Electronic Supplementary Information

Mechanistic insights into Ni-catalyzed hydrogen atom transfer (HAT)-triggered hydrodefluorination of CF_3-substituted alkenes

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Computational methods

All calculations were performed with Gaussian 09[1] with the ultrafine integration grid and the keywords acc2e=11 and 5D 7F. The hybrid functional B3LYP[2] was combined with the dispersion correction D3[3] to improve computational accuracy. Structures were optimized and characterized by frequency calculations to be energy minima (zero imaginary frequencies) or transition states (only one imaginary frequency) at the B3LYP-D3/BS1 level in the gas phase, BS1 designating a mixed basis set of SDD[4] for nickel and 6-31G(d,p) for other atoms. The energies were then refined by B3LYP-D3/BS2// B3LYP-D3/BS1 single-point energy calculations with the solvent (benzene) effects included using the SMD solvation model,[5] BS2 denoting a mixed basis set of SDD for nickel and 6-311++G(d,p) for other atoms. The refined energies were converted to zero-point energy-corrected Gibbs free energies at 298.15 K and 1 atm, using the B3LYP-D3/BS1 harmonic frequencies. Minimum energy crossing points (MECPs) were obtained using the MECP-locating program developed by the Harvey group.[6] Selected molecular structures were illustrated with CYLview.[7] For open-shell singlet structures whose S^2 values are not zero, the energy was corrected by applying Yamaguchi et al.'s equation[8–11] in the form:[12,13]

$$E = \frac{2E_{\mathrm{OS}} - E_{\mathrm{triplet}} < S^2 >_{\mathrm{OS}}}{2 - < S^2 >_{\mathrm{OS}}}$$

where E_{OS} is the energy of open-shell singlet calculation, E_{triplet} is the energy of the triplet state at the open-shell singlet geometry and $\langle S^2 \rangle_{\mathrm{OS}}$ is the S^2 value of the open-shell singlet calculation.

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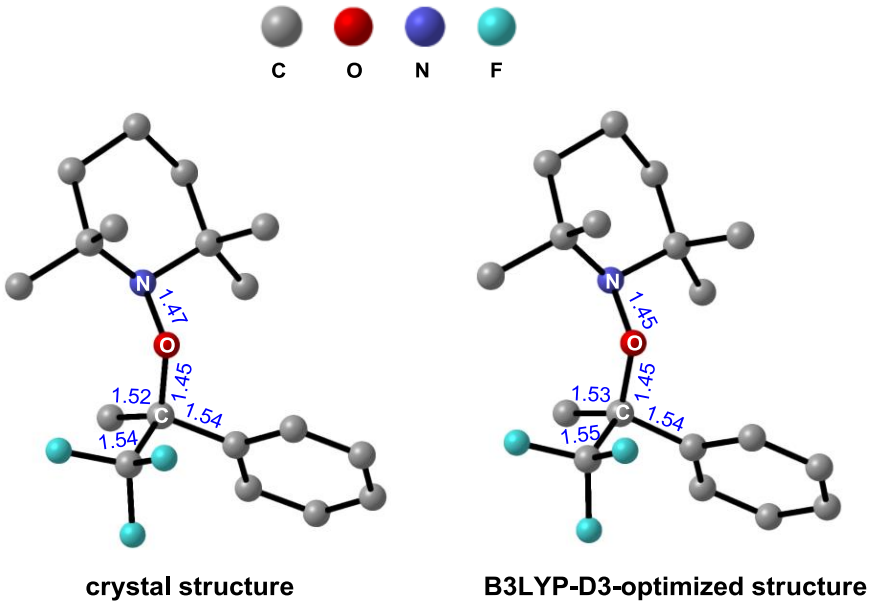

Fig. S1 Crystal structure (left) and DFT-computed structure (right) of the TEMPO-R1 compound showing a high degree of consistency. The numbers in blue font denote key bond distances in Å.

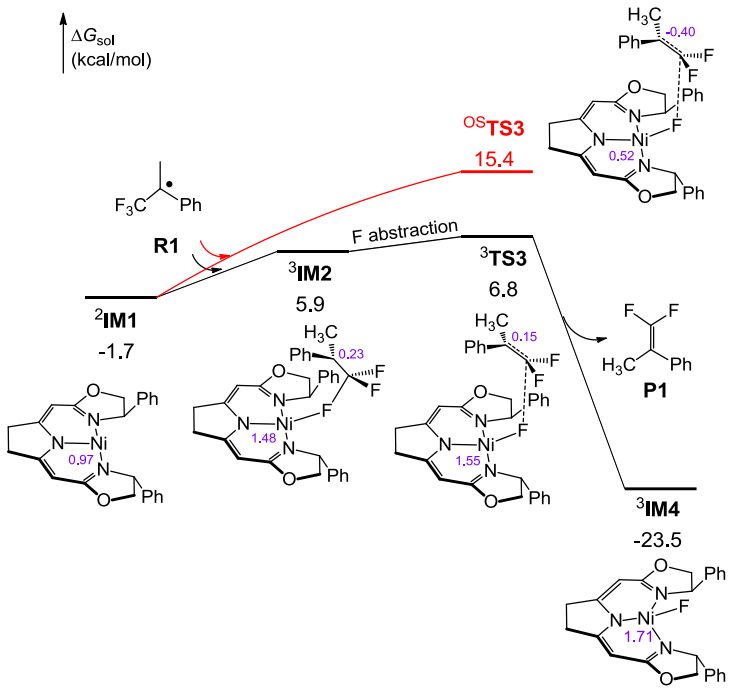

Fig. S2 Free energy profile of F atom abstraction: the open-shell singlet pathway (red) in comparison with the triplet pathway (black). The numbers in purple font on selected atoms in open-shell structures denote positive α-spin and negative β-spin densities (the same below).

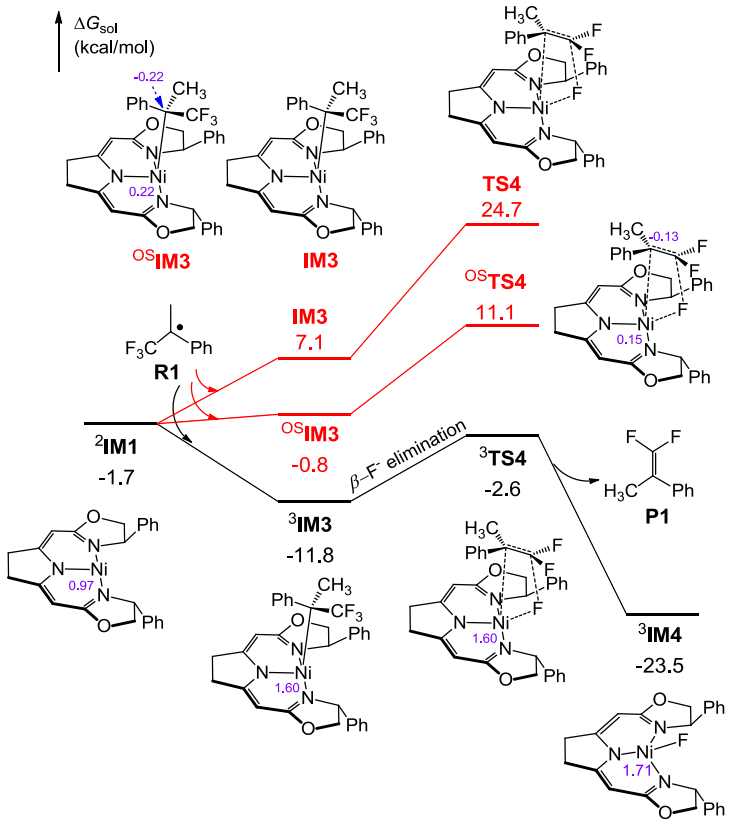

Fig. S3 Free energy profile of radical rebound and *β*-fluoride elimination: the (open-shell) singlet pathways (red) in comparison with the triplet pathway (black).

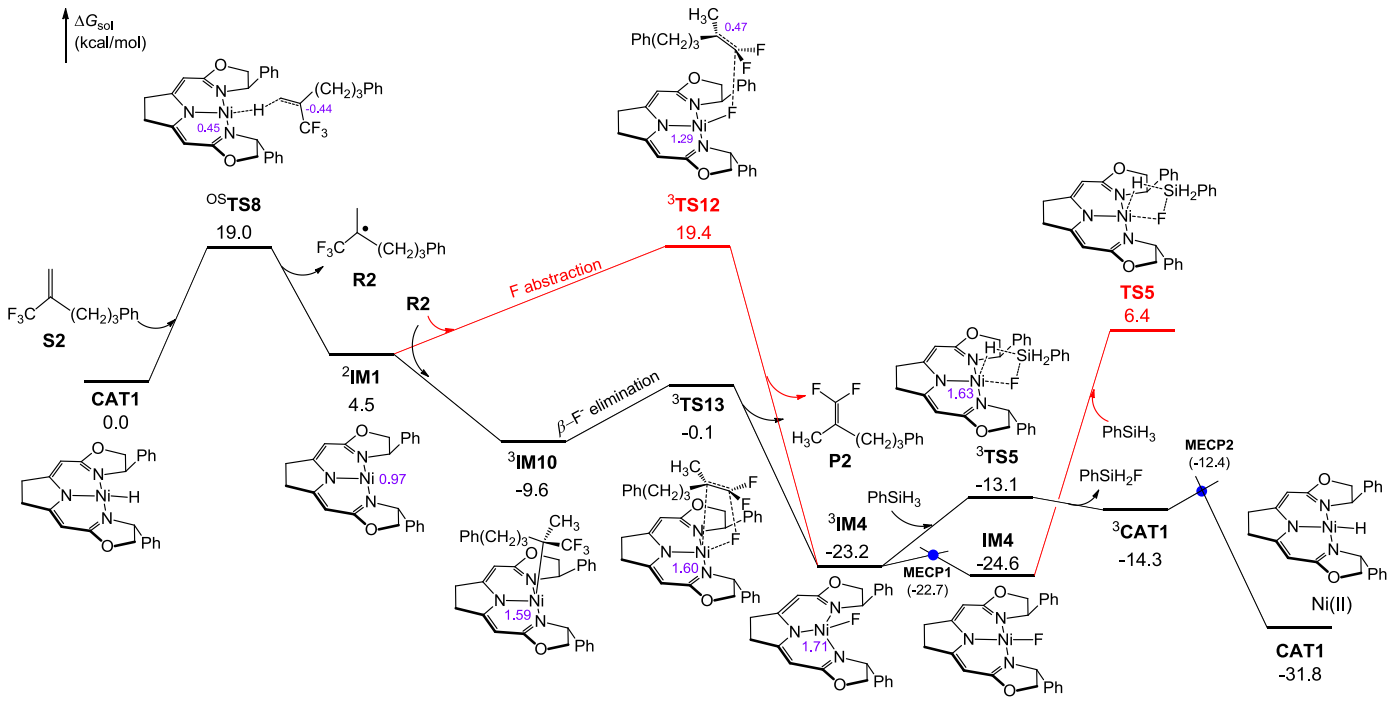

Fig. S4 Free energy profile for the hydrodefluorination of the aliphatic alkene **S2**.

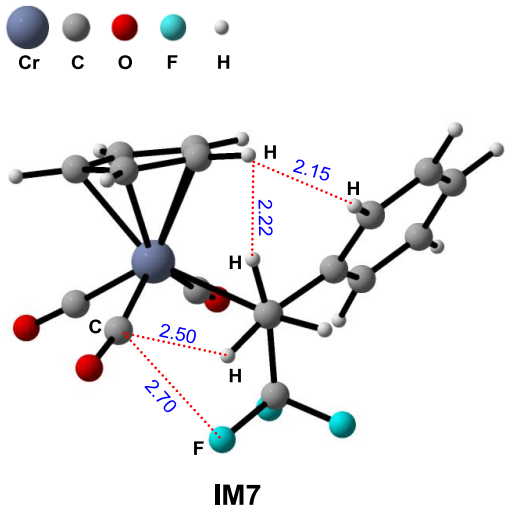

Fig. S5 Optimized geometry of **IM7** showing steric repulsions between non-bonded H···H, H···C, and C···F atoms at a distance less than the sum of the van der Waals radii (H 1.20 Å, C 1.70 Å, and F 1.47 Å).

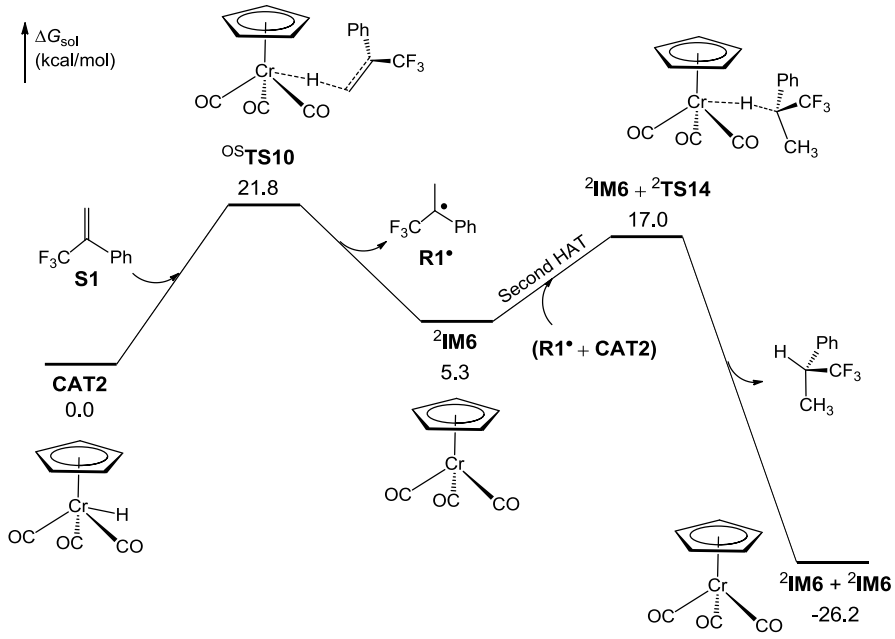

Fig. S6 Free energy profile for the $HCrCp(CO)_3$-mediated hydrogenation of **S1**. The calculations show the second HAT step to be kinetically viable and highly exergonic. Thus, the turnover of ^{2}**IM6** to **CAT2** by $PhSiH_3$ can be difficult and low-efficient (not a focus of this study). Experimentally, treatment of substrate **S1** with 20 mol% $HCrCp(CO)_3$ and $PhSiH_3$ (1 equiv) at 70 °C for 24 h only gave the hydrogenation product in 23% yield (see ref. 5 of main text).

DLPNO-CCSD(T) procedure

DLPNO-CCSD(T) calculations were performed on the key structures with reference to published studies.[1]

Using G09 program

The structures were optimized and characterized by frequency calculations at the B3LYP-D3/6-31G(d,p)−SDD level to give the geometries and free energy corrections (G_{corr}).

Using G09 program

Single-point calculations were then performed on the geometries at the B3LYP-D3/6-311++G(d,p)−SDD level in the gas phase and in benzene solution using the SMD solvation model to obtain solvation energies (E_{solv}) as follows:

$E_{solv} = E$[B3LYP-D3/6-311++G(d,p)−SDD/SMD(benzene)] – E[B3LYP-D3/6-311++G(d,p)−SDD]

Using ORCA 4.2.1 program[2]

Single-point calculations were performed again on the geometries at the DLPNO-CCSD(T)/def2-TZVP[3] level in the gas phase to give the E_{gas} values.

Free energies in solution (G_{sol}) were obtained as follows:

$G_{sol} = E_{gas} + E_{solv} + G_{corr}$

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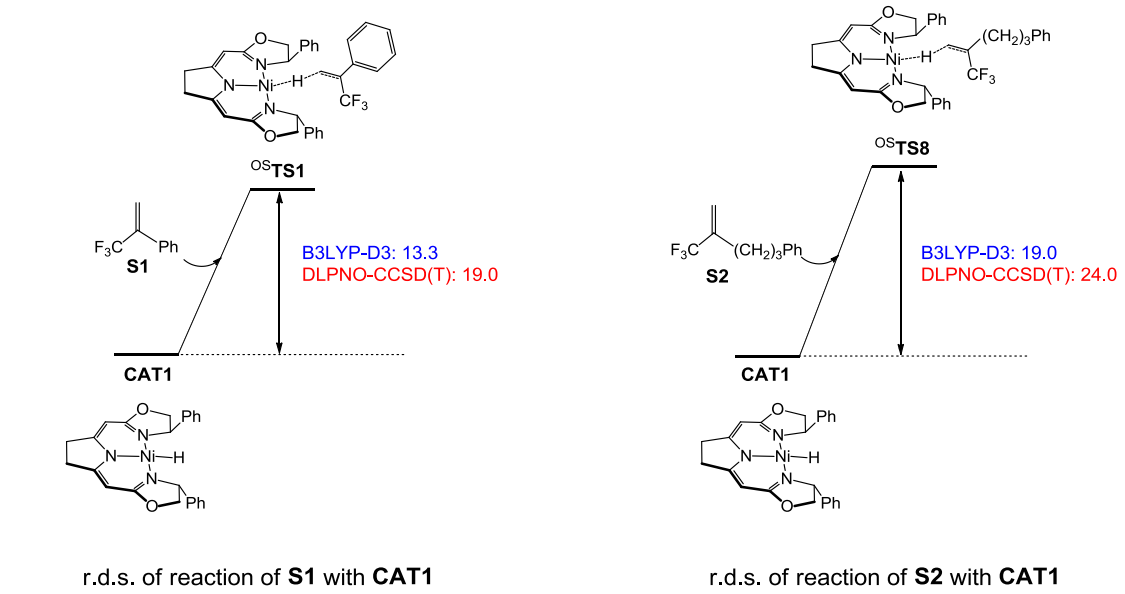

Fig. S7 Results of benchmark DLPNO-CCSD(T) calculations.

Cartesian coordinates (Å), SCF energies, and free energies at 298.15 K and 1 atm for the optimized structures

CAT1

E_{gas} optimization: -1414.19211157 a.u.

E_{sol} single-point: -1414.52716951 a.u.

G_{sol} thermo-corrected: -1414.15917951 a.u.

Ni	0.407688	-0.375557	0.138600
O	-1.046082	-3.831670	-1.466273
O	2.897238	2.547950	1.503199
N	-0.594274	-1.817110	-0.551592
N	2.134517	-1.391095	0.021788
N	1.258710	1.152664	0.827412
C	-2.018460	-1.739337	-0.948260
H	-2.081532	-1.109171	-1.843661
C	-2.337975	-3.212576	-1.292231
H	-2.858504	-3.717312	-0.470105
H	-2.910311	-3.335690	-2.213653
C	-0.127758	-2.988187	-0.921352
C	1.205208	-3.461915	-0.833059
H	1.385566	-4.482101	-1.146694
C	2.246166	-2.685877	-0.387811
C	3.678291	-3.178310	-0.271301
H	4.016221	-3.651759	-1.197515
H	3.745670	-3.934167	0.519387
C	4.459159	-1.899553	0.085801
H	5.110517	-2.015295	0.956776
H	5.088977	-1.558724	-0.743721
C	3.359052	-0.884317	0.344265
C	3.585042	0.381917	0.821980
H	4.591675	0.700504	1.060297
C	2.542631	1.319734	1.034919
C	1.672770	3.252119	1.809951
H	1.762593	4.274630	1.439048
H	1.549598	3.266540	2.898556
C	0.563694	2.430764	1.109480
H	-0.265270	2.227867	1.790370
C	0.016852	3.055397	-0.159987
C	-1.362339	3.133813	-0.373389
H	-2.042423	2.740622	0.377097
C	-1.866099	3.680585	-1.555312
H	-2.940283	3.733519	-1.710362
C	-0.992440	4.151308	-2.536970
H	-1.382796	4.576389	-3.457386
C	0.388065	4.070589	-2.332493
H	1.073570	4.430940	-3.094450
C	0.888224	3.524195	-1.151255
H	1.962360	3.451168	-0.998779
C	-2.926681	-1.158568	0.112530
C	-3.831521	-0.144065	-0.209587
H	-3.859822	0.244409	-1.224494
C	-4.676152	0.391211	0.765921
H	-5.372396	1.182743	0.502731
C	-4.619510	-0.085598	2.076171
H	-5.271934	0.331708	2.837952
C	-3.715117	-1.100277	2.405262
H	-3.660159	-1.470068	3.425377
C	-2.876274	-1.633389	1.428915
H	-2.151455	-2.399780	1.688757
H	-0.836004	0.369190	0.211886

^{3}CAT1

E_{gas} optimization: -1414.15930261 a.u.

E_{sol} single-point: -1414.4937556 a.u.

G_{sol} thermo-corrected: -1414.1314016 a.u.

Ni	0.001513	-0.016151	0.036665
O	-3.413422	-0.983061	-2.273190
O	3.534523	-0.795830	2.235380
N	-1.723203	-0.155390	-1.032160
N	0.112798	-2.147075	-0.047690
N	1.767538	-0.060305	1.043791
C	-2.624360	0.988813	-1.227597
H	-2.045370	1.840835	-1.591274
C	-3.592575	0.453003	-2.315414
H	-4.642814	0.673091	-2.116993
H	-3.323340	0.801646	-3.318995
C	-2.266779	-1.210046	-1.579252
C	-1.813307	-2.554222	-1.503319
H	-2.388354	-3.293725	-2.045969

C	-0.723986	-2.953222	-0.771570
C	-0.281291	-4.405695	-0.704060
H	0.198248	-4.680443	-1.651324
H	-1.124762	-5.085056	-0.557120
C	0.728053	-4.396595	0.452261
H	0.279682	-4.778720	1.377381
H	1.631424	-4.981678	0.262357
C	1.031098	-2.916502	0.617495
C	2.084698	-2.463501	1.368239
H	2.731249	-3.177419	1.862641
C	2.410006	-1.088961	1.524841
C	3.559926	0.646213	2.382473
H	4.585084	0.986894	2.229249
H	3.236278	0.890611	3.400434
C	2.563863	1.153899	1.314418
H	1.900577	1.925322	1.710251
C	3.214701	1.661261	0.039020
C	2.809097	2.870446	-0.532691
H	2.017452	3.442290	-0.058169
C	3.393874	3.326614	-1.716348
H	3.068407	4.267712	-2.150819
C	4.388404	2.573535	-2.342007
H	4.843420	2.927191	-3.262920
C	4.794550	1.359559	-1.780294
H	5.566171	0.766619	-2.263488
C	4.209512	0.906327	-0.598734
H	4.524115	-0.040653	-0.167141
C	-3.329406	1.391882	0.057416
C	-3.639726	2.736194	0.289496
H	-3.322803	3.489385	-0.427919
C	-4.335085	3.118861	1.437179
H	-4.562480	4.167668	1.606633
C	-4.726848	2.157118	2.370760
H	-5.263427	2.453242	3.267643
C	-4.417666	0.813527	2.148331
H	-4.714119	0.059756	2.872577
C	-3.724044	0.433239	0.998611
H	-3.475108	-0.611170	0.836535
H	-0.106894	1.568869	0.139177

S1

E_{gas} optimization: -646.699619916 a.u.

E_{sol} single-point: -646.89970708 a.u.

G_{sol} thermo-corrected: -646.79658408 a.u.

C	0.779305	0.745523	-0.232744
C	1.167475	1.962088	-0.633265
H	0.442578	2.704504	-0.948536
H	2.214003	2.239412	-0.664596
C	-0.638998	0.321291	-0.119696
C	-1.615220	1.250383	0.279486
C	-1.043979	-0.993802	-0.407113
C	-2.956946	0.885241	0.365314
H	-1.313920	2.258199	0.548424
C	-2.386772	-1.357176	-0.316668
H	-0.310437	-1.729457	-0.713801
C	-3.349043	-0.421039	0.065518
H	-3.694301	1.617943	0.680430
H	-2.680919	-2.376728	-0.548494
H	-4.393854	-0.708586	0.137982
C	1.838088	-0.271447	0.133669
F	3.066168	0.273454	0.253926
F	1.550893	-0.885980	1.300701
F	1.935536	-1.246548	-0.810008

P1

E_{gas} optimization: -547.449488446 a.u.

E_{sol} single-point: -547.614574765 a.u.

G_{sol} thermo-corrected: -547.502957765 a.u.

H	-1.251756	2.578212	0.549858
C	-1.023669	0.520674	-0.093058
C	-1.455527	1.952285	-0.326892
H	-0.908338	2.382205	-1.171823
H	-2.523603	2.016804	-0.537098
C	0.422827	0.198862	-0.044499
C	1.347135	1.216606	0.257248
C	0.931592	-1.085519	-0.322279
C	2.717192	0.960176	0.298963
H	0.997034	2.220718	0.470510
C	2.300642	-1.338109	-0.281716
H	0.254571	-1.889294	-0.582043
C	3.203206	-0.319455	0.031547
H	3.404671	1.765775	0.541212
H	2.664001	-2.337466	-0.504462
H	4.270109	-0.520155	0.061217

C	-1.977823	-0.397145	0.089053
F	-3.284557	-0.139734	0.046364
F	-1.793236	-1.689939	0.345016

$PhSiH_3$

E_{gas} optimization: -522.955455382 a.u.

E_{sol} single-point: -523.045361037 a.u.

G_{sol} thermo-corrected: -522.962269037 a.u.

Si	-2.347205	-0.000018	0.005901
H	-2.856233	-1.219024	-0.677747
H	-2.889596	0.007699	1.392903
C	-0.468741	0.000136	-0.011759
C	0.255893	1.205742	-0.009746
C	0.255764	-1.205624	-0.009769
C	1.651685	1.208043	0.003170
H	-0.272379	2.156502	-0.023622
C	1.651493	-1.208128	0.003202
H	-0.272824	-2.156193	-0.023653
C	2.351773	-0.000076	0.010859
H	2.192069	2.150646	0.003197
H	2.191872	-2.150739	0.003293
H	3.438189	-0.000261	0.018139
H	-2.857431	1.211076	-0.690852

$PhSiH_2F$

E_{gas} optimization: -622.258298788 a.u.

E_{sol} single-point: -622.385416049 a.u.

G_{sol} thermo-corrected: -622.306997049 a.u.

F	-2.720489	-0.000027	0.971196
Si	-1.935004	0.000013	-0.446893
H	-2.339098	1.228652	-1.175940
H	-2.339352	-1.228559	-1.175957
C	-0.092108	-0.000099	-0.198129
C	0.624122	-1.207895	-0.105931
C	0.624004	1.207812	-0.105994
C	2.006306	-1.210089	0.083104
H	0.097286	-2.156268	-0.185127
C	2.006143	1.210182	0.083172
H	0.097167	2.156165	-0.185403
C	2.697458	0.000064	0.178693
H	2.544505	-2.151174	0.152378
H	2.544203	2.151325	0.152663
H	3.774205	0.000075	0.323636

^{OS}TS1

E_{gas} optimization: -2060.90130910 a.u.

E_{sol} single-point: -2061.42881847 a.u.

G_{sol} thermo-corrected: -2060.93454147 a.u.

Ni	0.784496	-0.764022	0.017471
O	-2.673062	-2.564404	-1.156043
O	4.661804	-0.375552	1.236831
N	-0.966742	-1.393570	-0.279427
N	1.563254	-2.293270	-0.984426
N	2.483620	-0.210607	0.672890
C	-2.135871	-0.980725	0.515858
H	-2.196919	0.102981	0.530541
C	-3.303019	-1.556524	-0.319742
H	-4.072817	-2.045649	0.278572
H	-3.745877	-0.801243	-0.975370
C	-1.344886	-2.321866	-1.121456
C	-0.508218	-3.118637	-1.949447
H	-0.990893	-3.804300	-2.633391
C	0.854100	-3.109012	-1.827051
C	1.788062	-4.013373	-2.609150
H	1.885493	-3.635143	-3.633879
H	1.411262	-5.037095	-2.673969
C	3.112362	-3.881658	-1.835844
H	3.290165	-4.752304	-1.193519
H	3.991448	-3.764875	-2.474983
C	2.874342	-2.658174	-0.969794
C	3.853562	-2.039357	-0.233590
H	4.863612	-2.427635	-0.235927
C	3.608164	-0.886297	0.547589
C	4.123616	0.648689	2.100665
H	4.842971	1.466170	2.158841
H	3.962431	0.214990	3.095137
C	2.796053	1.028133	1.411277
H	2.011386	1.223629	2.146090
C	2.952523	2.238284	0.500000
C	2.826622	3.522326	1.045076
H	2.586752	3.636224	2.100287
C	2.982144	4.653652	0.244633
H	2.869411	5.642782	0.678969

C	3.267537	4.512550	-1.115620
H	3.379786	5.391515	-1.743437
C	3.400360	3.235913	-1.663999
H	3.618677	3.118436	-2.721661
C	3.245679	2.103891	-0.860809
H	3.326650	1.112893	-1.295127
C	-2.053797	-1.488083	1.944740
C	-2.465290	-0.662396	2.997785
H	-2.815470	0.342313	2.782353
C	-2.417803	-1.121745	4.315987
H	-2.736403	-0.469928	5.124777
C	-1.956728	-2.409457	4.594472
H	-1.916898	-2.765800	5.619989
C	-1.540228	-3.236372	3.547635
H	-1.174627	-4.237865	3.757384
C	-1.586920	-2.777700	2.231399
H	-1.244383	-3.416450	1.422652
H	0.136050	0.642502	0.420938
C	-1.537644	2.169904	-0.307118
C	-0.173826	1.958153	-0.070982
H	0.485953	1.908040	-0.929736
H	0.270115	2.486203	0.763486
C	-2.219781	1.696161	-1.507125
C	-1.549155	0.851458	-2.424242
C	-3.578162	1.989197	-1.777194
C	-2.203437	0.313627	-3.528144
H	-0.517879	0.572015	-2.242916
C	-4.225456	1.448882	-2.885159
H	-4.131185	2.641075	-1.112732
C	-3.549561	0.601091	-3.767392
H	-1.659501	-0.350065	-4.194832
H	-5.270147	1.692410	-3.059530
H	-4.062001	0.173811	-4.624068
C	-2.352066	2.771014	0.788669
F	-1.638480	2.988961	1.919163
F	-2.912554	3.963625	0.443390
F	-3.419362	1.985797	1.170195

TS2

E_{gas} optimization: -2060.89574745 a.u.

E_{sol} single-point: -2061.41887306 a.u.

G_{sol} thermo-corrected: -2060.91898706 a.u.

Ni	0.076725	-0.011998	-0.469120
O	1.544494	3.829579	-0.483036
O	-1.344051	-3.261090	-2.544304
N	0.398559	1.897327	-0.316673
N	1.558448	-0.288649	-1.623121
N	-0.936626	-1.521532	-1.166711
C	-0.483276	2.887680	0.305802
H	-0.488280	2.725959	1.392913
C	0.232885	4.224823	-0.028842
H	-0.270398	4.759624	-0.842018
H	0.346541	4.889501	0.829938
C	1.497832	2.490040	-0.706066
C	2.620431	1.880427	-1.319594
H	3.501509	2.489541	-1.466452
C	2.617156	0.569322	-1.718522
C	3.803704	-0.125654	-2.352481
H	4.562577	-0.280587	-1.577728
H	4.256881	0.479141	-3.142712
C	3.211389	-1.456634	-2.856879
H	3.191577	-1.516987	-3.950175
H	3.756691	-2.332639	-2.493714
C	1.798318	-1.446634	-2.303967
C	0.884294	-2.444837	-2.514631
H	1.151113	-3.305036	-3.114504
C	-0.448749	-2.374782	-2.029389
C	-2.592966	-3.047625	-1.852633
H	-2.751251	-3.877112	-1.156183
H	-3.399010	-3.041538	-2.589000
C	-2.407750	-1.690550	-1.136478
H	-2.841888	-0.882112	-1.740085
C	-2.998600	-1.595538	0.254849
C	-3.665653	-0.424894	0.632257
H	-3.784507	0.378819	-0.086655
C	-4.155838	-0.270601	1.930107
H	-4.660811	0.651137	2.203911
C	-3.991463	-1.293926	2.865260
H	-4.372155	-1.178548	3.876106
C	-3.329295	-2.468049	2.495504
H	-3.185767	-3.264194	3.220210
C	-2.831053	-2.614750	1.200661
H	-2.272908	-3.508527	0.943859
C	-1.914385	2.826572	-0.188033
C	-2.965788	3.191342	0.658771

H	-2.752673	3.475413	1.686783
C	-4.285041	3.185196	0.199139
H	-5.092021	3.471188	0.867729
C	-4.564861	2.803876	-1.114719
H	-5.590233	2.791207	-1.472438
C	-3.519113	2.427236	-1.963405
H	-3.730469	2.119492	-2.983648
C	-2.201907	2.438969	-1.503289
H	-1.387624	2.122176	-2.147391
H	-0.873692	0.063741	0.797778
C	1.120574	-0.781321	1.642303
C	-0.222108	-0.289334	1.817223
H	-0.314585	0.645849	2.366308
H	-0.944867	-1.023064	2.161453
C	2.317030	0.047311	1.763027
C	2.249536	1.400364	2.172897
C	3.607685	-0.445542	1.441868
C	3.375570	2.215278	2.214638
H	1.295431	1.829237	2.457791
C	4.732851	0.371542	1.494485
H	3.727765	-1.476281	1.135711
C	4.631992	1.714576	1.865908
H	3.268688	3.252823	2.520646
H	5.702267	-0.048767	1.237075
H	5.510981	2.351339	1.895443
C	1.298960	-2.257892	1.544457
F	0.120151	-2.934473	1.545877
F	1.957406	-2.679044	0.414123
F	2.034938	-2.770787	2.574147

[2]**IM1**

E_{gas} optimization: -1413.60705135 a.u.

E_{sol} single-point: -1413.94107816 a.u.

G_{sol} thermo-corrected: -1413.58214716 a.u.

Ni	-0.734310	0.039795	0.006473
O	-0.863901	4.060623	-0.678019
O	-1.645631	-3.874091	0.718520
N	-0.390417	1.873159	-0.369623
N	-2.706525	0.231349	0.001807
N	-0.770709	-1.816898	0.403810
C	0.905300	2.510994	-0.656475
H	1.165777	2.308234	-1.705412
C	0.563027	4.006644	-0.478380
H	0.793465	4.347695	0.539321
H	1.044144	4.665034	-1.203906
C	-1.328463	2.791136	-0.458345
C	-2.735064	2.624937	-0.369689
H	-3.333283	3.522498	-0.465970
C	-3.356726	1.411911	-0.163344
C	-4.862560	1.220247	-0.057940
H	-5.382568	1.652866	-0.917917
H	-5.244010	1.727970	0.835236
C	-5.015675	-0.314125	0.038992
H	-5.621091	-0.634715	0.892102
H	-5.479055	-0.737524	-0.859378
C	-3.578468	-0.798811	0.162065
C	-3.210641	-2.108826	0.380695
H	-3.974008	-2.871265	0.473815
C	-1.862671	-2.542258	0.487874
C	-0.228699	-4.092014	0.550091
H	-0.051410	-4.514672	-0.446830
H	0.107632	-4.799999	1.309781
C	0.387860	-2.682693	0.689323
H	0.701401	-2.508952	1.728158
C	1.558014	-2.382325	-0.221968
C	2.809587	-2.057070	0.307373
H	2.944483	-2.024374	1.385105
C	3.877510	-1.740825	-0.535321
H	4.838419	-1.473335	-0.107451
C	3.700369	-1.744362	-1.918610
H	4.528574	-1.493629	-2.575441
C	2.448609	-2.058469	-2.456809
H	2.300628	-2.050773	-3.533082
C	1.384080	-2.371367	-1.613567
H	0.402734	-2.583646	-2.028078
C	2.039800	2.023454	0.219281
C	3.343024	1.970270	-0.286488
H	3.526704	2.242247	-1.323196
C	4.404070	1.559058	0.521642
H	5.410245	1.522225	0.113640
C	4.169926	1.182545	1.845429
H	4.993552	0.854952	2.473626
C	2.869823	1.221695	2.355017
H	2.677650	0.922930	3.381842
C	1.811833	1.644512	1.549292

H	0.797311	1.660909	1.935994

R1$^{\bullet}$

E_{gas} optimization: -647.287856282 a.u.

E_{sol} single-point: -647.487625008 a.u.

G_{sol} thermo-corrected: -647.376272008 a.u.

H	-0.734740	2.681578	0.881186
C	-0.738210	0.712416	0.000194
C	-1.131948	2.160711	0.000071
H	-0.735010	2.681382	-0.881264
H	-2.214175	2.280640	0.000295
C	0.630161	0.297592	0.000140
C	1.673510	1.267289	0.000019
C	1.021754	-1.073810	0.000160
C	3.009545	0.891608	-0.000093
H	1.426227	2.322729	-0.000006
C	2.360659	-1.435439	0.000049
H	0.267695	-1.849482	0.000268
C	3.366828	-0.461461	-0.000083
H	3.780381	1.657022	-0.000210
H	2.626807	-2.488548	0.000045
H	4.412773	-0.752842	-0.000165
C	-1.821484	-0.327817	-0.000040
F	-3.061518	0.208204	-0.000054
F	-1.749978	-1.143910	-1.086552
F	-1.750155	-1.144185	1.086311

^{3}**IM2**

E_{gas} optimization: -2060.92111189 a.u.

E_{sol} single-point: -2061.44195974 a.u.

G_{sol} thermo-corrected: -2060.94635174 a.u.

Ni	0.589347	0.439836	-0.070133
O	4.500024	-0.003664	-1.468502
O	-1.462083	0.956213	3.486573
N	2.342716	-0.157799	-0.837477
N	1.474053	2.115869	0.657483
N	-0.735016	0.412738	1.421852
C	2.730729	-1.550904	-1.145404
H	2.020512	-1.967628	-1.858172
C	4.122576	-1.362089	-1.798231
H	4.886830	-2.033595	-1.402307
H	4.082711	-1.451029	-2.888843
C	3.390259	0.609655	-0.977699
C	3.520822	1.989015	-0.637805
H	4.433361	2.482829	-0.946175
C	2.622740	2.652760	0.160527
C	2.794291	4.086201	0.632461
H	2.610298	4.767352	-0.206283
H	3.809213	4.279320	0.990140
C	1.716975	4.223198	1.727542
H	2.153477	4.307579	2.728407
H	1.063916	5.089229	1.586055
C	0.932180	2.927011	1.604093
C	-0.114585	2.581588	2.422039
H	-0.395281	3.236204	3.237408
C	-0.751442	1.310584	2.381682
C	-1.698861	-0.464403	3.361099
H	-2.671916	-0.693585	3.795686
H	-0.905414	-0.994720	3.902823
C	-1.617741	-0.698153	1.835375
H	-1.142572	-1.651953	1.596665
C	-3.013384	-0.647681	1.232360
C	-3.758718	-1.831293	1.154854
H	-3.278925	-2.781733	1.377853
C	-5.110167	-1.800967	0.809512
H	-5.674870	-2.727213	0.753567
C	-5.731926	-0.581124	0.530105
H	-6.784047	-0.553204	0.262029
C	-4.985474	0.597960	0.573751
H	-5.453883	1.548238	0.333307
C	-3.633742	0.566365	0.922744
H	-3.055321	1.483032	0.935100
C	2.716107	-2.388443	0.121261
C	1.821210	-3.453934	0.260298
H	1.140033	-3.689270	-0.551260
C	1.776518	-4.189604	1.447425
H	1.076222	-5.014692	1.543710
C	2.625869	-3.864725	2.506118
H	2.591236	-4.436351	3.429250
C	3.522268	-2.799484	2.374318
H	4.185295	-2.540509	3.195016
C	3.564051	-2.065650	1.190001
H	4.252748	-1.229936	1.093265
H	-4.048049	-0.951172	-1.542031

C	-1.996369	-0.698758	-2.241827
C	-3.431912	-1.123788	-2.429661
H	-3.895051	-0.574207	-3.258733
H	-3.500036	-2.186766	-2.667227
C	-1.616294	0.647359	-2.124266
C	-2.607308	1.684408	-1.997668
C	-0.233765	1.090593	-2.102237
C	-2.259719	3.008606	-1.875164
H	-3.654730	1.408008	-1.981186
C	0.074054	2.475827	-2.060832
H	0.512710	0.436278	-2.535621
C	-0.904790	3.431932	-1.902466
H	-3.046554	3.752297	-1.767464
H	1.119034	2.761324	-2.138686
H	-0.655696	4.486332	-1.833271
C	-0.990790	-1.727588	-2.049173
F	0.057930	-1.761340	-2.944911
F	-0.268947	-1.573055	-0.794334
F	-1.455065	-2.987690	-1.981606

^{3}TS3

E_{gas} optimization: -2060.92069232 a.u.

E_{sol} single-point: -2061.44170434 a.u.

G_{sol} thermo-corrected: -2060.94498634 a.u.

Ni	0.556681	0.391390	-0.076443
O	4.470057	0.116838	-1.522219
O	-1.420153	0.631433	3.559289
N	2.318321	-0.108297	-0.897336
N	1.428263	2.037217	0.751694
N	-0.725136	0.251146	1.448623
C	2.743980	-1.483317	-1.239642
H	2.033181	-1.908356	-1.945655
C	4.113887	-1.232933	-1.912414
H	4.902986	-1.905050	-1.570500
H	4.047828	-1.266200	-3.004921
C	3.349075	0.685303	-1.004304
C	3.448439	2.048351	-0.594828
H	4.340291	2.585571	-0.890861
C	2.550982	2.635689	0.260949
C	2.692744	4.043039	0.812969
H	2.441485	4.764206	0.026486
H	3.715180	4.256593	1.135321
C	1.662254	4.070542	1.959218
H	2.142171	4.082118	2.943721
H	0.988670	4.931196	1.917562
C	0.897613	2.771005	1.766004
C	-0.119505	2.351620	2.586646
H	-0.389140	2.944241	3.451585
C	-0.736905	1.076398	2.471435
C	-1.644521	-0.779549	3.331339
H	-2.607319	-1.051240	3.764263
H	-0.835899	-1.338715	3.818699
C	-1.587298	-0.898341	1.791561
H	-1.104881	-1.824135	1.472088
C	-2.991249	-0.816641	1.212620
C	-3.730075	-1.997281	1.062012
H	-3.242894	-2.957191	1.218426
C	-5.083294	-1.953009	0.725683
H	-5.642516	-2.877159	0.610918
C	-5.714071	-0.721439	0.530437
H	-6.767555	-0.682900	0.269111
C	-4.975303	0.456998	0.649950
H	-5.450789	1.418077	0.475399
C	-3.621136	0.411076	0.987974
H	-3.048724	1.329014	1.056486
C	2.774489	-2.334811	0.017711
C	1.829899	-3.348896	0.207670
H	1.088718	-3.536889	-0.562006
C	1.813605	-4.086048	1.394464
H	1.075592	-4.871896	1.530181
C	2.740614	-3.814496	2.402035
H	2.728602	-4.388069	3.324546
C	3.686186	-2.800743	2.219292
H	4.409670	-2.583272	2.999989
C	3.700066	-2.064771	1.035365
H	4.427198	-1.267521	0.901297
H	-3.976999	-0.904639	-1.541257
C	-1.984058	-0.538720	-2.361481
C	-3.415450	-1.007166	-2.474235
H	-3.950889	-0.433304	-3.241255
H	-3.462192	-2.057369	-2.767467
C	-1.653784	0.815699	-2.123028
C	-2.681653	1.785424	-1.870024
C	-0.297106	1.314528	-2.073876
C	-2.388332	3.105177	-1.604502

H	-3.716565	1.465756	-1.871465
C	-0.041490	2.691352	-1.867675
H	0.486350	0.731224	-2.539954
C	-1.056889	3.585313	-1.594835
H	-3.205212	3.796291	-1.407261
H	0.990196	3.025951	-1.921735
H	-0.848816	4.634503	-1.409270
C	-0.956016	-1.518980	-2.262461
F	0.155463	-1.402645	-3.055090
F	-0.236494	-1.462410	-0.877718
F	-1.325451	-2.803681	-2.308488

^{OS}TS3

E_{gas} optimization: -2060.90564052 a.u.

E_{sol} single-point: -2061.42697008 a.u.

G_{sol} thermo-corrected: -2060.93135508 a.u.

Ni	0.674718	0.243608	0.236158
O	4.258046	0.896300	-1.715985
O	-1.381757	-0.123689	3.763776
N	2.257743	0.224096	-0.921331
N	1.209374	1.946020	1.070038
N	-0.579030	-0.199585	1.657454
C	2.842892	-0.998596	-1.512428
H	2.136503	-1.416506	-2.227363
C	4.090230	-0.442994	-2.240428
H	5.004865	-1.005481	-2.041931
H	3.933764	-0.369638	-3.321541
C	3.128797	1.191306	-1.016623
C	3.036312	2.491387	-0.440918
H	3.775453	3.221387	-0.744738
C	2.136324	2.801662	0.547053
C	2.056615	4.153196	1.233431
H	1.544905	4.861938	0.571096
H	3.045015	4.565454	1.451910
C	1.213652	3.851471	2.487178
H	1.831225	3.815852	3.391955
H	0.417409	4.579130	2.666273
C	0.650286	2.470600	2.195260
C	-0.229520	1.813538	3.019308
H	-0.536023	2.269910	3.951823
C	-0.703200	0.500561	2.760824
C	-1.490302	-1.507278	3.360511
H	-2.445869	-1.896737	3.712732
H	-0.661816	-2.066181	3.813921
C	-1.364379	-1.435436	1.820495
H	-0.805444	-2.285290	1.421416
C	-2.746049	-1.372331	1.184530
C	-3.420795	-2.568796	0.907132
H	-2.896774	-3.516138	1.015097
C	-4.759671	-2.558590	0.515382
H	-5.269600	-3.494812	0.306519
C	-5.441164	-1.344614	0.391858
H	-6.485112	-1.332290	0.092212
C	-4.763410	-0.147764	0.631866
H	-5.274262	0.802784	0.509813
C	-3.422218	-0.159625	1.020402
H	-2.897648	0.775178	1.182811
C	3.094757	-2.018568	-0.418001
C	2.231698	-3.110983	-0.277889
H	1.415280	-3.235870	-0.983199
C	2.394651	-4.010198	0.778425
H	1.719829	-4.856245	0.876140
C	3.422139	-3.822965	1.704870
H	3.551382	-4.522477	2.525887
C	4.284766	-2.730607	1.572985
H	5.083244	-2.577553	2.293541
C	4.118698	-1.832338	0.519493
H	4.777564	-0.971776	0.431798
H	-3.872818	-1.155569	-1.735772
C	-2.004952	-0.305055	-2.455179
C	-3.315469	-1.015697	-2.668033
H	-3.957959	-0.443950	-3.348443
H	-3.163367	-2.000766	-3.110889
C	-1.949111	1.072377	-2.057701
C	-3.153018	1.780590	-1.769663
C	-0.733946	1.803593	-1.894075
C	-3.138523	3.094137	-1.327855
H	-4.104445	1.272296	-1.867642
C	-0.736438	3.126262	-1.454657
H	0.211686	1.356155	-2.162664
C	-1.928502	3.784124	-1.157470
H	-4.080223	3.591631	-1.109186
H	0.216442	3.637514	-1.352313
H	-1.924401	4.814587	-0.814592
C	-0.812187	-1.098505	-2.443065

F	0.270204	-0.627062	-3.117756
F	-0.213772	-1.195433	-1.020494
F	-0.938835	-2.392542	-2.765599

^{3}IM3

E_{gas} optimization: -2060.95336121 a.u.

E_{sol} single-point: -2061.47452325 a.u.

G_{sol} thermo-corrected: -2060.97456725 a.u.

Ni	-0.187169	0.031583	0.331622
O	-0.487789	4.177432	0.456926
O	-0.148388	-3.497864	2.584121
N	0.121662	2.010615	0.372199
N	-1.850785	0.239831	1.438881
N	0.255706	-1.715977	1.261413
C	1.295166	2.738605	-0.130298
H	1.360801	2.579606	-1.210319
C	0.929452	4.212199	0.181750
H	1.446231	4.582906	1.074511
H	1.104850	4.893601	-0.652729
C	-0.825953	2.874237	0.640124
C	-2.147674	2.619545	1.099275
H	-2.799696	3.477672	1.198282
C	-2.596211	1.377760	1.475103
C	-3.985069	1.100179	2.019195
H	-4.727848	1.326755	1.248928
H	-4.199943	1.728829	2.888907
C	-3.941058	-0.403948	2.356558
H	-4.169107	-0.620641	3.404425
H	-4.633989	-0.978973	1.734835
C	-2.519140	-0.798989	2.006386
C	-1.974440	-2.034505	2.259865
H	-2.566404	-2.786792	2.765125
C	-0.618557	-2.367060	1.990417
C	1.190682	-3.715777	2.091451
H	1.159261	-4.557367	1.393525
H	1.830715	-3.978610	2.935680
C	1.574279	-2.377169	1.428809
H	2.153901	-1.769686	2.138653
C	2.361442	-2.429372	0.131604
C	3.036442	-1.265110	-0.257528
H	3.032819	-0.401687	0.398974
C	3.700347	-1.196536	-1.481117
H	4.197793	-0.275071	-1.765128
C	3.719880	-2.306301	-2.327309
H	4.236598	-2.258940	-3.281349
C	3.068364	-3.478384	-1.939848
H	3.076280	-4.346828	-2.592135
C	2.387568	-3.536875	-0.722366
H	1.862475	-4.450302	-0.463649
C	2.585714	2.276040	0.511495
C	3.771190	2.246847	-0.230944
H	3.753033	2.541626	-1.277216
C	4.965380	1.819525	0.353607
H	5.876797	1.793236	-0.236681
C	4.984033	1.410020	1.688412
H	5.909502	1.065079	2.139898
C	3.804372	1.438119	2.437387
H	3.810699	1.117370	3.475360
C	2.613224	1.871322	1.853179
H	1.689201	1.873091	2.423776
H	-0.343764	-2.500966	-1.199674
C	-0.844515	-0.414854	-1.614629
C	-0.234009	-1.773786	-2.004311
H	-0.701850	-2.186280	-2.908945
H	0.835329	-1.676249	-2.187196
C	-2.344150	-0.443088	-1.527704
C	-3.000009	-1.647593	-1.189131
C	-3.172361	0.689779	-1.695945
C	-4.381903	-1.717352	-1.017013
H	-2.419488	-2.548782	-1.036311
C	-4.555102	0.617789	-1.533476
H	-2.735167	1.644659	-1.947986
C	-5.178113	-0.583558	-1.186972
H	-4.836339	-2.669483	-0.753611
H	-5.150259	1.515720	-1.682108
H	-6.256197	-0.636399	-1.064001
C	-0.285321	0.601763	-2.568593
F	-0.584678	0.358292	-3.877023
F	-0.667038	1.897571	-2.351240
F	1.089954	0.635239	-2.512593

^{OS}IM3

E_{gas} optimization: -2060.93796687 a.u.

E_{sol} single-point: -2061.4583366 a.u.

G_{sol} thermo-corrected: -2060.9569516 a.u.

Ni	-0.228190	-0.002384	-0.277197
O	-0.191790	-4.114946	0.075589
O	-0.577355	3.394152	-2.644310
N	0.147006	-1.890505	0.020955
N	-1.853208	-0.487269	-1.437979
N	0.003370	1.686000	-1.290630
C	1.415172	-2.437345	0.519718
H	1.679754	-1.938053	1.451889
C	1.048396	-3.918503	0.791214
H	1.781877	-4.631934	0.411080
H	0.863265	-4.100901	1.854743
C	-0.664054	-2.884236	-0.250065
C	-1.952593	-2.831126	-0.845219
H	-2.514139	-3.755917	-0.873804
C	-2.486276	-1.688964	-1.390623
C	-3.868053	-1.608720	-2.014637
H	-4.624016	-1.903854	-1.281267
H	-3.950028	-2.289731	-2.868081
C	-3.986269	-0.125775	-2.418357
H	-4.222616	0.021483	-3.476316
H	-4.746928	0.395602	-1.828897
C	-2.621956	0.438101	-2.067920
C	-2.223382	1.723390	-2.347804
H	-2.889543	2.390218	-2.879961
C	-0.929400	2.219493	-2.046129
C	0.683274	3.786271	-2.058775
H	0.474975	4.499914	-1.252857
H	1.289506	4.265632	-2.828474
C	1.251597	2.462234	-1.541324
H	1.771704	1.955232	-2.369501
C	2.205941	2.499453	-0.368155
C	2.831984	1.298456	-0.007718
H	2.647619	0.402983	-0.593148
C	3.677703	1.236909	1.096695
H	4.134099	0.289774	1.365116
C	3.932925	2.387689	1.845505
H	4.591351	2.344643	2.708138
C	3.341552	3.595781	1.474617
H	3.541375	4.498127	2.045306
C	2.481095	3.651021	0.375247
H	2.021111	4.599729	0.118912
C	2.553388	-2.239813	-0.469372
C	3.874699	-2.241807	-0.003981
H	4.067287	-2.386077	1.057010
C	4.940048	-2.040629	-0.882159
H	5.958471	-2.034165	-0.504330
C	4.695099	-1.831645	-2.241567
H	5.522163	-1.664149	-2.925247
C	3.381399	-1.833352	-2.714394
H	3.182537	-1.670100	-3.769925
C	2.316362	-2.038563	-1.834428
H	1.293586	-2.013285	-2.196964
H	-0.400815	2.710890	0.996999
C	-0.704173	0.652142	1.649543
C	-0.216304	2.091775	1.873539
H	-0.716541	2.552226	2.736229
H	0.857622	2.109205	2.051175
C	-2.197483	0.527063	1.534152
C	-2.966256	1.636510	1.117265
C	-2.902696	-0.681383	1.741250
C	-4.340982	1.545124	0.905926
H	-2.481494	2.586978	0.934176
C	-4.277551	-0.769575	1.537840
H	-2.368524	-1.569328	2.044154
C	-5.013247	0.339831	1.113320
H	-4.887641	2.426350	0.579755
H	-4.776497	-1.719775	1.711417
H	-6.086119	0.268224	0.957909
C	-0.084806	-0.178574	2.745935
F	-0.450090	0.239798	3.991733
F	-0.358500	-1.516600	2.727648
F	1.283921	-0.102289	2.722263

IM3

E_{gas} optimization: -2060.92893421 a.u.

E_{sol} single-point: -2061.44841889 a.u.

G_{sol} thermo-corrected: -2060.94439589 a.u.

Ni	-0.330722	0.019798	0.239294
O	-0.354693	4.073750	-0.346139
O	-0.606036	-3.219786	2.781356
N	-0.038762	1.849901	-0.216619
N	-1.931088	0.570121	1.454559
N	-0.095449	-1.616846	1.277490
C	1.257208	2.390441	-0.660452

H	1.619914	1.825327	-1.515623
C	0.864025	3.821247	-1.083667
H	1.593901	4.585112	-0.812030
H	0.637582	3.873421	-2.154079
C	-0.837594	2.863544	0.034866
C	-2.107915	2.848329	0.664319
H	-2.682897	3.764677	0.635867
C	-2.598854	1.744179	1.318737
C	-3.966394	1.675677	1.974409
H	-4.744277	2.028801	1.291965
H	-3.991832	2.317632	2.862243
C	-4.102295	0.182391	2.329428
H	-4.426705	-0.002566	3.357196
H	-4.804353	-0.324900	1.658629
C	-2.711224	-0.361178	2.063199
C	-2.309986	-1.639557	2.364300
H	-2.975483	-2.305422	2.898333
C	-1.004785	-2.117524	2.085236
C	0.684669	-3.588242	2.250668
H	0.532504	-4.361425	1.487863
H	1.294740	-3.983986	3.063535
C	1.196523	-2.276254	1.657962
H	1.613136	-1.665797	2.474788
C	2.256860	-2.354832	0.584179
C	2.863010	-1.158773	0.179798
H	2.564597	-0.227970	0.648540
C	3.824006	-1.149931	-0.827293
H	4.263128	-0.206371	-1.135239
C	4.215345	-2.347551	-1.429970
H	4.964425	-2.345653	-2.216505
C	3.644103	-3.549218	-1.009249
H	3.950093	-4.487022	-1.463990
C	2.669786	-3.552748	-0.008155
H	2.230193	-4.499382	0.288819
C	2.313819	2.334216	0.434155
C	3.665957	2.412009	0.074973
H	3.935055	2.512891	-0.974391
C	4.666727	2.339588	1.044035
H	5.710724	2.390127	0.748167
C	4.325752	2.185755	2.390165
H	5.103241	2.118424	3.145487
C	2.980876	2.112772	2.756949
H	2.707186	1.991072	3.801282
C	1.979789	2.188930	1.785687
H	0.936025	2.101885	2.069860
H	-0.097070	-2.802890	-0.900872
C	-0.450927	-0.795098	-1.666811
C	0.108609	-2.218460	-1.794882
H	-0.330184	-2.734708	-2.658513
H	1.188647	-2.194951	-1.923925
C	-1.963461	-0.742537	-1.621910
C	-2.699942	-1.878668	-1.220225
C	-2.705918	0.438164	-1.859227
C	-4.082817	-1.837076	-1.050807
H	-2.184462	-2.808075	-1.015002
C	-4.087889	0.476542	-1.697188
H	-2.191526	1.343699	-2.142846
C	-4.791768	-0.658311	-1.286268
H	-4.606385	-2.734859	-0.732779
H	-4.616143	1.407391	-1.886418
H	-5.870498	-0.626013	-1.160563
C	0.157265	-0.017687	-2.814726
F	-0.145378	-0.573485	-4.022143
F	-0.204185	1.292434	-2.930781
F	1.523392	-0.005348	-2.747434

^{3}TS4

E_{gas} optimization: -2060.93878830 a.u.

E_{sol} single-point: -2061.45867612 a.u.

G_{sol} thermo-corrected: -2060.95995312 a.u.

Ni	-0.060126	0.037680	0.344002
O	-3.775675	1.826189	-0.318057
O	2.835770	-1.194700	3.109547
N	-1.631809	1.172020	-0.146425
N	-1.203561	-0.964268	1.712416
N	1.607351	-0.344066	1.421170
C	-1.567284	2.383639	-0.984672
H	-1.027620	2.138474	-1.901171
C	-3.064037	2.655335	-1.269162
H	-3.364226	3.693120	-1.113264
H	-3.353493	2.338207	-2.276121
C	-2.870091	0.957900	0.204088
C	-3.369687	-0.074727	1.047211
H	-4.445404	-0.163356	1.120408
C	-2.571453	-0.964326	1.715442

C	-3.104446	-2.096541	2.573475
H	-3.565703	-2.841700	1.916870
H	-3.872109	-1.750899	3.271149
C	-1.841125	-2.638740	3.271073
H	-1.848183	-2.456794	4.350910
H	-1.698602	-3.714230	3.127928
C	-0.715931	-1.855073	2.613232
C	0.610189	-1.989516	2.957467
H	0.885696	-2.668965	3.754063
C	1.645784	-1.159723	2.446646
C	3.607129	-0.073294	2.619320
H	4.649064	-0.383600	2.532490
H	3.521284	0.742744	3.346155
C	2.944321	0.278646	1.266485
H	2.816617	1.358907	1.156999
C	3.705959	-0.253186	0.066218
C	4.002042	0.581386	-1.013100
H	3.649621	1.608200	-1.003646
C	4.712685	0.095557	-2.111542
H	4.927826	0.753261	-2.948777
C	5.131725	-1.234658	-2.140938
H	5.679818	-1.615589	-2.997864
C	4.840623	-2.077170	-1.064429
H	5.162272	-3.114635	-1.081127
C	4.134552	-1.587605	0.033427
H	3.905551	-2.245046	0.868281
C	-0.815618	3.476431	-0.244590
C	0.515096	3.754261	-0.576732
H	0.984546	3.195884	-1.380038
C	1.240753	4.703032	0.147597
H	2.272878	4.912159	-0.120630
C	0.643018	5.381156	1.211533
H	1.205809	6.121336	1.773279
C	-0.683368	5.101812	1.553349
H	-1.152867	5.621728	2.383741
C	-1.405931	4.151997	0.831683
H	-2.430929	3.924242	1.114351
H	0.525258	-2.877094	0.161836
C	-0.115529	-1.522007	-1.417248
C	0.790334	-2.619206	-0.867421
H	0.727503	-3.534753	-1.471939
H	1.827929	-2.294182	-0.852479
C	-1.561920	-1.822503	-1.550610
C	-2.074066	-2.985403	-0.930895
C	-2.503350	-1.013490	-2.229143
C	-3.428863	-3.312355	-0.976887
H	-1.405508	-3.647426	-0.394588
C	-3.855465	-1.341810	-2.270724
H	-2.182331	-0.105095	-2.716646
C	-4.338211	-2.491930	-1.643132
H	-3.770460	-4.222104	-0.488428
H	-4.540753	-0.681952	-2.796723
H	-5.394167	-2.742833	-1.677828
C	0.548421	-0.577266	-2.243985
F	1.774440	-0.850061	-2.679538
F	-0.106828	0.095400	-3.192871
F	0.998170	0.811937	-1.313092

^{OS}**TS4**

E_{gas} optimization: -2060.91854935 a.u.

E_{sol} single-point: -2061.43815726 a.u.

G_{sol} thermo-corrected: -2060.93831426 a.u.

Ni	-0.095950	0.045763	0.416293
O	-3.659753	1.975894	-0.349237
O	2.732402	-1.343307	3.089222
N	-1.564830	1.192080	-0.141342
N	-1.277361	-0.926696	1.713381
N	1.525174	-0.454794	1.407200
C	-1.408434	2.403571	-0.970438
H	-0.870939	2.133625	-1.879977
C	-2.880619	2.766381	-1.280037
H	-3.119278	3.819362	-1.119774
H	-3.168952	2.473761	-2.294395
C	-2.821452	1.052086	0.184178
C	-3.391783	0.049793	1.015257
H	-4.471471	0.008519	1.063090
C	-2.643787	-0.874311	1.693093
C	-3.233737	-1.994932	2.526603
H	-3.714536	-2.710738	1.851654
H	-3.997239	-1.628084	3.217925
C	-2.003898	-2.598262	3.233649
H	-2.016334	-2.425654	4.315032
H	-1.906313	-3.677398	3.081711
C	-0.838248	-1.858015	2.598754
C	0.478219	-2.062826	2.941440

H	0.724341	-2.764946	3.727604
C	1.542939	-1.273043	2.431289
C	3.524377	-0.230242	2.612213
H	4.561328	-0.556706	2.527659
H	3.446970	0.581012	3.345402
C	2.876187	0.143384	1.257664
H	2.767419	1.226344	1.156602
C	3.646074	-0.390727	0.064401
C	4.018475	0.460513	-0.977599
H	3.711629	1.501770	-0.949277
C	4.748404	-0.024420	-2.063519
H	5.022290	0.646372	-2.872738
C	5.112009	-1.370125	-2.116548
H	5.674346	-1.750579	-2.964365
C	4.747706	-2.228388	-1.075481
H	5.026920	-3.277565	-1.110459
C	4.022469	-1.739741	0.010120
H	3.738100	-2.408523	0.818371
C	-0.608886	3.446580	-0.209613
C	0.726371	3.690357	-0.548915
H	1.168835	3.143406	-1.374979
C	1.491191	4.592805	0.194384
H	2.526769	4.775690	-0.079527
C	0.927457	5.258341	1.284388
H	1.520685	5.962069	1.861400
C	-0.404663	5.014622	1.631899
H	-0.848204	5.526333	2.481393
C	-1.165914	4.111207	0.891060
H	-2.196113	3.910759	1.175571
H	0.405987	-2.879886	0.118513
C	-0.168361	-1.479301	-1.448523
C	0.676578	-2.627393	-0.911607
H	0.559116	-3.535944	-1.519587
H	1.731297	-2.363842	-0.902757
C	-1.615908	-1.708249	-1.604115
C	-2.195087	-2.846439	-0.989962
C	-2.515029	-0.859495	-2.297714
C	-3.562736	-3.108275	-1.051307
H	-1.566098	-3.539277	-0.444717
C	-3.880094	-1.123573	-2.352974
H	-2.146560	0.027615	-2.790783
C	-4.426287	-2.247097	-1.727808
H	-3.952113	-4.000696	-0.566046
H	-4.526585	-0.434505	-2.890998
H	-5.492457	-2.447698	-1.774608
C	0.560000	-0.518869	-2.215570
F	1.768252	-0.862659	-2.672759
F	-0.058626	0.198038	-3.168214
F	1.038206	0.741702	-1.271213

TS4

E_{gas} optimization: -2060.89793373 a.u.

E_{sol} single-point: -2061.41805997 a.u.

G_{sol} thermo-corrected: -2060.91637697 a.u.

Ni	-0.178548	0.142445	0.341580
O	-3.914622	1.101124	-0.919256
O	2.710793	0.453210	3.150198
N	-1.739655	0.700090	-0.538193
N	-1.188099	-0.508596	1.872607
N	1.451472	0.207125	1.300159
C	-1.737433	1.809033	-1.523335
H	-1.078905	1.554943	-2.348455
C	-3.211497	1.800840	-1.976724
H	-3.650628	2.794486	-2.078527
H	-3.344150	1.234925	-2.904242
C	-2.975022	0.451927	-0.192197
C	-3.402562	-0.375103	0.876177
H	-4.447540	-0.646815	0.924478
C	-2.524186	-0.813667	1.825207
C	-2.897240	-1.713743	2.981724
H	-2.999660	-2.733604	2.593483
H	-3.850135	-1.431875	3.435886
C	-1.688377	-1.583652	3.925674
H	-1.908422	-0.933698	4.780545
H	-1.335031	-2.537861	4.325272
C	-0.640340	-0.927608	3.046194
C	0.660401	-0.713234	3.425087
H	0.987607	-0.963758	4.425487
C	1.575398	-0.033745	2.584077
C	3.252003	1.397559	2.193137
H	4.339767	1.358360	2.249422
H	2.894034	2.398098	2.463481
C	2.679357	0.920524	0.843001
H	2.380775	1.760771	0.214549
C	3.649276	0.031388	0.087198

C	3.956624	0.292183	-1.248951
H	3.452680	1.103734	-1.762013
C	4.857424	-0.520330	-1.940895
H	5.070923	-0.317536	-2.986168
C	5.462849	-1.599318	-1.297953
H	6.157927	-2.236364	-1.837269
C	5.167562	-1.861401	0.043723
H	5.633921	-2.701506	0.550348
C	4.268231	-1.050463	0.731523
H	4.035125	-1.262666	1.770940
C	-1.246607	3.082945	-0.857873
C	0.036752	3.565487	-1.138121
H	0.653591	3.036546	-1.857515
C	0.530165	4.690757	-0.473207
H	1.527161	5.058072	-0.700991
C	-0.255950	5.342747	0.478478
H	0.125752	6.218933	0.994822
C	-1.538434	4.864545	0.763937
H	-2.154431	5.367186	1.504214
C	-2.028807	3.739676	0.101850
H	-3.020353	3.361364	0.337514
H	1.421894	-2.410231	0.408363
C	0.266174	-1.674872	-1.300021
C	1.426270	-2.448153	-0.686494
H	1.393767	-3.506629	-0.980125
H	2.384728	-2.047495	-1.006775
C	-1.060201	-2.290741	-1.219815
C	-1.288188	-3.263008	-0.207878
C	-2.176684	-2.002939	-2.050363
C	-2.523522	-3.881676	-0.033017
H	-0.482828	-3.526188	0.467270
C	-3.408597	-2.623063	-1.867558
H	-2.080021	-1.286828	-2.852406
C	-3.606235	-3.566061	-0.855060
H	-2.635866	-4.622994	0.755699
H	-4.228845	-2.363485	-2.532878
H	-4.570362	-4.047462	-0.720918
C	0.656270	-0.704004	-2.285780
F	1.825521	-0.897817	-2.933647
F	-0.244696	-0.319215	-3.219468
F	0.961646	0.668045	-1.624413

^{3}IM4

E_{gas} optimization: -1513.47565783 a.u.

E_{sol} single-point: -1513.84887958 a.u.

G_{sol} thermo-corrected: -1513.49017658 a.u.

Ni	0.641070	0.365961	-0.713214
O	3.482077	-2.621580	-0.794395
O	-1.098858	3.076442	1.915135
N	1.690176	-1.306045	-0.480451
N	2.257372	1.418240	-0.104686
N	-0.483909	1.335292	0.627442
C	1.108043	-2.628994	-0.767808
H	0.672695	-2.570315	-1.770823
C	2.357890	-3.540911	-0.764930
H	2.450804	-4.157926	0.133355
H	2.423252	-4.182951	-1.645236
C	2.988054	-1.377968	-0.574167
C	3.927549	-0.303956	-0.469054
H	4.976904	-0.561157	-0.534211
C	3.551291	0.989194	-0.214270
C	4.516980	2.129842	0.069178
H	5.093875	2.372427	-0.829038
H	5.234439	1.846994	0.845120
C	3.588789	3.282966	0.511517
H	3.817948	3.652683	1.515011
H	3.634651	4.141990	-0.166258
C	2.205978	2.654054	0.461997
C	1.071833	3.214779	0.995856
H	1.121118	4.186405	1.469867
C	-0.155316	2.500740	1.133050
C	-2.149319	2.101209	2.107585
H	-3.109973	2.593628	1.947989
H	-2.086978	1.736847	3.138606
C	-1.846417	0.989230	1.061966
H	-1.821750	0.004189	1.539743
C	-2.873378	0.946926	-0.058155
C	-4.090641	0.293639	0.177002
H	-4.253642	-0.207815	1.128596
C	-5.088561	0.274694	-0.796910
H	-6.026249	-0.238435	-0.602025
C	-4.875906	0.909982	-2.023122
H	-5.647093	0.891402	-2.787916
C	-3.665370	1.561420	-2.262351
H	-3.487532	2.046887	-3.217475

C	-2.669762	1.582167	-1.284316
H	-1.720818	2.066040	-1.483735
C	-0.013484	-2.942674	0.207955
C	-1.316566	-2.568410	-0.150321
H	-1.475302	-2.068207	-1.101635
C	-2.377661	-2.768577	0.734125
H	-3.378809	-2.471420	0.438059
C	-2.148649	-3.333909	1.990796
H	-2.974633	-3.494637	2.678342
C	-0.849503	-3.687879	2.362072
H	-0.660428	-4.118180	3.341683
C	0.211686	-3.489009	1.476639
H	1.217345	-3.753217	1.791331
F	-0.411821	-0.273862	-2.074157

MECP1

E_{sol} single-point: -1513.84877668 a.u.

Ni	-0.008043	0.165438	-0.038028
O	3.505892	0.825613	-2.198433
O	-3.445034	0.971107	2.199572
N	1.741619	0.139568	-0.982753
N	0.047273	2.212652	-0.014172
N	-1.712768	0.204773	0.984438
C	2.517211	-1.094809	-1.260003
H	1.821358	-1.871565	-1.576445
C	3.429629	-0.612800	-2.400080
H	4.442627	-1.014518	-2.377699
H	2.982276	-0.791718	-3.384391
C	2.409828	1.151074	-1.462319
C	2.128850	2.531841	-1.265198
H	2.834525	3.243090	-1.675131
C	1.049277	2.983230	-0.556398
C	0.836900	4.451035	-0.231792
H	1.028788	5.097588	-1.091542
H	1.539308	4.741153	0.559410
C	-0.612014	4.485032	0.271453
H	-0.767351	5.116630	1.149478
H	-1.296629	4.836499	-0.510276
C	-0.904948	3.023228	0.556856
C	-1.997960	2.613359	1.270680
H	-2.661692	3.350057	1.705424
C	-2.335101	1.245456	1.464559
C	-3.455001	-0.469846	2.385261
H	-4.487128	-0.814351	2.315342
H	-3.055148	-0.685280	3.382810
C	-2.534684	-0.995464	1.263769
H	-1.877932	-1.794631	1.605667
C	-3.275465	-1.449523	0.016355
C	-2.922986	-2.643162	-0.619547
H	-2.088788	-3.218332	-0.233155
C	-3.606257	-3.062602	-1.762474
H	-3.325009	-3.994654	-2.244776
C	-4.639969	-2.285887	-2.288960
H	-5.170087	-2.611927	-3.179482
C	-4.986421	-1.082735	-1.668369
H	-5.783723	-0.467343	-2.076729
C	-4.309057	-0.669176	-0.521672
H	-4.583365	0.266992	-0.042143
C	3.242031	-1.541106	0.002368
C	2.630081	-2.468065	0.855439
H	1.639165	-2.829814	0.601292
C	3.263411	-2.865048	2.034337
H	2.779653	-3.585667	2.688166
C	4.509979	-2.337302	2.378119
H	5.001838	-2.649735	3.295218
C	5.116553	-1.398523	1.540818
H	6.081899	-0.974520	1.804114
C	4.484133	-0.999711	0.362340
H	4.956354	-0.252822	-0.270315
F	-0.114845	-1.672343	-0.166112

IM4

E_{gas} optimization: -1513.48778585 a.u.

E_{sol} single-point: -1513.85817592 a.u.

G_{sol} thermo-corrected: -1513.49253492 a.u.

Ni	-0.000025	0.116221	-0.000048
O	3.207815	0.694925	-2.467016
O	-3.207717	0.695591	2.466944
N	1.571363	0.064342	-1.061808
N	0.000086	2.066292	-0.000174
N	-1.571453	0.064670	1.061676
C	2.402187	-1.153707	-1.241536
H	1.737149	-1.993912	-1.431002
C	3.219627	-0.759265	-2.483084

H	4.257655	-1.092136	-2.463510
H	2.739655	-1.089647	-3.411054
C	2.147410	1.048728	-1.698193
C	1.789364	2.418669	-1.626693
H	2.348463	3.122847	-2.228366
C	0.797636	2.856649	-0.792945
C	0.416826	4.315377	-0.645156
H	-0.190599	4.616876	-1.507344
H	1.292090	4.968470	-0.614210
C	-0.416162	4.315469	0.644821
H	0.191301	4.616869	1.507014
H	-1.291302	4.968729	0.613844
C	-0.797259	2.856813	0.792629
C	-1.789062	2.419061	1.626407
H	-2.347998	3.123376	2.228071
C	-2.147326	1.049180	1.698021
C	-3.219814	-0.758598	2.483092
H	-4.257910	-1.091254	2.463372
H	-2.740060	-1.089040	3.411149
C	-2.402321	-1.153305	1.241645
H	-1.737318	-1.993496	1.431310
C	-3.222856	-1.420674	-0.011405
C	-2.775528	-2.360843	-0.946974
H	-1.831584	-2.863153	-0.768126
C	-3.505820	-2.598759	-2.112518
H	-3.149178	-3.332685	-2.830091
C	-4.685397	-1.894234	-2.361035
H	-5.253827	-2.081353	-3.267846
C	-5.127837	-0.941507	-1.440400
H	-6.039843	-0.382050	-1.629752
C	-4.399643	-0.705086	-0.273937
H	-4.745532	0.048034	0.429260
C	3.222722	-1.420848	0.011573
C	2.775251	-2.360697	0.947386
H	1.831222	-2.862900	0.768693
C	3.505521	-2.598461	2.112988
H	3.148739	-3.332159	2.830725
C	4.685200	-1.894068	2.361330
H	5.253618	-2.081034	3.268181
C	5.127774	-0.941619	1.440458
H	6.039862	-0.382255	1.629692
C	4.399625	-0.705366	0.273944
H	4.745615	0.047553	-0.429415
F	-0.000111	-1.696510	0.000106

TS5

E_{gas} optimization: -2036.42354216 a.u.

E_{sol} single-point: -2036.88041669 a.u.

G_{sol} thermo-corrected: -2036.40533369 a.u.

Ni	0.635643	0.299454	-0.125295
O	2.916691	-2.556408	-1.899925
O	-0.588938	3.946204	1.179238
N	1.690929	-1.177289	-0.624467
N	1.433968	1.373900	-1.521367
N	-0.210505	1.796501	0.647602
C	2.239916	-2.185797	0.326987
H	1.446192	-2.525189	0.984787
C	2.669572	-3.280794	-0.659400
H	3.588342	-3.798714	-0.383925
H	1.865140	-4.000947	-0.841497
C	2.249069	-1.386435	-1.786960
C	2.311125	-0.463975	-2.864275
H	2.750303	-0.789480	-3.797442
C	1.990686	0.849160	-2.663730
C	2.218335	1.946945	-3.681299
H	1.392427	1.945387	-4.403422
H	3.147809	1.809881	-4.237977
C	2.181475	3.214504	-2.810542
H	3.194077	3.515253	-2.514760
H	1.704365	4.074141	-3.286244
C	1.424518	2.741693	-1.587991
C	0.821712	3.569525	-0.683776
H	0.889502	4.643883	-0.787983
C	0.030267	3.057542	0.375079
C	-1.186143	3.176940	2.254299
H	-2.156631	3.613348	2.490565
H	-0.520270	3.236956	3.122808
C	-1.269547	1.747626	1.678728
H	-0.997577	1.001132	2.424958
C	-2.640546	1.424256	1.103412
C	-3.665033	1.054067	1.984909
H	-3.450373	0.959351	3.046808
C	-4.943870	0.776962	1.507523
H	-5.724773	0.474358	2.199039
C	-5.211746	0.856830	0.138967

H	-6.198216	0.607897	-0.238967
C	-4.195964	1.221199	-0.742975
H	-4.390393	1.256522	-1.810323
C	-2.917138	1.509124	-0.263291
H	-2.120705	1.761768	-0.955239
C	3.362230	-1.566670	1.145711
C	3.114576	-1.155620	2.460670
H	2.119963	-1.285967	2.872648
C	4.124604	-0.550330	3.211506
H	3.921038	-0.237596	4.231936
C	5.388702	-0.345327	2.656232
H	6.174038	0.123984	3.242133
C	5.639595	-0.745633	1.341175
H	6.620321	-0.588189	0.900845
C	4.632115	-1.350907	0.590102
H	4.834324	-1.651621	-0.434400
F	0.134382	-0.870661	1.896433
Si	-1.266849	-1.696299	1.064582
H	-0.832080	-0.678200	-0.058148
H	-2.002889	-1.597810	2.365066
H	-0.537592	-2.991202	0.910929
C	-2.832668	-2.038575	-0.031903
C	-2.803308	-1.902012	-1.429510
C	-4.041812	-2.451876	0.547833
C	-3.920211	-2.180795	-2.219158
H	-1.888738	-1.554222	-1.910621
C	-5.169537	-2.732372	-0.229596
H	-4.110825	-2.542321	1.630647
C	-5.111251	-2.597447	-1.617794
H	-3.867526	-2.067285	-3.299803
H	-6.094983	-3.047282	0.247438
H	-5.986938	-2.809433	-2.226133

^{3}TS5

E_{gas} optimization: -2036.45355577 a.u.

E_{sol} single-point: -2036.90975486 a.u.

G_{sol} thermo-corrected: -2036.43647386 a.u.

Ni	-0.643524	-0.180147	0.271038
O	-3.468206	-2.180233	-2.070885
O	0.865679	1.218598	3.902517
N	-2.029603	-0.799032	-1.033445
N	-1.094023	-1.768557	1.492924
N	0.153885	0.826657	1.803259
C	-2.586926	0.017745	-2.132663
H	-1.758820	0.453740	-2.691803
C	-3.328848	-1.047864	-2.968418
H	-4.325294	-0.745474	-3.293901
H	-2.739623	-1.372142	-3.832105
C	-2.608875	-1.968234	-1.041845
C	-2.461710	-3.019499	-0.089592
H	-2.974940	-3.947608	-0.306319
C	-1.770667	-2.887015	1.085942
C	-1.666929	-3.981969	2.133331
H	-0.968251	-4.750785	1.783448
H	-2.627847	-4.472067	2.309095
C	-1.117556	-3.234139	3.362298
H	-1.891721	-3.077276	4.121877
H	-0.283418	-3.743887	3.851959
C	-0.690573	-1.893274	2.787594
C	-0.045603	-0.927523	3.520518
H	0.187858	-1.116972	4.560446
C	0.299177	0.357699	3.020882
C	0.949849	2.499477	3.234538
H	1.903653	2.960174	3.493860
H	0.121650	3.124250	3.589107
C	0.816227	2.142966	1.733416
H	0.164826	2.850055	1.214341
C	2.160682	2.094641	1.026118
C	2.617185	3.225856	0.340011
H	1.976285	4.100948	0.261980
C	3.875666	3.230305	-0.260741
H	4.212460	4.110320	-0.801348
C	4.690142	2.098148	-0.186483
H	5.660239	2.089281	-0.674110
C	4.239343	0.964553	0.489730
H	4.845582	0.064560	0.510177
C	2.982222	0.963776	1.095622
H	2.624844	0.066787	1.590202
C	-3.443623	1.131242	-1.556072
C	-2.924316	2.427465	-1.463106
H	-1.918865	2.619857	-1.824302
C	-3.676973	3.448484	-0.878116
H	-3.265601	4.452126	-0.814388
C	-4.952690	3.181982	-0.377776
H	-5.539259	3.976655	0.074474

C	-5.472093	1.886770	-0.457948
H	-6.461853	1.671421	-0.065160
C	-4.719812	0.867072	-1.040489
H	-5.122298	-0.142043	-1.085640
F	-0.000952	1.287015	-1.165760
Si	1.266234	0.174093	-1.898069
H	0.816865	-0.710105	-0.618509
H	1.919943	1.430299	-2.385731
H	0.411026	-0.396810	-2.978895
C	2.875193	-0.892280	-1.863762
C	3.004060	-2.059326	-1.095467
C	3.994969	-0.477065	-2.603500
C	4.194979	-2.788830	-1.065887
H	2.161228	-2.393376	-0.490970
C	5.189783	-1.200115	-2.588181
H	3.940681	0.443629	-3.181404
C	5.294333	-2.358238	-1.813401
H	4.270183	-3.686671	-0.456764
H	6.042909	-0.855306	-3.167740
H	6.226215	-2.917153	-1.787688

MECP2

E_{sol} single-point: -1414.49239709 a.u.

Ni	0.051635	-0.054432	0.128994
O	3.459742	0.992944	-2.277826
O	-3.598738	0.862180	2.194747
N	1.762701	0.129726	-1.068205
N	-0.093034	2.135215	-0.041841
N	-1.841800	0.079180	1.017629
C	2.688737	-0.997349	-1.254888
H	2.136048	-1.860488	-1.633975
C	3.666131	-0.438881	-2.323574
H	4.716665	-0.640298	-2.107203
H	3.422360	-0.788320	-3.333375
C	2.300660	1.196161	-1.595821
C	1.835883	2.535703	-1.507063
H	2.406777	3.281324	-2.046044
C	0.745844	2.932356	-0.773974
C	0.306055	4.387445	-0.726579
H	-0.164640	4.651163	-1.681371
H	1.151052	5.065332	-0.581641
C	-0.711850	4.394973	0.420563
H	-0.270088	4.784475	1.345782
H	-1.611887	4.980295	0.216478
C	-1.022162	2.917412	0.597517
C	-2.098299	2.488161	1.329884
H	-2.739672	3.219926	1.804838
C	-2.462435	1.122722	1.489089
C	-3.657634	-0.578097	2.353299
H	-4.687113	-0.899223	2.187171
H	-3.356381	-0.819576	3.378706
C	-2.654418	-1.117573	1.306890
H	-2.001337	-1.886896	1.725234
C	-3.287526	-1.642422	0.029898
C	-2.862785	-2.852224	-0.527269
H	-2.078964	-3.418081	-0.032336
C	-3.419450	-3.316282	-1.721634
H	-3.078937	-4.257013	-2.145533
C	-4.404755	-2.571801	-2.371345
H	-4.836459	-2.930708	-3.301359
C	-4.830875	-1.358159	-1.823148
H	-5.594457	-0.771291	-2.326077
C	-4.273586	-0.896345	-0.631888
H	-4.600316	0.051934	-0.212164
C	3.374274	-1.392390	0.043385
C	3.668228	-2.735456	0.299645
H	3.362290	-3.495771	-0.414979
C	4.326548	-3.109107	1.471767
H	4.537916	-4.157643	1.661845
C	4.698061	-2.139177	2.405245
H	5.202828	-2.428733	3.322354
C	4.408989	-0.795718	2.156291
H	4.689744	-0.035168	2.879759
C	3.752935	-0.424836	0.982071
H	3.517724	0.619680	0.800298
H	0.228553	-1.645352	0.423134

^{2r}**TS6**

E_{gas} optimization: -2061.49994776 a.u.

E_{sol} single-point: -2062.02243359 a.u.

G_{sol} thermo-corrected: -2061.51663659 a.u.

Ni	0.032096	0.829764	-0.152625
O	4.005572	0.348192	-0.932933
O	-3.235689	2.984468	0.954040

N	1.851075	0.344801	-0.286454
N	0.356366	2.464996	-1.271206
N	-1.684230	1.447328	0.389658
C	2.542950	-0.473136	0.735622
H	2.014033	-1.415482	0.853433
C	3.923284	-0.688171	0.081435
H	4.761652	-0.554952	0.767240
H	3.989595	-1.657967	-0.416778
C	2.750505	0.834105	-1.099272
C	2.562846	1.850742	-2.075918
H	3.392629	2.071907	-2.734506
C	1.438035	2.632621	-2.092605
C	1.235896	3.829570	-3.003491
H	0.950595	3.482062	-4.003946
H	2.145749	4.425195	-3.111750
C	0.074974	4.577664	-2.320628
H	0.436843	5.440302	-1.748634
H	-0.687067	4.943975	-3.013641
C	-0.478637	3.534182	-1.366400
C	-1.635812	3.682922	-0.642665
H	-2.202614	4.602967	-0.702361
C	-2.131218	2.676147	0.221439
C	-3.395331	1.906490	1.904290
H	-4.461204	1.748871	2.071220
H	-2.901335	2.193013	2.841251
C	-2.682495	0.730415	1.209656
H	-2.172619	0.077296	1.918677
C	-3.661476	-0.084655	0.376689
C	-4.324263	-1.166959	0.968618
H	-4.082418	-1.448874	1.989633
C	-5.259948	-1.909319	0.248320
H	-5.753407	-2.756277	0.716505
C	-5.549300	-1.572718	-1.076423
H	-6.271168	-2.154459	-1.642332
C	-4.901122	-0.487692	-1.668927
H	-5.118524	-0.220871	-2.699406
C	-3.964630	0.253547	-0.946309
H	-3.446496	1.079823	-1.421259
C	2.555417	0.267077	2.061554
C	1.748657	-0.167880	3.117820
H	1.141943	-1.058209	2.990701
C	1.714393	0.542778	4.320296
H	1.085556	0.193631	5.134811
C	2.484188	1.696395	4.475770
H	2.458089	2.249075	5.410696
C	3.290222	2.138399	3.422299
H	3.890843	3.036641	3.535879
C	3.323018	1.428783	2.222864
H	3.941205	1.781894	1.401138
H	-0.247689	-0.579609	0.333554
C	-0.380473	-2.409961	-0.459019
C	-1.599847	-2.176477	-1.318107
H	-1.562752	-1.197364	-1.801472
H	-2.515048	-2.205465	-0.731224
C	0.883954	-2.692925	-1.128644
C	1.220091	-1.970861	-2.297753
C	1.789245	-3.691133	-0.697296
C	2.393545	-2.229743	-2.996637
H	0.565896	-1.172216	-2.629008
C	2.957312	-3.955942	-1.409461
H	1.563770	-4.280500	0.182701
C	3.270310	-3.229132	-2.562048
H	2.631145	-1.641820	-3.878514
H	3.624073	-4.741412	-1.064273
H	4.184818	-3.434676	-3.110319
C	-0.640099	-3.018537	0.879332
F	-1.690562	-2.448116	1.517214
F	-0.924616	-4.352634	0.800127
F	0.421914	-2.921524	1.731543
H	-1.662095	-2.940156	-2.103734

^{2}**IM5**

E_{gas} optimization: -2061.51634604 a.u.

E_{sol} single-point: -2062.03586222 a.u.

G_{sol} thermo-corrected: -2061.52769622 a.u.

Ni	-0.175931	-0.099634	-0.294455
O	-0.824392	-4.197322	-0.507048
O	0.316594	3.257915	-2.745379
N	-0.080852	-2.079316	-0.367475
N	-1.845063	-0.139622	-1.398537
N	0.464872	1.504548	-1.334386
C	1.026291	-2.882525	0.161275
H	1.043020	-2.760868	1.249373
C	0.589516	-4.319394	-0.220578
H	1.096000	-4.672695	-1.126460

H	0.718308	-5.049133	0.580589
C	-1.075398	-2.870831	-0.669036
C	-2.363997	-2.496784	-1.139258
H	-3.084831	-3.290582	-1.286088
C	-2.685689	-1.208084	-1.488794
C	-4.023731	-0.800114	-2.077610
H	-4.813666	-0.971845	-1.340831
H	-4.259242	-1.395295	-2.965334
C	-3.833355	0.697121	-2.391242
H	-4.019780	0.947781	-3.439475
H	-4.481715	1.326378	-1.774237
C	-2.387776	0.951304	-2.008673
C	-1.707740	2.108818	-2.296657
H	-2.202111	2.899269	-2.846500
C	-0.308331	2.252647	-2.076357
C	1.736896	3.110172	-2.522136
H	2.130382	4.058047	-2.149042
H	2.209096	2.886311	-3.483206
C	1.869362	1.936325	-1.514301
H	2.416725	1.103351	-1.968886
C	2.542632	2.264451	-0.195575
C	3.335322	1.289188	0.419956
H	3.494009	0.337441	-0.075891
C	3.908253	1.524929	1.670435
H	4.510975	0.751755	2.137897
C	3.702043	2.745700	2.315105
H	4.146651	2.932090	3.288410
C	2.917834	3.727510	1.703806
H	2.747545	4.677216	2.202661
C	2.337923	3.484660	0.458829
H	1.700734	4.243189	0.011432
C	2.373709	-2.469158	-0.391323
C	3.514334	-2.533030	0.415734
H	3.419738	-2.856971	1.449101
C	4.764585	-2.165910	-0.088039
H	5.640899	-2.217095	0.551788
C	4.884421	-1.719279	-1.405593
H	5.853713	-1.422902	-1.795587
C	3.747133	-1.643300	-2.215425
H	3.831068	-1.289726	-3.239468
C	2.500931	-2.018201	-1.711974
H	1.611131	-1.938637	-2.329513
H	-0.127719	2.466259	1.159951
C	-0.805662	0.448671	1.603029
C	-0.104564	1.759792	1.988333
H	-0.581350	2.228233	2.859389
H	0.945974	1.583956	2.212980
C	-2.300257	0.605941	1.467256
C	-2.841252	1.859975	1.113256
C	-3.220230	-0.450640	1.641753
C	-4.211720	2.049885	0.940846
H	-2.182498	2.703453	0.951243
C	-4.590867	-0.259224	1.475415
H	-2.866987	-1.437319	1.902258
C	-5.102829	0.991003	1.121343
H	-4.581557	3.035112	0.668159
H	-5.263575	-1.099495	1.627858
H	-6.171956	1.137696	0.996365
C	-0.414467	-0.593288	2.631795
F	-0.911061	-0.302484	3.866788
F	-0.836360	-1.865748	2.360608
F	0.934283	-0.698805	2.790964
H	1.015087	-0.075875	0.479188

^{2r}**TS7**

E_{gas} optimization: -2061.51313270 a.u.

E_{sol} single-point: -2062.0322395 a.u.

G_{sol} thermo-corrected: -2061.5248815 a.u.

Ni	0.281779	0.048028	-0.266005
O	0.862498	4.181847	-0.422857
O	-0.027046	-3.303627	-2.779475
N	0.155991	2.045816	-0.293700
N	1.980161	0.166111	-1.378638
N	-0.258611	-1.646657	-1.260317
C	-1.004038	2.829438	0.140932
H	-1.145842	2.672355	1.214764
C	-0.551210	4.288484	-0.144176
H	-1.046340	4.707342	-1.027285
H	-0.688044	4.962322	0.704262
C	1.140255	2.857720	-0.574266
C	2.448178	2.518849	-1.018555
H	3.156844	3.330636	-1.120336
C	2.804041	1.249142	-1.403778
C	4.171826	0.885693	-1.955657
H	4.929427	1.032609	-1.180178

H	4.436953	1.524539	-2.803718
C	4.013892	-0.597554	-2.343911
H	4.211495	-0.789953	-3.402730
H	4.671418	-1.247899	-1.759273
C	2.567949	-0.896965	-1.989704
C	1.933401	-2.076403	-2.294486
H	2.461240	-2.839374	-2.852567
C	0.548500	-2.301201	-2.056738
C	-1.400974	-3.403598	-2.351485
H	-1.511053	-4.322614	-1.768257
H	-2.034822	-3.471767	-3.237957
C	-1.640791	-2.118019	-1.530654
H	-2.118393	-1.359312	-2.165950
C	-2.491120	-2.251847	-0.281016
C	-3.198670	-1.123169	0.152696
H	-3.154234	-0.212072	-0.431626
C	-3.944788	-1.153532	1.330025
H	-4.472293	-0.259938	1.649604
C	-4.008884	-2.325322	2.086360
H	-4.591439	-2.355311	3.002632
C	-3.318299	-3.460432	1.656799
H	-3.359762	-4.376223	2.239528
C	-2.559890	-3.420798	0.485376
H	-2.005766	-4.306994	0.192040
C	-2.281120	2.434769	-0.572655
C	-3.510542	2.516372	0.090371
H	-3.537230	2.838500	1.128518
C	-4.695707	2.168239	-0.561871
H	-5.642292	2.230604	-0.032634
C	-4.661510	1.725294	-1.885746
H	-5.580592	1.442255	-2.390307
C	-3.436570	1.636700	-2.553332
H	-3.401030	1.286134	-3.581135
C	-2.254468	1.991591	-1.901600
H	-1.297916	1.900710	-2.407488
H	-0.060654	-2.534026	1.295069
C	0.555514	-0.504782	1.743317
C	-0.103039	-1.838413	2.130536
H	0.401735	-2.285920	2.994072
H	-1.156785	-1.696918	2.367196
C	2.060254	-0.624367	1.601209
C	2.621991	-1.856601	1.204011
C	2.958632	0.441225	1.825172
C	3.994586	-2.013788	1.026823
H	1.976743	-2.700704	0.998408
C	4.332109	0.279219	1.654901
H	2.588117	1.411373	2.119978
C	4.865393	-0.946336	1.251290
H	4.381921	-2.979172	0.711965
H	4.989290	1.124784	1.840394
H	5.937020	-1.068454	1.121417
C	0.129452	0.523032	2.781079
F	0.588682	0.204039	4.017759
F	0.547399	1.797755	2.542885
F	-1.225432	0.609134	2.884603
H	-0.755920	-0.079145	0.722169

S2

E_{gas} optimization: -764.655040636 a.u.

E_{sol} single-point: -764.886317754 a.u.

G_{sol} thermo-corrected: -764.706186754 a.u.

C	3.266354	1.176472	-0.183893
C	4.439739	0.747600	-0.806705
C	4.817315	-0.594896	-0.740190
H	5.731374	-0.930307	-1.221706
C	4.013980	-1.503187	-0.046968
C	2.842311	-1.069127	0.573915
C	2.452437	0.275875	0.515295
C	1.153998	0.728853	1.144117
H	1.222770	1.788361	1.422002
H	0.975563	0.172958	2.073650
C	-0.047142	0.527231	0.201968
H	-0.116652	-0.527915	-0.077674
H	0.120208	1.084102	-0.728005
C	-1.370766	0.990581	0.841668
H	-1.540029	0.429314	1.768844
H	-1.284727	2.046442	1.122524
C	-2.573505	0.829865	-0.058038
C	-3.142032	1.822630	-0.742978
H	-2.757476	2.835699	-0.673376
H	-3.999360	1.656825	-1.384958
H	4.301618	-2.549211	0.012997
H	2.221091	-1.780198	1.113888
H	2.978183	2.223963	-0.237204
H	5.060165	1.462079	-1.340723

C	-3.131653	-0.566655	-0.164351
F	-3.424198	-1.062149	1.063620
F	-2.235190	-1.422042	-0.720512
F	-4.256050	-0.638426	-0.904585

^{OS}TS8

E_{gas} optimization: -2061.51313270 a.u.

E_{sol} single-point: -2062.0322395 a.u.

G_{sol} thermo-corrected: -2061.5248815 a.u.

Ni	-0.488687	-0.769156	0.386050
O	-2.841154	-1.254336	-2.916188
O	1.878101	-1.752861	3.568493
N	-1.773618	-0.726566	-1.005127
N	0.330260	-2.434176	-0.351571
N	0.576273	-0.839550	1.966656
C	-3.053210	-0.004421	-0.915629
H	-2.854975	1.044248	-0.724368
C	-3.627065	-0.179357	-2.342253
H	-4.676501	-0.477739	-2.360413
H	-3.480371	0.720611	-2.945495
C	-1.777455	-1.446574	-2.099432
C	-0.823150	-2.426367	-2.488437
H	-0.930132	-2.863308	-3.472632
C	0.131686	-2.894554	-1.625453
C	1.124620	-3.992476	-1.955479
H	1.933008	-3.566228	-2.562470
H	0.674670	-4.808302	-2.526181
C	1.642515	-4.403053	-0.564872
H	1.148796	-5.314690	-0.207368
H	2.720746	-4.578786	-0.527467
C	1.224363	-3.227603	0.300287
C	1.668534	-3.013025	1.581106
H	2.339509	-3.720986	2.049928
C	1.323554	-1.861801	2.331121
C	1.268128	-0.597271	4.183401
H	2.019088	-0.092600	4.792040
H	0.434291	-0.935261	4.811275
C	0.785507	0.222967	2.971157
H	-0.160959	0.727117	3.180285
C	1.828644	1.243446	2.527568
C	1.837927	2.519625	3.107594
H	1.078149	2.782675	3.840701
C	2.796926	3.460735	2.734429
H	2.785352	4.450081	3.182997
C	3.761635	3.135838	1.775626
H	4.502199	3.872677	1.477996
C	3.762681	1.865629	1.197989
H	4.494323	1.600268	0.440764
C	2.802079	0.925043	1.575558
H	2.796070	-0.045834	1.097220
C	-3.935254	-0.530052	0.200321
C	-4.686494	0.372471	0.961574
H	-4.597087	1.437394	0.762911
C	-5.528555	-0.088105	1.975885
H	-6.105026	0.621431	2.562974
C	-5.622346	-1.455897	2.239973
H	-6.274063	-1.815371	3.031280
C	-4.868350	-2.360703	1.487345
H	-4.931443	-3.425513	1.693940
C	-4.028366	-1.900288	0.473536
H	-3.425160	-2.601511	-0.095736
H	-0.951828	0.756621	0.691635
C	-0.994668	2.668723	-0.689284
C	-0.754893	2.153971	0.590315
H	0.279544	2.076312	0.900709
H	-1.421877	2.479206	1.385704
C	-2.233511	3.425481	-0.989935
F	-3.137985	3.413357	0.027232
F	-1.988062	4.732444	-1.277443
F	-2.898477	2.947114	-2.096556
C	-0.136835	2.336573	-1.884091
H	-0.038125	3.214542	-2.537981
H	-0.669872	1.580008	-2.484681
C	1.239330	1.774410	-1.523036
H	1.849394	2.536835	-1.024645
H	1.111819	0.966806	-0.795495
C	2.005085	1.191895	-2.723484
H	2.237890	1.980053	-3.449634
H	1.353412	0.470011	-3.234413
C	3.270945	0.496108	-2.272012
C	4.539656	1.038822	-2.501247
C	3.178250	-0.695956	-1.536752
C	5.687764	0.412300	-2.005773
H	4.630370	1.963832	-3.065697
C	4.318438	-1.321447	-1.034502

H	2.197996	-1.111626	-1.326872
C	5.581258	-0.767361	-1.266842
H	6.664473	0.849931	-2.193734
H	4.216048	-2.229765	-0.446586
H	6.472011	-1.249744	-0.874757

R2$^{\bullet}$

E_{gas} optimization: -765.232374455 a.u.

E_{sol} single-point: -765.463904057 a.u.

G_{sol} thermo-corrected: -765.276100057 a.u.

H	-2.613130	2.855234	-0.466154
C	-2.545273	0.793129	0.112053
C	-2.818891	1.866794	-0.889108
H	-2.177468	1.755758	-1.779009
H	-3.855019	1.837065	-1.236264
C	-3.134809	-0.549644	-0.141518
F	-4.391139	-0.477525	-0.639755
F	-2.400097	-1.259355	-1.054745
F	-3.183088	-1.310790	0.977369
C	-1.362519	0.867926	1.024119
H	-1.508120	0.197772	1.878768
H	-1.274714	1.887780	1.420688
C	-0.036090	0.490908	0.315430
H	-0.123734	-0.517304	-0.103320
H	0.132256	1.165350	-0.533097
C	1.173637	0.555263	1.265283
H	0.999107	-0.122222	2.110840
H	1.249589	1.566594	1.684431
C	2.462761	0.187401	0.566206
C	2.849529	-1.154089	0.441941
C	3.269586	1.171586	-0.019696
C	4.011520	-1.503619	-0.246750
H	2.233656	-1.929423	0.892050
C	4.433183	0.827295	-0.709587
H	2.983784	2.217292	0.069706
C	4.807825	-0.512730	-0.825507
H	4.297125	-2.548675	-0.328914
H	5.048489	1.605216	-1.153217
H	5.714339	-0.782725	-1.359523

CAT2

E_{gas} optimization: -1578.58871350 a.u.

E_{sol} single-point: -1578.82452201 a.u.

G_{sol} thermo-corrected: -1578.74497401 a.u.

Cr	-0.066951	-0.000199	0.144093
O	-1.431457	-2.455333	1.187683
O	-1.428103	2.456296	1.188488
O	-2.095000	0.001710	-2.081292
C	-0.939624	-1.499141	0.757825
C	-0.937597	1.499513	0.758375
C	-1.328734	0.000933	-1.214669
C	1.499662	-0.715108	-1.216482
C	1.827758	-1.151259	0.097233
C	2.030970	-0.000656	0.906571
C	1.828102	1.149947	0.097111
C	1.499784	0.713646	-1.216595
H	1.303022	-1.352661	-2.067275
H	2.288100	-0.000724	1.956760
H	1.913928	2.177485	0.423333
H	1.303625	1.350987	-2.067650
H	-0.360011	-0.000258	1.697467
H	1.912704	-2.178697	0.423900

^{3}CAT2

E_{gas} optimization: -1578.52987858 a.u.

E_{sol} single-point: -1578.76650947 a.u.

G_{sol} thermo-corrected: -1578.70233647 a.u.

Cr	0.372524	0.004181	0.474169
O	-1.541653	-2.226594	1.273166
O	-1.522742	2.264515	1.233432
O	-3.348410	-0.030633	-1.337802
C	-0.841607	-1.370000	0.944509
C	-0.830066	1.396314	0.919853
C	-2.323123	0.011963	-1.827213
C	1.305782	-0.729104	-1.443209
C	2.098017	-1.161547	-0.338357
C	2.591616	0.000216	0.318923
C	2.099601	1.145621	-0.367805
C	1.306821	0.686310	-1.461362
H	0.775003	-1.371739	-2.133147
H	3.219601	0.010981	1.198949
H	2.305057	2.177662	-0.119293
H	0.776091	1.311528	-2.167080

H	0.542275	0.021536	2.081431
H	2.301587	-2.187252	-0.063306

^{OS}TS9

E_{gas} optimization: -2225.28404894 a.u.

E_{sol} single-point: -2225.70979975 a.u.

G_{sol} thermo-corrected: -2225.50675175 a.u.

Cr	2.051495	-0.234176	0.044513
O	1.077843	-2.509111	-1.662443
O	2.505226	2.122775	-1.765537
O	4.843442	-1.110693	-0.674402
C	1.481289	-1.632362	-1.014616
C	2.358163	1.193022	-1.088525
C	3.765651	-0.775554	-0.419435
C	1.483194	-1.240533	1.964102
C	0.498816	-0.278929	1.608367
C	1.120023	1.005197	1.587067
C	2.490378	0.834396	1.935454
C	2.711333	-0.554758	2.154729
H	1.328070	-2.306663	2.057548
H	0.626859	1.940379	1.366714
H	3.232258	1.616840	2.015588
H	3.654825	-1.010536	2.423889
H	0.461350	0.228086	-0.937156
H	-0.540900	-0.480797	1.394862
C	-1.725724	0.730297	-0.804870
C	-0.591872	0.601984	-1.627212
H	-0.597768	-0.216082	-2.344551
H	-0.182209	1.522862	-2.033714
C	-2.585624	-0.379224	-0.425087
C	-2.223490	-1.711496	-0.743496
C	-3.795119	-0.182647	0.286849
C	-3.028620	-2.782943	-0.372640
H	-1.297589	-1.916437	-1.266096
C	-4.595292	-1.260172	0.648614
H	-4.114923	0.818442	0.545095
C	-4.220383	-2.566971	0.324403
H	-2.719117	-3.792768	-0.625675
H	-5.520061	-1.078034	1.188270
H	-4.846905	-3.405314	0.613552
C	-1.917572	2.048737	-0.106151
F	-0.932291	2.932524	-0.389941
F	-3.090101	2.650103	-0.426172
F	-1.920136	1.904951	1.250235

^{2}IM6

E_{gas} optimization: -1577.98887964 a.u.

E_{sol} single-point: -1578.22411982 a.u.

G_{sol} thermo-corrected: -1578.15676682 a.u.

Cr	0.066699	0.007307	-0.109614
O	1.964410	-0.033124	2.237523
O	1.627257	-2.315611	-1.262081
O	1.512535	2.455859	-1.159738
C	1.250594	-0.013448	1.325970
C	1.062719	-1.405839	-0.825002
C	0.992785	1.503849	-0.759755
C	-1.858237	1.157611	0.050798
C	-1.629511	0.447450	1.256979
C	-1.605258	-0.948506	0.953587
C	-1.819708	-1.088444	-0.449430
C	-1.978087	0.210841	-1.003684
H	-1.923645	2.232502	-0.051427
H	-1.479425	-1.753797	1.663708
H	-1.874821	-2.021792	-0.993161
H	-2.145915	0.442195	-2.047483
H	-1.502365	0.887466	2.236696

^{OS}TS10

E_{gas} optimization: -2225.26145792 a.u.

E_{sol} single-point: -2225.69090276 a.u.

G_{sol} thermo-corrected: -2225.48970276 a.u.

Cr	2.166210	0.256987	0.186159
O	0.801094	2.849155	0.998257
O	1.358990	-2.074105	1.954549
O	4.101497	0.902459	2.399720
C	1.302734	1.847432	0.725676
C	1.659241	-1.162390	1.314089
C	3.340243	0.658350	1.562519
C	3.857056	0.731843	-1.154777
C	2.672766	1.157444	-1.817562
C	1.869833	0.014744	-2.053661
C	2.530279	-1.118287	-1.507714
C	3.776330	-0.681641	-0.968300

H	4.682095	1.366015	-0.859837
H	0.881579	0.016449	-2.487365
H	2.155645	-2.131632	-1.522609
H	4.531550	-1.307150	-0.512713
H	2.432583	2.173184	-2.100954
H	-2.585228	-1.881382	2.108842
C	-2.316948	-1.197523	0.083874
C	-2.261825	-2.272523	1.139272
H	-2.915837	-3.120623	0.892326
H	-1.249752	-2.664607	1.255257
C	-3.382417	-0.212578	0.069722
C	-4.607464	-0.498255	0.720029
C	-3.254709	1.056221	-0.549680
C	-5.652582	0.419627	0.727713
H	-4.745573	-1.458815	1.204999
C	-4.301896	1.969273	-0.532902
H	-2.316066	1.333358	-1.012170
C	-5.510331	1.659582	0.099693
H	-6.583993	0.165359	1.225885
H	-4.170015	2.938442	-1.005811
H	-6.324765	2.377720	0.110357
C	-1.226453	-1.116042	-0.791631
F	-1.345909	-0.510011	-1.979322
F	-0.087192	-0.070379	-0.084532
F	-0.437681	-2.189138	-0.934188

IM7

E_{gas} optimization: -2225.30357782 a.u.

E_{sol} single-point: -2225.72836051 a.u.

G_{sol} thermo-corrected: -2225.51563351 a.u.

Cr	-1.302466	-0.426999	0.047521
O	-0.149738	-0.183055	2.817695
O	-2.572423	1.743935	-1.616130
O	-3.684047	0.324157	1.711779
C	-0.522525	-0.168328	1.725720
C	-2.011295	0.981677	-0.955657
C	-2.754990	0.061714	1.073188
C	-0.408276	-2.458088	0.046805
C	-0.394132	-2.005778	-1.295983
C	-1.726121	-1.761471	-1.707744
C	-2.583831	-2.084635	-0.619291
C	-1.769720	-2.520453	0.467710
H	0.463491	-2.713457	0.633122
H	-2.037044	-1.404982	-2.680371
H	-3.663674	-2.022474	-0.620876
H	-2.124115	-2.846261	1.436219
H	1.588781	1.497815	-2.483965
H	0.492927	-1.858189	-1.887897
C	0.685998	0.800884	-0.622313
C	0.630246	1.091385	-2.138971
H	0.412842	0.199260	-2.727089
H	-0.136636	1.826105	-2.376382
C	1.921065	-0.008680	-0.257541
C	2.466085	-0.046315	1.044334
C	2.604573	-0.760318	-1.236515
C	3.582139	-0.822219	1.350781
H	2.030099	0.545833	1.833871
C	3.716790	-1.545389	-0.930093
H	2.283434	-0.729512	-2.270682
C	4.211285	-1.592141	0.371497
H	3.963169	-0.816918	2.368262
H	4.201873	-2.110697	-1.721209
H	5.077039	-2.200711	0.614926
C	0.714150	2.173545	0.052148
F	1.864672	2.835665	-0.244098
F	-0.297294	2.978844	-0.361600
F	0.631289	2.162106	1.408627

IM8

E_{gas} optimization: -2111.96647645 a.u.

E_{sol} single-point: -2112.35789017 a.u.

G_{sol} thermo-corrected: -2112.15288617 a.u.

Cr	-1.320914	-0.375057	-0.136416
O	-1.144740	1.017223	2.506795
O	-3.824372	1.252314	-0.373202
C	-1.199676	0.531654	1.456609
C	-2.830964	0.656029	-0.307377
C	-0.809721	-2.181685	0.981476
C	-0.295126	-2.370669	-0.329915
C	-1.391518	-2.371139	-1.228028
C	-2.585891	-2.188582	-0.485478
C	-2.234302	-2.077343	0.887969
H	-0.224525	-2.155304	1.890019
H	-1.328756	-2.468121	-2.304731

H	-3.586970	-2.142082	-0.892380
H	-2.921872	-1.953497	1.713235
H	-0.240329	1.459493	-2.424030
H	0.746895	-2.479603	-0.592411
C	0.491604	0.671389	-0.520656
C	-0.120567	0.520991	-1.877701
H	0.365177	-0.224164	-2.505394
H	-1.228394	0.181856	-1.840025
C	1.784969	-0.042310	-0.221010
C	2.141355	-0.312039	1.112380
C	2.671684	-0.443866	-1.231287
C	3.321332	-0.985384	1.419026
H	1.481389	0.008467	1.910428
C	3.849817	-1.130155	-0.926496
H	2.454776	-0.209466	-2.268810
C	4.178442	-1.409012	0.399640
H	3.569427	-1.185784	2.457549
H	4.515524	-1.434533	-1.729362
H	5.093955	-1.942261	0.637962
C	0.598904	2.140841	-0.161124
F	1.526345	2.763113	-0.940410
F	-0.566378	2.808686	-0.362497
F	0.966309	2.354617	1.119021

TS11

E_{gas} optimization: -2111.93746529 a.u.

E_{sol} single-point: -2112.32834391 a.u.

G_{sol} thermo-corrected: -2112.12431091 a.u.

Cr	1.163248	-0.423695	-0.061861
O	-0.526614	-1.986276	1.882071
O	0.378752	-2.686420	-1.881839
C	0.106687	-1.391521	1.119187
C	0.640977	-1.803891	-1.183373
C	2.603837	-0.334820	1.583907
C	2.811653	0.876711	0.861093
C	3.230870	0.539873	-0.439978
C	3.277801	-0.874546	-0.552573
C	2.916319	-1.424301	0.713119
H	2.321282	-0.413712	2.624948
H	3.383354	1.237943	-1.251055
H	3.565034	-1.433072	-1.432709
H	2.901506	-2.474145	0.972290
H	-1.146333	2.343050	2.242311
H	2.666964	1.879354	1.234853
C	-0.655389	1.116295	0.518622
C	-0.384403	1.614759	1.937093
H	-0.411186	0.790377	2.653392
H	0.586633	2.099380	2.020094
C	-1.970258	0.448437	0.247783
C	-2.267279	-0.090487	-1.021036
C	-2.922729	0.292507	1.266439
C	-3.475563	-0.736244	-1.259090
H	-1.534990	-0.009777	-1.815971
C	-4.133030	-0.362532	1.025248
H	-2.728797	0.674654	2.262082
C	-4.419290	-0.877277	-0.237007
H	-3.676066	-1.141848	-2.246726
H	-4.850401	-0.469594	1.834127
H	-5.359376	-1.388074	-0.423126
C	-0.165577	1.924466	-0.513847
F	0.818148	2.778257	-0.303870
F	0.776055	0.711551	-1.670216
F	-0.885364	2.326984	-1.535383

IM9

E_{gas} optimization: -1677.83203686 a.u.

E_{sol} single-point: -1678.11079297 a.u.

G_{sol} thermo-corrected: -1678.03850597 a.u.

Cr	0.042647	-0.000155	0.062830
O	1.458704	2.573441	0.877849
O	1.464425	-2.571200	0.875400
O	1.981471	0.003092	-2.251640
C	0.957036	1.606167	0.518805
C	0.960429	-1.604827	0.517109
C	1.245088	0.001846	-1.360896
C	-1.470096	0.712867	-1.329268
C	-1.871825	1.148718	-0.028562
C	-2.132254	-0.002119	0.751971
C	-1.869991	-1.151806	-0.029720
C	-1.468983	-0.714049	-1.329956
H	-1.241465	1.350572	-2.172229
H	-2.362837	-0.002837	1.807480
H	-1.970637	-2.177931	0.296090
H	-1.239146	-1.350499	-2.173540

H	-1.974242	2.174360	0.298222
F	0.270174	-0.001487	2.018477

^{3}TS12

E_{gas} optimization: -2178.85826230 a.u.

E_{sol} single-point: -2179.4081689 a.u.

G_{sol} thermo-corrected: -2178.8344979 a.u.

Ni	0.486194	0.512084	0.494563
O	-3.137350	2.235075	-0.536533
O	4.053179	0.937980	2.535749
N	-1.152888	1.179053	-0.364457
N	-0.199474	0.997964	2.336576
N	2.364496	0.451354	1.117593
C	-1.293582	1.483080	-1.807323
H	-1.098551	0.576388	-2.377200
C	-2.779164	1.888678	-1.897756
H	-2.969960	2.755211	-2.532588
H	-3.412532	1.050487	-2.208150
C	-2.176177	1.691678	0.266761
C	-2.407677	1.752456	1.668676
H	-3.373936	2.122751	1.986681
C	-1.461526	1.424378	2.610858
C	-1.682921	1.558531	4.109594
H	-2.521150	0.935278	4.435813
H	-1.934518	2.593213	4.364760
C	-0.330775	1.118846	4.707250
H	0.099605	1.855465	5.391501
H	-0.410674	0.175360	5.258573
C	0.541642	0.922610	3.478180
C	1.904564	0.766522	3.518311
H	2.421299	0.832929	4.467510
C	2.721980	0.695484	2.354766
C	4.594087	1.171607	1.214706
H	5.603452	0.760834	1.177346
H	4.623315	2.254426	1.043552
C	3.590726	0.462850	0.278446
H	3.394834	1.054182	-0.619171
C	4.057562	-0.924197	-0.126260
C	4.085774	-1.298416	-1.470846
H	3.697403	-0.617419	-2.221219
C	4.579980	-2.547913	-1.851343
H	4.584424	-2.827690	-2.900670
C	5.052058	-3.437164	-0.885957
H	5.437811	-4.408973	-1.180387
C	5.019155	-3.074760	0.464022
H	5.378687	-3.764571	1.222307
C	4.523392	-1.828004	0.840889
H	4.504914	-1.546830	1.890295
C	-0.283496	2.547695	-2.198725
C	0.884372	2.182636	-2.878158
H	1.036659	1.142196	-3.145156
C	1.860517	3.138162	-3.171121
H	2.762151	2.842946	-3.701044
C	1.677257	4.467959	-2.787744
H	2.434267	5.212364	-3.017830
C	0.514372	4.838359	-2.105930
H	0.366865	5.871001	-1.802310
C	-0.457555	3.883024	-1.810276
H	-1.352039	4.171786	-1.264068
H	2.035950	-2.955326	0.639749
C	0.315096	-2.764046	-0.651375
C	1.467710	-3.546459	-0.096168
H	1.110008	-4.444951	0.420583
H	2.174008	-3.851043	-0.869540
C	0.546758	-1.961900	-1.799861
F	-0.522741	-1.591384	-2.541544
F	1.055420	-0.510228	-1.379786
F	1.517621	-2.334414	-2.638298
C	-0.719617	-2.295348	0.296069
H	-0.718050	-2.950009	1.176108
H	-0.384781	-1.280919	0.710127
C	-2.161742	-2.119301	-0.207184
H	-2.467913	-3.029862	-0.735252
H	-2.209794	-1.304336	-0.932319
C	-3.158420	-1.831149	0.930297
H	-2.873325	-0.899641	1.431390
H	-3.091106	-2.632312	1.678343
C	-4.577079	-1.734939	0.414220
C	-5.358684	-2.889173	0.264305
C	-5.122497	-0.506824	0.014191
C	-6.646196	-2.822680	-0.269773
H	-4.950237	-3.849850	0.570442
C	-6.409999	-0.435908	-0.521990
H	-4.541772	0.402620	0.126394
C	-7.177127	-1.593364	-0.667029

H	-7.235658	-3.729734	-0.373810
H	-6.814259	0.527356	-0.822101
H	-8.179728	-1.538536	-1.081824

^{3}IM10

E_{gas} optimization: -2178.90127584 a.u.

E_{sol} single-point: -2179.45575022 a.u.

G_{sol} thermo-corrected: -2178.88065322 a.u.

Ni	-0.741674	-0.637083	0.080074
O	-0.322863	-0.842162	-4.057161
O	-2.332441	-2.440181	3.489713
N	-0.778552	-0.391987	-1.899999
N	-0.059603	-2.519876	-0.120691
N	-1.808416	-1.173551	1.701586
C	-1.444902	0.693308	-2.624718
H	-1.033736	1.645514	-2.281735
C	-1.032310	0.417770	-4.101179
H	-1.886666	0.305798	-4.773180
H	-0.352713	1.179401	-4.494103
C	-0.211007	-1.202160	-2.753119
C	0.490797	-2.414318	-2.480437
H	0.963963	-2.899431	-3.324531
C	0.533232	-3.009533	-1.243295
C	1.212297	-4.339630	-0.956240
H	2.261401	-4.318834	-1.264869
H	0.725322	-5.141290	-1.521937
C	1.026759	-4.510062	0.566690
H	0.621111	-5.484683	0.851183
H	1.971125	-4.381644	1.107796
C	0.081759	-3.376300	0.927374
C	-0.559670	-3.248810	2.136370
H	-0.414649	-3.999977	2.902287
C	-1.538652	-2.245701	2.400456
C	-3.162629	-1.261944	3.617751
H	-2.767068	-0.649115	4.434143
H	-4.175910	-1.581043	3.867037
C	-3.053473	-0.579054	2.239803
H	-3.878615	-0.918798	1.597691
C	-3.043048	0.934919	2.207232
C	-3.669028	1.586225	1.138032
H	-4.187227	1.004016	0.382023
C	-3.619706	2.975745	1.023415
H	-4.103387	3.457311	0.179438
C	-2.943892	3.732562	1.980029
H	-2.898338	4.814024	1.890642
C	-2.319303	3.092150	3.052319
H	-1.785023	3.673461	3.798095
C	-2.368435	1.703112	3.164375
H	-1.859908	1.221320	3.993779
C	-2.945799	0.701305	-2.386398
C	-3.656613	1.904284	-2.465868
H	-3.121278	2.828857	-2.667731
C	-5.038151	1.929374	-2.268589
H	-5.576047	2.871241	-2.330100
C	-5.725418	0.748081	-1.977857
H	-6.798919	0.767496	-1.814367
C	-5.022143	-0.456056	-1.890808
H	-5.548063	-1.378333	-1.660185
C	-3.641069	-0.479168	-2.095851
H	-3.090311	-1.410965	-2.010030
H	0.926448	-0.495897	2.615270
C	0.909857	0.443025	0.670610
C	0.929862	0.517329	2.200195
H	1.809652	1.045266	2.594031
H	0.043336	1.029815	2.577308
C	0.742079	1.811584	0.094587
F	-0.553772	2.270069	0.201174
F	1.503715	2.789450	0.676826
F	1.041496	1.876496	-1.240587
C	2.155306	-0.255089	0.103496
H	2.007716	-0.450788	-0.964616
H	2.216225	-1.241186	0.581899
C	3.505592	0.461405	0.285103
H	3.479877	1.440012	-0.206299
H	3.698305	0.656710	1.346667
C	4.673877	-0.361121	-0.291220
H	4.479694	-0.556385	-1.354298
H	4.702105	-1.340371	0.205077
C	6.007479	0.331687	-0.132738
C	6.440846	1.273362	-1.076551
C	6.816542	0.092824	0.986151
C	7.646844	1.954996	-0.909935
H	5.823419	1.471295	-1.949890
C	8.024175	0.771496	1.158339
H	6.494564	-0.634199	1.728477

C	8.444136	1.705897	0.209606
H	7.965864	2.678868	-1.655094
H	8.638218	0.568801	2.031819
H	9.384725	2.233619	0.340052

^{3}TS13

E_{gas} optimization: -2178.88471245 a.u.

E_{sol} single-point: -2179.43909402 a.u.

G_{sol} thermo-corrected: -2178.86550702 a.u.

Ni	-0.822142	0.670999	0.151560
O	0.473449	0.360699	4.147679
O	-2.906010	2.987977	-2.701804
N	-0.408496	0.209871	2.082472
N	-0.089695	2.588723	0.498314
N	-2.074289	1.432452	-1.295109
C	-0.789403	-1.061728	2.715271
H	-0.237409	-1.866870	2.222162
C	-0.310655	-0.857164	4.179570
H	-1.146603	-0.707047	4.870645
H	0.325192	-1.665085	4.547956
C	0.285357	0.924604	2.926051
C	0.863024	2.208550	2.708509
H	1.450823	2.619510	3.519442
C	0.661686	2.956866	1.574102
C	1.218151	4.361060	1.388928
H	2.294657	4.392566	1.578420
H	0.744190	5.043090	2.103753
C	0.835001	4.700626	-0.064182
H	0.389428	5.691599	-0.182980
H	1.703150	4.652205	-0.732129
C	-0.136410	3.589718	-0.426521
C	-0.956930	3.617579	-1.525752
H	-0.950084	4.486633	-2.171532
C	-1.945604	2.627429	-1.808604
C	-3.757790	1.836423	-2.894780
H	-3.554593	1.415740	-3.884779
H	-4.797534	2.166401	-2.852431
C	-3.370356	0.873080	-1.748237
H	-4.078787	0.977699	-0.915680
C	-3.315498	-0.589599	-2.129819
C	-3.955938	-1.535523	-1.325912
H	-4.474783	-1.215026	-0.426864
C	-3.893269	-2.892243	-1.640260
H	-4.384578	-3.614853	-0.995208
C	-3.186671	-3.317333	-2.765448
H	-3.132379	-4.374326	-3.010444
C	-2.538698	-2.378276	-3.571008
H	-1.973127	-2.702835	-4.439722
C	-2.602995	-1.022983	-3.253434
H	-2.077622	-0.302425	-3.874521
C	-2.273493	-1.343745	2.580143
C	-2.724457	-2.613995	2.213281
H	-2.000935	-3.393743	1.994456
C	-4.089941	-2.874344	2.091487
H	-4.425918	-3.866547	1.803623
C	-5.021107	-1.858824	2.320209
H	-6.083994	-2.058917	2.218205
C	-4.577106	-0.581324	2.673280
H	-5.294031	0.216482	2.847043
C	-3.211048	-0.328082	2.805724
H	-2.863696	0.668085	3.066849
H	0.987450	1.546651	-2.290456
C	1.012523	-0.173788	-0.994518
C	0.955523	0.455662	-2.374577
H	1.793490	0.143073	-3.014398
H	0.027802	0.195809	-2.886432
C	0.477850	-1.461007	-0.860335
F	-1.177264	-1.344999	-0.164869
F	0.093448	-2.161171	-1.919972
F	0.952208	-2.277273	0.087508
C	2.191948	0.189857	-0.105582
H	1.990179	-0.108210	0.927627
H	2.281100	1.282674	-0.088687
C	3.531639	-0.422570	-0.548564
H	3.450731	-1.516508	-0.536546
H	3.756175	-0.138216	-1.584106
C	4.701058	0.009680	0.356133
H	4.472488	-0.273994	1.391790
H	4.776072	1.104917	0.343419
C	6.017251	-0.600967	-0.066446
C	6.401670	-1.866171	0.398602
C	6.857336	0.056519	-0.975140
C	7.590819	-2.457749	-0.029397
H	5.760718	-2.389454	1.104652
C	8.048030	-0.530145	-1.406766

H	6.573944	1.039408	-1.345150
C	8.419195	-1.790824	-0.934767
H	7.872499	-3.437798	0.346134
H	8.687346	-0.001767	-2.108914
H	9.346785	-2.248238	-1.267053

^{2}TS14

E_{gas} optimization: -2225.89076607 a.u.

E_{sol} single-point: -2226.315798 a.u.

G_{sol} thermo-corrected: -2226.102728 a.u.

Cr	1.754558	-0.335424	0.026707
O	0.380356	-1.885747	-2.137356
O	2.088002	2.497994	-0.906514
O	4.257823	-0.801722	-1.580540
C	0.925537	-1.280661	-1.309714
C	1.947228	1.401982	-0.560769
C	3.288317	-0.617182	-0.975721
C	1.288079	-1.920088	1.535449
C	0.568302	-0.740816	1.861066
C	1.508220	0.299138	2.112316
C	2.815027	-0.242133	1.949695
C	2.673789	-1.614658	1.582046
H	0.854025	-2.877744	1.282310
H	1.261634	1.314586	2.384689
H	3.747944	0.287836	2.083260
H	3.482171	-2.305264	1.383408
H	-0.506186	-0.646215	1.891909
C	-1.422081	0.922553	-0.701750
C	-1.166818	1.272462	-2.149754
H	-0.820387	0.406040	-2.714792
H	-2.087578	1.636296	-2.625513
C	-2.295749	-0.194327	-0.357971
C	-2.534454	-1.227385	-1.297531
C	-2.926539	-0.318141	0.908426
C	-3.332422	-2.322379	-0.985209
H	-2.078172	-1.182441	-2.277030
C	-3.727267	-1.413591	1.210899
H	-2.803839	0.454535	1.655157
C	-3.933240	-2.428255	0.271663
H	-3.486149	-3.097639	-1.730114
H	-4.199564	-1.472212	2.187329
H	-4.556681	-3.283659	0.513685
C	-1.408178	2.108505	0.231971
F	-0.564603	3.076571	-0.173649
F	-2.639801	2.674911	0.333963
F	-1.035538	1.790343	1.506680
H	0.235256	0.294888	-0.400266
H	-0.408357	2.050396	-2.233337

^{3}TS$_{REB}$

E_{gas} optimization: -2060.92842935 a.u.

E_{sol} single-point: -2061.44889070 a.u.

G_{sol} thermo-corrected: -2060.9515627 a.u.

Ni	0.347159	0.387897	-1.050552
O	-0.563937	-3.518264	-1.764874
O	0.308038	4.457083	-0.718439
N	0.268548	-1.506871	-1.174141
N	-1.513413	0.673521	-1.648095
N	0.735152	2.242098	-0.857385
C	1.266161	-2.486961	-0.712740
H	1.123464	-2.641045	0.362375
C	0.830146	-3.755090	-1.475857
H	1.375998	-3.864846	-2.422175
H	0.913083	-4.673598	-0.892587
C	-0.751921	-2.167896	-1.672861
C	-2.008398	-1.656078	-2.089946
H	-2.731125	-2.380440	-2.443873
C	-2.349621	-0.322861	-2.043751
C	-3.713379	0.231430	-2.420786
H	-4.475986	-0.172216	-1.748056
H	-3.988712	-0.054223	-3.440921
C	-3.537432	1.755533	-2.247830
H	-3.644868	2.301636	-3.191218
H	-4.255503	2.180396	-1.540871
C	-2.117298	1.885790	-1.721172
C	-1.515308	3.080886	-1.383291
H	-2.074566	4.004029	-1.471058
C	-0.156877	3.198239	-0.987517
C	1.737144	4.356758	-0.555164
H	2.030401	4.935030	0.323452
H	2.216808	4.788140	-1.440604
C	2.019792	2.839317	-0.436135
H	2.791149	2.537746	-1.152536
C	2.419899	2.317146	0.932741

C	3.245452	1.189120	1.013265
H	3.636895	0.739704	0.104329
C	3.559022	0.625526	2.251324
H	4.194307	-0.253995	2.289888
C	3.056910	1.190600	3.425083
H	3.303599	0.757165	4.390043
C	2.229335	2.314363	3.352513
H	1.827351	2.753809	4.261115
C	1.906034	2.867842	2.113217
H	1.235157	3.721737	2.066401
C	2.692080	-2.040111	-0.941612
C	3.678611	-2.329134	0.007664
H	3.408773	-2.877552	0.906941
C	4.994990	-1.902108	-0.179127
H	5.749503	-2.132028	0.567999
C	5.336673	-1.167843	-1.317174
H	6.357327	-0.824258	-1.458649
C	4.357098	-0.872978	-2.269628
H	4.614154	-0.298616	-3.155291
C	3.044124	-1.309295	-2.084804
H	2.273721	-1.059609	-2.808185
H	-0.184708	0.983618	1.512873
C	-1.388228	-0.739120	1.956773
C	-0.335611	0.261749	2.321438
H	-0.618796	0.830861	3.218031
H	0.627799	-0.205324	2.513970
C	-2.702653	-0.342032	1.556675
C	-3.021680	1.040008	1.437433
C	-3.748717	-1.272988	1.292427
C	-4.305534	1.459324	1.117565
H	-2.249742	1.784265	1.588192
C	-5.026865	-0.841045	0.967636
H	-3.552252	-2.335079	1.351072
C	-5.322458	0.525997	0.884816
H	-4.514310	2.522846	1.043448
H	-5.804848	-1.575812	0.780261
H	-6.326799	0.857026	0.637751
C	-1.097562	-2.192749	2.171347
F	-1.866173	-2.733824	3.156162
F	-1.327438	-2.957456	1.066184
F	0.192932	-2.423200	2.523438