Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Nickel Catalyzed Regio- and Stereoselective Arylation and Methylation of Allenamides via Coupling Reactions. An Experimental and Computational Study

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Contents

1 Alternative mechanism: Allenamide first and phenylboronate second

A mechanism in which the order of participation of the reagents is inverted was also considered. However, the key transition state in which the phenyl fragment migrates onto the cumulene carbon atom of the allenamide is very high in energy (43.1 kcal/mol with respect to the resting state of the catalyst, **A**) and the corresponding mechanism is therefore not competitive.

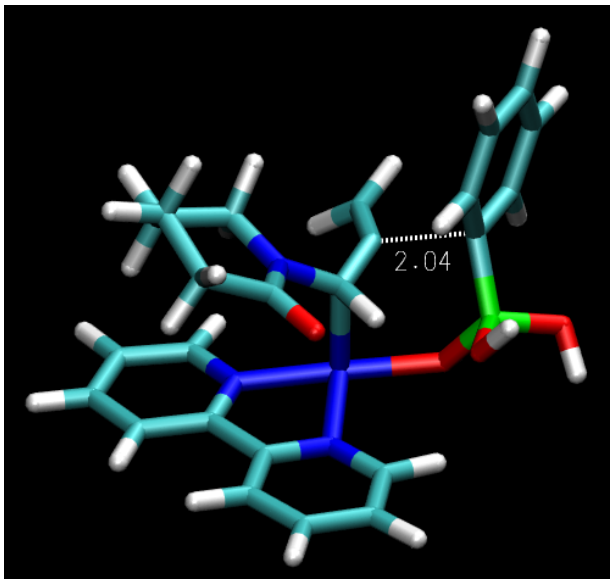

Figure S6: Computed the phenyl migration transition state for the alternative mechanism where allenamide is complexed to nickel prior to the participation of the phenylboronate. Key bond lenght for the forming C—C bond is given in Å.

2 α- vs. γ-attack in the PhB(OH)$_2$-mediated three-component variant with acetaldehyde

The two alternative nucleophilic attacks for the Ni-allenyl derivative **D** onto acetaldehyde are represented in Figure S7. It can be observed that the α-product is kinetically more favoured but thermodynamically unstable given the 2.6 kcal/mol barrier to revert from the adduct to **D**.

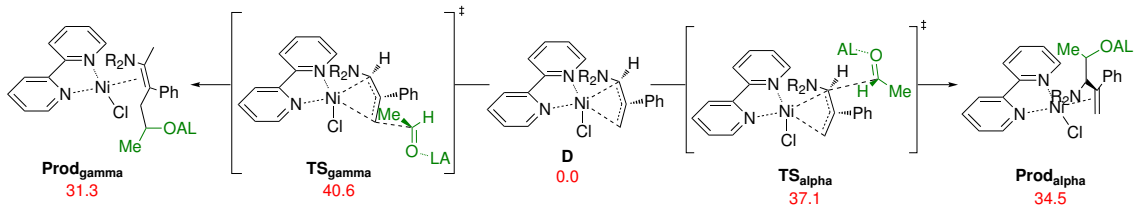

Figure S7: Computed mechanism for the $ZnMe_2$-mediated organonickel insertion onto N-allenyl amines (Gibbs free energies in kcal/mol).

3 $ZnMe_2$ vs. $PhB(OH)_2$ in the three-component variant with aldehydes

The computed pathway for the three-component non-redox catalytic cycle of the $ZnMe_2$-mediated insertion to N-allenyl amines is provided below. A comparative analysis with the mechanism found for the phenylboronic transmetallating agent (Scheme 4 in the manuscript) suggests that the main differences between these two reagents are not due to different intermediates or chemical steps. actually, most steps found for $ZnMe_2$ are essentially mimics of what was described earlier with the phenylboronic acid. however, all the steps where $ZnMe_2$ participates (A to C) display reduced energy requirements compared to the boronic analog (14.0 vs. 20.6 kcal/mol), in good agreement with the enhanced reactivity observed in the former. The main differences between the two reaction mechanisms appear in the electronic structure of the intermediates. With $ZnMe_2$ all the steps occur in the singlet spin state up to the late attack onto the aldehyde (TS_{EF}). In this step the reactivity trends seem to revert due to boron derivatives being better Lewis acids than zinc complexes. This explains why we could not find a transition state for such a nucleophilic attack in the singlet surface. On the triplet surface, however, a transition state corresponding to this process could be located. It is noteworthy that, unlike in the boron mechanism, this is not an irrelevant step in terms of the energy barrier (18.6 kcal/mol) and therefore small spin-orbit couplings could render this attack unfeasible under the thermal conditions used. This last finding increased the urgency for an alternative redox mechanism. We considered also that the improved kinetics could be a consequence of a completely different mechanism operating in this case since $ZnMe_2$ could access redox chemistry that is not available to boron derivatives. This line of thinking was supported by a sudden color change in the reaction flask that was never observed when phenylboronic acid was employed.

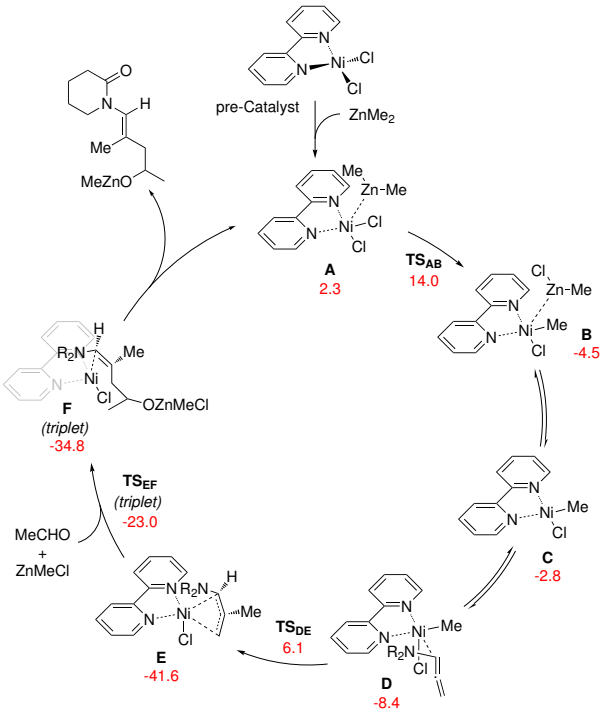

Figure S8: Computed mechanism for the $ZnMe_2$-mediated organonickel insertion onto N-allenyl amines (Gibbs free energies in kcal/mol).

4 Energy Span Model

We used the Energy Span Model by Kozuch and Shaik to account for the degree of competition between the two alternative mechanisms computed for the $ZnMe_2$-mediated three-component variant of the reaction. This model assumes an adiabatic energy profile for the mechanism and relies on the transition state theory (TST). Using TST on adiabatic surfaces also implies that all the intermediates are considered to be fully relaxed at each step of the reaction profile (no dynamic effects are considered in the model). These assumptions have to be taken with some care for the non-redox pathway since it involves singlet-triplet surface crosses that are spin forbidden. Here we have used the triplet transition state in the energy span model taking no consideration of the spin flip event. This is to say that we are therefore obtaining an upper limit for the reaction rate for that mechanism, since we are considering that the spin flip event does not affect the rate of the reaction. The results thus obtained suggest that the most favourable profile is the non-redox one, with an energy span of 20.7 kcal/mol vs 36.5 kcal/mol for the redox one.

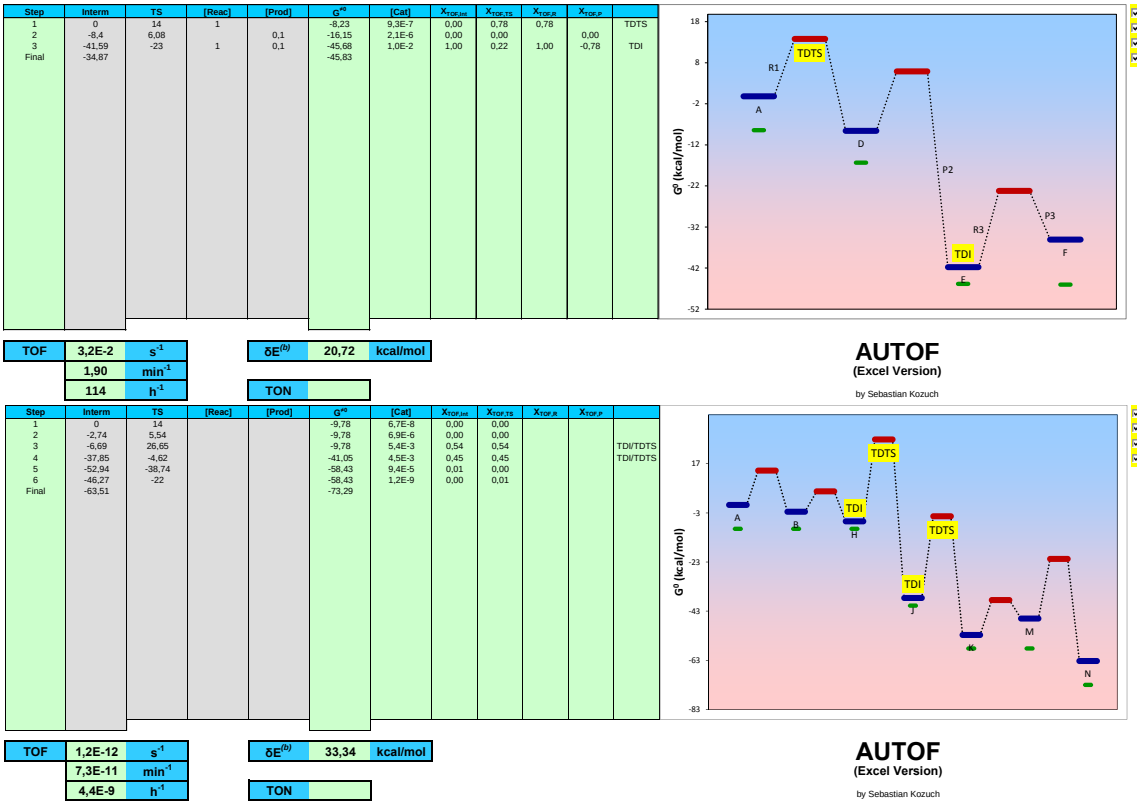

Figure S9: Energy Span Model results for the $ZnMe_2$-mediated three-component variant of the cross-coupling reaction (the non-redox version at the top and the redox alternative at the bottom.

5 Ni(II) vs. Ni(I) activation

In a previous communication on this chemistry (Org. Lett., 2017, 19, 5034) a referee asked for the possibility of Ni(I) species being actually activating this chemistry. At the time we had not considered this option due to the absence of an obvious reducing agent in the reaction mixture, but we rationalized that the inertness of the catalyst with respect to the addition of iodo-aranes suggested that these species were not present/participating in the reaction mechanism. Nevertheless, in the current work we decided to explore the Ni(I) chemistry computationally to determine whether this catalyst could also activate the coupling process. The energy profiles obtained suggest that indeed Ni(I)-based catalyst could promote the formation of the enamide however at a significantly slower rate than Ni(II) complexes (see the energy profiles in Figure S10).

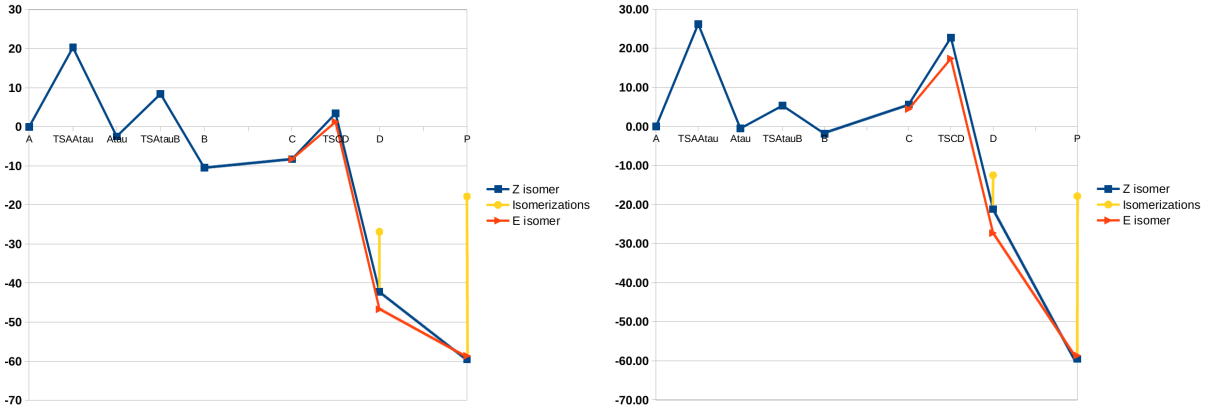

Figure S10: Gibbs free energy profiles (in kcal/mol, 1 Atm, 298K) for the allenamide formation with Ni(II) (left) and Ni(I) catalysts (right).

6 Cartesian Coordinates

Structure names correspond to the labels in the manuscript with a few exceptions where self explanatory names have been used for structures with no label in the main manuscript (like boronate, precatalyst or solvated pre-catalyst).

6.1 Isomers of the pre-catalyst

Pre-catalyst 2
SCF Energy: -3075.59494063
ZPE-corrected Energy: -3075.38374
ΔU: -3075.36392
ΔH: -3075.36297
ΔG: -3075.43582
Num. Imaginary Frequencies: 0

N	0.562927	-1.286963	-0.020986
C	0.446831	-2.617963	-0.029465
C	1.553390	-3.460960	-0.021887
C	2.825023	-2.900619	-0.004204
C	2.947411	-1.515325	0.004212
C	1.795477	-0.733413	-0.004913
H	-0.580936	-2.998051	-0.044234
H	1.405375	-4.544781	-0.029256
H	3.718613	-3.533359	0.003581
H	3.935895	-1.048198	0.020123
C	1.796109	0.732185	0.002622
N	0.564011	1.286801	0.016129
C	0.449033	2.617916	0.022453
C	1.556319	3.459956	0.015563
C	2.827507	2.898509	0.001310
C	2.948734	1.513104	-0.005130
Ni	-0.885883	0.000530	-0.000374
H	-0.578403	2.998930	0.035633
H	1.409211	4.543913	0.021010
H	3.721645	3.530486	-0.005426
H	3.936855	1.045127	-0.018531
O	-1.452317	-0.129646	2.696548
H	-1.904231	0.651775	2.327247
H	-1.916448	-0.860077	2.246623
O	-1.475971	0.129053	-2.694773
Cl	-2.464399	1.559309	0.080733
Cl	-2.466200	-1.557134	-0.071831
H	-1.935707	0.859903	-2.241053
H	-1.924227	-0.651948	-2.320133

Pre-catalyst 3
SCF Energy: -3075.59792136
ZPE-corrected Energy: -3075.38617
ΔU: -3075.36813
ΔH: -3075.36718
ΔG: -3075.43318
Num. Imaginary Frequencies: 0

N	1.641917	-0.196198	0.164101
C	2.778363	-0.876854	-0.002284
C	3.958094	-0.256455	-0.400515
C	3.948441	1.112751	-0.641506
C	2.763043	1.820192	-0.468502
C	1.621161	1.137110	-0.061142
H	2.715669	-1.954337	0.185747
H	4.867276	-0.852434	-0.521828
H	4.857464	1.631846	-0.962747
H	2.727312	2.897999	-0.650434
C	0.320319	1.767574	0.185693
N	-0.627888	0.905722	0.612033
C	-1.852813	1.347270	0.898228
C	-2.192790	2.692481	0.774713
C	-1.229121	3.588976	0.332141
C	0.050040	3.122663	0.034459
Ni	-0.086085	-0.935379	0.520227
H	-2.579387	0.602329	1.231848
H	-3.209145	3.015793	1.016158
H	-1.466424	4.651669	0.216799
H	0.825190	3.810893	-0.314668
O	-1.837410	-1.533955	0.908387
H	-1.807508	-2.508805	0.962264
H	-2.502325	-1.266484	0.137905
O	-0.462760	-0.778031	-1.949574
Cl	0.534810	-3.041868	0.481449
Cl	-3.468840	-0.527922	-1.241857
H	-1.441811	-0.614019	-1.913510
H	-0.382701	-1.742436	-2.038115

Pre-catalyst
SCF Energy: -3075.60141207
ZPE-corrected Energy: -3075.38971
ΔU: -3075.37084
ΔH: -3075.36990
ΔG: -3075.43721
S^2 before (0.9953) and after higher multiplicity projection (0.0137)
Num. Imaginary Frequencies: 0

N	-0.976891	-1.048339	-0.259675
C	-1.337317	-2.324739	-0.322607
C	-2.671691	-2.718619	-0.288789
C	-3.646142	-1.731237	-0.172792
C	-3.259740	-0.397007	-0.091325
C	-1.900165	-0.083296	-0.135250
H	-0.519684	-3.053706	-0.399040
H	-2.935993	-3.778719	-0.346587
H	-4.707933	-1.997459	-0.137255
H	-4.014199	0.387704	0.015544
C	-1.369113	1.295154	-0.033493
N	-0.029699	1.397702	-0.006073
C	0.555389	2.587559	0.093289
C	-0.182042	3.766539	0.171221
C	-1.570069	3.680891	0.142076
C	-2.175045	2.431411	0.038337
Ni	0.963367	-0.389723	-0.075465
H	1.653779	2.574148	0.106032
H	0.329499	4.730167	0.253617
H	-2.186416	4.584498	0.199931
H	-3.265572	2.349981	0.011189
O	1.113909	-0.296958	-2.277448
H	1.270198	-1.218757	-2.549331
H	2.011809	0.099589	-2.174769
O	1.907124	-2.343474	-0.237105
H	2.804569	-1.948727	-0.302791
H	1.755038	-2.430829	0.739480
Cl	3.181841	0.428122	-0.294549
Cl	0.879577	-1.001515	2.192764

SolvatedPre-catalyst
SCF Energy: -2691.68255479
ZPE-corrected Energy: -2691.44724
ΔU: -2691.42718
ΔH: -2691.42623
ΔG: -2691.49528
S^2 before (1.0002) and after higher multiplicity projection (0.0114)
Num. Imaginary Frequencies: 0

N	0.227688	1.353324	-0.177337
C	-0.063560	2.651997	-0.157291
C	0.917775	3.627411	-0.008102
C	2.240251	3.216243	0.126388
C	2.538211	1.856556	0.109648
C	1.499751	0.937919	-0.041359
H	-1.124707	2.912124	-0.262902
H	0.644140	4.686319	0.005722
H	3.042825	3.950877	0.248494
H	3.573680	1.522738	0.218648
C	1.697488	-0.529533	-0.054181
N	0.584525	-1.266355	-0.227622
C	0.655648	-2.594815	-0.217188
C	1.856508	-3.277280	-0.056442
C	3.018648	-2.529790	0.108070
C	2.940487	-1.140367	0.112341
Ni	-1.154417	-0.157912	-0.211055
H	-0.291575	-3.134768	-0.336016
H	1.873870	-4.370842	-0.055852
H	3.986103	-3.024797	0.240931
H	3.845149	-0.542941	0.254044
O	-1.297522	-0.124737	-2.315995
H	-1.800436	0.633966	-2.663326
H	-0.457683	-0.147547	-2.807900
O	-2.829258	1.160108	-0.158584
H	-3.625966	0.653176	-0.404682
H	-2.832121	1.173956	0.828621
O	-2.613321	-1.677703	-0.214225
Cl	-1.456751	-0.251101	2.087543
H	-2.668249	-2.477433	-0.764987
H	-2.648519	-1.924759	0.734331

6.2 Ni/B mechanism

A.3
SCF Energy: -3022.63183798
ZPE-corrected Energy: -3022.30595
ΔU: -3022.27991
ΔH: -3022.27896
ΔG: -3022.36720
S^2 before (2.0073) and after higher multiplicity projection (2.0000)
Num. Imaginary Frequencies: 0

N	1.478088	1.634776	0.412550
C	0.862992	2.782898	0.679959
C	1.500840	4.009611	0.519785
C	2.812596	4.014895	0.054388
C	3.440421	2.808631	-0.245695
C	2.735049	1.620502	-0.057694
H	-0.176194	2.703796	1.021914
H	0.973069	4.939446	0.750776
H	3.348093	4.959549	-0.087691
H	4.462458	2.801894	-0.635191
C	3.262149	0.276551	-0.382353
N	2.380305	-0.736508	-0.257617
C	2.745099	-1.980314	-0.571774
C	4.028355	-2.282374	-1.020041
C	4.953568	-1.251395	-1.133966
C	4.566431	0.047257	-0.814831
Ni	0.588934	-0.186080	0.571100
H	1.979637	-2.760419	-0.485829
H	4.285838	-3.314884	-1.272769
H	5.974797	-1.451415	-1.475012
H	5.279312	0.872170	-0.901942
O	-0.072288	-3.494122	-0.588365
H	0.143384	-3.100009	0.285563
H	-0.907661	-3.967752	-0.368102
O	-0.943874	0.397090	-0.308639
B	-2.049011	-0.273818	-0.639763
O	-2.505575	-3.657545	0.711797
Cl	0.175166	-1.840259	2.055378
O	-2.064637	-1.588367	-1.072440
C	-3.468734	0.423498	-0.550101
H	-1.180377	-2.019599	-1.094120
C	-4.655702	-0.273747	-0.821160
C	-5.901896	0.343243	-0.719240
C	-5.985704	1.684702	-0.345411
C	-4.818983	2.400516	-0.074030
C	-3.580092	1.770311	-0.174950
H	-4.597518	-1.328683	-1.119784
H	-6.816185	-0.224097	-0.933226
H	-6.964185	2.174307	-0.265042
H	-4.880291	3.456096	0.219515
H	-2.660649	2.331489	0.039466
H	-2.044892	-3.179828	1.426001
H	-2.737645	-2.941379	0.081405

Allenamide
SCF Energy: -440.745600425
ZPE-corrected Energy: -440.570139
ΔU: -440.560440
ΔH: -440.559496
ΔG: -440.605314
Num. Imaginary Frequencies: 0

C	0.133418	-0.881568	-0.053652
N	-0.063563	0.485386	-0.034677
O	-0.802780	-1.654592	-0.078265
C	1.008154	1.478000	0.080016
C	-1.370050	1.007520	0.019221
C	2.362019	0.933180	-0.315083
H	0.741993	2.342729	-0.556284
H	1.043978	1.850721	1.126416
C	2.607582	-0.389426	0.384187
H	2.404168	0.785479	-1.413705
H	3.132370	1.684321	-0.062266
C	1.561826	-1.382001	-0.086165
H	3.623563	-0.773525	0.180426
H	2.536144	-0.246864	1.482193
H	1.761669	-1.671076	-1.138867
H	1.572055	-2.324797	0.488590
C	-2.533533	0.390263	0.030723
H	-1.381043	2.107322	0.054198
C	-3.763413	-0.052261	0.042942
H	-4.321760	-0.239123	-0.888012
H	-4.281973	-0.298388	0.983034

A
SCF Energy: -3022.63656517
ZPE-corrected Energy: -3022.30973
ΔU: -3022.28439
ΔH: -3022.28344
ΔG: -3022.36719
S^2 before (0.1694) and after higher multiplicity projection (0.0005)
Num. Imaginary Frequencies: 0

N	-1.021795	1.522789	-0.035862
C	-0.090775	2.472285	0.072196
C	-0.409782	3.767843	0.467879
C	-1.735561	4.073545	0.756158
C	-2.704200	3.081046	0.632928
C	-2.313308	1.807789	0.228591
H	0.928831	2.153918	-0.175667
H	0.380201	4.520286	0.546553
H	-2.020298	5.082263	1.073106
H	-3.754042	3.300712	0.847113
C	-3.225695	0.673436	0.031429
N	-2.622415	-0.455144	-0.405561
C	-3.361036	-1.544213	-0.635902
C	-4.737807	-1.564429	-0.436755
C	-5.365578	-0.410910	0.018888
C	-4.598522	0.726039	0.254711
Ni	-0.676192	-0.305277	-0.565575
H	-2.807230	-2.421825	-0.990817
H	-5.300107	-2.480781	-0.638030
H	-6.446697	-0.391353	0.190993
H	-5.067641	1.646890	0.612832
O	-0.643320	-2.302755	1.985097
H	-0.947604	-2.403057	1.061833
H	0.043631	-3.010961	2.031592
O	1.108364	0.041629	-0.652027
B	2.030807	-0.305266	0.246549
O	1.560867	-3.759736	1.173454
Cl	-0.369916	-2.411559	-1.194476
O	1.788778	-0.977658	1.431978
C	3.534284	0.128592	0.001844
H	0.842234	-1.193271	1.602394
C	4.544618	-0.140068	0.937240
C	5.862411	0.259373	0.718270
C	6.197116	0.943979	-0.450483
C	5.208500	1.224878	-1.394443
C	3.894790	0.818849	-1.165041
H	4.284755	-0.675198	1.859716
H	6.636538	0.036434	1.463155
H	7.233098	1.259021	-0.627001
H	5.467695	1.760742	-2.316272
H	3.115240	1.032397	-1.908268
H	1.198939	-3.593131	0.280700
H	2.075611	-2.946070	1.352404

Boronic
SCF Energy: -328.500064142
ZPE-corrected Energy: -328.427816
ΔU: -328.421101
ΔH: -328.420157
ΔG: -328.457940
Num. Imaginary Frequencies: 1
Imaginary Frequency: -267.6752

B	0.745197	-0.023908	-0.000458
O	0.082322	-1.200661	-0.000983
O	0.057513	1.173432	-0.000891
H	-0.894376	-1.072592	-0.001302
O	2.111368	0.022413	0.001161
H	2.487118	-0.870355	0.001307
H	0.664463	1.928415	-0.000810
O	-2.349401	-0.084301	0.000957
H	-3.304620	0.067809	0.000393
H	-1.892981	0.779206	0.000752

C.3
SCF Energy: -2694.11056465
ZPE-corrected Energy: -2693.86085
ΔU: -2693.84300
ΔH: -2693.84206
ΔG: -2693.91026
S^2 before (2.0110) and after higher multiplicity projection (2.0001)
Num. Imaginary Frequencies: 0

N	1.642365	-0.983110	0.410149
C	2.160382	-2.180670	0.665633
C	3.513965	-2.359267	0.935860
C	4.342580	-1.240629	0.917417
C	3.800846	0.006374	0.619525
C	2.431943	0.100905	0.364016
H	1.459401	-3.024190	0.631769
H	3.907120	-3.357805	1.148799
H	5.414380	-1.337965	1.120716
H	4.445509	0.888997	0.573254
C	1.747410	1.358424	-0.012916
N	0.448751	1.227714	-0.339802
C	-0.252828	2.286849	-0.738885
C	0.311175	3.556213	-0.830810
C	1.648664	3.711183	-0.479231
C	2.378862	2.601112	-0.064317
Ni	-0.364385	-0.646280	-0.099683
H	-1.305942	2.098656	-0.984763
H	-0.293300	4.403109	-1.168679
H	2.127603	4.694918	-0.528273
H	3.431060	2.708002	0.215304
C	-2.259884	-0.301788	0.271387
Cl	-0.257652	-2.034532	-1.858498
C	-3.274955	-1.112499	-0.265883
C	-4.621870	-0.907734	0.037498
C	-4.999174	0.124770	0.897867
C	-4.016993	0.946712	1.448224
C	-2.672191	0.731418	1.132441
H	-2.997687	-1.926436	-0.951025
H	-5.388508	-1.558576	-0.403774
H	-6.057466	0.289098	1.137004
H	-4.299649	1.762046	2.127710
H	-1.925069	1.402550	1.588150

C
SCF Energy: -2694.13063104
ZPE-corrected Energy: -2693.87946
ΔU: -2693.86242
ΔH: -2693.86148
ΔG: -2693.92593
Num. Imaginary Frequencies: 0

N	1.805755	-0.833963	-0.011957
C	2.516577	-1.961063	0.019821
C	3.905798	-1.958758	0.108832
C	4.568305	-0.736806	0.171149
C	3.825009	0.439163	0.135887
C	2.436322	0.354003	0.040614
H	1.919412	-2.881979	-0.028254
H	4.453067	-2.906066	0.130946
H	5.660157	-0.694640	0.246664
H	4.327064	1.409764	0.184264
C	1.535459	1.514850	-0.026366
N	0.215703	1.209944	-0.084150
C	-0.666700	2.212542	-0.191441
C	-0.288006	3.550001	-0.228571
C	1.063126	3.868234	-0.151408
C	1.985901	2.833441	-0.052099
Ni	-0.189737	-0.683285	-0.045600
H	-1.721679	1.923166	-0.246271
H	-1.055248	4.324905	-0.317175
H	1.399604	4.909982	-0.174245
H	3.056347	3.051996	-0.001974
C	-2.040345	-0.424418	0.036498
Cl	-0.537485	-2.820260	-0.105203
C	-2.871598	-0.563956	-1.081959
C	-4.234212	-0.266425	-1.010383
C	-4.801352	0.152131	0.194309
C	-3.992798	0.265516	1.325220
C	-2.627325	-0.019877	1.243037
H	-2.450925	-0.920570	-2.032701
H	-4.863680	-0.373097	-1.903697
H	-5.872885	0.379609	0.253343
H	-4.429194	0.579673	2.282619
H	-2.007324	0.090324	2.145644

D1
SCF Energy: -3134.90077995
ZPE-corrected Energy: -3134.47125
ΔU: -3134.44409
ΔH: -3134.44315
ΔG: -3134.52778
Num. Imaginary Frequencies: 0

Ni	-0.829995	-0.480239	-0.466125
N	1.034088	-0.545100	-1.252417
C	1.617262	-1.663265	-1.677954
C	2.907931	-1.676718	-2.195638
C	3.597119	-0.469423	-2.285701
C	2.968049	0.701714	-1.879961
C	1.668463	0.632419	-1.368072
C	0.865616	1.816674	-1.008124
H	1.011993	-2.575328	-1.604777
H	3.355038	-2.617161	-2.531378
H	4.613337	-0.435273	-2.693192
H	3.474930	1.665112	-1.987319
N	-0.434622	1.571412	-0.766535
C	-1.255668	2.595594	-0.556569
C	-0.819672	3.917741	-0.522590
C	0.533294	4.174736	-0.712171
C	1.388467	3.109675	-0.972548
H	-2.311671	2.344482	-0.400818
H	-1.535788	4.725128	-0.342257
H	0.921971	5.197870	-0.671184
H	2.454526	3.288388	-1.143233
Cl	-1.540150	-1.224599	-2.529151
C	-2.594212	-0.301477	0.258026
C	-2.811199	0.616694	1.294923
C	-4.089185	0.813341	1.828580
C	-5.170086	0.079252	1.347145
C	-4.958947	-0.852740	0.330875
C	-3.685145	-1.043730	-0.206628
H	-1.975455	1.199443	1.708246
H	-4.231677	1.544601	2.634793
H	-6.172907	0.227109	1.766232
H	-5.800030	-1.443289	-0.054926
H	-3.536023	-1.767708	-1.015389
C	-0.137751	-0.958599	1.410290
C	-0.612035	-2.017521	0.650641
C	-0.874816	-3.288755	0.410693
H	-1.324535	-3.589010	-0.547389
H	-0.675462	-4.070630	1.160665
N	1.235202	-0.714569	1.669465
C	1.560858	0.558998	2.086171
C	3.014336	0.842752	2.396320
C	3.862410	-0.377429	2.702791
C	3.606295	-1.429708	1.640992
C	2.154351	-1.852108	1.672492
O	0.722072	1.440549	2.157350
H	3.414591	1.366463	1.501559
H	3.023884	1.590870	3.208583
H	3.594918	-0.786997	3.698489
H	4.931529	-0.101638	2.752004
H	4.239298	-2.323982	1.788086
H	3.856023	-1.020074	0.639054
H	1.954578	-2.468990	2.575768
H	1.916563	-2.490862	0.802865
H	-0.810889	-0.468953	2.126280

D
SCF Energy: -3134.90006342
ZPE-corrected Energy: -3134.47044
ΔU: -3134.44320
ΔH: -3134.44226
ΔG: -3134.52779
Num. Imaginary Frequencies: 0

N	-2.246694	-0.637136	-0.614444
C	-2.785908	-1.564641	-1.402186
C	-3.980573	-1.355652	-2.082780
C	-4.626388	-0.132470	-1.925439
C	-4.079566	0.817660	-1.070742
C	-2.882621	0.529339	-0.411180
H	-2.231790	-2.508033	-1.477098
H	-4.392195	-2.141981	-2.722489
H	-5.563907	0.076818	-2.451658
H	-4.591106	1.770512	-0.908603
C	-2.281808	1.396751	0.619111
N	-1.204878	0.883241	1.240587
C	-0.714513	1.509903	2.307252
C	-1.229415	2.715152	2.777186
C	-2.295579	3.290426	2.094576
C	-2.839005	2.615762	1.007472
Ni	-0.440667	-0.818629	0.276531
H	0.131576	1.022796	2.806495
H	-0.791966	3.189314	3.661011
H	-2.717447	4.248683	2.416106
H	-3.698933	3.032642	0.475347
O	0.442791	2.285459	-1.421780
C	1.256177	-0.845229	1.143906
Cl	-1.325032	-2.511428	1.563872
C	1.837021	-2.013430	1.649946
C	3.090262	-1.983753	2.263643
C	3.787723	-0.782557	2.397427
C	3.215664	0.389874	1.908691
C	1.966916	0.353617	1.278984
H	1.288644	-2.959378	1.578572
H	3.523974	-2.915203	2.649772
H	4.769419	-0.760580	2.886035
H	3.743649	1.347547	2.012774
H	1.552562	1.293944	0.889840
C	1.515761	1.740035	-1.617522
C	2.781867	2.546191	-1.802201
C	4.073961	1.771748	-1.615234
H	2.733588	2.962811	-2.830132
H	2.698055	3.415989	-1.125885
C	3.984419	0.479587	-2.403666
H	4.937010	2.383520	-1.935705
H	4.227425	1.535070	-0.542734
C	2.863161	-0.380259	-1.860711
H	3.803409	0.709494	-3.474258
H	4.926027	-0.097029	-2.353698
N	1.613564	0.367158	-1.709378
H	2.662155	-1.233311	-2.534626
H	3.148679	-0.809966	-0.878048
C	0.412159	-0.351282	-1.565487
C	0.347467	-1.695688	-1.234711
H	-0.434196	0.137370	-2.069559
C	0.482477	-2.982996	-1.495451
H	0.235929	-3.732505	-0.729461
H	0.829418	-3.337682	-2.479118

E1
SCF Energy: -3134.96271929
ZPE-corrected Energy: -3134.53095
ΔU: -3134.50417
ΔH: -3134.50323
ΔG: -3134.58901
Num. Imaginary Frequencies: 0

Ni	-0.449482	-0.422800	0.813892
N	-0.096369	-1.849634	-0.498998
C	-1.093088	-2.444908	-1.149894
C	-0.875416	-3.483922	-2.048062
C	0.432431	-3.915323	-2.251478
C	1.466190	-3.302195	-1.552340
C	1.169330	-2.259047	-0.673403
H	-2.103479	-2.076327	-0.928299
H	-1.718927	-3.945707	-2.569939
H	0.648642	-4.734437	-2.945852
H	2.496697	-3.644105	-1.684647
C	2.190233	-1.552686	0.133026
N	1.712557	-0.701632	1.049218
C	2.553567	-0.014480	1.811791
C	3.937331	-0.135495	1.707458
C	4.445931	-1.016963	0.755739
C	3.564405	-1.737751	-0.041824
H	2.099947	0.663652	2.549601
H	4.597050	0.444675	2.360659
H	5.527302	-1.142666	0.632447
H	3.948693	-2.421434	-0.804445
Cl	-1.248840	-1.896055	2.321548
C	-1.468737	1.192488	0.477131
C	-1.010148	1.156916	1.823661
C	-0.437226	1.104629	-0.504864
H	-1.742459	1.039163	2.633259
H	-0.078402	1.666856	2.116250
N	0.724402	1.940335	-0.497157
H	-0.728783	0.781534	-1.519062
C	0.565492	3.336790	-0.075565
C	1.893138	4.018208	0.166868
C	2.774965	3.878036	-1.058363
C	3.010119	2.403926	-1.330963
C	1.778965	1.523387	-1.277188
O	1.760389	0.451465	-1.859701
H	-0.049963	3.362028	0.837557
H	-0.008571	3.886772	-0.855125
H	1.710982	5.078742	0.420689
H	2.391449	3.556149	1.045371
H	2.268716	4.348754	-1.926159
H	3.737691	4.406206	-0.930791
H	3.703041	1.984754	-0.570193
H	3.488465	2.218579	-2.308569
C	-2.889598	1.022538	0.088100
C	-3.394626	1.752517	-0.995884
C	-4.731605	1.637917	-1.374637
C	-5.583849	0.788544	-0.672451
C	-5.088140	0.051279	0.404938
C	-3.753894	0.163017	0.784859
H	-2.726549	2.434022	-1.539084
H	-5.109791	2.220722	-2.222983
H	-6.635722	0.695347	-0.967458
H	-5.749475	-0.631589	0.951497
H	-3.352631	-0.460071	1.596202

EnamideE
SCF Energy: -672.691073334
ZPE-corrected Energy: -672.410745
ΔU: -672.396312
ΔH: -672.395368
ΔG: -672.452781
Num. Imaginary Frequencies: 0

C	-0.722903	-0.295563	0.406939
C	-0.379627	-1.457415	1.284862
C	0.221627	0.470942	-0.168845
N	1.617849	0.303334	-0.029702
H	-0.061192	1.322955	-0.807401
C	2.337721	1.554392	0.221333
C	3.781787	1.339574	0.616850
C	4.450160	0.398737	-0.366184
C	3.733102	-0.937898	-0.323737
C	2.225971	-0.865070	-0.459409
O	1.590537	-1.810729	-0.880853
H	1.795342	2.099415	1.016180
H	2.286188	2.190000	-0.691359
H	4.289576	2.320622	0.659489
H	3.830608	0.906655	1.636928
H	4.394079	0.829282	-1.387285
H	5.523532	0.268601	-0.136513
H	3.931725	-1.438042	0.647310
H	4.080865	-1.638438	-1.102511
C	-2.154704	-0.019779	0.148541
C	-3.079902	-1.074264	0.104883
C	-4.429402	-0.838519	-0.148249
C	-4.889662	0.461018	-0.350748
C	-3.986044	1.522378	-0.293991
C	-2.637968	1.284425	-0.044838
H	-2.733054	-2.103813	0.253165
H	-5.128477	-1.682206	-0.188109
H	-5.952197	0.648477	-0.544071
H	-4.337853	2.551472	-0.433485
H	-1.947784	2.133617	0.028362
H	-0.326601	-2.397723	0.703127
H	0.613368	-1.320322	1.748334
H	-1.128305	-1.585814	2.088131

EnamideZ
SCF Energy: -672.691818573
ZPE-corrected Energy: -672.411701
ΔU: -672.397169
ΔH: -672.396225
ΔG: -672.454156
Num. Imaginary Frequencies: 0

C	0.926707	1.666326	-0.197210
C	1.721069	2.926322	-0.358543
C	-0.415193	1.694444	-0.267493
N	-1.247657	0.546227	-0.259695
H	-0.943547	2.655930	-0.346049
C	-1.085810	-0.424174	-1.345730
C	-1.808786	-1.721846	-1.062013
C	-3.246270	-1.435491	-0.671815
C	-3.252522	-0.616054	0.605326
C	-2.299885	0.559647	0.626609
O	-2.426476	1.459720	1.437880
H	-0.006201	-0.610425	-1.490280
H	-1.464726	0.023352	-2.290498
H	-1.746901	-2.368811	-1.956273
H	-1.295075	-2.259008	-0.237136
H	-3.742844	-0.873799	-1.489823
H	-3.823973	-2.367786	-0.533965
H	-2.957609	-1.254408	1.464216
H	-4.251192	-0.218976	0.860133
C	1.678528	0.415272	0.061074
C	2.789963	0.061063	-0.715998
C	3.485864	-1.121613	-0.470807
C	3.090813	-1.964027	0.566858
C	1.999273	-1.612369	1.362031
C	1.301075	-0.434062	1.112887
H	3.106884	0.713687	-1.539170
H	4.345979	-1.386372	-1.096980
H	3.639825	-2.892354	0.762858
H	1.694846	-2.259536	2.193114
H	0.455895	-0.147940	1.751541
H	2.356858	2.897722	-1.265612
H	1.063871	3.810055	-0.441892
H	2.404367	3.076675	0.499594

E
SCF Energy: -3134.95501756
ZPE-corrected Energy: -3134.52310
ΔU: -3134.49639
ΔH: -3134.49545
ΔG: -3134.58187
Num. Imaginary Frequencies: 0

Ni	0.274741	-1.232098	-0.140669
N	2.378304	-1.082857	-0.749026
C	2.962987	-1.551722	-1.845505
C	4.233313	-1.153758	-2.254044
C	4.907691	-0.217024	-1.475194
C	4.298471	0.271814	-0.325249
C	3.023882	-0.189950	0.013165
H	2.390527	-2.288914	-2.426283
H	4.679302	-1.570109	-3.162850
H	5.904875	0.134743	-1.761726
H	4.809252	1.017865	0.290586
C	2.301326	0.252334	1.224872
N	1.027448	-0.156381	1.329281
C	0.315476	0.146069	2.413923
C	0.822026	0.934618	3.440599
C	2.134103	1.389816	3.335631
C	2.887409	1.030453	2.225130
H	-0.690938	-0.288295	2.461901
H	0.200907	1.170619	4.310044
H	2.576908	2.006753	4.125149
H	3.930195	1.349475	2.142893
Cl	0.063678	-3.013563	1.201237
C	-1.317466	-0.899991	-1.226706
C	-0.657782	-2.095955	-1.630032
C	-0.457696	0.229012	-1.363598
H	-1.114563	-3.067137	-1.403177
H	0.004065	-2.074171	-2.511556
N	-0.861686	1.553207	-1.002916
H	0.275968	0.199347	-2.189640
C	-2.105732	2.049104	-1.615087
C	-2.619681	3.302448	-0.943984
C	-1.536766	4.363605	-0.936120
C	-0.318151	3.825490	-0.208097
C	0.125619	2.437236	-0.623239
O	1.297123	2.111542	-0.544787
H	-2.863533	1.251314	-1.563313
H	-1.920715	2.244930	-2.694847
H	-3.524749	3.649290	-1.476039
H	-2.927537	3.063390	0.095617
H	-1.268421	4.618289	-1.981988
H	-1.886339	5.299936	-0.463509
H	-0.536571	3.752690	0.879014
H	0.562600	4.483753	-0.302216
C	-2.604253	-0.955181	-0.490234
C	-3.584767	-1.871478	-0.890904
C	-4.801497	-1.963496	-0.216470
C	-5.061747	-1.139677	0.875302
C	-4.094820	-0.219591	1.285288
C	-2.882513	-0.128792	0.611015
H	-3.392306	-2.517634	-1.755492
H	-5.552990	-2.688407	-0.550468
H	-6.016314	-1.212797	1.409064
H	-4.287072	0.431675	2.146344
H	-2.129864	0.600300	0.934350

PhBoronic
SCF Energy: -560.344941699
ZPE-corrected Energy: -560.170986
ΔU: -560.157777
ΔH: -560.156833
ΔG: -560.211978
Num. Imaginary Frequencies: 0

B	-0.561162	-0.147135	-0.116041
O	-1.167593	-1.290791	0.223092
O	-1.320339	0.941199	-0.536926
H	-2.157832	-1.321595	0.080489
C	1.005062	-0.038005	-0.042325
H	-0.777344	1.663099	-0.887939
O	-3.803543	-1.258725	-0.168404
H	-4.040219	-1.334460	-1.106117
H	-4.033576	-0.328071	0.095035
O	-3.863598	1.358389	0.440105
H	-2.948228	1.396257	0.076408
H	-3.775850	1.528680	1.391535
C	1.681233	1.191040	-0.061438
C	3.071532	1.260410	0.005795
C	3.818615	0.086311	0.090826
C	3.169533	-1.148604	0.115465
C	1.779224	-1.204965	0.054093
H	1.117313	2.134663	-0.110550
H	3.575149	2.234230	-0.004411
H	4.912929	0.134023	0.141855
H	3.754464	-2.073455	0.185569
H	1.268382	-2.175399	0.080909

Pre-catalyst
SCF Energy: -3075.60141207
ZPE-corrected Energy: -3075.38971
ΔU: -3075.37084
ΔH: -3075.36990
ΔG: -3075.43721
S^2 before (0.9953) and after higher multiplicity projection (0.0137)
Num. Imaginary Frequencies: 0

N	-0.976891	-1.048339	-0.259675
C	-1.337317	-2.324739	-0.322607
C	-2.671691	-2.718619	-0.288789
C	-3.646142	-1.731237	-0.172792
C	-3.259740	-0.397007	-0.091325
C	-1.900165	-0.083296	-0.135250
H	-0.519684	-3.053706	-0.399040
H	-2.935993	-3.778719	-0.346587
H	-4.707933	-1.997459	-0.137255
H	-4.014199	0.387704	0.015544
C	-1.369113	1.295154	-0.033493
N	-0.029699	1.397702	-0.006073
C	0.555389	2.587559	0.093289
C	-0.182042	3.766539	0.171221
C	-1.570069	3.680891	0.142076
C	-2.175045	2.431411	0.038337
Ni	0.963367	-0.389723	-0.075465
H	1.653779	2.574148	0.106032
H	0.329499	4.730167	0.253617
H	-2.186416	4.584498	0.199931
H	-3.265572	2.349981	0.011189
O	1.113909	-0.296958	-2.277448
H	1.270198	-1.218757	-2.549331
H	2.011809	0.099589	-2.174769
O	1.907124	-2.343474	-0.237105
H	2.804569	-1.948727	-0.302791
H	1.755038	-2.430829	0.739480
Cl	3.181841	0.428122	-0.294549
Cl	0.879577	-1.001515	2.192764

TS AB.3
SCF Energy: -3022.59978125
ZPE-corrected Energy: -3022.27811
ΔU: -3022.25327
ΔH: -3022.25232
ΔG: -3022.33437
S^2 before (2.0072) and after higher multiplicity projection (2.0000)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -1206.9196

N	0.084002	1.443232	-0.748711
C	1.092152	2.315479	-0.740139
C	0.889197	3.665776	-0.459389
C	-0.398917	4.100658	-0.169782
C	-1.445561	3.181794	-0.176277
C	-1.168408	1.848846	-0.474686
H	2.099512	1.920708	-0.942451
H	1.739335	4.354260	-0.464459
H	-0.595044	5.152849	0.063395
H	-2.463878	3.507746	0.054174
C	-2.197764	0.784435	-0.491799
N	-1.741890	-0.449621	-0.759152
C	-2.577522	-1.485130	-0.795720
C	-3.940951	-1.340294	-0.557002
C	-4.431020	-0.068089	-0.276924
C	-3.552752	1.011132	-0.246229
Ni	0.324537	-0.624560	-0.919796
H	-2.110790	-2.451075	-1.035109
H	-4.601349	-2.211751	-0.595022
H	-5.498042	0.089004	-0.085431
H	-3.926247	2.017036	-0.034671
O	2.254543	-0.522299	-0.647177
B	2.399351	-0.568602	0.787361
Cl	0.312369	-2.655263	-1.906451
O	3.375330	0.326942	1.311986
C	0.992477	-0.657642	1.582283
H	3.323761	0.391857	2.276138
C	0.207994	-1.826847	1.579296
C	-1.046824	-1.865491	2.195213
C	-1.550226	-0.732009	2.827200
C	-0.789564	0.441434	2.850703
C	0.459548	0.470315	2.238072
H	0.593654	-2.727408	1.084697
H	-1.633331	-2.792668	2.181028
H	-2.535390	-0.759828	3.309099
H	-1.177189	1.337035	3.352719
H	1.043663	1.402746	2.256611
O	3.046591	-2.108514	0.680265
H	2.810155	-1.711250	-0.379657
H	4.004303	-2.057545	0.851396
H	4.242074	1.316326	-0.227416
O	4.208216	1.315263	-1.202812
H	3.567359	0.579496	-1.329875

TS AB
SCF Energy: -3022.60445685
ZPE-corrected Energy: -3022.28145
ΔU: -3022.25731
ΔH: -3022.25636
ΔG: -3022.33483
S^2 before (0.3367) and after higher multiplicity projection (0.0018)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -1231.9181

N	0.105604	1.241602	-0.892027
C	1.132356	2.088773	-0.986059
C	0.954594	3.463828	-0.849264
C	-0.320993	3.956256	-0.597112
C	-1.387581	3.065724	-0.506032
C	-1.139635	1.705512	-0.666415
H	2.124968	1.652292	-1.165458
H	1.817909	4.129626	-0.938155
H	-0.491888	5.031354	-0.476649
H	-2.401009	3.431343	-0.316793
C	-2.169821	0.657242	-0.610153
N	-1.713331	-0.586585	-0.868085
C	-2.555555	-1.621568	-0.836678
C	-3.907510	-1.463672	-0.548648
C	-4.390360	-0.186850	-0.280855
C	-3.510613	0.890535	-0.314216
Ni	0.240372	-0.710769	-0.947924
H	-2.099483	-2.597545	-1.046564
H	-4.565159	-2.337814	-0.533975
H	-5.447670	-0.026320	-0.044815
H	-3.865655	1.903202	-0.102588
O	2.076264	-0.668503	-0.608575
B	2.327735	-0.520972	0.828336
Cl	0.304651	-2.874377	-1.387872
O	3.414763	0.364683	1.105092
C	1.012202	-0.349730	1.741419
H	3.450692	0.601113	2.042590
C	0.097338	-1.400637	1.927863
C	-1.116966	-1.201751	2.586090
C	-1.447564	0.059580	3.083192
C	-0.545454	1.113666	2.933111
C	0.666428	0.902464	2.274384
H	0.335272	-2.394087	1.525617
H	-1.813756	-2.040257	2.713369
H	-2.402849	0.218275	3.598919
H	-0.788676	2.107160	3.331429
H	1.357799	1.749534	2.149635
O	2.863587	-2.074750	0.897418
H	2.572265	-1.832343	-0.205729
H	3.831527	-2.063066	1.007233
H	4.240490	0.990384	-0.575176
O	4.165667	0.877836	-1.542848
H	3.463696	0.192466	-1.560571

TS BC.3
SCF Energy: -3022.64053556
ZPE-corrected Energy: -3022.31584
ΔU: -3022.29127
ΔH: -3022.29033
ΔG: -3022.37128
S^2 before (2.0093) and after higher multiplicity projection (2.0000)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -179.7328

N	-0.912155	1.636457	-0.309811
C	-0.633314	2.906280	-0.020597
C	-1.624190	3.811851	0.351283
C	-2.938640	3.363269	0.422725
C	-3.223145	2.033473	0.123056
C	-2.177595	1.186436	-0.243328
H	0.425743	3.183404	-0.081564
H	-1.360240	4.847984	0.582764
H	-3.746253	4.044264	0.712330
H	-4.252452	1.666693	0.173302
C	-2.358420	-0.247309	-0.565745
N	-1.247544	-0.888829	-0.960764
C	-1.286730	-2.185005	-1.253523
C	-2.461693	-2.927260	-1.162624
C	-3.622849	-2.277836	-0.755607
C	-3.576096	-0.919053	-0.455928
Ni	0.519692	0.214178	-0.778900
H	-0.334487	-2.624407	-1.579667
H	-2.459066	-3.993449	-1.407965
H	-4.567385	-2.825748	-0.669439
H	-4.480566	-0.396446	-0.131621
O	2.020675	1.571029	-0.423206
B	2.204735	1.042020	0.890645
Cl	1.662301	-0.994207	-2.370794
O	1.704767	1.896141	1.878870
C	0.883436	-0.590773	1.122727
H	1.733496	1.495228	2.758067
C	1.441777	-1.879177	1.017601
C	1.031850	-2.936187	1.831395
C	0.034332	-2.734424	2.786337
C	-0.527391	-1.465339	2.932116
C	-0.098029	-0.418380	2.115204
H	2.212698	-2.063093	0.255919
H	1.488963	-3.927547	1.716665
H	-0.297477	-3.563125	3.424097
H	-1.301718	-1.291754	3.690729
H	-0.546079	0.577385	2.259218
O	3.435090	0.363267	1.034257
H	2.829142	1.395631	-0.984224
H	3.527892	-0.082124	1.887533
H	3.665491	-0.088175	-1.996713
O	4.237737	0.605148	-1.596171
H	4.380039	0.298236	-0.676479

TS BC
SCF Energy: -3022.62336288
ZPE-corrected Energy: -3022.29912
ΔU: -3022.27441
ΔH: -3022.27347
ΔG: -3022.35377
S^2 before (0.9100) and after higher multiplicity projection (0.0238)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -264.7478

N	1.150477	-1.574444	-0.206425
C	1.055882	-2.862357	0.111906
C	2.162755	-3.605597	0.515549
C	3.396865	-2.967506	0.590793
C	3.488159	-1.616734	0.265716
C	2.333581	-0.942849	-0.133487
H	0.050646	-3.295199	0.043533
H	2.051437	-4.664660	0.766699
H	4.291007	-3.517351	0.903983
H	4.451427	-1.101217	0.321335
C	2.298954	0.491600	-0.492945
N	1.103786	0.953227	-0.900822
C	0.954678	2.231926	-1.238282
C	2.007124	3.139738	-1.170403
C	3.250077	2.681697	-0.744371
C	3.402812	1.340282	-0.407284
Ni	-0.450117	-0.333470	-0.735179
H	-0.047710	2.515936	-1.583411
H	1.847858	4.185431	-1.449604
H	4.103400	3.364944	-0.675501
H	4.374126	0.963612	-0.073834
O	-1.767465	-1.789422	-0.341522
B	-2.039100	-1.279720	0.958963
Cl	-1.567699	0.510013	-2.588749
O	-1.374944	-1.975006	1.966846
C	-0.999214	0.593705	1.039199
H	-1.488213	-1.565622	2.835191
C	-1.787824	1.732349	0.794944
C	-1.635290	2.907355	1.531670
C	-0.671888	2.977016	2.540032
C	0.117835	1.859667	2.814601
C	-0.054937	0.688781	2.074028
H	-2.534930	1.699016	-0.012127
H	-2.266814	3.778696	1.315266
H	-0.542140	3.900710	3.117468
H	0.870466	1.902487	3.612684
H	0.572978	-0.185165	2.309343
O	-3.353741	-0.800188	1.104730
H	-2.584835	-1.722372	-0.920589
H	-3.505121	-0.347879	1.946148
H	-3.505838	-0.391857	-2.031853
O	-4.023888	-1.093850	-1.572531
H	-4.225054	-0.732158	-0.685262

TS D1E1
SCF Energy: -3134.88552465
ZPE-corrected Energy: -3134.45660
ΔU: -3134.42997
ΔH: -3134.42903
ΔG: -3134.51254
Num. Imaginary Frequencies: 1
Imaginary Frequency: -268.6897

Ni	0.881607	-0.275456	0.513352
N	-0.951414	-0.358894	1.345771
C	-1.363810	-1.448029	1.990918
C	-2.607659	-1.517449	2.607912
C	-3.427527	-0.390945	2.566539
C	-2.973698	0.756465	1.927319
C	-1.713064	0.743690	1.319802
C	-1.106044	1.926719	0.669784
H	-0.651214	-2.282964	2.021943
H	-2.917817	-2.432153	3.122018
H	-4.409943	-0.398408	3.051155
H	-3.584125	1.664485	1.925354
N	0.198237	1.814886	0.385409
C	0.835618	2.837026	-0.169619
C	0.201508	4.036770	-0.485570
C	-1.156969	4.156268	-0.210915
C	-1.823239	3.089222	0.381267
H	1.907051	2.689502	-0.368061
H	0.765600	4.856079	-0.942039
H	-1.698426	5.076279	-0.456393
H	-2.893955	3.160326	0.597418
Cl	1.665088	-0.345021	2.645609
C	2.634151	-0.464918	-0.311718
C	0.204681	-0.716247	-1.316956
C	1.123229	-1.643408	-0.773200
C	1.400046	-2.953302	-0.773123
H	2.098500	-3.391322	-0.047854
H	0.985681	-3.619924	-1.542749
N	-1.178637	-0.942565	-1.516780
C	-1.893653	0.110853	-2.055905
C	-3.381261	-0.075118	-2.259463
C	-3.866123	-1.511246	-2.288904
C	-3.245136	-2.254010	-1.122603
C	-1.739658	-2.268160	-1.264326
O	-1.364158	1.176398	-2.321130
H	-3.863374	0.471056	-1.419886
H	-3.645891	0.490047	-3.170701
H	-3.562694	-1.997946	-3.238556
H	-4.970246	-1.547151	-2.254511
H	-3.603405	-3.298105	-1.061966
H	-3.529207	-1.760884	-0.168522
H	-1.446810	-2.946922	-2.094210
H	-1.266880	-2.673422	-0.352868
H	0.564109	0.070232	-1.990258
C	2.996527	0.407205	-1.349298
C	4.339531	0.648927	-1.657996
C	5.347887	0.014050	-0.943486
C	5.001513	-0.865236	0.089527
C	3.670388	-1.099140	0.399895
H	2.235219	0.924098	-1.945930
H	4.588840	1.343500	-2.469801
H	6.401268	0.198198	-1.185484
H	5.786344	-1.369075	0.667054
H	3.412438	-1.772493	1.224602

TS DE
SCF Energy: -3134.88136703
ZPE-corrected Energy: -3134.45261
ΔU: -3134.42591
ΔH: -3134.42497
ΔG: -3134.50909
Num. Imaginary Frequencies: 1
Imaginary Frequency: -301.3293

Ni	-0.268780	-1.009556	-0.160988
N	-2.132153	-0.558328	-0.724439
C	-2.692924	-1.161507	-1.769374
C	-4.003246	-0.906032	-2.155456
C	-4.743525	0.004540	-1.404877
C	-4.155868	0.614289	-0.302754
C	-2.830706	0.308959	0.019849
C	-2.121034	0.861633	1.193234
H	-2.061597	-1.885038	-2.303487
H	-4.432808	-1.417752	-3.021881
H	-5.781741	0.232179	-1.669728
H	-4.731720	1.314307	0.309267
N	-0.923088	0.321348	1.445528
C	-0.229619	0.727888	2.500038
C	-0.680522	1.728578	3.358225
C	-1.914547	2.314476	3.091425
C	-2.652337	1.869558	2.000258
H	0.733862	0.225293	2.668830
H	-0.075127	2.035402	4.217015
H	-2.306153	3.111833	3.732579
H	-3.624193	2.318648	1.775173
Cl	-1.146569	-2.916732	0.713513
C	1.569379	-1.511327	0.219298
C	0.434903	0.220730	-1.552288
C	0.963723	-1.096399	-1.607293
C	1.384959	-1.960878	-2.535000
H	1.604637	-3.010990	-2.304095
H	1.552069	-1.621854	-3.567701
N	1.265243	1.354717	-1.310029
C	0.665374	2.475153	-0.782418
C	1.550605	3.662303	-0.467105
C	3.040515	3.402785	-0.587247
C	3.285846	2.676483	-1.895562
C	2.627873	1.312929	-1.853503
O	-0.531720	2.516488	-0.554651
H	1.243784	4.475381	-1.156181
H	1.251779	4.004453	0.541446
H	3.396592	2.775714	0.256890
H	3.604477	4.351778	-0.534452
H	4.363303	2.542536	-2.102348
H	2.871795	3.278430	-2.730676
H	3.240171	0.617000	-1.245223
H	2.573610	0.872998	-2.868173
H	-0.428674	0.452918	-2.195778
C	2.352022	-0.533424	0.850331
C	3.481177	-0.878893	1.599358
C	3.851931	-2.213063	1.728840
C	3.074623	-3.200301	1.113088
C	1.949185	-2.856036	0.377007
H	2.077705	0.523960	0.762276
H	4.069616	-0.090440	2.086097
H	4.738364	-2.489304	2.311956
H	3.345362	-4.257706	1.221726
H	1.329423	-3.638449	-0.074250

TS EE1
SCF Energy: -3134.92777299
ZPE-corrected Energy: -3134.49887
ΔU: -3134.47204
ΔH: -3134.47109
ΔG: -3134.55739
S^2 before (1.0347) and after higher multiplicity projection (0.2806)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -36.7345

Ni	1.446796	0.061265	-1.285798
N	1.144317	2.038324	-0.785385
C	1.299201	2.298482	0.527106
C	0.897133	3.518218	1.074225
C	0.336627	4.480063	0.240921
C	0.199496	4.206314	-1.117645
C	0.615205	2.963180	-1.583562
H	1.009767	3.714875	2.144357
H	0.007168	5.439473	0.653479
H	-0.232009	4.937661	-1.807563
H	0.515667	2.689093	-2.642020
C	1.899109	1.200790	1.316657
C	2.144925	1.260447	2.689049
C	2.730151	0.160818	3.312004
C	3.064992	-0.957649	2.553373
C	2.783163	-0.940247	1.189648
N	2.208927	0.105992	0.604023
H	1.885280	2.150420	3.270147
H	2.928503	0.183622	4.389081
H	3.535494	-1.835224	3.007389
H	3.023694	-1.781202	0.524121
Cl	3.054607	-1.114736	-2.329727
C	-0.488962	-0.581052	-1.020739
C	-0.157961	-0.460806	-2.384536
C	-1.392340	0.416602	-0.407938
C	-0.249354	-1.823393	-0.233731
H	-0.608417	0.371625	-2.948365
H	0.169601	-1.313959	-2.992932
C	0.299546	-2.986265	-0.800958
C	0.551159	-4.112244	-0.021643
C	0.258364	-4.113539	1.342454
C	-0.283279	-2.966294	1.921778
C	-0.532058	-1.838111	1.145243
H	0.567818	-3.006783	-1.862481
H	0.984638	-5.003488	-0.490839
H	0.454744	-5.004086	1.950866
H	-0.511718	-2.945841	2.994383
H	-0.934810	-0.932667	1.620554
N	-2.729937	0.120148	-0.164223
C	-3.391540	0.882507	0.787972
C	-4.865201	0.627056	1.008303
C	-5.565761	-0.150903	-0.088776
C	-4.709789	-1.349053	-0.448100
C	-3.385660	-0.883395	-1.009081
O	-2.797278	1.716422	1.452717
H	-5.327770	1.612195	1.200283
H	-4.938533	0.075356	1.968792
H	-6.576559	-0.454327	0.239606
H	-5.701634	0.486691	-0.986607
H	-4.537161	-1.970573	0.454996
H	-5.200184	-1.999121	-1.195402
H	-2.696528	-1.738351	-1.128223
H	-3.528376	-0.449944	-2.022185
H	-1.055225	1.317870	0.111482

TS enamide Z-E
SCF Energy: -672.620672804
ZPE-corrected Energy: -672.344915
ΔU: -672.330281
ΔH: -672.329337
ΔG: -672.387751
S^2 before (1.0393) and after higher multiplicity projection (0.3167)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -564.4642

C	0.839158	1.268393	-0.147666
C	0.937411	2.608413	0.521051
C	-0.398352	0.929334	-0.855881
N	-1.476412	0.327637	-0.214242
H	-0.602047	1.222523	-1.893811
C	-1.282878	-0.131125	1.165262
C	-2.579433	-0.460197	1.870784
C	-3.432318	-1.354638	0.993797
C	-3.788466	-0.588867	-0.265480
C	-2.629819	0.095243	-0.954963
O	-2.715938	0.458065	-2.115278
H	-0.734621	0.657463	1.713865
H	-0.618808	-1.021539	1.152574
H	-2.340167	-0.935863	2.839416
H	-3.134463	0.472791	2.099571
H	-2.863991	-2.272738	0.738485
H	-4.347940	-1.684276	1.517746
H	-4.525528	0.206727	-0.027539
H	-4.273705	-1.221359	-1.030304
C	1.945369	0.359242	-0.131125
C	3.168579	0.677828	0.515900
C	4.228632	-0.217762	0.528603
C	4.117373	-1.461939	-0.099613
C	2.923137	-1.797939	-0.747074
C	1.859475	-0.909249	-0.765309
H	3.284025	1.647456	1.013456
H	5.161411	0.056567	1.035800
H	4.957715	-2.165451	-0.087225
H	2.826570	-2.768970	-1.247288
H	0.928599	-1.176583	-1.282797
H	1.721453	3.248190	0.063598
H	-0.019176	3.155710	0.449208
H	1.195844	2.520948	1.597447

6.3 3 component extension of the Ni/B mechanism

AcH
SCF Energy: -153.609254569
ZPE-corrected Energy: -153.554229
ΔU: -153.550318
ΔH: -153.549373
ΔG: -153.579193
Num. Imaginary Frequencies: 0

C	-0.231741	0.393598	-0.000015
O	-1.231736	-0.273839	-0.000007
H	-0.297043	1.518142	0.000020
C	1.161829	-0.147763	-0.000021
H	1.710989	0.224120	-0.885825
H	1.710555	0.224009	0.886091
H	1.148865	-1.250571	-0.000008

PFalpha.NA
SCF Energy: -3288.57191515
ZPE-corrected Energy: 0
ΔU: 0
ΔH: 0
ΔG: 0
Num. Imaginary Frequencies: 0

Ni	0.240040	-1.348861	-1.301147
N	0.171036	-2.653204	0.203309
C	1.233812	-3.247331	0.747903
C	1.230008	-3.698152	2.065115
C	0.091852	-3.492120	2.841360
C	-1.016335	-2.870167	2.272643
C	-0.944385	-2.473756	0.940061
H	2.106512	-3.336345	0.086200
H	2.117531	-4.188899	2.476655
H	0.068240	-3.806132	3.890451
H	-1.912603	-2.659455	2.864437
C	-2.042647	-1.837367	0.197132
N	-1.651559	-1.203309	-0.928929
C	-2.577297	-0.689768	-1.743594
C	-3.938153	-0.772007	-1.472354
C	-4.348190	-1.396735	-0.295838
C	-3.386841	-1.935267	0.551928
H	-2.208640	-0.194872	-2.649135
H	-4.660619	-0.349747	-2.177626
H	-5.411797	-1.475364	-0.046143
H	-3.675265	-2.451936	1.472338
Cl	2.134015	-2.025139	-2.149431
C	0.886181	0.879644	-0.587173
C	0.442323	0.463606	-1.925548
C	0.068223	1.369673	0.371505
H	1.207299	0.532172	-2.714139
H	-0.509447	0.916753	-2.253704
N	-1.286806	1.743284	0.179869
H	0.437798	1.509564	1.397753
C	-1.532789	2.911058	-0.678460
C	-3.007247	3.150938	-0.913338
C	-3.737642	3.195327	0.415269
C	-3.580544	1.853864	1.108060
C	-2.178836	1.281515	1.114301
O	-1.874860	0.399621	1.902836
H	-1.008564	2.747868	-1.637970
H	-1.064880	3.802468	-0.209858
H	-3.127996	4.094146	-1.477270
H	-3.429640	2.340280	-1.544781
H	-3.306029	4.002105	1.041876
H	-4.808575	3.436244	0.282611
H	-4.217390	1.091003	0.611161
H	-3.910163	1.874561	2.162318
C	2.306859	0.649705	-0.202411
C	3.353240	1.062543	-1.036016
C	4.681488	0.854862	-0.674492
C	4.991133	0.219355	0.527577
C	3.958860	-0.203781	1.364666
C	2.630847	0.011623	1.002998
H	3.120514	1.553706	-1.989195
H	5.485028	1.185484	-1.343378
H	6.036707	0.045424	0.807670
H	4.189452	-0.718144	2.305672
H	1.820448	-0.348794	1.651890
C	1.754245	4.199406	0.530876
C	2.964619	3.890247	1.345114
H	1.754184	3.750463	-0.501201
O	0.829108	4.850372	0.906167
H	3.881611	4.170966	0.793260
H	2.922980	4.409688	2.317429
H	3.024543	2.793429	1.499661

PFalpha
SCF Energy: -3696.25625734
ZPE-corrected Energy: -3695.63710
ΔU: -3695.59863
ΔH: -3695.59769
ΔG: -3695.70667
S^2 before (0.4938) and after higher multiplicity projection (0.0137)
Num. Imaginary Frequencies: 0

Ni	2.308988	-0.988780	-0.427421
N	2.118925	-1.525809	1.448767
C	2.657993	-0.861503	2.472455
C	2.243327	-1.081836	3.781923
C	1.240794	-2.017964	4.016825
C	0.689993	-2.713977	2.944689
C	1.151299	-2.436876	1.662867
H	3.447857	-0.146287	2.211962
H	2.699999	-0.517366	4.599857
H	0.881495	-2.204338	5.034152
H	-0.111791	-3.440563	3.104438
C	0.673214	-3.095948	0.439892
N	1.067143	-2.502092	-0.707037
C	0.780025	-3.072691	-1.877850
C	0.065259	-4.261810	-1.973161
C	-0.371447	-4.866743	-0.798602
C	-0.063758	-4.277751	0.424116
H	1.144995	-2.562072	-2.776720
H	-0.141563	-4.697272	-2.955142
H	-0.940648	-5.801593	-0.830552
H	-0.372435	-4.749474	1.361338
Cl	4.391080	-0.321468	-0.249709
C	1.357333	1.106497	-1.300457
C	1.854022	0.127222	-2.156811
C	-0.069233	1.211657	-0.904888
H	2.870877	0.232131	-2.559931
H	1.142455	-0.461101	-2.750887
N	-0.910239	0.104381	-1.350705
H	-0.118685	1.224986	0.199725
C	-1.496803	0.187476	-2.689337
C	-2.070693	-1.137616	-3.136304
C	-3.130921	-1.570157	-2.142840
C	-2.538351	-1.672953	-0.746256
C	-1.416556	-0.722271	-0.389511
O	-0.956418	-0.756917	0.750946
H	-0.711849	0.532691	-3.388380
H	-2.296402	0.954981	-2.689918
H	-2.494801	-1.022986	-4.150956
H	-1.264570	-1.898926	-3.208363
H	-3.939813	-0.813158	-2.139935
H	-3.597464	-2.529839	-2.433922
H	-2.134743	-2.687618	-0.550733
H	-3.309217	-1.511196	0.032330
C	2.284338	2.070685	-0.683078
C	3.311113	2.653644	-1.439573
C	4.200404	3.546411	-0.854049
C	4.094858	3.844516	0.504242
C	3.080384	3.266334	1.267569
C	2.168731	2.399427	0.677443
H	3.396863	2.420702	-2.507291
H	4.987453	4.008888	-1.459980
H	4.803651	4.538882	0.969799
H	2.988280	3.506114	2.332702
H	1.359884	1.975934	1.286379
C	-0.845045	2.582667	-1.229380
C	-0.181506	3.858090	-0.735041
H	-0.868783	2.648708	-2.342518
O	-2.120717	2.420494	-0.781753
H	-0.888317	4.681902	-0.940095
H	-0.013583	3.843070	0.354360
H	0.769495	4.079758	-1.252860
B	-2.499296	2.478326	0.700094
C	-3.800097	1.482423	0.826400
C	-4.170792	0.959455	2.077316
C	-5.279718	0.128240	2.238434
C	-6.072038	-0.202634	1.136851
C	-5.738726	0.312361	-0.115954
C	-4.617836	1.134421	-0.259565
H	-3.563297	1.221057	2.956319
H	-5.535714	-0.262154	3.232722
H	-6.949356	-0.851202	1.257127
H	-6.357472	0.066476	-0.990504
H	-4.361600	1.527477	-1.254536
O	-2.799442	3.850561	1.068285
O	-1.412858	2.032186	1.575478
H	-1.476165	1.072093	1.693555
H	-3.401309	4.201730	0.397832

PFgamma
SCF Energy: -3696.25683417
ZPE-corrected Energy: -3695.63872
ΔU: -3695.59896
ΔH: -3695.59801
ΔG: -3695.71178
S^2 before (0.9761) and after higher multiplicity projection (0.0274)
Num. Imaginary Frequencies: 0

Ni	-1.815629	0.366497	0.814366
N	-3.250445	-0.710638	-0.047793
C	-4.262665	-0.220994	-0.758917
C	-5.227862	-1.048085	-1.321706
C	-5.123014	-2.420142	-1.110314
C	-4.069675	-2.919721	-0.352335
C	-3.130205	-2.031353	0.167752
H	-4.297471	0.871491	-0.873863
H	-6.045101	-0.619603	-1.908741
H	-5.863347	-3.105473	-1.535968
H	-3.975449	-3.996116	-0.185760
C	-1.950569	-2.448791	0.959075
N	-1.093797	-1.465917	1.297428
C	0.000633	-1.729983	2.010580
C	0.302025	-3.022419	2.433231
C	-0.570425	-4.051685	2.095441
C	-1.708897	-3.766254	1.345863
H	0.674520	-0.889614	2.236836
H	1.211157	-3.206126	3.013314
H	-0.368196	-5.080127	2.412872
H	-2.403483	-4.566305	1.075375
Cl	-2.794103	0.981005	2.674936
C	-0.518055	1.407468	-0.527848
C	0.443086	1.603086	0.611766
C	-0.592497	0.274118	-1.315029
H	-0.138998	1.896348	1.516541
H	0.949580	0.664402	0.879578
N	0.279869	-0.786628	-1.445366
H	-1.453980	0.176914	-1.990984
C	1.752015	-0.673529	-1.375145
C	2.369572	-1.861158	-0.653867
C	1.698244	-3.186341	-1.040790
C	0.784354	-3.022468	-2.254265
C	-0.244879	-1.957271	-1.998995
O	-1.434946	-2.093297	-2.210243
H	2.038294	0.279894	-0.899564
H	2.123137	-0.619455	-2.418629
H	3.447294	-1.864620	-0.899060
H	2.325462	-1.683847	0.437711
H	2.447061	-3.971533	-1.248150
H	1.086543	-3.567555	-0.198579
H	0.242900	-3.949082	-2.507680
H	1.381486	-2.738338	-3.144700
C	-1.467278	2.507065	-0.859162
C	-1.903567	2.714204	-2.181740
C	-2.838838	3.697345	-2.486724
C	-3.354679	4.512412	-1.479108
C	-2.910870	4.344316	-0.169231
C	-1.972466	3.362755	0.138250
H	-1.475862	2.115881	-2.994084
H	-3.153288	3.840760	-3.526802
H	-4.089140	5.289653	-1.718437
H	-3.297917	4.984743	0.630953
H	-1.662412	3.251585	1.182279
C	1.583542	2.661172	0.410120
O	2.750712	2.043531	0.021027
H	1.259942	3.313902	-0.434807
C	1.697280	3.544929	1.644198
H	1.877658	2.942069	2.551746
H	2.545035	4.243038	1.538212
H	0.766299	4.130444	1.782983
B	3.636618	1.292116	0.969082
C	4.695356	0.478756	0.018619
C	5.468714	-0.554281	0.572654
C	6.402931	-1.269462	-0.175494
C	6.594593	-0.965909	-1.525788
C	5.848612	0.061748	-2.102697
C	4.919934	0.769919	-1.334798
H	5.317781	-0.813325	1.631480
H	6.988076	-2.072634	0.292641
H	7.326974	-1.524721	-2.122578
H	5.995432	0.314972	-3.161584
H	4.331277	1.572504	-1.800746
O	4.347363	2.163706	1.904123
O	2.832067	0.372386	1.810967
H	5.051134	2.621664	1.425296
H	3.194217	0.473623	2.702889

TSalpha
SCF Energy: -3696.24928642
ZPE-corrected Energy: -3695.63287
ΔU: -3695.59418
ΔH: -3695.59324
ΔG: -3695.70260
S^2 before (0.3341) and after higher multiplicity projection (0.0118)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -316.4569

Ni	2.615521	-0.957578	-0.701032
N	2.757936	-1.228398	1.271223
C	3.515780	-0.493628	2.085423
C	3.244034	-0.396638	3.447528
C	2.134963	-1.065849	3.958273
C	1.351152	-1.839821	3.105893
C	1.702650	-1.907416	1.761630
H	4.352081	0.029947	1.603144
H	3.887175	0.211840	4.090563
H	1.874796	-0.983425	5.018816
H	0.460118	-2.358125	3.473120
C	1.007685	-2.719991	0.752429
N	1.286178	-2.378058	-0.521806
C	0.809736	-3.121069	-1.523179
C	0.023125	-4.245403	-1.304520
C	-0.294959	-4.589210	0.007811
C	0.200356	-3.815453	1.050904
H	1.078586	-2.804351	-2.537911
H	-0.335494	-4.834421	-2.154159
H	-0.918231	-5.464698	0.219070
H	-0.012575	-4.074646	2.092109
Cl	4.636491	-0.156041	-0.992707
C	1.232481	0.881690	-1.304192
C	1.806030	-0.001803	-2.269883
C	-0.094866	0.826491	-0.813890
H	2.665976	0.356950	-2.851873
H	1.120007	-0.652032	-2.831524
N	-0.998008	-0.218050	-1.195848
H	-0.225718	1.104130	0.239029
C	-1.552803	-0.198363	-2.554459
C	-2.256170	-1.490467	-2.902655
C	-3.358369	-1.724473	-1.888168
C	-2.763762	-1.823916	-0.494131
C	-1.600025	-0.912001	-0.179180
O	-1.182408	-0.853008	0.977037
H	-0.732621	0.017434	-3.261742
H	-2.283068	0.631751	-2.632440
H	-2.660906	-1.411232	-3.928553
H	-1.537137	-2.336878	-2.902690
H	-4.063339	-0.869948	-1.924528
H	-3.947187	-2.631156	-2.119970
H	-2.389897	-2.849210	-0.292526
H	-3.517823	-1.623530	0.291694
C	2.094392	1.931248	-0.705886
C	2.937226	2.709743	-1.509896
C	3.743022	3.693997	-0.949542
C	3.738069	3.901392	0.430063
C	2.909695	3.127931	1.241940
C	2.085856	2.159135	0.678119
H	2.952657	2.548162	-2.593979
H	4.388773	4.301009	-1.594159
H	4.381985	4.669575	0.873457
H	2.898929	3.283217	2.327276
H	1.436359	1.560554	1.331211
C	-1.181117	2.495744	-1.203823
C	-0.497090	3.666001	-0.567142
H	-1.049567	2.441755	-2.305456
O	-2.340025	2.120629	-0.799028
H	-1.190777	4.522524	-0.672591
H	-0.350706	3.516016	0.514891
H	0.458468	3.912650	-1.058225
B	-2.858323	2.279134	0.755400
C	-4.121596	1.257818	0.786246
C	-4.384226	0.475218	1.921034
C	-5.489506	-0.373531	1.994841
C	-6.379221	-0.456610	0.922874
C	-6.150787	0.319070	-0.214228
C	-5.035370	1.156166	-0.275314
H	-3.697317	0.534467	2.777012
H	-5.663650	-0.972316	2.898353
H	-7.252588	-1.118621	0.976334
H	-6.846163	0.265234	-1.062312
H	-4.861596	1.749543	-1.185520
O	-3.198426	3.657668	0.928401
O	-1.777888	1.929053	1.626069
H	-1.687972	0.963756	1.687659
H	-4.085992	3.814070	0.579985

TSgamma
SCF Energy: -3696.23735932
ZPE-corrected Energy: -3695.62326
ΔU: -3695.58301
ΔH: -3695.58206
ΔG: -3695.69702
S^2 before (0.5608) and after higher multiplicity projection (0.0229)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -498.2717

Ni	1.642317	0.197162	-0.704838
N	3.198822	-0.814034	-0.106584
C	4.270512	-0.215693	0.405222
C	5.358244	-0.937611	0.881431
C	5.311296	-2.326798	0.800896
C	4.194932	-2.941316	0.245454
C	3.136040	-2.151595	-0.202595
H	4.250151	0.882530	0.422556
H	6.222428	-0.416550	1.303544
H	6.145973	-2.934036	1.166840
H	4.146997	-4.031374	0.174622
C	1.897257	-2.695582	-0.803316
N	0.958586	-1.786866	-1.114204
C	-0.179316	-2.171931	-1.686201
C	-0.448538	-3.508325	-1.977498
C	0.510036	-4.462357	-1.650833
C	1.699830	-4.055014	-1.054022
H	-0.918360	-1.386921	-1.911107
H	-1.396649	-3.786239	-2.448129
H	0.337320	-5.523364	-1.861331
H	2.465985	-4.792662	-0.798262
Cl	2.574936	0.788012	-2.669936
C	0.687970	1.554024	0.426896
C	-0.092173	1.513250	-0.784050
C	0.848904	0.445532	1.276299
H	0.285062	2.113277	-1.620339
H	-0.730280	0.655368	-1.047884
N	-0.058463	-0.583963	1.581634
H	1.665899	0.511742	2.012118
C	-1.516108	-0.408233	1.593176
C	-2.241735	-1.649536	1.088015
C	-1.592500	-2.948594	1.584990
C	-0.568617	-2.680530	2.683610
C	0.468606	-1.693274	2.215283
O	1.668611	-1.851338	2.361645
H	-1.785874	0.469770	0.986556
H	-1.831446	-0.175812	2.632610
H	-3.294716	-1.573436	1.415573
H	-2.277477	-1.623536	-0.017151
H	-2.353656	-3.662135	1.948839
H	-1.074165	-3.458430	0.748563
H	-0.036764	-3.593884	2.998425
H	-1.072446	-2.269654	3.583069
C	1.480889	2.776132	0.728702
C	1.446825	3.308461	2.025652
C	2.134382	4.480583	2.334912
C	2.868026	5.138015	1.349754
C	2.913469	4.614083	0.056901
C	2.225033	3.445645	-0.257089
H	0.854910	2.801296	2.797938
H	2.090751	4.884688	3.352873
H	3.410279	6.059925	1.589805
H	3.502969	5.117103	-0.718328
H	2.315695	3.011150	-1.262435
C	-1.749878	2.737612	-0.590325
O	-2.726813	2.001261	-0.232954
H	-1.290210	3.312730	0.239119
C	-1.719122	3.428097	-1.920715
H	-1.790316	2.720354	-2.762564
H	-2.607222	4.085139	-1.981255
H	-0.805977	4.040461	-2.021207
B	-3.621356	1.072465	-1.204898
C	-4.637849	0.330719	-0.193849
C	-5.288979	-0.832486	-0.633399
C	-6.219959	-1.501152	0.159885
C	-6.527246	-1.015672	1.432489
C	-5.899655	0.141642	1.892065
C	-4.971053	0.801909	1.083953
H	-5.041285	-1.230059	-1.628001
H	-6.709815	-2.410433	-0.211901
H	-7.257339	-1.538045	2.063300
H	-6.136509	0.533088	2.889943
H	-4.477931	1.707306	1.463342
O	-4.258809	1.910193	-2.179746
O	-2.699021	0.167301	-1.858105
H	-5.138792	2.169897	-1.876347
H	-2.680680	0.406345	-2.797330

6.4 Ni/Zn mechanism via a non-redox pathway

A
SCF Energy: -4781.74641788
ZPE-corrected Energy: -4781.51348
ΔU: -4781.49234
ΔH: -4781.49140
ΔG: -4781.56605
S^2 before (0.4796) and after higher multiplicity projection (0.0032)
Num. Imaginary Frequencies: 0

Ni	-0.175386	-0.081391	-0.675307
Cl	-1.642155	-1.755293	-0.966166
Cl	-1.718925	1.399447	-1.347446
N	1.326230	-1.292141	-0.217872
C	1.293949	-2.627284	-0.215989
C	2.409028	-3.397037	0.098367
C	3.596698	-2.751826	0.422873
C	3.629717	-1.360790	0.426359
C	2.473749	-0.655547	0.101854
C	2.387492	0.810898	0.081372
H	0.329550	-3.077687	-0.474996
H	2.335164	-4.488062	0.085407
H	4.495797	-3.323457	0.673784
H	4.552671	-0.832290	0.678845
C	3.439933	1.654842	0.427328
C	3.244560	3.031701	0.386464
C	2.002382	3.524877	0.003926
C	0.997925	2.622149	-0.328154
N	1.186786	1.300306	-0.295020
H	4.405851	1.244187	0.732488
H	4.059635	3.710722	0.655988
H	1.801120	4.598947	-0.039063
H	-0.001624	2.948841	-0.635939
Zn	-2.654113	0.020509	0.942608
C	-4.560136	-0.082212	0.458366
H	-5.118655	0.831248	0.745429
H	-4.649017	-0.200604	-0.639599
H	-5.073002	-0.943096	0.932381
C	-1.052746	0.266324	2.095698
H	-1.379709	0.182869	3.152768
H	-0.248432	-0.484869	1.958489
H	-0.603203	1.272617	1.975222

B
SCF Energy: -4781.76118596
ZPE-corrected Energy: -4781.52636
ΔU: -4781.50599
ΔH: -4781.50504
ΔG: -4781.57686
Num. Imaginary Frequencies: 0

N	1.233386	-1.367251	-0.381241
C	1.381962	-2.694348	-0.295396
C	2.507417	-3.297673	0.252597
C	3.528003	-2.490128	0.740071
C	3.385861	-1.110659	0.649218
C	2.231932	-0.574806	0.081123
H	0.564165	-3.307854	-0.681438
H	2.569221	-4.388807	0.292240
H	4.429184	-2.925336	1.183276
H	4.177204	-0.451845	1.015865
C	2.012489	0.869578	-0.078953
N	0.874995	1.189834	-0.720944
C	0.579041	2.472948	-0.922157
C	1.405533	3.507084	-0.494611
C	2.577346	3.185288	0.181240
C	2.888724	1.845760	0.391582
Ni	-0.312751	-0.399346	-1.027825
H	-0.372831	2.670440	-1.427916
H	1.121956	4.546543	-0.683836
H	3.248292	3.969671	0.546202
H	3.803117	1.572352	0.924733
Cl	-2.081827	0.844559	-1.516167
Cl	-0.721844	1.103876	2.078744
Zn	-2.191905	-0.066905	0.862879
C	-3.768565	-1.224825	1.067069
C	-1.302586	-1.992738	-1.396963
H	-4.345347	-1.239381	0.122188
H	-3.472059	-2.265785	1.300723
H	-4.435747	-0.871309	1.876539
H	-0.719763	-2.526090	-2.178505
H	-2.317005	-1.799830	-1.787695
H	-1.395417	-2.648277	-0.507071

C
SCF Energy: -2502.68823929
ZPE-corrected Energy: -2502.49036
ΔU: -2502.47674
ΔH: -2502.47580
ΔG: -2502.53112
Num. Imaginary Frequencies: 0

N	-1.243291	-0.616126	0.000407
C	-2.311898	-1.422861	0.000736
C	-3.620124	-0.954560	0.000382
C	-3.840266	0.418047	-0.000446
C	-2.739233	1.266053	-0.000780
C	-1.455140	0.723852	-0.000261
H	-2.114337	-2.497692	0.001164
H	-4.448520	-1.668858	0.000718
H	-4.855152	0.827897	-0.000844
H	-2.880414	2.350050	-0.001456
C	-0.236360	1.544945	-0.000220
N	0.907612	0.833349	0.000196
C	2.076053	1.477821	0.000658
C	2.163859	2.866237	0.000615
C	0.987187	3.608794	0.000071
C	-0.232495	2.939638	-0.000334
Ni	0.620593	-1.148616	0.000169
H	2.962662	0.831179	0.000899
H	3.144644	3.351113	0.000989
H	1.013738	4.703327	-0.000015
H	-1.168627	3.504560	-0.000706
Cl	2.763468	-1.604586	-0.000726
C	0.210877	-3.016622	0.000016
H	1.105832	-3.662874	-0.000272
H	-0.389977	-3.264167	0.901421
H	-0.390408	-3.263952	-0.901139

D1
SCF Energy: -2943.46818547
ZPE-corrected Energy: -2943.09277
ΔU: -2943.06866
ΔH: -2943.06772
ΔG: -2943.14545
Num. Imaginary Frequencies: 0

Ni	1.534395	-0.219272	-0.379645
N	0.316602	-0.663608	1.163247
C	0.211430	-1.873060	1.711624
C	-0.643419	-2.134248	2.776927
C	-1.399874	-1.083200	3.290814
C	-1.264287	0.185259	2.737623
C	-0.385597	0.367080	1.666190
C	-0.122071	1.673710	1.033584
H	0.845220	-2.654853	1.274828
H	-0.708242	-3.143117	3.194557
H	-2.082992	-1.245467	4.131008
H	-1.825297	1.028163	3.150789
N	0.907159	1.692438	0.163887
C	1.219369	2.835482	-0.441949
C	0.531777	4.023833	-0.214982
C	-0.537884	4.010875	0.673913
C	-0.869488	2.819332	1.309404
H	2.060173	2.802842	-1.145473
H	0.832194	4.938129	-0.735357
H	-1.112901	4.920941	0.873708
H	-1.711208	2.783557	2.007324
Cl	3.334614	-0.948173	0.898078
C	2.777384	0.386261	-1.709052
C	0.140317	-0.678100	-1.806564
C	1.053919	-1.681531	-1.520947
C	1.576855	-2.886225	-1.662129
H	2.448957	-3.184575	-1.061119
H	1.171570	-3.616117	-2.381069
N	-1.213145	-0.698724	-1.389814
C	-1.919953	0.477129	-1.525167
C	-3.369633	0.476903	-1.098346
C	-4.035162	-0.885540	-1.056184
C	-3.128731	-1.847946	-0.313840
C	-1.814969	-1.990263	-1.048613
O	-1.385162	1.497673	-1.929522
H	-3.381923	0.933508	-0.085262
H	-3.893922	1.192859	-1.755742
H	-4.204855	-1.259270	-2.086558
H	-5.027949	-0.811902	-0.577135
H	-3.586523	-2.848788	-0.214492
H	-2.947340	-1.474303	0.716323
H	-1.958944	-2.569850	-1.985686
H	-1.089888	-2.559226	-0.440882
H	0.319557	0.014187	-2.640314
H	3.402819	-0.446902	-2.075139
H	2.263755	0.878809	-2.558730
H	3.423339	1.113312	-1.181751

E1
SCF Energy: -2943.52423314
ZPE-corrected Energy: -2943.14561
ΔU: -2943.12207
ΔH: -2943.12113
ΔG: -2943.19834
Num. Imaginary Frequencies: 0

Ni	0.848697	-1.015032	0.473609
N	1.854914	0.371876	-0.482406
C	2.865402	0.068767	-1.296479
C	3.612816	1.042688	-1.948581
C	3.294407	2.379480	-1.722009
C	2.249291	2.691076	-0.859105
C	1.536130	1.656564	-0.250579
H	3.087410	-0.999699	-1.411470
H	4.431109	0.753625	-2.614569
H	3.862894	3.179267	-2.208000
H	2.000651	3.736049	-0.653314
C	0.408502	1.878185	0.680215
N	-0.025324	0.786203	1.328347
C	-1.059800	0.887299	2.158180
C	-1.721939	2.088505	2.398487
C	-1.273484	3.228650	1.735231
C	-0.193474	3.125527	0.864688
H	-1.376300	-0.037368	2.661609
H	-2.567971	2.125169	3.091690
H	-1.765087	4.195010	1.889731
H	0.158424	4.007216	0.321169
Cl	2.666259	-1.577327	1.740429
C	-0.041029	-2.571706	-0.278456
C	-0.257853	-2.505440	1.123255
C	-0.473194	-1.429261	-1.007984
H	0.224425	-3.259128	1.761374
H	-1.172115	-2.057862	1.544010
N	-1.763180	-0.832653	-0.856395
H	-0.039947	-1.275801	-2.011341
C	-2.921781	-1.706753	-0.622433
C	-4.125355	-0.938154	-0.126954
C	-4.446775	0.185960	-1.092062
C	-3.252582	1.117586	-1.182626
C	-1.903601	0.448798	-1.332126
O	-0.956767	1.066726	-1.798506
H	-2.636440	-2.483196	0.103407
H	-3.170671	-2.234463	-1.568953
H	-4.975169	-1.636484	-0.018114
H	-3.911949	-0.524540	0.881258
H	-4.668770	-0.244319	-2.089947
H	-5.347320	0.745764	-0.780831
H	-3.172694	1.720213	-0.251838
H	-3.340186	1.847304	-2.006667
C	0.886063	-3.579657	-0.887043
H	0.343104	-4.501632	-1.175865
H	1.365253	-3.182412	-1.801990
H	1.680219	-3.857735	-0.170208

F1.3
SCF Energy: -5376.22167373
ZPE-corrected Energy: -5375.74466
ΔU: -5375.71163
ΔH: -5375.71069
ΔG: -5375.80983
S^2 before (2.0084) and after higher multiplicity projection (2.0000)
Num. Imaginary Frequencies: 1

Ni	-1.503409	1.350407	0.518493
N	-3.279373	0.562674	0.019991
C	-4.208542	1.192087	-0.695122
C	-5.419913	0.587257	-1.011276
C	-5.656349	-0.702032	-0.541102
C	-4.681350	-1.349081	0.211774
C	-3.482101	-0.688151	0.466174
H	-3.969455	2.216062	-1.009896
H	-6.163421	1.124438	-1.606584
H	-6.602027	-1.207983	-0.760432
H	-4.854546	-2.362373	0.583802
C	-2.350398	-1.278750	1.209872
N	-1.252933	-0.497847	1.311460
C	-0.182462	-0.929429	1.980089
C	-0.139952	-2.185668	2.576458
C	-1.259106	-3.005097	2.475567
C	-2.379257	-2.547597	1.784094
H	0.689945	-0.264711	2.041732
H	0.768876	-2.496639	3.100748
H	-1.267499	-4.000245	2.931689
H	-3.268381	-3.178098	1.700249
Cl	-2.020253	3.400587	1.166300
C	0.082670	1.711637	-1.074187
C	1.210803	1.729025	-0.078911
C	-0.535069	0.607905	-1.615339
H	0.885334	2.414353	0.737291
H	1.389757	0.738934	0.377554
N	-0.143078	-0.726468	-1.594853
H	-1.413905	0.782352	-2.255960
C	1.262830	-1.143452	-1.752250
C	1.579667	-2.357841	-0.894243
C	0.453518	-3.401041	-0.953175
C	-0.567447	-3.076751	-2.041614
C	-1.109383	-1.679455	-1.902242
O	-2.285172	-1.391871	-2.028362
H	1.927188	-0.288982	-1.533757
H	1.417050	-1.385125	-2.823331
H	2.535830	-2.780344	-1.256541
H	1.766517	-2.037159	0.150257
H	0.854056	-4.416698	-1.118428
H	-0.075057	-3.440694	0.018518
H	-1.428316	-3.765956	-2.026037
H	-0.102453	-3.168776	-3.044603
C	-0.292297	3.045439	-1.665110
C	2.599451	2.238475	-0.584371
O	3.352129	1.227517	-1.121740
H	2.389266	3.004577	-1.373988
C	3.318182	2.959711	0.551077
H	3.454409	2.269510	1.407591
H	4.317785	3.284588	0.204620
H	2.764632	3.852853	0.901926
Zn	4.260669	-0.109223	-0.099786
C	5.746387	-1.263377	-0.717409
Cl	3.284947	-0.456032	1.999557
H	0.383069	3.272510	-2.514107
H	-1.326294	3.050040	-2.058535
H	-0.196476	3.861459	-0.929030
H	5.486634	-2.336254	-0.619261
H	6.002798	-1.076957	-1.778724
H	6.662987	-1.093407	-0.118444

F1
SCF Energy: -5376.20463059
ZPE-corrected Energy: -5375.72744
ΔU: -5375.69362
ΔH: -5375.69267
ΔG: -5375.79306
S^2 before (0.9127) and after higher multiplicity projection (0.0259)
Num. Imaginary Frequencies: 0

Ni	-1.548221	1.297456	0.566238
N	-3.317656	0.562223	0.094304
C	-4.246660	1.216513	-0.599996
C	-5.450625	0.615042	-0.949586
C	-5.681895	-0.694999	-0.538362
C	-4.704997	-1.369375	0.187722
C	-3.511987	-0.712961	0.475406
H	-4.013524	2.254528	-0.865825
H	-6.193657	1.173054	-1.526015
H	-6.623004	-1.196558	-0.785397
H	-4.868083	-2.401620	0.509084
C	-2.371379	-1.325410	1.178606
N	-1.271812	-0.544196	1.269637
C	-0.185934	-0.986129	1.906443
C	-0.131707	-2.253137	2.478583
C	-1.250754	-3.073570	2.384566
C	-2.385863	-2.605482	1.725666
H	0.687013	-0.321870	1.965050
H	0.786734	-2.572210	2.980565
H	-1.247426	-4.076816	2.822510
H	-3.277823	-3.233067	1.649216
Cl	-2.098989	3.370439	1.030772
C	0.109197	1.744224	-1.040696
C	1.214464	1.740779	-0.020746
C	-0.501916	0.655047	-1.608400
H	0.863565	2.398062	0.807499
H	1.394454	0.738082	0.406347
N	-0.106282	-0.683406	-1.600128
H	-1.370014	0.840908	-2.260851
C	1.299179	-1.085640	-1.796437
C	1.640490	-2.322537	-0.980259
C	0.522217	-3.374025	-1.046198
C	-0.529737	-3.022719	-2.095741
C	-1.072529	-1.631809	-1.903436
O	-2.254376	-1.348061	-1.991109
H	1.960135	-0.233920	-1.556844
H	1.438964	-1.292152	-2.877217
H	2.593378	-2.726650	-1.371208
H	1.843374	-2.028752	0.069229
H	0.927222	-4.379595	-1.256812
H	0.019813	-3.452448	-0.062822
H	-1.387024	-3.716412	-2.076658
H	-0.091386	-3.083572	-3.113163
C	-0.241859	3.087298	-1.621507
C	2.606142	2.277228	-0.477481
O	3.371190	1.295180	-1.052773
H	2.408601	3.081433	-1.231536
C	3.303960	2.943424	0.703787
H	3.419900	2.215405	1.531453
H	4.311539	3.280555	0.393998
H	2.745488	3.821607	1.083495
Zn	4.282442	-0.068934	-0.075058
C	5.774237	-1.200437	-0.722637
Cl	3.275505	-0.547376	1.983758
H	0.456440	3.318343	-2.450830
H	-1.265711	3.105171	-2.038904
H	-0.156955	3.894753	-0.874737
H	5.529322	-2.276447	-0.620391
H	6.007699	-1.009975	-1.788593
H	6.700603	-1.019880	-0.141998

TS AB.3
SCF Energy: -4781.75483894
ZPE-corrected Energy: 0
ΔU: 0
ΔH: 0
ΔG: 0
S^2 before (2.0071) and after higher multiplicity projection (2.0000)
Num. Imaginary Frequencies: 0

N	1.546755	-1.271820	0.039535
C	1.661127	-2.596809	0.107258
C	2.896225	-3.238392	0.103680
C	4.044335	-2.457240	0.019850
C	3.923509	-1.071960	-0.050570
C	2.650233	-0.503479	-0.034768
H	0.717509	-3.154869	0.162712
H	2.949774	-4.329204	0.163741
H	5.036113	-2.920910	0.010092
H	4.818370	-0.447338	-0.116304
C	2.412061	0.958350	-0.082317
N	1.122271	1.333777	-0.066315
C	0.797992	2.624490	-0.058807
C	1.758068	3.630413	-0.091120
C	3.098991	3.258737	-0.127795
C	3.434302	1.907921	-0.118013
Ni	-0.295312	-0.187151	-0.081873
H	-0.274299	2.851400	-0.012459
H	1.455146	4.681375	-0.086461
H	3.887479	4.017791	-0.156290
H	4.484839	1.605451	-0.132120
C	-1.354769	0.643366	-1.726403
Zn	-2.803882	0.079738	-0.167937
C	-4.758520	0.287695	-0.234996
Cl	-1.689098	-2.148399	-0.093341
H	-1.439621	1.745447	-1.794086
H	-0.412542	0.359760	-2.243687
H	-2.142353	0.200585	-2.374440
Cl	-1.445882	0.745881	1.776169
H	-5.045827	1.355512	-0.279584
H	-5.181949	-0.212883	-1.127278
H	-5.237314	-0.153488	0.660124

TS AB
SCF Energy: -4781.73966616
ZPE-corrected Energy: 0
ΔU: 0
ΔH: 0
ΔG: 0
S^2 before (0.9124) and after higher multiplicity projection (0.0205)
Num. Imaginary Frequencies: 0

N	1.516331	-1.264076	0.086320
C	1.617376	-2.591144	0.080067
C	2.844178	-3.239367	-0.031753
C	3.994005	-2.461511	-0.132884
C	3.883322	-1.073368	-0.131959
C	2.616163	-0.500001	-0.025534
H	0.669292	-3.139057	0.169221
H	2.892311	-4.332192	-0.035702
H	4.979544	-2.931103	-0.216355
H	4.779288	-0.452705	-0.218925
C	2.367658	0.958143	-0.043491
N	1.074495	1.329195	0.038504
C	0.748785	2.621510	-0.003552
C	1.703927	3.625395	-0.120266
C	3.044198	3.258845	-0.192369
C	3.381739	1.909466	-0.155791
Ni	-0.279408	-0.174562	0.193917
H	-0.320531	2.852002	0.079160
H	1.394399	4.673995	-0.150362
H	3.828093	4.018182	-0.278506
H	4.430249	1.605284	-0.213200
C	-0.923426	0.088230	-1.764424
Zn	-2.671908	-0.033056	-0.402659
C	-4.583998	0.049004	-0.845046
Cl	-1.641476	-2.024172	0.613691
H	-1.007401	1.153147	-2.060913
H	0.071405	-0.256734	-2.107768
H	-1.655716	-0.509940	-2.348825
Cl	-1.856387	1.240287	1.509305
H	-4.892438	1.078023	-1.107063
H	-4.853990	-0.635764	-1.669836
H	-5.169527	-0.244709	0.046480

TS D1E1
SCF Energy: -2943.44606498
ZPE-corrected Energy: -2943.07062
ΔU: -2943.04726
ΔH: -2943.04632
ΔG: -2943.12238
Num. Imaginary Frequencies: 1
Imaginary Frequency: -392.5909

Ni	1.536662	-0.443754	-0.206103
N	0.233404	-0.376447	1.295663
C	0.007552	-1.460167	2.039296
C	-0.897747	-1.463175	3.093510
C	-1.571751	-0.279083	3.386851
C	-1.311453	0.855915	2.627882
C	-0.393513	0.778177	1.575301
C	-0.025906	1.937422	0.730340
H	0.589134	-2.353259	1.775333
H	-1.063911	-2.375614	3.673490
H	-2.287649	-0.234414	4.214202
H	-1.805041	1.801836	2.868225
N	1.054674	1.766749	-0.044095
C	1.438245	2.750266	-0.848967
C	0.777517	3.974996	-0.916731
C	-0.338806	4.164109	-0.107257
C	-0.750972	3.131573	0.728467
H	2.323117	2.557974	-1.473737
H	1.133949	4.759554	-1.591344
H	-0.893249	5.108267	-0.130382
H	-1.639953	3.254166	1.354718
Cl	3.235318	-0.884983	1.258653
C	2.779147	-0.684385	-1.761877
C	0.190649	-0.692817	-1.639098
C	1.175721	-1.710134	-1.533884
C	1.344141	-3.035935	-1.648153
H	2.241604	-3.520871	-1.238283
H	0.614471	-3.666332	-2.174855
N	-1.178314	-0.825546	-1.305214
C	-1.974335	0.278358	-1.529287
C	-3.427064	0.197704	-1.120361
C	-3.983685	-1.201691	-0.946315
C	-3.005845	-2.009025	-0.116262
C	-1.683871	-2.118495	-0.841497
O	-1.521540	1.312713	-1.997482
H	-3.491604	0.752257	-0.159063
H	-3.995359	0.800513	-1.850796
H	-4.116019	-1.686412	-1.935160
H	-4.982241	-1.161923	-0.475166
H	-3.381075	-3.028679	0.085735
H	-2.856967	-1.519844	0.869809
H	-1.787841	-2.795920	-1.715575
H	-0.917726	-2.569962	-0.188144
H	0.346050	0.115253	-2.368284
H	3.162169	0.295783	-1.395540
H	3.562987	-1.442608	-1.616715
H	2.534054	-0.556603	-2.831040

TS DE
SCF Energy: -2943.44260696
ZPE-corrected Energy: -2943.06770
ΔU: -2943.04397
ΔH: -2943.04303
ΔG: -2943.12105
Num. Imaginary Frequencies: 1
Imaginary Frequency: -377.9460

Ni	-0.761894	-1.126264	0.456480
N	-1.890131	0.151313	-0.540004
C	-2.844984	-0.298233	-1.352891
C	-3.738537	0.554041	-1.990665
C	-3.628397	1.921661	-1.750659
C	-2.631861	2.383583	-0.897885
C	-1.762087	1.466427	-0.303268
C	-0.652100	1.857258	0.594396
H	-2.892079	-1.387222	-1.488208
H	-4.506615	0.148937	-2.655897
H	-4.318292	2.628746	-2.222939
H	-2.540239	3.453399	-0.689973
N	-0.065689	0.853817	1.259196
C	0.984385	1.106331	2.032372
C	1.509404	2.385871	2.200151
C	0.891348	3.439369	1.530227
C	-0.206474	3.176010	0.718056
H	1.431019	0.244834	2.552209
H	2.378778	2.548774	2.844698
H	1.266769	4.463128	1.632381
H	-0.687350	3.989110	0.166410
Cl	-2.554767	-1.553524	1.834475
C	0.311431	-2.508435	1.430022
C	0.536687	-1.216696	-1.010567
C	0.107814	-2.480613	-0.532315
C	-0.157059	-3.698684	-1.016756
H	-0.725886	-4.440611	-0.439312
H	0.210234	-3.996871	-2.008910
N	1.837998	-0.666632	-0.859506
C	2.001009	0.635277	-1.280543
C	3.384210	1.245204	-1.218362
C	4.408854	0.494122	-0.390181
C	4.288929	-0.985129	-0.699089
C	2.918328	-1.468881	-0.281206
O	1.070249	1.279810	-1.742693
H	3.722857	1.311755	-2.273102
H	3.248711	2.291122	-0.886871
H	4.224528	0.658119	0.691751
H	5.424329	0.875767	-0.599745
H	5.050995	-1.580049	-0.163861
H	4.441613	-1.159535	-1.783801
H	2.854019	-1.437361	0.826414
H	2.755165	-2.518349	-0.587813
H	0.040659	-0.831040	-1.912147
H	0.274047	-1.781560	2.271242
H	-0.310941	-3.377564	1.693791
H	1.359112	-2.817090	1.304888

TS E1F1.3
SCF Energy: -5376.19417916
ZPE-corrected Energy: -5375.72195
ΔU: -5375.68724
ΔH: -5375.68630
ΔG: -5375.79092
S^2 before (2.0279) and after higher multiplicity projection (2.0003)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -311.3118

Ni	-1.499036	1.285638	0.342179
N	-3.380414	0.569189	0.052815
C	-4.326595	1.225454	-0.610920
C	-5.550219	0.640086	-0.919723
C	-5.778872	-0.667715	-0.498147
C	-4.787357	-1.343930	0.205591
C	-3.579649	-0.693128	0.456147
H	-4.090133	2.261197	-0.889169
H	-6.307652	1.202966	-1.472930
H	-6.730690	-1.163528	-0.715263
H	-4.955739	-2.370803	0.541554
C	-2.438588	-1.309561	1.165889
N	-1.326845	-0.549338	1.254179
C	-0.264512	-1.011760	1.914118
C	-0.239541	-2.269737	2.508097
C	-1.372576	-3.070580	2.408445
C	-2.487139	-2.584034	1.730972
H	0.615814	-0.359384	1.974553
H	0.662109	-2.602171	3.032057
H	-1.396059	-4.068593	2.858084
H	-3.390641	-3.194749	1.653356
Cl	-2.065100	3.230980	1.367711
C	0.029338	1.826712	-1.028582
C	0.958142	1.766640	0.043377
C	-0.636160	0.737121	-1.613050
H	0.981065	2.635990	0.712581
H	1.290295	0.810508	0.467875
N	-0.195259	-0.606771	-1.628450
H	-1.383554	0.959748	-2.391099
C	1.219674	-0.965202	-1.796709
C	1.584899	-2.194737	-0.976535
C	0.496644	-3.275516	-1.054077
C	-0.541232	-2.953713	-2.124617
C	-1.123242	-1.573820	-1.943121
O	-2.314015	-1.329119	-2.064985
H	1.848064	-0.104334	-1.522265
H	1.408999	-1.154712	-2.874001
H	2.555277	-2.573174	-1.351304
H	1.760378	-1.897176	0.076296
H	0.932890	-4.271910	-1.246730
H	-0.022807	-3.355078	-0.079218
H	-1.381258	-3.668688	-2.119390
H	-0.081314	-3.008142	-3.133231
C	-0.315307	3.188736	-1.572779
C	3.018508	2.271117	-0.667827
O	3.546541	1.189544	-1.026706
H	2.567408	2.904974	-1.461679
C	3.491844	2.978979	0.562504
H	3.484377	2.293266	1.430329
H	4.542713	3.287135	0.385476
H	2.900762	3.882421	0.787446
Zn	4.441258	-0.287814	0.065205
C	5.915927	-1.204407	-0.858096
Cl	3.259014	-0.416795	1.993282
H	0.396242	3.453480	-2.381049
H	-1.331368	3.216795	-2.008702
H	-0.256217	3.964312	-0.790301
H	6.538810	-1.798415	-0.163257
H	5.522824	-1.893130	-1.631303
H	6.571633	-0.470383	-1.364791

TS E1F1
SCF Energy: -5376.18305563
ZPE-corrected Energy: -5375.71060
ΔU: -5375.67681
ΔH: -5375.67587
ΔG: -5375.77619
S^2 before (0.8906) and after higher multiplicity projection (0.0506)
Num. Imaginary Frequencies: 2
Imaginary Frequency: -466.2237

Ni	-1.393314	1.245624	0.400228
N	-3.244727	0.595207	0.085789
C	-4.156231	1.292984	-0.587089
C	-5.397854	0.758523	-0.912943
C	-5.686486	-0.540944	-0.502181
C	-4.732039	-1.260785	0.208593
C	-3.501769	-0.662745	0.478097
H	-3.875067	2.320076	-0.853169
H	-6.123993	1.355567	-1.472147
H	-6.655226	-0.995604	-0.733712
H	-4.943668	-2.282474	0.535954
C	-2.394100	-1.326623	1.192777
N	-1.257014	-0.605590	1.283837
C	-0.214110	-1.107116	1.945455
C	-0.236530	-2.366089	2.538304
C	-1.398045	-3.125037	2.437354
C	-2.492710	-2.598481	1.756760
H	0.691055	-0.489027	2.007182
H	0.652177	-2.730882	3.063011
H	-1.458789	-4.121051	2.887885
H	-3.418481	-3.174869	1.676489
Cl	-1.983357	3.258722	1.309278
C	-0.025209	1.792196	-1.090936
C	0.856309	1.734153	0.043693
C	-0.626885	0.690036	-1.693142
H	0.784788	2.577502	0.743583
H	1.192502	0.775050	0.460926
N	-0.193749	-0.643860	-1.680577
H	-1.423131	0.884130	-2.427973
C	1.224841	-1.008532	-1.808261
C	1.565625	-2.237534	-0.977202
C	0.466916	-3.307079	-1.058022
C	-0.546382	-2.995119	-2.155389
C	-1.126985	-1.614033	-1.994708
O	-2.313644	-1.360032	-2.119260
H	1.846507	-0.143182	-1.527267
H	1.434954	-1.202700	-2.880398
H	2.533844	-2.628805	-1.343679
H	1.740979	-1.938563	0.074845
H	0.896367	-4.310942	-1.224243
H	-0.072602	-3.364694	-0.092542
H	-1.387273	-3.708720	-2.162200
H	-0.062992	-3.057753	-3.152347
C	-0.362786	3.146301	-1.651272
C	2.793651	2.323057	-0.498890
O	3.393573	1.303495	-0.952961
H	2.391813	3.036658	-1.251911
C	3.248638	2.941663	0.790689
H	3.251227	2.190271	1.601912
H	4.292937	3.285244	0.645586
H	2.636697	3.811778	1.083348
Zn	4.365932	-0.198974	0.010460
C	5.832817	-1.054729	-0.982464
Cl	3.262951	-0.530853	1.967076
H	0.386714	3.432959	-2.416639
H	-1.351789	3.146860	-2.146249
H	-0.372554	3.919123	-0.864334
H	6.479361	-1.663600	-0.322821
H	5.432984	-1.722256	-1.770785
H	6.467338	-0.294518	-1.477416

TS EE1
SCF Energy: -2943.48417437
ZPE-corrected Energy: -2943.10942
ΔU: -2943.08522
ΔH: -2943.08428
ΔG: -2943.16529
S^2 before (1.0216) and after higher multiplicity projection (0.2027)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -116.6088

Ni	-1.291349	-1.091553	0.738725
N	-1.326392	0.869670	1.370534
C	-1.663681	1.756492	0.413536
C	-1.598493	3.131544	0.645666
C	-1.187123	3.588395	1.893494
C	-0.853198	2.662829	2.878661
C	-0.934258	1.309964	2.565468
H	-1.863172	3.845399	-0.139387
H	-1.128817	4.663331	2.093070
H	-0.529399	2.978699	3.874686
H	-0.674158	0.542760	3.305803
C	-2.094602	1.163379	-0.870899
C	-2.525079	1.910915	-1.968562
C	-2.926345	1.243087	-3.121735
C	-2.899872	-0.149184	-3.146528
C	-2.461667	-0.821791	-2.009971
N	-2.061311	-0.180673	-0.913126
H	-2.554389	3.003513	-1.929501
H	-3.265261	1.811054	-3.994370
H	-3.216941	-0.710215	-4.030743
H	-2.442634	-1.918432	-1.950357
Cl	-2.604832	-2.981458	0.702271
C	0.708623	-1.392951	0.395472
C	0.345235	-1.816514	1.681356
C	1.403667	-0.109058	0.173363
C	0.758719	-2.378401	-0.752857
H	0.633175	-1.205109	2.551901
H	0.148416	-2.880625	1.879434
N	2.754956	-0.076737	-0.171748
C	3.219699	1.010911	-0.892834
C	4.694401	1.072360	-1.219194
C	5.602949	0.229404	-0.344728
C	4.993884	-1.150536	-0.195804
C	3.651062	-1.038196	0.487173
O	2.455811	1.873388	-1.301748
H	4.973117	2.141426	-1.219593
H	4.779970	0.742445	-2.276001
H	6.617163	0.182996	-0.780727
H	5.707728	0.692776	0.657484
H	4.871011	-1.620235	-1.193555
H	5.638718	-1.821404	0.400210
H	3.145829	-2.017932	0.521353
H	3.785841	-0.720485	1.543002
H	0.880551	0.837202	-0.002642
H	1.781765	-2.773859	-0.925469
H	0.088668	-3.236572	-0.560742
H	0.441944	-1.897288	-1.698861

TS EF.3
SCF Energy: -5376.19500948
ZPE-corrected Energy: 0
ΔU: 0
ΔH: 0
ΔG: 0
S^2 before (2.0221) and after higher multiplicity projection (2.0002)
Num. Imaginary Frequencies: 0

Ni	-1.468547	-0.826384	1.186445
N	-2.807017	0.390084	0.271721
C	-3.307879	1.486680	0.835305
C	-4.084778	2.391304	0.120051
C	-4.349177	2.113298	-1.220033
C	-3.831759	0.958135	-1.797321
C	-3.041496	0.112503	-1.017946
H	-3.082456	1.625961	1.901231
H	-4.478373	3.288227	0.607169
H	-4.961237	2.796602	-1.817948
H	-4.031417	0.734066	-2.848761
C	-2.399325	-1.121941	-1.516753
N	-1.598669	-1.761935	-0.638787
C	-0.992548	-2.891074	-1.001714
C	-1.146652	-3.451219	-2.266352
C	-1.966838	-2.799414	-3.180115
C	-2.602535	-1.619927	-2.801809
H	-0.355771	-3.368656	-0.247645
H	-0.626853	-4.379286	-2.520914
H	-2.117144	-3.205015	-4.185923
H	-3.256729	-1.098377	-3.505801
Cl	-2.655273	-1.269569	3.070919
C	0.457482	-0.281286	1.914267
C	0.892187	-1.621857	1.964303
C	0.321824	0.309391	0.653170
H	0.788167	-2.194172	2.896592
H	1.082211	-2.174891	1.033252
N	0.285305	1.695348	0.385022
H	0.581388	-0.294536	-0.227367
C	0.978226	2.678763	1.225868
C	1.969386	3.478438	0.399666
C	1.293455	4.198999	-0.769347
C	-0.076781	3.584048	-1.083173
C	-0.133969	2.093411	-0.862985
O	-0.533654	1.304262	-1.707785
H	1.524209	2.129776	2.004172
H	0.243980	3.340924	1.729463
H	2.496985	4.191377	1.059703
H	2.739445	2.767631	0.039780
H	1.153877	5.271500	-0.542366
H	1.939923	4.156754	-1.665135
H	-0.398677	3.783957	-2.118279
H	-0.837740	4.034421	-0.413729
C	0.265841	0.444149	3.219064
C	3.086587	-0.949837	1.979590
O	3.143243	-0.033364	1.124977
H	2.925094	-0.649831	3.037633
C	3.724202	-2.283894	1.771040
H	3.573641	-2.630059	0.732721
H	4.815740	-2.169910	1.939245
H	3.350579	-3.037943	2.484600
Zn	3.406993	-0.109024	-0.908416
C	4.232422	1.433233	-1.804649
Cl	2.317495	-2.003493	-1.548054
H	-0.157485	-0.244871	3.969522
H	1.232597	0.821146	3.610097
H	-0.422946	1.303427	3.131520
H	4.745042	2.089727	-1.078091
H	4.966832	1.120173	-2.571111
H	3.457571	2.040339	-2.314306

TS EF
SCF Energy: -5376.18321846
ZPE-corrected Energy: 0
ΔU: 0
ΔH: 0
ΔG: 0
S^2 before (0.9308) and after higher multiplicity projection (0.0674)
Num. Imaginary Frequencies: 0

Ni	-1.310305	-0.899264	1.201668
N	-2.625727	0.330374	0.356912
C	-3.083218	1.427097	0.960024
C	-3.849502	2.371735	0.286950
C	-4.152498	2.139101	-1.054148
C	-3.683593	0.985212	-1.672613
C	-2.901271	0.095132	-0.936094
H	-2.828246	1.531653	2.023484
H	-4.206793	3.265135	0.807186
H	-4.756732	2.856126	-1.619621
H	-3.911482	0.793896	-2.724875
C	-2.307433	-1.140583	-1.483633
N	-1.498678	-1.811761	-0.638941
C	-0.931782	-2.947766	-1.039598
C	-1.134503	-3.481552	-2.309106
C	-1.960350	-2.792902	-3.190025
C	-2.557025	-1.605741	-2.773139
H	-0.285881	-3.454445	-0.312673
H	-0.644520	-4.417092	-2.594463
H	-2.145075	-3.175768	-4.199079
H	-3.215804	-1.054427	-3.449934
Cl	-2.410431	-1.492918	3.096134
C	0.594647	-0.311435	1.919106
C	1.021820	-1.653565	1.895301
C	0.428395	0.320828	0.676827
H	0.915730	-2.269713	2.799216
H	1.119321	-2.177977	0.934149
N	0.289950	1.697753	0.439113
H	0.656122	-0.247891	-0.233231
C	0.836836	2.727795	1.329214
C	1.710807	3.678362	0.531710
C	0.930990	4.378431	-0.582130
C	-0.322053	3.578932	-0.957081
C	-0.147619	2.088891	-0.810549
O	-0.403161	1.289234	-1.698368
H	1.450660	2.224516	2.088630
H	0.021312	3.265102	1.857681
H	2.187695	4.405547	1.212894
H	2.510856	3.059062	0.084292
H	0.633895	5.399672	-0.281963
H	1.576834	4.495598	-1.472007
H	-0.655582	3.780436	-1.988202
H	-1.158943	3.859274	-0.284642
C	0.440581	0.355545	3.258924
C	3.263279	-1.148551	1.801740
O	3.328854	-0.196267	0.998509
H	3.218206	-0.891637	2.883958
C	3.720902	-2.534528	1.492229
H	3.423919	-2.838582	0.474416
H	4.829512	-2.545247	1.547865
H	3.339810	-3.261086	2.229698
Zn	3.123392	0.041434	-1.026325
C	3.652225	1.770259	-1.810235
Cl	2.084791	-1.838558	-1.699438
H	0.048210	-0.373447	3.988127
H	1.414165	0.728487	3.638080
H	-0.265154	1.204331	3.234614
H	4.287099	2.373550	-1.131118
H	4.226209	1.606843	-2.743114
H	2.755129	2.367064	-2.072904

6.5 Ni/Zn mechanism via a redox pathway

A
SCF Energy: -4781.74641788
ZPE-corrected Energy: -4781.51348
ΔU: -4781.49234
ΔH: -4781.49140
ΔG: -4781.56605
S^2 before (0.4796) and after higher multiplicity projection (0.0032)
Num. Imaginary Frequencies: 0

Ni	-0.175386	-0.081391	-0.675307
Cl	-1.642155	-1.755293	-0.966166
Cl	-1.718925	1.399447	-1.347446
N	1.326230	-1.292141	-0.217872
C	1.293949	-2.627284	-0.215989
C	2.409028	-3.397037	0.098367
C	3.596698	-2.751826	0.422873
C	3.629717	-1.360790	0.426359
C	2.473749	-0.655547	0.101854
C	2.387492	0.810898	0.081372
H	0.329550	-3.077687	-0.474996
H	2.335164	-4.488062	0.085407
H	4.495797	-3.323457	0.673784
H	4.552671	-0.832290	0.678845
C	3.439933	1.654842	0.427328
C	3.244560	3.031701	0.386464
C	2.002382	3.524877	0.003926
C	0.997925	2.622149	-0.328154
N	1.186786	1.300306	-0.295020
H	4.405851	1.244187	0.732488
H	4.059635	3.710722	0.655988
H	1.801120	4.598947	-0.039063
H	-0.001624	2.948841	-0.635939
Zn	-2.654113	0.020509	0.942608
C	-4.560136	-0.082212	0.458366
H	-5.118655	0.831248	0.745429
H	-4.649017	-0.200604	-0.639599
H	-5.073002	-0.943096	0.932381
C	-1.052746	0.266324	2.095698
H	-1.379709	0.182869	3.152768
H	-0.248432	-0.484869	1.958489
H	-0.603203	1.272617	1.975222

B
SCF Energy: -4781.76118596
ZPE-corrected Energy: -4781.52636
ΔU: -4781.50599
ΔH: -4781.50504
ΔG: -4781.57686
Num. Imaginary Frequencies: 0

N	1.233386	-1.367251	-0.381241
C	1.381962	-2.694348	-0.295396
C	2.507417	-3.297673	0.252597
C	3.528003	-2.490128	0.740071
C	3.385861	-1.110659	0.649218
C	2.231932	-0.574806	0.081123
H	0.564165	-3.307854	-0.681438
H	2.569221	-4.388807	0.292240
H	4.429184	-2.925336	1.183276
H	4.177204	-0.451845	1.015865
C	2.012489	0.869578	-0.078953
N	0.874995	1.189834	-0.720944
C	0.579041	2.472948	-0.922157
C	1.405533	3.507084	-0.494611
C	2.577346	3.185288	0.181240
C	2.888724	1.845760	0.391582
Ni	-0.312751	-0.399346	-1.027825
H	-0.372831	2.670440	-1.427916
H	1.121956	4.546543	-0.683836
H	3.248292	3.969671	0.546202
H	3.803117	1.572352	0.924733
Cl	-2.081827	0.844559	-1.516167
Cl	-0.721844	1.103876	2.078744
Zn	-2.191905	-0.066905	0.862879
C	-3.768565	-1.224825	1.067069
C	-1.302586	-1.992738	-1.396963
H	-4.345347	-1.239381	0.122188
H	-3.472059	-2.265785	1.300723
H	-4.435747	-0.871309	1.876539
H	-0.719763	-2.526090	-2.178505
H	-2.317005	-1.799830	-1.787695
H	-1.395417	-2.648277	-0.507071

Ethane
SCF Energy: -79.6793951925
ZPE-corrected Energy: -79.605997
ΔU: -79.602497
ΔH: -79.601553
ΔG: -79.629117
Num. Imaginary Frequencies: 0

C	-0.758776	0.000001	0.000000
H	-1.165811	0.936540	-0.424255
H	-1.165830	-0.835678	-0.598939
H	-1.165834	-0.100851	1.023181
C	0.758776	-0.000001	0.000000
H	1.165830	0.835677	0.598940
H	1.165811	-0.936541	0.424253
H	1.165834	0.100853	-1.023181

H
SCF Energy: -4781.76624895
ZPE-corrected Energy: -4781.53047
ΔU: -4781.51066
ΔH: -4781.50971
ΔG: -4781.58041
Num. Imaginary Frequencies: 0

N	-1.112531	1.445434	-0.458164
C	-1.038786	2.778580	-0.419250
C	-1.987632	3.571916	0.215813
C	-3.057972	2.950060	0.848429
C	-3.146874	1.563193	0.805435
C	-2.162302	0.836283	0.137676
H	-0.178796	3.238093	-0.916148
H	-1.876195	4.659922	0.212305
H	-3.822598	3.536043	1.368168
H	-3.984507	1.053960	1.288831
C	-2.198312	-0.627886	-0.007427
N	-1.183587	-1.151698	-0.724818
C	-1.171685	-2.464641	-0.958530
C	-2.149912	-3.327790	-0.477683
C	-3.181776	-2.798502	0.289358
C	-3.210085	-1.427853	0.521746
Ni	0.264668	0.174254	-1.101527
H	-0.341760	-2.851974	-1.558287
H	-2.091687	-4.396675	-0.701996
H	-3.965886	-3.443307	0.698818
H	-4.019736	-0.990020	1.111186
C	1.567236	-1.194980	-1.613211
C	1.529344	1.557554	-1.513950
H	2.501411	1.246221	-1.936473
H	0.966764	2.104771	-2.302818
H	1.744185	2.268703	-0.688545
H	1.097215	-1.320188	-2.614534
H	2.635749	-0.971408	-1.797001
H	1.507065	-2.174684	-1.094043
Zn	1.952194	-0.203864	0.469004
Cl	4.088611	0.335491	0.628776
Cl	0.686543	-0.998690	2.136730

I
SCF Energy: -4702.05079363
ZPE-corrected Energy: -4701.88890
ΔU: -4701.87239
ΔH: -4701.87145
ΔG: -4701.93716
S^2 before (0.8056) and after higher multiplicity projection (0.0845)
Num. Imaginary Frequencies: 0

N	-0.704514	1.139096	-0.053227
C	-0.004726	2.279244	-0.006498
C	-0.598291	3.507706	0.263540
C	-1.969332	3.550717	0.498908
C	-2.699618	2.367227	0.445742
C	-2.041307	1.171410	0.160816
H	1.075961	2.195607	-0.193064
H	0.014610	4.413689	0.289640
H	-2.472111	4.497882	0.719716
H	-3.778965	2.381384	0.621717
C	-2.726789	-0.133912	0.058376
N	-1.923562	-1.175015	-0.246205
C	-2.449615	-2.394992	-0.372347
C	-3.806231	-2.649209	-0.202642
C	-4.643363	-1.582480	0.116083
C	-4.097652	-0.309112	0.250157
Ni	-0.012092	-0.628051	-0.423427
H	-1.749532	-3.201637	-0.622360
H	-4.194401	-3.665326	-0.320186
H	-5.717675	-1.737389	0.259146
H	-4.742193	0.538327	0.500457
Zn	2.348133	-0.380814	-0.004526
Cl	3.570270	1.442951	-0.608413
Cl	3.493081	-2.090060	0.935466

J
SCF Energy: -2443.55163088
ZPE-corrected Energy: -2443.21510
ΔU: -2443.19458
ΔH: -2443.19363
ΔG: -2443.26613
Num. Imaginary Frequencies: 0

N	-2.280089	-0.793123	-0.049244
C	-3.053449	-1.870205	0.104514
C	-4.373130	-1.790059	0.538675
C	-4.902266	-0.534390	0.824811
C	-4.100098	0.591917	0.662867
C	-2.788276	0.430219	0.219698
H	-2.588165	-2.835068	-0.130009
H	-4.969672	-2.700315	0.650317
H	-5.935482	-0.428369	1.171129
H	-4.499086	1.587507	0.878171
C	-1.845206	1.545076	-0.003556
N	-0.640808	1.165677	-0.484119
C	0.287266	2.093413	-0.740185
C	0.064844	3.449137	-0.518188
C	-1.169950	3.848477	-0.012741
C	-2.140569	2.884482	0.245788
Ni	-0.396831	-0.764920	-0.591603
H	1.237995	1.728834	-1.152272
H	0.851002	4.176242	-0.742445
H	-1.380965	4.905795	0.177852
H	-3.117465	3.178426	0.640979
C	1.395487	-1.228697	-0.987424
C	0.552377	-2.332974	-0.640967
C	0.590443	-3.657683	-0.471976
H	-0.304828	-4.241403	-0.197451
H	1.518876	-4.246396	-0.591739
N	2.444485	-0.736751	-0.117936
H	1.695049	-1.097429	-2.039818
C	2.250401	-0.945691	1.312677
C	3.473144	-0.622333	2.140709
H	1.389759	-0.319787	1.644168
H	1.942764	-1.996545	1.461254
C	4.005747	0.742432	1.752711
H	3.200105	-0.669954	3.210950
H	4.258617	-1.387931	1.973806
C	4.409845	0.697620	0.292055
H	3.211331	1.503551	1.903087
H	4.861299	1.044187	2.384332
C	3.357740	0.128813	-0.639229
H	4.677951	1.691523	-0.108255
H	5.315868	0.067207	0.172218
O	3.374389	0.428717	-1.832967

K
SCF Energy: -2597.21519638
ZPE-corrected Energy: -2596.81566
ΔU: -2596.79246
ΔH: -2596.79152
ΔG: -2596.86936
Num. Imaginary Frequencies: 0

C	-3.150866	2.874922	0.267115
C	-2.665483	1.574834	0.151363
N	-1.366759	1.319773	-0.151187
C	-0.549329	2.354215	-0.391800
C	-0.970187	3.677508	-0.304197
C	-2.290169	3.944339	0.042557
C	-3.506854	0.376359	0.291010
N	-2.862212	-0.767681	-0.003499
C	-3.502696	-1.934705	0.051840
C	-4.845037	-2.017441	0.408752
C	-5.524716	-0.842227	0.721819
C	-4.850522	0.374590	0.662792
Ni	-0.935867	-0.555096	-0.317182
O	-0.756948	-2.327928	-0.702685
C	0.542449	-2.792547	-0.885754
C	1.061955	-3.486665	0.365847
C	1.408841	-1.593651	-1.283774
C	0.942207	-0.479516	-0.390330
C	1.750856	0.280244	0.360281
N	3.186416	0.210565	0.330413
C	3.825719	-0.846313	1.112856
C	5.286906	-1.019310	0.761828
C	5.987026	0.325294	0.817790
C	5.356873	1.251718	-0.206275
C	3.842251	1.279833	-0.205710
H	1.166358	-1.335591	-2.336104
H	2.501419	-1.800214	-1.242665
H	0.550527	-3.544936	-1.713166
H	1.103777	-2.771025	1.211417
H	0.378135	-4.307273	0.655037
H	2.073002	-3.915956	0.218053
H	1.360323	1.060311	1.035412
H	3.265819	-1.783120	0.939988
H	3.721331	-0.613129	2.195757
H	5.376343	-1.445037	-0.259708
H	5.742174	-1.747912	1.457377
H	7.072029	0.227066	0.631070
H	5.877106	0.752005	1.836052
H	5.695752	2.297985	-0.102025
H	5.653717	0.939350	-1.229249
O	3.241447	2.218157	-0.718862
H	-2.885332	-2.804995	-0.203942
H	-5.345713	-2.989644	0.442174
H	-6.579984	-0.869395	1.012643
H	-5.368659	1.306303	0.907700
H	0.486313	2.109641	-0.654390
H	-0.258867	4.483101	-0.508481
H	-2.653824	4.973505	0.125796
H	-4.200930	3.052313	0.516578

L
SCF Energy: -4456.01228286
ZPE-corrected Energy: -4455.54265
ΔU: -4455.51205
ΔH: -4455.51111
ΔG: -4455.60531
Num. Imaginary Frequencies: 0

C	2.343108	3.772366	0.494645
C	2.004172	2.483263	0.092740
N	0.828611	1.910870	0.454132
C	0.006143	2.585934	1.265480
C	0.285781	3.872148	1.715743
C	1.468600	4.481411	1.312078
C	2.890721	1.614581	-0.696204
N	2.435644	0.353848	-0.824632
C	3.149862	-0.549629	-1.496417
C	4.375351	-0.235133	-2.075985
C	4.855034	1.066550	-1.954917
C	4.104728	2.008361	-1.255997
Ni	0.607829	0.095040	-0.134721
O	0.668526	-1.719604	-0.497097
C	-0.586620	-2.349998	-0.590485
C	-1.094822	-2.347450	-2.020678
C	-1.529250	-1.609563	0.356400
C	-1.248466	-0.150117	0.120371
C	-2.210679	0.737674	-0.171351
N	-3.612563	0.428937	-0.143834
C	-4.317114	0.579976	-1.303590
C	-5.808505	0.316963	-1.264356
C	-6.446372	0.388387	0.110837
C	-5.592134	-0.395529	1.088854
C	-4.216844	0.227565	1.173618
H	-1.266323	-1.885304	1.400782
H	-2.590999	-1.896474	0.191291
H	-0.471325	-3.410124	-0.264651
H	-1.260388	-1.310838	-2.375011
H	-0.358305	-2.827162	-2.692074
H	-2.051558	-2.898143	-2.107671
H	-1.988114	1.771990	-0.480716
O	-3.766547	0.871010	-2.358914
H	-5.946420	-0.698254	-1.691401
H	-6.272924	1.010606	-1.988052
H	-7.481691	0.003115	0.075126
H	-6.511328	1.443656	0.447284
H	-6.040378	-0.418644	2.098978
H	-5.503843	-1.448599	0.748033
H	-4.275267	1.206012	1.699748
H	-3.535866	-0.407046	1.769172
H	2.698961	-1.548417	-1.556963
H	4.938495	-1.001568	-2.616414
H	5.811272	1.352508	-2.404914
H	4.462376	3.037150	-1.156716
H	-0.914084	2.069018	1.555022
H	-0.422993	4.379944	2.376106
H	1.720031	5.494620	1.641354
H	3.294853	4.214561	0.186956
Zn	1.780098	-2.422250	1.219739
C	1.801318	-0.946773	2.560380
C	2.193271	-4.281390	0.654447
H	2.178843	-1.280305	3.548881
H	2.446804	-0.104753	2.233612
H	0.784638	-0.529919	2.717136
H	2.325921	-4.325896	-0.446340
H	3.107148	-4.701117	1.120608
H	1.358911	-4.968639	0.905591

M
SCF Energy: -4456.00626494
ZPE-corrected Energy: -4455.53528
ΔU: -4455.50535
ΔH: -4455.50441
ΔG: -4455.59539
Num. Imaginary Frequencies: 0

C	3.819145	1.457874	0.133558
N	3.381043	0.353175	0.804581
C	4.239997	-0.508558	1.617305
C	5.694539	-0.464248	1.204681
C	6.148344	0.977311	1.086194
C	5.317142	1.657911	0.015497
C	1.974747	0.119879	0.998390
C	1.103192	-0.260891	0.050660
C	1.529270	-0.515797	-1.367251
C	1.555679	-1.997902	-1.791086
C	2.581770	-2.781673	-0.979372
O	0.326017	-2.617652	-1.773863
Ni	-0.693697	-0.204689	0.616241
N	-2.579549	0.056046	1.241967
C	-3.227540	1.036522	0.579183
C	-4.591424	1.264409	0.761204
C	-5.293916	0.478639	1.668418
C	-4.610747	-0.504625	2.376911
C	-3.254574	-0.681949	2.124435
C	-2.371395	1.863800	-0.288909
C	-2.844955	2.934472	-1.045400
C	-1.935566	3.718098	-1.749481
C	-0.580222	3.422077	-1.656317
C	-0.181808	2.323731	-0.897997
N	-1.058341	1.547997	-0.250690
H	0.836972	-0.000962	-2.070040
H	2.536481	-0.093217	-1.562677
H	1.944664	-1.974620	-2.844942
H	2.319065	-2.776764	0.096963
H	2.606489	-3.834482	-1.319664
H	3.601171	-2.358793	-1.088634
H	1.671459	0.241418	2.055290
H	3.843406	-1.538100	1.539861
H	4.139501	-0.211493	2.685551
H	5.821446	-0.974850	0.227366
H	6.295293	-1.026538	1.942896
H	7.224111	1.046953	0.841763
H	6.008575	1.489388	2.060491
H	5.485629	2.748438	-0.029669
H	5.599701	1.265899	-0.984136
O	3.060024	2.250070	-0.414774
H	-2.685780	-1.456932	2.649848
H	-5.115777	-1.134498	3.114904
H	-6.364653	0.643222	1.826366
H	-5.104448	2.056684	0.209427
H	0.882973	2.070516	-0.782620
H	0.172779	4.029472	-2.167268
H	-2.286942	4.562194	-2.351866
H	-3.913342	3.164428	-1.082824
Zn	-1.256454	-1.908867	-1.141659
C	-3.211120	-1.863214	-1.324447
H	-3.557154	-0.845446	-1.592875
H	-3.558570	-2.559374	-2.112372
H	-3.699343	-2.147340	-0.371301
C	-0.463022	-1.914105	1.469661
H	0.365086	-2.556097	1.120234
H	-0.243257	-1.624099	2.523419
H	-1.384024	-2.538161	1.484583

N
SCF Energy: -4456.03486123
ZPE-corrected Energy: -4455.56179
ΔU: -4455.53213
ΔH: -4455.53118
ΔG: -4455.62286
Num. Imaginary Frequencies: 0

C	-1.473784	-2.064598	-1.111986
N	-2.208516	-1.367281	-0.059154
C	-3.542622	-1.525861	0.181470
C	-4.343371	-2.402993	-0.760962
C	-3.528682	-3.341067	-1.630695
C	-2.371412	-2.561232	-2.222903
C	-1.483103	-0.526694	0.874930
C	-1.446363	0.911767	0.690790
C	-2.075433	1.496939	-0.562054
C	-1.665949	2.948279	-0.914680
C	-2.596167	3.988844	-0.292995
O	-0.336357	3.231618	-0.636395
Ni	0.271865	-0.103661	0.358114
N	1.361918	-1.686446	0.700632
C	2.613165	-1.616133	0.197623
C	3.607056	-2.516431	0.579624
C	3.296835	-3.513929	1.498651
C	2.001885	-3.586674	2.005978
C	1.067357	-2.648658	1.581250
C	2.808134	-0.540047	-0.789194
C	3.884988	-0.500023	-1.673131
C	3.930228	0.498526	-2.641198
C	2.893568	1.424125	-2.698880
C	1.862069	1.336994	-1.768621
N	1.822647	0.386669	-0.823224
H	-1.810075	0.844496	-1.419132
H	-3.186496	1.449055	-0.477553
H	-1.824883	3.039354	-2.019472
H	-2.563980	3.970547	0.812610
H	-2.286010	5.000515	-0.617457
H	-3.647693	3.835287	-0.605958
H	-1.639958	-0.871423	1.914511
O	-4.105645	-0.954668	1.109252
H	-4.923473	-1.705060	-1.399879
H	-5.091225	-2.931809	-0.142765
H	-4.163809	-3.790052	-2.416149
H	-3.131924	-4.180632	-1.023380
H	-1.773202	-3.175765	-2.920351
H	-2.761883	-1.698126	-2.802289
H	-0.912334	-2.918339	-0.672692
H	-0.707575	-1.371977	-1.513548
H	0.036429	-2.666253	1.954492
H	1.712914	-4.358069	2.725787
H	4.063447	-4.227781	1.816858
H	4.620063	-2.432400	0.175200
H	1.041957	2.074704	-1.741438
H	2.879973	2.219240	-3.450370
H	4.763677	0.542055	-3.349916
H	4.669404	-1.261231	-1.626404
Zn	0.520023	2.325748	0.777801
C	1.875631	2.357045	2.205479
H	2.670352	1.618066	1.979528
H	2.353707	3.347070	2.336186
H	1.415897	2.070473	3.172119
C	-1.763636	1.654619	1.986936
H	-1.424849	2.709728	2.040522
H	-2.866305	1.680123	2.126516
H	-1.323773	1.135309	2.859992

TS AB.3
SCF Energy: -4781.75483894
ZPE-corrected Energy: 0
ΔU: 0
ΔH: 0
ΔG: 0
S^2 before (2.0071) and after higher multiplicity projection (2.0000)
Num. Imaginary Frequencies: 0

N	1.546755	-1.271820	0.039535
C	1.661127	-2.596809	0.107258
C	2.896225	-3.238392	0.103680
C	4.044335	-2.457240	0.019850
C	3.923509	-1.071960	-0.050570
C	2.650233	-0.503479	-0.034768
H	0.717509	-3.154869	0.162712
H	2.949774	-4.329204	0.163741
H	5.036113	-2.920910	0.010092
H	4.818370	-0.447338	-0.116304
C	2.412061	0.958350	-0.082317
N	1.122271	1.333777	-0.066315
C	0.797992	2.624490	-0.058807
C	1.758068	3.630413	-0.091120
C	3.098991	3.258737	-0.127795
C	3.434302	1.907921	-0.118013
Ni	-0.295312	-0.187151	-0.081873
H	-0.274299	2.851400	-0.012459
H	1.455146	4.681375	-0.086461
H	3.887479	4.017791	-0.156290
H	4.484839	1.605451	-0.132120
C	-1.354769	0.643366	-1.726403
Zn	-2.803882	0.079738	-0.167937
C	-4.758520	0.287695	-0.234996
Cl	-1.689098	-2.148399	-0.093341
H	-1.439621	1.745447	-1.794086
H	-0.412542	0.359760	-2.243687
H	-2.142353	0.200585	-2.374440
Cl	-1.445882	0.745881	1.776169
H	-5.045827	1.355512	-0.279584
H	-5.181949	-0.212883	-1.127278
H	-5.237314	-0.153488	0.660124

TS AB
SCF Energy: -4781.73966616
ZPE-corrected Energy: 0
ΔU: 0
ΔH: 0
ΔG: 0
S^2 before (0.9124) and after higher multiplicity projection (0.0205)
Num. Imaginary Frequencies: 0

N	1.516331	-1.264076	0.086320
C	1.617376	-2.591144	0.080067
C	2.844178	-3.239367	-0.031753
C	3.994005	-2.461511	-0.132884
C	3.883322	-1.073368	-0.131959
C	2.616163	-0.500001	-0.025534
H	0.669292	-3.139057	0.169221
H	2.892311	-4.332192	-0.035702
H	4.979544	-2.931103	-0.216355
H	4.779288	-0.452705	-0.218925
C	2.367658	0.958143	-0.043491
N	1.074495	1.329195	0.038504
C	0.748785	2.621510	-0.003552
C	1.703927	3.625395	-0.120266
C	3.044198	3.258845	-0.192369
C	3.381739	1.909466	-0.155791
Ni	-0.279408	-0.174562	0.193917
H	-0.320531	2.852002	0.079160
H	1.394399	4.673995	-0.150362
H	3.828093	4.018182	-0.278506
H	4.430249	1.605284	-0.213200
C	-0.923426	0.088230	-1.764424
Zn	-2.671908	-0.033056	-0.402659
C	-4.583998	0.049004	-0.845046
Cl	-1.641476	-2.024172	0.613691
H	-1.007401	1.153147	-2.060913
H	0.071405	-0.256734	-2.107768
H	-1.655716	-0.509940	-2.348825
Cl	-1.856387	1.240287	1.509305
H	-4.892438	1.078023	-1.107063
H	-4.853990	-0.635764	-1.669836
H	-5.169527	-0.244709	0.046480

TS BH
SCF Energy: -4781.74660541
ZPE-corrected Energy: -4781.51241
ΔU: -4781.49289
ΔH: -4781.49194
ΔG: -4781.56093
S^2 before (0.0680) and after higher multiplicity projection (0.0001)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -128.7071

N	1.744562	-1.241436	0.076384
C	2.065960	-2.537784	0.120369
C	3.376288	-2.995982	0.043673
C	4.402448	-2.066775	-0.088035
C	4.077718	-0.715821	-0.132880
C	2.740445	-0.331199	-0.045703
H	1.237358	-3.245487	0.222038
H	3.578046	-4.070151	0.087154
H	5.447165	-2.386484	-0.154352
H	4.865759	0.035295	-0.234810
C	2.301015	1.072705	-0.065988
N	0.967561	1.241058	0.026860
C	0.457177	2.474142	0.045049
C	1.253300	3.610016	-0.041714
C	2.632223	3.448712	-0.147021
C	3.165272	2.164533	-0.155606
Ni	-0.074449	-0.438378	0.089192
H	-0.630637	2.546213	0.154006
H	0.793127	4.602084	-0.023945
H	3.293309	4.318458	-0.216971
H	4.246256	2.018570	-0.228116
C	-1.191583	0.170788	-1.924849
Zn	-2.463695	0.085835	-0.345910
Cl	-4.589476	-0.507148	-0.213667
C	-0.958110	-2.151105	0.167276
H	-0.668249	-2.752188	-0.719013
H	-2.068802	-2.161103	0.214825
H	-0.608034	-2.655560	1.091481
H	-1.155240	1.225868	-2.257913
H	-0.163529	-0.237850	-2.020650
H	-1.801912	-0.413878	-2.641671
Cl	-1.603875	0.508621	1.815885

TS HI
SCF Energy: -4781.71227047
ZPE-corrected Energy: -4781.47740
ΔU: -4781.45771
ΔH: -4781.45677
ΔG: -4781.52756
Num. Imaginary Frequencies: 1
Imaginary Frequency: -451.8164

N	-2.075890	-1.037818	-0.159344
C	-2.661824	-2.222024	-0.308893
C	-4.043259	-2.389398	-0.293672
C	-4.837204	-1.261882	-0.109113
C	-4.227075	-0.020983	0.044851
C	-2.832977	0.058658	0.012234
H	-1.997435	-3.086495	-0.448077
H	-4.480242	-3.384077	-0.421320
H	-5.928776	-1.342813	-0.084989
H	-4.842341	0.870985	0.188380
C	-2.084319	1.325217	0.153658
N	-0.733204	1.238480	0.077162
C	-0.018199	2.368116	0.180117
C	-0.595311	3.619027	0.373246
C	-1.977920	3.710674	0.463130
C	-2.729049	2.546763	0.347165
Ni	-0.023495	-0.624975	-0.058865
H	1.069717	2.280966	0.077326
H	0.045467	4.502496	0.447568
H	-2.473050	4.674884	0.616740
H	-3.819031	2.595870	0.408029
C	0.664358	-2.118312	-1.067233
C	0.470862	-2.199391	0.925627
H	1.477473	-2.611508	1.089572
H	0.277548	-1.463381	1.754629
H	-0.292490	-2.996212	0.976767
H	0.471503	-1.377539	-1.892063
H	1.716414	-2.439894	-1.129941
H	0.010849	-2.991892	-1.245561
Zn	2.267378	-0.080339	0.005207
Cl	3.873701	-1.437580	0.864039
Cl	3.202540	1.718442	-1.016773

TS JK
SCF Energy: -2597.12916249
ZPE-corrected Energy: -2596.73582
ΔU: -2596.71131
ΔH: -2596.71037
ΔG: -2596.79235
S^2 before (0.0853) and after higher multiplicity projection (0.0006)
Num. Imaginary Frequencies: 1
Imaginary Frequency: -432.3070

N	-1.501664	-0.350928	-1.264399
C	-1.665566	-0.246820	-2.584735
C	-2.635204	-0.967607	-3.274544
C	-3.459469	-1.828249	-2.554204
C	-3.290735	-1.936667	-1.176569
C	-2.298783	-1.179233	-0.555793
H	-0.987651	0.442955	-3.102191
H	-2.735913	-0.853527	-4.357809
H	-4.232407	-2.415372	-3.060608
H	-3.928058	-2.608408	-0.594157
C	-2.019817	-1.200993	0.894200
N	-0.978398	-0.431065	1.268083
C	-0.633324	-0.352175	2.552970
C	-1.313390	-1.053992	3.544252
C	-2.386952	-1.858597	3.171131
C	-2.748621	-1.935144	1.828574
Ni	-0.165901	0.616577	-0.184761
H	0.230966	0.284377	2.779056
H	-1.000933	-0.969510	4.589221
H	-2.946008	-2.426168	3.922275
H	-3.593871	-2.556809	1.519141
C	1.752231	1.098046	0.169654
C	1.025654	1.821890	-0.774750
C	0.799235	3.198137	-0.944301
H	0.066926	3.484523	-1.717282
H	1.667944	3.882376	-0.893529
N	2.528851	-0.061906	-0.142260
H	2.090757	1.580415	1.104776
C	2.633169	-0.445843	-1.548088
C	3.739385	-1.444501	-1.803703
H	1.657111	-0.862255	-1.881470
H	2.789409	0.480327	-2.133041
C	3.625144	-2.596273	-0.824202
H	3.672065	-1.788956	-2.851822
H	4.727341	-0.953625	-1.687418
C	3.790085	-2.054632	0.583443
H	2.630204	-3.075042	-0.933435
H	4.378872	-3.378769	-1.026793
C	2.946001	-0.839646	0.903337
H	3.565272	-2.806987	1.360091
H	4.845835	-1.754143	0.749782
O	2.695973	-0.544996	2.066588
O	-1.276798	2.702949	0.525880
C	-0.301877	3.519328	0.543963
C	-0.610231	4.999954	0.386027
H	0.502621	3.366639	1.324273
H	0.297809	5.622283	0.278022
H	-1.269881	5.158140	-0.488475
H	-1.159713	5.345144	1.285001

TS LM
SCF Energy: -4455.99042197
ZPE-corrected Energy: -4455.52228
ΔU: -4455.49228
ΔH: -4455.49134
ΔG: -4455.58338
Num. Imaginary Frequencies: 1
Imaginary Frequency: -101.7623

C	-3.292394	3.110636	-0.354220
C	-2.756840	1.823693	-0.308551
N	-1.420389	1.608335	-0.221575
C	-0.599839	2.667291	-0.155128
C	-1.067533	3.976364	-0.189828
C	-2.436847	4.204530	-0.297989
C	-3.572376	0.601957	-0.328150
N	-2.855384	-0.540332	-0.319771
C	-3.481409	-1.718151	-0.278308
C	-4.867237	-1.820956	-0.266262
C	-5.620965	-0.649063	-0.299056
C	-4.968111	0.578128	-0.326659
Ni	-0.918678	-0.295422	-0.241402
O	-0.604237	-1.635010	1.399832
C	0.124192	-0.879302	2.316757
C	-0.825434	-0.048121	3.165289
C	1.161081	0.022321	1.592933
C	0.904903	0.029163	0.110015
C	1.860802	0.228143	-0.810536
N	3.230449	0.491844	-0.519844
C	3.590642	1.636235	0.141350
C	5.062250	1.825476	0.444164
C	6.012314	1.096842	-0.488485
C	5.563754	-0.346123	-0.614885
C	4.171870	-0.399035	-1.203733
H	2.202853	-0.315759	1.789701
H	1.120060	1.065512	1.975166
H	0.686489	-1.560314	3.006376
H	-1.374650	0.664530	2.514684
H	-1.569572	-0.697322	3.664506
H	-0.291922	0.534155	3.941932
H	1.648321	0.143728	-1.891002
O	2.772061	2.463662	0.522021
H	5.208844	1.465116	1.484072
H	5.241678	2.914572	0.472253
H	7.048941	1.167565	-0.111829
H	6.003732	1.574752	-1.489647
H	6.247037	-0.934271	-1.254293
H	5.563652	-0.825259	0.385943
H	4.203413	-0.129051	-2.282698
H	3.760090	-1.423936	-1.144927
H	-2.838480	-2.605203	-0.252263
H	-5.343116	-2.805261	-0.232164
H	-6.715083	-0.688797	-0.295863
H	-5.543367	1.508175	-0.336771
H	0.475562	2.454860	-0.067615
H	-0.354776	4.804558	-0.132135
H	-2.837736	5.222570	-0.333915
H	-4.373261	3.258251	-0.433407
Zn	0.470938	-2.369467	-0.156416
C	-0.586588	-1.751877	-1.890043
C	2.020875	-3.563092	0.162389
H	0.306905	-1.974881	-2.511276
H	-1.332816	-2.553850	-2.063093
H	-1.006591	-0.829750	-2.347304
H	1.772416	-4.418952	0.821223
H	2.457405	-3.972698	-0.769986
H	2.820840	-2.985730	0.673186

TS MN
SCF Energy: -4455.96310702
ZPE-corrected Energy: -4455.49418
ΔU: -4455.46407
ΔH: -4455.46312
ΔG: -4455.55672
Num. Imaginary Frequencies: 1
Imaginary Frequency: -419.7991

C	-3.308197	-1.433287	-0.699605
N	-3.267544	-0.675449	0.553163
C	-4.306016	-0.639784	1.447347
C	-5.640526	-1.215799	1.017209
C	-5.585350	-2.213318	-0.123941
C	-4.712083	-1.641142	-1.222465
C	-1.988347	-0.238861	1.015554
C	-1.207604	0.713209	0.403098
C	-1.727745	1.438047	-0.815642
C	-1.263173	2.881529	-1.113000
C	-2.056208	3.927617	-0.332498
O	0.089223	3.088004	-0.966758
Ni	0.569089	0.213861	0.568953
N	2.293672	-0.353274	1.488148
C	3.017890	-1.234288	0.769826
C	4.298916	-1.623099	1.169142
C	4.826533	-1.100864	2.344994
C	4.064939	-0.200258	3.088461
C	2.807092	0.149885	2.611340
C	2.346588	-1.735443	-0.442704
C	2.851139	-2.770321	-1.233865
C	2.147012	-3.168406	-2.363621
C	0.945719	-2.528689	-2.667874
C	0.503446	-1.516880	-1.826430
N	1.182943	-1.118246	-0.745258
H	-1.408428	0.838728	-1.698352
H	-2.840055	1.422535	-0.833377
H	-1.572354	3.035708	-2.182519
H	-1.913202	3.845322	0.761775
H	-1.720852	4.938802	-0.631195
H	-3.140809	3.850131	-0.540786
H	-1.693357	-0.668658	1.983625
O	-4.191459	-0.122458	2.551247
H	-6.265534	-0.346102	0.725057
H	-6.112593	-1.630865	1.925838
H	-6.604092	-2.440628	-0.487799
H	-5.150893	-3.172040	0.226881
H	-4.670917	-2.305765	-2.104884
H	-5.130385	-0.671742	-1.565759
H	-2.810783	-2.416025	-0.541119
H	-2.702504	-0.894179	-1.448940
H	2.177726	0.869792	3.153778
H	4.439156	0.229495	4.022561
H	5.828490	-1.393096	2.676183
H	4.886952	-2.321028	0.565784
H	-0.437270	-0.988288	-2.027989
H	0.356263	-2.805846	-3.546938
H	2.529263	-3.975097	-2.997441
H	3.785432	-3.271318	-0.964029
Zn	1.419214	1.811401	-1.196011
C	3.126934	1.253008	-1.989097
H	2.958816	0.410726	-2.689572
H	3.615169	2.074096	-2.548651
H	3.828212	0.905229	-1.205156
C	-0.274193	1.595214	1.681744
H	-0.881229	2.502877	1.549644
H	-0.481777	1.169358	2.682588
H	0.774459	1.993708	1.634284