Supplementary Information

DFT Studies on Ni-catalyzed Intermolecular Cycloaddition of Diynes with Methyleneaziridines

Xiaoling Lai,[a,b] Mengwei Hu [a,b] and Yang Li *[a.b]

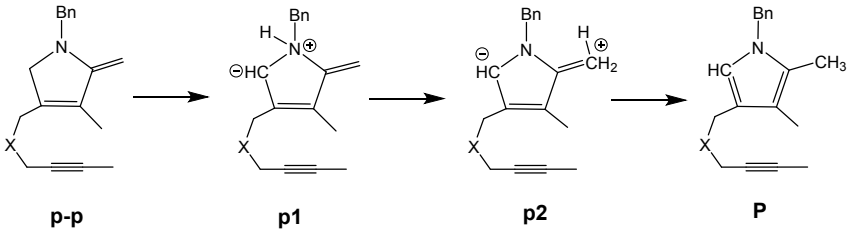
[a.] *State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116023 (P. R. China)*

[b.]*School of Chemical Engineering, Dalian University of Technology, Panjin 124221 (P. R. China)*

Author Email Address: *E-mail: chyangli@dlut.edu.cn*

Contents:

(1)



X = $C(CO_2Me)_2$

Scheme S1 Proposed mechanism for the isomerization of **p-p** to **P**.

(2) Cartesian coordinates for all of the calculated structures.

methyleneaziridines

absolute energy -442.347657 a.u.
enthalpy -442.152847 a.u.
free energy -442.200185 a.u.

C	-2.472461	0.510392	-0.385389
C	-3.244315	-0.588536	0.187904
H	-3.908835	-1.209702	-0.410799
H	-3.512506	-0.515789	1.244827
C	-2.324289	1.776762	-0.746875
H	-1.352956	2.171276	-1.028861
H	-3.177925	2.445298	-0.788147
N	-1.797848	-0.685293	-0.161193
C	-0.800195	-0.775345	0.914053
H	-0.801469	-1.817699	1.259671
H	-1.082116	-0.144541	1.773675
C	0.582863	-0.388063	0.430309
C	1.411627	0.414828	1.221965
C	1.066955	-0.852621	-0.800647
C	2.703206	0.740816	0.801698
H	1.043290	0.790203	2.174278
C	2.353649	-0.522546	-1.225281
H	0.421029	-1.461063	-1.426817
C	3.177647	0.272758	-0.424124
H	3.333371	1.366081	1.428880
H	2.714617	-0.886492	-2.183855
H	4.180325	0.528798	-0.756176

diynes

absolute energy -805.784479 a.u.
enthalpy -805.496560 a.u.
free energy -805.571088 a.u.

C	1.286551	-1.804819	-0.743873
C	2.473079	-2.031385	-0.778447
C	3.914068	-2.263283	-0.807568
H	4.420075	-1.677157	-0.030110
H	4.155790	-3.319480	-0.635052
H	4.346273	-1.977084	-1.774340
C	-0.160530	-1.608543	-0.716718
C	-0.667837	-0.296584	-0.036087
C	-0.092816	-0.086610	1.402448
C	1.253537	0.485988	1.454867
C	2.339880	1.010185	1.539714
C	3.662827	1.624452	1.623586
H	4.310861	1.083262	2.324271
H	4.160424	1.625984	0.645900
H	3.603256	2.665104	1.966117
H	-0.773521	0.574605	1.949410
H	-0.119081	-1.051612	1.921817
H	-0.554193	-1.616366	-1.739355
H	-0.626983	-2.449183	-0.184959
C	-2.198701	-0.431835	-0.001902
O	-2.931544	-0.100658	-0.907684
O	-2.630710	-1.029983	1.127049
C	-0.361212	0.914537	-0.931805
O	-0.769149	2.051557	-0.334069
O	0.160194	0.868824	-2.020364
C	-0.544984	3.254452	-1.085583
C	-4.050748	-1.251607	1.201866
H	-0.936152	4.062985	-0.467369
H	0.523551	3.393040	-1.270102
H	-1.072450	3.209635	-2.041874
H	-4.219251	-1.735677	2.163995
H	-4.587323	-0.301131	1.147474
H	-4.380280	-1.894542	0.381746

cod

absolute energy -312.024465 a.u.
enthalpy -311.834901 a.u.
free energy -311.874794 a.u.

C	-1.083485	1.107083	0.665646
C	-1.923449	0.010472	-0.024332
C	1.923437	-0.010443	-0.024313
C	-1.214822	-1.236310	-0.495375
C	1.083542	-1.107105	0.665579
C	0.008586	-1.704579	-0.218203
H	-0.666196	0.723655	1.600164
H	-2.425257	0.455351	-0.896624
H	2.741430	0.284408	0.653104
H	0.666345	-0.723859	1.600236
H	-1.772014	1.909271	0.959785
H	-2.741473	-0.284329	0.653069
H	2.425304	-0.455283	-0.896597
H	-1.821439	-1.842141	-1.170889
H	1.772099	-1.909330	0.959575
H	0.292311	-2.634794	-0.711642
C	-0.008609	1.704597	-0.218181
H	-0.292404	2.634750	-0.711702
C	1.214789	1.236319	-0.495400
H	1.821357	1.842090	-1.171012

a

absolute energy -1417.497562 a.u.
enthalpy -1417.010883 a.u.
free energy -1417.111650 a.u.

Ni	-0.293245	-1.524341	0.347564
C	-1.853417	-1.550485	-0.916952
C	-0.967508	-2.324983	-1.351249
C	-0.380613	-3.279659	-2.314463
H	-0.249276	-4.271060	-1.862098
H	-1.018609	-3.396077	-3.199523
H	0.608469	-2.946832	-2.651075
C	-3.165512	-0.867511	-0.929699
C	-3.211089	0.441873	-0.096703
C	-2.797109	0.163374	1.376322
C	-1.416697	-0.345325	1.510186
C	-0.295436	-0.499784	2.052862
C	0.725554	-0.248822	3.090943
H	1.562440	0.320492	2.668791
H	0.312016	0.325263	3.929969
H	1.135577	-1.183610	3.492568
H	-3.430353	-0.628900	-1.966056
H	-3.936411	-1.539789	-0.534765
C	-4.638330	1.003968	-0.136768
O	-4.966749	2.041622	-0.669031
O	-5.508504	0.182186	0.488884
C	-2.313073	1.502301	-0.759102
O	-2.017522	2.500187	0.093434
O	-1.936829	1.462304	-1.908416
C	-1.237848	3.570521	-0.462970
C	-6.879195	0.618366	0.485452
H	-1.099663	4.283999	0.349923
H	-0.273367	3.196144	-0.815633
H	-1.771611	4.033889	-1.296730
H	-7.430963	-0.151497	1.025278
H	-6.973245	1.584991	0.986851
H	-7.247868	0.711707	-0.539270
H	-2.903589	1.085303	1.958880
H	-3.506619	-0.565030	1.785797
C	1.720613	-1.630311	-0.073252
C	2.354972	-1.121864	-1.295328
H	1.805544	-0.508456	-2.004651
H	3.184515	-1.694844	-1.716099
C	1.371453	-2.740769	0.661448
H	1.117796	-3.673302	0.167808
H	1.609994	-2.798388	1.720181
N	2.559884	-0.508621	0.045377
C	3.866515	-0.691279	0.690254
C	4.879456	0.339108	0.234449
C	6.214804	-0.027531	0.030696
C	4.509658	1.676886	0.039955
C	7.166807	0.921299	-0.348948
H	6.513289	-1.064705	0.169185
C	5.457448	2.624885	-0.345721
H	3.471366	1.963108	0.179291
C	6.790113	2.251436	-0.538668
H	8.199191	0.618327	-0.503379
H	5.155161	3.658066	-0.496938
H	7.527372	2.991110	-0.839394
H	3.700921	-0.603744	1.772324
H	4.257020	-1.708811	0.513914

a1

absolute energy -1287.167340 a.u.
enthalpy -1286.685904 a.u.
free energy -1286.780871 a.u.

Ni	1.889837	-0.033537	0.080184
C	4.173044	-0.592567	-1.829894
C	4.387837	0.803000	-1.186397
C	3.409534	-2.463351	0.625944
C	3.775461	0.955258	0.191559
C	4.380752	-1.367313	1.141371
C	3.748472	0.013381	1.195973
H	4.954169	-1.284838	-1.501124
H	3.931311	1.561117	-1.834146
H	3.986836	-3.349017	0.314573
H	5.284080	-1.342469	0.524146
H	4.296855	-0.496899	-2.915285
H	5.464982	1.035202	-1.162482
H	2.779318	-2.793245	1.460584
H	3.486704	1.971433	0.456175
H	4.715177	-1.646940	2.147571
H	3.408059	0.343416	2.175755
C	2.801956	-1.178557	-1.537874
H	2.059388	-1.070743	-2.326602
C	2.485600	-2.007006	-0.485495
H	1.530529	-2.528484	-0.530730
C	-2.154149	2.361623	-1.075069
C	-1.455387	3.342546	-1.181522
C	-0.589062	4.513996	-1.282678
H	0.461472	4.239343	-1.126084
H	-0.664246	4.984421	-2.271045
H	-0.850453	5.272003	-0.533938
C	-3.058977	1.215105	-1.032696
C	-2.566455	-0.053522	-0.261945
C	-1.130250	-0.514986	-0.670503
C	0.004803	0.172740	0.001586
C	0.500658	1.033598	0.808587
C	0.344798	2.174048	1.749100
H	1.018970	2.998778	1.485654
H	-0.682734	2.553684	1.750488
H	0.602729	1.873786	2.773164
H	-1.049550	-1.588713	-0.471005
H	-1.037983	-0.410548	-1.758253
H	-4.014365	1.515516	-0.587835
H	-3.271359	0.900176	-2.063810
C	-3.619369	-1.126250	-0.586255
O	-4.666304	-1.253627	0.010794
O	-3.283792	-1.864579	-1.664217
C	-2.648514	0.180576	1.253065
O	-2.288473	-0.933660	1.920098
O	-2.991547	1.208672	1.790678
C	-2.350186	-0.842027	3.351671
C	-4.261071	-2.839160	-2.069524
H	-2.048830	-1.822808	3.720614
H	-1.667407	-0.069140	3.714131
H	-3.367170	-0.604161	3.674196
H	-3.837224	-3.329068	-2.946445
H	-4.433394	-3.562388	-1.268357
H	-5.207332	-2.351612	-2.317905

a2

absolute energy -1417.478512 a.u.
enthalpy -1416.991897 a.u.
free energy -1417.098628 a.u.

Ni	-0.837280	1.730329	0.053005
C	3.268741	0.672528	2.115735
C	3.108697	1.720890	2.696244
C	2.894425	2.999853	3.368068
H	1.931984	3.438413	3.076084
H	2.886397	2.883004	4.458845
H	3.681191	3.722059	3.117365
C	3.488146	-0.636032	1.504152
C	2.706395	-0.940869	0.184622
C	1.181229	-0.617129	0.276159
C	0.845519	0.811400	0.060077
C	1.036883	2.022848	-0.227355
C	1.811015	3.244405	-0.543145
H	1.547353	4.066995	0.130700
H	2.883884	3.041468	-0.445347
H	1.610681	3.585021	-1.565902
H	0.651087	-1.214546	-0.471101
H	0.809568	-0.950779	1.250887
H	4.553290	-0.774880	1.288649
H	3.206640	-1.411825	2.230144
C	2.962697	-2.434370	-0.076189
O	3.996600	-2.864726	-0.539328

O	1.946887	-3.216262	0.337098
C	3.335992	-0.182209	-0.994425
O	2.737475	-0.539052	-2.147823
O	4.234444	0.623642	-0.918105
C	3.249388	0.091876	-3.332717
C	2.158020	-4.631684	0.183629
H	2.673908	-0.327097	-4.158380
H	3.110147	1.174756	-3.278460
H	4.313188	-0.129123	-3.451100
H	1.255437	-5.103695	0.571999
H	2.303194	-4.882187	-0.870165
H	3.036729	-4.949848	0.750315
C	-2.652056	1.958911	-0.623501
C	-3.133633	2.412745	-1.939316
H	-2.459183	2.549617	-2.781679
H	-4.027013	3.041789	-1.955598
C	-2.630471	2.278615	0.732820
H	-2.979792	1.565417	1.478179
H	-2.558008	3.317173	1.051798
N	-3.290837	1.014755	-1.471085
C	-4.640156	0.570851	-1.101026
H	-5.175548	0.365127	-2.038134
H	-5.192662	1.367646	-0.573476
C	-4.608489	-0.677959	-0.241726
C	-5.425707	-0.785037	0.889271
C	-3.785068	-1.760136	-0.583910
C	-5.429342	-1.949319	1.661640
H	-6.065080	0.049625	1.168700
C	-3.783069	-2.921419	0.188522
H	-3.139905	-1.677308	-1.453700
C	-4.607001	-3.021232	1.313277
H	-6.070186	-2.014482	2.537197
H	-3.138456	-3.751847	-0.088599
H	-4.605318	-3.926970	1.914069

a3

absolute energy -923.722462 a.u.
enthalpy -923.334840 a.u.
free energy -923.405557 a.u.

Ni	1.680470	-0.566227	0.016049
C	-0.138796	-1.089521	0.363815
C	-1.079043	-0.926553	1.489051
H	-0.870686	-0.259153	2.323860
H	-1.730862	-1.767900	1.735835
C	0.495158	-2.109711	-0.377029
H	0.843026	-3.009314	0.131189
H	0.294397	-2.225940	-1.442849
N	-1.301202	-0.263180	0.182861
C	-2.378209	-0.803473	-0.651446
C	-3.720240	-0.171052	-0.339680
C	-4.882145	-0.950806	-0.307034
C	-3.829393	1.207630	-0.109930
C	-6.128707	-0.369885	-0.061839
H	-4.811064	-2.023526	-0.475067
C	-5.071754	1.789828	0.140759
H	-2.928410	1.813777	-0.116825
C	-6.227171	1.003741	0.162772
H	-7.019827	-0.992212	-0.039942
H	-5.139401	2.860169	0.319624
H	-7.194961	1.458547	0.357739
C	3.109100	0.977901	-1.983720
C	2.835089	2.051161	-0.892732
C	4.587942	0.079584	0.687594
C	1.897171	1.575209	0.203259
C	3.665839	0.596013	1.825384
C	2.266670	0.973020	1.383102
H	3.994419	1.273602	-2.568651
H	2.392913	2.927457	-1.381177
H	5.044111	0.922440	0.160783
H	4.155275	1.442772	2.332539
H	2.271191	0.975227	-2.691311
H	3.778285	2.395749	-0.458657
H	5.417944	-0.474440	1.142162
H	0.854724	1.874987	0.108995
H	3.570330	-0.190024	2.585023
H	1.502549	0.883767	2.154101
C	3.264923	-0.436304	-1.461942
H	2.964131	-1.220852	-2.153886
C	3.874177	-0.825721	-0.298582
H	3.976737	-1.896481	-0.127801
H	-2.104461	-0.596523	-1.695972
H	-2.448793	-1.901874	-0.559931

a4

absolute energy -481.315439 a.u.
enthalpy -481.125743 a.u.
free energy -481.168472 a.u.

Ni	0.000201	-0.000076	-1.176591
C	-0.928060	1.233524	1.172511
C	-1.927930	0.079595	0.819319
C	1.927686	-0.079465	0.819753
C	-1.358711	-1.029019	-0.051807
C	0.927738	-1.233379	1.172846
C	-0.072491	-1.572430	0.069468
H	-0.385102	0.979715	2.088872
H	-2.786075	0.508455	0.285699
H	2.334825	0.322662	1.762128
H	0.384577	-0.979481	2.089062
H	-1.516040	2.127799	1.413085
H	-2.335352	-0.322406	1.761622
H	2.785996	-0.508393	0.286452
H	-2.087594	-1.576780	-0.650155
H	1.515693	-2.127612	1.413641
H	0.124893	-2.491695	-0.486950
C	0.072391	1.572409	0.069283
H	-0.124892	2.491646	-0.487217
C	1.358666	1.029000	-0.051687
H	2.087702	1.576810	-0.649808

a5

absolute energy -793.398188 a.u.
enthalpy -793.015753 a.u.
free energy -793.075503 a.u.

C	2.636824	0.582664	-1.420205
C	2.246256	1.836460	-0.602093
C	2.243757	-1.837509	0.603330
C	1.394315	1.537760	0.614934
C	2.634561	-0.583876	1.421648
C	1.536304	0.470440	1.481591
H	3.553545	0.139809	-1.017172
H	1.674751	2.514085	-1.249314
H	3.152631	-2.394479	0.319609
H	3.551936	-0.141771	1.019326
H	2.886834	0.894426	-2.441887
H	3.155274	2.392504	-0.317028
H	1.670785	-2.514439	1.250000
H	0.780160	2.369627	0.956350
H	2.883412	-0.895622	2.443618
H	1.001577	0.534508	2.426232
C	1.537758	-0.470696	-1.481313
H	1.004417	-0.534553	-2.426794
C	1.393623	-1.538085	-0.614778
H	0.780065	-2.369662	-0.957946
Ni	0.000226	-0.000047	-0.001554
C	-2.634771	0.584530	1.421372
C	-2.243450	1.837851	0.602820
C	-2.245945	-1.836748	-0.602026
C	-1.393630	1.537886	-0.615316
C	-2.637083	-0.582979	-1.419822
C	-1.537974	0.470322	-1.481488
H	-3.552381	0.142812	1.019110
H	-1.670095	2.514579	1.249351

H	-3.154642	-2.393448	-0.317217
H	-3.553534	-0.140139	-1.016162
H	-2.883495	0.896649	2.443259
H	-3.152112	2.395184	0.319135
H	-1.673854	-2.513862	-1.249272
H	-0.779538	2.369045	-0.958573
H	-2.887709	-0.894639	-2.441387
H	-1.004712	0.533651	-2.427046
C	-1.537060	-0.470251	1.481665
H	-1.002464	-0.534252	2.426393
C	-1.394540	-1.537641	0.615238
H	-0.780851	-2.369449	0.957586

1ts(a-b)

absolute energy -1417.464746 a.u.
enthalpy -1416.978702 a.u.
free energy -1417.074878 a.u.
imaginary frequency -205.98 cm^{-1}

Ni	0.231831	1.357967	-0.451247
C	-1.791060	0.840148	-0.834126
C	-2.920764	0.560038	-1.755996
H	-2.855877	-0.141415	-2.581639
H	-3.616651	1.385196	-1.916638
C	-1.494676	2.151262	-0.271563
H	-1.789310	2.328861	0.762183
H	-1.622372	3.010460	-0.929179
N	-2.858996	-0.028014	-0.409710
C	-3.797698	0.448401	0.608066
H	-4.005516	1.525768	0.500074
H	-3.307718	0.313377	1.581275
C	-5.093856	-0.334283	0.563752
C	-6.315986	0.316641	0.365308
C	-5.091347	-1.727148	0.727432
C	-7.514115	-0.402517	0.336054
H	-6.331604	1.396604	0.234663
C	-6.283701	-2.448410	0.695434
H	-4.145429	-2.241771	0.873629
C	-7.500481	-1.787371	0.500732
H	-8.454578	0.120203	0.181701
H	-6.265886	-3.527623	0.824569
H	-8.430064	-2.350051	0.477423
C	2.056960	1.913242	-0.081686
C	1.271172	2.827805	0.285269
C	0.948137	4.150363	0.859813
C	3.352989	1.253067	-0.343248
C	3.298929	-0.294245	-0.242551
C	-1.031488	-1.699286	-1.813292
C	-0.340177	-0.472398	-1.292226
C	0.917455	-0.235949	-1.092045
C	2.247679	-0.875874	-1.231824
H	2.626842	-0.712080	-2.250515
H	2.176223	-1.958642	-1.075581
H	-1.268242	-1.613493	-2.881326
H	-1.950131	-1.917802	-1.266262
H	3.703142	1.501595	-1.352081
H	4.109925	1.628103	0.352923
C	2.964349	-0.746229	1.188358
O	2.087214	-1.518071	1.498539
O	3.804041	-0.170642	2.077229
C	4.677593	-0.851645	-0.625856
O	4.807513	-2.136557	-0.237489
O	5.529105	-0.245860	-1.237800
C	6.051289	-2.768843	-0.586890
C	3.589748	-0.535516	3.450648
H	5.980714	-3.784348	-0.197087
H	6.182427	-2.779806	-1.672008
H	6.890415	-2.236851	-0.131312
H	4.348947	0.003494	4.018036
H	2.587202	-0.240555	3.771091
H	3.703310	-1.614931	3.581168
H	1.859006	4.684089	1.160507
H	0.409067	4.771320	0.135019
H	0.302270	4.049166	1.739592
H	-0.343082	-2.544320	-1.698551

1b

absolute energy -1417.511874 a.u.
enthalpy -1417.024162 a.u.
free energy -1417.121762 a.u.

Ni	-0.844965	-1.948876	0.653800
C	1.447518	-1.689074	-0.946027
C	2.221788	-2.715533	-1.722523
H	2.027012	-2.893848	-2.780250
H	2.539288	-3.602982	-1.169991
C	1.062182	-1.948644	0.501434
H	1.412715	-1.144762	1.161671
H	1.405599	-2.914220	0.906083
N	2.842976	-1.438812	-1.397456
C	3.917178	-1.437551	-0.405416
H	4.806465	-1.852180	-0.901551
H	3.706918	-2.086407	0.460139
C	4.215932	-0.030871	0.079383
C	4.418106	1.008582	-0.840703
C	4.316098	0.255168	1.445530
C	4.717606	2.298601	-0.403202
H	4.328369	0.794626	-1.901853
C	4.616046	1.546857	1.888377
H	4.155501	-0.539377	2.170911
C	4.818521	2.572813	0.964559
H	4.875855	3.092102	-1.129683
H	4.686983	1.749303	2.953992
H	5.053204	3.577924	1.305547
C	-2.749215	-1.443975	1.210797
C	-2.736520	-2.668255	1.027564
C	-3.072127	-4.095713	0.880406
H	-2.440745	-4.730166	1.512135
H	-4.117585	-4.271832	1.161770
H	-2.936908	-4.419090	-0.157622
C	-3.118230	-0.020559	1.263396
C	-2.377260	0.852316	0.189121
C	0.675505	-0.077360	-2.830655
C	0.383481	-0.844200	-1.567510
C	-0.760901	-0.838308	-0.853045
C	-1.977028	0.031316	-1.080765
H	-2.849871	-0.561039	-1.380122
H	-1.779637	0.741154	-1.890333
H	-0.196604	0.463587	-3.206416
H	1.017914	-0.753267	-3.625513
H	-4.201171	0.042650	1.095567
H	-2.903003	0.400320	2.248842
C	-1.124806	1.484072	0.829904
O	-0.787963	1.344451	1.985250
O	-0.451899	2.213826	-0.070699
C	-3.332088	2.007217	-0.142744
O	-4.188149	1.686790	-1.134556
O	-3.360141	3.062814	0.451296
C	-5.153966	2.701068	-1.464241
C	0.759281	2.829919	0.407590
H	-5.751891	2.281039	-2.273293
H	-5.780557	2.929203	-0.598017
H	-4.650696	3.614945	-1.789608
H	1.151835	3.392013	-0.439452
H	0.538074	3.495221	1.245701
H	1.474709	2.067416	0.723021
H	1.489057	0.637513	-2.663590

1ts(b-c)

absolute energy -1417.461947 a.u.
enthalpy -1416.977017 a.u.
free energy -1417.073725 a.u.
imaginary frequency -289.54 cm^{-1}

Ni	0.149186	1.526186	0.265285

C	-1.651216	0.478926	-0.118588
C	-1.861580	2.281048	-0.208417
C	-1.247457	0.045357	1.192240
H	-0.718976	-0.890678	1.297519
H	-1.712971	0.461955	2.083258
N	-2.818223	1.204935	-0.444594
C	-3.993805	1.146911	0.429924
H	-4.615894	2.006271	0.146484
H	-3.740742	1.282706	1.494161
C	-4.768299	-0.142736	0.249678
C	-5.184910	-0.548134	-1.026806
C	-5.097341	-0.941749	1.349820
C	-5.915307	-1.723875	-1.195106
H	-4.924174	0.062686	-1.886486
C	-5.833253	-2.118143	1.185240
H	-4.775715	-0.641355	2.344590
C	-6.243502	-2.512492	-0.088296
H	-6.231919	-2.025052	-2.190473
H	-6.079546	-2.726746	2.051443
H	-6.813614	-3.428378	-0.219923
C	1.969235	2.014042	0.161380
C	1.291730	3.088829	0.074559
C	1.177165	4.546968	-0.160302
H	2.120327	4.979444	-0.520658
H	0.397805	4.764489	-0.900954
C	3.195853	1.203115	-0.036225
C	2.937883	-0.311886	-0.275194
H	0.895251	5.071139	0.761111
C	-1.417712	-0.900567	-2.357417
C	-0.801355	-0.195627	-1.178974
C	0.481265	-0.023428	-0.823702
C	1.792206	-0.541729	-1.310978
H	2.091063	-0.032868	-2.239390
H	1.727003	-1.615036	-1.524381
H	-1.945277	-0.189921	-3.006805
H	-2.156085	-1.646188	-2.034636
H	3.747872	1.579191	-0.905364
H	3.859126	1.312039	0.827830
C	2.600407	-1.064236	1.024325
O	1.733644	-1.899111	1.150662
O	3.437564	-0.706953	2.022592
C	4.224015	-0.919530	-0.867980
O	4.296423	-2.245397	-0.638336
O	5.050107	-0.306607	-1.507760
C	5.437076	-2.913707	-1.204897
C	3.233466	-1.389895	3.269957
H	5.330261	-3.960776	-0.921404
H	5.440752	-2.806310	-2.292623
H	6.363057	-2.495711	-0.801754
H	3.988955	-0.991926	3.948001
H	2.229347	-1.191084	3.653221
H	3.359601	-2.467994	3.139825
H	-0.653501	-1.406874	-2.955858
H	-1.660883	2.894826	-1.086599
H	-2.060040	2.854182	0.701306

1c

absolute energy -1417.528990 a.u.
enthalpy -1417.040620 a.u.
free energy -1417.137235 a.u.

Ni	-0.069490	1.211398	-0.337975
C	1.113967	-0.265007	-0.397977
C	1.789228	0.464137	1.824296
N	2.005178	0.510296	0.416756
C	3.273124	0.972973	-0.141720
H	3.058258	1.420028	-1.119514
C	4.368403	-0.074986	-0.321582
C	4.307899	-1.343711	0.264314
C	5.481779	0.250341	-1.109721
C	5.339888	-2.265764	0.068138
H	3.458385	-1.608990	0.885152
C	6.514481	-0.666193	-1.302607
H	5.538587	1.231180	-1.579001
C	6.445805	-1.931398	-0.713270
H	5.276151	-3.247283	0.530678
H	7.369425	-0.395677	-1.916994
H	7.247212	-2.649504	-0.864857
C	0.366513	0.262660	2.215730
C	-0.589323	0.347135	1.265510
C	0.089749	-0.025592	3.675849
C	-2.870195	-0.147204	0.158201
C	-3.002542	1.154471	-0.693148
C	-1.710406	1.831837	-0.958306
C	-0.896494	2.766898	-1.236988
H	-3.654507	1.848745	-0.144274
H	-3.502549	0.912859	-1.635918
H	-0.948843	-0.326769	3.833441
H	0.272536	0.856048	4.305621
C	-2.257502	-1.324712	-0.619519
O	-1.824891	-2.321577	-0.081258
O	-2.291992	-1.158447	-1.955027
C	-4.308339	-0.538717	0.551128
O	-4.920917	-1.234822	-0.428969
O	-4.849219	-0.225432	1.587657
C	-6.281457	-1.617196	-0.159492
C	-1.789458	-2.262572	-2.723840
H	-6.609000	-2.167975	-1.041350
H	-6.903519	-0.732025	-0.003463
H	-6.329614	-2.249169	0.730811
H	-1.896237	-1.964161	-3.767065
H	-2.370386	-3.165602	-2.518357
H	-0.740149	-2.450937	-2.482817
C	-2.057957	0.068045	1.467160
H	-2.199007	-0.823645	2.087730
H	-2.536286	0.897015	2.005781
C	-0.627333	4.142998	-1.725472
H	0.029729	4.126912	-2.603119
H	-0.115935	4.734134	-0.956746
H	-1.550210	4.669264	-2.002792
H	0.736952	-0.828388	4.051222
H	0.884325	-1.265788	-0.036868
H	1.429568	-0.258906	-1.447742
C	2.799281	0.597936	2.709415
H	3.838426	0.660595	2.410293
H	2.596777	0.643141	3.771530
H	3.630871	1.787623	0.498809

1ts(c-a)

absolute energy -1417.523723 a.u.
enthalpy -1417.036418 a.u.
free energy -1417.131434 a.u.
imaginary frequency -317.51 cm^{-1}

Ni	0.094007	1.382840	-0.380248
C	1.796443	0.136703	1.780277
C	1.516140	-0.036442	-0.573921
N	2.221195	0.609938	0.510356
C	3.569267	1.123278	0.266840
C	4.608929	0.095583	-0.163180
C	4.770043	-1.126102	0.508240
C	5.439131	0.373451	-1.256488
C	5.739679	-2.039985	0.093473
H	4.133549	-1.359179	1.356349
C	6.415869	-0.535995	-1.667361
H	5.320252	1.312682	-1.793137
C	6.568042	-1.747889	-0.992929
H	5.850537	-2.982455	0.623686
H	7.050340	-0.300027	-2.517781
H	7.323580	-2.460852	-1.312146
C	-0.091648	-0.364879	0.413704
C	0.460349	-0.478199	1.657551
C	-1.203066	-1.217710	-0.161469
C	-2.546821	-0.531124	-0.590054

C	-2.383092	0.570297	-1.681253
C	-1.534210	1.682338	-1.209209
C	-1.139428	2.823417	-0.812753
H	-3.378897	0.925236	-1.969462
H	-1.463463	-2.009689	0.547240
C	-3.418022	-1.648831	-1.193117
O	-3.547956	-1.864425	-2.377453
O	-3.986734	-2.404253	-0.230694
C	-3.270813	0.035332	0.641042
O	-4.399626	0.680258	0.275194
O	-2.916168	-0.082791	1.791479
C	-5.168578	1.235537	1.354324
C	-4.788092	-3.504120	-0.696840
H	-6.036038	1.700776	0.885359
H	-5.478973	0.448519	2.046675
H	-4.579745	1.978593	1.898247
H	-5.167692	-3.989069	0.202589
H	-5.610951	-3.139777	-1.317055
H	-4.179746	-4.198289	-1.282387
C	-0.122144	-1.207575	2.835946
H	-1.091061	-1.647611	2.602142
H	-0.285009	-0.517948	3.674369
C	-1.358657	4.284756	-0.666343
H	-2.336729	4.593239	-1.059155
H	-1.304252	4.583917	0.387323
H	-0.586308	4.854628	-1.196957
H	-0.813329	-1.714542	-1.061170
H	1.741512	-1.097042	-0.739859
H	1.678564	0.497799	-1.524939
C	2.514873	0.208169	2.921306
H	3.530068	0.584538	2.959728
H	2.073971	-0.099196	3.860833
H	-1.949642	0.094264	-2.567210
H	3.492955	1.890096	-0.512696
H	3.885066	1.644095	1.177493
H	0.559595	-1.992168	3.191449

p-p

absolute energy -1248.252263 a.u.
enthalpy -1247.764137 a.u.
free energy -1247.858747 a.u.

C	1.428081	-2.157707	-1.064342
C	1.210234	0.066862	-0.372743
H	1.594451	0.995683	-0.821868
H	1.070417	0.265011	0.702883
C	1.857568	-3.436233	-1.145087
H	1.222401	-4.194141	-1.586418
H	2.838447	-3.753473	-0.810277
N	2.130330	-1.046660	-0.580371
C	3.284744	-1.178844	0.286209
H	2.985863	-1.392599	1.328314
H	3.857091	-2.047212	-0.058679
C	4.186946	0.043070	0.260493
C	4.648070	0.614961	1.450656
C	4.603139	0.596347	-0.958856
C	5.515172	1.710622	1.429136
H	4.326064	0.199264	2.403127
C	5.464401	1.692588	-0.984141
H	4.238931	0.162626	-1.886595
C	5.925685	2.252585	0.211025
H	5.863853	2.141924	2.364004
H	5.778592	2.110417	-1.937286
H	6.597422	3.106743	0.190912
C	-0.064765	-0.399671	-1.036946
C	0.088599	-1.671038	-1.463799
C	-1.220208	0.546991	-1.230184
C	-2.264257	0.715169	-0.064464
C	-1.640805	0.753983	1.368555
C	-1.183508	-0.549467	1.853077
C	-0.812522	-1.633420	2.241169
H	-2.392813	1.151703	2.058657
H	-0.817304	1.476511	1.363561
H	-1.793210	0.269018	-2.118503
H	-0.800829	1.544230	-1.415042
C	-2.994456	2.038967	-0.350961
O	-4.048384	2.130878	-0.941011
O	-2.291120	3.102909	0.088904
C	-3.354587	-0.369852	-0.143080
O	-4.156231	-0.312870	0.936168
O	-3.509663	-1.153883	-1.051068
C	-5.250408	-1.243885	0.941693
C	-2.875872	4.387472	-0.192661
H	-5.783048	-1.062383	1.875503
H	-4.876889	-2.270380	0.903918
H	-5.903099	-1.065894	0.083305
H	-2.185059	5.119432	0.226144
H	-3.858963	4.469934	0.277571
H	-2.983235	4.529223	-1.271027
C	-0.868008	-2.543290	-2.216405
H	-0.413462	-2.892847	-3.152188
H	-1.803912	-2.029878	-2.436482
H	-1.117718	-3.437487	-1.630614
C	-0.333951	-2.950387	2.656121
H	0.270562	-3.407808	1.862726
H	-1.167026	-3.628332	2.878551
H	0.287611	-2.883868	3.557671

2b

absolute energy -1729.505557 a.u.
enthalpy -1728.827236 a.u.
free energy -1728.947840 a.u.

Ni	-0.465682	1.604493	0.462122
C	1.436080	1.265971	1.087932
C	1.957722	-0.023614	1.558503
H	1.362292	-0.930958	1.514301
H	2.734789	0.000333	2.326718
C	1.166074	2.578043	1.417203
H	1.569169	3.394364	0.826855
H	0.812264	2.828269	2.412798
N	2.309247	0.563011	0.233868
C	3.661243	1.078849	0.034395
H	3.602267	1.855829	-0.739906
H	4.027774	1.582361	0.947955
C	4.651465	0.009677	-0.393192
C	5.993506	0.369460	-0.584169
C	4.274145	-1.321540	-0.602773
C	6.938001	-0.575322	-0.981636
H	6.300911	1.401029	-0.420355
C	5.222639	-2.270081	-0.998323
H	3.241192	-1.619760	-0.455698
C	6.554184	-1.903000	-1.190516
H	7.973223	-0.276585	-1.126113
H	4.913816	-3.300660	-1.154017
H	7.288611	-2.642716	-1.498169
C	-1.068324	4.964061	-0.974738
C	0.079834	4.060780	-1.485568
C	-3.398157	2.907880	-0.310971
C	-0.126826	2.557612	-1.448763
C	-2.721377	2.433146	-1.621780
C	-1.312895	1.848957	-1.523962
H	-1.886043	4.968042	-1.700361
H	0.991089	4.302616	-0.923648
H	-4.308096	3.470365	-0.576775
H	-2.720285	3.248526	-2.353673
H	-0.691308	5.994577	-0.946326
H	0.300760	4.351739	-2.525966
H	-3.750171	2.022699	0.230619
H	0.774029	2.000177	-1.709849
H	-3.375576	1.666386	-2.055371
H	-1.230202	0.815520	-1.846558
C	-1.583753	4.588718	0.391594
H	-1.085450	5.061648	1.237700

C	-2.566076	3.716562	0.658878
H	-2.824106	3.565503	1.706945
C	-1.326410	-2.877587	2.320965
C	-0.745518	-2.751858	3.374681
C	-0.009863	-2.605891	4.629184
C	-2.073799	-3.226189	1.112529
C	-2.035111	-2.262860	-0.117091
C	-1.059809	0.724601	3.401742
C	-1.270163	0.598618	1.945147
C	-1.754018	0.094121	0.899406
C	-2.636248	-0.846568	0.162219
H	-2.917428	-0.415761	-0.800617
H	-3.572207	-0.997051	0.716925
H	-0.000060	0.600580	3.655905
H	-1.629666	-0.036747	3.947201
H	-1.721403	-4.200824	0.756168
H	-3.133250	-3.355871	1.376830
C	-2.840139	-3.015240	-1.199471
O	-2.468844	-4.061596	-1.686602
O	-4.012240	-2.429663	-1.507281
C	-0.601001	-2.161937	-0.667220
O	-0.599545	-1.536165	-1.859964
O	0.391424	-2.597576	-0.129985
C	0.692124	-1.388072	-2.486099
C	-4.804496	-3.123011	-2.488616
H	0.493393	-0.902661	-3.442018
H	1.341516	-0.771905	-1.859549
H	1.146818	-2.369661	-2.641052
H	-5.710089	-2.527244	-2.604178
H	-4.261970	-3.190818	-3.434838
H	-5.044522	-4.131318	-2.142160
H	0.879866	-1.977790	4.498565
H	-0.625838	-2.148484	5.413315
H	0.329327	-3.580540	5.001757
H	-1.365646	1.714199	3.763870

2ts(b-c)

absolute energy -1729.477964 a.u.
enthalpy -1728.800482 a.u.
free energy -1728.917835 a.u.
imaginary frequency -251.58 cm^{-1}

Ni	1.235472	0.829313	0.423944
C	1.614043	-0.443596	1.926972
C	1.339481	-1.557972	2.888166
H	0.331787	-1.891968	3.120744
H	2.065287	-1.668192	3.697525
C	2.606930	0.590268	1.861862
H	3.580423	0.363002	1.437097
H	2.599500	1.362014	2.629780
N	1.790568	-1.822791	1.526424
C	3.141543	-2.353616	1.339422
H	3.098068	-3.412490	1.632400
H	3.868173	-1.867083	2.011582
C	3.624456	-2.244857	-0.094329
C	4.971125	-1.970496	-0.362333
C	2.752632	-2.456368	-1.171771
C	5.442590	-1.912143	-1.675909
H	5.657724	-1.799177	0.464315
C	3.220570	-2.393741	-2.485189
H	1.704241	-2.654575	-0.972574
C	4.567262	-2.123011	-2.742515
H	6.491151	-1.696270	-1.864049
H	2.531522	-2.556203	-3.310146
H	4.929791	-2.074115	-3.765854
C	3.058325	4.044139	-0.512620
C	3.572483	2.598642	-0.691883
C	-0.140839	3.659468	-0.599647
C	2.571146	1.500811	-1.005554
C	0.464727	2.872722	-1.784753
C	1.267235	1.604256	-1.494003
H	2.643484	4.404929	-1.457891
H	4.148614	2.311302	0.196731
H	-0.625719	4.561001	-1.009913
H	1.067007	3.545574	-2.406634
H	3.933500	4.676561	-0.314300
H	4.299631	2.612353	-1.520257
H	-0.959960	3.062548	-0.180193
H	3.065577	0.551641	-1.215133
H	-0.381135	2.581816	-2.419946
H	0.916910	0.736271	-2.050255
C	2.068148	4.227022	0.610157
H	2.497555	4.500414	1.574500
C	0.740962	4.063862	0.558377
H	0.187811	4.247559	1.480694
C	-4.432684	1.317570	0.459129
C	-4.944025	2.297979	-0.032293
C	-5.570462	3.479877	-0.620634
C	-3.814628	0.124255	1.039263
C	-2.967279	-0.685097	0.015198
C	-0.730178	0.485197	3.021005
C	-0.196842	0.220041	1.639243
C	-0.611560	0.265587	0.413443
C	-1.752043	0.125288	-0.525967
H	-1.412794	-0.360252	-1.446443
H	-2.119503	1.111827	-0.836595
H	0.070309	0.604983	3.757301
H	-1.381995	-0.330298	3.353941
H	-3.163528	0.400483	1.873423
H	-4.582217	-0.536547	1.455119
C	-3.860245	-1.087649	-1.170267
O	-3.701068	-0.754673	-2.322039
O	-4.881381	-1.866220	-0.750878
C	-2.446650	-1.955876	0.703768
O	-1.866862	-2.774751	-0.192379
O	-2.514944	-2.189404	1.891752
C	-1.208106	-3.934247	0.350681
C	-5.799224	-2.284480	-1.774255
H	-0.948977	-4.550860	-0.510620
H	-0.305876	-3.620580	0.883012
H	-1.875482	-4.473228	1.026927
H	-6.544925	-2.896103	-1.265702
H	-6.267938	-1.415523	-2.243351
H	-5.279056	-2.866596	-2.539536
H	-5.469814	3.478457	-1.712820
H	-6.641352	3.521593	-0.386470
H	-5.112807	4.403818	-0.246527
H	-1.321474	1.408069	3.016492

2c

absolute energy -1729.546029 a.u.
enthalpy -1728.865514 a.u.
free energy -1728.980622 a.u.

Ni	-1.856125	-1.143315	0.076731
C	0.331145	-2.334062	-1.168615
C	0.343729	-3.586915	-1.995767
H	0.234377	-3.553204	-3.079813
H	-0.079168	-4.483169	-1.533610
C	-0.316964	-2.316569	0.198069
H	0.338032	-1.839053	0.937067
H	-0.605353	-3.306253	0.570460
N	1.594926	-3.068714	-1.463039
C	2.243018	-3.839080	-0.408012
H	2.778378	-4.663969	-0.899651
H	1.517475	-4.314101	0.276841
C	3.228375	-3.025929	0.415590
C	3.379429	-1.644518	0.257045
C	4.005442	-3.677281	1.384926
C	4.276682	-0.926455	1.053440
H	2.795544	-1.120507	-0.489528
C	4.906742	-2.966457	2.176306
H	3.902748	-4.753008	1.520388
C	5.043851	-1.584387	2.014577

H	4.360211	0.147577	0.912886
H	5.501527	-3.490612	2.920676
H	5.743341	-1.028607	2.633985
C	-3.996483	-1.393365	2.387411
C	-3.642021	0.098444	2.185796
C	-4.459382	-2.468510	-0.593023
C	-3.316013	0.491436	0.761294
C	-4.973909	-1.011467	-0.508553
C	-3.859175	0.008117	-0.390725
H	-5.043405	-1.574515	2.129204
H	-2.766828	0.339347	2.801296
H	-5.294784	-3.164283	-0.417739
H	-5.673946	-0.902551	0.324230
H	-3.904502	-1.628474	3.454022
H	-4.459469	0.728633	2.569817
H	-4.116651	-2.663185	-1.616153
H	-2.666052	1.357399	0.674542
H	-5.550081	-0.797021	-1.415980
H	-3.553243	0.481886	-1.320770
C	-3.093386	-2.324630	1.603338
H	-2.264717	-2.762188	2.156151
C	-3.312004	-2.793413	0.337603
H	-2.670313	-3.598133	-0.011148
C	1.046453	2.670160	1.821216
C	1.572061	3.463223	2.568047
C	2.237478	4.412973	3.456551
H	3.165065	3.992950	3.864763
H	2.499437	5.335062	2.923110
H	1.598290	4.690486	4.304252
C	0.376374	1.724951	0.927178
C	0.234602	2.220579	-0.546729
C	1.071927	-0.620606	-2.952166
C	0.212636	-0.967058	-1.760433
C	-0.658981	-0.167144	-1.096717
C	-0.775668	1.322340	-1.367684
H	-1.775484	1.690657	-1.133885
H	-0.614703	1.552779	-2.428024
H	0.798760	0.338487	-3.397488
H	0.981141	-1.393081	-3.726658
H	0.916184	0.774382	0.904004
H	-0.625353	1.508293	1.310562
C	1.620694	2.197085	-1.211920
O	2.633411	1.775506	-0.696486
O	1.574995	2.676019	-2.469174
C	-0.255732	3.677161	-0.508152
O	-1.517615	3.746805	-0.013489
O	0.381305	4.657014	-0.817752
C	-2.027088	5.077778	0.166600
C	2.838246	2.751677	-3.147296
H	-3.033939	4.954488	0.567268
H	-1.398131	5.632759	0.867444
H	-2.054480	5.611091	-0.787145
H	2.621343	3.199035	-4.117762
H	3.533797	3.377109	-2.582145
H	3.268681	1.754392	-3.270377
H	2.134045	-0.588300	-2.682257

2ts(c-d)

absolute energy -1729.479416 a.u.
enthalpy -1728.801780 a.u.
free energy -1728.917416 a.u.
imaginary frequency -263.94 cm^{-1}

Ni	-0.516246	1.657362	0.279273
C	-1.822472	-0.137802	0.088812
C	-1.414102	0.513859	-1.556947
C	-2.434613	0.755252	0.992567
H	-2.258228	0.589063	2.046970
H	-3.344686	1.287531	0.735733
N	-2.342358	-0.518049	-1.195190
C	-3.754453	-0.241288	-1.500047
H	-3.834076	-0.328536	-2.591672
H	-4.058009	0.787638	-1.248174
C	-4.683780	-1.232651	-0.832284
C	-4.461699	-2.611208	-0.960601
C	-5.796318	-0.794237	-0.106201
C	-5.333737	-3.527285	-0.373551
H	-3.596283	-2.957908	-1.517997
C	-6.675122	-1.709690	0.478010
H	-5.978529	0.272810	0.002332
C	-6.444785	-3.079319	0.346646
H	-5.148203	-4.592974	-0.480178
H	-7.534504	-1.351214	1.038680
H	-7.124874	-3.794175	0.802339
C	-1.443597	4.560039	0.718932
C	-1.467511	3.866585	2.104428
C	1.389643	3.803912	-0.464497
C	-0.504576	2.704872	2.229076
C	1.507085	3.819693	1.075530
C	0.783943	2.659762	1.741598
H	-0.695099	5.359604	0.710925
H	-2.476178	3.484465	2.294367
H	1.605152	4.809065	-0.864344
H	1.134816	4.765169	1.482227
H	-2.407603	5.059892	0.565499
H	-1.267379	4.606547	2.897716
H	2.165727	3.141244	-0.855052
H	-0.789693	1.929488	2.934620
H	2.567508	3.773277	1.350767
H	1.409639	1.844037	2.085769
C	-1.192419	3.601844	-0.438213
H	-2.063774	3.372256	-1.047141
C	0.053732	3.293587	-0.969422
H	0.079967	2.861691	-1.969008
C	2.418971	-3.549715	0.167245
C	2.644987	-4.406999	0.991242
C	2.911407	-5.453331	1.976082
H	3.731359	-6.106774	1.653267
H	3.190981	-5.025894	2.946953
H	2.028187	-6.084100	2.135648
C	2.166380	-2.519429	-0.841370
C	2.668377	-1.104458	-0.416867
C	-0.820511	-2.373764	0.927063
C	-0.619477	-0.923991	0.551181
C	0.464021	-0.124323	0.534166
C	1.887180	-0.545749	0.819835
H	1.940202	-1.328103	1.591104
H	2.465043	0.300427	1.201656
H	-1.194173	-2.956416	0.074518
H	-1.570634	-2.470809	1.724243
H	2.670117	-2.789976	-1.775079
H	1.098757	-2.443166	-1.066986
C	2.504193	-0.189651	-1.641869
O	1.769465	-0.406301	-2.581230
O	3.319978	0.885428	-1.577012
C	4.183483	-1.240257	-0.171600
O	4.567454	-0.901773	1.072141
O	4.951138	-1.640346	-1.021464
C	5.969910	-1.060870	1.340545
C	3.378098	1.680267	-2.774332
H	6.104402	-0.756538	2.379020
H	6.268142	-2.103100	1.200855
H	6.561217	-0.429086	0.672580
H	4.085475	2.481558	-2.559362
H	3.731809	1.070401	-3.609860
H	2.394908	2.088344	-3.018782
H	0.105477	-2.839151	1.273490
H	-0.501800	0.183880	-2.040979
H	-1.881492	1.411725	-1.960407

2d

absolute energy -1729.563815 a.u.
enthalpy -1728.882504 a.u.

free energy -1728.999513 a.u.

Ni	-0.373458	-1.420186	-0.185316
C	-1.670867	1.177327	-1.458757
C	-1.554865	-0.129951	0.633117
C	-2.382753	1.948558	-2.321193
H	-1.898586	2.475431	-3.130658
H	-3.451537	2.094419	-2.225792
N	-2.305548	0.423109	-0.464761
C	-3.725572	0.152892	-0.549125
H	-3.911627	-0.843624	-0.124266
H	-4.003575	0.092598	-1.609831
C	-4.648564	1.144049	0.159468
C	-4.157584	2.269728	0.826368
C	-6.031246	0.911767	0.155576
C	-5.030198	3.145099	1.478813
H	-3.089211	2.461421	0.825732
C	-6.904288	1.783494	0.805220
H	-6.427568	0.038392	-0.360654
C	-6.404504	2.905632	1.472024
H	-4.631684	4.016334	1.992466
H	-7.973653	1.587589	0.792575
H	-7.082252	3.586276	1.980593
C	-1.856030	-3.930249	-1.288243
C	-1.101564	-3.255676	-2.460144
C	0.407604	-4.085070	1.021910
C	0.263084	-2.700961	-2.116170
C	1.032152	-4.413108	-0.355186
C	1.168495	-3.192117	-1.235319
H	-1.493469	-4.950700	-1.138106
H	-1.709149	-2.425921	-2.839480
H	0.179975	-5.024066	1.551311
H	0.457314	-5.193513	-0.859242
H	-2.909080	-4.028681	-1.576318
H	-1.013146	-3.969203	-3.294270
H	1.161781	-3.572160	1.630005
H	0.576516	-1.855505	-2.724077
H	2.028736	-4.836734	-0.183427
H	2.129023	-2.686205	-1.182528
C	-1.786304	-3.141274	0.007431
H	-2.685748	-2.582144	0.249268
C	-0.828345	-3.211969	0.986285
H	-1.060610	-2.728939	1.934851
C	3.209483	3.130146	-0.414158
C	3.941390	3.668364	-1.213676
C	4.814326	4.334393	-2.178023
H	5.543255	4.982680	-1.676167
H	5.375639	3.607046	-2.777571
H	4.237944	4.958678	-2.871901
C	2.341677	2.485950	0.573431
C	2.536588	0.940571	0.654897
C	0.472157	2.187257	-2.360602
C	-0.175111	1.119645	-1.492523
C	0.513669	0.178645	-0.795265
C	2.026993	0.201535	-0.627248
H	2.544765	0.666393	-1.474610
H	2.412577	-0.817084	-0.564290
H	0.107044	3.187778	-2.099344
H	0.226038	2.029128	-3.419452
H	2.539218	2.904252	1.565407
H	1.286808	2.679418	0.352504
C	1.794155	0.451722	1.908045
O	1.009859	1.105045	2.558293
O	2.149982	-0.813413	2.232104
C	4.033199	0.703715	0.932906
O	4.672468	0.045651	-0.051464
O	4.583331	1.100826	1.938203
C	6.084559	-0.128353	0.150969
C	1.591514	-1.299876	3.463696
H	6.441645	-0.663437	-0.729581
H	6.577263	0.843235	0.239355
H	6.273400	-0.707351	1.058716
H	2.032205	-2.285396	3.617704
H	1.851497	-0.631002	4.287810
H	0.503404	-1.369733	3.388231
H	1.557792	2.201145	-2.276378
H	-1.031512	0.624230	1.220847
H	-2.240396	-0.677787	1.288507

2ts(d-a)

absolute energy -1729.550352 a.u.
enthalpy -1728.870682 a.u.
free energy -1728.986024 a.u.
imaginary frequency -124.91 cm^{-1}

Ni	-0.083743	1.670563	0.146167
C	2.084133	-0.203906	1.606960
C	1.062735	0.256349	-0.547714
N	2.240574	0.254341	0.301192
C	3.517281	0.720692	-0.183889
C	4.474368	-0.349133	-0.709687
C	4.044864	-1.647062	-1.002691
C	5.815993	-0.014979	-0.939015
C	4.937861	-2.589852	-1.518410
H	3.010707	-1.922106	-0.818316
C	6.709026	-0.953466	-1.455816
H	6.165342	0.990329	-0.708139
C	6.271067	-2.247583	-1.748461
H	4.587981	-3.595111	-1.739683
H	7.746776	-0.676897	-1.625319
H	6.964708	-2.982340	-2.148937
C	-1.830240	3.601985	-1.290683
C	-2.165604	4.022636	0.164482
C	0.851840	4.623870	0.140096
C	-1.627411	3.061400	1.205114
C	0.696406	4.125202	1.600369
C	-0.406937	3.111013	1.815800
H	-2.030462	4.447758	-1.967855
H	-3.256726	4.070817	0.261097
H	0.129606	5.417995	-0.067832
H	0.547309	4.990659	2.265222
H	-2.515205	2.800733	-1.590269
H	-1.803687	5.035853	0.359619
H	1.841377	5.085211	0.039524
H	-2.335681	2.328116	1.583963
H	1.637380	3.661339	1.919141
H	-0.244400	2.430638	2.648503
C	-0.421269	3.089472	-1.501168
H	-0.308400	2.413452	-2.348238
C	0.724786	3.513005	-0.883878
H	1.664905	3.110403	-1.256637
C	-0.247885	0.006652	1.009627
C	0.662252	-0.493055	1.894055
C	-1.693054	-0.496220	0.971616
C	-2.040440	-1.577646	-0.100702
C	-2.130424	-0.983377	-1.541007
C	-3.289380	-0.107535	-1.728909
C	-4.271996	0.582458	-1.884150
H	-2.170774	-1.809074	-2.258386
H	-2.394219	0.323417	0.786078
C	-1.001222	-2.707219	-0.103863
O	-0.195659	-2.919593	-0.984872
O	-1.091503	-3.448566	1.016498
C	-3.408836	-2.191686	0.256874
O	-3.719600	-3.181085	-0.609114
O	-4.129172	-1.846312	1.164455
C	-4.991992	-3.812093	-0.394406
C	-0.144814	-4.526102	1.126702
H	-5.068698	-4.583969	-1.160696
H	-5.036552	-4.253386	0.604713
H	-5.800060	-3.083395	-0.499865
H	-0.357799	-5.002797	2.083501
H	-0.277116	-5.233109	0.303604
H	0.876184	-4.137677	1.108181

C	0.380436	-1.383401	3.083789
H	-0.669932	-1.661957	3.172431
H	0.665314	-0.874773	4.015225
C	-5.465452	1.404209	-2.077386
H	-6.043579	1.068366	-2.947011
H	-6.124349	1.354920	-1.201895
H	-5.207358	2.458069	-2.239401
H	-1.976411	-0.912364	1.941306
H	0.773389	-0.743383	-0.879000
H	1.335960	0.792263	-1.473304
C	3.110833	-0.433020	2.463017
H	4.149249	-0.354317	2.165148
H	2.917080	-0.734834	3.484172
H	-1.205086	-0.436312	-1.743730
H	3.329918	1.443879	-0.989672
H	4.015162	1.277222	0.623609
H	0.974850	-2.304970	3.042388

3b

absolute energy -1729.499358 a.u.
enthalpy -1728.820579 a.u.
free energy -1728.942897 a.u.

Ni	-0.613482	-1.424845	-0.371083
C	-2.065315	-0.824569	-1.712324
C	-2.939528	-1.578397	-2.624233
H	-3.197552	-2.621478	-2.449196
H	-2.963454	-1.275145	-3.673797
C	-0.955719	0.006011	-1.785007
H	-1.010832	1.003114	-1.353142
H	-0.183811	-0.158621	-2.533167
N	-3.475882	-0.620521	-1.625706
C	-4.011843	0.642172	-2.154505
H	-4.986683	0.407967	-2.603178
H	-3.364547	1.043263	-2.953004
C	-4.188463	1.688203	-1.072489
C	-3.542396	2.926413	-1.156411
C	-5.025502	1.440338	0.025245
C	-3.723381	3.898063	-0.167967
H	-2.893847	3.133211	-2.004853
C	-5.206644	2.405655	1.015297
H	-5.531703	0.481635	0.099694
C	-4.555001	3.639485	0.921610
H	-3.214291	4.854895	-0.251337
H	-5.860113	2.198703	1.859028
H	-4.698162	4.392570	1.692043
C	-3.196404	-1.545834	2.396049
C	-3.326368	-2.304406	1.055754
C	-0.047361	-1.496495	2.916125
C	-2.068980	-2.831669	0.393468
C	-0.421622	-2.912823	2.415687
C	-0.825948	-3.091915	0.951222
H	-2.888915	-2.230194	3.191822
H	-3.843682	-1.665782	0.331371
H	0.073913	-1.547779	4.010918
H	-1.208275	-3.333476	3.051949
H	-4.203395	-1.205394	2.670921
H	-3.988597	-3.170519	1.223039
H	0.943503	-1.247584	2.521413
H	-2.286361	-3.380291	-0.523096
H	0.454686	-3.548248	2.598114
H	-0.236653	-3.836097	0.419874
C	-2.280464	-0.349113	2.343307
H	-2.750718	0.595218	2.071511
C	-0.959852	-0.343672	2.565718
H	-0.451090	0.618958	2.499977
C	3.529161	-0.119489	-2.438392
C	3.307096	-1.051178	-3.176441
C	3.023527	-2.196602	-4.037236
H	2.089436	-2.689232	-3.739383
H	2.917320	-1.893311	-5.086205
H	3.825446	-2.943497	-3.987637
C	3.831554	1.062223	-1.633726
C	3.177547	1.143377	-0.214821
C	1.638480	0.879775	-0.229433
C	1.266303	-0.550815	-0.237659
C	1.440512	-1.779686	-0.159306
C	2.211832	-3.035533	-0.070992
H	2.134610	-3.489667	0.924085
H	1.865714	-3.779881	-0.797423
H	3.268853	-2.824560	-0.269276
H	1.194253	1.353134	0.652041
H	1.214669	1.397687	-1.094792
H	4.915024	1.150656	-1.497009
H	3.506742	1.954598	-2.187066
C	3.506765	2.563403	0.275988
O	4.578739	2.880064	0.744135
O	2.501585	3.433387	0.057345
C	3.888530	0.182789	0.750602
O	3.404750	0.328667	2.001229
O	4.765871	-0.594347	0.452654
C	4.043641	-0.475306	3.006885
C	2.774613	4.795880	0.432548
H	3.540313	-0.228023	3.941660
H	3.929127	-1.537706	2.777440
H	5.107705	-0.232270	3.064783
H	1.869985	5.351832	0.185925
H	2.988628	4.859706	1.502273
H	3.631246	5.181037	-0.126337

3ts(b-c)

absolute energy -1729.476740 a.u.
enthalpy -1728.797422 a.u.
free energy -1728.915291 a.u.
imaginary frequency -197.75 cm^{-1}

Ni	-1.680938	-0.550845	0.045017
C	-1.940524	0.620641	-1.437281
C	-2.786781	0.861251	-2.624308
H	-3.731888	0.343711	-2.775729
H	-2.294772	1.169974	-3.551126
C	-0.496972	0.503304	-1.312553
H	0.005552	1.417573	-0.999979
H	-0.018162	0.016443	-2.159442
N	-2.753614	1.819731	-1.502881
C	-2.104025	3.098699	-1.780203
H	-2.821989	3.701691	-2.355108
H	-1.212275	2.976881	-2.423606
C	-1.710518	3.858266	-0.525517
C	-0.740536	4.867135	-0.604184
C	-2.328194	3.615325	0.707209
C	-0.401248	5.623323	0.518866
H	-0.251271	5.066797	-1.555898
C	-1.980938	4.362432	1.835377
H	-3.080890	2.836596	0.772267
C	-1.019350	5.370100	1.746303
H	0.343615	6.411100	0.434987
H	-2.466867	4.157307	2.785940
H	-0.753408	5.953543	2.623759
C	-4.467537	-1.617342	-0.784097
C	-3.640912	-2.557778	-1.690481
C	-3.206878	-2.442655	2.116041
C	-2.636040	-3.503578	-1.075250
C	-3.529850	-3.715422	1.300917
C	-2.577766	-3.998698	0.166316
H	-5.229182	-2.191735	-0.243997
H	-3.093049	-1.931435	-2.404528
H	-3.992899	-2.342551	2.882826
H	-4.559113	-3.667729	0.935822
H	-5.037180	-0.965715	-1.457318
H	-4.348545	-3.142278	-2.301766
H	-2.282377	-2.605433	2.676291
H	-1.858392	-3.823415	-1.770374
H	-3.505417	-4.559923	2.001711

H	-1.743417	-4.660327	0.400900
C	-3.725175	-0.714449	0.201359
H	-4.004214	0.333707	0.122137
C	-3.129851	-1.101123	1.407232
H	-2.971303	-0.287565	2.118570
C	3.277804	1.482193	1.305174
C	3.335359	2.675316	1.112744
C	3.394625	4.119757	0.900410
H	2.388168	4.545811	0.809614
H	3.897118	4.622240	1.736181
H	3.948046	4.367442	-0.014003
C	3.196309	0.039957	1.540250
C	3.054163	-0.783890	0.225904
C	1.809441	-0.386144	-0.604474
C	0.448223	-0.561922	0.029672
C	-0.142837	-1.133040	1.028699
C	0.146884	-1.890242	2.278593
H	-0.394669	-1.451562	3.125773
H	1.206906	-1.939970	2.539761
H	1.953819	0.660938	-0.884477
H	1.835985	-0.954968	-1.540335
H	4.089291	-0.316158	2.063805
H	2.340775	-0.182886	2.183195
C	3.077409	-2.283868	0.566517
O	3.207717	-2.756418	1.672885
O	2.965718	-3.026053	-0.554000
C	4.358986	-0.560248	-0.575261
O	4.178286	0.066557	-1.749643
O	5.442885	-0.911811	-0.161735
C	5.380876	0.320154	-2.497721
C	3.033717	-4.449744	-0.361553
H	5.055914	0.827308	-3.406434
H	6.059128	0.953866	-1.921089
H	5.885668	-0.619071	-2.737166
H	2.951065	-4.882758	-1.358596
H	3.984011	-4.724865	0.102815
H	2.211622	-4.787950	0.274309
H	-0.207868	-2.923545	2.181740

3c

absolute energy -1729.546187 a.u.
enthalpy -1728.864995 a.u.
free energy -1728.981598 a.u.

Ni	-1.487087	1.480794	0.117147
C	-1.117765	-0.294735	0.779507
C	-1.106732	-0.522726	2.258109
H	-1.393975	0.252946	2.968455
H	-0.366032	-1.224876	2.650356
C	-0.044632	-0.958474	-0.069091
H	-0.482420	-1.389291	-0.983835
H	0.442921	-1.798770	0.444339
N	-2.185300	-1.065896	1.427541
C	-2.260742	-2.526678	1.292154
H	-2.673510	-2.903734	2.238336
H	-1.272633	-2.997340	1.169989
C	-3.160214	-2.949626	0.146953
C	-2.658766	-3.690068	-0.929506
C	-4.523391	-2.617973	0.155995
C	-3.495347	-4.092715	-1.974332
H	-1.604379	-3.956067	-0.949445
C	-5.361351	-3.015514	-0.885736
H	-4.922199	-2.042677	0.987652
C	-4.849069	-3.755858	-1.955481
H	-3.087221	-4.668274	-2.801196
H	-6.416277	-2.753535	-0.861173
H	-5.502223	-4.068854	-2.765926
C	-3.963492	3.029505	1.346259
C	-2.710353	3.937291	1.386468
C	-3.912829	1.822566	-1.633105
C	-1.751249	3.748228	0.231309
C	-3.424853	3.291072	-1.672406
C	-2.048080	3.459356	-1.065792
H	-4.723604	3.459888	0.688122
H	-2.155561	3.730572	2.309717
H	-4.989249	1.785858	-1.862677
H	-4.143585	3.947238	-1.174848
H	-4.407923	3.014336	2.348387
H	-3.017626	4.992780	1.451904
H	-3.417218	1.263722	-2.436090
H	-0.715908	3.985017	0.459293
H	-3.390157	3.617771	-2.718319
H	-1.221535	3.436453	-1.770856
C	-3.643594	1.607030	0.932997
H	-3.525075	0.874458	1.727682
C	-3.637017	1.099420	-0.334647
H	-3.555354	0.018995	-0.414511
C	4.399223	1.584044	0.536024
C	5.027038	2.507126	0.069020
C	5.777775	3.628947	-0.491032
H	5.703255	3.652576	-1.585305
H	5.400850	4.588036	-0.114580
H	6.842230	3.567480	-0.232753
C	3.676541	0.450656	1.119429
C	3.364565	-0.677363	0.089675
C	2.289231	-0.242995	-0.961550
C	0.918817	0.148938	-0.427798
C	0.410721	1.399289	-0.315285
C	1.220603	2.647422	-0.590353
H	0.743218	3.308372	-1.325719
H	2.230215	2.436715	-0.958568
H	2.172138	-1.083333	-1.656056
H	4.275344	0.023755	1.929465
H	2.727716	0.783366	1.555260
C	2.920161	-1.982800	0.770762
O	2.767698	-3.022741	0.165092
O	2.717867	-1.861146	2.096629
C	4.710582	-1.067724	-0.559839
O	4.758604	-0.853136	-1.884117
O	5.637795	-1.512367	0.083394
C	6.008766	-1.186010	-2.510189
C	2.361121	-3.076757	2.776785
H	5.875426	-0.954606	-3.567368
H	6.818710	-0.590000	-2.081806
H	6.233587	-2.246503	-2.371386
H	2.280167	-2.807531	3.830210
H	1.408114	-3.460983	2.403248
H	3.134090	-3.834718	2.628189
H	2.729153	0.574847	-1.535389
H	1.352323	3.242820	0.324480

3ts(c-d)

absolute energy -1729.476220 a.u.
enthalpy -1728.798441 a.u.
free energy -1728.917102 a.u.
imaginary frequency -215.19 cm^{-1}

Ni	1.895909	-1.478607	0.124146
C	1.168824	0.329867	-0.329517
C	0.682108	1.149842	0.739773
H	1.300428	1.386014	1.600363
H	-0.254913	1.695247	0.648148
C	0.020693	-0.115731	-1.258695
H	0.420454	-0.543840	-2.190086
H	-0.568826	0.760518	-1.571480
N	1.867204	1.433505	-0.857939
C	3.155045	1.854105	-0.340476
H	3.918406	1.537434	-1.074716
H	3.425991	1.365999	0.609752
C	3.294085	3.361978	-0.166110
C	4.490745	3.882835	0.346057
C	2.266501	4.245829	-0.506450
C	4.656586	5.256297	0.519858
H	5.300395	3.205120	0.613982

C	2.430686	5.623192	-0.334417
H	1.344613	3.837952	-0.906422
C	3.623159	6.133711	0.179220
H	5.590128	5.642175	0.921995
H	1.622007	6.298289	-0.603993
H	3.748953	7.204990	0.313664
C	4.976286	-2.375547	0.489767
C	4.128156	-3.059823	1.585926
C	3.234312	-2.769765	-2.181354
C	2.726229	-3.428812	1.157787
C	3.143436	-4.047514	-1.310280
C	2.305882	-3.843869	-0.066446
H	5.390461	-3.120961	-0.194136
H	4.045604	-2.379503	2.442724
H	4.022464	-2.900379	-2.939605
H	4.142513	-4.404706	-1.049234
H	5.839389	-1.899442	0.969933
H	4.654938	-3.950754	1.961817
H	2.298010	-2.655235	-2.740488
H	1.996788	-3.459564	1.963503
H	2.687118	-4.840697	-1.913638
H	1.263488	-4.134339	-0.159304
C	4.205197	-1.318350	-0.274665
H	4.381665	-0.301583	0.053547
C	3.470472	-1.486433	-1.415497
H	3.141975	-0.585565	-1.930892
C	-4.410726	1.819511	-0.928811
C	-5.346187	2.577020	-0.812143
C	-6.471896	3.496503	-0.662764
H	-6.447197	4.005941	0.308572
H	-6.460587	4.269143	-1.441600
H	-7.431719	2.970171	-0.735661
C	-3.270165	0.918681	-1.110703
C	-3.334533	-0.423252	-0.312276
C	-2.215637	-1.432505	-0.769514
C	-0.758647	-1.135881	-0.452764
C	0.004018	-1.777631	0.462338
C	-0.516940	-2.756276	1.489194
H	-0.183262	-3.787504	1.304548
H	-1.610337	-2.769877	1.550451
H	-2.340891	-1.543433	-1.853629
H	-3.185132	0.652481	-2.171959
H	-2.350955	1.442950	-0.839879
C	-4.684303	-1.074127	-0.670402
O	-4.872661	-1.699059	-1.692438
O	-5.643244	-0.821151	0.234950
C	-3.217110	-0.251275	1.204222
O	-2.858608	0.995318	1.571253
O	-3.379773	-1.154928	1.996204
C	-2.706503	1.196440	2.985745
C	-6.945618	-1.333962	-0.086444
H	-2.449604	2.249483	3.104455
H	-3.640180	0.965812	3.504794
H	-1.912053	0.556929	3.379318
H	-7.582711	-1.056834	0.753791
H	-7.312522	-0.886960	-1.014313
H	-6.911159	-2.420301	-0.201795
H	-2.485385	-2.398857	-0.336167
H	-0.154898	-2.491643	2.492426

3d

absolute energy -1729.554691 a.u.
enthalpy -1728.873833 a.u.
free energy -1728.991475 a.u.

Ni	-1.068732	1.772012	0.316883
C	-2.017263	0.230644	0.921678
C	-0.337556	-1.041706	-0.250755
H	-0.388312	-0.540703	-1.228435
H	-0.077002	-2.081888	-0.452353
C	-3.018401	0.426231	1.810597
H	-3.207577	1.413846	2.221883
H	-3.690296	-0.363129	2.142852
N	-1.671224	-1.002232	0.372371
C	-2.124023	-2.210596	1.061186
C	-3.528611	-2.667302	0.685852
C	-4.038100	-2.475459	-0.603536
C	-4.315123	-3.351514	1.621036
C	-5.301652	-2.955742	-0.950179
H	-3.435412	-1.935210	-1.328186
C	-5.578196	-3.837544	1.277699
H	-3.935597	-3.501100	2.630178
C	-6.076810	-3.640959	-0.011406
H	-5.683136	-2.794134	-1.955684
H	-6.174898	-4.362934	2.019392
H	-7.061821	-4.013545	-0.280674
C	-1.681633	4.730739	0.586958
C	-2.822705	4.372726	-0.395857
C	-0.397855	3.611113	-2.133994
C	-2.988284	2.878316	-0.559067
C	-1.395096	2.500005	-2.555763
C	-2.384918	2.086601	-1.487954
H	-1.453611	5.805862	0.514492
H	-3.756422	4.791861	-0.003149
H	-0.859953	4.595930	-2.241838
H	-1.928539	2.817615	-3.465065
H	-2.038497	4.571213	1.611849
H	-2.660601	4.854796	-1.363606
H	0.443757	3.599360	-2.836640
H	-3.707720	2.393373	0.095991
H	-0.826350	1.606188	-2.839149
H	-2.718838	1.052954	-1.544496
C	-0.407301	3.930127	0.421335
H	0.195368	3.860907	1.322958
C	0.142404	3.440258	-0.727244
H	1.124458	2.980108	-0.642837
C	0.710952	-0.370309	0.638078
C	0.423125	0.859534	1.110150
C	1.927562	-1.189914	1.038311
C	3.070726	-1.382571	-0.018158
C	4.441277	-1.654801	0.703373
C	4.820081	-0.705596	1.748379
C	5.165578	0.028915	2.644840
C	2.811590	-2.619482	-0.896920
O	1.900794	-3.409023	-0.771264
O	3.791181	-2.770433	-1.814669
C	3.197215	-0.141833	-0.910481
O	2.408271	-0.246254	-2.005901
O	3.894732	0.820257	-0.686560
C	2.487218	0.847955	-2.928800
C	3.656814	-3.907437	-2.682882
H	1.814503	0.589873	-3.747537
H	3.510711	0.966209	-3.295066
H	2.172743	1.778751	-2.450699
H	4.521870	-3.872323	-3.345687
H	2.728577	-3.840465	-3.256372
H	3.651685	-4.834796	-2.104183
C	1.232187	1.609563	2.143156
H	1.961866	0.978452	2.664137
H	1.804543	2.435380	1.697224
C	5.585129	0.941917	3.705290
H	4.937414	1.826376	3.743350
H	6.612156	1.292223	3.544213
H	5.548554	0.460916	4.690639
H	0.576970	2.046600	2.907476
H	-1.425237	-3.019250	0.815498
H	1.611003	-2.199737	1.327250
H	5.226054	-1.705731	-0.058659
H	2.400865	-0.736099	1.909355
H	4.375289	-2.658537	1.147176
H	-2.075307	-2.067584	2.152697

3ts(d-a)

absolute energy -1729.548071 a.u.
enthalpy -1728.869386 a.u.
free energy -1728.986601 a.u.
imaginary frequency -239.86 cm^{-1}

Ni	-1.251163	1.414555	0.397596
C	-2.011388	-0.212366	1.073028
C	-0.508182	-1.426603	-0.324564
H	-0.403793	-0.952631	-1.310662
H	-0.284945	-2.485331	-0.484312
C	-2.922470	-0.105545	2.071972
H	-2.904497	0.754807	2.734540
H	-3.722265	-0.822672	2.235925
N	-1.903325	-1.283648	0.166526
C	-2.609442	-2.521296	0.505548
C	-4.069294	-2.548215	0.075758
C	-4.453760	-2.080891	-1.187616
C	-5.046888	-3.101737	0.910016
C	-5.782508	-2.160811	-1.604321
H	-3.699170	-1.650211	-1.840213
C	-6.378832	-3.186032	0.496587
H	-4.763713	-3.466406	1.895515
C	-6.751410	-2.714256	-0.762624
H	-6.063189	-1.792401	-2.588077
H	-7.124544	-3.614619	1.161510
H	-7.787400	-2.774775	-1.085782
C	-1.535488	4.369153	0.645854
C	-2.753029	4.071775	-0.269310
C	-0.472953	3.054594	-2.064643
C	-3.056145	2.592778	-0.391691
C	-1.604045	2.065423	-2.459202
C	-2.580808	1.743306	-1.348717
H	-1.206603	5.408496	0.486069
H	-3.628920	4.580539	0.150602
H	-0.823991	4.085778	-2.164482
H	-2.134815	2.458535	-3.340321
H	-1.861078	4.317951	1.692323
H	-2.597622	4.511212	-1.258515
H	0.344367	2.944877	-2.787465
H	-3.801055	2.193252	0.292476
H	-1.149544	1.120724	-2.781944
H	-3.013429	0.746405	-1.382535
C	-0.369097	3.416727	0.485577
H	0.257235	3.315861	1.369656
C	0.078676	2.825830	-0.668445
H	1.000983	2.253104	-0.606541
C	0.423884	-0.827696	0.722093
C	-0.111533	0.224131	1.393595
C	1.679936	-1.580769	1.095920
C	3.042523	-1.165973	0.427214
C	4.080387	-2.282367	0.801837
C	5.435837	-2.100635	0.285217
C	6.565744	-1.984104	-0.129201
C	2.916287	-1.159729	-1.097098
O	2.132960	-1.858409	-1.708543
O	3.835007	-0.384768	-1.697173
C	3.517465	0.150322	1.051412
O	3.089821	1.249592	0.399591
O	4.161580	0.201179	2.077439
C	3.527115	2.496831	0.967649
C	3.858267	-0.452603	-3.131295
H	3.090006	3.272810	0.339252
H	4.618409	2.555964	0.953615
H	3.179405	2.592536	1.999343
H	4.651276	0.228180	-3.441763
H	2.896742	-0.139255	-3.546577
H	4.074110	-1.471939	-3.462076
C	0.378276	0.759369	2.717934
H	1.000053	0.039135	3.266390
H	0.971381	1.675150	2.603215
C	7.931378	-1.829391	-0.624172
H	8.631155	-1.620953	0.194455
H	8.003306	-1.000322	-1.339148
H	8.278268	-2.736715	-1.134174
H	-0.474026	1.007100	3.360948
H	-2.091963	-3.346272	0.001645
H	1.541326	-2.641352	0.855279
H	3.670869	-3.235663	0.444509
H	1.853871	-1.520919	2.177135
H	4.110166	-2.328422	1.896148
H	-2.546493	-2.719623	1.589272

4ts(a-b)

absolute energy -1417.466578 a.u.
enthalpy -1416.982183 a.u.
free energy -1417.082553 a.u.
imaginary frequency -216.49 cm^{-1}

Ni	0.107892	-0.009498	0.189874
C	1.629820	0.876798	-0.741646
C	2.227709	-0.036193	0.661887
H	2.114807	-1.090629	0.914623
H	2.503920	0.619563	1.489782
C	1.283734	2.024977	-1.352714
H	0.288583	2.444211	-1.269855
H	1.974302	2.507065	-2.044816
N	2.855589	0.246893	-0.615447
C	4.095451	1.023770	-0.668209
C	5.285845	0.224659	-0.183644
C	6.129469	0.730481	0.811265
C	5.571541	-1.032535	-0.735859
C	7.241904	0.003200	1.242982
H	5.916046	1.702637	1.250409
C	6.677537	-1.762872	-0.303585
H	4.915036	-1.435849	-1.502198
C	7.518251	-1.245678	0.686594
H	7.887353	0.411742	2.016161
H	6.886307	-2.736079	-0.740402
H	8.381169	-1.814740	1.022194
H	4.236253	1.321348	-1.714948
H	3.989444	1.955121	-0.084222
C	-1.174827	-1.311416	-0.676738
C	-0.039325	-1.487202	-1.173278
C	0.954577	-2.074996	-2.094224
H	1.831690	-2.450960	-1.556079
H	0.515006	-2.902106	-2.665747
H	1.313645	-1.318254	-2.800176
C	-2.615857	-1.584471	-0.484864
C	-3.428096	-0.395331	0.095455
C	-2.828450	0.069561	1.452493
C	-1.437972	0.556378	1.349754
C	-0.446474	1.271019	1.625604
C	0.291997	2.346637	2.319119
H	0.965481	1.933214	3.080668
H	0.904478	2.918696	1.613581
H	-0.395911	3.037869	2.822454
H	-3.459806	0.861680	1.870193
H	-2.873610	-0.781525	2.141870
H	-3.051504	-1.859866	-1.451944
H	-2.743748	-2.436205	0.193401
C	-4.880746	-0.845882	0.305728
O	-5.841165	-0.410023	-0.290156
O	-4.963788	-1.815553	1.241745
C	-3.480907	0.743763	-0.938882
O	-3.815257	1.915421	-0.367197
O	-3.274987	0.604039	-2.122476
C	-3.969404	3.017639	-1.275754
C	-6.288167	-2.318288	1.493027
H	-4.244108	3.871176	-0.655387
H	-3.032522	3.210571	-1.804831
H	-4.755146	2.800038	-2.003655
H	-6.167844	-3.085506	2.258136
H	-6.939693	-1.516131	1.848956
H	-6.713809	-2.744589	0.581097

4b

absolute energy -1417.476400 a.u.
enthalpy -1416.990790 a.u.
free energy -1417.092304 a.u.

Ni	0.241088	-0.069689	0.103843
C	1.516956	0.682379	-1.102557
C	2.116019	-0.157870	0.696960
H	2.244548	-1.225499	0.908838
H	2.366898	0.469180	1.559144
C	1.191327	1.521293	-2.099102
H	0.158967	1.658758	-2.401742
H	1.950528	2.078860	-2.648821
N	2.710118	0.282443	-0.553755
C	3.939181	1.062354	-0.621720
C	5.137428	0.298386	-0.095432
C	5.988893	0.867878	0.857364
C	5.424811	-0.989277	-0.570487
C	7.109535	0.174361	1.321935
H	5.773417	1.863716	1.238905
C	6.539572	-1.686186	-0.106581
H	4.760905	-1.441461	-1.302633
C	7.387658	-1.105215	0.841055
H	7.759992	0.632905	2.062362
H	6.749112	-2.683657	-0.484671
H	8.256631	-1.648603	1.202795
H	4.092280	1.323348	-1.676720
H	3.832710	2.015381	-0.072149
C	-1.192926	-1.342331	-0.758084
C	-0.068138	-1.597113	-1.232424
C	0.950620	-2.244818	-2.080054
H	1.840727	-2.513868	-1.501798
H	0.542068	-3.152595	-2.541054
H	1.268576	-1.559660	-2.872136
C	-2.644749	-1.539163	-0.564688
C	-3.382873	-0.362820	0.126884
C	-2.714214	-0.022718	1.487689
C	-1.328446	0.464432	1.345906
C	-0.346736	1.210589	1.552288
C	0.400428	2.325670	2.166933
H	1.155212	1.956310	2.870530
H	0.919639	2.914478	1.403214
H	-0.278943	2.987768	2.718469
H	-3.311618	0.740203	1.998990
H	-2.736159	-0.925689	2.107573
H	-3.104258	-1.704164	-1.545498
H	-2.812826	-2.439334	0.038587
C	-4.845436	-0.776203	0.343628
O	-5.791643	-0.333774	-0.269103
O	-4.950753	-1.730783	1.291893
C	-3.406518	0.855668	-0.814073
O	-3.766299	1.972437	-0.156879
O	-3.150599	0.816835	-1.995668
C	-3.876515	3.153678	-0.969411
C	-6.285077	-2.210767	1.539167
H	-4.182765	3.948063	-0.288426
H	-2.914097	3.389620	-1.430505
H	-4.625165	3.005024	-1.751545
H	-6.182216	-2.968098	2.316448
H	-6.927052	-1.393647	1.877651
H	-6.708851	-2.644128	0.629767

4ts(b-1c)

absolute energy -1417.480964 a.u.
enthalpy -1416.995794 a.u.
free energy -1417.094104 a.u.
imaginary frequency -124.27 cm^{-1}

Ni	-0.120312	1.227111	0.180976
C	1.179456	-0.098395	-0.304538
C	1.905420	-0.602122	1.949695
N	2.150707	0.001589	0.739413
C	3.355542	0.802824	0.531243
H	3.081486	1.722608	-0.002285
C	4.472833	0.101590	-0.232836
C	4.557841	-1.293237	-0.305699
C	5.460008	0.871785	-0.862059
C	5.611997	-1.904333	-0.989117
H	3.795384	-1.899876	0.173873
C	6.515640	0.263366	-1.541320
H	5.401061	1.958107	-0.820841
C	6.594598	-1.129808	-1.607339
H	5.662972	-2.989043	-1.037720
H	7.271835	0.876412	-2.025041
H	7.413260	-1.606421	-2.139910
C	-0.012234	-0.745407	2.273066
C	-0.775402	-0.106486	1.407197
C	-0.300753	-1.618036	3.448506
C	-2.952742	-0.079119	-0.010247
C	-2.975178	1.380178	-0.569478
C	-1.707258	2.122307	-0.392562
C	-0.891741	3.053677	-0.178817
H	-3.760346	1.934748	-0.035545
H	-3.257890	1.355040	-1.625119
H	-1.366043	-1.873719	3.499986
H	-0.034447	-1.126710	4.394292
C	-2.281752	-1.097203	-0.946601
O	-2.100328	-2.253556	-0.633684
O	-1.948510	-0.590661	-2.149760
C	-4.431021	-0.498316	0.111242
O	-4.965738	-0.740323	-1.105302
O	-5.058840	-0.561154	1.143064
C	-6.353331	-1.120317	-1.106804
C	-1.362836	-1.528904	-3.067979
H	-6.609570	-1.284054	-2.153669
H	-6.968124	-0.324366	-0.678461
H	-6.497147	-2.034846	-0.526155
H	-1.170376	-0.962651	-3.979546
H	-2.054390	-2.352842	-3.262105
H	-0.432299	-1.931765	-2.660564
C	-2.294617	-0.175725	1.398813
H	-2.634728	-1.111165	1.854300
H	-2.717796	0.636954	2.003945
C	-0.428475	4.451425	-0.031489
H	0.281042	4.714855	-0.824786
H	0.086261	4.596372	0.924969
H	-1.266152	5.159032	-0.078698
H	0.272606	-2.551605	3.396399
H	0.813242	-1.113095	-0.453414
H	1.580782	0.321863	-1.236442
C	2.781223	-1.042852	2.859295
H	3.851726	-1.081542	2.669312
H	2.441924	-1.384380	3.830114
H	3.713548	1.106046	1.522297

5b

absolute energy -923.722462 a.u.
enthalpy -923.334840 a.u.
free energy -923.405557 a.u.

Ni	1.680470	-0.566227	0.016049
C	-0.138796	-1.089521	0.363815
C	-1.079043	-0.926553	1.489051
H	-0.870686	-0.259153	2.323860
H	-1.730862	-1.767900	1.735835
C	0.495158	-2.109711	-0.377029
H	0.843026	-3.009314	0.131189
H	0.294397	-2.225940	-1.442849
N	-1.301202	-0.263180	0.182861
C	-2.378209	-0.803473	-0.651446
C	-3.720240	-0.171052	-0.339680
C	-4.882145	-0.950806	-0.307034
C	-3.829393	1.207630	-0.109930
C	-6.128707	-0.369885	-0.061839

H	-4.811064	-2.023526	-0.475067
C	-5.071754	1.789828	0.140759
H	-2.928410	1.813777	-0.116825
C	-6.227171	1.003741	0.162772
H	-7.019827	-0.992212	-0.039942
H	-5.139401	2.860169	0.319624
H	-7.194961	1.458547	0.357739
C	3.109100	0.977901	-1.983720
C	2.835089	2.051161	-0.892732
C	4.587942	0.079584	0.687594
C	1.897171	1.575209	0.203259
C	3.665839	0.596013	1.825384
C	2.266670	0.973020	1.383102
H	3.994419	1.273602	-2.568651
H	2.392913	2.927457	-1.381177
H	5.044111	0.922440	0.160783
H	4.155275	1.442772	2.332539
H	2.271191	0.975227	-2.691311
H	3.778285	2.395749	-0.458657
H	5.417944	-0.474440	1.142162
H	0.854724	1.874987	0.108995
H	3.570330	-0.190024	2.585023
H	1.502549	0.883767	2.154101
C	3.264923	-0.436304	-1.461942
H	2.964131	-1.220852	-2.153886
C	3.874177	-0.825721	-0.298582
H	3.976737	-1.896481	-0.127801
H	-2.104461	-0.596523	-1.695972
H	-2.448793	-1.901874	-0.559931

5ts(b-c)

absolute energy -923.680088 a.u.
enthalpy -923.294727 a.u.
free energy -923.366821 a.u.
imaginary frequency -215.64 cm^{-1}

Ni	1.440509	-0.140817	0.106912
C	-0.116858	-1.183523	-0.503294
C	-0.634451	-0.140050	0.623442
H	-0.460005	0.938367	0.710033
H	-0.988540	-0.605618	1.546460
C	0.126344	-2.506098	-0.699060
H	1.061649	-2.971616	-0.408583
H	-0.580052	-3.126044	-1.248265
N	-1.332866	-0.505406	-0.614602
C	-2.577330	-1.267889	-0.527287
C	-3.766885	-0.388567	-0.200598
C	-4.737015	-0.819738	0.711507
C	-3.933395	0.857162	-0.822180
C	-5.855508	-0.031656	0.992931
H	-4.616297	-1.780986	1.206551
C	-5.045819	1.649145	-0.537903
H	-3.177513	1.201995	-1.521902
C	-6.012683	1.206468	0.368973
H	-6.598496	-0.383015	1.704377
H	-5.159499	2.613994	-1.025860
H	-6.879434	1.824152	0.589283
C	3.986093	-0.813145	1.338257
C	4.374007	-0.749778	-0.166870
C	3.421046	2.138341	0.285220
C	3.174869	-0.647360	-1.092048
C	2.999422	1.931928	-1.198322
C	2.599309	0.514661	-1.555775
H	4.875544	-0.594945	1.950681
H	4.936599	-1.658623	-0.411812
H	4.477404	1.884990	0.412358
H	3.814005	2.282328	-1.852076
H	3.700566	-1.843170	1.585007
H	5.062745	0.081930	-0.342154
H	3.340074	3.206860	0.517939
H	2.841384	-1.575114	-1.552006
H	2.143217	2.582529	-1.415626
H	1.888480	0.425894	-2.375981
C	2.834134	0.087857	1.737924
H	2.250698	-0.256608	2.591883
C	2.577833	1.354532	1.273260
H	1.785653	1.912465	1.771447
H	-2.720729	-1.749871	-1.503950
H	-2.480300	-2.082905	0.211809

5c

absolute energy -923.720180 a.u.
enthalpy -923.332391 a.u.
free energy -923.402336 a.u.

Ni	-1.328502	-0.218435	-0.138365
C	0.419511	-0.146009	0.599676
C	-0.026797	-1.095164	-1.268943
H	-0.050687	-0.746535	-2.310411
H	-0.167643	-2.187271	-1.212837
C	0.872312	0.163300	1.831568
H	0.200934	0.515645	2.609219
H	1.928570	0.110547	2.093537
N	1.116110	-0.615551	-0.500768
C	2.361004	-1.361470	-0.409922
H	2.457653	-1.918479	-1.352671
H	2.309223	-2.110234	0.401661
C	3.599973	-0.500399	-0.214156
C	4.690628	-0.991161	0.514062
C	3.697165	0.770110	-0.794950
C	5.857775	-0.237047	0.651553
H	4.623637	-1.972183	0.980614
C	4.860161	1.528237	-0.655973
H	2.844229	1.160188	-1.342775
C	5.946619	1.026775	0.065395
H	6.693620	-0.634056	1.222406
H	4.917879	2.514791	-1.109615
H	6.851707	1.618726	0.175059
C	-3.953561	-1.492579	0.356056
C	-4.008836	-0.370135	1.423154
C	-3.809697	1.359101	-1.110899
C	-2.682558	0.342281	1.607021
C	-2.983132	2.232616	-0.132345
C	-2.263417	1.469162	0.959455
H	-4.977200	-1.808645	0.101048
H	-4.299861	-0.821206	2.378839
H	-4.789218	1.129823	-0.682607
H	-3.635171	3.001482	0.310493
H	-3.469377	-2.372517	0.796436
H	-4.795204	0.348844	1.178458
H	-4.007598	1.949630	-2.012945
H	-2.054987	-0.022787	2.417100
H	-2.223198	2.779120	-0.703400
H	-1.349863	1.934322	1.320863
C	-3.189747	-1.137816	-0.901500
H	-2.754560	-1.986591	-1.425302
C	-3.103510	0.078669	-1.517256
H	-2.570952	0.111599	-2.465547

5ts(c-2d)

absolute energy -1729.514887 a.u.
enthalpy -1728.836573 a.u.
free energy -1728.952548 a.u.
imaginary frequency -76.70 cm^{-1}

Ni	0.043016	1.510354	0.158825
C	1.482872	0.340929	-0.434170
C	2.213335	-0.235874	1.837399
N	2.496449	0.272243	0.597086
C	3.866090	0.635574	0.250050
H	3.848357	1.557686	-0.348296
C	4.645782	-0.417918	-0.528667
C	4.517000	-1.784303	-0.242667
C	5.529367	-0.024034	-1.540939
C	5.261197	-2.729183	-0.950451

H	3.834411	-2.101320	0.540136
C	6.278234	-0.967546	-2.247478
H	5.631507	1.032817	-1.781144
C	6.145813	-2.325326	-1.953773
H	5.152377	-3.785155	-0.715419
H	6.957469	-0.641787	-3.031300
H	6.724016	-3.063197	-2.503749
C	0.928237	4.094741	1.353983
C	-0.587556	4.322173	1.578567
C	-0.500105	4.239410	-1.510001
C	-1.425772	3.103926	1.255798
C	-1.859355	3.550205	-1.254727
C	-1.968783	2.795526	0.050440
H	1.448100	5.065710	1.370023
H	-0.739523	4.587812	2.630988
H	-0.454371	5.196711	-0.983341
H	-2.666673	4.296772	-1.320218
H	1.328722	3.525362	2.200791
H	-0.932630	5.182004	0.997582
H	-0.430383	4.480161	-2.577344
H	-1.679224	2.460267	2.095274
H	-2.053682	2.830175	-2.058211
H	-2.658438	1.958898	0.005788
C	1.296383	3.340403	0.094249
H	2.248084	2.822975	0.158259
C	0.685987	3.379108	-1.126564
H	1.172925	2.851759	-1.944077
C	0.300348	-0.506023	2.101974
C	-0.545732	0.003298	1.204483
C	0.104958	-1.375755	3.305056
C	-2.281785	-1.533273	0.064786
C	-2.188738	-0.939138	-1.374906
C	-3.308675	-0.055818	-1.710687
C	-4.261077	0.637742	-1.990392
H	-2.151605	-1.761214	-2.096422
H	-1.238004	-0.399921	-1.454234
H	-0.940492	-1.666644	3.438362
H	0.428279	-0.855233	4.216412
C	-1.316524	-2.710533	0.270764
O	-1.378765	-3.452494	1.227815
O	-0.391814	-2.825061	-0.700452
C	-3.699428	-2.097887	0.275662
O	-3.943224	-3.097866	-0.599416
O	-4.505401	-1.705537	1.086674
C	-5.244223	-3.698088	-0.502433
C	0.574592	-3.873702	-0.508113
H	-5.261456	-4.483560	-1.258627
H	-6.022036	-2.955764	-0.700774
H	-5.396668	-4.119379	0.494558
H	1.242738	-3.813837	-1.367253
H	0.076984	-4.845937	-0.467446
H	1.126364	-3.710982	0.420660
C	-1.994567	-0.477647	1.178596
H	-2.276318	-0.947065	2.125483
H	-2.709042	0.336040	1.030747
C	-5.418289	1.465335	-2.326612
H	-5.144087	2.523319	-2.421000
H	-6.192743	1.391756	-1.553463
H	-5.867971	1.154166	-3.277539
H	0.698722	-2.293670	3.231626
H	1.115708	-0.644753	-0.726800
H	1.925941	0.823678	-1.312745
C	3.057620	-0.627690	2.807862
H	4.135509	-0.673064	2.672861
H	2.681043	-0.916287	3.780676
H	4.388897	0.880965	1.182972

5ts(c-3d)

absolute energy -1729.525565 a.u.
enthalpy -1728.847701 a.u.
free energy -1728.967197 a.u.

imaginary frequency -111.55 cm^{-1}

Ni	1.107593	1.870864	-0.296252
C	2.267801	0.439227	-0.817121
C	0.794227	-1.022829	0.381588
H	0.781835	-0.450634	1.309359
H	0.555302	-2.071058	0.557788
C	3.348757	0.739568	-1.572102
H	3.470707	1.733634	-1.992473
H	4.143535	0.026534	-1.789934
N	1.992123	-0.857473	-0.367335
C	2.417988	-1.984023	-1.199835
C	3.750188	-2.610493	-0.804949
C	4.289679	-2.458049	0.476274
C	4.439116	-3.403434	-1.733063
C	5.486894	-3.087091	0.825109
H	3.768772	-1.829637	1.192589
C	5.633237	-4.036434	-1.387350
H	4.036378	-3.523409	-2.737252
C	6.162061	-3.880806	-0.103633
H	5.894172	-2.953711	1.824482
H	6.154267	-4.645527	-2.121876
H	7.094678	-4.368935	0.167178
C	0.944459	2.565894	2.604054
C	-0.026451	3.642851	2.055094
C	2.581817	4.573172	0.707857
C	-0.335491	3.475837	0.580625
C	1.591724	4.872873	-0.443070
C	0.352465	4.004168	-0.471937
H	1.301613	2.873167	3.599304
H	-0.963965	3.569480	2.617289
H	2.236238	5.031828	1.637891
H	1.297002	5.933642	-0.410472
H	0.379708	1.639113	2.759857
H	0.366104	4.644646	2.249182
H	3.538676	5.052869	0.470907
H	-1.267033	2.964686	0.351454
H	2.112083	4.738469	-1.399419
H	-0.103495	3.914805	-1.454652
C	2.121669	2.247204	1.707290
H	2.518996	1.239478	1.808628
C	2.812360	3.090132	0.892236
H	3.655345	2.662236	0.355368
C	-0.627533	-0.254272	-0.709481
C	-0.275072	0.915925	-1.233191
C	-1.826486	-1.133074	-0.915093
C	-2.900398	-1.018528	0.214777
C	-3.587888	0.378365	0.212855
C	-4.404641	0.621378	-0.976815
C	-5.084947	0.808428	-1.959823
C	-3.961795	-2.111363	0.011352
O	-4.003777	-2.897564	-0.905947
O	-4.879010	-2.071083	1.004542
C	-2.241478	-1.216130	1.584909
O	-1.896727	-2.508349	1.774276
O	-2.030061	-0.343082	2.398999
C	-1.281972	-2.811495	3.037703
C	-5.938785	-3.035197	0.902325
H	-1.135157	-3.891792	3.038317
H	-1.933610	-2.508763	3.861228
H	-0.322926	-2.295087	3.129935
H	-6.574658	-2.864734	1.771618
H	-5.534722	-4.051044	0.912779
H	-6.502238	-2.885144	-0.022313
C	-1.029260	1.604306	-2.352991
H	-1.758611	0.938330	-2.831233
H	-1.591773	2.481446	-2.004853
C	-5.907507	1.036588	-3.145800
H	-6.023396	0.115127	-3.729334
H	-5.459709	1.791089	-3.804184
H	-6.911497	1.386117	-2.875004
H	-0.338718	1.954356	-3.130354

H	1.640347	-2.758084	-1.156331
H	-1.531719	-2.184872	-0.982542
H	-2.791955	1.126341	0.294164
H	-2.341707	-0.892841	-1.853614
H	-4.199898	0.471358	1.115738
H	2.471740	-1.650920	-2.244544

a1-H

absolute energy -1132.403249 a.u.
enthalpy -1131.992691 a.u.
free energy -1132.076113 a.u.

Ni	1.704575	-0.037168	-0.223005
C	-3.972897	1.962479	-0.060822
C	-4.162165	1.093808	-1.332807
C	-3.302992	-0.144392	2.221875
C	-3.570470	-0.297960	-1.231329
C	-4.250122	-0.829473	1.200713
C	-3.581551	-1.125387	-0.131263
H	-4.776773	1.765018	0.654695
H	-3.675185	1.596434	-2.177083
H	-3.900341	0.321076	3.022390
H	-5.143695	-0.217749	1.043696
H	-4.076019	3.017249	-0.342300
H	-5.232939	1.043582	-1.588228
H	-2.696039	-0.916304	2.709912
H	-3.257031	-0.733598	-2.178568
H	-4.606440	-1.770313	1.636872
H	-3.244527	-2.150052	-0.277918
C	-2.623077	1.758448	0.605056
H	-1.864047	2.507034	0.384693
C	-2.347793	0.863180	1.612294
H	-1.406021	0.984677	2.144855
C	2.704682	0.158664	-0.489999
C	1.376315	0.714514	0.092361
C	0.178795	-0.013514	-0.405774
C	-0.315104	-0.932367	-1.152140
C	-0.140242	-2.028164	-2.142826
H	-0.533830	-1.730927	-3.123582
H	0.915615	-2.298205	-2.264947
H	-0.689559	-2.928737	-1.841977
H	1.419514	0.667010	1.187133
H	1.307501	1.775955	-0.169763
C	3.922698	0.972779	-0.061014
O	4.929388	0.524927	0.442082
O	3.748492	2.282263	-0.344025
C	2.932201	-1.308195	-0.142726
O	2.803074	-1.528345	1.178112
O	3.191612	-2.173213	-0.951071
C	3.043599	-2.878663	1.602917
C	4.856327	3.135340	-0.010068
H	2.898177	-2.875554	2.683489
H	2.339849	-3.562654	1.121151
H	4.064518	-3.178588	1.352747
H	4.550417	4.139527	-0.304785
H	5.062357	3.094080	1.062738
H	5.752897	2.829485	-0.555663
H	2.649961	0.210620	-1.582902

a2-H

absolute energy -1262.713049 a.u.
enthalpy -1262.297325 a.u.
free energy -1262.392176 a.u.

Ni	-0.732379	-1.627175	-0.877635
C	3.141645	0.424122	-0.524371
C	1.589967	0.433324	-0.480673
C	1.035158	-0.921881	-0.717275
C	1.109626	-2.166478	-0.911247
C	1.757302	-3.484201	-1.103798
H	1.602829	-3.850980	-2.125043
H	2.835839	-3.403042	-0.921851
H	1.343950	-4.234309	-0.420467
H	1.254536	0.808167	0.492703
H	1.219657	1.135416	-1.233216
C	3.764204	1.807048	-0.342079
O	4.752969	2.041114	0.316439
O	3.097910	2.740530	-1.051992
C	3.734443	-0.543681	0.495847
O	3.323931	-0.244791	1.741414
O	4.458940	-1.475452	0.223391
C	3.840820	-1.089940	2.781887
C	3.646168	4.069136	-0.988868
H	3.411861	-0.708032	3.708458
H	3.538735	-2.127407	2.616043
H	4.931898	-1.032644	2.809444
H	2.992266	4.683453	-1.608102
H	3.653778	4.430416	0.042626
H	4.667826	4.079078	-1.377324
H	3.458619	0.058812	-1.507911
C	-2.509789	-1.923254	-0.119827
C	-2.932267	-2.772501	1.006706
H	-2.212712	-3.261445	1.659602
H	-3.893858	-3.283053	0.913448
C	-2.631205	-1.735357	-1.493660
H	-2.943649	-0.773597	-1.897848
H	-2.708394	-2.591945	-2.161142
N	-2.947231	-1.291453	1.072665
C	-4.251964	-0.619141	1.052468
H	-4.671955	-0.710405	2.063527
H	-4.949584	-1.120002	0.359126
C	-4.126638	0.844354	0.676509
C	-5.019956	1.424936	-0.230953
C	-3.135677	1.649120	1.256749
C	-4.933859	2.782350	-0.550371
H	-5.789840	0.810052	-0.692227
C	-3.044043	3.003135	0.934884
H	-2.432997	1.200873	1.953138
C	-3.944423	3.575378	0.031641
H	-5.636005	3.216212	-1.257654
H	-2.269852	3.614539	1.391719
H	-3.872798	4.630899	-0.217376

a6

absolute energy -1471.396808 a.u.
enthalpy -1470.958227 a.u.
free energy -1471.066518 a.u.

C	-4.230457	-0.177486	-0.086369
C	-2.760980	-0.646868	0.082117
C	-1.847675	0.058258	-0.852599
C	-1.590044	0.909799	-1.756133
C	-1.904289	1.982951	-2.730028
H	-1.832902	1.606233	-3.757025
H	-2.920825	2.361248	-2.568242
H	-1.200995	2.818036	-2.641209
H	-2.440684	-0.475676	1.115794
H	-2.715977	-1.726953	-0.085751
C	-5.211188	-0.929010	0.812106
O	-6.110963	-0.417552	1.440533
O	-4.976650	-2.257315	0.784725
C	-4.385064	1.324020	0.135722
O	-3.911005	1.688717	1.340653
O	-4.854686	2.095368	-0.671736
C	-4.043599	3.083354	1.659503
C	-5.885703	-3.058667	1.560223
H	-3.621393	3.196062	2.658255
H	-3.495249	3.694449	0.937714
H	-5.096905	3.374679	1.650953
H	-5.552129	-4.088024	1.427578
H	-5.844527	-2.771533	2.613980
H	-6.909041	-2.934160	1.196806
H	-4.538226	-0.364374	-1.121494
Ni	-0.001183	-0.017715	-1.271857
C	4.226431	0.182445	-0.088213

C	2.753042	0.640027	0.078467	H	3.656331	-3.164105	2.697581
C	1.843925	-0.084412	-0.845488	H	3.529260	-3.683618	0.983377
C	1.590248	-0.952126	-1.734645	H	5.130230	-3.341338	1.687661
C	1.909072	-2.042317	-2.687945	H	5.514944	4.122852	1.376159
H	1.827407	-1.688259	-3.722175	H	5.821248	2.823789	2.578124
H	2.930190	-2.407436	-2.524755	H	6.881657	2.978304	1.156969
H	1.214465	-2.882056	-2.576895	H	4.529893	0.360000	-1.126256
H	2.436888	0.477779	1.114885				
H	2.697603	1.717615	-0.101659				
C	5.202178	0.953712	0.798878				
O	6.108579	0.458206	1.430547				
O	4.954591	2.279293	0.757098				
C	4.395748	-1.314823	0.151135				
O	3.928314	-1.669736	1.361585				
O	4.870320	-2.091243	-0.648536				
C	4.074402	-3.059301	1.696232				
C	5.857930	3.098214	1.520811				