761272	-0.464587
C	0.494320	-0.994652	-1.276629
C	-0.476271	-1.857306	-0.891271
H	0.472718	-0.524021	-2.259839
H	-1.950704	0.261258	-1.813756
H	-0.407757	-2.395674	0.056142
H	-1.265984	-2.148537	-1.581893
O	2.584009	0.031031	-1.116756
O	1.923311	-1.206906	0.646023
C	3.799547	0.364039	-0.436202
H	4.178313	1.264096	-0.938113
H	3.587328	0.599277	0.617183
I	-3.883344	-1.177290	-0.211203
N	-1.069877	2.210957	-0.608744
H	-1.594904	-1.494861	2.214461
C	-0.841105	-0.704457	2.332066
N	-1.312308	0.509546	1.643321
H	-0.687006	-0.510762	3.410159
H	0.105533	-1.040409	1.894955
C	-0.256573	1.549677	1.622987
C	-2.526474	1.001975	2.325990
C	-0.691167	2.708554	0.746034

H	0.658105	1.091534	1.223502
H	-0.029936	1.904605	2.646421
H	-2.277470	1.384535	3.333464
H	-3.244100	0.179701	2.421637
H	-3.011375	1.797415	1.747606
H	0.111150	3.461720	0.674267
H	-1.560164	3.213028	1.186172
C	-2.208639	2.984615	-1.145543
C	0.078147	2.318259	-1.528544
H	-2.447144	2.628794	-2.155186
H	-1.966181	4.063182	-1.188920
H	-3.091002	2.836452	-0.508829
H	0.352346	3.378110	-1.687513
H	-0.178669	1.862775	-2.492634
H	0.940109	1.786641	-1.112743
C	4.810025	-0.775140	-0.533698
H	4.424646	-1.673681	-0.031916
H	5.016613	-1.018400	-1.586335
C	6.121016	-0.424075	0.120260
F	7.011523	-1.426764	0.016014
F	6.688306	0.669515	-0.433455
F	5.973745	-0.159469	1.436126

ts-4-6H
Geometry with 45 atoms:
Thermal correction to Gibbs Free Energy: 0.306633
Total energy: -2837.693326

Ni	0.905782	0.408266	-0.234573
C	-1.793248	0.291173	-0.358914
C	-0.705723	-0.636946	-0.731155
C	0.098412	-0.346974	-1.862384
H	-0.787951	-1.643831	-0.314090
H	1.215803	-0.901284	0.270837
H	-0.219373	0.450841	-2.541513
H	0.680408	-1.154085	-2.318739
O	-2.530331	-0.193114	0.665563
O	-2.011171	1.379569	-0.863859
C	-3.621433	0.608583	1.138511
H	-3.897636	0.165385	2.104340
H	-3.286761	1.644116	1.299959
I	3.106394	-2.102381	-0.012743
N	1.187942	1.173279	1.634318
H	1.040190	2.240887	-2.919363
C	1.109992	2.841578	-2.003941
N	1.882470	2.106497	-0.986500
H	1.597324	3.802500	-2.254176
H	0.092419	3.027253	-1.633710
C	2.110568	2.965817	0.202603
C	3.157423	1.631982	-1.559867
C	2.313396	2.122862	1.450040
H	1.231427	3.613131	0.323328
H	2.979502	3.630355	0.047527
H	3.754514	2.478418	-1.949367
H	2.950125	0.928360	-2.376973
H	3.740482	1.098053	-0.799155
H	2.423790	2.773977	2.337303
H	3.230776	1.523745	1.359809
C	1.510481	0.208303	2.700978
C	-0.073052	1.866866	1.968829
H	0.694948	-0.521412	2.791114
H	1.643467	0.725306	3.669153
H	2.431503	-0.329651	2.445924
H	0.045904	2.490336	2.874304
H	-0.848251	1.113320	2.153585
H	-0.406661	2.499092	1.137157
C	-4.813735	0.613328	0.189371
H	-5.637623	1.167679	0.663655
H	-4.561709	1.113633	-0.755539
C	-5.337742	-0.759876	-0.150839
F	-6.510250	-0.682750	-0.811801
F	-4.491481	-1.453061	-0.939558
F	-5.553855	-1.512150	0.949169

2I
Geometry with 48 atoms:
Thermal correction to Gibbs Free Energy: 0.339484
Total energy: -2877.035532

C	0.783875	-0.469762	-0.746223
C	-3.806917	-1.790479	1.507713
H	-4.290101	-1.682303	2.495488
H	-3.931165	-2.837274	1.197168
C	-4.450596	-0.861966	0.497007
H	-4.366181	0.179365	0.835592
H	-5.524142	-1.087695	0.375136
Ni	-1.823094	-1.058282	-0.383415
O	2.041019	-0.185633	-0.531866
O	0.062544	-0.959998	0.141777
C	-4.094522	0.247321	-1.619152
H	-3.687228	0.152647	-2.631198
H	-5.191157	0.359501	-1.685896
H	-3.658459	1.137143	-1.145078
C	-4.154233	-2.174831	-1.556441
H	-5.238883	-2.163163	-1.766099
H	-3.603413	-2.222248	-2.503714
H	-3.911876	-3.069975	-0.969643
C	-1.600670	-2.681662	2.040521
H	-0.529610	-2.443270	2.042618
H	-1.907716	-2.983266	3.059269
H	-1.770582	-3.521818	1.351899
C	-2.058029	-0.340655	2.433505
H	-2.318268	-0.544710	3.488976
H	-0.988884	-0.106500	2.357241
H	-2.613057	0.538531	2.085397
C	2.571182	-0.360946	0.811891

```
H   1.991449   0.279589   1.492861
H   2.428742  -1.411466   1.109290
I  -1.117948   2.947157   0.221857
C  -1.126599  -0.911917  -2.196356
H  -1.779034  -0.438709  -2.944298
H  -0.942973  -1.954764  -2.525985
C   0.202903  -0.156358  -2.082972
H   0.947394  -0.342001  -2.877441
H   0.030444   0.935498  -2.059332
N  -3.752908  -0.954403  -0.823035
N  -2.356286  -1.505322   1.581626
C   4.032320   0.030438   0.788282
H   4.123870   1.080997   0.469578
H   4.406427  -0.028532   1.822762
C   4.871658  -0.868088  -0.120311
H   4.525754  -0.807064  -1.162797
H   4.805843  -1.921301   0.194746
C   6.332032  -0.500631  -0.118156
F   7.049751  -1.312501  -0.920022
F   6.542455   0.761700  -0.546126
F   6.875809  -0.587449   1.115633
H   3.231817   2.876764   2.202152
H   1.551884   2.462685   1.802061
C   2.339091   0.224258   2.551378
C   4.369919   0.713391   1.338882
H   2.593726  -0.841350   2.501593
H   2.732005   0.646615   3.495557
H   1.246274   0.320562   2.530280
H   4.859034   1.146058   2.232237
H   4.584248  -0.360475   1.296413
H   4.796292   1.176661   0.439549
N   1.845215   2.308294  -0.874561
N   2.911237   0.921665   1.385256
C  -4.542877  -0.375191   1.204952
H  -5.036831  -0.055450   2.136479
H  -4.665260  -1.467783   1.129626
C  -5.205322   0.302722   0.005393
H  -4.719427  -0.003925  -0.932614
H  -5.131131   1.399094   0.079543
C  -6.666777  -0.031458  -0.127511
F  -7.221463   0.580543  -1.193488
F  -6.875947  -1.356130  -0.282907
F  -7.379078   0.347843   0.956221
```

3I

```
Geometry with 48 atoms:
Thermal correction to Gibbs Free Energy:
0.339256
Total energy: -2877.049039
Ni   1.923051   0.331739  -0.375955
 I   2.781254  -2.179358  -0.221573
 C   0.701693  -0.187882  -1.801170
 C  -0.501429  -0.936642  -1.216352
 H   1.181376  -0.833302  -2.557422
 H   0.325237   0.693734  -2.347182
 C  -1.099797  -0.291202   0.007621
 H  -0.194326  -1.941441  -0.872374
 H  -1.310427  -1.100908  -1.950166
 O  -2.409882  -0.541091   0.137214
 O  -0.480203   0.355399   0.832981
 C  -3.068402  -0.042231   1.317541
 H  -2.619986  -0.512347   2.207301
 H  -2.901076   1.044822   1.392403
 H   1.688282   2.046713  -2.972002
 C   2.364274   2.507805  -2.243040
 H   2.453785   3.585758  -2.472939
 H   3.351948   2.036206  -2.333896
 C   2.750683   2.985314   0.092333
 C   0.485895   2.875421  -0.763263
 C   2.591304   2.364135   1.460559
 H   3.781923   2.857832  -0.262453
 H   2.546571   4.070210   0.119291
 H   0.499038   3.956090  -0.994286
 H  -0.186937   2.371094  -1.465243
 H   0.094426   2.718229   0.247365
```

4I

```
Geometry with 48 atoms:
Thermal correction to Gibbs Free Energy:
0.337580
Total energy: -2877.029453
Ni  -1.462173  -0.073391  -0.148758
 C   1.526510   0.167083   0.104803
 C   0.489938  -0.738869  -0.431064
 C  -0.263830  -1.610871   0.372519
 H   0.628936  -0.959340  -1.491862
 H  -1.516714  -0.579119  -1.471685
 H  -0.094512  -1.632959   1.451933
 H  -0.648607  -2.536755  -0.062198
 O   2.220604   0.735805  -0.906426
 O   1.771372   0.389254   1.277099
 C   3.300219   1.636120  -0.599264
 H   3.206515   2.467207  -1.313414
 H   3.177643   2.025363   0.421692
 I  -3.772200  -1.550940  -0.369881
 N  -1.799619   1.815745  -0.987052
 H  -1.254967  -0.633062   3.137972
 C  -0.924931   0.385920   2.894470
 N  -1.705539   0.891418   1.749968
 H  -1.083367   1.024933   3.783517
 H   0.140248   0.369912   2.643869
 C  -1.240961   2.251900   1.385264
 C  -3.127725   0.905082   2.147111
 C  -1.964871   2.759588   0.151033
 H  -0.158999   2.190040   1.199734
 H  -1.395994   2.956717   2.225064
```

H	-3.287364	1.604176	2.989797
H	-3.423965	-0.104611	2.455522
H	-3.772964	1.192522	1.310887
H	-1.593238	3.762947	-0.120062
H	-3.037160	2.866125	0.357808
C	-2.983610	1.844328	-1.863135
C	-0.600521	2.174242	-1.769742
H	-2.833185	1.153966	-2.703108
H	-3.157620	2.862392	-2.258731
H	-3.867640	1.513540	-1.304036
H	-0.734122	3.157305	-2.259263
H	-0.414609	1.411619	-2.536021
H	0.275961	2.221137	-1.115549
C	4.645184	0.946767	-0.770489
H	5.431876	1.703887	-0.618024
H	4.739384	0.584810	-1.807203
C	4.853329	-0.217712	0.198169
H	4.762173	0.110496	1.244273
H	4.107790	-1.009980	0.033053
C	6.204569	-0.864744	0.050552
F	6.362158	-1.888422	0.913097
F	6.399500	-1.363295	-1.189851
F	7.215281	0.001481	0.282066

H	-2.946558	3.915371	-1.753004
H	-2.181522	2.553278	-2.633667
H	-4.790100	2.279259	-1.351458
H	-3.858923	0.907941	-2.051239
H	-4.447474	0.808900	-0.380893
H	-0.176558	-0.551273	2.199164
H	-1.122142	0.222578	3.519698
H	-1.938531	-0.796253	2.285700
H	-0.288856	2.524417	2.787181
H	-0.261637	2.856238	1.025212
H	0.728599	1.543116	1.689158
I	-3.507174	-2.148223	0.004635
N	-2.779891	2.079358	-0.666108
N	-1.326512	1.096070	1.579941
C	4.288659	-0.517457	0.094834
H	4.148578	-0.037859	-0.885650
H	4.340942	-1.605624	-0.069571
C	5.586963	-0.023327	0.730063
H	5.559804	1.065169	0.896293
H	5.765686	-0.504812	1.704551
C	6.798158	-0.301541	-0.120342
F	7.927911	0.147261	0.463901
F	6.971146	-1.621296	-0.346562
F	6.720361	0.292052	-1.330418

6I
Geometry with 48 atoms:
Thermal correction to Gibbs Free Energy:
0.332446
Total energy: -2877.025981

C	-0.730441	-0.076555	-2.088405
H	-1.421009	-0.726847	-2.637736
H	-0.256656	0.703658	-2.700820
C	0.020695	-0.633686	-1.001832
H	-0.138122	-1.660401	-0.660223
C	1.268318	-0.003340	-0.560653
O	1.716263	1.063799	-0.952964
O	1.875337	-0.724908	0.418370
C	3.087336	-0.200723	0.975956
H	2.992944	0.887112	1.121154
H	3.183723	-0.681209	1.960982
Ni	-1.351216	0.644560	-0.409677
C	-2.660870	1.708068	1.776791
H	-3.399911	0.894493	1.747462
H	-2.732988	2.196709	2.766911
C	-2.950357	2.713546	0.671000
H	-2.257480	3.562706	0.740062
H	-3.968967	3.122242	0.783273
C	-4.044784	1.490014	-1.139263
C	-2.269679	3.045779	-1.656526
C	-1.131885	-0.071860	2.453299
C	-0.232459	2.062768	1.783547
H	-2.285709	-0.522093	-0.236584
H	-1.273528	3.399882	-1.353819

7I
Geometry with 46 atoms:
Thermal correction to Gibbs Free Energy:
0.330119
Total energy: -2578.522294

C	1.573398	-2.187290	-0.762280
H	2.050165	-2.788263	-1.554582
H	1.240441	-2.818768	0.079030
C	0.670133	-1.126881	-1.192934
H	0.586485	-0.839472	-2.249376
C	-0.431335	-0.689952	-0.354457
O	-0.745408	-1.101177	0.755602
O	-1.125113	0.351270	-0.938848
C	-2.209565	0.909967	-0.200619
H	-1.939890	0.994826	0.864644
H	-2.353528	1.923544	-0.607095
Ni	2.284070	-0.477661	-0.307546
C	3.779639	1.862961	0.178977
H	4.286137	1.878132	-0.796398
H	3.919829	2.861839	0.635134
C	4.396463	0.789357	1.067916
H	3.931924	0.819190	2.063369
H	5.477444	0.979983	1.206213
C	5.088705	-0.865863	-0.596687
C	4.249907	-1.596117	1.544865
C	1.851093	2.257403	-1.267677
C	1.511333	1.921332	1.094657
H	3.499676	-1.403069	2.324206

H	5.256248	-1.618688	2.008044
H	4.037361	-2.576927	1.099761
H	6.137401	-0.895881	-0.240175
H	4.826200	-1.839435	-1.031005
H	5.004694	-0.109335	-1.388025
H	0.808281	1.957293	-1.437489
H	1.905470	3.359743	-1.167173
H	2.446961	1.948585	-2.138129
H	1.559902	3.005290	1.319331
H	1.831926	1.359605	1.981845
H	0.470029	1.648703	0.881653
N	2.348334	1.576053	-0.064357
N	4.158011	-0.561892	0.503304
C	-3.481212	0.083105	-0.353568
H	-3.299867	-0.921365	0.057426
H	-3.711956	-0.030628	-1.425173
C	-4.661149	0.732318	0.367303
H	-4.451044	0.857890	1.441368
H	-4.885487	1.728321	-0.046371
C	-5.928240	-0.074620	0.267744
F	-6.954130	0.530507	0.902081
F	-6.317026	-0.262917	-1.011958
F	-5.798179	-1.301011	0.817008

$CF_3C_3H_6I$
Geometry with 14 atoms:
Thermal correction to Gibbs Free Energy: 0.062737
Total energy: -753.584164

C	-2.796017	-0.199856	-0.030290
C	-1.387909	0.029289	-0.511777
C	-0.656540	1.106650	0.286525
H	-0.866187	-0.937579	-0.443158
H	-1.452614	0.300657	-1.577119
C	0.737388	1.419980	-0.222863
H	-1.228012	2.050663	0.224054
H	-0.622705	0.828170	1.351669
H	1.199516	2.243987	0.333773
H	0.756671	1.642209	-1.298114
I	2.171977	-0.240736	0.014361
F	-3.415010	-1.158753	-0.747363
F	-2.836805	-0.587563	1.262655
F	-3.557405	0.912372	-0.124384

$CH_2CHCOOCH_2CH_2CH_2CF_3$
Geometry with 21 atoms:
Thermal correction to Gibbs Free Energy: 0.117302
Total energy: -722.336508

C	-2.666229	-0.064794	-0.185355
C	-3.930879	0.025917	0.590490
C	-4.829798	0.982373	0.333093
H	-4.082602	-0.722238	1.373253
H	-4.647635	1.717198	-0.457646
H	-5.762947	1.057101	0.898261
O	-1.916551	-1.098503	0.241211
O	-2.336925	0.678754	-1.085607
C	-0.650275	-1.314858	-0.404225
H	-0.411699	-2.372801	-0.221897
H	-0.757957	-1.155926	-1.488530
C	0.423921	-0.402657	0.172500
H	0.129539	0.645484	0.011930
H	0.494964	-0.567548	1.259552
C	1.779672	-0.658857	-0.483475
H	1.737197	-0.475182	-1.568437
H	2.109556	-1.698847	-0.332713
C	2.866277	0.227544	0.066112
F	3.058148	0.038851	1.389404
F	2.588589	1.537988	-0.101865
F	4.049181	-0.003201	-0.537921

ts-1-2I
Geometry with 48 atoms:
Thermal correction to Gibbs Free Energy: 0.335821
Total energy: -2877.010332

Ni	-2.871151	-0.649809	-0.053510
O	-0.985628	-0.743937	-0.138578
C	-0.465156	-1.902945	-0.335574
O	0.756366	-2.076313	-0.519027
C	-2.841357	-2.498369	-0.653137
H	-2.971627	-2.490166	-1.753417
H	-3.646040	-3.128659	-0.235518
C	-1.456061	-3.047780	-0.288924
H	-1.442879	-3.399993	0.759036
H	-1.095440	-3.889629	-0.905574
C	-2.206951	2.097939	-0.602439
H	-1.230133	1.681685	-0.879042
H	-2.884296	1.992809	-1.460742
H	-2.090884	3.172356	-0.366862
C	-1.819333	1.489860	1.701992
H	-2.172557	0.859302	2.530541
H	-0.818779	1.151623	1.406674
H	-1.762572	2.539651	2.045066
C	-5.559530	-1.041603	-1.140039
H	-5.136878	-0.651432	-2.075374
H	-5.433985	-2.129631	-1.122777
H	-6.638140	-0.805476	-1.101347
C	-5.337813	-1.050528	1.266216
H	-4.816240	-0.617587	2.129057
H	-6.425282	-0.893762	1.386952
H	-5.127126	-2.126764	1.243404
C	-4.109857	1.751419	0.906361
H	-4.286621	1.472106	1.954022
H	-4.244715	2.845910	0.834597

C	-5.095277	1.037710	-0.000332
H	-6.136060	1.258361	0.296713
H	-4.968545	1.378301	-1.037247
C	1.820227	-0.183079	-0.524494
H	1.358704	-0.064819	0.448391
H	1.223911	0.068457	-1.395526
I	2.392507	2.483828	-0.286409
N	-4.856449	-0.435663	0.009954
N	-2.730005	1.351591	0.555107
C	3.170435	-0.798991	-0.691736
H	3.016202	-1.770591	-1.188737
H	3.776911	-0.194115	-1.381816
C	3.899618	-1.003153	0.632466
H	3.306683	-1.639224	1.307191
H	4.073084	-0.038701	1.133986
C	5.240262	-1.665282	0.463626
F	5.140860	-2.880339	-0.119079
F	6.076355	-0.936135	-0.306031
F	5.856862	-1.848963	1.648198
H	2.634517	-1.016030	1.434768
I	-1.726448	2.517419	-0.307787
C	-0.984873	-0.507834	-1.982710
H	-1.553779	0.089418	-2.716488
H	-0.924282	-1.533001	-2.385692
C	0.438085	0.048677	-1.843347
H	1.167718	-0.367626	-2.560669
H	0.455393	1.142348	-1.991380
N	-3.027745	-2.106248	-0.689527
N	-2.747187	-0.510131	1.644163
C	4.296331	0.302653	0.933951
H	4.697666	0.332706	1.959460
H	4.428981	1.308393	0.503615
C	5.067988	-0.723317	0.103907
H	4.675776	-0.771490	-0.922754
H	4.986496	-1.729990	0.542950
C	6.535738	-0.405656	-0.000341
F	7.196237	-1.333491	-0.721964
F	6.759527	0.785735	-0.594414
F	7.133133	-0.352279	1.210422

ts-2-3I

Geometry with 48 atoms:

Thermal correction to Gibbs Free Energy: 0.340736

Total energy: -2877.034556

C	0.963590	-0.150250	-0.452451
C	-3.246006	-1.898233	1.749536
H	-3.924385	-2.015502	2.615084
H	-2.383443	-2.557932	1.918176
C	-3.954847	-2.270398	0.464154
H	-4.816668	-1.610698	0.302337
H	-4.338476	-3.304636	0.506273
Ni	-1.878212	-0.500991	-0.252181
O	2.267067	0.055981	-0.311906
O	0.242806	-0.438686	0.496476
C	-3.806617	-1.924890	-1.930596
H	-4.380852	-0.991163	-1.867301
H	-4.499915	-2.772280	-2.085039
H	-3.129015	-1.863093	-2.789715
C	-2.170647	-3.306915	-0.802794
H	-2.787950	-4.209248	-0.965979
H	-1.478465	-3.195339	-1.643723
H	-1.578632	-3.439476	0.111512
C	-1.751986	-0.228822	2.692543
H	-1.334992	0.773052	2.527428
H	-2.210167	-0.277630	3.697932
H	-0.932578	-0.954236	2.628219
C	-3.866644	0.446692	1.763870
H	-4.445571	0.252800	2.686286
H	-3.471173	1.466891	1.791835
H	-4.533920	0.375224	0.895871
C	2.817070	-0.009831	1.023486
H	2.291790	0.718428	1.660139

ts-3-4I

Geometry with 48 atoms:

Thermal correction to Gibbs Free Energy: 0.336335

Total energy: -2877.008399

Ni	1.382320	0.185435	-0.105443
I	4.101038	-1.620596	-0.025068
C	0.780911	-0.841518	-1.742464
C	-0.067760	-1.137904	-0.667674
H	1.513539	-1.585777	-2.064466
H	0.444883	-0.126520	-2.494239
C	-1.301067	-0.331953	-0.437789
H	1.180447	-0.959466	0.718219
H	-0.070032	-2.120446	-0.191043
O	-1.966137	-0.776965	0.643100
O	-1.673701	0.607040	-1.114587
H	3.321013	0.969665	-2.291990
C	3.268412	1.801843	-1.578622
H	3.605922	2.732942	-2.070040
H	3.940538	1.565884	-0.745745
C	1.775154	2.979376	-0.038396
C	1.011096	2.338818	-2.227951
C	2.254117	2.441991	1.293669
H	2.352617	3.878238	-0.320157
H	0.720946	3.281795	0.028984
H	1.231790	3.376918	-2.535532
H	1.196168	1.684359	-3.088133
H	-0.043230	2.251118	-1.936590
H	3.324548	2.199737	1.246504
H	2.118893	3.197779	2.088292
C	0.143206	1.456725	2.065854
C	2.252842	0.480570	2.712778

H	-0.350865	0.502819	2.286061
H	0.128616	2.095268	2.967945
H	-0.418747	1.954013	1.266139
H	2.339038	1.125856	3.605773
H	1.706884	-0.433223	2.979088
H	3.252410	0.196925	2.361639
N	1.877073	1.941223	-1.098582
N	1.533153	1.189099	1.634839
C	-3.170242	-0.087027	1.020253
H	-3.028863	0.996934	0.889510
H	-3.299962	-0.302975	2.090562
C	-4.362169	-0.581786	0.213039
H	-4.449635	-1.673528	0.331928
H	-4.187174	-0.374608	-0.853661
C	-5.654231	0.095993	0.665588
H	-5.603195	1.186868	0.523786
H	-5.852943	-0.093366	1.732274
C	-6.863242	-0.385911	-0.092873
F	-7.061537	-1.713043	0.054436
F	-6.760229	-0.154052	-1.418826
F	-7.988082	0.227545	0.326782
H	-3.722429	0.044137	2.365252
H	-3.630266	1.651979	1.635810
H	-0.627603	3.606432	0.674605
H	-2.286115	3.218398	1.138735
C	-2.849892	2.869670	-1.197885
C	-0.496081	2.449219	-1.514513
H	-3.022025	2.473779	-2.206086
H	-2.724274	3.967318	-1.255295
H	-3.727237	2.636428	-0.580199
H	-0.333548	3.530136	-1.685366
H	-0.679512	1.955100	-2.476231
H	0.408066	2.019671	-1.071792
C	4.545123	-0.068365	-0.399786
H	4.253892	-1.021653	0.066929
H	4.720571	-0.259831	-1.470399
C	5.823734	0.455504	0.252267
H	5.682872	0.619310	1.332159
H	6.135778	1.413345	-0.192945
C	6.985258	-0.491930	0.102223
F	7.290221	-0.723863	-1.192440
F	6.738576	-1.694097	0.664007
F	8.099756	-0.006822	0.685832

ts-4-5I

Geometry with 48 atoms:

Thermal correction to Gibbs Free Energy:

0.337757

Total energy: -2877.012592

Ni	-2.046394	0.243192	-0.383027
C	1.418017	-0.397111	-0.290672
C	0.277243	-0.788565	-1.140942
C	-0.602920	-1.749789	-0.772708
H	0.247011	-0.350400	-2.138952
H	-2.260686	0.178287	-1.822882
H	-0.515714	-2.254602	0.191351
H	-1.322470	-2.147431	-1.486661
O	2.225382	0.472130	-0.935799
O	1.640871	-0.787695	0.840770
C	3.404930	0.929471	-0.253828
H	3.655641	1.888204	-0.730461
H	3.173137	1.108611	0.807451
I	-4.092527	-1.442105	-0.267978
N	-1.648473	2.231999	-0.620106
H	-1.916460	-1.458261	2.267364
C	-1.247846	-0.595754	2.392207
N	-1.803695	0.549419	1.650841
H	-1.159979	-0.361369	3.469645
H	-0.254793	-0.846570	2.003367
C	-0.854053	1.687492	1.651796
C	-3.091182	0.934133	2.265135
C	-1.361475	2.785773	0.736294
H	0.117285	1.315086	1.300864
H	-0.707157	2.079578	2.676302
H	-2.927983	1.375627	3.266009

19

Geometry with 27 atoms:

Thermal correction to Gibbs Free Energy:

0.185392

Total energy: -2452.001598

I	-1.550379	1.758027	0.186647
I	-1.386089	-1.890443	-0.186317
Ni	0.421651	0.019069	0.000288
C	3.093091	0.707823	-0.492881
H	3.114525	0.324536	-1.521416
H	3.953556	1.387866	-0.375318
C	3.143001	-0.425682	0.496032
H	3.126995	-0.040686	1.524151
H	4.062029	-1.024299	0.379871
C	1.735732	-2.080684	1.537118
H	0.913239	-2.788450	1.392297
H	2.657754	-2.637298	1.780937
H	1.485497	-1.409946	2.370253
C	2.133608	-2.179190	-0.855421
H	3.031830	-2.803773	-0.706532
H	1.255337	-2.822612	-0.970401
H	2.250883	-1.590303	-1.773338
C	1.926662	2.367099	0.852074
H	2.762504	3.072118	0.699759
H	0.992956	2.927020	0.965129
H	2.099094	1.795412	1.772540
C	1.537985	2.222696	-1.539347
H	0.655190	2.852896	-1.392471
H	2.405156	2.859829	-1.787214
H	1.347203	1.528691	-2.369503

```
 N   1.939975  -1.281258   0.307108
 N   1.816078   1.449940  -0.307067
```

20A
Geometry with 38 atoms:
Thermal correction to Gibbs Free Energy:
0.289114
Total energy: -2163.125043

```
 C  -1.662076  -0.335672  -0.935049
 H  -0.970944   0.612511  -0.914376
 H  -2.004519  -0.328166  -1.978001
 C  -2.759565   0.039640   0.036688
 O  -2.565478   0.517991   1.132558
 O  -3.962022  -0.261593  -0.450751
 C  -5.087913  -0.011147   0.406156
 H  -5.009817  -0.602920   1.330989
 H  -5.146920   1.056600   0.666583
 H  -5.975974  -0.312266  -0.163080
Ni   0.375663  -0.178783  -0.312365
 C   2.758480   1.184051   0.121775
 H   3.201814   1.074997  -0.877437
 H   3.318751   1.976889   0.647560
 C   2.841803  -0.125413   0.884339
 H   2.490655   0.011421   1.915841
 H   3.882141  -0.489749   0.933395
 C   2.578787  -1.701025  -0.983171
 C   1.693926  -2.246040   1.203927
 C   1.178658   2.492967  -1.194536
 C   0.759760   2.160321   1.168658
 H   3.532795  -2.204173  -0.744877
 H   2.769120  -0.899397  -1.707971
 H   1.889725  -2.423247  -1.437655
 H   2.643364  -2.688819   1.553246
 H   1.093755  -3.021946   0.714743
 H   1.136682  -1.853911   2.064581
 H   0.892672   1.480424   2.020731
 H  -0.318064   2.314194   1.026106
 H   1.244755   3.125419   1.402204
 H   0.120358   2.769791  -1.296998
 H   1.507360   2.000381  -2.120129
 H   1.773023   3.411930  -1.041792
 C  -0.888981  -1.561246  -0.548348
 H  -1.209874  -2.058826   0.378472
 H  -0.715067  -2.280582  -1.361407
 N   1.334129   1.566047  -0.057934
 N   1.962782  -1.150967   0.246279
```

20B
Geometry with 41 atoms:
Thermal correction to Gibbs Free Energy:
0.316783
Total energy: -2202.452101

```
 C  -1.337386  -0.209505  -0.907071
 H  -0.599976   0.703356  -0.873914
 H  -1.690760  -0.166359  -1.945643
 C  -2.403285   0.197292   0.087381
 O  -2.167922   0.695151   1.167028
 O  -3.620546  -0.105622  -0.355024
 C  -4.733597   0.157616   0.534963
 H  -4.559080  -0.377711   1.482181
 H  -4.754412   1.235953   0.760858
Ni   0.710347  -0.164953  -0.307747
 C   3.164316   1.070132   0.109819
 H   3.603294   0.930124  -0.887477
 H   3.767016   1.833980   0.631631
 C   3.173428  -0.237641   0.879696
 H   2.814882  -0.077953   1.905542
 H   4.193259  -0.654122   0.942582
 C   2.838837  -1.802275  -0.987970
 C   1.923769  -2.298051   1.198112
 C   1.653702   2.436382  -1.230709
 C   1.234048   2.182342   1.143505
 H   3.764471  -2.354521  -0.746855
 H   3.072777  -1.012232  -1.712668
 H   2.113913  -2.487856  -1.443509
 H   2.848703  -2.790729   1.546648
 H   1.282870  -3.041675   0.710504
 H   1.389514  -1.876657   2.059620
 H   1.354195   1.521647   2.012137
 H   0.161402   2.379352   1.014588
 H   1.764552   3.131248   1.341739
 H   0.612218   2.769432  -1.336448
 H   1.950342   1.905855  -2.146217
 H   2.298846   3.324058  -1.100857
 C  -0.623992  -1.479298  -0.549982
 H  -0.961041  -1.975066   0.371834
 H  -0.492856  -2.192611  -1.376205
 N   1.762438   1.528218  -0.073425
 N   2.248861  -1.219663   0.239201
 C  -5.995186  -0.304303  -0.156024
 H  -6.862609  -0.117792   0.496370
 H  -6.149178   0.239612  -1.101387
 H  -5.951338  -1.382906  -0.374924
```

22A
Geometry with 35 atoms:
Thermal correction to Gibbs Free Energy:
0.268006
Total energy: -2123.842193

```
 C   2.803072   0.046993   0.000987
 C   2.616147  -1.409836   0.278771
 C   1.201111  -1.796226  -0.177743
 H   3.439428  -2.000084  -0.163245
 H   2.720810  -1.505762   1.376144
 H   1.219976  -2.099678  -1.241578
```

```
 H   0.830610  -2.654566   0.404796
 C  -2.321101   1.251651   0.322703
 H  -3.016782   2.042517  -0.009112
 H  -2.430056   1.160303   1.412043
 C  -2.651813  -0.063881  -0.354244
 H  -2.623140   0.052158  -1.446147
 H  -3.665500  -0.406006  -0.083007
Ni   0.106100  -0.190081  -0.052341
 O   1.803928   0.767439  -0.141877
 C  -1.767611  -2.231380  -0.953223
 H  -1.087939  -3.041883  -0.670331
 H  -2.801776  -2.617323  -0.954882
 H  -1.508056  -1.882433  -1.961230
 C  -1.858056  -1.605759   1.383349
 H  -2.858643  -2.063218   1.478705
 H  -1.092093  -2.353740   1.620247
 H  -1.771220  -0.781040   2.101843
 C  -0.362138   2.489955   1.082691
 H   0.686066   2.715786   0.851038
 H  -0.930830   3.435186   1.153505
 H  -0.403746   1.972351   2.051625
 C  -0.763942   2.248166  -1.290218
 H   0.303925   2.401243  -1.494709
 H  -1.174432   1.596164  -2.072761
 H  -1.285769   3.222036  -1.326208
 N  -0.914254   1.615850   0.033845
 N  -1.644406  -1.109257   0.004024
 O   3.985837   0.613568  -0.064591
 H   4.696842  -0.042043   0.067018


ethyl propionate
Geometry with 17 atoms:
Thermal correction to Gibbs Free Energy:
0.111254
Total energy: -347.106534
 C  -3.011938  -0.173213  -0.001632
 C  -1.631315  -0.815645   0.001334
 H  -3.152779   0.460490  -0.891237
 H  -3.154690   0.464541   0.884753
 C  -0.503496   0.192841   0.000612
 H  -1.484357  -1.470524  -0.874895
 H  -1.486440  -1.466499   0.880940
 O   0.693438  -0.414006   0.000581
 O  -0.637979   1.396571   0.000289
 C   1.862766   0.430037   0.000325
 H   1.833026   1.083809  -0.887177
 H   1.834254   1.082554   0.888808
 H  -3.798203  -0.943934  -0.000745
 C   3.080687  -0.466641  -0.001126
 H   3.094160  -1.110081  -0.895322
 H   3.995863   0.146320  -0.001215
 H   3.095265  -1.111469   0.892050


methyl propionate
Geometry with 14 atoms:
Thermal correction to Gibbs Free Energy:
0.085793
Total energy: -307.780740
 C  -1.214974  -0.738394  -0.000008
 C   0.050668   0.089040  -0.000002
 H  -1.169048  -1.405844  -0.877871
 H  -1.169039  -1.405864   0.877840
 O   1.144071  -0.691969   0.000007
 O   0.102172   1.298508  -0.000003
 C   2.410449  -0.024474  -0.000001
 H   2.522827   0.607818  -0.894962
 H   3.174354  -0.812884   0.000000
 H   2.522826   0.607818   0.894961
 C  -2.482976   0.104851   0.000006
 H  -2.527297   0.754598  -0.888077
 H  -3.376302  -0.538717   0.000031
 H  -2.527262   0.754629   0.888068


ts-14-20A
Geometry with 38 atoms:
Thermal correction to Gibbs Free Energy:
0.289728
Total energy: -2163.119412
 C  -0.727007  -1.754555  -0.660668
 H  -0.333232  -2.433095  -1.435055
 H  -1.094567  -2.344213   0.195137
 C  -2.580321  -0.182817  -0.112674
 O  -2.018055   0.380720   0.813199
 O  -3.892185  -0.309067  -0.221768
 C  -4.695980   0.266681   0.824627
 H  -5.739081   0.081156   0.541357
 H  -4.471645  -0.212505   1.789504
 H  -4.508011   1.348070   0.903516
Ni   0.308479  -0.225575  -0.275754
 C   2.565708   1.346181   0.038507
 H   2.998711   1.177529  -0.956640
 H   3.085591   2.213365   0.481832
 C   2.743897   0.114003   0.907023
 H   2.368049   0.308730   1.920407
 H   3.808113  -0.163907   0.994261
 C   2.650333  -1.644538  -0.804667
 C   1.728550  -2.041891   1.400781
 C   0.842044   2.365781  -1.370835
 C   0.543315   2.317631   1.031550
 H   1.191631  -2.897053   0.975379
 H   2.693472  -2.387961   1.811618
 H   1.124497  -1.606817   2.207631
 H   0.992137   3.320748   1.147621
 H   0.717686   1.737457   1.947043
 H  -0.540891   2.409447   0.895320
```

```
 H   1.322683   3.361090  -1.355631
 H   1.214413   1.801657  -2.237514
 H  -0.244011   2.497961  -1.475131
 H   2.037104  -2.462558  -1.199917
 H   2.799625  -0.904412  -1.600606
 H   3.632233  -2.042212  -0.491836
 C  -1.779420  -0.795744  -1.227301
 H  -2.400520  -1.211732  -2.035263
 H  -1.265295   0.087950  -1.699652
 N   1.117035   1.615695  -0.133125
 N   1.955695  -1.027155   0.348586
```

ts-14-20B

Geometry with 41 atoms:

Thermal correction to Gibbs Free Energy: 0.315548

Total energy: -2202.446957

```
 C  -0.363886  -1.766918  -0.669394
 H   0.046825  -2.453085  -1.428002
 H  -0.747282  -2.347088   0.185891
 C  -2.235625  -0.194706  -0.177368
 O  -1.695598   0.373565   0.759827
 O  -3.542139  -0.319751  -0.322729
 C  -4.393191   0.265359   0.698496
 H  -4.151792  -0.207250   1.663920
 H  -4.153237   1.337552   0.779093
Ni   0.656327  -0.229185  -0.278147
 C   2.895988   1.360496   0.070100
 H   3.346224   1.194149  -0.917795
 H   3.401854   2.232075   0.521003
 C   3.069957   0.130554   0.942813
 H   2.675454   0.322932   1.949600
 H   4.134925  -0.138254   1.047973
 C   3.016620  -1.627958  -0.770932
 C   2.067336  -2.034593   1.420965
 C   1.187140   2.367049  -1.366449
 C   0.850601   2.315291   1.030800
 H   1.543238  -2.893854   0.987878
 H   3.029322  -2.373085   1.844861
 H   1.448769  -1.604975   2.219660
 H   1.291681   3.320766   1.155752
 H   1.012932   1.734632   1.948153
 H  -0.231621   2.401033   0.876515
 H   1.658447   3.366678  -1.342819
 H   1.579099   1.806695  -2.226924
 H   0.101783   2.489298  -1.488585
 H   2.416154  -2.451382  -1.174588
 H   3.169616  -0.886242  -1.564712
 H   3.997862  -2.016597  -0.444796
 C  -1.403385  -0.813640  -1.266564
 H  -2.001162  -1.232779  -2.090307
 H  -0.877483   0.068771  -1.729554
 N   1.448228   1.618552  -0.124994
 N   2.300465  -1.017285   0.372789
 C  -5.828012   0.030117   0.289398
 H  -6.043441  -1.046937   0.208941
 H  -6.501906   0.463184   1.045004
 H  -6.043624   0.505248  -0.680599
```

ts-2-19A

Geometry with 41 atoms:

Thermal correction to Gibbs Free Energy: 0.288675

Total energy: -2759.676081

```
 C   0.415755  -1.352115   2.364958
 C   1.142350  -1.916589   1.180447
 C   0.926368  -1.066839  -0.063680
 H   2.198611  -2.028737   1.478767
 H   0.754446  -2.937373   1.016036
 H   0.925335   0.035893   0.002449
 H   1.152738  -1.538261  -1.018709
 C  -3.583189  -1.496932  -1.193914
 H  -4.653571  -1.271641  -1.331807
 H  -3.468248  -2.586218  -1.264898
 C  -2.742462  -0.802132  -2.237424
 H  -2.869747   0.286587  -2.170396
 H  -3.021314  -1.113684  -3.257913
 O  -0.707470  -0.653195   1.935297
 O   0.699976  -1.431490   3.523577
 C  -0.476534  -0.138924  -2.759231
 H   0.587478  -0.375952  -2.650728
 H  -0.745523  -0.195202  -3.827696
 H  -0.653553   0.876955  -2.384722
 C  -0.975747  -2.488096  -2.397297
 H  -1.223625  -2.634343  -3.462396
 H   0.094471  -2.675321  -2.253857
 H  -1.535292  -3.212450  -1.793047
 C  -3.420504  -2.104428   1.156433
 H  -3.083204  -1.777227   2.146568
 H  -4.504699  -2.309614   1.200180
 H  -2.890450  -3.030708   0.894178
 C  -3.778960   0.212790   0.518232
 H  -3.487899   0.506873   1.529833
 H  -3.469954   1.008373  -0.170464
 H  -4.876874   0.100101   0.487529
 C  -1.321790   0.257611   2.887298
 H  -0.563776   0.576897   3.611503
 H  -2.144857  -0.247957   3.408962
 H  -1.667653   1.119102   2.308008
 I  -0.730954   2.971868  -0.035270
Ni  -1.092864  -0.889541  -0.043720
 N  -1.301009  -1.099705  -1.985912
 N  -3.123360  -1.062611   0.152658
 I   4.153077  -0.215516  -0.316179
 H   2.293669  -0.567999  -0.219586
```

ts-2-19B
Geometry with 44 atoms:
Thermal correction to Gibbs Free Energy: 0.313876
Total energy: -2799.000636

C	0.618030	-1.527550	2.115539
C	1.464414	-1.886115	0.932090
C	1.241825	-0.885363	-0.195145
H	2.506737	-1.952675	1.284939
H	1.173134	-2.899285	0.602787
H	1.114338	0.187033	0.028048
H	1.564805	-1.185221	-1.190575
C	-3.034359	-1.717743	-1.862375
H	-4.115227	-1.634259	-2.060595
H	-2.726006	-2.726823	-2.165132
C	-2.259737	-0.669244	-2.623576
H	-2.579753	0.338047	-2.323747
H	-2.406628	-0.762979	-3.712649
O	-0.608267	-1.029886	1.685121
O	0.898107	-1.587870	3.277096
C	-0.105659	0.427723	-2.746956
H	0.969866	0.338767	-2.558226
H	-0.267550	0.565443	-3.829489
H	-0.493997	1.297012	-2.201402
C	-0.224542	-1.987081	-2.952500
H	-0.405938	-1.939438	-4.039426
H	0.856757	-2.016196	-2.778966
H	-0.660743	-2.910249	-2.553336
C	-2.856967	-2.848377	0.291076
H	-2.604484	-2.715125	1.348657
H	-3.879576	-3.257826	0.211657
H	-2.148896	-3.564383	-0.148574
C	-3.691056	-0.569971	0.170367
H	-3.533514	-0.486699	1.248352
H	-3.531000	0.418237	-0.277822
H	-4.732828	-0.892080	-0.002574
C	-1.338079	-0.193583	2.660372
H	-1.933608	0.479531	2.035249
H	-0.580575	0.410739	3.176523
I	-1.527506	2.973236	0.157844
Ni	-0.783529	-0.977235	-0.336473
N	-0.809688	-0.795679	-2.289031
N	-2.750034	-1.553031	-0.409635
C	-2.158334	-1.006824	3.634794
H	-1.518679	-1.672561	4.230161
H	-2.667098	-0.309839	4.320167
H	-2.930197	-1.606926	3.131400
I	4.387325	0.247468	-0.148552
H	2.565175	-0.269209	-0.195806

ts-20-21A
Geometry with 77 atoms:
Thermal correction to Gibbs Free Energy: 0.599263
Total energy: -4624.366389

C	-2.270427	1.723516	-1.052671
H	-1.403184	1.686604	-1.712126
C	-2.175395	2.758757	0.004602
O	-3.070205	3.119391	0.742374
O	-0.933336	3.295982	0.053467
Ni	-3.132353	-0.055447	-0.431220
C	-4.023346	-2.417091	0.995616
H	-3.589563	-3.218386	0.382177
H	-4.318810	-2.871683	1.958559
C	-5.232562	-1.829331	0.303915
H	-5.730211	-1.097604	0.955725
H	-5.966111	-2.626222	0.079255
C	-4.374082	-2.041387	-1.985786
C	-5.998569	-0.351883	-1.427287
C	-1.702014	-2.098416	1.467682
C	-3.298128	-0.520403	2.352419
H	-5.173186	-2.751084	-2.271478
H	-3.499664	-2.610419	-1.644605
H	-4.077068	-1.458522	-2.867359
H	-6.861123	-1.024062	-1.590186
H	-5.754440	0.138328	-2.376409
H	-6.276218	0.415414	-0.692734
H	-4.261130	-0.018317	2.189473
H	-2.527019	0.253216	2.451624
H	-3.354395	-1.100850	3.292674
H	-0.939641	-1.391846	1.794871
H	-1.354000	-2.602133	0.556292
H	-1.827901	-2.852903	2.265810
C	-3.539343	1.400979	-1.612512
H	-4.420903	1.944616	-1.249193
H	-3.579091	1.131894	-2.676867
N	-4.837960	-1.115982	-0.932330
N	-2.968189	-1.394714	1.206893
C	0.194917	0.223266	0.004577
H	-0.048463	-0.818257	-0.217892
H	0.144385	0.974992	-0.767616
H	-1.314854	0.329415	-0.228150
Ni	2.162301	-0.295538	-0.575720
I	2.139104	-2.319757	1.142281
C	0.278738	0.751285	1.422700
C	1.413205	1.722528	1.639041
H	0.471887	-0.065905	2.135753
H	-0.647119	1.239302	1.765013
O	1.222447	2.477140	2.721666
O	2.412024	1.802393	0.947241
H	-0.023864	0.382365	-2.716430
C	0.960600	0.223180	-3.170754
H	0.969550	0.704890	-4.164761
H	1.117133	-0.857104	-3.292186
C	3.341963	0.575700	-2.985725
C	1.814668	2.229996	-2.095206

C	4.438109	0.587733	-1.949936
H	3.314009	-0.393404	-3.500181
H	3.506102	1.349457	-3.754580
H	1.823613	2.764294	-3.061083
H	0.855070	2.417139	-1.601172
H	2.598567	2.629376	-1.442877
H	5.428618	0.446758	-2.417501
H	4.458473	1.550333	-1.421737
C	4.961412	-0.194182	0.270075
C	4.547753	-1.798729	-1.495159
H	4.835115	-1.010725	0.989582
H	6.033222	-0.095697	0.020122
H	4.600861	0.736878	0.724809
H	5.612337	-1.807267	-1.791242
H	4.376457	-2.567821	-0.734680
H	3.929805	-2.040093	-2.369232
N	2.028814	0.780587	-2.313262
N	4.174738	-0.476228	-0.949572
C	-0.721496	4.334059	1.017409
H	0.321138	4.653285	0.896705
H	-1.398992	5.181132	0.829482
H	-0.884613	3.962434	2.039123
C	2.259602	3.406327	3.064254
H	1.901224	3.950535	3.946878
H	3.193896	2.874653	3.301320
H	2.446186	4.107390	2.236822

ts-20-21B
Geometry with 80 atoms:
Thermal correction to Gibbs Free Energy:
0.626612
Total energy: -4663.694159

C	2.296309	1.318718	1.525886
H	1.469303	1.044389	2.181821
C	2.103144	2.601339	0.805646
O	2.944268	3.197123	0.163258
O	0.843422	3.071274	0.961551
Ni	3.204421	-0.163266	0.399285
C	4.124407	-2.043352	-1.605005
H	3.755546	-2.987379	-1.180747
H	4.377902	-2.241499	-2.662335
C	5.350403	-1.578472	-0.854186
H	5.782632	-0.690409	-1.336450
H	6.124139	-2.368647	-0.863688
C	4.665683	-2.373205	1.362817
C	6.156963	-0.494328	1.128675
C	1.777197	-1.728403	-1.909701
C	3.270570	0.099211	-2.407637
H	5.516948	-3.077231	1.423104
H	3.797206	-2.901781	0.949489
H	4.406622	-2.033766	2.374263
H	7.065179	-1.122227	1.071265
H	5.958858	-0.265169	2.181651
H	6.335968	0.444726	0.588357
H	4.220351	0.587512	-2.152859
H	2.467707	0.834953	-2.278939
H	3.307129	-0.219272	-3.466586
H	0.969570	-1.003868	-2.012765
H	1.493592	-2.471721	-1.152706
H	1.900031	-2.238847	-2.882321
C	3.608081	0.935865	1.921117
H	4.437846	1.614969	1.687625
H	3.723205	0.381652	2.862444
N	5.005702	-1.198930	0.534238
N	3.023301	-1.052326	-1.514144
C	-0.151286	0.066295	0.132429
H	0.111619	-0.989431	0.046500
H	-0.101658	0.567766	1.086200
H	1.369450	0.154553	0.356923
Ni	-2.100061	-0.647637	0.564950
I	-2.069850	-2.122642	-1.644923
C	-0.286045	0.973257	-1.074075
C	-1.461262	1.916784	-0.983538
H	-0.464644	0.387761	-1.989876
H	0.612571	1.578498	-1.273151
O	-1.332490	2.960083	-1.798979
O	-2.440753	1.743918	-0.279167
H	0.121904	-0.601224	2.755605
C	-0.844853	-0.910228	3.168802
H	-0.828536	-0.747817	4.261433
H	-0.983916	-1.980420	2.964472
C	-3.237777	-0.571599	3.143339
C	-1.757761	1.307913	2.772142
C	-4.355151	-0.264086	2.178243
H	-3.184492	-1.650757	3.335469
H	-3.397914	-0.073951	4.115004
H	-1.747388	1.524401	3.854689
H	-0.815852	1.657985	2.336209
H	-2.567656	1.866618	2.290820
H	-5.335420	-0.552360	2.596927
H	-4.391228	0.812791	1.965783
C	-4.917004	-0.358071	-0.167647
C	-4.450588	-2.405698	1.033413
H	-4.763510	-0.901374	-1.106976
H	-5.988597	-0.390594	0.100264
H	-4.602385	0.683287	-0.307356
H	-5.499118	-2.516292	1.363855
H	-4.322825	-2.905060	0.067392
H	-3.790877	-2.896558	1.759688
N	-1.943855	-0.143437	2.544289
N	-4.101757	-0.974445	0.900056
C	0.553066	4.332725	0.347237
H	-0.500360	4.543798	0.568430
H	1.191874	5.123811	0.769272
H	0.709752	4.285458	-0.739238
C	-2.413072	3.920713	-1.839141
H	-3.308483	3.422373	-2.245154

```
 H  -2.646229   4.236031  -0.809810
 C  -1.968234   5.079505  -2.701311
 H  -1.720522   4.740542  -3.719484
 H  -2.778946   5.821609  -2.770595
 H  -1.082460   5.572914  -2.271045
```

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ts-20-22A
Geometry with 72 atoms:
Thermal correction to Gibbs Free Energy:
0.565133
Total energy: -4286.592132
 C  -1.873682   1.043370  -1.434543
 H  -1.294355   1.324124  -0.103521
 H  -1.000197   1.639180  -1.729624
 C  -3.123562   1.851862  -1.407151
 O  -4.259013   1.421165  -1.496609
 O  -2.867959   3.161756  -1.213536
 C  -4.001074   4.019220  -1.064516
 H  -4.633602   4.003648  -1.966183
 H  -4.614766   3.716343  -0.200890
 H  -3.603842   5.030229  -0.904013
Ni  -2.087116  -0.581924  -0.158013
 C  -2.871433  -1.770757   2.317652
 H  -1.982592  -2.348672   2.606044
 H  -3.523822  -1.717113   3.208126
 C  -3.590570  -2.466595   1.180517
 H  -4.525728  -1.941050   0.941048
 H  -3.854704  -3.501126   1.468298
 C  -1.598582  -3.372099   0.062868
 C  -3.587296  -2.868199  -1.197445
 C  -1.297118  -0.017993   2.791598
 C  -3.506794   0.573259   2.004908
 H  -1.927178  -4.410768   0.255228
 H  -0.929112  -3.053529   0.870908
 H  -1.038262  -3.341071  -0.878662
 H  -4.023704  -3.869322  -1.024747
 H  -2.973293  -2.897643  -2.104760
 H  -4.396045  -2.140359  -1.342166
 H  -4.352108   0.267562   1.374792
 H  -3.143897   1.542699   1.638757
 H  -3.859950   0.687316   3.047642
 H  -1.081304   1.044175   2.654216
 H  -0.399787  -0.599607   2.534574
 H  -1.548852  -0.190447   3.854450
 C  -1.967032  -0.310312  -2.007481
 H  -2.879576  -0.531134  -2.579418
 H  -1.061687  -0.678821  -2.515863
 C   0.567679   1.760627   0.694566
 C   1.551901   2.387317   1.642446
 C   2.972811   2.112823   1.128083
 H   1.294828   3.447660   1.810673
 H   1.376866   1.874294   2.606642
 H   3.294806   2.921950   0.443933
 H   3.696837   2.082749   1.959794
 C   3.880643  -1.949198  -1.066172
 H   4.017050  -2.601958  -1.947109
 H   3.850584  -2.599297  -0.180898
 C   5.031150  -0.965128  -0.955959
 H   5.107788  -0.369342  -1.875724
 H   5.991073  -1.493909  -0.821643
Ni   2.879978   0.479074   0.074064
 O   1.022242   0.852287  -0.068053
 O  -0.659082   2.078578   0.696442
 C   5.729025   1.138285   0.005863
 H   5.619598   1.828858   0.849014
 H   6.775599   0.787845  -0.035517
 H   5.488318   1.671797  -0.923114
 C   5.041309  -0.653271   1.480023
 H   6.081194  -1.018865   1.555935
 H   4.854001   0.076136   2.277700
 H   4.353097  -1.497063   1.616566
 C   1.474844  -2.024873  -0.645912
 H   0.553829  -1.428782  -0.681858
 H   1.346181  -2.934900  -1.260323
 H   1.657790  -2.320340   0.397074
 C   2.308751  -0.704881  -2.484697
 H   1.419137  -0.063112  -2.437188
 H   3.148496  -0.103073  -2.857083
 H   2.124403  -1.535557  -3.191484
 N   2.599335  -1.212083  -1.132534
 N   4.808388  -0.007341   0.168645
 N  -2.755748  -2.462360  -0.047111
 N  -2.414628  -0.416925   1.914870
```

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ts-20-22B
Geometry with 75 atoms:
Thermal correction to Gibbs Free Energy:
0.590903
Total energy: -4325.918420
 C  -1.866687   0.947358  -1.136636
 H  -1.267363   1.049745   0.212698
 H  -1.053622   1.653767  -1.347957
 C  -3.172632   1.636240  -0.942699
 O  -4.271696   1.122548  -1.055739
 O  -3.005100   2.919103  -0.562895
 C  -4.181198   3.687539  -0.245471
 H  -4.888521   3.054284   0.312517
 H  -3.821823   4.486328   0.420027
Ni  -1.890617  -0.879876  -0.149813
 C  -2.525967  -2.521115   2.103619
 H  -1.597419  -3.073310   2.302592
 H  -3.175785  -2.657695   2.986776
 C  -3.199882  -3.075867   0.865576
 H  -4.172928  -2.588763   0.708904
 H  -3.384902  -4.160136   0.982203
 C  -1.141102  -3.617735  -0.363649
```

C	-3.175772	-3.112479	-1.546055
C	-1.059106	-0.763156	2.838586
C	-3.325237	-0.210083	2.196536
H	-1.372151	-4.699179	-0.334733
H	-0.498440	-3.367022	0.488921
H	-0.592710	-3.391346	-1.285391
H	-3.509714	-4.166523	-1.534667
H	-2.570984	-2.938994	-2.443757
H	-4.053908	-2.454972	-1.580195
H	-4.163367	-0.464703	1.534840
H	-3.038632	0.830582	1.996203
H	-3.658990	-0.298727	3.248146
H	-0.913598	0.319474	2.869586
H	-0.133651	-1.236979	2.480004
H	-1.274078	-1.118072	3.863612
C	-1.874384	-0.295076	-1.928066
H	-2.791797	-0.500594	-2.497925
H	-0.966171	-0.494864	-2.519136
C	0.576286	1.522367	1.029064
C	1.540615	2.088550	2.033674
C	2.953222	2.046932	1.431943
H	1.191611	3.076273	2.381712
H	1.465452	1.412794	2.906057
H	3.157553	2.980881	0.872838
H	3.719679	1.966336	2.221136
C	4.140613	-1.498663	-1.412926
H	4.294633	-2.001942	-2.384593
H	4.219691	-2.267920	-0.632537
C	5.193404	-0.425842	-1.200827
H	5.160347	0.304006	-2.021287
H	6.206490	-0.864793	-1.188793
Ni	2.966835	0.596613	0.134341
O	1.078171	0.790535	0.120420
O	-0.672929	1.716702	1.115385
C	5.714034	1.585184	0.040183
H	5.587482	2.118491	0.988657
H	6.787691	1.375024	-0.111726
H	5.349533	2.221896	-0.776675
C	5.332619	-0.474364	1.248553
H	6.413626	-0.701256	1.224424
H	5.100476	0.091474	2.159009
H	4.770345	-1.416420	1.274910
C	1.772561	-1.886925	-0.946013
H	0.796875	-1.390030	-0.865384
H	1.708861	-2.697899	-1.694843
H	2.022769	-2.323162	0.031716
C	2.396696	-0.216045	-2.568729
H	1.450905	0.314403	-2.397212
H	3.157640	0.520038	-2.859446
H	2.266832	-0.939822	-3.395045
N	2.792084	-0.896692	-1.323527
N	4.940883	0.324822	0.066197
N	-2.376797	-2.811496	-0.341700
N	-2.170787	-1.090436	1.925498
C	-4.830159	4.261117	-1.491955
H	-5.205256	3.454978	-2.140245
H	-5.679810	4.904551	-1.210941
H	-4.109789	4.869044	-2.062673

ts-22-23A
Geometry with 74 atoms:
Thermal correction to Gibbs Free Energy:
0.571245
Total energy: -4585.103847

Ni	3.202381	0.132499	-0.497288
I	2.021523	-2.210188	0.047951
C	1.412843	1.148243	0.046636
C	1.253657	0.984243	1.544380
H	1.187981	0.350788	-0.680672
H	1.661147	2.147012	-0.303999
C	2.538043	1.076873	2.336729
H	0.831313	-0.005253	1.783993
H	0.547469	1.721162	1.963493
O	2.320462	1.339765	3.623769
O	3.654456	0.907921	1.878592
C	3.468912	1.393020	4.482878
H	3.992737	0.424883	4.492489
H	3.089067	1.626686	5.485353
H	4.167195	2.176381	4.150503
H	2.077903	2.560494	-2.169037
C	3.023265	2.177280	-2.569047
H	3.494502	2.969244	-3.177291
H	2.809806	1.309273	-3.207100
C	5.224766	1.332872	-2.055418
C	4.155997	2.901234	-0.541753
C	5.926886	0.425059	-1.078802
H	5.012930	0.799091	-2.990587
H	5.845162	2.208328	-2.311153
H	4.634925	3.739356	-1.076703
H	3.204032	3.245678	-0.124202
H	4.790129	2.581814	0.292585
H	6.889488	0.068901	-1.484678
H	6.140541	0.958467	-0.143288
C	5.524463	-1.362856	0.486927
C	5.048874	-1.706601	-1.864236
H	4.931117	-2.259180	0.697551
H	6.585909	-1.648240	0.377906
H	5.412421	-0.659657	1.321158
H	6.081395	-2.039735	-2.071193
H	4.436617	-2.571361	-1.587347
H	4.622667	-1.265174	-2.773876
C	-2.011610	1.007449	-0.266914
C	-1.810771	-0.359794	0.339201
C	-3.028742	-1.224541	-0.005238
H	-0.835597	-0.785534	0.048396
H	-1.754039	-0.183871	1.429192
H	-2.887378	-1.702398	-0.994613

H	-3.161256	-2.035028	0.731373
C	-7.294917	0.724196	0.022272
H	-8.183173	1.200900	-0.430034
H	-7.397841	0.814615	1.112443
C	-7.218285	-0.737388	-0.377237
H	-7.195800	-0.830487	-1.471646
H	-8.101935	-1.291963	-0.015218
Ni	-4.534841	-0.011198	-0.154128
O	-3.217601	1.334476	-0.493857
C	-5.741236	-2.640620	-0.569084
H	-4.860055	-3.145138	-0.158680
H	-6.617448	-3.303823	-0.456590
H	-5.571874	-2.440770	-1.635379
C	-6.055542	-1.614790	1.598150
H	-6.887023	-2.306426	1.824687
H	-5.112617	-2.054904	1.945001
H	-6.215830	-0.673278	2.138444
C	-5.789665	2.593059	0.465005
H	-4.831306	3.038091	0.170607
H	-6.594031	3.345188	0.361336
H	-5.720852	2.284891	1.518041
C	-6.049154	1.793004	-1.800483
H	-5.060788	2.193938	-2.060791
H	-6.239195	0.912382	-2.428756
H	-6.823090	2.554881	-2.011195
N	-6.048204	1.414577	-0.376691
N	-5.966545	-1.364098	0.142225
N	3.926047	1.769362	-1.469514
N	5.040227	-0.723150	-0.757297
O	-1.065711	1.814788	-0.512223
H	0.112602	1.401226	-0.287390

ts-22-23B
Geometry with 77 atoms:
Thermal correction to Gibbs Free Energy:
0.596443
Total energy: -4624.430040

Ni	-3.126708	-0.547554	0.473219
I	-1.932603	-1.501801	-1.735577
C	-1.350047	0.517672	0.955707
C	-1.225401	1.634680	-0.060060
H	-1.102068	-0.532945	0.733696
H	-1.591561	0.814179	1.973417
C	-2.524395	2.323518	-0.414755
H	-0.830580	1.246563	-1.013267
H	-0.512214	2.409757	0.268343
O	-2.328330	3.518972	-0.962960
O	-3.633038	1.842684	-0.252258
C	-3.491910	4.251807	-1.413061
H	-4.016107	3.648306	-2.171790
H	-4.177481	4.384508	-0.560605
H	-1.978996	-0.482106	3.411700
C	-2.916231	-1.044426	3.331725
H	-3.379381	-1.097293	4.332821
H	-2.690541	-2.061040	2.983041
C	-5.128759	-1.131076	2.368041
C	-4.074996	1.017819	2.769770
C	-5.842005	-0.868163	1.066568
H	-4.906668	-2.200503	2.475063
H	-5.745511	-0.836243	3.233678
H	-4.539210	1.057059	3.770250
H	-3.129338	1.568317	2.796582
H	-4.726019	1.508404	2.038173
H	-6.801390	-1.411779	1.019268
H	-6.063643	0.201972	0.958781
C	-5.444724	-0.633696	-1.303445
C	-4.964200	-2.743166	-0.212664
H	-4.841719	-0.975286	-2.151829
H	-6.502262	-0.900196	-1.477888
H	-5.345623	0.454738	-1.215114
H	-5.994618	-3.106209	-0.374480
H	-4.341314	-3.020967	-1.068963
H	-4.548679	-3.223758	0.681778
C	2.082842	0.261258	1.000696
C	1.884244	-0.024029	-0.467786
C	3.120414	-0.767802	-0.986802
H	0.920940	-0.530263	-0.648922
H	1.801725	0.970267	-0.944043
H	3.009593	-1.856508	-0.814098
H	3.242376	-0.621910	-2.073365
C	7.360762	0.501796	0.579534
H	8.253219	0.421568	1.226036
H	7.438301	1.455017	0.039032
C	7.313177	-0.655963	-0.400457
H	7.322698	-1.610746	0.142626
H	8.193236	-0.644640	-1.067547
Ni	4.614677	-0.154668	0.087651
O	3.290271	0.290726	1.393913
C	5.875557	-1.932912	-1.861712
H	4.982657	-1.913177	-2.495585
H	6.753521	-2.173297	-2.487446
H	5.751396	-2.711520	-1.097502
C	6.100144	0.446226	-2.228139
H	6.941132	0.283421	-2.926481
H	5.158111	0.444792	-2.789833
H	6.214577	1.428224	-1.752260
C	5.810619	1.882571	1.863108
H	4.856113	1.861814	2.403160
H	6.606247	2.258369	2.533268
H	5.710477	2.565488	1.007426
C	6.152099	-0.423783	2.501916
H	5.165272	-0.441322	2.982737
H	6.373874	-1.436147	2.137587
H	6.919298	-0.135545	3.244867
N	6.115060	0.527834	1.377760
N	6.055768	-0.621024	-1.204349
N	-3.835418	-0.389232	2.374809

```
 N  -4.958676  -1.270387  -0.059094
 O   1.134209   0.496697   1.806956
 H  -0.049217   0.419321   1.343462
 C  -3.016311   5.573854  -1.970223
 H  -2.329315   5.419601  -2.817285
 H  -3.879559   6.158020  -2.325784
 H  -2.494224   6.161255  -1.198347
```

ts-3-19A
Geometry with 41 atoms:
Thermal correction to Gibbs Free Energy: 0.284719
Total energy: -2759.715027

```
Ni   1.037805   0.493219  -0.156800
 I   1.179893  -1.716269  -1.654784
 C  -0.935765   0.102740   0.188467
 C  -1.077905  -1.130069   1.066014
 H  -1.101596   0.001281  -0.894540
 H  -1.270183   1.028385   0.656263
 C  -0.010668  -1.254533   2.127329
 H  -1.011770  -2.049700   0.463174
 H  -2.055576  -1.180217   1.577683
 O  -0.298644  -2.209931   3.012352
 O   1.009954  -0.592046   2.185346
 C   0.671861  -2.463516   4.036737
 H   1.626237  -2.790869   3.595842
 H   0.253463  -3.261749   4.662720
 H   0.847311  -1.560840   4.642028
 H  -1.144051   2.787620  -0.195687
 C  -0.130712   3.161807  -0.381308
 H  -0.107633   4.240704  -0.144975
 H   0.108389   3.018517  -1.443555
 C   2.198155   3.030628   0.232498
 C   0.489131   2.529398   1.879630
 C   3.260508   2.029082   0.610779
 H   2.284496   3.294857  -0.829517
 H   2.300938   3.963687   0.812547
 H   0.489668   3.585406   2.202195
 H  -0.509667   2.111528   2.047341
 H   1.195260   1.954744   2.488703
 H   4.271955   2.448211   0.464510
 H   3.169754   1.756244   1.670765
 C   3.796828  -0.317387   0.459000
 C   3.595766   0.993727  -1.565601
 H   3.718169  -1.219606  -0.157884
 H   4.863750  -0.061997   0.593296
 H   3.338422  -0.519217   1.435057
 H   4.666753   1.265895  -1.540479
 H   3.468903   0.068765  -2.138832
 H   3.035666   1.787885  -2.075118
 I  -4.263871   0.302183  -0.393740
 H  -2.402502   0.197833  -0.206021
 N   0.852853   2.430970   0.448203
 N   3.078928   0.796687  -0.194805
```

14A
Geometry with 38 atoms:
Thermal correction to Gibbs Free Energy: 0.293432
Total energy: -2163.156903

```
 C  -2.487209  -0.624763   0.067388
 C   2.280394   1.647798  -0.167792
 H   2.766686   2.552560   0.237951
 H   2.489966   1.620987  -1.245765
 C   2.824796   0.404733   0.506092
 H   2.678486   0.466302   1.593406
 H   3.907387   0.295032   0.321879
Ni   0.194762  -0.281784  -0.066408
 O  -3.774730  -0.416912   0.080723
 O  -1.670219   0.305264  -0.070214
 C   2.382586  -1.916199   0.981634
 H   1.964202  -2.854603   0.604293
 H   3.472879  -2.040068   1.103044
 H   1.931725  -1.688525   1.956721
 C   2.533167  -1.208033  -1.326702
 H   3.614199  -1.434157  -1.337447
 H   1.973215  -2.098568  -1.637773
 H   2.328001  -0.402041  -2.042115
 C   0.170105   2.484137  -1.058170
 H  -0.916079   2.482080  -0.906485
 H   0.535928   3.527170  -1.059925
 H   0.388137   2.025603  -2.033056
 C   0.431357   2.231090   1.332024
 H   0.718399   3.294125   1.430998
 H  -0.655253   2.135425   1.458609
 H   0.922464   1.655828   2.128003
 C  -0.558917  -2.060744  -0.317204
 H  -0.001790  -2.907208   0.108672
 H  -0.599426  -2.208340  -1.414805
 C  -1.983769  -2.016008   0.251079
 H  -2.700485  -2.744436  -0.165607
 H  -1.975074  -2.178592   1.345041
 N   2.098723  -0.814804   0.034103
 N   0.810921   1.699325   0.010742
 C  -4.252400   0.940595  -0.055236
 H  -5.345346   0.877131  -0.001418
 H  -3.861687   1.563785   0.762078
 H  -3.938467   1.356369  -1.023539
```

14B
Geometry with 41 atoms:
Thermal correction to Gibbs Free Energy: 0.319172
Total energy: -2202.484909

```
 C  -2.120776  -0.812738   0.077086
```

C	2.486688	1.764603	-0.207698
H	2.925026	2.704299	0.172979
H	2.660871	1.738960	-1.291953
C	3.132179	0.567966	0.458908
H	3.016077	0.635658	1.549165
H	4.213442	0.526405	0.242200
Ni	0.533028	-0.293259	-0.061529
O	-3.417328	-0.690663	0.084163
O	-1.363911	0.167925	-0.062493
C	2.834161	-1.767846	0.980475
H	2.457969	-2.733917	0.628603
H	3.931671	-1.830689	1.082056
H	2.390545	-1.546353	1.960395
C	2.909773	-1.088694	-1.340983
H	4.001427	-1.254379	-1.363902
H	2.396723	-2.013178	-1.632707
H	2.649809	-0.304917	-2.063615
C	0.306895	2.483846	-1.018131
H	-0.772393	2.415119	-0.836863
H	0.610849	3.546548	-1.011776
H	0.524069	2.053954	-2.006315
C	0.651992	2.202660	1.360431
H	0.887328	3.276448	1.478723
H	-0.425267	2.049263	1.509161
H	1.189516	1.633364	2.130663
C	-4.000982	0.639791	-0.064852
H	-3.625342	1.270011	0.755883
H	-3.644334	1.063139	-1.016376
C	-0.100428	-2.119637	-0.299042
H	0.515352	-2.920123	0.135134
H	-0.130941	-2.281182	-1.394940
C	-1.525617	-2.166840	0.269215
H	-2.192316	-2.943278	-0.143740
H	-1.507170	-2.322076	1.364137
N	2.472273	-0.700696	0.020312
N	1.023834	1.721289	0.017724
C	-5.501688	0.484200	-0.030939
H	-5.831592	0.047233	0.924340
H	-5.971817	1.473797	-0.140949
H	-5.850307	-0.158963	-0.853921

15A
Geometry with 38 atoms:
Thermal correction to Gibbs Free Energy:
0.294103
Total energy: -2163.130192

C	2.769931	-0.549536	0.287839
C	2.021032	-1.790519	0.669528
C	0.823514	-1.973234	-0.263118
H	2.748553	-2.620527	0.671221
H	1.690634	-1.663915	1.717122
H	1.164996	-2.169218	-1.297616
H	0.218696	-2.832990	0.058205
C	-2.235250	1.313168	0.670171
H	-2.878308	2.207419	0.598709
H	-2.224509	1.005257	1.724148
C	-2.768857	0.197823	-0.199573
H	-2.805401	0.516657	-1.249594
H	-3.792414	-0.088453	0.095913
O	1.872025	0.357433	-0.282158
O	3.934637	-0.293929	0.382076
C	-2.135236	-1.876166	-1.270208
H	-1.522442	-2.780809	-1.199959
H	-3.200623	-2.164874	-1.281087
H	-1.892169	-1.351049	-2.203419
C	-2.084288	-1.718550	1.150838
H	-3.136928	-2.042595	1.223044
H	-1.435872	-2.599601	1.187690
H	-1.844606	-1.078717	2.008973
C	-0.111013	2.241996	1.385272
H	0.914835	2.478356	1.079678
H	-0.603765	3.173392	1.718086
H	-0.070628	1.537867	2.228105
C	-0.842573	2.526726	-0.907494
H	0.183450	2.810016	-1.161354
H	-1.288810	2.024214	-1.776006
H	-1.413477	3.448152	-0.692747
C	2.434526	1.465964	-1.025824
H	3.417779	1.176097	-1.415307
H	2.541094	2.343654	-0.374718
H	1.747541	1.666520	-1.853998
Ni	-0.045765	-0.250403	-0.164177
N	-1.860708	-0.985463	-0.118667
N	-0.842177	1.625799	0.262659

15B
Geometry with 41 atoms:
Thermal correction to Gibbs Free Energy:
0.320776
Total energy: -2202.457257

C	2.399650	-1.243859	0.359880
C	1.383457	-2.244858	0.815751
C	0.197362	-2.192994	-0.150807
H	1.890960	-3.221467	0.887689
H	1.069843	-1.971550	1.840093
H	0.513637	-2.494708	-1.167690
H	-0.591593	-2.885626	0.174745
C	-2.166646	1.647903	0.616037
H	-2.595646	2.661395	0.533371
H	-2.331585	1.310251	1.647633
C	-2.826783	0.702167	-0.361033
H	-2.672558	1.050362	-1.391398
H	-3.914803	0.638040	-0.190220
O	1.734552	-0.120993	-0.140776
O	3.593415	-1.326125	0.323193
C	-2.539992	-1.442782	-1.447963

H	-2.140880	-2.458165	-1.352639
H	-3.635131	-1.497586	-1.576572
H	-2.095221	-0.965245	-2.330964
C	-2.722264	-1.340677	0.968247
H	-3.822475	-1.415365	0.923035
H	-2.298624	-2.348072	1.028874
H	-2.434707	-0.790635	1.872427
C	0.034913	2.022738	1.582057
H	1.112072	1.962627	1.391406
H	-0.217681	3.044650	1.918737
H	-0.213266	1.311801	2.382620
C	-0.392961	2.609755	-0.731780
H	0.689605	2.683142	-0.871684
H	-0.844105	2.266841	-1.672793
H	-0.776989	3.618858	-0.496361
C	2.499425	0.710173	-1.082600
H	1.736133	1.151457	-1.733328
H	3.111200	0.024182	-1.684249
Ni	-0.281195	-0.323787	-0.098520
N	-2.207806	-0.652039	-0.240147
N	-0.703926	1.663889	0.357571
C	3.357202	1.746533	-0.393177
H	4.086319	1.266656	0.274216
H	3.910065	2.309858	-1.162250
H	2.757067	2.463729	0.184882

17A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy:
0.286001
Total energy: -2461.239399

C	-1.290851	-2.616203	-0.460159
H	-0.875024	-3.399699	-1.115350
H	-2.296289	-2.938545	-0.157904
C	-0.414288	-2.400199	0.758162
H	0.618635	-2.178012	0.456474
H	-0.392796	-3.304802	1.391285
N	-1.440314	-1.334823	-1.215365
N	-0.917261	-1.228710	1.518967
C	0.120220	-0.701504	2.426576
H	-0.262675	0.194652	2.929209
H	0.395803	-1.460489	3.180328
H	1.010487	-0.429172	1.844918
C	-2.146914	-1.533946	2.277905
H	-1.950188	-2.294301	3.055281
H	-2.507789	-0.614100	2.757477
H	-2.932123	-1.905005	1.606407
C	-2.660853	-1.389097	-2.045982
H	-2.738536	-0.475513	-2.646615
H	-2.624250	-2.260650	-2.722726
H	-3.544372	-1.470909	-1.399078
C	-0.259889	-1.077111	-2.074964
H	-0.157135	-1.873978	-2.832470
H	-0.386482	-0.110628	-2.578294
H	0.654740	-1.031918	-1.471149
Ni	-1.445859	0.082010	0.123813
C	-1.260935	2.191637	0.030114
C	-2.162228	1.634955	-0.936848
C	-3.653067	1.648457	-0.652065
H	-1.875976	1.808724	-1.980558
H	-3.860992	1.546793	0.423896
H	-4.108869	2.596097	-0.993673
H	-4.172597	0.832213	-1.175041
O	-0.297617	3.019962	-0.332865
O	-1.315644	1.684989	1.201150
C	0.793190	3.218723	0.588868
H	1.469811	3.930428	0.100492
H	1.319205	2.268684	0.767904
H	0.428328	3.632372	1.540285
I	3.326339	-0.130333	-0.245075

17B
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy:
0.312396
Total energy: -2500.565321

C	-1.876230	-2.622176	-0.001571
H	-1.655400	-3.594614	-0.472782
H	-2.929644	-2.638375	0.308767
C	-0.973037	-2.375830	1.191325
H	0.082278	-2.458179	0.897742
H	-1.159804	-3.118877	1.986505
N	-1.719221	-1.517884	-0.995349
N	-1.187118	-0.994310	1.690587
C	-0.040701	-0.540767	2.502433
H	-0.210616	0.496542	2.814886
H	0.079237	-1.181211	3.394526
H	0.875568	-0.582022	1.898396
C	-2.439023	-0.858228	2.461943
H	-2.405172	-1.474411	3.378674
H	-2.572299	0.195451	2.741897
H	-3.302232	-1.165918	1.857811
C	-2.906150	-1.468457	-1.872725
H	-2.766521	-0.694406	-2.636028
H	-3.053319	-2.442216	-2.371866
H	-3.797638	-1.230157	-1.277861
C	-0.499999	-1.707620	-1.817073
H	-0.579320	-2.636752	-2.408608
H	-0.385086	-0.852253	-2.494470
H	0.389585	-1.758631	-1.178462
Ni	-1.429976	0.103582	0.051104
C	-0.829601	2.098943	-0.405728
C	-1.799811	1.539166	-1.305328
C	-3.261964	1.902649	-1.113454
H	-1.464589	1.460873	-2.346217
H	-3.508655	2.041080	-0.049818

```
 H  -3.504942   2.844773  -1.638902
 H  -3.929184   1.126590  -1.515737
 O   0.267387   2.677263  -0.854062
 O  -1.005052   1.822668   0.828866
 C   1.363580   2.907831   0.075374
 H   2.250242   2.981096  -0.568155
 H   1.474383   2.022156   0.716610
 I   3.165230  -0.762611  -0.263802
 C   1.146221   4.172198   0.881357
 H   0.267310   4.076144   1.536692
 H   2.029626   4.359386   1.512863
 H   1.004337   5.041675   0.219715
```

18A
Geometry with 38 atoms:
Thermal correction to Gibbs Free Energy:
0.292409
Total energy: -2163.153353

```
 C   2.678493  -0.331547  -0.323545
 H   3.492952  -0.658672  -0.992052
 H   2.984810  -0.554013   0.707692
 C   2.399554   1.150080  -0.484073
 H   2.207191   1.391806  -1.537847
 H   3.266895   1.750577  -0.161010
 N   1.436609  -1.116336  -0.594783
 N   1.182396   1.507360   0.290792
 C   0.531248   2.709995  -0.263819
 H  -0.381199   2.922048   0.306288
 H   1.209325   3.580289  -0.214033
 H   0.257648   2.526655  -1.312111
 C   1.470370   1.698366   1.728412
 H   2.147929   2.557129   1.881990
 H   0.527713   1.880633   2.261563
 H   1.936136   0.795934   2.145816
 C   1.592473  -2.484817  -0.059373
 H   0.692812  -3.070584  -0.279606
 H   2.466480  -2.976311  -0.520724
 H   1.737022  -2.440323   1.027763
 C   1.133382  -1.178483  -2.045091
 H   1.951975  -1.681270  -2.589031
 H   0.201262  -1.739250  -2.190837
 H   0.999544  -0.168244  -2.452257
Ni  -0.008503  -0.082967   0.196172
 C  -2.118640  -0.239499   0.168149
 C  -1.441750  -1.478066   0.416818
 C  -1.287869  -1.970233   1.843561
 H  -1.616787  -2.254087  -0.337230
 H  -1.199123  -1.134871   2.554414
 H  -2.163006  -2.575240   2.143364
 H  -0.398614  -2.607767   1.955147
 O  -3.032650  -0.141160  -0.783687
 O  -1.642161   0.789198   0.756277
 C  -3.385760   1.181419  -1.229149
 H  -4.119975   1.042190  -2.032059
 H  -2.498156   1.707149  -1.613766
 H  -3.828303   1.764537  -0.408392
```

18B
Geometry with 41 atoms:
Thermal correction to Gibbs Free Energy:
0.318697
Total energy: -2202.480715

```
 C   2.947472   0.186984  -0.406369
 H   3.778198   0.036890  -1.116394
 H   3.347655   0.046179   0.606743
 C   2.348945   1.572232  -0.548589
 H   2.054253   1.760226  -1.589824
 H   3.083054   2.347277  -0.268760
 N   1.892446  -0.850054  -0.614497
 N   1.126318   1.667134   0.290774
 C   0.220670   2.721187  -0.205831
 H  -0.682192   2.743615   0.415997
 H   0.714791   3.708391  -0.174432
 H  -0.069713   2.496736  -1.241466
 C   1.440606   1.898310   1.716947
 H   1.935091   2.876264   1.855721
 H   0.507176   1.879312   2.295150
 H   2.099626   1.106834   2.097161
 C   2.348833  -2.134651  -0.043085
 H   1.599790  -2.911335  -0.234222
 H   3.305925  -2.436240  -0.502744
 H   2.487036  -2.025707   1.040260
 C   1.577611  -1.027625  -2.051651
 H   2.469106  -1.377582  -2.601077
 H   0.774750  -1.768827  -2.152526
 H   1.235550  -0.081839  -2.490736
Ni   0.276789  -0.128640   0.199483
 C  -1.765935  -0.709662   0.195149
 C  -0.841860  -1.785161   0.413745
 C  -0.582253  -2.256627   1.832762
 H  -0.868576  -2.571894  -0.349452
 H  -0.656036  -1.429911   2.555322
 H  -1.317541  -3.027300   2.128193
 H   0.416456  -2.705560   1.933160
 O  -2.703943  -0.794001  -0.731654
 O  -1.489676   0.385969   0.791545
 C  -3.371974   0.424570  -1.158668
 H  -3.775097   0.175336  -2.149911
 H  -2.619020   1.219939  -1.270001
 C  -4.471133   0.825093  -0.195928
 H  -4.055882   1.090351   0.787744
 H  -5.006487   1.701687  -0.594754
 H  -5.196304   0.005866  -0.068644
```

ts-16-17A

Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.287166
Total energy: -2461.212123

C	1.021846	-2.116373	1.481478
H	0.459696	-2.442631	2.372650
H	1.963443	-2.681750	1.458943
C	0.224441	-2.358150	0.214852
H	-0.749449	-1.853707	0.271838
H	0.035558	-3.435778	0.068317
N	1.373297	-0.667636	1.595235
N	0.961443	-1.783828	-0.941894
C	0.052386	-1.503201	-2.072674
H	0.619541	-1.014688	-2.876404
H	-0.393957	-2.437534	-2.457116
H	-0.749238	-0.830915	-1.740920
C	2.072066	-2.652743	-1.381393
H	1.692514	-3.633834	-1.718810
H	2.600567	-2.168829	-2.213880
H	2.785392	-2.807508	-0.561322
C	2.550112	-0.509669	2.476622
H	2.764218	0.555174	2.618662
H	2.352873	-0.969391	3.461392
H	3.422874	-0.993814	2.018107
C	0.236120	0.123613	2.123433
H	-0.003752	-0.195086	3.153128
H	0.503543	1.187193	2.122404
H	-0.650187	-0.013036	1.491343
Ni	1.717290	-0.096948	-0.237680
C	1.326913	2.182033	-0.477712
C	2.586292	1.621187	-0.020143
C	3.501916	1.122084	-1.104617
H	3.009298	1.999477	0.912996
H	3.064240	0.216248	-1.624533
H	3.630959	1.829387	-1.941382
H	4.479391	0.814903	-0.711624
O	0.705646	3.009787	0.372818
O	0.811866	1.794400	-1.536664
C	-0.656314	3.346631	0.061974
H	-1.001625	3.993570	0.878352
H	-1.281503	2.441880	0.005529
H	-0.715973	3.884213	-0.896593
I	-3.432085	-0.104429	-0.009615

ts-16-17B
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.311029
Total energy: -2500.538498

C	1.406966	-2.272783	1.331848
H	0.919202	-2.731575	2.208179
H	2.413084	-2.705132	1.249219
C	0.611305	-2.532213	0.067022
H	-0.422338	-2.177188	0.180989
H	0.571365	-3.612717	-0.156039
N	1.570039	-0.801991	1.544477
N	1.226692	-1.779166	-1.057487
C	0.262239	-1.571427	-2.157145
H	0.730219	-0.952473	-2.934350
H	-0.044242	-2.537388	-2.596382
H	-0.624634	-1.051922	-1.773064
C	2.448052	-2.437172	-1.566450
H	2.213570	-3.438847	-1.969293
H	2.881003	-1.823053	-2.367543
H	3.194814	-2.539193	-0.768622
C	2.748646	-0.552505	2.401669
H	2.823016	0.517236	2.625723
H	2.653955	-1.109070	3.351057
H	3.661130	-0.873492	1.881647
C	0.360312	-0.209408	2.164616
H	0.194530	-0.642894	3.166597
H	0.494681	0.875277	2.253274
H	-0.521760	-0.399922	1.539868
Ni	1.739690	-0.050031	-0.248026
C	1.017214	2.155526	-0.273316
C	2.369049	1.755655	0.075615
C	3.285320	1.486865	-1.088265
H	2.787094	2.125759	1.014216
H	2.934260	0.593694	-1.685849
H	3.285971	2.287337	-1.848050
H	4.311739	1.271997	-0.764688
O	0.346241	2.846222	0.655017
O	0.500950	1.742925	-1.324773
C	-1.079065	3.032792	0.461021
H	-1.465934	3.233885	1.470047
H	-1.518964	2.092024	0.097890
I	-3.293473	-0.666030	0.024144
C	-1.368563	4.183457	-0.482819
H	-0.997728	3.960653	-1.494403
H	-2.456922	4.345568	-0.542284
H	-0.897891	5.114099	-0.126663

ts-4-16A
Geometry with 39 atoms:
Thermal correction to Gibbs Free Energy: 0.283448
Total energy: -2461.215985

Ni	-0.091634	0.002612	-0.393941
C	2.729636	-1.131909	-0.580388
C	1.632381	-0.553737	-1.379826
C	0.546852	-1.382103	-1.740759
H	1.941083	0.256909	-2.045512
H	-0.721394	-0.136745	-1.648507
H	0.460023	-2.365153	-1.264552
H	0.138698	-1.340848	-2.755360
O	3.792163	-0.294631	-0.528785

O	2.734110	-2.222308	-0.044615
C	4.950722	-0.778632	0.155641
H	5.705607	0.015061	0.082447
H	4.729202	-0.989647	1.213944
H	5.327325	-1.701160	-0.313508
I	-2.534723	-1.098690	0.068982
N	-0.411288	2.193970	-0.658491
H	1.450883	-1.294521	2.073347
C	1.683108	-0.223939	2.123556
N	0.574550	0.561177	1.551199
H	1.864097	0.063789	3.175716
H	2.599121	-0.029567	1.560936
C	1.025970	1.958772	1.333344
C	-0.544281	0.514087	2.514481
C	-0.035660	2.793019	0.636705
H	1.935418	1.914337	0.716953
H	1.299020	2.428621	2.297596
H	-0.256635	1.007416	3.462119
H	-0.799052	-0.532792	2.718300
H	-1.438137	0.998413	2.109888
H	0.332670	3.828611	0.508754
H	-0.935552	2.855928	1.263134
C	-1.795232	2.518457	-1.018669
C	0.501445	2.626112	-1.723783
H	-2.043475	2.053281	-1.982832
H	-1.948875	3.612837	-1.102677
H	-2.482628	2.114730	-0.263702
H	0.397754	3.710460	-1.928558
H	0.285516	2.070259	-2.646812
H	1.542732	2.425942	-1.440393

ts-4-16B
Geometry with 42 atoms:
Thermal correction to Gibbs Free Energy: 0.308473
Total energy: -2500.543258

Ni	-0.320972	-0.028593	-0.370940
C	2.586704	-0.877568	-0.411008
C	1.466850	-0.460365	-1.274131
C	0.473299	-1.403700	-1.629315
H	1.720091	0.340566	-1.973242
H	-0.866408	-0.293390	-1.647692
H	0.454776	-2.365083	-1.102889
H	0.117197	-1.459378	-2.663226
O	3.517648	0.102681	-0.320198
O	2.700823	-1.951279	0.147036
C	4.725260	-0.183027	0.413755
H	5.114951	0.803129	0.705145
H	4.473739	-0.747183	1.325088
I	-2.730157	-1.199275	0.019430
N	-0.707580	2.163734	-0.727628
H	1.076816	-1.194016	2.216571
C	1.289110	-0.118534	2.258297
N	0.218838	0.634054	1.577526
H	1.377267	0.197846	3.313858
H	2.248979	0.073948	1.774194
C	0.677887	2.020735	1.311410
C	-0.957727	0.629347	2.471273
C	-0.364959	2.822005	0.548607
H	1.603901	1.947626	0.722091
H	0.922378	2.533796	2.261404
H	-0.734557	1.182671	3.403042
H	-1.213583	-0.406924	2.722578
H	-1.830054	1.075380	1.983886
H	0.009553	3.849665	0.382843
H	-1.279273	2.918202	1.149190
C	-2.100264	2.412870	-1.110567
C	0.196393	2.598771	-1.798044
H	-2.318615	1.900447	-2.058118
H	-2.303445	3.495110	-1.238583
H	-2.777103	2.006755	-0.347352
H	0.039190	3.666864	-2.049714
H	0.025353	1.995221	-2.700596
H	1.242029	2.468328	-1.490252
C	5.725256	-0.943164	-0.438195
H	6.663718	-1.083483	0.122240
H	5.332263	-1.935119	-0.707719
H	5.952960	-0.388749	-1.362666

10
Geometry with 36 atoms:
Thermal correction to Gibbs Free Energy: 0.263925
Total energy: -2421.927628

C	-0.533889	2.770844	0.154321
C	-1.049208	2.336357	1.524404
C	-0.177660	1.287342	2.192914
H	-1.149381	3.233512	2.153078
H	-2.064581	1.935188	1.365912
H	0.854513	1.632223	2.364516
H	-0.243206	0.313239	1.628406
C	2.439562	-1.357275	-1.319495
H	3.257512	-1.485279	-2.046476
H	1.644681	-2.068025	-1.578564
C	2.911166	-1.580924	0.098838
H	3.755846	-0.920691	0.336603
H	3.241902	-2.620564	0.256525
Ni	0.962343	0.372547	0.266456
O	0.326759	1.967998	-0.429104
O	-0.916795	3.803236	-0.369858
C	2.334240	-0.958933	2.380816
H	1.507703	-0.765684	3.075294
H	2.911355	-1.824491	2.747711
H	2.989206	-0.078018	2.340016
C	0.804918	-2.343134	1.107165
H	1.283821	-3.251635	1.509924

```
 H  -0.022166  -2.041649   1.761233
 H   0.388454  -2.551759   0.115358
 C   0.896687   0.085276  -2.544142
 H   0.492034   1.100585  -2.600970
 H   1.404894  -0.178911  -3.486820
 H   0.073142  -0.615011  -2.353603
 C   2.919183   1.046201  -1.596299
 H   2.444602   2.033906  -1.585632
 H   3.645617   0.989948  -0.775622
 H   3.441449   0.888790  -2.554884
 I  -2.649243  -0.951282  -0.304526
 H  -0.570391   0.952643   3.164815
 N   1.865265   0.016709  -1.424494
 N   1.795821  -1.241863   1.030620


11
Geometry with 27 atoms:
Thermal correction to Gibbs Free Energy:
0.185392
Total energy: -2452.001598
 I  -1.550379   1.758027   0.186647
 I  -1.386089  -1.890443  -0.186317
Ni   0.421651   0.019069   0.000288
 C   3.093091   0.707823  -0.492881
 H   3.114525   0.324536  -1.521416
 H   3.953556   1.387866  -0.375318
 C   3.143001  -0.425682   0.496032
 H   3.126995  -0.040686   1.524151
 H   4.062029  -1.024299   0.379871
 C   1.735732  -2.080684   1.537118
 H   0.913239  -2.788450   1.392297
 H   2.657754  -2.637298   1.780937
 H   1.485497  -1.409946   2.370253
 C   2.133608  -2.179190  -0.855421
 H   3.031830  -2.803773  -0.706532
 H   1.255337  -2.822612  -0.970401
 H   2.250883  -1.590303  -1.773338
 C   1.926662   2.367099   0.852074
 H   2.762504   3.072118   0.699759
 H   0.992956   2.927020   0.965129
 H   2.099094   1.795412   1.772540
 C   1.537985   2.222696  -1.539347
 H   0.655190   2.852896  -1.392471
 H   2.405156   2.859829  -1.787214
 H   1.347203   1.528691  -2.369503
 N   1.939975  -1.281258   0.307108
 N   1.816078   1.449940  -0.307067


12
Geometry with 36 atoms:
Thermal correction to Gibbs Free Energy:
0.256816
Total energy: -2421.931054
 C  -0.224382   2.945086   0.007925
 C   0.052889   2.818616  -1.487072
 C   0.221317   1.341742  -1.854774
 H  -0.721777   3.355957  -2.061280
 H   1.000294   3.364128  -1.653396
 H  -0.747682   0.889970  -2.132422
 H   0.910160   1.199492  -2.706774
 C   2.374468  -1.627258   1.163382
 H   2.382124  -2.359450   1.990486
 H   3.424093  -1.402433   0.930694
 C   1.677010  -2.222800  -0.047999
 H   0.652790  -2.520605   0.218763
 H   2.208142  -3.125164  -0.401021
Ni   0.893711   0.455014  -0.259391
 O   0.284325   1.945221   0.692272
 O  -0.808088   3.886573   0.523042
 C   0.664331  -1.766440  -2.194802
 H   0.588638  -1.055550  -3.025299
 H   1.051240  -2.726874  -2.579698
 H  -0.335594  -1.921864  -1.771238
 C   2.881397  -0.921681  -1.754311
 H   3.354799  -1.838714  -2.149632
 H   2.742999  -0.206226  -2.574543
 H   3.549005  -0.465488  -1.013005
 C   2.636704   0.608613   2.132091
 H   2.088524   1.535825   2.341892
 H   3.100097   0.232378   3.063913
 H   3.429432   0.832090   1.403406
 C   0.579314  -0.605242   2.482984
 H   0.006201   0.325467   2.583340
 H  -0.087937  -1.376824   2.078551
 H   0.941136  -0.932604   3.476350
 I  -2.592361  -0.815581   0.151688
 H  -1.016880  -0.206203  -0.053265
 N   1.564217  -1.227587  -1.154597
 N   1.701954  -0.370991   1.561830


13
Geometry with 36 atoms:
Thermal correction to Gibbs Free Energy:
0.260824
Total energy: -2421.913137
 C   0.870680   2.539093  -0.605153
 C  -0.097198   3.065268   0.408775
 C  -0.610534   1.897157   1.259283
 H   0.399940   3.873617   0.969073
 H  -0.929419   3.522193  -0.158335
 H   0.186283   1.544757   1.939364
 H  -1.466413   2.221753   1.872188
 C  -2.695318  -1.603844  -0.954264
 H  -2.807220  -2.587333  -1.442794
 H  -3.603387  -1.028033  -1.176603
```

```
 C  -2.524824  -1.768927   0.541324
 H  -1.639755  -2.382765   0.757994
 H  -3.399365  -2.270228   0.991220
Ni  -1.030559   0.469817   0.012900
 O   1.917095   2.967385  -0.990968
 C  -1.770361  -0.655648   2.549483
 H  -1.670068   0.302746   3.069249
 H  -2.450272  -1.306490   3.126616
 H  -0.781493  -1.127144   2.479516
 C  -3.571711   0.329186   1.258761
 H  -4.330598  -0.230696   1.833359
 H  -3.385345   1.290364   1.750738
 H  -3.957119   0.529077   0.251266
 C  -1.898769  -0.100671  -2.703077
 H  -1.023954   0.453699  -3.066784
 H  -2.259578  -0.768527  -3.506589
 H  -2.688945   0.621825  -2.454128
 C  -0.412931  -1.781146  -1.795340
 H   0.462976  -1.212996  -2.133525
 H  -0.119522  -2.330493  -0.892808
 H  -0.695393  -2.499528  -2.586580
 N  -2.308217  -0.438660   1.186941
 N  -1.529328  -0.864508  -1.498409
 O   0.369145   1.330098  -1.100452
 H   1.102744   0.804243  -1.491522
 I   2.806608  -0.893498   0.352090
```

CH3CH2COOH
Geometry with 11 atoms:
Thermal correction to Gibbs Free Energy: 0.060435
Total energy: -268.471745

```
 C  -0.566866   0.102278   0.000397
 O  -0.610745   1.311553   0.000135
 O  -1.672465  -0.664157  -0.000381
 H  -2.449850  -0.073679  -0.000648
 C   0.690765  -0.734341   0.000433
 H   0.636384  -1.401750   0.878025
 H   0.635900  -1.402848  -0.876274
 C   1.967740   0.094171  -0.000386
 H   2.020271   0.743740   0.887201
 H   2.853196  -0.559828  -0.000127
 H   2.019939   0.742547  -0.888873
```

ts-1-10
Geometry with 36 atoms:
Thermal correction to Gibbs Free Energy: 0.252731
Total energy: -2421.901385

```
 C  -0.358951   2.725753   0.077977
 C   0.854280   1.890365   0.479278
 C   0.636111   0.415226   0.164123
 H   1.756370   2.322046   0.012974
 H   0.978740   2.027360   1.567404
 H   0.804821   0.096746  -0.876095
 H   0.852533  -0.317209   0.951302
 C  -3.788574  -1.356124   0.054071
 H  -4.748371  -1.584360  -0.441805
 H  -3.928909  -1.535885   1.128260
 C  -2.684027  -2.240614  -0.490567
 H  -2.602510  -2.116903  -1.579306
 H  -2.895566  -3.306048  -0.290385
Ni  -1.361804   0.162685   0.042419
 O  -1.455633   2.021236  -0.056720
 O  -0.313124   3.937793  -0.067836
 C  -0.288105  -2.485039  -0.692221
 H   0.687192  -2.256469  -0.246499
 H  -0.417575  -3.581547  -0.713005
 H  -0.308810  -2.099557  -1.720208
 C  -1.262666  -2.273539   1.509603
 H  -1.372764  -3.369095   1.601496
 H  -0.281485  -1.977954   1.901479
 H  -2.034375  -1.782728   2.115729
 C  -4.054237   0.926562   0.883113
 H  -3.704693   1.955715   0.740043
 H  -5.155872   0.887236   0.799628
 H  -3.756680   0.592855   1.887304
 C  -3.733164   0.550747  -1.485295
 H  -3.330839   1.565014  -1.598846
 H  -3.261058  -0.096369  -2.236988
 H  -4.825593   0.558943  -1.655833
 I   3.948149  -0.276306  -0.081795
 H   2.137281   0.019417   0.028675
 N  -3.415381   0.066901  -0.128016
 N  -1.368502  -1.853247   0.094882
```

ts-10-11
Geometry with 38 atoms:
Thermal correction to Gibbs Free Energy: 0.264466
Total energy: -2720.409415

```
 C   0.387523  -2.175642   0.233746
 C  -0.056440  -2.314366  -1.213433
 C  -0.059128  -0.997507  -1.970798
 H   0.622054  -3.041792  -1.686769
 H  -1.061394  -2.764492  -1.207010
 H   0.940720  -0.537483  -2.023142
 H  -0.851266  -0.324259  -1.542305
 C  -0.647862   2.896740   1.269244
 H  -0.351522   3.614875   2.050036
 H  -1.734573   2.757074   1.331884
 C  -0.248655   3.365107  -0.109886
 H   0.830543   3.559719  -0.161585
 H  -0.772123   4.292072  -0.394126
Ni  -0.061477   0.618332  -0.173297
```

O	0.685225	-0.920794	0.632955
O	0.532374	-3.117234	0.975442
C	0.263234	2.413909	-2.301031
H	-0.008825	1.630523	-3.019234
H	0.088928	3.399602	-2.763855
H	1.326591	2.317780	-2.041782
C	-2.003368	2.271513	-1.436091
H	-2.263060	3.217167	-1.940140
H	-2.212604	1.429452	-2.106557
H	-2.617603	2.146517	-0.537577
C	-0.774798	0.807953	2.538397
H	-0.290421	-0.161127	2.697115
H	-0.798401	1.380036	3.480933
H	-1.797307	0.639822	2.176902
C	1.401711	1.714457	1.953041
H	1.829731	0.719994	2.113881
H	1.987216	2.233576	1.184815
H	1.441213	2.287129	2.894357
I	-3.631250	-1.027199	0.084978
H	-0.421398	-1.092437	-3.004784
N	-0.009319	1.569254	1.520846
N	-0.562929	2.273404	-1.079465
I	3.826822	-0.609057	-0.099579
H	2.161174	-0.782869	0.389134

ts-12-13
Geometry with 36 atoms:
Thermal correction to Gibbs Free Energy:
0.253232
Total energy: -2421.927271

C	-0.755277	2.607946	0.129226
C	-0.276815	2.713432	-1.314790
C	0.267058	1.356328	-1.771808
H	-1.080548	3.138189	-1.942609
H	0.534786	3.464861	-1.300163
H	-0.553326	0.722737	-2.160749
H	1.006647	1.463526	-2.585994
C	2.785578	-1.241636	1.231277
H	2.950714	-2.017903	2.000581
H	3.718579	-0.667979	1.146771
C	2.442942	-1.884892	-0.100379
H	1.546829	-2.512137	0.005921
H	3.265094	-2.536993	-0.446306
Ni	0.988300	0.500531	-0.185164
O	-0.146527	1.643585	0.787000
O	-1.582387	3.349414	0.637411
C	1.454192	-1.494881	-2.270210
H	1.265742	-0.756566	-3.057342
H	2.078049	-2.307682	-2.683854
H	0.492405	-1.908712	-1.938381
C	3.361192	-0.170142	-1.596918
H	4.059791	-0.892839	-2.057162
H	3.089323	0.591768	-2.337745
H	3.864105	0.331599	-0.760720
C	2.208973	0.771434	2.487126
H	1.387006	1.468681	2.691382
H	2.607196	0.374827	3.440353
H	3.007095	1.319651	1.966138
C	0.577788	-0.994993	2.269011
H	-0.231874	-0.270063	2.419683
H	0.201063	-1.798927	1.622881
H	0.875603	-1.428668	3.242675
I	-2.751357	-0.972771	-0.027970
H	-1.399537	-0.054514	0.163472
N	2.134452	-0.849319	-1.128693
N	1.708737	-0.307883	1.624069

ts-13-11
Geometry with 38 atoms:
Thermal correction to Gibbs Free Energy:
0.259674
Total energy: -2720.372860

C	0.341778	-1.754075	0.887233
C	-1.097941	-1.408956	1.140077
C	-1.558127	-0.181265	0.375108
H	-1.689455	-2.316157	0.934748
H	-1.179648	-1.225348	2.225382
H	-1.585610	-0.228606	-0.724053
H	-2.199033	0.523507	0.906477
C	1.260806	3.590721	0.129590
H	2.020883	4.267485	-0.295785
H	1.126363	3.868281	1.183413
C	-0.044914	3.698480	-0.621499
H	0.102059	3.484587	-1.688259
H	-0.473989	4.711107	-0.541620
Ni	0.057188	1.052740	0.203782
O	0.878726	-2.814181	1.012476
C	-2.103769	2.518184	-1.078913
H	-2.883776	1.861957	-0.678342
H	-2.554697	3.497848	-1.310031
H	-1.699319	2.078268	-1.999719
C	-1.573746	3.144133	1.204813
H	-2.075963	4.117693	1.075904
H	-2.305304	2.414809	1.571358
H	-0.778840	3.243703	1.953550
C	2.644078	1.915155	1.211433
H	3.045281	0.897959	1.142290
H	3.490741	2.623533	1.194716
H	2.098072	2.024947	2.158548
C	2.387947	1.886364	-1.209557
H	2.664520	0.826660	-1.253022
H	1.706260	2.104601	-2.041202
H	3.302792	2.493939	-1.322406
N	-1.010732	2.688643	-0.091106
N	1.727770	2.181053	0.082421
O	1.045511	-0.627382	0.489029

```
H   2.004876  -0.866621   0.260715
I   4.202612  -1.599137  -0.339802
I  -4.632441  -1.349099  -0.276617
H  -2.906416  -0.632192   0.030712
```