Supporting Information

DFT insights into the Ni-Catalyzed Regioselective Hydrocarboxylation of Unsaturated Alkenes with CO_2

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1. The formation of carbonic acid.

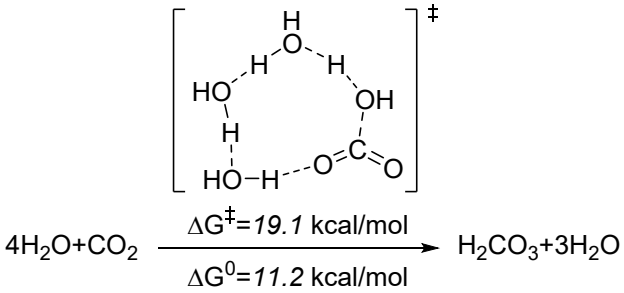

Figure S1. The energy changes for formation of carbonic acid (in kcal/mol).

2. Relative energies for (L)Ni(0)X (X, Y=H_2O/styrene/CO_2/DMA).

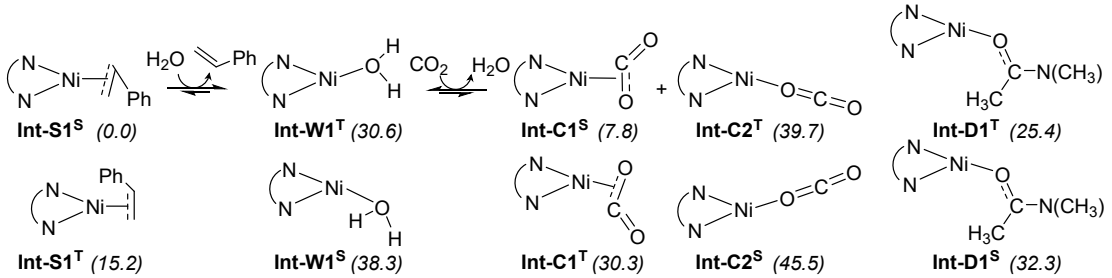

Figure S2. The relative Gibbs free energies of **(L)NiX (X, Y= H_2O/styrene/CO_2/DMA)** in kcal/mol (in parenthesis and italic).

3. Relative energies for (L)Ni(0)XY (X, Y=H_2O/styrene/CO_2/DMA/H_2CO_3).

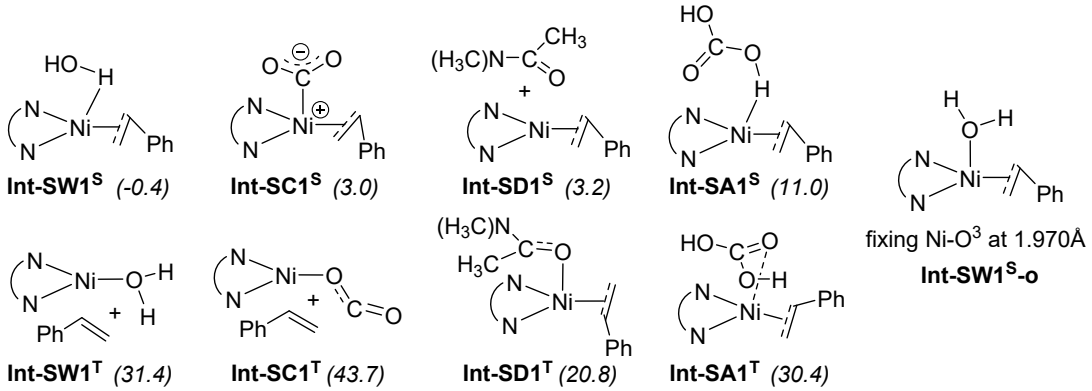

Figure S3. The relative Gibbs free energies of **(L)Ni(0)XY (X, Y=H_2O/styrene/CO_2/DMA/H_2CO_3)** in kcal/mol (in parenthesis and italic). Note that the possibility for an O-coordination of water molecule in **Int-SW1^S** were also examine, but the assumed structure does not correspond to a local minimum. Partial optimization by fixing the Ni-O distance at 1.970 Å results in a species with much higher energy than **Int-SW1^S** (electronic energy gap: 12.6 kcal/mol).

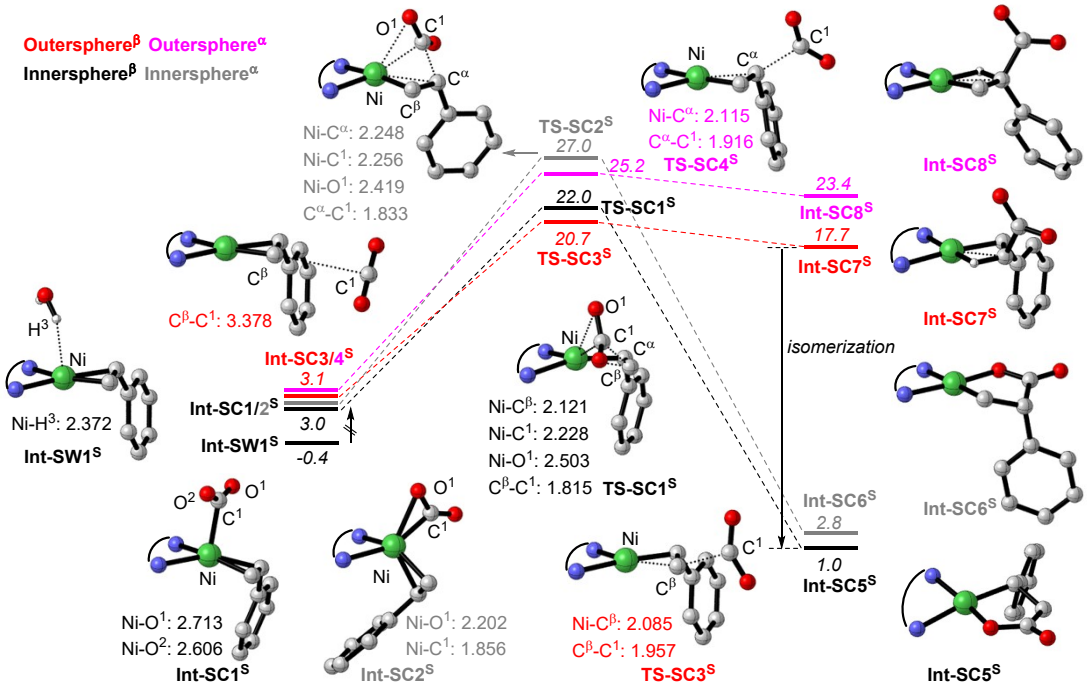

Figure S4. Gibbs free energy profiles for the singlet state carboxylation process in carboxylation/H-transfer pathway (in kcal/mol). The bond distances in the optimized geometries of the transition states (All H atoms were omitted for clarity reasons) are given in Å.

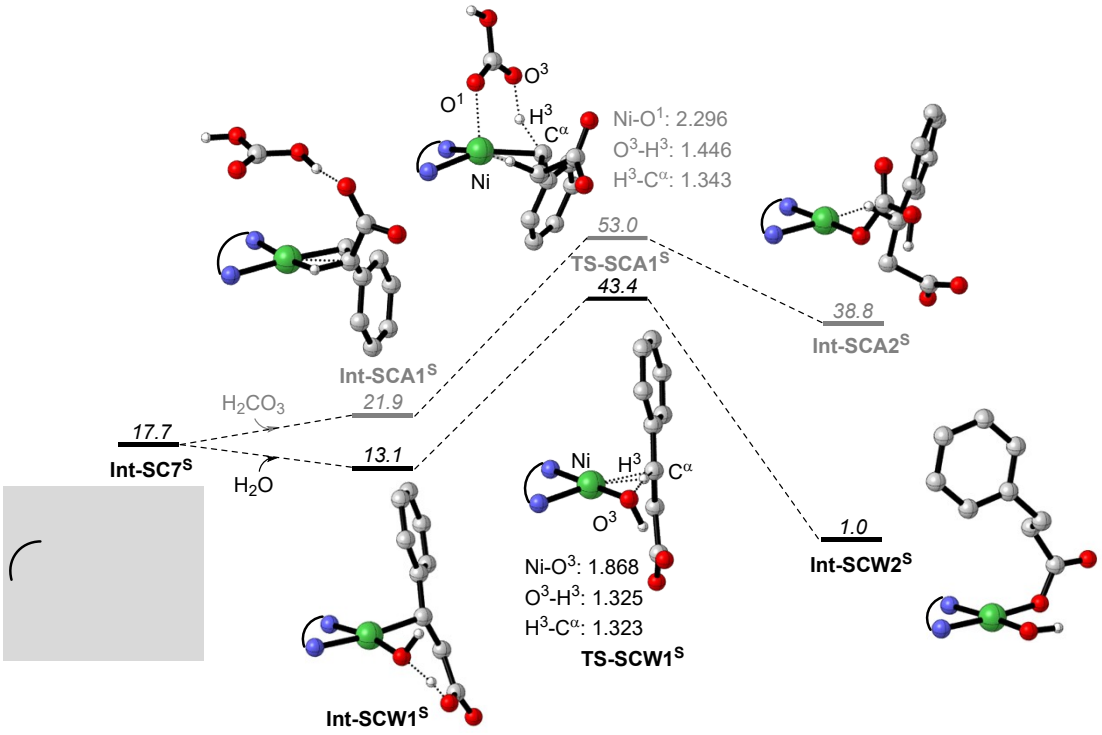

Figure S5. Gibbs energy profiles for the direct H-transfer on **Int-SC7^S** (in kcal/mol). The bond distances in the optimized geometries of the transition states are given in Å. Only selected H atoms are shown.

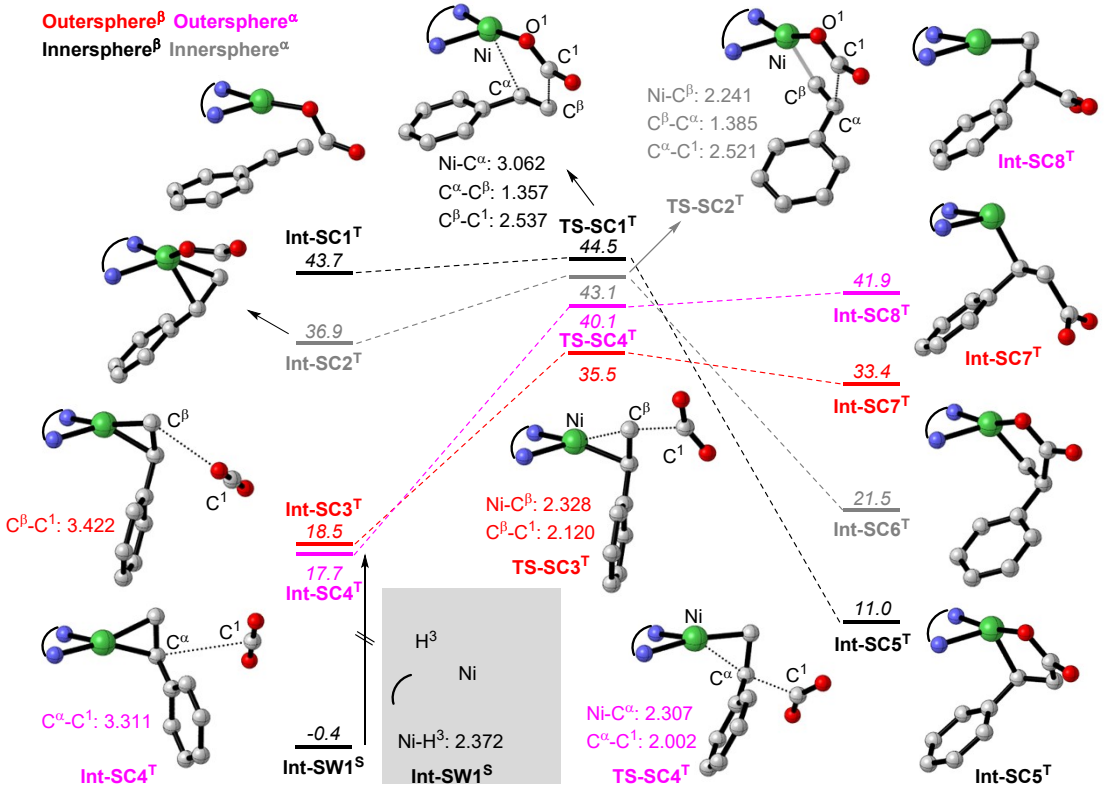

Figure S6. Gibbs free energy profiles for the triplet state carboxylation process in carboxylation/H-transfer pathway (in kcal/mol). The bond distances in the optimized

geometries of the transition states are given in Å. All H atoms were omitted for clarity reasons.

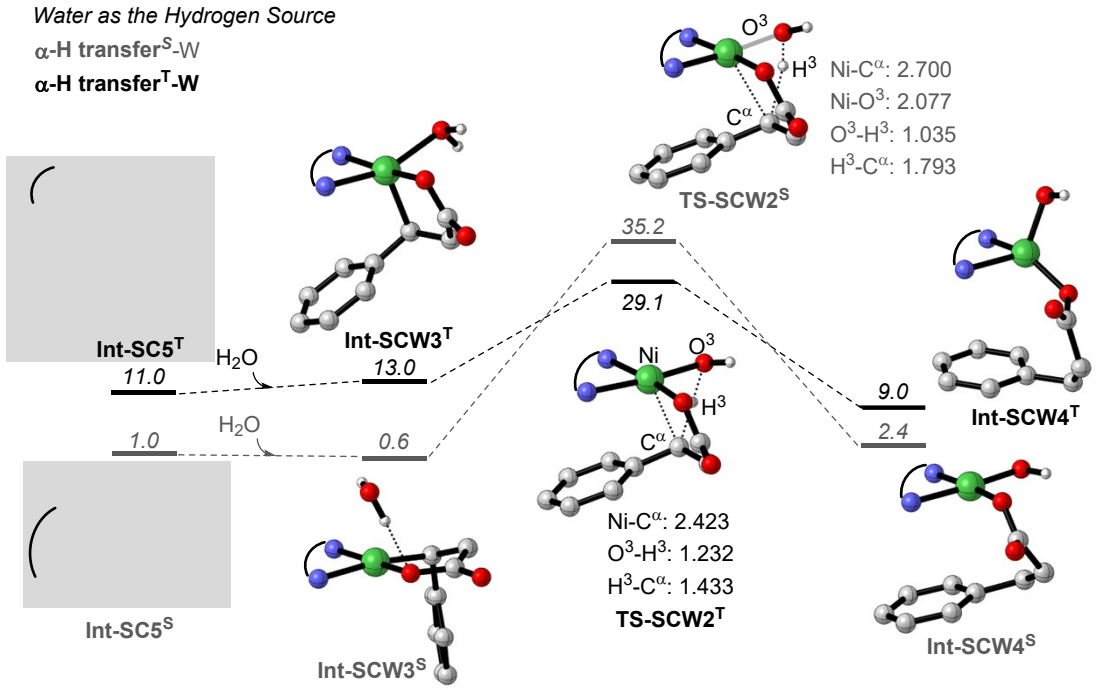

Figure S7. Gibbs free energy profiles (in kcal/mol) for the water mediated H-transfer step in carboxylation/H-transfer pathway along the singlet and triplet potential energy surface. The bond distances in selected structures are given in Å. Only selected H atoms were shown for clarity reasons.

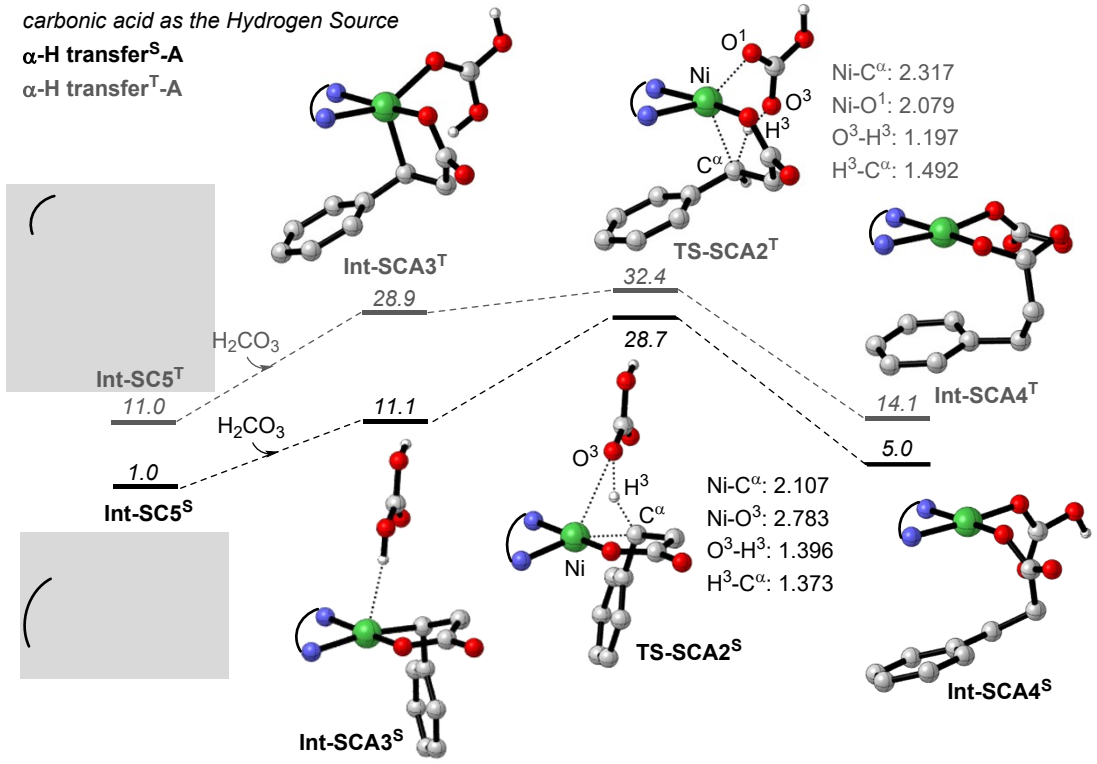

Figure S8. Gibbs free energy profiles (in kcal/mol) for the H_2CO_3 mediated H-transfer step in carboxylation/H-transfer pathway along the singlet and triplet potential energy surface. The bond distances in selected structures are given in Å. Only selected H atoms were shown for clarity reasons.

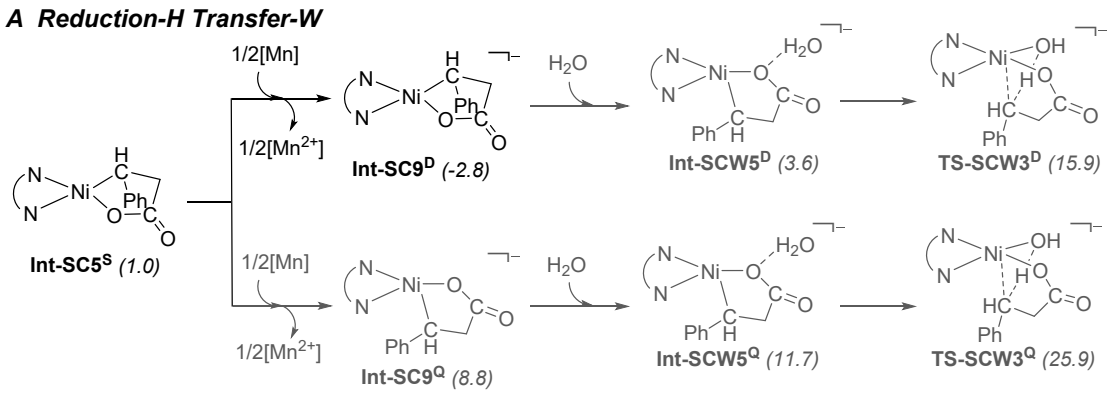

Figure S9. Gibbs free energies (in kcal/mol) for the reduction-H-transfer processes from the intermediate **Int-SC5^S** involving quartet Ni(I) intermediates (A), or Ni(0) intermediates (B).

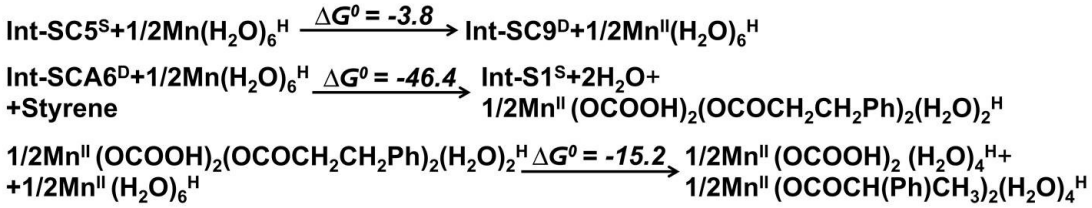

Figure S10. The reduction involved in the carboxylation/H-transfer pathway, and the reaction Gibbs free energy (in kcal/mol).

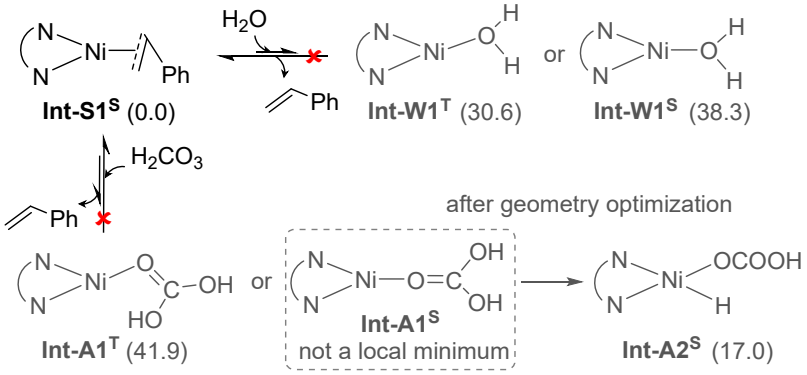

Figure S11. The relative Gibbs free energy of possible precursors in the hydrometallation/carboxylation mechanism (kcal/mol).

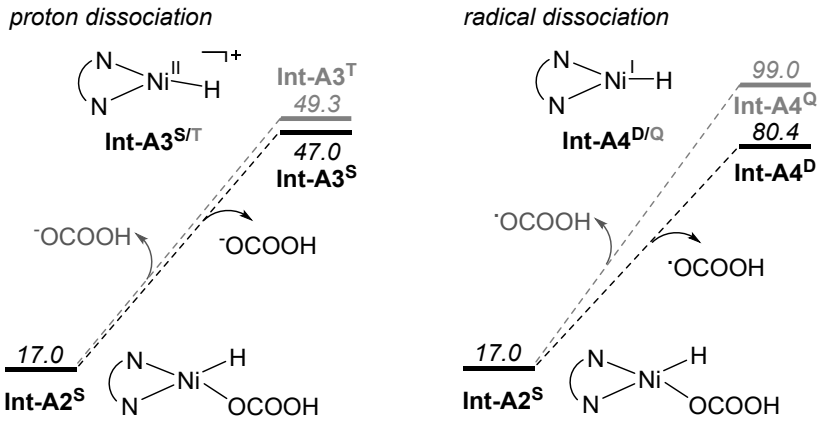

Figure S12. Gibbs free energy profiles for Ni-H intermediate formed from **Int-A2^S** by proton or radical dissociation.

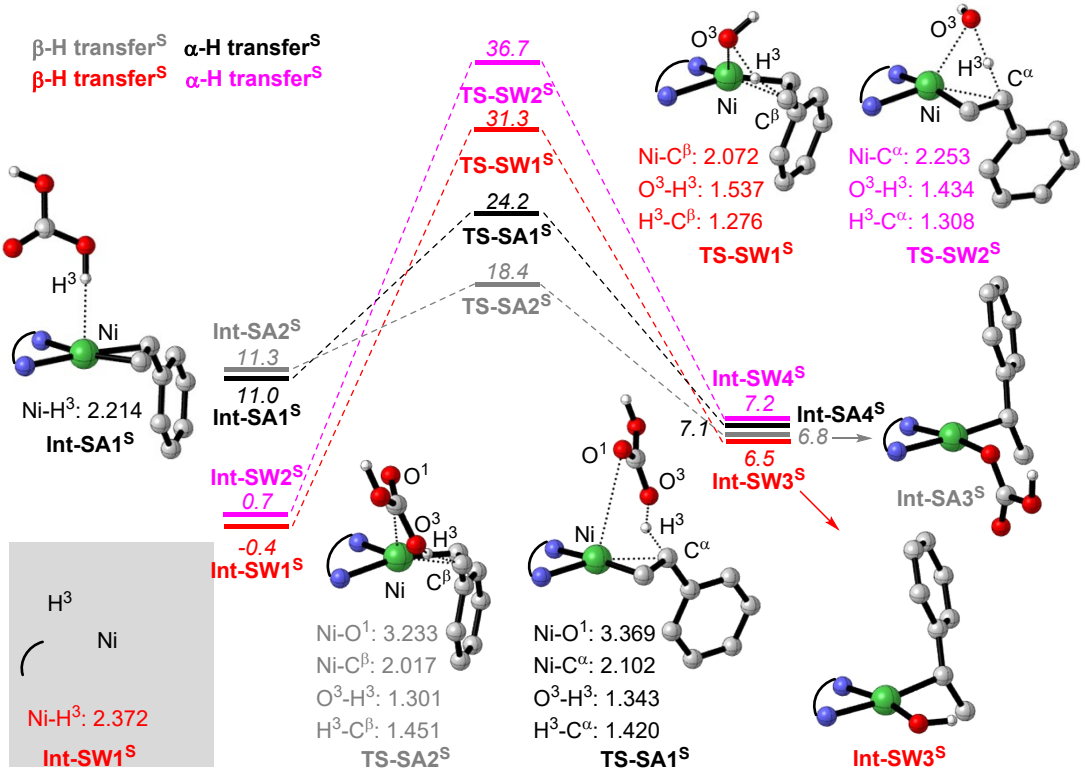

Figure S13. Gibbs free energy profiles for singlet H-transfer process in the H_2O/H_2CO_3 mediated H-transfer-carboxylation pathway. The relative free energies are given in kcal/mol. The bond distances in transition states are given in Å. Only selected H atoms were shown for clarity reasons.

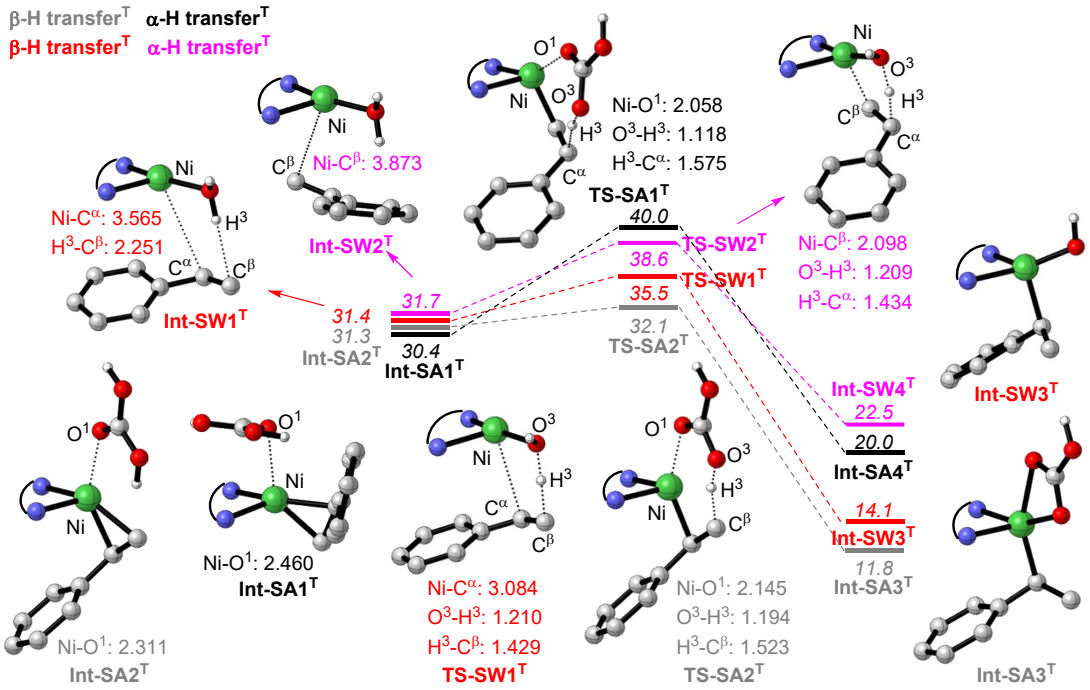

Figure S14. Gibbs free energy profiles for triplet H-transfer process in the H_2O/H_2CO_3 mediated H-transfer-carboxylation pathway. The relative free energies are given in kcal/mol. The bond distances in transition states are given in Å. Only selected H atoms were shown for clarity reasons.

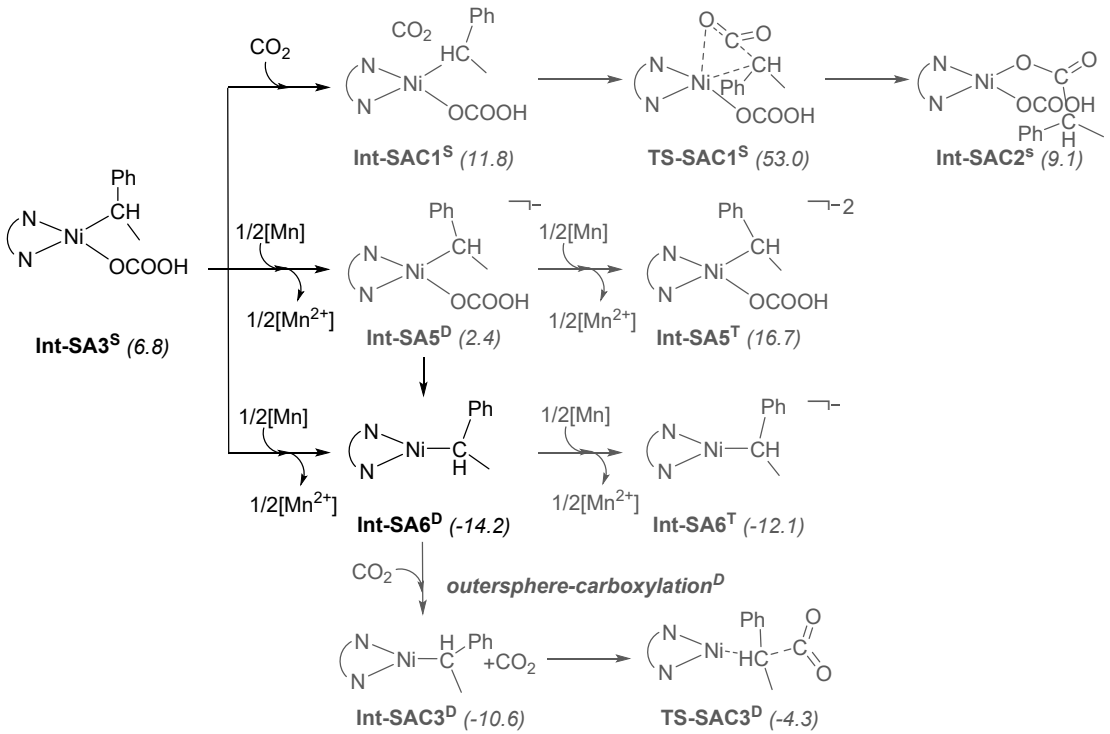

Figure S15. Gibbs free energies (in kcal/mol) for the related reactions of intermediate **Int-SA3^S**.

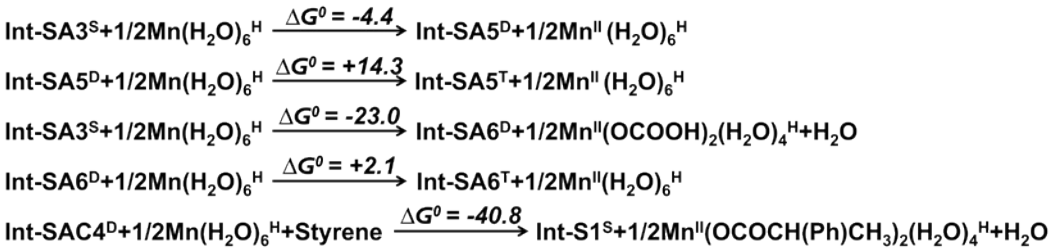

Figure S16. The reduction of the selected species, and the reaction Gibbs free energy (in kcal/mol).

Each transition state structure was separated into two fragments, namely Ni-Sty and H_2CO_3. For each segment, the energy difference between the warped structure of the transition state and the unrestricted optimized structural element is the strain energy(Ni-Sty: ΔE_{dist}(Ni-Sty), H_2CO_3: $\Delta E_{dist}(H_2CO_3)$). The interaction energy (ΔE_{int}) is the difference between the activation energy ($\Delta E^{‡}$) and the total distortion energy (ΔE_{dist}(Ni-Sty)+$\Delta E_{dist}(H_2CO_3)$).

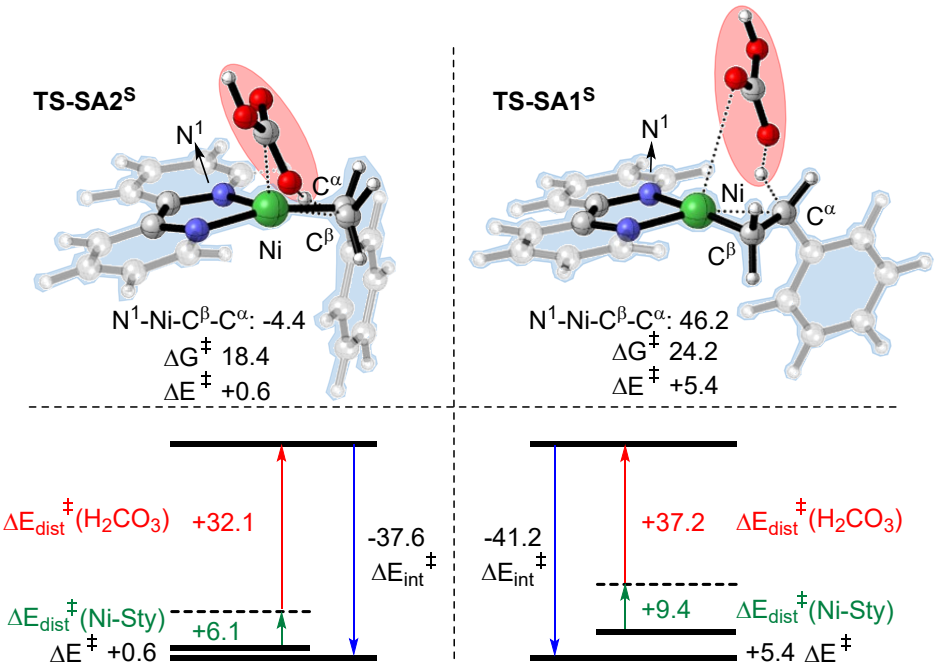

Figure S17. Optimized structures, relative Gibbs free energies and electronic energies, and distortion/interaction analysis of the competing insertion transition states **TS-SA2^{S}** and **TS- SA1^{S}**. Energies are in kcal/mol.

Table S1. Gibbs free energies of intermediate and different transition states calculated at **MN**//B3LYP-D3/SDD+f-6-311G(d,p)-IEFPCM methods (in kcal/mol).

Method	**A**	β-carboxylation inner	β-carboxylation outer	α-H-transfer	β-H-transfer	ΔΔG‡
		TS-SC1^{S}-F	**TS-SC3^{S}-F**	**TS-SA1^{S}-F**	**TS-SA2^{S}-F**	
M1	-1.4	23.6	18.7	21.4	18.5	0.2
M2	-0.7	23.1	20.1	20.7	18.1	2.0
M3	0.3	24.1	24.1	21.3	19.4	1.9
M4	-0.6	29.1	26.9	27.1	23.9	3.0
M5	-5.0	23.3	19.5	17.4	14.2	3.2
M6	-4.3	23.3	19.2	17.8	14.4	3.4

M1: PBE/SDD+f-def2-TZVP; **M2**: B3PW91/SDD+f-def2-TZVP; **M3**: ωB97XD/SDD+f-def2-TZVP; **M4**: M06/SDD+f-def2-TZVP; **M5**: PBE/SDD+f-6-311G(d,p); **M6**: PBE/LanL2DZ+f-6-311G(d,p); **A**: **Int-SW1^{S}-F**.

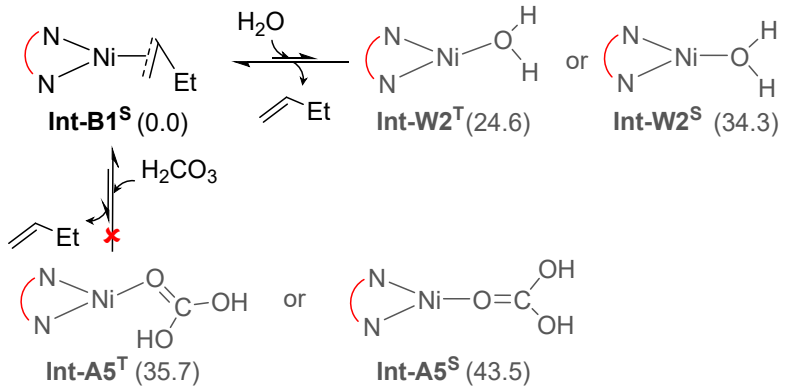

Figure S18. The relative Gibbs free energy of possible precursors in the hydrometallation/carboxylation mechanism for aliphatic alkenes (kcal/mol).

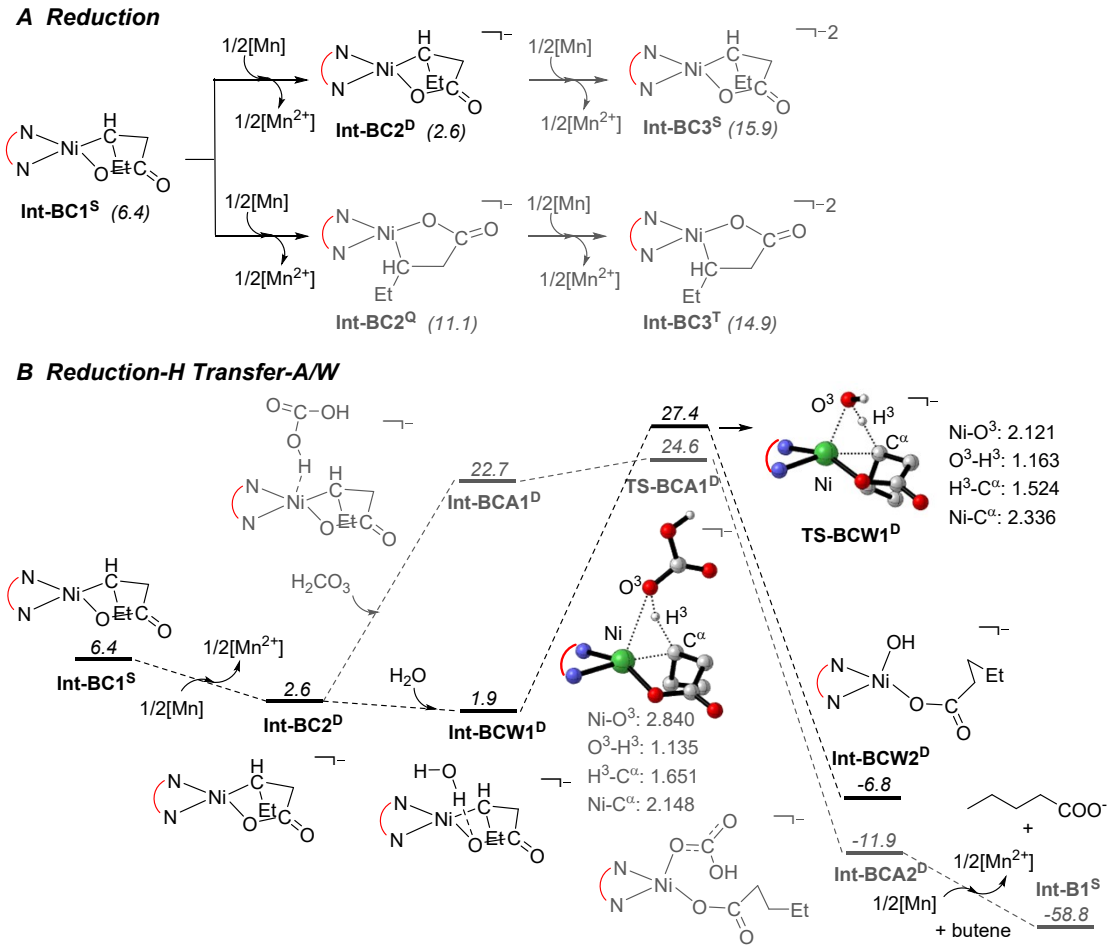

Figure S19. The Gibbs free energy profiles of the H transfer process of 1-butene substrate. The relative free energies are given in kcal/mol. The selected bond distances are given in Å.

The optimized geometries, electronic energies (SCF D), and Cartesian coordinates for the calculated structures

Butene

PBE SCF Energy: -157.050356789 a.u.

C 0.855721 0.559005 -0.00019400
C 1.533079 -0.587382 0.00004600
C -0.641461 0.721154 -0.00003400
H -0.918842 1.331392 0.86981800
C -1.454023 -0.574146 0.00005600
H -1.234913 -1.180605 -0.88330800
H -1.235145 -1.180444 0.88360400
H -2.524485 -0.355482 -0.00012400
H -0.918955 1.331462 -0.86983100
H 1.415254 1.493566 0.00072500
H 1.039475 -1.553477 -0.00024400
H 2.617718 -0.598203 0.00011500

CO_2

PBE SCF Energy: -188.480898997 a.u.

C 0.000000 0.000000 0.00000000
O 0.000000 0.000000 1.16036900
O 0.000000 0.000000 -1.16036900

H_2CO_3

PBE SCF Energy: -264.862773545 a.u.

C 0.000052 0.102964 -0.00000000
O -0.000009 1.309258 -0.00000000

O -0.000009 -0.680277 1.08410900
H -0.000044 -0.103710 1.86051200
O -0.000009 -0.680277 -1.08410900
H -0.000044 -0.103710 -1.86051200

H_2O

PBE SCF Energy: -76.3836758756 a.u.
O 0.000000 -0.000000 0.11945700
H 0.000000 0.755340 -0.47782800
H -0.000000 -0.755340 -0.47782800

Int-A1-T

PBE SCF Energy: -930.808173357 a.u.
C 1.976002 0.113943 0.08550700
C 2.116386 -2.237258 -0.09351200
C 3.471564 -2.244878 0.16160800
C 4.110088 -0.999639 0.39639300
C 3.369435 0.156749 0.35774000
C 1.120294 1.256584 0.01004700
C -1.063340 2.038581 -0.42175300
C -0.689596 3.359766 -0.30438700
C 0.666355 3.640823 0.01150700
C 1.551373 2.601421 0.16112400
H 1.577663 -3.161042 -0.27649600
H 4.018898 -3.178023 0.18170900
H 5.173184 -0.959409 0.60432500
H 3.851152 1.109663 0.53580900
H -2.089853 1.776039 -0.65740500
H -1.416242 4.148826 -0.44647800
H 1.002307 4.664968 0.12621700
H 2.589605 2.808678 0.38775200
N 1.365829 -1.117085 -0.13635600
N -0.223020 0.994695 -0.25697700
Ni -0.537800 -0.976668 -0.41741000
C -3.303112 -0.812770 0.32083200
O -2.518790 -1.274777 -0.50514600
O -4.597962 -1.059717 0.31743100
O -2.981265 -0.008822 1.31487900
H -4.799360 -1.650798 -0.42346300
H -2.017163 0.151133 1.28089400

Int-A2-S

PBE SCF Energy: -930.849018085 a.u.
C 2.000329 0.103425 0.05229100
C 2.000076 -2.222037 -0.10795900
C 3.379394 -2.273743 0.04370900
C 4.081980 -1.084946 0.20406300
C 3.382976 0.117122 0.20836500
C 1.151309 1.310015 0.03794000
C -1.044847 2.045333 -0.18317700
C -0.659692 3.373208 -0.03775000
C 0.688564 3.659045 0.15456400
C 1.609452 2.616004 0.19279900
H 1.405938 -3.113777 -0.23534200
H 3.881776 -3.231624 0.03434300
H 5.157991 -1.089382 0.32414400
H 3.909481 1.052921 0.33111800
H -2.072991 1.745616 -0.33847800
H -1.403074 4.158289 -0.07474400
H 1.023625 4.681879 0.27346200
H 2.660154 2.822246 0.34099000
N 1.318847 -1.064153 -0.10592700
N -0.161036 1.044013 -0.14381500
Ni -0.566252 -0.901620 -0.30636000
C -3.307780 -0.868066 0.30489100
O -2.401312 -0.586423 -0.57064500
O -4.571120 -0.516411 -0.10718900
O -3.184177 -1.371562 1.41014000
H -4.490918 -0.144519 -0.99490000
H -0.759283 -2.352310 -0.41117300

Int-A3-S

PBE SCF Energy: -666.37779939 a.u.
C -0.680192 0.805694 -0.00001000
C -2.616394 -0.509481 0.00019800
C -3.426497 0.617731 -0.00006000
C -2.831001 1.873558 -0.00033300
C -1.443035 1.967801 -0.00031300
C 0.793315 0.765949 -0.00000800
C 2.624705 -0.673894 -0.00063400
C 3.515633 0.393465 -0.00018200
C 3.004573 1.687288 0.00046600
C 1.625737 1.880017 0.00055800
H -3.022231 -1.508484 0.00038400
H -4.501345 0.499209 -0.00007200
H -3.435989 2.771146 -0.00058500
H -0.962351 2.935691 -0.00061700
H 2.963324 -1.702271 -0.00104600

H 4.580856 0.206883 -0.00028200
H 3.669633 2.541591 0.00092000
H 1.214268 2.879200 0.00115700
N -1.276631 -0.418161 0.00021300
N 1.300797 -0.488084 -0.00053800
Ni -0.102847 -1.867327 0.00010800
H -1.196674 -2.842839 0.00130200

Int-A3-T

PBE SCF Energy: -666.372570347 a.u.
C 0.720970 -0.822886 -0.00118500
C 2.644708 0.492396 -0.01648500
C 3.467777 -0.627242 0.01129700
C 2.872989 -1.884488 0.03142600
C 1.484896 -1.987361 0.02553000
C -0.762104 -0.798642 0.00313000
C -2.648807 0.566200 0.06972400
C -3.502993 -0.527974 0.01807000
C -2.943762 -1.799691 -0.04893200
C -1.559317 -1.939377 -0.05489700
H 3.040386 1.499813 -0.03189500
H 4.542837 -0.509385 0.01897500
H 3.480782 -2.780292 0.05477600
H 1.014248 -2.959785 0.04838800
H -3.024426 1.580660 0.11504900
H -4.574140 -0.379134 0.02416900
H -3.576041 -2.677192 -0.09943100
H -1.115143 -2.922612 -0.11252100
N 1.312489 0.391188 -0.02343200
N -1.317030 0.432664 0.06125900
Ni 0.024834 2.002806 -0.01522400
H 0.901793 3.276771 -0.08211000

Int-A4-D

PBE SCF Energy: -666.527441973 a.u.
C -0.747218 -0.803628 -0.00024200
C -2.640873 0.537462 0.00682800
C -3.485834 -0.566432 0.00176500
C -2.915978 -1.836412 -0.00632300
C -1.530452 -1.958159 -0.00771300
C 0.734073 -0.804266 0.00050000
C 2.636632 0.528804 -0.00624000
C 3.474906 -0.578302 -0.00149100
C 2.900339 -1.846495 0.00610200
C 1.514421 -1.960165 0.00741700
H -3.027719 1.549282 0.01188900
H -4.559082 -0.428432 0.00339900
H -3.539433 -2.721963 -0.01179500
H -1.074198 -2.938179 -0.01575400
H 3.031775 1.537089 -0.01110000
H 4.548515 -0.443570 -0.00304500
H 3.519803 -2.734682 0.01121800
H 1.052983 -2.937709 0.01499200
N -1.307213 0.427235 0.00562800
N 1.298491 0.427580 -0.00500500
Ni 0.034737 1.978600 -0.00035100
H -0.504311 3.459203 0.00204300

Int-A4-Q

PBE SCF Energy: -666.49667306 a.u.
C 0.714687 0.797067 0.00623900
C 2.660182 -0.550137 0.04799800
C 3.495526 0.543607 0.03981000
C 2.903632 1.834176 -0.00437300
C 1.535241 1.953501 -0.02216800
C -0.714646 0.797087 0.00633700
C -2.660212 -0.550075 0.04880500
C -3.495496 0.543662 0.03992800
C -2.903576 1.834226 -0.00515400
C -1.535192 1.953481 -0.02297900
H 3.052623 -1.561244 0.07244000
H 4.569015 0.412537 0.06398300
H 3.527233 2.720268 -0.02336000
H 1.078487 2.934238 -0.05521900
H -3.052639 -1.561174 0.07393900
H -4.568995 0.412675 0.06414700
H -3.527175 2.720300 -0.02488000
H -1.078426 2.934188 -0.05695100
N 1.314542 -0.455670 0.02805100
N -1.314513 -0.455705 0.02893500
Ni -0.000067 -1.950136 -0.08651800
H 0.000687 -2.967916 1.10283900

Int-A5-S

PBE SCF Energy: -1547.21737163 a.u.
C -0.481871 0.282728 -0.18253000
C -2.768372 0.581940 -0.51186500
C -2.618173 1.955865 -0.32939500

C -1.367792 2.541656 -0.09828500
C -0.246001 1.673968 -0.04983300
C 0.595766 -0.640982 -0.05091200
C 1.220823 -2.890775 0.03135000
C 2.563635 -2.517510 -0.03446900
C 2.960735 -1.176593 -0.05056100
C 1.939258 -0.193686 -0.04314700
H -3.495265 2.588593 -0.39734700
H 3.317367 -3.294859 -0.05216000
N -1.718061 -0.267040 -0.44755200
N 0.240345 -1.964687 0.08888300
Ni -1.633866 -2.168431 0.27415800
C -4.241528 -3.284886 0.18093500
O -3.402115 -2.710370 0.86838500
O -5.469795 -3.549481 0.58950500
O -4.049071 -3.724002 -1.05032800
H -5.574018 -3.212360 1.49156000
H -3.130008 -3.507421 -1.30061900
C -4.112906 -0.021917 -0.80391100
H -4.017480 -0.809220 -1.55551000
H -4.525388 -0.482796 0.09943400
H -4.822585 0.726738 -1.15793300
C 0.801903 -4.329435 0.06912600
H 0.015045 -4.457045 0.82200700
H 0.365308 -4.622744 -0.89027900
H 1.640708 -4.992916 0.28427400
C 1.121225 2.106432 0.04946800
C 2.158335 1.224273 0.02432200
H 1.329787 3.165700 0.11643200
H 3.173076 1.594745 0.07904000
C -1.269583 4.010353 0.07272200
C -1.891838 4.873112 -0.84403300
C -0.598367 4.576862 1.16860700
C -1.834496 6.254216 -0.67781800
H -2.409658 4.454474 -1.69974100
C -0.542430 5.958336 1.33482700
H -0.136954 3.928368 1.90416000
C -1.157807 6.803465 0.41151400
H -2.314535 6.902333 -1.40250300
H -0.024576 6.374341 2.19177000
H -1.113282 7.878702 0.54114300
C 4.405577 -0.844551 -0.08634000
C 4.933241 0.018803 -1.05941000
C 5.286785 -1.430170 0.83558100
C 6.297666 0.294398 -1.10192000
H 4.272125 0.459349 -1.79647900
C 6.650405 -1.151062 0.79469500
H 4.894115 -2.095780 1.59598900
C 7.161290 -0.286689 -0.17359700
H 6.686957 0.958229 -1.86561300
H 7.313611 -1.606156 1.52168800
H 8.222891 -0.070203 -0.20626100

Int-A5-T

PBE SCF Energy: -1547.22747741 a.u.

C 0.578413 -0.638803 -0.19095800
C 1.263890 -2.887801 -0.28078800
C 2.592068 -2.505791 -0.18686000
C 2.960425 -1.142103 -0.07174100
C 1.926757 -0.182961 -0.09592200
C -0.504171 0.268400 -0.20965700
C -2.825521 0.564288 -0.38674300
C -2.669718 1.943712 -0.32795200
C -1.395892 2.535568 -0.17193600
C -0.279238 1.675957 -0.14132100
H 3.358131 -3.270269 -0.16441400
H -3.550911 2.571881 -0.36184500
N 0.259744 -1.985022 -0.27735400
N -1.777700 -0.280714 -0.31119000
Ni -1.654956 -2.281548 -0.35091200
C -4.127270 -3.291081 0.73018300
O -3.407412 -3.268288 -0.26559900
O -5.246961 -3.979722 0.80914600
O -3.901373 -2.632476 1.85040300
H -5.385112 -4.445996 -0.02897600
H -3.056176 -2.151299 1.75466600
C -4.193677 -0.051207 -0.50056100
H -4.177786 -0.888876 -1.20106000
H -4.519229 -0.440015 0.46980000
H -4.932018 0.679397 -0.83214500
C 0.853082 -4.329940 -0.37730600
H 0.190449 -4.587395 0.45611400
H 0.284035 -4.497115 -1.29787200
H 1.711901 -5.001369 -0.36608700
C 1.089312 2.116950 -0.12755700
C 2.129813 1.240828 -0.10736000
H 1.294389 3.178760 -0.16437200
H 3.141788 1.622987 -0.12875000

C -1.292820 4.007994 -0.05738100
C -0.550995 4.615564 0.97029700
C -1.984102 4.840668 -0.95382700
C -0.489452 6.001749 1.08601100
H -0.037850 3.993355 1.69403900
C -1.920809 6.226679 -0.83895100
H -2.560374 4.392882 -1.75566400
C -1.171218 6.814840 0.18046800
H 0.084574 6.447114 1.89103900
H -2.453945 6.848893 -1.54928500
H -1.122819 7.893976 0.27079300
C 4.393090 -0.796341 0.06063800
C 5.344372 -1.383816 -0.79199400
C 4.855893 0.074820 1.06242400
C 6.700525 -1.099291 -0.65948200
H 5.010457 -2.055998 -1.57455800
C 6.212670 0.358564 1.19514100
H 4.146971 0.512624 1.75530100
C 7.142374 -0.224589 0.33382800
H 7.413404 -1.557778 -1.33600400
H 6.545233 1.028360 1.98049500
H 8.198492 -0.003856 0.43834000

Int-AS1-S

PBE SCF Energy: -1240.21339859 a.u.

C -0.919064 -0.335943 -1.30808800
C -0.770471 -2.600164 -0.77969700
C -2.008970 -2.856909 -1.35262300
C -2.714416 -1.805158 -1.92438500
C -2.162716 -0.530078 -1.89912000
C -0.244925 0.970897 -1.20109000
C 1.637562 2.038400 -0.34893200
C 1.191541 3.275853 -0.79606000
C -0.020036 3.340683 -1.47988600
C -0.750956 2.175689 -1.68423400
H -0.180452 -3.379406 -0.32231700
H -2.403438 -3.864027 -1.34205400
H -3.685098 -1.969156 -2.37477200
H -2.702793 0.305052 -2.32053000
H 2.564771 1.909183 0.19385300
H 1.783085 4.162620 -0.61131600
H -0.396744 4.288029 -1.84502300
H -1.699983 2.210371 -2.19986500
N -0.227981 -1.372277 -0.75841600
N 0.938525 0.917770 -0.55349700
Ni 1.460199 -0.930265 0.01143100
C 4.223609 -0.462052 0.16436600
O 3.091401 -0.339320 0.76979200
O 5.265503 0.103826 0.86121300
O 4.471644 -0.984993 -0.91188500
H 4.900066 0.465189 1.67889100
H 1.773260 -2.332196 0.32962900
C -3.890795 -0.745229 1.13951200
C -2.632715 -0.729185 1.72717000
C -1.888824 0.461542 1.80463700
C -2.459164 1.630990 1.27703900
C -3.718246 1.614848 0.68266600
C -4.440243 0.425383 0.61104000
H -4.443344 -1.676016 1.08190600
H -2.223418 -1.649701 2.12534100
H -1.897538 2.557991 1.31941400
H -4.131841 2.529266 0.27263600
H -5.419391 0.406623 0.14660700
C -0.540220 0.527992 2.38313100
C 0.222551 -0.502219 2.76507900
H -0.123306 1.529655 2.45510800
H 1.222640 -0.340414 3.14611100
H -0.105261 -1.532255 2.69359400

Int-AS2-S

PBE SCF Energy: -1240.21560903 a.u.

C -0.269909 1.287598 1.01400500
C 0.251215 2.891740 -0.58066800
C -0.382789 3.891785 0.14628800
C -0.988296 3.554264 1.35322900
C -0.931382 2.237229 1.79265700
C -0.138601 -0.136164 1.38588500
C 0.660839 -2.207181 0.70228900
C 0.301052 -2.801465 1.90474000
C -0.316685 -2.014553 2.87198400
C -0.533085 -0.665916 2.61427000
H 0.727178 3.095857 -1.53027900
H -0.401926 4.905183 -0.23247600
H -1.501006 4.303535 1.94350700
H -1.405855 1.954538 2.72159500
H 1.148334 -2.766932 -0.08506700
H 0.501055 -3.851466 2.07130500
H -0.617720 -2.441265 3.82069700

H -0.989456 -0.037819 3.36608400
N 0.307914 1.622747 -0.16096300
N 0.430798 -0.918313 0.44486400
Ni 0.959539 0.035006 -1.23524700
C 3.474477 -0.084171 0.21248200
O 2.893155 -0.407099 -0.88190000
O 4.748186 -0.617982 0.33565200
O 3.073198 0.610277 1.13889800
H 4.912129 -1.130367 -0.46597800
H 1.371876 0.841221 -2.34286600
C 0.287228 -1.311547 -2.59704500
C -0.735775 -0.388338 -2.34771200
H 0.878144 -1.226307 -3.50123900
H -0.830070 0.453980 -3.02705200
H 0.268156 -2.301561 -2.15299700
C -1.912600 -0.591297 -1.47866200
C -2.711884 0.516136 -1.15210400
C -2.256435 -1.838380 -0.93429000
C -3.798285 0.389846 -0.29207000
H -2.457568 1.488668 -1.55987100
C -3.342037 -1.966340 -0.07397300
H -1.669466 -2.714409 -1.18042400
C -4.115494 -0.852513 0.25677500
H -4.392969 1.262127 -0.04518500
H -3.585875 -2.938416 0.33981700
H -4.958680 -0.953738 0.93035300

Int-B1-S

PBE SCF Energy: -1439.45914029 a.u.

C -0.451899 1.648496 -0.03900900
C -1.627377 2.447409 -0.13718100
C -2.817382 1.798949 -0.41574200
C -2.880149 0.404309 -0.59160800
C 2.966893 -0.922922 -0.05098100
C 2.713136 -2.257416 -0.31664000
C 1.409025 -2.735550 -0.53867200
H -3.727081 2.375819 -0.52609200
H 3.538981 -2.954522 -0.38464700
N -1.785613 -0.358024 -0.48864600
N 0.352100 -1.915419 -0.49392200
Ni -1.600201 -2.350771 -0.42143600
C -3.195816 -3.352134 0.00446400
C -2.049241 -4.203533 -0.16485000
H -1.961501 -4.820693 -1.06179700
H -1.600497 -4.676215 0.71359100
H -3.954860 -3.363186 -0.78486600
C -3.782772 -3.120210 1.38769800
H -2.968526 -3.109248 2.12210200
C -4.189109 -0.254513 -0.91298100
H -4.026936 -1.122528 -1.54973000
H -4.669572 -0.610643 0.00221500
H -4.867819 0.447039 -1.40060200
C 1.175486 -4.186494 -0.83928800
H 0.798383 -4.698676 0.05012300
H 0.411310 -4.293257 -1.60861100
H 2.097570 -4.674605 -1.15763000
C -1.614263 3.923171 0.02196200
C -0.756609 4.727178 -0.74304400
C -2.501398 4.540148 0.91490300
C -0.782861 6.113097 -0.61255700
H -0.082090 4.264901 -1.45410300
C -2.520911 5.926226 1.04956400
H -3.165891 3.927954 1.51389400
C -1.661738 6.716465 0.28675200
H -0.119797 6.721516 -1.21677600
H -3.205553 6.388121 1.75161700
H -1.678435 7.795240 0.39054200
C 4.365291 -0.467780 0.15119000
C 4.906787 0.578215 -0.61019700
C 5.184290 -1.117950 1.08499700
C 6.232862 0.965952 -0.43707700
H 4.292152 1.074743 -1.35175900
C 6.508292 -0.723952 1.26190600
H 4.774232 -1.924253 1.68231800
C 7.036256 0.319024 0.50177500
H 6.639550 1.770363 -1.03908800
H 7.126108 -1.230192 1.99469100
H 8.067221 0.624469 0.63829400
C 1.850423 -0.039949 0.00078200
C 0.572386 -0.591295 -0.24290800
C -0.590107 0.258539 -0.25127400
C 0.843379 2.158925 0.30048300
C 1.939862 1.353588 0.32284700
H 0.942545 3.204482 0.55820500
H 2.900409 1.765999 0.59985600
C -4.819035 -4.181091 1.79428200
H -5.656360 -4.195061 1.08833000
H -4.369522 -5.178926 1.79340900

H -5.226072 -3.992490 2.79371400
H -4.249935 -2.129891 1.44339700

Int-BC1-S

PBE SCF Energy: -1627.95042995 a.u.
C 0.645368 1.778351 -0.11102100
C 0.002408 3.032048 -0.32651300
C -1.298660 3.009905 -0.79320700
C -2.004611 1.806438 -0.97768800
C 2.482472 -2.076958 -0.08964700
C 1.680899 -3.119750 -0.51491700
C 0.326771 -2.929561 -0.85904600
H -1.797337 3.939726 -1.03555700
H 2.107666 -4.108190 -0.62870900
N -1.432942 0.631800 -0.69634300
N -0.242228 -1.726315 -0.75676000
Ni -2.235780 -1.137234 -0.46307000
C -3.839742 -0.605565 0.53924500
C -4.423165 -1.912478 1.10134500
H -5.507200 -1.896116 1.25341200
H -3.975985 -2.124996 2.08206500
H -4.561025 -0.181055 -0.16890500
C -3.543776 0.407274 1.65030000
H -3.059651 1.298699 1.24752600
H -2.818120 -0.034819 2.34509200
C -4.792192 0.848235 2.43351900
H -4.538529 1.584468 3.20283700
H -5.527119 1.303643 1.76113300
H -5.276705 0.002362 2.92878000
C -3.401508 1.845124 -1.52278900
H -3.671136 0.884015 -1.95519700
H -4.122068 2.085760 -0.73713500
H -3.475093 2.621129 -2.28694200
C -0.481433 -4.081687 -1.37585200
H -1.112373 -4.485561 -0.58212600
H -1.158214 -3.749937 -2.16200100
H 0.172261 -4.869106 -1.75256300
C -4.037759 -3.080661 0.21638900
O -2.943145 -2.854787 -0.46333000
O -4.654829 -4.140660 0.16736900
C 0.682998 4.333547 -0.11562700
C 1.901226 4.627671 -0.74462500
C 0.079563 5.310832 0.68766600
C 2.502532 5.871018 -0.56878800
H 2.365676 3.890214 -1.38843700
C 0.688461 6.549784 0.87009900
H -0.860460 5.089969 1.18016200
C 1.900876 6.833013 0.24220500
H 3.439009 6.089278 -1.06881600
H 0.216280 7.292513 1.50258500
H 2.373026 7.798593 0.38163000
C 3.910753 -2.330541 0.22597800
C 4.932419 -1.609437 -0.40842300
C 4.256172 -3.337963 1.13695500
C 6.268399 -1.888192 -0.13287500
H 4.679241 -0.844042 -1.13251000
C 5.593125 -3.608544 1.41787300
H 3.472973 -3.898483 1.63437100
C 6.602369 -2.884812 0.78387100
H 7.048002 -1.329276 -0.63741500
H 5.845624 -4.383639 2.13216600
H 7.642808 -3.097471 1.00070500
C 1.890482 -0.783390 -0.00528000
C 0.527392 -0.675596 -0.35459700
C -0.108037 0.614079 -0.36450400
C 1.989841 1.623147 0.35941300
C 2.579702 0.398115 0.42130100
H 2.538140 2.500160 0.67418800
H 3.592051 0.309198 0.79047300

Int-BC2-D

PBE SCF Energy: -1628.05596658 a.u.
C 0.840348 1.725386 -0.15035400
C 0.324169 3.028760 -0.31911200
C -1.026917 3.132252 -0.74120300
C -1.825044 2.021401 -0.93941700
C 2.281984 -2.307016 -0.07737000
C 1.338140 -3.294556 -0.39893800
C 0.007416 -2.974222 -0.67944600
H -1.435996 4.109364 -0.96764700
H 1.648391 -4.330240 -0.45709700
N -1.361015 0.760306 -0.72854700
N -0.441475 -1.706998 -0.65234500
Ni -2.358376 -0.884230 -0.53053500
C -3.820716 -0.270817 0.65047000
C -4.438669 -1.586489 1.14327100
H -5.453792 -1.499420 1.54983900
H -3.814450 -2.001824 1.94752800

H -4.569429 0.253445 0.04047800
C -3.363015 0.639333 1.79053400
H -2.851880 1.518302 1.38720000
H -2.609830 0.106208 2.38657800
C -4.496241 1.112942 2.71797900
H -4.123424 1.780628 3.50230700
H -5.256692 1.657378 2.14726500
H -4.993169 0.269922 3.20689400
C -3.235941 2.180589 -1.43836200
H -3.524654 1.320775 -2.04518300
H -3.943828 2.245334 -0.60885500
H -3.331331 3.091032 -2.03298300
C -0.964582 -4.062673 -1.03586100
H -1.765643 -4.114678 -0.29725400
H -1.454201 -3.840613 -1.98606300
H -0.461714 -5.028241 -1.10310100
C -4.423136 -2.615422 0.02088100
O -3.432513 -2.452040 -0.80545600
O -5.254279 -3.522405 -0.07037400
C 1.108608 4.263677 -0.11702300
C 2.398667 4.431253 -0.65475700
C 0.547322 5.347819 0.58411100
C 3.101925 5.619925 -0.47990800
H 2.839727 3.631430 -1.23746800
C 1.250477 6.536231 0.75772000
H -0.444291 5.244218 1.01049700
C 2.534508 6.678960 0.22990900
H 4.091792 5.723904 -0.91088800
H 0.797307 7.351288 1.31154900
H 3.082940 7.604242 0.36477300
C 3.682929 -2.706025 0.19989100
C 4.764041 -2.096703 -0.45732900
C 3.954473 -3.747101 1.10198400
C 6.072056 -2.505978 -0.21012100
H 4.573205 -1.311290 -1.17903300
C 5.262623 -4.153754 1.35145300
H 3.132015 -4.227274 1.62015900
C 6.327618 -3.533933 0.69734500
H 6.891874 -2.026257 -0.73308600
H 5.450822 -4.952990 2.05965600
H 7.346037 -3.851421 0.89007500
C 1.838846 -0.969495 -0.04645700
C 0.472593 -0.706506 -0.36723300
C -0.018675 0.617768 -0.40366700
C 2.170266 1.422392 0.30662200
C 2.645673 0.148044 0.35052100
H 2.806178 2.234209 0.63390500
H 3.649836 -0.032839 0.71100200

Int-BC2-Q

PBE SCF Energy: -1628.03807423 a.u.

C -1.901846 -0.949775 -0.05728300
C -2.342091 -2.290848 -0.08270400
C -1.348983 -3.303155 -0.20199200
C -0.009712 -2.983529 -0.33242800
C -0.339894 3.047446 -0.09680400
C 1.054789 3.164371 -0.24794700
C 1.862392 2.033978 -0.38940500
H -1.646721 -4.343654 -0.22846300
H 1.511624 4.144939 -0.28655700
N 0.423833 -1.703838 -0.34837600
N 1.354183 0.795384 -0.38984300
Ni 2.321746 -1.012236 -0.60766100
C 3.503001 -1.475252 0.98072200
C 4.900598 -1.032760 0.53596300
H 5.738765 -1.565242 1.00559300
H 5.042527 0.026797 0.79259500
H 3.487857 -2.574812 1.07092700
C 3.026748 -0.859066 2.29093000
H 1.990199 -1.171872 2.47313200
H 2.987068 0.232757 2.17088600
C 3.874019 -1.195804 3.53162700
H 3.475589 -0.730941 4.44111700
H 3.905677 -2.279000 3.69448700
H 4.906336 -0.853042 3.40769100
C 1.047435 -4.044631 -0.46794700
H 1.649013 -3.869833 -1.36604300
H 1.733857 -4.001913 0.38235800
H 0.612468 -5.043124 -0.52266300
C 3.353451 2.168735 -0.52774400
H 3.830390 1.977281 0.43855500
H 3.740538 1.427818 -1.22831600
H 3.633746 3.171472 -0.85298900
C 5.096393 -1.100800 -0.98767800
O 4.015276 -0.955798 -1.69618300
O 6.222904 -1.245192 -1.47395800
C -3.761829 -2.688016 0.00942700
C -4.759120 -2.071324 -0.76927500

C -4.150926 -3.749567 0.84804900
C -6.086482 -2.484343 -0.69737900
H -4.482911 -1.279316 -1.45527100
C -5.478208 -4.161961 0.91961800
H -3.403375 -4.240774 1.46089500
C -6.455834 -3.530175 0.14949400
H -6.832783 -1.995793 -1.31440000
H -5.751446 -4.975784 1.58252700
H -7.489483 -3.852107 0.20417600
C -1.155659 4.279915 0.02186800
C -2.278652 4.500888 -0.79197800
C -0.784547 5.285620 0.92901700
C -3.012139 5.680602 -0.69176000
H -2.563945 3.750046 -1.51936900
C -1.520301 6.463135 1.03166500
H 0.078665 5.131126 1.56655500
C -2.638492 6.665716 0.22223600
H -3.871949 5.833469 -1.33449800
H -1.222225 7.222073 1.74649700
H -3.210387 7.583277 0.30054200
C -0.892501 1.751588 -0.06231000
C -0.012113 0.635689 -0.21717200
C -0.506271 -0.688990 -0.20650200
C -2.751120 0.186166 0.18864900
C -2.275651 1.461335 0.18629800
H -3.796920 0.016119 0.40807000
H -2.951370 2.278609 0.40159900

Int-BC3-S

PBE SCF Energy: -1628.13747379 a.u.

C 0.377538 1.871075 -0.14005300
C -0.455231 2.994769 -0.31594600
C -1.799634 2.714125 -0.78550800
C -2.260223 1.442271 -0.99321300
C 2.861610 -1.630560 -0.09884400
C 2.201259 -2.843166 -0.43560700
C 0.826617 -2.888361 -0.65714100
H -2.423992 3.543287 -1.09799900
H 2.775541 -3.756482 -0.52891300
N -1.496865 0.323636 -0.74240600
N 0.034384 -1.801824 -0.57654100
Ni -2.009416 -1.485932 -0.44639800
C -3.687966 -1.222009 0.54579700
C -3.976703 -2.610962 1.13917900
H -5.014771 -2.778945 1.45392900
H -3.352640 -2.761691 2.03253900
H -4.502697 -0.985218 -0.15510000
C -3.627107 -0.135182 1.62284000
H -3.301859 0.811488 1.18300800
H -2.846919 -0.406131 2.34776800
C -4.950994 0.099250 2.37230800
H -4.860769 0.899848 3.11532100
H -5.742764 0.383949 1.66979100
H -5.285970 -0.802010 2.89505900
C -3.619864 1.229906 -1.60644000
H -3.565241 0.452617 -2.37601700
H -4.351872 0.889518 -0.87235600
H -3.992939 2.153176 -2.05492400
C 0.184356 -4.208680 -0.99003400
H -0.533643 -4.492254 -0.21915800
H -0.394804 -4.133221 -1.91307800
H 0.937371 -4.991687 -1.09776500
C -3.560972 -3.689206 0.14908500
O -2.583545 -3.321833 -0.61754800
O -4.092447 -4.805695 0.10971300
C -0.062242 4.383705 -0.09652000
C 1.223431 4.899740 -0.40753100
C -1.008557 5.327664 0.38535800
C 1.545057 6.237656 -0.21199400
H 1.963235 4.246556 -0.85254900
C -0.684146 6.665478 0.57510100
H -2.005760 4.985848 0.63958800
C 0.599409 7.139665 0.28680300
H 2.539385 6.586708 -0.47365700
H -1.437789 7.345532 0.96065900
H 0.852050 8.183511 0.43427900
C 4.313599 -1.650728 0.17139700
C 5.195030 -0.703382 -0.38600000
C 4.875718 -2.670722 0.96465100
C 6.564413 -0.758424 -0.13987200
H 4.800071 0.067602 -1.03655400
C 6.244262 -2.726230 1.20943900
H 4.221534 -3.414035 1.40674000
C 7.099824 -1.768028 0.66118900
H 7.217970 -0.017199 -0.58759600
H 6.645033 -3.516964 1.83486600
H 8.166550 -1.812208 0.84951600
C 2.075722 -0.469143 -0.04277900

C 0.674433 -0.563856 -0.34910200
C -0.141708 0.560965 -0.40249400
C 1.727644 1.911923 0.36572600
C 2.537020 0.815815 0.39456300
H 2.112796 2.849320 0.74511500
H 3.542268 0.910517 0.78581200

Int-BC3-T

PBE SCF Energy: -1628.13603743 a.u.

C 0.687980 1.844707 -0.09118000
C 0.018611 3.117105 -0.25000100
C -1.345526 3.054864 -0.63903500
C -2.014960 1.870737 -0.85817400
C 2.532952 -2.081125 0.00415700
C 1.623215 -3.149850 -0.22267600
C 0.284503 -2.957554 -0.48897300
H -1.872142 3.978430 -0.85260800
H 1.998642 -4.166460 -0.24591100
N -1.400847 0.655980 -0.68629800
N -0.274662 -1.705937 -0.54714400
Ni -2.237697 -1.090255 -0.55428100
C -3.785074 -0.720482 0.64052100
C -4.229267 -2.134492 1.03447200
H -5.233938 -2.208647 1.47202200
H -3.533675 -2.540365 1.78397600
H -4.597109 -0.259647 0.05912400
C -3.446954 0.173313 1.83054100
H -3.025760 1.117148 1.46967400
H -2.646899 -0.303571 2.41413500
C -4.631005 0.485115 2.76431400
H -4.337746 1.148886 3.58564800
H -5.437698 0.976676 2.20872200
H -5.045698 -0.426393 3.20608600
C -3.434284 1.872348 -1.36150300
H -3.582839 1.071621 -2.09114300
H -4.152183 1.701964 -0.55562600
H -3.675418 2.828325 -1.83182100
C -0.619410 -4.133729 -0.73385200
H -1.404514 -4.188030 0.02562800
H -1.145919 -4.039250 -1.68619900
H -0.051117 -5.066401 -0.72525000
C -4.140766 -3.057880 -0.17874300
O -3.212105 -2.719706 -1.01675700
O -4.879135 -4.040175 -0.31746100
C 0.654928 4.422981 -0.09056400
C 1.984655 4.696125 -0.50098900
C -0.074165 5.520407 0.43755200
C 2.540136 5.964764 -0.38495000
H 2.571162 3.907298 -0.95450400
C 0.485234 6.787183 0.55223000
H -1.088348 5.359306 0.78605400
C 1.801656 7.026892 0.14685800
H 3.557181 6.131170 -0.72634200
H -0.106702 7.593805 0.97360900
H 2.239769 8.013950 0.24124200
C 3.950677 -2.366622 0.19173300
C 4.983873 -1.516635 -0.28517600
C 4.376205 -3.567972 0.82185100
C 6.326660 -1.839885 -0.13706900
H 4.719594 -0.609905 -0.81442200
C 5.720192 -3.885819 0.96854400
H 3.631214 -4.243604 1.22694800
C 6.716853 -3.025916 0.49513600
H 7.080138 -1.165422 -0.53246300
H 5.995692 -4.809142 1.46906800
H 7.765682 -3.272759 0.61387500
C 1.947443 -0.757437 0.01788200
C 0.558734 -0.632229 -0.30367400
C -0.058805 0.654628 -0.35799700
C 2.015209 1.670490 0.36554900
C 2.618045 0.423033 0.41561000
H 2.577419 2.531130 0.70184100
H 3.629938 0.353386 0.79197900

Int-BCA1-D

PBE SCF Energy: -1892.91826022 a.u.

C 2.014814 -1.349266 0.04305900
C 2.039856 -2.768173 0.17807500
C 0.839132 -3.409317 0.41887800
C -0.368845 -2.692371 0.52913700
C 1.728765 2.916391 -0.01822600
C 0.454483 3.438050 0.13414000
C -0.678489 2.610418 0.22342000
H 0.821772 -4.483207 0.56218300
H 0.321526 4.510540 0.20641300
N -0.413135 -1.371604 0.35711100
N -0.566547 1.278167 0.16411200
Ni -2.059905 -0.052433 -0.22828800

C -3.706774 -1.193783 -0.68754200
C -4.747844 -0.177330 -1.17778100
H -5.239705 0.288476 -0.31413700
H -5.553126 -0.594224 -1.80235300
H -4.202657 -1.869208 0.02718600
C -3.207769 -2.074518 -1.85568300
H -2.295942 -2.610447 -1.56860600
H -2.908453 -1.420901 -2.68539100
C -4.223851 -3.110089 -2.37247600
H -3.829511 -3.689935 -3.21572600
H -4.486246 -3.815875 -1.57615100
H -5.150408 -2.632280 -2.70526600
C -1.629289 -3.413979 0.91296500
H -2.483158 -2.748699 0.82783300
H -1.786514 -4.294556 0.28514000
H -1.549455 -3.761543 1.94837100
C -2.046100 3.200182 0.39979200
H -2.646464 2.576803 1.06514900
H -1.986302 4.217617 0.79036000
H -2.563241 3.202270 -0.56154500
C -4.118097 0.982865 -1.97028400
O -2.882188 1.224496 -1.72153300
O -4.819351 1.629875 -2.77129100
C 3.291469 -3.564005 0.09317600
C 4.384688 -3.292235 0.92818700
C 3.376293 -4.638873 -0.80220800
C 5.535063 -4.074463 0.86459500
H 4.324746 -2.477079 1.63981100
C 4.530340 -5.415987 -0.86971300
H 2.537871 -4.854618 -1.45465800
C 5.612994 -5.136079 -0.03680200
H 6.368704 -3.857116 1.52252000
H 4.583729 -6.238431 -1.57388100
H 6.510357 -5.741909 -0.08792500
C 2.892015 3.834834 -0.10527000
C 3.984180 3.710527 0.76601000
C 2.892175 4.878526 -1.04132900
C 5.049747 4.604356 0.69842700
H 3.987935 2.921589 1.50894100
C 3.961818 5.767757 -1.11240900
H 2.055642 4.981378 -1.72309200
C 5.043884 5.633309 -0.24328200
H 5.882469 4.499441 1.38447200
H 3.950578 6.563822 -1.84813200
H 5.875596 6.326294 -0.29760200
C 1.858976 1.498844 -0.05974900
C 0.677046 0.731692 0.07068800
C 0.757589 -0.707964 0.14668500
C 3.172076 -0.547944 -0.22353700
C 3.098861 0.810267 -0.26491600
H 4.120389 -1.037934 -0.39779100
H 3.990604 1.387530 -0.46862400
C -4.306130 0.430257 2.67603100
O -4.590802 1.407474 2.01456400
O -4.599081 0.312839 3.98975900
O -3.687543 -0.657732 2.27159600
H -3.404107 -0.575532 1.28875300
H -5.058260 1.122926 4.25015400

Int-BCA2-D

PBE SCF Energy: -1892.97571676 a.u.

C -2.046195 1.542403 -0.14150200
C -1.895961 2.948359 -0.10260800
C -0.584274 3.462663 -0.10938900
C 0.525737 2.629724 -0.12782500
C -2.203226 -2.743972 -0.21386000
C -0.959491 -3.395080 -0.24211600
C 0.241071 -2.689086 -0.20897000
H -0.432894 4.534233 -0.07170100
H -0.925320 -4.477195 -0.25381900
N 0.397383 1.285141 -0.15615200
N 0.257189 -1.341703 -0.16772500
Ni 1.831702 -0.100047 -0.00820800
C 5.329827 0.985369 0.03151000
C 5.488234 -0.539661 -0.01037200
H 5.329235 -0.947001 0.99348200
H 6.500609 -0.828883 -0.30114400
H 6.091135 1.393518 0.70851200
C 5.446693 1.675784 -1.33479600
H 5.290682 2.751992 -1.19677800
H 4.630206 1.324970 -1.97451800
C 6.788102 1.445002 -2.03950800
H 6.849932 2.016489 -2.97010700
H 7.624983 1.750857 -1.40242200
H 6.931246 0.390582 -2.29140700
C 1.930890 3.157754 -0.10632200
H 2.459875 2.759498 0.76429100
H 2.476313 2.811773 -0.99050200

H 1.956943 4.247023 -0.07873600
C 1.567057 -3.391190 -0.18634900
H 2.070018 -3.197783 0.76527700
H 1.447274 -4.466845 -0.31983800
H 2.226915 -2.989589 -0.95850500
C 4.518209 -1.284886 -0.93730200
O 3.331786 -0.797400 -1.08193800
O 4.907781 -2.311570 -1.50569100
C -3.040591 3.886934 -0.05128800
C -4.065902 3.742821 0.89799800
C -3.098127 4.980697 -0.93048900
C -5.117742 4.653375 0.95661200
H -4.024367 2.923964 1.60660900
C -4.151435 5.889405 -0.87288300
H -2.317931 5.106018 -1.67290400
C -5.167175 5.728995 0.06985500
H -5.895145 4.527121 1.70183600
H -4.181238 6.721315 -1.56767700
H -5.986835 6.436882 0.11525500
C -3.444244 -3.554604 -0.20344100
C -4.446713 -3.347180 0.75744700
C -3.617973 -4.589704 -1.13569600
C -5.589467 -4.142803 0.77781500
H -4.317611 -2.572145 1.50377800
C -4.762748 -5.381932 -1.11725700
H -2.855250 -4.761198 -1.88688500
C -5.753940 -5.161288 -0.16087000
H -6.348557 -3.971359 1.53273600
H -4.882184 -6.170086 -1.85217300
H -6.644401 -5.779207 -0.14508600
C -2.201706 -1.330699 -0.19462100
C -0.944375 -0.669350 -0.16721600
C -0.868949 0.747714 -0.15117300
C -3.303274 0.851731 -0.23880800
C -3.376555 -0.507155 -0.26608500
H -4.212559 1.432440 -0.31825200
H -4.342133 -0.984311 -0.36820900
C 3.295128 -0.411301 2.60278800
O 4.027751 0.000456 3.50046700
O 3.242084 -1.779756 2.36621400
O 2.547140 0.268753 1.83286700
H 4.361654 1.221736 0.47485900
H 3.852100 -2.184468 2.99597400

Int-BCW1-D

PBE SCF Energy: -1704.45352248 a.u.

C 1.335799 1.534274 -0.10614700
C 1.097476 2.917254 -0.25522100
C -0.223932 3.310631 -0.58012600
C -1.252365 2.394958 -0.71944000
C 1.868336 -2.716477 -0.02407100
C 0.706604 -3.477567 -0.24113300
C -0.535598 -2.877808 -0.44400900
H -0.430630 4.355460 -0.77746200
H 0.775719 -4.557585 -0.27539000
N -1.050518 1.064369 -0.53926600
N -0.689949 -1.539643 -0.44501500
Ni -2.368479 -0.339608 -0.30001400
C -3.610411 0.500789 0.99134300
C -4.481351 -0.684427 1.42893100
H -5.411974 -0.413450 1.94246400
H -3.909891 -1.318828 2.12156700
H -4.251209 1.220579 0.46406700
C -2.891462 1.196533 2.14345200
H -2.218436 1.962335 1.74479600
H -2.243841 0.466320 2.64781400
C -3.821942 1.848801 3.18158000
H -3.254620 2.355961 3.96956100
H -4.469411 2.591668 2.70284700
H -4.469259 1.108873 3.66166700
C -2.630166 2.848519 -1.11983600
H -3.120006 2.088712 -1.73152400
H -3.260167 3.014066 -0.24269200
H -2.578783 3.784317 -1.67912700
C -1.756738 -3.721502 -0.67230700
H -2.479983 -3.563310 0.13042000
H -2.265034 -3.419600 -1.58944200
H -1.498382 -4.779721 -0.72667200
C -4.804058 -1.550433 0.21787800
O -3.830988 -1.584952 -0.65370700
O -5.862928 -2.162472 0.08565900
C 2.142656 3.954133 -0.12034000
C 3.385134 3.851404 -0.77185800
C 1.889718 5.116133 0.63119700
C 4.339891 4.858605 -0.65988800
H 3.590720 2.986569 -1.39127300
C 2.844462 6.123002 0.74255500
H 0.939861 5.217378 1.14438500

C 4.076943 5.998835 0.10005500
H 5.287369 4.757823 -1.17784800
H 2.627929 7.004139 1.33663600
H 4.820810 6.782629 0.18626300
C 3.163428 -3.410304 0.17129300
C 4.302949 -3.063967 -0.57317500
C 3.264097 -4.473474 1.08333000
C 5.503670 -3.748151 -0.40103800
H 4.238767 -2.266262 -1.30383200
C 4.465353 -5.155801 1.25675800
H 2.395830 -4.752585 1.66959300
C 5.591445 -4.795275 0.51627500
H 6.369435 -3.468132 -0.99077900
H 4.523255 -5.967357 1.97356400
H 6.526497 -5.327068 0.65023000
C 1.731562 -1.313727 -0.00909700
C 0.438072 -0.762154 -0.24983900
C 0.244906 0.637237 -0.28876600
C 2.599174 0.953387 0.26224000
C 2.788369 -0.393380 0.30255800
H 3.417722 1.609964 0.52590000
H 3.752740 -0.785719 0.59749500
O -3.878172 -0.304294 -3.13954000
H -2.968511 0.004004 -3.06027700
H -3.991276 -0.841783 -2.33080600

Int-BCW2-D

PBE SCF Energy: -1704.46825071 a.u.
C 1.288032 1.743996 -0.13233200
C 0.784017 3.064202 -0.17588300
C -0.598346 3.223233 -0.44000900
C -1.415835 2.138841 -0.70923500
C 2.542004 -2.362024 -0.03559300
C 1.531040 -3.311816 -0.27209100
C 0.220049 -2.925375 -0.54610000
H -1.023126 4.218821 -0.47171100
H 1.774421 -4.366801 -0.26267900
N -0.935275 0.873999 -0.73372900
N -0.126708 -1.630520 -0.62110700
Ni -1.971440 -0.843832 -0.95420200
C -5.628757 -0.682242 -0.30215300
C -5.006005 -1.846044 0.49375000
H -4.591153 -2.580571 -0.20297900
H -5.763441 -2.349523 1.09671000
H -6.462507 -1.074810 -0.89723400
C -6.131445 0.482262 0.56307000
H -6.543551 1.252554 -0.09870200
H -5.279574 0.944451 1.07533300
C -7.180343 0.079854 1.60486000
H -7.578665 0.956784 2.12338700
H -8.021041 -0.443186 1.13638300
H -6.741730 -0.582171 2.35485200
C -2.880407 2.290465 -1.00754900
H -3.101474 1.923918 -2.01557900
H -3.463165 1.676329 -0.31498900
H -3.207587 3.327429 -0.92923800
C -0.874904 -3.937490 -0.74382100
H -1.422492 -4.071514 0.19567700
H -1.594474 -3.579489 -1.48373000
H -0.474257 -4.906667 -1.04412800
C -3.888568 -1.369476 1.42634700
O -2.794365 -0.965625 0.88129700
O -4.089006 -1.356865 2.64955300
C 1.617366 4.263372 0.05798800
C 2.847803 4.449107 -0.59700100
C 1.168359 5.282111 0.91699300
C 3.605057 5.598549 -0.38784200
H 3.198822 3.695588 -1.29215700
C 1.925910 6.431046 1.12568300
H 0.225560 5.158724 1.43798000
C 3.150202 6.594742 0.47658500
H 4.547630 5.721008 -0.90992900
H 1.562498 7.197661 1.80119500
H 3.740313 7.489420 0.63893600
C 3.923346 -2.827725 0.23274300
C 5.022371 -2.306362 -0.46901600
C 4.156092 -3.843061 1.17439700
C 6.310914 -2.775986 -0.22748500
H 4.859890 -1.543383 -1.22111200
C 5.445026 -4.309770 1.41784900
H 3.320129 -4.254014 1.72908000
C 6.528549 -3.777261 0.71891800
H 7.144840 -2.364464 -0.78500900
H 5.603934 -5.087127 2.15687200
H 7.531994 -4.141455 0.90738800
C 2.179753 -0.997297 -0.05417300
C 0.829331 -0.670537 -0.36487400
C 0.392781 0.674961 -0.41425100

C 2.626045 1.385828 0.25727500
C 3.049949 0.092185 0.29002400
H 3.307282 2.170171 0.55945100
H 4.059277 -0.125921 0.61320000
O -3.051881 -1.679905 -2.27890300
H -3.843195 -2.121156 -1.96088300
H -4.885249 -0.312235 -1.01287500

Int-C1-S

PBE SCF Energy: -854.464955465 a.u.
C 1.644842 0.290525 -0.00001800
C 3.025505 0.477429 0.00027700
C 3.856891 -0.638564 0.00025900
C 3.290701 -1.909806 -0.00004700
C 1.904537 -2.018280 -0.00031800
C 0.649096 1.384864 0.00000400
C 0.958852 2.742423 -0.00010000
C -0.073188 3.675442 -0.00013700
C -1.392166 3.231311 -0.00005800
C -1.635944 1.864370 0.00005800
H 3.450134 1.471453 0.00054800
H 4.932568 -0.513949 0.00049200
H 3.903623 -2.801332 -0.00006400
H 1.408639 -2.981165 -0.00056700
H 1.988391 3.071964 -0.00017100
H 0.152569 4.734420 -0.00022700
H -2.222320 3.924914 -0.00010500
H -2.636692 1.452835 0.00015500
N 1.101524 -0.948958 -0.00031300
N -0.640927 0.963008 0.00008700
Ni -0.913121 -0.904434 0.00001400
C -2.638817 -1.418258 0.00014600
O -1.948141 -2.506910 -0.00000700
O -3.823802 -1.145848 0.00009900

Int-C1-T

PBE SCF Energy: -854.423884183 a.u.
C 0.696126 1.352339 0.03090800
C 1.057146 2.687501 0.22035200
C 0.071870 3.667063 0.17204200
C -1.251588 3.296546 -0.06219000
C -1.539897 1.949726 -0.23277000
C 1.645933 0.217159 0.04820800
C 3.013493 0.349105 0.29049200
C 3.820151 -0.782458 0.27758000
C 3.243758 -2.026481 0.02799900
C 1.875984 -2.088506 -0.19446200
H 2.086811 2.963731 0.39863600
H 0.335027 4.707860 0.31437100
H -2.043973 4.031664 -0.10942000
H -2.545691 1.587507 -0.40825600
H 3.446981 1.319640 0.48657400
H 4.883603 -0.693799 0.46118900
H 3.836932 -2.930929 0.00657100
H 1.373253 -3.028528 -0.38426800
N -0.592004 1.006221 -0.18678300
N 1.093135 -0.998827 -0.18856600
Ni -0.906417 -0.981501 -0.37821300
C -2.605205 -1.452027 0.49344200
O -2.942902 -1.163610 -0.71399900
O -3.265574 -1.779726 1.46679800

Int-C2-S

PBE SCF Energy: -854.398241635 a.u.
C 1.775259 0.262807 -0.05326000
C 3.157185 0.483535 -0.01773100
C 4.027698 -0.592767 0.01592200
C 3.490972 -1.892036 0.03346200
C 2.122642 -2.053298 -0.04561500
C 0.768122 1.306513 0.03628400
C 0.955707 2.621165 -0.40847400
C -0.089692 3.527846 -0.34265800
C -1.327244 3.089318 0.16235300
C -1.454053 1.779208 0.57644500
H 3.533723 1.497794 0.02699900
H 5.098501 -0.435267 0.05240600
H 4.131659 -2.763902 0.07290800
H 1.670830 -3.035768 -0.09433400
H 1.909175 2.912757 -0.83189600
H 0.039070 4.545893 -0.68883000
H -2.168585 3.766036 0.24964900
H -2.389899 1.413133 0.98548600
N 1.255326 -1.011377 -0.13016700
N -0.442497 0.874530 0.53897400
Ni -0.611143 -1.058992 0.05485800
C -3.681768 -1.285573 -0.17708600
O -4.823452 -1.133756 -0.29151800

O -2.535451 -1.462656 -0.06447100

Int-C2-T

PBE SCF Energy: -854.405292934 a.u.

C -1.797704 -0.016187 0.05033200
C -3.209983 -0.097083 0.17785600
C -3.843455 -1.315851 0.19106500
C -3.073301 -2.503409 0.07563200
C -1.705461 -2.376796 -0.04510600
C -1.047565 1.201524 0.02680000
C -1.604501 2.504814 0.12778600
C -0.793873 3.613833 0.09563000
C 0.609548 3.451013 -0.04047800
C 1.101629 2.164961 -0.13446500
H -3.791628 0.811865 0.26567600
H -4.921763 -1.368949 0.28874400
H -3.533449 -3.482714 0.08104300
H -1.070449 -3.251987 -0.13552500
H -2.675497 2.625017 0.23093100
H -1.224925 4.605511 0.17367000
H 1.280762 4.299226 -0.07035800
H 2.166204 1.979814 -0.23939500
N -1.057571 -1.193854 -0.06029300
N 0.330453 1.062545 -0.10496200
Ni 0.839752 -0.838349 -0.20619700
C 3.979661 -0.984943 0.15263600
O 2.948078 -0.785836 -0.35419800
O 5.009117 -1.173678 0.63787100

Int-D1-S

PBE SCF Energy: -953.538523747 a.u.

C -2.684553 -2.205306 0.11425000
C -2.560592 0.139780 0.04078600
C -3.960268 0.222101 0.12942600
C -4.719130 -0.929509 0.19884000
C -4.060731 -2.178334 0.15259900
H -4.437569 1.193994 0.09591000
H -5.799398 -0.876371 0.25748200
H -4.615696 -3.107493 0.18357600
C -1.668865 1.252006 -0.16444000
C -1.935196 2.576233 0.22305900
C -0.977720 3.556717 0.04849300
H -2.884701 2.813770 0.68851500
C 0.489299 1.872717 -0.84182300
C 0.271963 3.188110 -0.50135800
H -1.171321 4.579626 0.34738200
H 1.046066 3.925508 -0.67678100
N -1.914384 -1.084301 0.11494900
N -0.442975 0.890158 -0.71017500
Ni -0.059724 -0.965025 -0.14509600
N 4.017574 -0.562946 -0.00295700
C 4.383718 -1.467464 -1.09274800
H 5.103549 -2.207232 -0.73165200
H 3.497070 -1.974302 -1.46004500
H 4.842196 -0.899390 -1.90631300
C 5.130774 0.135752 0.63853900
H 4.805237 1.070486 1.08780100
H 5.600687 -0.489587 1.40414400
H 5.875597 0.370549 -0.12270300
C 2.745302 -0.474659 0.42368900
C 2.418542 0.404240 1.60408400
H 2.430001 1.457580 1.30958200
H 1.409411 0.155492 1.93069200
H 3.119007 0.268111 2.42876200
O 1.836997 -1.115967 -0.16246000
H 1.436171 1.552862 -1.26424600
H -2.136795 -3.139830 0.13717500

Int-D1-T

PBE SCF Energy: -953.546225931 a.u.

C -2.239958 -2.502874 0.06081500
C -2.611983 -0.171116 0.04136600
C -4.002571 -0.410846 0.20474800
C -4.486524 -1.693493 0.29156300
C -3.581377 -2.785510 0.21720600
H -4.686093 0.427227 0.26127300
H -5.549113 -1.869028 0.41569500
H -3.920372 -3.811228 0.28065900
C -2.008194 1.119093 -0.06376100
C -2.706875 2.356525 -0.03222500
C -2.025159 3.543396 -0.15403000
H -3.783224 2.363442 0.08662300
C 0.014528 2.296644 -0.33633300
C -0.614618 3.525989 -0.31462100
H -2.562160 4.485018 -0.12959900
H -0.041991 4.438548 -0.41701900
N -1.735919 -1.254963 -0.02738200
N -0.625680 1.120901 -0.21385700

Ni 0.119642 -0.730436 -0.21410200
N 4.273062 -0.439205 -0.03910400
C 4.619770 -1.173340 -1.25705700
H 5.107522 -2.116913 -0.99712800
H 3.722011 -1.375346 -1.83221000
H 5.311037 -0.573251 -1.85334600
C 5.417175 0.065653 0.71785700
H 5.120204 0.442867 1.69081800
H 6.131362 -0.747188 0.86839500
H 5.912460 0.866396 0.16122600
C 2.992135 -0.255068 0.31101400
C 2.668490 0.542062 1.55284100
H 3.123997 1.533529 1.52376400
H 1.587107 0.644460 1.61741000
H 3.027900 0.027133 2.44688400
O 2.071929 -0.742129 -0.39333600
H 1.091281 2.224360 -0.45641500
H -1.506588 -3.300597 0.00061700

Int-S1-S-F

PBE SCF Energy: -1328.81453293 a.u.
C -1.82231600 1.313453 -0.69489300
C 0.40027300 0.829937 -0.28394400
C 0.68247100 2.181136 -0.11499000
C -0.32338500 3.147738 -0.23849100
C -1.60451200 2.676331 -0.53813400
H 1.69099900 2.48771400 0.12231600
H -2.44514500 3.345736 -0.64949600
C 1.40276400 -0.253899 -0.15101800
C 2.74786300 -0.0135510 0.09030900
C 3.64914200 -1.0763820 0.21742500
H 3.09814900 1.0042880 0.17840200
C 1.75262700 -2.5511950 -0.15705600
C 3.11485100 -2.3566100 0.09000000
H 3.74174300 -3.2318720 0.17828900
N -0.85123800 0.399704 -0.57457200
N 0.90351500 -1.512565 -0.28017700
Ni -1.06068700 -1.551713 -0.70345000
C -5.74825100 -0.1904410 0.45256600
C -4.86055400 -0.726631 -0.47766900
C -3.83831100 -1.620859 -0.09846500
C -3.76553100 -1.9610810 1.26973700
C -4.65496200 -1.4297470 2.19783500
C -5.65355400 -0.535941 1.80076900
H -6.51998800 0.4972090 0.12160200
H -4.95262400 -0.45027 -1.52408000
H -2.98765600 -2.6375290 1.60495100
H -4.56727600 -1.7116370 3.24237700
H -6.34310000 -0.1211180 2.52722300
C -2.88070100 -2.115043 -1.10208100
C -1.97515400 -3.227228 -0.90882500
H -3.17744300 -1.881733 -2.12716200
H -1.70888500 -3.815784 -1.78874300
H -2.06233900 -3.847380 -0.01424700
C 0.00714200 4.630990 -0.04032200
C -1.23242600 5.5272150 -0.20485200
H -0.94737000 6.5710670 -0.05408100
H -1.66358100 5.4423600 -1.20585700
H -2.00682100 5.2849230 0.52772100
C 1.06375700 5.0564470 -1.08592000
H 1.30937200 6.1139300 -0.95526600
H 1.98833700 4.4835790 -0.98626700
H 0.6836420 4.91620500 -2.10134300
C 0.5757310 4.83558200 1.38309900
H 0.81035200 5.8919870 1.53942800
H -0.15205700 4.5305140 2.13968500
H 1.491913 4.26255700 1.54261100
C 5.133199 -0.80139400 0.48213600
C 5.70459200 0.0389610 -0.68333500
H 5.19153200 0.9979470 -0.78424800
H 6.76436700 0.2433730 -0.50795800
H 5.61163400 -0.4982480 -1.63096700
C 5.95376400 -2.0973480.0.59798100
H 7.00029300 -1.8468980 0.78674500
H 5.60755600 -2.7236520 1.42443900
H 5.91357400 -2.6852990 -0.32273100
C 5.27134400 -0.0132430 1.80524100
H 4.75045300 0.945808 1.76468800
H 4.86436800 -0.5860530 2.64280100
H 6.32676600 0.18784400 2.00847300
H -2.80889800 0.924310 -0.91124400
C 1.19022900 -3.9359920 -0.2928170
H 0.38523500 -4.0862640 0.42863000
H 0.74356300 -4.0655470 -1.2805490
H 1.96207700 -4.6912990 -0.1420250

Int-S1-S

PBE SCF Energy: -975.351310966 a.u.

C -0.459842 2.081667 -0.58975700
C 1.684628 1.427896 0.02546500
C 2.056612 2.754107 0.24209500
C 1.124948 3.764361 0.02729700
C -0.157730 3.423614 -0.39390900
H 3.054790 2.999946 0.57730000
H 1.397129 4.799732 0.19096400
H -0.914239 4.177838 -0.56738800
C 2.576176 0.265013 0.23318200
C 3.911559 0.359145 0.62289100
C 4.653522 -0.804416 0.79597100
H 4.370680 1.324024 0.78801100
C 2.709252 -2.055288 0.18228200
C 4.042152 -2.035304 0.57326800
H 5.691708 -0.748653 1.09894100
H 4.581974 -2.964987 0.69743600
N 0.435603 1.102991 -0.39197900
N 1.985897 -0.937662 0.01356100
Ni 0.113081 -0.840720 -0.60143100
H 2.185038 -2.982584 -0.00766500
H -1.444360 1.758815 -0.90397000
C -4.585719 0.683634 0.07643300
C -3.618417 0.133807 -0.76132900
C -2.710075 -0.843827 -0.30441700
C -2.835583 -1.250650 1.04124100
C -3.804451 -0.704236 1.87676900
C -4.687674 0.270770 1.40538700
H -5.265743 1.435079 -0.31196500
H -3.556889 0.463542 -1.79444900
H -2.154234 -1.996106 1.43476900
H -3.871155 -1.040044 2.90678600
H -5.440146 0.696079 2.05971000
C -1.664751 -1.354190 -1.20752000
C -0.808961 -2.491334 -0.93860700
H -1.839288 -1.095267 -2.25400800
H -0.464418 -3.070505 -1.79728400
H -1.001498 -3.122667 -0.06865600

Int-S1-T

PBE SCF Energy: -975.322463311 a.u.

C -2.639852 -2.013592 0.08160500
C -2.279874 0.301547 0.35874500
C -3.468183 0.382234 1.12385300
C -4.225091 -0.742431 1.35449900
C -3.802021 -1.986464 0.81862400
H -3.778962 1.334968 1.53317300
H -5.133775 -0.678603 1.94145000
H -4.368570 -2.894364 0.97853800
C -1.418255 1.406502 0.05288800
C -1.655009 2.749496 0.43343200
C -0.763154 3.737122 0.08465500
H -2.544005 2.999813 0.99808800
C 0.567072 2.075658 -1.01694800
C 0.390948 3.395796 -0.66283200
H -0.944729 4.764991 0.37614600
H 1.119816 4.140965 -0.95340000
N -1.881623 -0.921409 -0.16231300
N -0.288552 1.089613 -0.68445800
Ni -0.180801 -0.857861 -1.13777100
H 1.431993 1.766233 -1.59057400
H -2.271057 -2.937749 -0.35071600
C 1.447875 -1.231190 -2.34939500
C 1.671431 -1.740467 -1.07301000
H 1.131071 -1.900473 -3.14359500
H 1.432937 -2.789614 -0.89579400
C 2.434123 -1.092374 0.01061100
C 3.275962 0.010053 -0.20884400
C 2.313766 -1.583768 1.32265300
C 3.943637 0.618852 0.84961900
H 3.418459 0.387242 -1.21418000
C 2.982497 -0.976696 2.37987400
H 1.671339 -2.438312 1.50825300
C 3.796586 0.134240 2.14987900
H 4.585918 1.471217 0.65798400
H 2.868167 -1.367894 3.38470200
H 4.316939 0.610447 2.97288300
H 1.883358 -0.293294 -2.67741300

Int-SA1-S

PBE SCF Energy: -1240.22809588 a.u.

C -0.531378 1.604750 1.20531600
C 1.415707 0.355167 1.44311700
C 1.868181 1.203612 2.45204100
C 1.082379 2.286260 2.83234000
C -0.141536 2.491020 2.20113100
H 2.817630 1.027136 2.93799900
H 1.420939 2.956473 3.61277300
H -0.785037 3.318465 2.46993500

C 2.155539 -0.830634 0.95637500
C 3.417974 -1.205914 1.41236700
C 4.022795 -2.340782 0.88272400
H 3.928596 -0.621857 2.16524800
C 2.094537 -2.642323 -0.49816900
C 3.350217 -3.075131 -0.08971400
H 5.004570 -2.644216 1.22471400
H 3.784063 -3.964492 -0.52770700
N 0.226617 0.564953 0.82825900
N 1.506375 -1.548726 0.00739800
Ni -0.218954 -0.761268 -0.59366700
H 1.527639 -3.171544 -1.25288300
H -1.473939 1.710362 0.68319800
O 0.586881 1.966647 -2.05522000
C -4.803754 0.852637 0.39560100
C -5.183764 -0.258823 1.14900400
C -4.485773 -1.457372 0.98248500
C -3.424741 -1.543567 0.08631500
C -3.020624 -0.431071 -0.68074000
C -3.744207 0.765787 -0.50386000
H -5.337230 1.791147 0.50602300
H -6.008928 -0.194601 1.84910700
H -4.770369 -2.332456 1.55788200
H -2.890654 -2.481112 -0.01580400
H -3.463006 1.638893 -1.08538600
C -1.866180 -0.459170 -1.59788900
C -1.159102 -1.649958 -2.01444400
H -1.833009 0.403615 -2.26548600
H 0.359207 1.091983 -1.65824900
H -1.552717 -2.636422 -1.76149800
H -0.685948 -1.631450 -2.99692600
C 1.873842 2.216630 -1.82896200
O 2.661693 1.488189 -1.27252800
O 2.167744 3.428452 -2.32500200
H 3.106731 3.588983 -2.15807500

Int-SA2-S

PBE SCF Energy: -1240.22781848 a.u.

C -1.060041 1.976464 -0.94201000
C 0.945616 1.872208 0.22848000
C 1.184800 3.225179 -0.00706000
C 0.259174 3.960587 -0.74017900
C -0.886686 3.328329 -1.21407800
H 2.075835 3.704275 0.37403800
H 0.430453 5.012439 -0.93307800
H -1.634520 3.865220 -1.78295400
C 1.845197 0.990583 1.00636800
C 3.047591 1.405251 1.57586700
C 3.811222 0.491968 2.29475800
H 3.390638 2.423725 1.45942200
C 2.146606 -1.160699 1.83583700
C 3.352606 -0.815275 2.43176100
H 4.749563 0.798356 2.74022800
H 3.914280 -1.557083 2.98412900
N -0.166998 1.261240 -0.24483500
N 1.407652 -0.286049 1.13733500
Ni -0.263330 -0.696782 0.14401000
H 1.745544 -2.163627 1.89889200
H -1.935603 1.434926 -1.27802900
O 2.126206 -2.169448 -1.40411500
C -5.081501 0.173889 -0.70617000
C -5.461413 0.162099 0.63634200
C -4.634575 -0.474181 1.56563200
C -3.448838 -1.081152 1.16405900
C -3.042345 -1.075569 -0.18701900
C -3.896236 -0.436481 -1.10908800
H -5.712868 0.657296 -1.44463200
H -6.383697 0.635680 0.95298900
H -4.916229 -0.495246 2.61354500
H -2.817529 -1.556516 1.90583100
H -3.617368 -0.422294 -2.15864100
C -1.766123 -1.651719 -0.64650200
C -0.904513 -2.511088 0.13685200
H -1.696414 -1.732948 -1.73275400
H 1.338215 -1.747876 -0.98479800
H -1.239896 -2.875361 1.11006200
H -0.327838 -3.265363 -0.40024100
C 2.918344 -1.216950 -1.88807100
O 2.704916 -0.027299 -1.87706100
O 4.016088 -1.793860 -2.40182300
H 4.575122 -1.087850 -2.75447300

Int-SA3-S

PBE SCF Energy: -1240.23988759 a.u.

C 1.322337 1.654778 -1.12112500
C -0.798920 2.185954 -0.35303200
C -0.615117 3.521539 -0.70159200
C 0.583676 3.923085 -1.27797300

C 1.569333 2.969112 -1.49410800
H -1.402379 4.241798 -0.53188000
H 0.738377 4.958555 -1.55393400
H 2.520371 3.224277 -1.94211700
C -2.042412 1.667815 0.24424100
C -3.137918 2.451331 0.60433700
C -4.251241 1.834514 1.16451300
H -3.127656 3.522082 0.45853900
C -3.111064 -0.259301 0.97397200
C -4.239802 0.456200 1.35460600
H -5.112523 2.425053 1.45110100
H -5.084032 -0.061063 1.79070000
N 0.173807 1.254252 -0.55729400
N -2.041760 0.331266 0.42780100
Ni -0.316266 -0.575431 -0.09013100
H -3.032551 -1.329580 1.10376100
H 2.073379 0.897962 -1.26103000
O -1.754628 -2.722419 -1.80561500
C 3.499147 -0.108816 2.42233000
C 4.692368 0.249825 1.78631200
C 4.824932 0.021584 0.41966800
C 3.779097 -0.551607 -0.30819300
C 2.566511 -0.904892 0.30744100
C 2.460718 -0.674834 1.69412800
H 3.381309 0.058378 3.48788400
H 5.502867 0.696556 2.35107100
H 5.746677 0.286791 -0.08768800
H 3.914474 -0.724551 -1.36977600
H 1.531306 -0.937891 2.19041000
C 1.406558 -1.503310 -0.42563500
C 1.589668 -1.768556 -1.91829500
H 1.166045 -2.447257 0.07048600
H 1.740642 -0.850366 -2.49531400
H 2.449015 -2.422735 -2.12460200
H 0.693578 -2.253455 -2.30867500
C -1.650693 -2.975563 -0.61282200
O -1.094621 -2.280204 0.31809200
O -2.203168 -4.148485 -0.15562000
H -2.031496 -4.195409 0.79368100

Int-SA4-S

PBE SCF Energy: -1240.23946681 a.u.

C -1.048252 2.216325 0.05481500
C -2.897193 1.049141 0.83717900
C -3.522692 2.221524 1.24330000
C -2.869404 3.432366 1.03395500
C -1.614609 3.432566 0.43434300
C 0.276614 2.065028 -0.57435100
C 1.812699 0.578156 -1.47168300
C 2.720937 1.596526 -1.72700500
C 2.381764 2.898520 -1.38419800
C 1.141829 3.131783 -0.80196900
H -3.341557 0.074079 0.98140200
H -4.497105 2.178948 1.71151300
H -3.327433 4.366373 1.33491800
H -1.093517 4.364670 0.26768200
H 2.054806 -0.443031 -1.70961100
H 3.674439 1.356740 -2.17758400
H 3.065864 3.718880 -1.56126800
H 0.854539 4.134850 -0.52125500
N -1.694330 1.048331 0.25177100
N 0.614964 0.787999 -0.90620900
Ni -0.684975 -0.572677 -0.39500600
C -2.907279 -2.307159 -0.40546200
O -2.019824 -1.720797 0.32164900
O -3.796199 -3.054848 0.33240800
O -3.058861 -2.272845 -1.61795800
H -3.533334 -2.978803 1.25861400
H 0.340289 -2.945075 1.04803900
C 0.298928 -2.153218 -0.95541100
C 1.057023 -2.763929 0.24076400
H -0.447551 -2.867532 -1.31693200
H 1.477668 -3.741123 -0.03436100
H 0.988533 -1.965691 -1.78709700
C 2.172788 -1.872666 0.73895800
C 3.465588 -1.979069 0.21479400
C 1.917911 -0.853101 1.66466500
C 4.468893 -1.083439 0.58580100
H 3.683654 -2.763163 -0.50399100
C 2.914655 0.044369 2.04044400
H 0.917234 -0.749684 2.07250300
C 4.195226 -0.063864 1.49677200
H 5.462330 -1.179986 0.16122700
H 2.690956 0.832019 2.75181000
H 4.971558 0.636944 1.78256800

Int-SA6-D

PBE SCF Energy: -975.919931894 a.u.

C -0.383751 2.045923 0.48112200
C 1.780202 1.361443 -0.00973700
C 2.210319 2.686165 -0.09775700
C 1.293739 3.710364 0.11430800
C -0.028812 3.387613 0.40768800
H 3.240085 2.920684 -0.32922300
H 1.609085 4.744459 0.04896300
H -0.773523 4.154713 0.57564500
C 2.651962 0.185081 -0.22389400
C 4.008299 0.263319 -0.54021500
C 4.732206 -0.908108 -0.73174700
H 4.497042 1.222776 -0.63795400
C 2.731377 -2.136109 -0.27976200
C 4.081778 -2.133020 -0.60166600
H 5.785619 -0.863973 -0.97882900
H 4.605590 -3.069196 -0.74393200
N 0.495454 1.055511 0.28111800
N 2.024785 -1.009905 -0.09215200
Ni 0.098192 -0.943679 0.42245600
H 2.180238 -3.060934 -0.16142800
H -1.398071 1.734134 0.69648500
C -3.715847 -0.679211 -2.09333400
C -4.465379 0.429907 -1.67873300
C -4.340651 0.858047 -0.35920300
C -3.484013 0.204830 0.52955700
C -2.694171 -0.896358 0.12873300
C -2.857071 -1.321905 -1.21349500
H -3.805418 -1.040923 -3.11332400
H -5.132500 0.936385 -2.36709600
H -4.921196 1.706517 -0.00903400
H -3.424817 0.560604 1.55181200
H -2.272119 -2.170633 -1.55788700
C -1.726767 -1.568841 1.02368100
C -1.940366 -1.348135 2.52529500
H -1.736951 -2.646864 0.80566500
H -1.735468 -0.314483 2.82417600
H -2.968086 -1.576763 2.85655400
H -1.258884 -1.978774 3.10279600

Int-SA6-Q

PBE SCF Energy: -975.897811942 a.u.

C 2.652207 -1.195077 -0.17522400
C 1.637911 0.893831 0.27167900
C 2.647249 1.158201 1.23390500
C 3.632387 0.233432 1.48074300
C 3.641736 -0.991322 0.76111000
H 2.636033 2.092962 1.77957800
H 4.397589 0.438214 2.22047300
H 4.397262 -1.746142 0.93314900
C 0.556336 1.771576 -0.04968100
C 0.321096 3.035550 0.55190400
C -0.769947 3.785986 0.18648400
H 1.001240 3.405077 1.30849800
C -1.382469 2.069534 -1.36914400
C -1.662857 3.293232 -0.80171600
H -0.949046 4.747606 0.65338300
H -2.538661 3.850951 -1.10518300
N 1.677024 -0.302917 -0.43244100
N -0.317048 1.321161 -1.03007000
Ni 0.161946 -0.490992 -1.70983400
H -2.027224 1.639776 -2.12852200
H 2.611185 -2.108158 -0.75956400
C -2.985960 -0.276516 1.68660200
C -2.255299 -0.697495 2.80080800
C -1.176173 -1.560662 2.61059400
C -0.827748 -1.992039 1.33224800
C -1.543056 -1.570601 0.19423400
C -2.637016 -0.708575 0.41234800
H -3.831220 0.392320 1.81344100
H -2.523880 -0.360796 3.79581400
H -0.597235 -1.899341 3.46396600
H 0.027923 -2.646069 1.21384800
H -3.204639 -0.359100 -0.44454700
C -1.138634 -1.939599 -1.18444900
C -0.472151 -3.306760 -1.36293400
H -1.995675 -1.843157 -1.86258600
H -0.286054 -3.507400 -2.42137700
H 0.494218 -3.366452 -0.85413800
H -1.091816 -4.126394 -0.97037000

Int-SA6-S

PBE SCF Energy: -976.009691361 a.u.

C -0.329435 2.034831 -0.37839700
C 1.877519 1.183080 -0.33716300
C 2.373404 2.507073 -0.28294700
C 1.518031 3.582875 -0.31416400
C 0.114900 3.331971 -0.36870000
H 3.442575 2.663358 -0.18691200

H 1.898255 4.596933 -0.27291900
H -0.598501 4.145973 -0.42536300
C 2.670977 0.008368 -0.25692000
C 4.055095 -0.091264 -0.54365700
C 4.672589 -1.319025 -0.56478600
H 4.611051 0.805435 -0.79312500
C 2.572043 -2.332014 0.02061400
C 3.895165 -2.486836 -0.31926600
H 5.728388 -1.400903 -0.79659900
H 4.336149 -3.475207 -0.35488400
N 0.486027 0.939329 -0.38351000
N 1.957380 -1.126930 0.13641200
Ni 0.115979 -0.694746 0.55169200
H 1.954290 -3.187688 0.27690000
H -1.387416 1.806809 -0.41557200
C -3.912157 -1.776499 -1.29897600
C -4.699468 -0.652288 -1.58123000
C -4.500686 0.504553 -0.83150800
C -3.534526 0.548412 0.17641600
C -2.708755 -0.560917 0.46254600
C -2.946011 -1.728853 -0.30414100
H -4.057468 -2.693573 -1.86194300
H -5.452225 -0.685866 -2.36094100
H -5.108871 1.383700 -1.02313900
H -3.422488 1.460243 0.75154900
H -2.336101 -2.605817 -0.10372400
C -1.628601 -0.539237 1.47292100
C -1.695781 0.586284 2.50322200
H -1.620500 -1.512949 1.99371600
H -1.481087 1.561603 2.05195500
H -2.678410 0.671440 2.99756400
H -0.944724 0.429522 3.28255400

Int-SA6-T

PBE SCF Energy: -976.018596771 a.u.

C -3.034353 -1.880410 0.23278400
C -2.634356 0.429430 0.00821800
C -4.037748 0.656557 0.00750300
C -4.915224 -0.394505 0.12001800
C -4.406085 -1.715773 0.23812100
H -4.416578 1.667532 -0.08149100
H -5.984861 -0.216125 0.11930400
H -5.061233 -2.572437 0.33014900
C -1.636144 1.443379 -0.09777300
C -1.892981 2.836575 -0.22106500
C -0.851614 3.729047 -0.31078100
H -2.914770 3.195666 -0.24319600
C 0.675850 1.882434 -0.15821000
C 0.482429 3.246935 -0.27784200
H -1.050270 4.791181 -0.40478500
H 1.331412 3.915446 -0.34363500
N -2.148800 -0.872258 0.12280800
N -0.323254 0.985667 -0.07128200
Ni -0.165419 -1.024269 0.09308700
H 1.674513 1.462448 -0.12848300
H -2.593551 -2.869239 0.32062600
C 3.918009 0.529841 1.46555600
C 4.529899 1.033551 0.30991000
C 4.200755 0.456565 -0.91656000
C 3.275622 -0.583951 -0.99673400
C 2.613387 -1.084215 0.15021900
C 2.993965 -0.501920 1.38684900
H 4.166266 0.951534 2.43521700
H 5.247158 1.844369 0.36944900
H 4.670044 0.819793 -1.82646000
H 3.038779 -0.998246 -1.97004200
H 2.515917 -0.862344 2.29374600
C 1.564528 -2.116622 0.08777600
C 1.626253 -3.064031 -1.11775600
H 1.579397 -2.701096 1.01746300
H 0.888783 -3.864877 -1.01060500
H 1.396147 -2.557354 -2.06029300
H 2.615817 -3.537900 -1.24550100

Int-SAC3-D

PBE SCF Energy: -1164.42290811 a.u.

C 1.712117 1.394286 1.45996100
C -0.223889 2.065952 0.36477900
C 0.235135 3.380734 0.30153400
C 1.476280 3.691048 0.84889100
C 2.230782 2.683497 1.44059600
H -0.353936 4.150909 -0.17619100
H 1.849647 4.706701 0.80553000
H 3.202764 2.882678 1.87174500
C -1.522510 1.613099 -0.19046800
C -2.507806 2.476311 -0.66938800
C -3.701058 1.942321 -1.14472800
H -2.357691 3.546667 -0.66162200

C -2.864603 -0.235034 -0.62040100
C -3.888099 0.563640 -1.11692100
H -4.477367 2.597508 -1.52021500
H -4.807124 0.110973 -1.46507000
N 0.516541 1.093589 0.94112000
N -1.708503 0.275442 -0.18335000
Ni -0.140770 -0.818219 0.55472300
H -2.954907 -1.309690 -0.54236700
H 2.262849 0.566640 1.88804200
C 0.312754 -2.469181 -0.50046100
C -1.036974 -2.079743 1.73551300
O -0.219394 -2.060191 2.65797600
O -2.142042 -2.527831 1.49468100
C 1.441694 -1.628141 -0.94637500
C 1.304681 -0.640169 -1.95270900
C 2.685859 -1.680938 -0.26657300
C 2.333161 0.255296 -2.23219400
H 0.372713 -0.563983 -2.49902900
C 3.706741 -0.785471 -0.55024000
H 2.822029 -2.428731 0.50794100
C 3.537089 0.197525 -1.53102200
H 2.188982 1.008350 -2.99962300
H 4.641744 -0.848680 -0.00376500
H 4.333056 0.900661 -1.74664200
H 0.658068 -3.305638 0.10870400
C -0.749025 -2.900596 -1.49414900
H -0.365198 -3.638325 -2.21224200
H -1.586864 -3.350291 -0.95771400
H -1.145954 -2.061274 -2.06925200

C -0.753090 1.644207 -0.54433900
C -0.655766 3.016901 -0.58305100
H 0.750859 4.679199 -0.51501200
H -1.550326 3.620677 -0.65777300
N 2.305182 -0.890963 -0.39625000
N 0.314200 0.822544 -0.44374200
Ni 0.327865 -1.210010 -0.39497200
H -1.714592 1.153370 -0.58122400
H 2.895378 -2.865723 -0.39677900
C -4.042537 0.090186 -1.83941300
C -4.633915 0.712420 -0.73567900
C -4.215146 0.349691 0.54348800
C -3.215801 -0.606965 0.72079600
C -2.586558 -1.224073 -0.37685800
C -3.044622 -0.860910 -1.66086000
H -4.361537 0.351155 -2.84332900
H -5.408285 1.458516 -0.87275900
H -4.665231 0.817146 1.41332500
H -2.902740 -0.854852 1.72781600
H -2.584030 -1.324076 -2.52872100
C -1.448815 -2.165836 -0.22329700
C -1.409957 -2.952882 1.09486300
H -1.460580 -2.869978 -1.06662500
H -0.632845 -3.721260 1.05702900
H -1.175151 -2.314069 1.95262200
H -2.364668 -3.451772 1.31679700
C -0.276146 0.756825 2.69255100
O 0.598554 -0.001951 2.78073600
O -1.152260 1.513056 2.62460000

Int-SAC3-Q

PBE SCF Energy: -1164.37561191 a.u.

C 3.260038 -1.843907 -0.37038900
C 2.671094 0.446195 -0.36229700
C 4.048705 0.783119 -0.30309400
C 5.004081 -0.202938 -0.27937000
C 4.607222 -1.566820 -0.31444600
H 4.346586 1.823380 -0.27614500
H 6.054857 0.058691 -0.23423700
H 5.331797 -2.369853 -0.29672100
C 1.590828 1.377452 -0.40043200
C 1.737267 2.788442 -0.41274200
C 0.634308 3.601704 -0.50258500
H 2.727137 3.222967 -0.35885500

Int-SAC4-D

PBE SCF Energy: -1164.44525279 a.u.

C -2.140986 -2.591414 -0.09972500
C -2.456561 -0.286401 -0.12403200
C -3.704529 -0.429143 0.48072300
C -4.169126 -1.700369 0.79905100
C -3.373399 -2.804078 0.50201700
H -4.307568 0.439211 0.70621600
H -5.135609 -1.825588 1.27110500
H -3.695166 -3.811476 0.73120600
C -1.860042 1.016962 -0.49347700
C -2.487199 2.250624 -0.31992100
C -1.817552 3.408090 -0.70275200
H -3.478829 2.314560 0.10613000

C 0.022159 2.043634 -1.38396800
C -0.538950 3.307045 -1.24379100
H -2.288493 4.375119 -0.57592900
H 0.017705 4.184297 -1.54637700
N -1.683262 -1.366299 -0.40652200
N -0.622026 0.928889 -1.02550800
Ni 0.100108 -0.949965 -1.09054700
H 1.017570 1.897897 -1.78449900
H -1.482502 -3.414727 -0.34612100
C 2.882618 -1.112845 0.51920500
C 3.011962 -0.793382 -0.99615400
O 1.929532 -0.905646 -1.69601600
O 4.101411 -0.461368 -1.46501600
C 1.954876 -0.112779 1.18668700
C 2.231891 1.258246 1.13412800
C 0.794166 -0.532769 1.84541500
C 1.362234 2.184520 1.70362400
H 3.119223 1.601204 0.61222800
C -0.077405 0.391051 2.42127000
H 0.561698 -1.591002 1.88778600
C 0.200179 1.753782 2.34552200
H 1.581363 3.244011 1.63275300
H -0.982978 0.045412 2.90727700
H -0.485139 2.475703 2.77452900
H 2.397023 -2.093090 0.57166500
C 4.245879 -1.188359 1.21539500
H 4.123256 -1.458710 2.26772100
H 4.883091 -1.933195 0.73423000
H 4.760500 -0.227120 1.16254300

C -0.065118 2.038500 0.28564400
C 0.279103 3.325940 0.62726200
H 1.967856 4.647571 1.00293100
H -0.490203 4.067143 0.79684900
N 2.459671 -0.974107 -0.29135300
N 0.848149 1.069524 0.06891500
Ni 0.508818 -0.787715 -0.48838800
H -1.097835 1.737139 0.17342800
H 2.648334 -2.986460 -0.70460400
C -3.115391 1.701216 -1.71330800
C -3.656666 2.402878 -0.63793000
C -3.867281 1.746573 0.57651900
C -3.544864 0.398267 0.70987100
C -3.005524 -0.319001 -0.36628100
C -2.790496 0.350705 -1.57615500
H -2.939025 2.203928 -2.65748700
H -3.905138 3.452839 -0.74064200
H -4.278439 2.287537 1.42138200
H -3.698163 -0.106406 1.65723800
H -2.367631 -0.189364 -2.41659600
C -2.684006 -1.799959 -0.22287400
C -3.961874 -2.643614 -0.12027400
H -2.124407 -2.109887 -1.10976800
H -3.718111 -3.707107 -0.06135200
H -4.524339 -2.377348 0.77562900
H -4.595739 -2.478598 -0.99502600
C -1.757654 -2.015087 0.99465700
O -0.488231 -1.774716 0.82170700
O -2.222822 -2.386515 2.06682800

Int-SAC4-Q

PBE SCF Energy: -1164.40012499 a.u.
C 3.206392 -2.083137 -0.48425600
C 3.078947 0.235067 0.00575300
C 4.493988 0.280429 0.07533800
C 5.236204 -0.857563 -0.12573000
C 4.579005 -2.085809 -0.40857000
H 4.988524 1.218877 0.29026600
H 6.317542 -0.818533 -0.06872100
H 5.132337 -3.002045 -0.56395500
C 2.201800 1.343755 0.20990700
C 2.601253 2.663268 0.53928600
C 1.658411 3.641352 0.74591700
H 3.653832 2.895983 0.63542300

Int-SAC5-D

PBE SCF Energy: -1164.40453775 a.u.
C 0.539980 2.225274 0.04631000
C 2.581217 1.126412 -0.07725100
C 3.264081 2.340846 -0.15147600
C 2.539792 3.527807 -0.12465900
C 1.152713 3.471120 -0.02535200
H 4.341980 2.366474 -0.23036300
H 3.052904 4.479927 -0.18225600
H 0.549742 4.369584 -0.00387700
C 3.241402 -0.198125 -0.10733400
C 4.620589 -0.384452 -0.20483700
C 5.133167 -1.676624 -0.23232900
H 5.289401 0.463251 -0.25921800

C 2.893778 -2.494593 -0.06375200
C 4.254054 -2.754609 -0.16174900
H 6.201365 -1.837694 -0.30785400
H 4.609423 -3.776532 -0.18113700
N 1.232706 1.077809 0.02400900
N 2.391210 -1.250432 -0.03567200
Ni 0.449219 -0.815650 0.14234800
H 2.166875 -3.295400 -0.00407000
H -0.533962 2.127008 0.12361700
C -3.045995 1.834977 -1.27405000
C -3.380197 2.653578 -0.18839800
C -3.147052 2.173050 1.10024300
C -2.582197 0.914632 1.30584600
C -2.205276 0.083219 0.22635400
C -2.479187 0.584023 -1.07068600
H -3.228448 2.180137 -2.28723800
H -3.817369 3.632898 -0.34609100
H -3.407401 2.784344 1.95922500
H -2.409220 0.578967 2.32159300
H -2.211928 -0.028534 -1.92650600
C -1.525029 -1.214807 0.40922000
C -1.776576 -1.922758 1.74821500
H -1.799258 -1.882952 -0.41766600
H -1.323988 -1.393964 2.59269400
H -2.849328 -2.034003 1.97529400
H -1.334095 -2.922990 1.73682500
C -4.617384 -1.972392 -0.69799400
O -4.185383 -2.250150 -1.73897700
O -5.066307 -1.707778 0.33835200

Int-SC1-S

PBE SCF Energy: -1163.83950854 a.u.

C -1.189717 1.673142 0.14971000
C -1.249274 3.063727 0.23691900
C -0.246035 3.742224 0.92133500
C 0.787437 3.018355 1.50865600
C 0.781468 1.634681 1.38272100
C -2.203352 0.837627 -0.54134800
C -3.366792 1.343658 -1.12127400
C -4.255690 0.464331 -1.73049000
C -3.964178 -0.896513 -1.74520900
C -2.784725 -1.326610 -1.14836900
H -2.060161 3.613165 -0.22021000
H -0.275472 4.822260 0.99588400
H 1.583030 3.508890 2.05373300
H 1.547588 1.012149 1.82337700
H -3.583795 2.402346 -1.09657600
H -5.164487 0.839157 -2.18493000
H -4.630757 -1.612648 -2.20740600
H -2.503741 -2.371846 -1.12978100
N -0.174067 0.982178 0.71317100
N -1.926690 -0.484210 -0.56417100
Ni -0.141314 -0.971363 0.29079000
C 1.613494 -1.863325 0.28066100
H 1.961560 -2.090240 1.28473500
C 0.592215 -2.684505 -0.27614600
C -0.605763 -1.451166 2.19515000
O 0.217138 -1.037457 2.97902400
O -1.659012 -2.044722 2.11679300
H 0.499695 -2.814349 -1.35362800
C 2.509514 -0.974871 -0.48248800
C 3.544621 -0.298175 0.18987600
C 2.349982 -0.717575 -1.85831600
C 4.370500 0.604479 -0.47297600
H 3.692432 -0.484031 1.24894400
C 3.176366 0.185379 -2.52072000
H 1.562750 -1.218581 -2.40944600
C 4.190199 0.855794 -1.83391200
H 5.157506 1.113140 0.07341900
H 3.028590 0.367190 -3.57992100
H 4.831466 1.559485 -2.35215100
H 0.249256 -3.540217 0.29963600

Int-SC1-T

PBE SCF Energy: -1163.76855112 a.u.

C -0.850186 1.715576 -0.57949100
C -1.544055 2.838100 -0.12926000
C -0.828316 3.923696 0.36384500
C 0.562590 3.864295 0.39493400
C 1.185478 2.714964 -0.07581300
C -1.496333 0.482953 -1.08594100
C -2.874650 0.323215 -1.21651800
C -3.379972 -0.886427 -1.67844800
C -2.493868 -1.910774 -1.99906800
C -1.132969 -1.682375 -1.84904100
H -2.624360 2.866326 -0.14760100
H -1.351296 4.800999 0.72392000
H 1.155283 4.685624 0.77571100

H 2.263247 2.606508 -0.07280800
H -3.548862 1.126660 -0.95616300
H -4.448820 -1.026743 -1.78080900
H -2.843371 -2.870404 -2.35654600
H -0.402092 -2.448645 -2.06966900
N 0.499428 1.669113 -0.55076600
N -0.639260 -0.517073 -1.40507700
Ni 1.254174 -0.120516 -1.08284000
C -0.004305 -3.114186 1.01886700
H -0.741472 -3.911112 0.94504300
C 1.224787 -3.341018 0.54334100
H 1.483249 -4.300396 0.11034900
C 3.792297 -0.457095 0.15669000
O 3.182989 -0.189423 -0.92721300
O 4.968787 -0.471798 0.44583200
H 2.003466 -2.585185 0.55591900
C -0.503678 -1.865264 1.61487400
C -1.882103 -1.715835 1.82864300
C 0.339545 -0.791934 1.95237000
C -2.406767 -0.533065 2.34548800
H -2.550167 -2.529717 1.56687600
C -0.182784 0.384703 2.47545500
H 1.408396 -0.868633 1.78791000
C -1.558068 0.523107 2.67119400
H -3.477221 -0.435176 2.48688100
H 0.483759 1.205833 2.71373500
H -1.961851 1.448190 3.06599000

Int-SC2-S

PBE SCF Energy: -1163.84276081 a.u.

C 0.393128 0.990826 -1.39176400
C 0.940749 2.202073 -1.81565200
C 0.183757 3.363483 -1.71801100
C -1.103777 3.290328 -1.19577000
C -1.584323 2.052689 -0.78800400
C 1.124157 -0.297955 -1.43226300
C 2.385379 -0.456350 -2.00843400
C 2.984319 -1.710725 -1.99443300
C 2.309431 -2.780063 -1.41325100
C 1.058460 -2.545026 -0.85645800
H 1.948313 2.246473 -2.20393900
H 0.598260 4.311243 -2.03844600
H -1.725316 4.170355 -1.09618900
H -2.569506 1.939627 -0.35363400
H 2.895516 0.379777 -2.46507500
H 3.963508 -1.849864 -2.43564000
H 2.738059 -3.773117 -1.38648500
H 0.493391 -3.338391 -0.38286900
N -0.860568 0.929337 -0.88587700
N 0.482411 -1.339086 -0.85928400
Ni -1.316066 -0.818074 0.01272900
C -0.921996 -0.475063 1.95645900
C -1.244651 -1.827399 1.74024000
H -2.219726 -2.190569 2.04999300
C -3.162279 -0.627412 0.01919800
O -3.932320 0.017970 0.70584600
O -3.203069 -1.387541 -0.96802500
H -0.470064 -2.588090 1.70025100
C 0.433480 0.101182 2.05847500
C 0.571868 1.498954 2.10804300
C 1.603250 -0.675888 2.05586200
C 1.826689 2.098728 2.12747200
H -0.320398 2.115975 2.10616300
C 2.859249 -0.077451 2.07514600
H 1.532347 -1.756059 2.02715800
C 2.979531 1.312744 2.10532100
H 1.905775 3.179881 2.15354700
H 3.748164 -0.698535 2.06568300
H 3.959096 1.776789 2.11569600
H -1.715900 0.179319 2.30787100

Int-SC2-T

PBE SCF Energy: -1163.78255514 a.u.

C -0.715655 1.291993 -1.10069100
C -1.385193 2.516215 -1.12810500
C -0.678827 3.680366 -0.84689300
C 0.678525 3.597824 -0.54824400
C 1.277672 2.343969 -0.53944000
C -1.372639 -0.013106 -1.36492700
C -2.702246 -0.138005 -1.76984500
C -3.229045 -1.404202 -1.99569900
C -2.415833 -2.519561 -1.81913100
C -1.103789 -2.318459 -1.40937300
H -2.441477 2.566869 -1.35107000
H -1.184638 4.637984 -0.85731400
H 1.262317 4.480635 -0.32273700
H 2.326526 2.202491 -0.30889400
H -3.321459 0.736411 -1.91074900

H -4.260271 -1.515882 -2.30704900
H -2.784618 -3.522662 -1.98747700
H -0.431032 -3.150650 -1.24265100
N 0.599687 1.223184 -0.80801800
N -0.594891 -1.102876 -1.18347700
Ni 1.300759 -0.685087 -0.39203600
C 1.374111 -2.167093 1.18904700
H 0.646740 -2.939381 0.96451300
H 2.411386 -2.477993 1.23572300
C 1.003556 -0.947023 1.72246800
H 1.791302 -0.309596 2.11978900
C -0.366609 -0.479009 2.00370100
C -1.496366 -1.305415 1.88871900
C -0.565961 0.866950 2.35427600
C -2.775502 -0.796002 2.08431500
H -1.376824 -2.350499 1.63132700
C -1.844669 1.376800 2.55262600
H 0.294417 1.522055 2.44122500
C -2.958495 0.548412 2.41262400
H -3.633800 -1.450045 1.97870800
H -1.972802 2.422620 2.80816500
H -3.956823 0.943952 2.56017000
C 4.277488 -0.643667 0.10775200
O 3.301969 -0.142972 -0.52063400
O 5.469666 -0.407271 0.10897300

Int-SC3-S

PBE SCF Energy: -1163.83661212 a.u.

C 0.795769 2.346930 -0.65678600
C 2.648490 1.057218 -0.10050100
C 3.448377 2.195715 -0.00990000
C 2.884490 3.443033 -0.25702300
C 1.533156 3.522242 -0.58328500
H 4.493992 2.116533 0.25389700
H 1.053679 4.472927 -0.77713100
C 3.123254 -0.320672 0.15724500
C 4.440287 -0.651239 0.47356700
C 4.771089 -1.982106 0.70503400
H 5.200353 0.115052 0.53763100
C 2.485458 -2.552340 0.29012700
C 3.776242 -2.951798 0.61321800
H 3.989760 -3.998459 0.78657300
N 1.334769 1.140369 -0.42804200
N 2.157605 -1.270530 0.06589900
Ni 0.380691 -0.595927 -0.46597300
H 1.673994 -3.262671 0.20250700
C -3.525378 2.448874 0.22408000
C -2.839399 1.548851 -0.58708000
C -2.262606 0.371989 -0.06661700
C -2.425113 0.139270 1.31548500
C -3.115370 1.035936 2.12511800
C -3.669554 2.201442 1.58994100
H -3.954632 3.344538 -0.21339800
H -2.745306 1.751201 -1.64991500
H -1.996764 -0.753334 1.75549400
H -3.221448 0.824787 3.18445300
H -4.205115 2.898917 2.22390400
C -1.501159 -0.524886 -0.95258600
C -1.055781 -1.861660 -0.61361200
H -1.653024 -0.305433 -2.01126600
H -0.987327 -2.584410 -1.42877800
H -1.388318 -2.324473 0.31679500
C -4.421823 -2.083587 -0.42992700
O -4.676475 -1.528671 -1.41638800
O -4.189604 -2.650040 0.55586900
H -0.260479 2.350090 -0.89489000
H 3.491248 4.337593 -0.19049300
H 5.789483 -2.255364 0.95204200

Int-SC3-T

PBE SCF Energy: -1163.80767367 a.u.

C -2.667298 -2.490779 0.12763900
C -2.963040 -0.150576 0.08116200
C -4.254280 -0.314874 0.63689800
C -4.731472 -1.571176 0.92900700
C -3.915024 -2.702075 0.66876800
H -4.866587 0.554837 0.83808200
H -5.719775 -1.694632 1.35593000
H -4.252995 -3.706783 0.88594600
C -2.365724 1.107832 -0.26140100
C -3.002067 2.366568 -0.14061500
C -2.339855 3.516682 -0.50300300
H -4.015566 2.422745 0.23536200
C -0.449605 2.174827 -1.11098800
C -1.017887 3.425549 -1.00389400
H -2.827016 4.480243 -0.41013100
H -0.460528 4.305217 -1.29796800
N -2.178770 -1.266513 -0.17288000

N -1.073557 1.034481 -0.75619600
Ni -0.393101 -0.845325 -0.86645400
H 0.556129 2.054890 -1.49376700
H -2.001997 -3.319402 -0.09029400
C 1.464241 -0.867203 -1.75803300
C 1.577075 -1.183117 -0.40521200
H 1.476931 -1.665570 -2.49385200
H 1.588768 -2.238378 -0.13228000
C 1.956531 -0.267510 0.68620200
C 2.466728 1.021125 0.45637400
C 1.811801 -0.694549 2.01809500
C 2.791833 1.858912 1.51873600
H 2.628854 1.365317 -0.55694200
C 2.137437 0.142638 3.07933300
H 1.428021 -1.690568 2.21305200
C 2.624366 1.428377 2.83529100
H 3.183292 2.849860 1.31759100
H 2.012401 -0.206699 4.09816700
H 2.878485 2.082901 3.66098600
H 1.705324 0.118440 -2.14006700
C 4.802850 -0.964311 -1.01519000
O 4.788683 -0.063386 -1.74659600
O 4.823782 -1.866255 -0.28597900

Int-SC4-S

PBE SCF Energy: -1163.83661318 a.u.

C 0.796000 2.347056 -0.65661900
C 2.648606 1.057101 -0.10050700
C 3.448685 2.195483 -0.01014100
C 2.884954 3.442863 -0.25728400
C 1.533582 3.522257 -0.58333400
H 4.494334 2.116164 0.25348000
H 1.054229 4.473003 -0.77718900
C 3.123202 -0.320845 0.15725300
C 4.440167 -0.651558 0.47370400
C 4.770804 -1.982464 0.70517600
H 5.200312 0.114645 0.53786900
C 2.485151 -2.552444 0.29006000
C 3.775861 -2.952046 0.61326200
H 3.989248 -3.998733 0.78662500
N 1.334839 1.140432 -0.42782900
N 2.157457 -1.270597 0.06581400
Ni 0.380626 -0.595763 -0.46602500
H 1.673616 -3.262683 0.20236800
C -3.525171 2.449228 0.22429800
C -2.839217 1.549222 -0.58690500
C -2.262695 0.372178 -0.06654400
C -2.425440 0.139265 1.31549000
C -3.115647 1.035928 2.12516900
C -3.669553 2.201619 1.59010500
H -3.954219 3.345033 -0.21309600
H -2.744944 1.751718 -1.64969600
H -1.997335 -0.753496 1.75542000
H -3.221920 0.824618 3.18445300
H -4.205080 2.899086 2.22410400
C -1.501249 -0.524665 -0.95255000
C -1.055870 -1.861456 -0.61365600
H -1.653068 -0.305128 -2.01122200
H -0.987506 -2.584199 -1.42882400
H -1.388289 -2.324271 0.31679600
C -4.421722 -2.083670 -0.43000100
O -4.676434 -1.528664 -1.41640100
O -4.189364 -2.650514 0.55553900
H 3.491864 4.337335 -0.19094400
H 5.789145 -2.255833 0.95228200
H -0.260284 2.350360 -0.89455900

Int-SC4-T

PBE SCF Energy: -1163.80890897 a.u.

C -1.627579 2.536251 -0.77540200
C -2.968550 0.718993 -0.08842300
C -4.081199 1.587754 -0.00243900
C -3.946454 2.923445 -0.30315500
C -2.678440 3.420896 -0.70040000
H -5.043803 1.197932 0.30299800
H -2.530212 4.465554 -0.94039600
C -2.992236 -0.685418 0.20972000
C -4.129480 -1.410151 0.64026700
C -4.032686 -2.757985 0.90103900
H -5.077194 -0.902451 0.76644700
C -1.712882 -2.657703 0.30943300
C -2.787052 -3.410956 0.73344700
H -2.670683 -4.468782 0.92936100
N -1.736452 1.218341 -0.48882200
N -1.783890 -1.338597 0.04811900
Ni -0.320401 -0.123657 -0.56914100
H -0.736499 -3.108247 0.16327700
C 3.186381 1.404856 2.41504400

C 2.475269 0.337657 1.87690000
C 2.266492 0.228816 0.49040000
C 2.802064 1.232100 -0.33970800
C 3.510852 2.299774 0.20058300
C 3.707561 2.393943 1.57958900
H 3.335700 1.465235 3.48729000
H 2.072912 -0.427770 2.53203400
H 2.662245 1.177481 -1.41232100
H 3.914782 3.061021 -0.45753100
H 4.261898 3.226643 1.99669600
C 1.499463 -0.918821 -0.02792400
C 1.241289 -1.203731 -1.36616000
H 1.293057 -1.691066 0.70963600
H 0.896977 -2.192498 -1.64816500
H 1.677855 -0.617191 -2.16890700
C 4.611263 -1.646507 -0.89358600
O 4.623090 -1.138102 -1.93664800
O 4.605885 -2.159139 0.14709100
H -4.800013 3.587566 -0.23628600
H -4.902367 -3.313394 1.23212400
H -0.637285 2.862793 -1.07428700

Int-SC5-S

PBE SCF Energy: -1163.84990273 a.u.

C -1.440173 -1.833926 -0.24201900
C -1.568956 -3.216506 -0.34576400
C -0.519343 -3.964153 -0.86680400
C 0.628943 -3.303929 -1.28720800
C 0.697306 -1.924354 -1.14471900
C -2.521413 -0.942052 0.21879100
C -3.747944 -1.367126 0.72592800
C -4.689829 -0.411993 1.09474400
C -4.385124 0.938352 0.94929300
C -3.138155 1.289524 0.44572900
H -2.483238 -3.703822 -0.03808000
H -0.606115 -5.039875 -0.95423700
H 1.465656 -3.837502 -1.71778700
H 1.575409 -1.378881 -1.44885900
H -3.967813 -2.419611 0.83680200
H -5.648830 -0.721352 1.49149000
H -5.093453 1.709203 1.22242300
H -2.823123 2.316476 0.31478600
N -0.297128 -1.196548 -0.61669800
N -2.233018 0.370829 0.09022200
Ni -0.322426 0.754318 -0.42087800
C 1.598349 1.192319 -0.65571400
H 1.806758 1.103926 -1.73040700
C 1.719295 2.675239 -0.24508000
C 0.403767 3.404461 -0.44825500
O -0.630846 2.600218 -0.40167100
O 0.309316 4.617320 -0.59442100
H 1.928606 2.744842 0.82873300
C 2.545956 0.320866 0.11200800
C 3.651140 -0.290434 -0.50047300
C 2.356983 0.088309 1.48610900
C 4.522165 -1.109139 0.22021600
H 3.826547 -0.123483 -1.55906300
C 3.224180 -0.722313 2.21066800
H 1.499122 0.538526 1.97625600
C 4.312954 -1.330397 1.57978900
H 5.364918 -1.571749 -0.28245400
H 3.048040 -0.890071 3.26796000
H 4.985959 -1.967727 2.14218700
H 2.532125 3.203449 -0.75453700

Int-SC5-T

PBE SCF Energy: -1163.83098045 a.u.

C -1.378628 0.797638 -1.09747300
C -1.917774 2.046300 -1.40577300
C -1.091525 3.019085 -1.95892000
C 0.249985 2.727406 -2.19162300
C 0.717947 1.462981 -1.85842000
C -2.144051 -0.318802 -0.49518800
C -3.463833 -0.208602 -0.05647300
C -4.087331 -1.315870 0.50543300
C -3.379690 -2.510324 0.62245100
C -2.066282 -2.545351 0.17535800
H -2.960912 2.261413 -1.22228200
H -1.493365 3.994369 -2.20433200
H 0.922530 3.460767 -2.61608100
H 1.749164 1.165064 -1.99982400
H -3.995848 0.728541 -0.13869800
H -5.110674 -1.245167 0.85242800
H -3.829287 -3.394699 1.05387500
H -1.462137 -3.440461 0.25688900
N -0.078648 0.528187 -1.33331900
N -1.464239 -1.481783 -0.37213500
Ni 0.543625 -1.305997 -0.70440500

C 1.224217 -1.128706 1.24260300
H 0.679627 -1.876835 1.82406900
C 2.704699 -1.468547 1.08085100
H 2.836980 -2.546946 1.22710100
C 3.272499 -1.187766 -0.32249200
O 2.412732 -1.269183 -1.29833800
O 4.467677 -0.940458 -0.48085000
H 3.354560 -0.974750 1.81319600
C 0.868206 0.234237 1.65402200
C -0.396267 0.503387 2.22621600
C 1.713922 1.342721 1.42961800
C -0.799736 1.797362 2.53087400
H -1.070863 -0.326691 2.41249600
C 1.308283 2.638319 1.73788000
H 2.691478 1.187259 0.98669200
C 0.047572 2.881924 2.28571600
H -1.782882 1.963957 2.95973900
H 1.981140 3.467428 1.54259200
H -0.267343 3.892623 2.51922100

Int-SC6-S

PBE SCF Energy: -1163.84752177 a.u.

C -2.799275 -0.642748 0.47484900
C -3.837377 -1.320732 1.11083700
C -3.733907 -2.697525 1.28431700
C -2.601305 -3.361257 0.82180000
C -1.603061 -2.620173 0.20006400
C -2.770176 0.809696 0.21155900
C -3.812461 1.677756 0.52608100
C -3.698843 3.026479 0.20979700
C -2.543888 3.473359 -0.42151300
C -1.538692 2.557886 -0.70302500
H -4.710227 -0.792721 1.46785400
H -4.529952 -3.242587 1.77617800
H -2.486895 -4.430686 0.93875300
H -0.691436 -3.062470 -0.18049800
H -4.706077 1.306803 1.00750300
H -4.502197 3.712139 0.44803900
H -2.413048 4.511558 -0.69569400
H -0.625898 2.862621 -1.19195100
N -1.703835 -1.297230 0.03235100
N -1.633679 1.256231 -0.39172000
Ni -0.290911 -0.106116 -0.75934300
C 2.444274 0.237608 -1.32670100
C 1.129383 1.022123 -1.45558900
H 0.899804 1.193227 -2.51602900
C 2.107828 -1.261584 -1.44859500
O 2.925528 -2.106109 -1.78977300
O 0.871631 -1.538537 -1.11613200
H 1.199719 1.996459 -0.96135500
C 3.175104 0.423572 -0.00334100
C 4.555918 0.194285 0.06266900
C 2.505021 0.771792 1.17573800
C 5.248093 0.314537 1.26556500
H 5.087870 -0.086162 -0.83999900
C 3.194617 0.890881 2.38264300
H 1.435804 0.947944 1.14948000
C 4.569005 0.664153 2.43352000
H 6.317993 0.137912 1.29119900
H 2.655393 1.163540 3.28354900
H 5.105936 0.761157 3.37051900
H 3.152497 0.476033 -2.12717800

Int-SC6-T

PBE SCF Energy: -1163.81404116 a.u.

C 1.726413 1.395790 0.46684200
C 1.872023 2.777117 0.59256400
C 0.834770 3.516444 1.15286200
C -0.321286 2.865451 1.57464700
C -0.399360 1.488349 1.41326900
C 2.755820 0.494047 -0.10589200
C 3.952864 0.938279 -0.66758000
C 4.849364 0.005825 -1.17798200
C 4.530091 -1.348161 -1.12255100
C 3.315579 -1.717320 -0.55876900
H 2.776455 3.272089 0.26845900
H 0.932199 4.589714 1.25972700
H -1.148109 3.407815 2.01315700
H -1.269333 0.914264 1.70440600
H 4.184495 1.993109 -0.71320000
H 5.783428 0.334625 -1.61629000
H 5.201059 -2.104069 -1.50829400
H 3.007474 -2.753954 -0.49986000
N 0.597323 0.779686 0.87438500
N 2.453570 -0.823253 -0.06095100
Ni 0.537447 -1.238797 0.57827800
C -0.492028 -1.939944 -1.01054100
H -0.273596 -1.529109 -2.00007400

H -0.241934 -3.011443 -1.03831600
C -1.958856 -1.774366 -0.60273800
H -2.617426 -2.514331 -1.07661600
C -2.559511 -0.401934 -0.91081200
C -1.795546 0.663159 -1.39714300
C -3.928239 -0.183058 -0.68963800
C -2.374045 1.908846 -1.64856600
H -0.735645 0.526266 -1.56240800
C -4.509488 1.056632 -0.93993500
H -4.526614 -0.997344 -0.29756100
C -3.732408 2.113113 -1.42099600
H -1.755947 2.720559 -2.01726100
H -5.569592 1.200485 -0.75979600
H -4.182578 3.080290 -1.61563100
C -2.109199 -2.014586 0.92925500
O -1.068395 -1.716267 1.64581600
O -3.170460 -2.433704 1.39367800

Int-SC7-S

PBE SCF Energy: -1163.82023949 a.u.

C 0.121414 -2.109156 -1.15448100
C -1.976158 -1.501008 -0.34729100
C -2.488502 -2.756884 -0.65873800
C -1.654780 -3.708318 -1.23711600
C -0.328130 -3.379701 -1.49012100
H -3.523607 -2.992676 -0.45669700
H 0.356027 -4.087487 -1.93838700
C -2.763569 -0.409593 0.26137800
C -4.105115 -0.508870 0.61999000
C -4.738850 0.594263 1.18289400
H -4.651687 -1.428307 0.46594900
C -2.682145 1.797313 0.99406000
C -4.018311 1.768415 1.37335500
H -4.473863 2.648647 1.80650300
N -0.677465 -1.189350 -0.59681100
N -2.067749 0.736403 0.45273500
Ni -0.196831 0.597927 -0.10922300
H -2.079380 2.686434 1.12195900
C 4.263800 -1.867172 0.28724300
C 3.447598 -0.982817 -0.41551100
C 2.563760 -0.118802 0.25377300
C 2.537204 -0.169175 1.66063600
C 3.353184 -1.049130 2.36226500
C 4.220136 -1.906301 1.67971900
H 4.937741 -2.521923 -0.25413500
H 3.498753 -0.950998 -1.49922500
H 1.858508 0.479870 2.20296200
H 3.311603 -1.071235 3.44572000
H 4.854731 -2.592522 2.22859000
C 1.669229 0.764978 -0.51975200
C 1.299659 2.116919 -0.02338800
H 1.822575 0.718238 -1.59806000
H 0.157650 2.160533 0.25426000
H 1.768996 2.392304 0.91967400
C 1.391953 3.250664 -1.10562000
O 0.707162 3.057676 -2.13614700
O 2.154195 4.192690 -0.81791500
H 1.145892 -1.813663 -1.32194300
H -2.039525 -4.689495 -1.48508600
H -5.781774 0.534270 1.46740700

Int-SC7-T

PBE SCF Energy: -1163.79226546 a.u.

C -2.250400 -2.254042 -0.91142000
C -2.278496 -0.012795 -0.28025500
C -3.426427 -0.218308 0.48349600
C -3.987631 -1.489253 0.53623400
C -3.394172 -2.528852 -0.17381300
H -3.877124 0.593728 1.03539400
H -4.876973 -1.664270 1.12864800
H -3.800067 -3.531283 -0.15644200
C -1.586163 1.294223 -0.39591300
C -1.989174 2.447238 0.27558200
C -1.259500 3.619172 0.10954900
H -2.851994 2.437008 0.92573300
C 0.204916 2.431447 -1.35435900
C -0.143567 3.617237 -0.72130300
H -1.558444 4.521182 0.62865800
H 0.451131 4.507730 -0.87378400
N -1.712271 -1.031019 -0.96410800
N -0.498192 1.305191 -1.19734100
Ni 0.102318 -0.554095 -1.74810700
H 1.072778 2.363035 -1.99776800
H -1.734131 -3.023753 -1.47135700
C 2.835104 -0.402217 -0.98574800
C 1.558893 -1.049976 -0.45548500
H 3.051871 -0.818638 -1.97682900
H 1.635745 -2.141136 -0.50018900

C 1.068682 -0.618417 0.87466700
C 1.380703 0.638697 1.42820700
C 0.188060 -1.440030 1.60753500
C 0.810645 1.063474 2.62594900
H 2.081015 1.285613 0.91559200
C -0.379072 -1.018704 2.80434600
H -0.068679 -2.415818 1.20725700
C -0.078557 0.243993 3.32162000
H 1.064506 2.042523 3.01923900
H -1.061854 -1.674537 3.33448100
H -0.523878 0.578113 4.25190400
H 2.719420 0.677484 -1.11367800
C 4.095501 -0.662147 -0.09093500
O 4.768923 0.347560 0.23186900
O 4.314697 -1.860806 0.20970000

Int-SC8-S

PBE SCF Energy: -1163.80952671 a.u.

C -1.130968 2.563845 0.38686400
C -2.704277 0.946848 -0.18285000
C -3.688187 1.918638 -0.34182000
C -3.361756 3.253648 -0.12455000
C -2.063300 3.584471 0.24793100
H -4.694112 1.644936 -0.62658500
H -1.769956 4.609642 0.42931600
C -2.920421 -0.502744 -0.36707700
C -4.130247 -1.074949 -0.74819800
C -4.217974 -2.456888 -0.87978400
H -4.993934 -0.454533 -0.94078200
C -1.914507 -2.602676 -0.25217300
C -3.093647 -3.234263 -0.62567100
H -3.118540 -4.311964 -0.71378200
N -1.440397 1.277455 0.17536200
N -1.825403 -1.270263 -0.12660100
Ni -0.267745 -0.283438 0.33348600
H -1.013910 -3.161284 -0.04571200
C 3.580026 1.300873 -2.22235700
C 2.652541 1.039623 -1.21264200
C 2.827647 -0.038428 -0.34134000
C 3.954040 -0.855737 -0.49890600
C 4.880849 -0.596729 -1.50444000
C 4.698044 0.483199 -2.37117800
H 3.425207 2.140478 -2.89095600
H 1.780131 1.676521 -1.10750900
H 4.101111 -1.680680 0.18586600
H 5.748664 -1.238111 -1.61346200
H 5.419839 0.682139 -3.15534400
C 1.840640 -0.342202 0.75702300
C 1.065637 -1.602250 0.59004600
H 1.077312 0.561104 0.72945200
H 0.884170 -2.187180 1.49216700
H 1.320572 -2.213339 -0.27538100
C 2.342796 -0.156240 2.25946000
O 1.426439 0.102515 3.07044200
O 3.556768 -0.330635 2.45277200
H -4.114753 4.022546 -0.24309000
H -5.152619 -2.916317 -1.17556400
H -0.108985 2.768683 0.67668800

Int-SC8-T

PBE SCF Energy: -1163.77897662 a.u.

C 2.087731 -2.118145 -1.12352000
C 2.395241 -0.004958 -0.20322600
C 3.610216 -0.397117 0.35590400
C 4.060445 -1.697168 0.15311600
C 3.290366 -2.576458 -0.60165100
H 4.197276 0.293103 0.94440300
H 3.605222 -3.595684 -0.78039200
C 1.816135 1.352685 -0.05176100
C 2.431520 2.395220 0.63822600
C 1.786941 3.626057 0.71565500
H 3.393808 2.258217 1.11045400
C -0.005471 2.707521 -0.56686200
C 0.549669 3.792019 0.10115700
H 0.020145 4.734403 0.13949500
N 1.654410 -0.867551 -0.93210200
N 0.612749 1.526022 -0.63580300
Ni -0.222189 -0.176958 -1.43897100
H -0.970411 2.763038 -1.05358000
C -0.060969 -0.388587 2.61062900
C -1.010395 0.260595 1.82799900
C -1.643286 -0.398317 0.76112900
C -1.309212 -1.746384 0.52818300
C -0.365559 -2.402260 1.32301100
C 0.270229 -1.723094 2.35788700
H 0.431045 0.148162 3.41427400
H -1.248524 1.301226 2.02013000
H -1.832457 -2.273782 -0.25939600

H -0.122011 -3.439362 1.12159200
H 1.018513 -2.222682 2.96225800
C -2.620976 0.316616 -0.15532800
C -2.157575 0.165334 -1.62789700
H -2.619066 1.371590 0.12577200
H -2.446072 1.036103 -2.22670300
H -2.643462 -0.716658 -2.06056700
C -4.077569 -0.222129 0.09094400
O -4.308225 -1.391735 -0.30623000
O -4.867755 0.563302 0.66603000
H 5.001168 -2.017791 0.58299600
H 2.249737 4.445842 1.25079000
H 1.439227 -2.761303 -1.70495100

Int-SC9-D

PBE SCF Energy: -1163.95612655 a.u.
C -1.471995 -1.819414 -0.22660400
C -1.540221 -3.234761 -0.27814700
C -0.510917 -3.964189 -0.81959700
C 0.621684 -3.279465 -1.33389100
C 0.661842 -1.906452 -1.22401800
C -2.517304 -0.959549 0.20940300
C -3.797971 -1.361393 0.67125500
C -4.720820 -0.415949 1.04971400
C -4.385994 0.960287 0.96988300
C -3.127213 1.297592 0.51157400
H -2.419226 -3.736644 0.10696900
H -0.567332 -5.045873 -0.86083300
H 1.444511 -3.808093 -1.79701100
H 1.514577 -1.352670 -1.58610400
H -4.046138 -2.414327 0.71943000
H -5.699522 -0.721446 1.40241800
H -5.086965 1.732203 1.25941200
H -2.801011 2.327181 0.42339800
N -0.316690 -1.163815 -0.66708400
N -2.207003 0.389531 0.14289000
Ni -0.335651 0.751462 -0.41373600
C 1.606752 1.169575 -0.66742900
H 1.827763 1.070922 -1.73931500
C 1.740754 2.656507 -0.27263500
C 0.431997 3.406417 -0.46376700
O -0.616357 2.633646 -0.39187100
O 0.373077 4.624738 -0.62270200
H 1.963249 2.736052 0.79832800
C 2.549195 0.302595 0.10905500
C 3.628174 -0.360344 -0.49832200
C 2.386105 0.120728 1.49548200
C 4.492540 -1.176516 0.23341300
H 3.787956 -0.235853 -1.56540500
C 3.247690 -0.684431 2.23242200
H 1.547203 0.605717 1.98539700
C 4.308415 -1.344071 1.60428600
H 5.312158 -1.679013 -0.27003000
H 3.087995 -0.809331 3.29857700
H 4.976652 -1.978291 2.17612400
H 2.552173 3.178442 -0.79327200

Int-SCA1-S

PBE SCF Energy: -1428.71119118 a.u.
C -0.211761 -2.090787 0.97412100
C 1.729936 -1.603725 -0.21587000
C 2.327251 -2.779254 0.22814200
C 1.617196 -3.626893 1.07211800
C 0.325763 -3.279305 1.44937500
H 3.333313 -3.030967 -0.07532500
H -0.262464 -3.907887 2.10408500
C 2.380155 -0.623973 -1.10852700
C 3.657893 -0.768262 -1.64095000
C 4.161233 0.228187 -2.47115600
H 4.255716 -1.639881 -1.41519900
C 2.108952 1.419531 -2.18555200
C 3.375661 1.340961 -2.75112200
H 3.729403 2.137550 -3.39161800
N 0.468647 -1.271075 0.16277800
N 1.622554 0.462850 -1.38473500
Ni -0.093431 0.448794 -0.45121600
H 1.460830 2.265851 -2.36999500
C -4.563582 -1.872163 0.02956300
C -3.623907 -0.992630 0.56289400
C -2.862540 -0.150296 -0.26587700
C -3.089749 -0.214749 -1.65414900
C -4.029727 -1.090193 -2.18587600
C -4.770344 -1.927214 -1.34786500
H -5.138230 -2.510184 0.69176000
H -3.482763 -0.946437 1.63801100
H -2.513527 0.418236 -2.31991800
H -4.184081 -1.123876 -3.25871200
H -5.501774 -2.609564 -1.76519300

C -1.825889 0.720059 0.32201800
C -1.502943 2.041120 -0.28181500
H -1.793556 0.699469 1.40942700
H -0.451019 2.012795 -0.81257000
H -2.144691 2.327967 -1.11265000
C -1.325958 3.219744 0.71763600
O -0.547337 3.021722 1.70507100
O -1.962052 4.247066 0.46939900
H -1.210293 -1.779606 1.23925400
H 2.070156 -4.543628 1.42788200
H 5.154210 0.133553 -2.89224300
C 1.647740 0.669210 2.42080300
O 2.383006 1.271233 1.66169500
O 0.425821 0.982589 2.76468800
O 2.014449 -0.481607 3.03423500
H 0.071489 1.814320 2.24272500
H 2.921583 -0.670618 2.75987500

Int-SCA2-S

PBE SCF Energy: -1428.68523249 a.u.

C -0.030890 2.282955 -0.16869700
C 2.263867 1.898066 0.02656300
C 2.522008 3.262744 0.03999300
C 1.456387 4.153092 -0.05347100
C 0.162091 3.657843 -0.16356500
H 3.535947 3.627763 0.11941000
H -0.692809 4.314897 -0.24373300
C 3.278770 0.838763 0.10239600
C 4.649925 1.033713 0.20818200
C 5.486988 -0.077262 0.26566000
H 5.060081 2.032755 0.24540700
C 3.556575 -1.485555 0.11220500
C 4.935432 -1.352720 0.21779300
H 5.553612 -2.238774 0.26157800
N 0.994318 1.425815 -0.06939000
N 2.758736 -0.412927 0.05354000
Ni 0.870588 -0.472633 -0.06549400
H 3.058321 -2.443229 0.07500400
C -3.910313 0.366427 -2.56722700
C -2.957817 -0.266722 -1.77684300
C -2.837184 0.048149 -0.41508100
C -3.689741 1.008973 0.13923800
C -4.648925 1.639139 -0.65588800
C -4.759351 1.324963 -2.00809100
H -3.992532 0.115220 -3.61873100
H -2.289035 -1.007089 -2.20400500
H -3.631748 1.241779 1.19553900
H -5.310158 2.375562 -0.21325100
H -5.502034 1.819629 -2.62370900
C -1.771118 -0.651228 0.39711200
C -1.648060 -0.288704 1.86525500
H -1.855736 -1.732295 0.29845500
H -0.757409 -0.775619 2.27345700
H -1.536277 0.786586 2.01367600
C -2.874085 -0.823758 2.67764000
O -3.183636 -2.018076 2.45525700
O -3.411261 -0.014110 3.46822700
H -1.020399 1.857337 -0.25633400
H 1.639156 5.219932 -0.04357000
H 6.558042 0.056250 0.34768100
C 0.271989 -2.853812 -1.10523500
O 0.786525 -2.323229 -0.03073100
O -0.132843 -2.250661 -2.08665700
O 0.200260 -4.203820 -1.06664100
H -0.833822 -0.413218 -0.20534200
H 0.557308 -4.505203 -0.22003800

Int-SCA3-S

PBE SCF Energy: -1428.72885736 a.u.

C 2.189194 -0.052921 1.19802200
C 2.941307 0.178263 2.34586900
C 2.377807 0.886579 3.40106200
C 1.078376 1.360640 3.27152300
C 0.377945 1.086485 2.10441100
C 2.708338 -0.731992 -0.00279500
C 3.987290 -1.269258 -0.13100200
C 4.349937 -1.858736 -1.33797800
C 3.430882 -1.896525 -2.38232600
C 2.170846 -1.345044 -2.18229100
H 3.958251 -0.181022 2.41298000
H 2.951441 1.074736 4.29987400
H 0.603493 1.936805 4.05416000
H -0.620432 1.460802 1.95516600
H 4.690083 -1.232108 0.68940500
H 5.339236 -2.282306 -1.45837500
H 3.677945 -2.344919 -3.33538400
H 1.400646 -1.343525 -2.94181700
N 0.902661 0.379739 1.09269400

N 1.823566 -0.778616 -1.02139900
Ni 0.022267 -0.104626 -0.56047800
C -1.849049 0.243234 -0.06651200
H -1.963418 1.110925 0.58286100
C -2.596337 0.468167 -1.38631300
C -1.867259 -0.199602 -2.54151500
O -0.617514 -0.486681 -2.26100600
O -2.380418 -0.431439 -3.62796500
H -3.637997 0.131037 -1.36631600
C -2.209489 -1.006476 0.67125800
C -2.326326 -1.006635 2.07366900
C -2.426707 -2.231961 0.01039300
C -2.619668 -2.169027 2.78221500
H -2.196040 -0.077480 2.61662400
C -2.726132 -3.394156 0.71617900
H -2.348010 -2.278458 -1.06899400
C -2.818708 -3.373983 2.10846500
H -2.702376 -2.130849 3.86330500
H -2.885940 -4.321119 0.17566000
H -3.048995 -4.279932 2.65748600
H -2.617773 1.538411 -1.61926600
O -0.184563 3.036330 -1.24254300
H -0.251532 2.111164 -0.92382300
C -0.707171 3.848461 -0.32341000
O -1.199475 3.514691 0.72935600
O -0.600505 5.108518 -0.75885100
H -0.986314 5.685093 -0.08469700

Int-SCA3-T

PBE SCF Energy: -1428.70258173 a.u.
C 1.852026 0.572321 -1.18102200
C 3.205042 0.413942 -1.47994700
C 3.647083 -0.803498 -1.98612700
C 2.733093 -1.834002 -2.18185900
C 1.403338 -1.608575 -1.84866300
C 1.259222 1.825482 -0.65345300
C 2.007038 2.964058 -0.34797100
C 1.359720 4.090690 0.14270900
C -0.022160 4.060142 0.31459700
C -0.699961 2.892759 -0.00861100
H 3.907196 1.220343 -1.32439300
H 4.694784 -0.942764 -2.22269900
H 3.039314 -2.795092 -2.57323200
H 0.638201 -2.367655 -1.94847900
H 3.079590 2.972018 -0.47877700
H 1.927168 4.979661 0.38894400
H -0.565482 4.916877 0.69050000
H -1.772801 2.809698 0.10458900
N 0.979940 -0.438428 -1.36422900
N -0.079846 1.804039 -0.47745500
Ni -0.936272 -0.089406 -0.63004100
C -0.824572 -0.733361 1.37878400
H -1.304814 -0.024456 2.06886800
C -1.549328 -2.083110 1.34019700
H -2.606951 -1.941069 1.59072600
C -1.570532 -2.754190 -0.04612200
O -1.572582 -1.942752 -1.05643800
O -1.620634 -3.983144 -0.14216000
H -1.162947 -2.808611 2.06513500
C 0.613756 -0.759107 1.70850100
C 1.252919 0.388454 2.22462000
C 1.427301 -1.886112 1.46778200
C 2.621451 0.417641 2.46520600
H 0.657266 1.275454 2.41879600
C 2.799062 -1.853746 1.70261200
H 0.984084 -2.789574 1.06460900
C 3.411615 -0.703397 2.20115400
H 3.076430 1.322940 2.85417200
H 3.395691 -2.734840 1.48923700
H 4.480564 -0.680410 2.38005600
C -3.891568 0.697212 -0.04208400
O -2.961506 0.749261 -0.83501000
O -5.156334 0.910264 -0.36090500
O -3.778594 0.433774 1.24639400
H -5.207975 1.090467 -1.31111800
H -2.834447 0.280258 1.43914000

Int-SCA4-S

PBE SCF Energy: -1428.74386397 a.u.
C -1.397279 2.263035 -0.02814300
C -2.016135 3.391673 0.49794000
C -3.360500 3.324092 0.84853800
C -4.054930 2.135292 0.65252800
C -3.376552 1.040952 0.13203600
C -0.003327 2.200924 -0.49348600
C 0.888199 3.267328 -0.50030500
C 2.161388 3.078524 -1.02808100
C 2.508626 1.833499 -1.53697900

C 1.577807 0.804525 -1.48790400
H -1.461612 4.310120 0.62779100
H -3.858350 4.192797 1.26036100
H -5.104738 2.046433 0.89653800
H -3.864164 0.095691 -0.05238700
H 0.595146 4.230327 -0.10694000
H 2.870512 3.896454 -1.03927500
H 3.488773 1.644511 -1.95085100
H 1.787712 -0.189063 -1.85194300
N -2.077044 1.098746 -0.18702200
N 0.353915 0.984759 -0.97565300
Ni -0.993028 -0.393746 -0.78905000
C 1.001567 -1.619627 1.50693300
H 0.971559 -1.949105 2.55248200
C 0.796194 -2.861704 0.63144100
C 0.868171 -2.663762 -0.88436300
O 0.177114 -1.707349 -1.44216300
O 1.570342 -3.413147 -1.56092200
H 1.524819 -3.635562 0.87736400
C 2.269394 -0.819124 1.29273500
C 2.352969 0.468754 1.84080800
C 3.372005 -1.307617 0.58387700
C 3.499709 1.241612 1.69412400
H 1.499584 0.869831 2.37887400
C 4.524208 -0.532840 0.43185200
H 3.331906 -2.288335 0.12578200
C 4.594940 0.741671 0.98732500
H 3.535223 2.239306 2.11728300
H 5.364646 -0.928488 -0.12794900
H 5.487090 1.344881 0.86299500
H -0.195028 -3.258781 0.86586100
O -2.409587 -1.650910 -0.63658900
H 0.137524 -0.958283 1.40554000
C -2.724532 -2.185398 0.49196600
O -2.242200 -1.970741 1.59902200
O -3.745752 -3.082580 0.33771900
H -3.934781 -3.435421 1.21701700

Int-SCA4-T

PBE SCF Energy: -1428.72725042 a.u.
C 2.470297 -0.595567 -0.62949500
C 3.554854 -1.469268 -0.61921300
C 3.340945 -2.815152 -0.90275400
C 2.053842 -3.256819 -1.18726900
C 1.017960 -2.329807 -1.18154700
C 2.563695 0.847691 -0.30176800
C 3.753403 1.504781 0.00381400
C 3.710572 2.853758 0.34376200
C 2.485622 3.511814 0.37808800
C 1.336917 2.798752 0.05377300
H 4.549120 -1.115969 -0.38642200
H 4.172921 -3.508349 -0.89486000
H 1.847281 -4.296217 -1.40424700
H -0.011451 -2.592651 -1.38291700
H 4.698359 0.981091 -0.01873000
H 4.626060 3.379949 0.58432200
H 2.413488 4.556264 0.65059300
H 0.345576 3.233522 0.07921200
N 1.226966 -1.038018 -0.91335000
N 1.384952 1.505214 -0.28278800
Ni -0.258250 0.373663 -0.80320700
C -3.049469 -1.332677 1.25074600
H -3.578013 -1.946775 1.98621800
C -3.375720 -1.887862 -0.15988800
H -4.456420 -1.999060 -0.25809900
C -2.869374 -0.914314 -1.21631800
O -1.596626 -0.951834 -1.42002200
O -3.658307 -0.125143 -1.75818100
H -2.902206 -2.862838 -0.29397000
C -1.578654 -1.318593 1.60481900
C -0.899459 -0.112166 1.84067800
C -0.865756 -2.514802 1.74447400
C 0.444030 -0.111431 2.23994300
H -1.435263 0.829845 1.79623600
C 0.473695 -2.512298 2.12403700
H -1.367460 -3.458738 1.56038900
C 1.135189 -1.309747 2.37886100
H 0.938874 0.831639 2.43537500
H 1.005109 -3.452000 2.22203400
H 2.176765 -1.309659 2.67655900
C -2.250171 2.438328 0.01831000
O -1.459994 1.935918 -0.86873600
O -3.560016 2.072829 -0.09456600
O -1.938531 3.201376 0.92813700
H -3.627173 1.404335 -0.81040900
H -3.454724 -0.320229 1.33011200

Int-SCA5-D

PBE SCF Energy: -1428.82470688 a.u.
C 2.539598 2.838014 0.71214900
C 1.766329 3.731928 1.44172300
C 0.399213 3.488767 1.57448000
C -0.135131 2.353463 0.98110500
C 4.583708 -0.233418 -1.74536900
C 3.769883 -1.258845 -2.22900000
C 2.419762 -1.242473 -1.90959600
H -0.242607 4.162711 2.12761100
H 4.171939 -2.056026 -2.84126000
N 0.605226 1.482165 0.27897800
N 1.865703 -0.279831 -1.15428800
Ni -0.066103 -0.286168 -0.53958200
C -1.822947 -0.845305 0.48838500
C -2.529678 -1.852545 -0.41413900
H -3.350515 -1.350512 -0.94065200
H -2.989768 -2.692685 0.12755300
H -2.503833 -0.082199 0.87060400
C -1.651122 -2.464041 -1.52764000
O -0.577831 -1.820955 -1.82233700
O -2.023844 -3.509822 -2.08432300
C 4.016384 0.765612 -0.96403100
C 2.648541 0.718509 -0.68132200
C 1.930969 1.720669 0.13358500
C -3.350463 2.109487 -0.90271700
O -3.414098 2.266892 0.29817000
O -4.062973 2.824500 -1.79210900
O -2.597093 1.241162 -1.55390600
H -2.059049 0.683181 -0.91200700
H -4.601378 3.452042 -1.29061200
H 1.726506 -2.001920 -2.24895300
H -1.189692 2.120109 1.05366500
H 3.600675 3.010862 0.59464500
H 4.632451 1.568065 -0.58168100
H 2.221561 4.603706 1.89576700
H 5.642427 -0.212436 -1.97340600
C -1.017093 -1.394970 1.58854600
C -0.482892 -2.710842 1.58088000
C -0.717258 -0.614995 2.73849700
C 0.323956 -3.182416 2.61403300
H -0.693277 -3.364422 0.74235800
C 0.087676 -1.088907 3.76425100
H -1.123037 0.389519 2.80154700
C 0.629056 -2.380065 3.71496800
H 0.716433 -4.193923 2.55868700
H 0.293041 -0.449584 4.61823200
H 1.258253 -2.750093 4.51667700

Int-SCA6-D
PBE SCF Energy: -1428.8659814 a.u.
C 2.056319 2.934696 -0.30386300
C 1.362326 4.038637 0.17334000
C -0.024438 3.956066 0.30754200
C -0.660684 2.778960 -0.05854100
C 3.865562 -0.860823 -1.68010500
C 2.976984 -1.921863 -1.85834300
C 1.622298 -1.699007 -1.65695000
H -0.603514 4.786332 0.69181200
H 3.325765 -2.906172 -2.14438500
N 0.003619 1.712946 -0.53570500
N 1.133111 -0.501477 -1.29552100
Ni -0.814791 -0.075207 -0.96324500
C -1.423800 -1.508903 2.02296800
C -1.541235 -2.894636 1.38374900
H -2.597775 -3.187259 1.40070600
H -0.999170 -3.646543 1.96263000
H -1.872211 -1.545656 3.02407200
C -1.085117 -2.996184 -0.08643400
O -1.414616 -2.034838 -0.86157100
O -0.467136 -4.017988 -0.43763200
C 3.365884 0.375688 -1.29408100
C 1.990806 0.527642 -1.10071600
C 1.352701 1.777339 -0.64456800
C -3.600108 0.883396 -0.47062000
O -3.459611 1.168791 0.72850400
O -4.885903 0.938494 -1.00065000
O -2.735648 0.550497 -1.32567000
H -2.026580 -0.796433 1.45166200
H -5.456977 1.213605 -0.27278500
H 0.887390 -2.488993 -1.74808700
H -1.728533 2.643102 0.05210700
H 3.133205 2.970318 -0.39496700
H 4.039640 1.207127 -1.13843800
H 1.893473 4.942314 0.44662300
H 4.929563 -0.996977 -1.83169600
C -0.020279 -0.944199 2.15125100
C 1.129083 -1.670502 1.82601300
C 0.139844 0.375006 2.59913600

C 2.396195 -1.096075 1.93731300
H 1.042860 -2.678148 1.43893500
C 1.400124 0.951217 2.71366400
H -0.741752 0.963070 2.83309300
C 2.538833 0.215108 2.38113800
H 3.270258 -1.670882 1.65169000
H 1.494727 1.980913 3.04050900
H 3.522167 0.666746 2.45077800

Int-SCW1-S

PBE SCF Energy: -1240.23078761 a.u.

C 0.493807 -1.455235 1.52066000
C -1.718104 -1.406960 0.83313300
C -1.992183 -2.569005 1.54950600
C -0.976552 -3.183687 2.27208000
C 0.287273 -2.607111 2.26782800
H -2.990646 -2.982555 1.55511700
H 1.109451 -3.033848 2.82648100
C -2.740251 -0.639018 0.10110700
C -4.071976 -1.019457 -0.05351700
C -4.935179 -0.173858 -0.74309300
H -4.432894 -1.954577 0.35086800
C -3.105577 1.333661 -1.07199000
C -4.448276 1.024732 -1.25657200
H -5.090680 1.709918 -1.79378400
N -0.469435 -0.865819 0.79962700
N -2.276160 0.519387 -0.41084000
Ni -0.298967 0.772013 -0.26505800
H -2.641911 2.238214 -1.44407000
C 2.413898 -2.086450 -2.54619000
C 1.885882 -0.896847 -2.06231100
C 2.317910 -0.333464 -0.84430800
C 3.324277 -1.020624 -0.14613200
C 3.854727 -2.220948 -0.62666100
C 3.403082 -2.763573 -1.82533600
H 2.054374 -2.492025 -3.48605200
H 1.107969 -0.384604 -2.62061000
H 3.706817 -0.624756 0.78762600
H 4.626911 -2.727823 -0.05757200
H 3.813774 -3.695209 -2.19776700
C 1.683535 0.944775 -0.37908700
C 2.306423 1.574686 0.86570200
H 1.797259 1.653168 -1.20590200
H 2.104891 0.985630 1.76695500
H 3.402285 1.603779 0.79082500
C 1.933261 3.009438 1.25141100
O 1.004290 3.670279 0.58153900
O 2.517284 3.540537 2.18202000
H 1.465074 -0.994764 1.48534400
H -1.175179 -4.086784 2.83542400
H -5.973995 -0.449914 -0.87540200
O -0.430692 2.460552 -1.08473200
H 0.011970 2.461144 -1.94061400
H 0.471864 3.146402 -0.14476400

Int-SCW2-S

PBE SCF Energy: -1240.25191185 a.u.

C 1.624031 -2.107070 1.36629900
C 2.215601 0.124173 1.05059100
C 2.853832 0.162162 2.28614400
C 2.866591 -0.983356 3.07524300
C 2.247392 -2.137859 2.60701600
H 3.335977 1.067275 2.62752800
H 2.242154 -3.050953 3.18677700
C 2.142081 1.246209 0.10040500
C 2.668899 2.516468 0.31210500
C 2.523964 3.480318 -0.68074200
H 3.180612 2.752819 1.23438300
C 1.353661 1.866668 -2.00721000
C 1.858302 3.152176 -1.85793400
H 1.725426 3.875339 -2.65124200
N 1.600628 -1.001941 0.60979200
N 1.494361 0.940593 -1.05067300
Ni 0.733442 -0.833925 -1.13030100
H 0.813706 1.531460 -2.88269800
C -2.371446 2.641196 0.98178100
C -2.079986 1.486376 0.25997500
C -3.027748 0.462598 0.12512400
C -4.276283 0.626063 0.73226800
C -4.573374 1.781854 1.45605500
C -3.621833 2.792838 1.58392100
H -1.625544 3.423599 1.07125600
H -1.108091 1.370185 -0.20807100
H -5.021653 -0.157187 0.63612900
H -5.548398 1.892685 1.91799000
H -3.852234 3.691516 2.14503300
C -2.664416 -0.798576 -0.62155100
C -1.885924 -1.786410 0.28332500

H -3.561367 -1.293676 -1.00334600
H -1.136850 -1.228758 0.85026500
H -2.568496 -2.258825 0.99185300
C -1.192827 -2.875866 -0.53383600
O -0.050530 -2.566152 -1.09447600
O -1.702171 -3.986440 -0.65596200
H 1.127842 -2.969762 0.94557800
H 3.358377 -0.972980 4.03976800
H 2.925987 4.474826 -0.53338500
O 0.007168 -0.500463 -2.77739300
H -2.037464 -0.538263 -1.47781300
H -0.450115 -1.305272 -3.04663000

Int-SCW3-S

PBE SCF Energy: -1240.24685875 a.u.

C 1.884001 1.635738 -0.14347400
C 2.449529 2.902179 -0.26642900
C 1.781478 3.884248 -0.98814000
C 0.563273 3.570875 -1.57858300
C 0.051797 2.290898 -1.41304000
C 2.529383 0.515664 0.56976300
C 3.748821 0.594413 1.23988700
C 4.247526 -0.544349 1.86436500
C 3.519278 -1.728822 1.80596500
C 2.310270 -1.733872 1.12088800
H 3.404351 3.120201 0.19030700
H 2.211274 4.872620 -1.09120600
H 0.009774 4.296439 -2.15926100
H -0.887977 2.006885 -1.85692100
H 4.302370 1.521764 1.27857600
H 5.193238 -0.503737 2.39031900
H 3.874426 -2.634071 2.28010600
H 1.689444 -2.615597 1.03741800
N 0.679866 1.340269 -0.70675000
N 1.832355 -0.639391 0.51925300
Ni 0.048876 -0.494298 -0.41898300
C -1.818318 -0.341939 -1.07817900
H -1.870870 0.265007 -1.98554200
C -2.267743 -1.779582 -1.39033000
C -1.484868 -2.797840 -0.57799300
O -0.327900 -2.329495 -0.14521300
O -1.857684 -3.942221 -0.37154700
H -3.340727 -1.945839 -1.25016300
C -2.577303 0.324074 0.02635600
C -3.097805 1.621541 -0.12242100
C -2.787655 -0.313352 1.26569600
C -3.772086 2.261541 0.91626300
H -2.989095 2.132791 -1.07292300
C -3.467343 0.319658 2.30162300
H -2.394658 -1.311425 1.42198700
C -3.959853 1.616016 2.13737600
H -4.160273 3.263414 0.76579000
H -3.609659 -0.198742 3.24397500
H -4.485911 2.110646 2.94597300
H -2.044765 -2.008624 -2.43862000
O 1.727739 -2.791674 -2.10233600
H 1.632653 -1.895983 -2.44450400
H 1.060794 -2.816969 -1.39610900

Int-SCW3-T

PBE SCF Energy: -1240.22852954 a.u.

C -1.406866 0.653966 -1.21272200
C -2.059145 1.818372 -1.61956800
C -1.319306 2.832569 -2.21806100
C 0.051440 2.665604 -2.39612700
C 0.633602 1.481352 -1.96246200
C -2.082087 -0.494299 -0.56158400
C -3.433999 -0.502220 -0.21313000
C -3.971408 -1.628346 0.39708900
C -3.149805 -2.726219 0.64525000
C -1.814314 -2.645765 0.27624300
H -3.123329 1.938959 -1.47468500
H -1.809928 3.743278 -2.53888900
H 0.659662 3.434756 -2.85340900
H 1.694402 1.282584 -2.05006700
H -4.057991 0.359210 -0.40391800
H -5.017500 -1.647875 0.67665000
H -3.530590 -3.623783 1.11425000
H -1.127342 -3.465311 0.44548100
N -0.079417 0.505218 -1.39418800
N -1.292108 -1.561302 -0.30870200
Ni 0.735996 -1.193368 -0.54080700
C 1.234706 -0.618492 1.40894800
H 0.837664 -1.409546 2.05126300
C 2.762572 -0.626229 1.34589500
H 3.122196 -1.630463 1.60042300
C 3.349843 -0.338845 -0.04991100
O 2.644534 -0.778475 -1.04861800

O 4.433173 0.237978 -0.16864800
H 3.236695 0.058915 2.05918100
C 0.574182 0.661545 1.68055800
C -0.742831 0.698795 2.19389800
C 1.174294 1.906851 1.38691500
C -1.418630 1.896694 2.39105800
H -1.237608 -0.239159 2.42785100
C 0.495493 3.105868 1.58517000
H 2.179536 1.930852 0.98107700
C -0.807111 3.116630 2.08751800
H -2.431323 1.880796 2.78181200
H 0.987566 4.042210 1.34092400
H -1.334002 4.051983 2.23854900
O 1.389390 -3.294693 -0.31736500
H 1.490993 -3.545157 0.60950100
H 2.293136 -3.220820 -0.65598000

Int-SCW4-S

PBE SCF Energy: -1240.25047771 a.u.

C -2.271676 0.120935 -0.39545900
C -3.589686 0.278019 0.02144100
C -4.311999 -0.844024 0.41398500
C -3.701140 -2.093974 0.37965100
C -2.381911 -2.183735 -0.04577800
C -1.379681 1.209763 -0.82398200
C -1.745510 2.547694 -0.92971300
C -0.800313 3.472583 -1.35866900
C 0.483354 3.036290 -1.66793100
C 0.784400 1.686323 -1.53836200
H -4.044043 1.258457 0.04687400
H -5.337828 -0.740334 0.74480200
H -4.229891 -2.988863 0.67921400
H -1.828107 -3.112091 -0.09083500
H -2.748698 2.864126 -0.68152800
H -1.064895 4.518848 -1.44706300
H 1.248299 3.724532 -2.00151300
H 1.764716 1.286186 -1.75717300
N -1.689191 -1.102599 -0.42361500
N -0.126455 0.794535 -1.12801800
Ni 0.177714 -1.128203 -0.90205200
C 2.129172 -1.405065 1.66322600
H 2.510435 -1.779087 2.62124000
C 3.316278 -1.315081 0.69484100
C 3.082133 -0.686862 -0.68702100
O 2.010529 -0.987160 -1.36269700
O 3.958448 0.039693 -1.15805900
H 4.147570 -0.769068 1.14402200
C 1.367021 -0.116646 1.90799600
C 0.047846 -0.185288 2.37791400
C 1.913887 1.146374 1.66231300
C -0.706021 0.965812 2.58195200
H -0.399751 -1.158092 2.55302000
C 1.159814 2.304024 1.86006700
H 2.921942 1.235016 1.27543700
C -0.152857 2.219530 2.31676200
H -1.731746 0.884504 2.92412400
H 1.596278 3.271672 1.63956200
H -0.744000 3.117859 2.45233500
H 3.678696 -2.332633 0.50849300
O 0.271881 -2.943258 -0.67166700
H 1.424055 -2.156446 1.30167100
H 1.184970 -3.192688 -0.85381700

Int-SCW4-T

PBE SCF Energy: -1240.23390246 a.u.

C -1.424198 1.046763 -0.93996400
C -1.741816 2.358516 -1.28651500
C -0.814012 3.116414 -1.99219300
C 0.406340 2.547114 -2.33699900
C 0.656644 1.231173 -1.96469100
C -2.330230 0.157669 -0.17288900
C -3.582610 0.542423 0.30462200
C -4.339914 -0.371564 1.02972900
C -3.836146 -1.648616 1.25777500
C -2.582853 -1.962850 0.74680700
H -2.692242 2.790214 -1.00780900
H -1.043795 4.139343 -2.26373000
H 1.156968 3.104641 -2.88119800
H 1.590310 0.731320 -2.19088600
H -3.965715 1.535977 0.12162700
H -5.312821 -0.087243 1.41099500
H -4.395402 -2.386929 1.81659600
H -2.136735 -2.939387 0.88746300
N -0.236915 0.502793 -1.28502000
N -1.854024 -1.082336 0.05524200
Ni 0.033345 -1.443634 -0.68686800
C 3.182195 -0.512798 1.94762200
H 3.913128 -0.181421 2.69468700

C 3.893150 -0.630264 0.58975300
H 4.658503 -1.412260 0.64951300
C 2.960952 -0.978216 -0.57433900
O 1.924645 -1.679549 -0.25466600
O 3.238054 -0.591677 -1.71431400
H 4.416407 0.290718 0.32519300
C 1.994992 0.430167 1.95135500
C 0.778501 0.035744 2.52032700
C 2.074075 1.708006 1.38510300
C -0.327487 0.883852 2.51955700
H 0.691677 -0.957589 2.94824600
C 0.970549 2.559600 1.37954700
H 3.001408 2.040310 0.93143600
C -0.235544 2.151331 1.94718900
H -1.264654 0.547792 2.94954900
H 1.049234 3.538560 0.92028800
H -1.098038 2.807359 1.92910700
O -0.445622 -2.790793 -1.92149500
H 2.841713 -1.502854 2.25578900
H 0.340832 -3.070641 -2.40309800

Int-SCW5-D

PBE SCF Energy: -1240.34346735 a.u.

C -1.609250 0.447270 -1.18126200
C -2.359603 1.569354 -1.59760200
C -1.733665 2.622509 -2.22771500
C -0.335700 2.568948 -2.44385600
C 0.348921 1.456900 -2.00649600
C -2.139083 -0.705233 -0.50223700
C -3.495616 -0.887359 -0.14937500
C -3.895940 -2.031703 0.50165000
C -2.929244 -3.019364 0.81838000
C -1.620033 -2.787195 0.46400600
H -3.425883 1.605258 -1.41383400
H -2.305909 3.485297 -2.54809700
H 0.191898 3.380116 -2.92897000
H 1.423312 1.361798 -2.11603300
H -4.220008 -0.119189 -0.38866000
H -4.935449 -2.173098 0.77302000
H -3.202517 -3.934589 1.32762700
H -0.837779 -3.501801 0.69798300
N -0.249912 0.409125 -1.40618500
N -1.206240 -1.676624 -0.18628800
Ni 0.665569 -1.040142 -0.40532200
C 1.374366 -0.409784 1.43543700
H 1.077727 -1.164294 2.16945700
C 2.888890 -0.345114 1.23987500
H 3.326769 -1.303975 1.54429600
C 3.312399 -0.167077 -0.22815300
O 2.584027 -0.827979 -1.08656700
O 4.284163 0.523563 -0.53660600
H 3.387565 0.428249 1.83728000
C 0.663166 0.853436 1.65349900
C -0.634282 0.862740 2.22078200
C 1.186219 2.106990 1.25921300
C -1.356558 2.037726 2.37988100
H -1.076275 -0.082932 2.51999300
C 0.457807 3.283064 1.41702300
H 2.167380 2.153341 0.79967500
C -0.820890 3.266109 1.97721400
H -2.350819 1.997969 2.81503000
H 0.892453 4.223805 1.09230100
H -1.386585 4.183379 2.09668000
O 2.397054 -3.547393 -0.35860400
H 2.258372 -3.399824 0.58289000
H 2.639509 -2.661867 -0.69166100

Int-SCW6-D

PBE SCF Energy: -1240.35811987 a.u.

C -1.411715 1.497752 -0.50185100
C -1.811714 2.799730 -0.16207800
C -0.900657 3.837775 -0.20026300
C 0.427957 3.552944 -0.58353300
C 0.767697 2.261017 -0.91549600
C -2.279000 0.334229 -0.44824800
C -3.617747 0.333746 -0.01429500
C -4.316958 -0.857804 0.03736100
C -3.679493 -2.050399 -0.34918600
C -2.365233 -1.979012 -0.77576600
H -2.835333 2.988373 0.13563400
H -1.200237 4.845250 0.06189000
H 1.180661 4.331076 -0.61685100
H 1.776498 1.987823 -1.19642600
H -4.095470 1.256122 0.28877200
H -5.345843 -0.870375 0.37767400
H -4.194176 -3.002108 -0.31619300
H -1.802900 -2.851306 -1.08857000
N -0.116619 1.230167 -0.89144300

N -1.679865 -0.827224 -0.83006800
Ni 0.309593 -0.639026 -1.31106500
C 2.413895 -1.837855 1.05726700
H 2.774777 -2.607678 1.75073100
C 3.613054 -1.051994 0.52265900
H 4.311511 -1.764894 0.06829600
C 3.292275 -0.003302 -0.56405900
O 2.410066 -0.318637 -1.43479300
O 3.936136 1.061440 -0.55077100
H 4.158792 -0.554721 1.32830800
C 1.335866 -1.026343 1.75384500
C 0.114546 -1.644568 2.05805200
C 1.486365 0.324378 2.08100800
C -0.920608 -0.942034 2.66515600
H -0.031925 -2.684413 1.78347600
C 0.450306 1.034352 2.68969000
H 2.399800 0.846062 1.82355200
C -0.756226 0.406446 2.98520400
H -1.863558 -1.438384 2.86706300
H 0.582648 2.087764 2.91141400
H -1.567021 0.963377 3.44152900
O 0.549036 -2.431896 -1.89691600
H 1.942351 -2.366464 0.22379300
H 1.498648 -2.514961 -2.03664200

Int-SD1-S

PBE SCF Energy: -1262.95650743 a.u.

C 0.917898 2.047909 -0.17737800
C -0.940613 1.161215 -1.25666000
C -1.286685 2.418624 -1.75002100
C -0.495013 3.516547 -1.42957500
C 0.628286 3.329629 -0.62853200
H -2.160670 2.545228 -2.37361200
H -0.752558 4.500547 -1.80123800
H 1.272435 4.155715 -0.35680800
C -1.707165 -0.077429 -1.51461000
C -2.885071 -0.130162 -2.25823800
C -3.538009 -1.348086 -2.41317200
H -3.297132 0.764724 -2.70364600
C -1.814701 -2.360994 -1.09992900
C -2.996662 -2.484798 -1.81971800
H -4.456899 -1.404908 -2.98332400
H -3.474396 -3.451585 -1.91028100
N 0.153808 0.986384 -0.47492200
N -1.176112 -1.191335 -0.95022700
Ni 0.477749 -0.892284 0.09036900
N -2.783018 0.750733 1.60543300
C -4.062548 0.403408 0.99670900
H -4.184507 0.957674 0.06538700
H -4.080947 -0.662183 0.78488500
H -4.897991 0.649203 1.66313200
C -2.467140 2.173786 1.67377900
H -1.395346 2.334056 1.76322900
H -2.793920 2.651311 0.74961900
H -2.971975 2.663893 2.51454200
C -2.112331 -0.199354 2.32100100
C -0.867135 0.245983 3.06549000
H -1.089854 1.039094 3.78366900
H -0.464415 -0.616654 3.59135300
H -0.110620 0.610620 2.36771000
O -2.490621 -1.371543 2.36179200
H -1.348245 -3.211094 -0.62030500
H 1.786594 1.842418 0.43548700
C 5.117082 0.899795 0.42944300
C 3.991923 0.372063 1.05772400
C 3.286706 -0.724585 0.51922200
C 3.784375 -1.274659 -0.68150200
C 4.911164 -0.750002 -1.30668600
C 5.587660 0.344502 -0.76113500
H 5.631165 1.746108 0.87381400
H 3.641665 0.813813 1.98621700
H 3.268395 -2.114629 -1.13232300
H 5.265192 -1.197340 -2.23016100
H 6.463872 0.751995 -1.25249900
C 2.064251 -1.204113 1.18429700
C 1.349680 -2.421158 0.86138300
H 1.946797 -0.811665 2.19594600
H 0.810571 -2.913146 1.67280600
H 1.782312 -3.136078 0.15840900

Int-SD1-T

PBE SCF Energy: -1262.92821686 a.u.

N 3.503350 -0.159593 -0.58276500
C 3.580440 1.244253 -0.97901100
H 4.595805 1.473532 -1.31556400
H 2.873750 1.431492 -1.78022600
H 3.333634 1.883082 -0.12889200
C 4.316993 -0.505143 0.57832600

H 4.365682 -1.578137 0.73186000
H 5.333343 -0.131570 0.43286300
H 3.896985 -0.037952 1.47512800
C 2.635060 -0.998305 -1.18112300
C 2.611364 -2.446518 -0.73933500
H 2.314973 -2.536043 0.30734400
H 1.881578 -2.969497 -1.35160100
H 3.589666 -2.916789 -0.86327800
O 1.867036 -0.611616 -2.08807800
C 0.658036 2.738764 -0.21142900
C 0.785514 0.865239 1.21326800
C 1.393188 1.682222 2.20555300
C 1.604081 3.019672 1.97207200
C 1.211995 3.583820 0.73016600
H 1.680553 1.249644 3.15546500
H 2.064540 3.638656 2.73374700
H 1.350353 4.634521 0.51246600
C 0.463665 -0.516834 1.37581800
C 0.742106 -1.287486 2.53797800
C 0.349938 -2.602232 2.61021400
H 1.264457 -0.834543 3.37107200
C -0.547659 -2.407034 0.39749600
C -0.334489 -3.190410 1.51457500
H 0.563781 -3.185400 3.49881600
H -0.665286 -4.220257 1.53562700
N 0.460493 1.425245 -0.01607700
N -0.166614 -1.125499 0.29669800
Ni -0.214123 0.073155 -1.35337000
H -1.034046 -2.815451 -0.48192300
H 0.366338 3.109535 -1.18925600
C -1.569932 -0.658082 -2.73042800
C -2.131175 0.419952 -2.03326600
H -1.181485 -0.497323 -3.73182400
H -2.078505 1.403759 -2.49960500
C -3.063776 0.341772 -0.89224200
C -3.593402 -0.869983 -0.41976400
C -3.433161 1.524726 -0.22877700
C -4.441759 -0.897746 0.68289600
H -3.339684 -1.798889 -0.91501100
C -4.282219 1.498249 0.87281000
H -3.030390 2.470563 -0.57643400
C -4.789300 0.284097 1.33897300
H -4.835290 -1.846552 1.03113800
H -4.547077 2.424884 1.37027500
H -5.449497 0.259615 2.19842400
H -1.828666 -1.685324 -2.49522400

Int-SW1-S-F

PBE SCF Energy: -1405.20943201 a.u.

C 1.79050800 1.42135500 0.51748100
C -0.4248210 0.8809080 0.13252800
C -0.7537330 2.22762300 0.02489100
C 0.22298500 3.22114100 0.16863100
C 1.52552900 2.78131100 0.41999000
H -1.7768940 2.51022400 -0.17615000
H 2.34608100 3.47344300 0.54114900
C -1.3966470 -0.2291080 -0.01936700
C -2.7495690 -0.0224210 -0.24645700
C -3.6210160 -1.1083320 -0.38921700
H -3.1293470 0.98652000 -0.31192400
C -1.6806730 -2.5350910 -0.05970000
C -3.0498120 -2.3751830 -0.29292000
H -3.6518160 -3.2663080 -0.39433300
N 0.8458980 0.4824900 0.38258900
N -0.86244200 -1.475200 0.07933400
Ni 1.1104220 -1.4718740 0.51338400
O 0.0441570 -1.2579040 3.42281500
H 0.1612600 -0.3457780 3.13340500
C 5.7632740 -0.03748600 -0.64357300
C 5.6765850 -0.41799100 -1.98283900
C 4.6975760 -1.34180400 -2.35904400
C 3.8189040 -1.86923400 -1.41854500
C 3.8853490 -1.49488800 -0.05932600
C 4.8864820 -0.56947600 0.29929700
H 6.5200780 0.67418600 -0.32961500
H 6.3578990 -0.00652500 -2.71887000
H 4.6165060 -1.65013300 -3.39653100
H 3.0545290 -2.56853800 -1.73729600
H 4.9716670 -0.26708000 1.33896600
C 2.9358320 -1.9829680 0.95553200
C 2.0583480 -3.1211440 0.79294500
H 3.2167790 -1.7074320 1.97402800
H 0.3778880 -1.7509230 2.65288000
H 2.1605160 -3.76384200 -0.08367000
H 1.8034070 -3.69109100 1.68815500
C -0.1612320 4.6992890 0.04478200
C 1.0503740 5.6297420 0.22695600
H 1.8166440 5.4502030 -0.53181800

H 0.7263200 6.6687600 0.13190200
H 1.5056300 5.5131740 1.21400500
C -1.2100220 5.0394020 1.12891700
H -1.4942030 6.0923540 1.05158100
H -2.1164240 4.43961500 1.02062700
H -0.8045960 4.86685500 2.12946700
C -0.7657280 4.94807400 -1.35667900
H -1.0395950 6.00157300 -1.45915500
H -0.0437120 4.70385400 -2.14040100
H -1.6648420 4.35102200 -1.52478000
C -5.1139330 -0.8703980 -0.63832100
C -5.2832520 -0.0663470 -1.94818800
H -6.3453220 0.1077730 -2.14133000
H -4.7893190 0.90632100 -1.89584900
H -4.8660460 -0.6145190 -2.79711200
C -5.6988860 -0.06372600 0.54407300
H -6.7653990 0.11306000 0.38008100
H -5.5827950 -0.61191600 1.48278200
H -5.2124730 0.9078360 0.65497600
C -5.8993890 -2.1866040 -0.76730500
H -5.5434820 -2.7905600 -1.60615000
H -5.834300 -2.7867370 0.14404000
H -6.9540370 -1.9623500 -0.94318700
C -1.07491600 -3.9037410 0.04671400
H -0.2762970 -4.0189540 -0.68846700
H -0.6105610 -4.0320570 1.02630700
H -1.8248320 -4.6804250 -0.10525000
H 2.7931130 1.0556820 0.69927300

Int-SW1-S

PBE SCF Energy: -1051.74504237 a.u.

C 0.520790 2.100527 0.49956000
C -1.601913 1.474926 -0.21657200
C -1.971934 2.809946 -0.37326800
C -1.051113 3.809180 -0.07556200
C 0.219585 3.450234 0.36593700
H -2.959911 3.071701 -0.72577400
H -1.322566 4.851086 -0.19190700
H 0.967187 4.196134 0.60218300
C -2.483279 0.322618 -0.51274400
C -3.805367 0.436442 -0.94021200
C -4.539824 -0.717053 -1.19401600
H -4.260654 1.408164 -1.07211900
C -2.615147 -1.997402 -0.58095100
C -3.934774 -1.957638 -1.01332700
H -5.567960 -0.645909 -1.52651000
H -4.469542 -2.879699 -1.20005600
N -0.365082 1.132412 0.22246800
N -1.899996 -0.889703 -0.33399600
Ni -0.046962 -0.828687 0.36212100
H -2.096746 -2.932982 -0.41769100
H 1.495915 1.762493 0.82712600
O -1.461941 -0.589258 3.13792400
H -1.123380 0.264018 2.84252700
C 4.682716 0.684295 -0.04798000
C 4.834591 0.315391 -1.38505500
C 3.963049 -0.633958 -1.92524100
C 2.956524 -1.198957 -1.14866200
C 2.782014 -0.837331 0.20409000
C 3.677619 0.116008 0.73084300
H 5.352741 1.415525 0.39266100
H 5.616591 0.755086 -1.99359600
H 4.068359 -0.934702 -2.96276200
H 2.284664 -1.923317 -1.59439900
H 3.576939 0.410002 1.77158800
C 1.695532 -1.366673 1.04615700
C 0.849336 -2.492436 0.71134900
H 1.820061 -1.132548 2.10513400
H -1.127965 -1.180426 2.44447200
H 1.074411 -3.100850 -0.16696100
H 0.467454 -3.094145 1.53792900

Int-SW2-S

PBE SCF Energy: -1051.74459716 a.u.

C 0.526407 2.025320 0.33194000
C -1.635681 1.409851 -0.26540600
C -1.955094 2.730997 -0.57564100
C -0.987502 3.717940 -0.41890300
C 0.277258 3.360224 0.04022900
H -2.938956 2.989972 -0.94161500
H -1.218493 4.748877 -0.65691400
H 1.059850 4.096073 0.17109100
C -2.567594 0.269072 -0.40900000
C -3.906367 0.391210 -0.77807900
C -4.688766 -0.753575 -0.88710900
H -4.337729 1.363117 -0.97353000
C -2.774598 -2.041791 -0.25674900
C -4.113783 -1.993703 -0.62337900

H -5.730571 -0.676027 -1.17224700
H -4.686034 -2.909130 -0.69772000
N -0.403556 1.069391 0.18822200
N -2.013412 -0.942268 -0.14927900
Ni -0.136863 -0.886071 0.46261100
H -2.275885 -2.976809 -0.03844000
H 1.491364 1.689360 0.68745700
C 4.549770 0.565248 -0.26661100
C 4.596736 0.213344 -1.61615300
C 3.682197 -0.725215 -2.10044500
C 2.735257 -1.296869 -1.25611100
C 2.666390 -0.950730 0.10920000
C 3.604102 -0.008744 0.57914200
H 5.254542 1.288560 0.13057900
H 5.331841 0.658380 -2.27702300
H 3.706773 -1.013008 -3.14661900
H 2.027967 -2.013106 -1.65799100
H 3.580260 0.276031 1.62707900
C 1.640963 -1.481134 1.02670200
C 0.734399 -2.572367 0.73564700
H 1.893207 -1.317192 2.07665500
H 0.869371 -3.168580 -0.16917200
H 0.395793 -3.174413 1.58019500
O 0.254892 0.707435 3.30975200
H -0.531492 1.131364 2.94979000
H 0.515424 0.112715 2.58904500

Int-SW3-S

PBE SCF Energy: -1051.7425687 a.u.

C 0.849114 1.523240 -1.08043800
C -1.302266 1.555077 -0.22208400
C -1.340116 2.945495 -0.30138800
C -0.236427 3.634378 -0.78852300
C 0.874158 2.906004 -1.19861700
H -2.226670 3.484200 0.00190900
H -0.251337 4.714936 -0.85655300
H 1.753803 3.390021 -1.60174400
C -2.444697 0.731739 0.20830100
C -3.657927 1.226922 0.68660400
C -4.660512 0.327111 1.03097400
H -3.820868 2.290240 0.79308000
C -3.191406 -1.459246 0.41488300
C -4.427565 -1.038840 0.88998500
H -5.609980 0.689627 1.40535300
H -5.184695 -1.768595 1.14543800
N -0.198337 0.845764 -0.58708100
N -2.227293 -0.593375 0.08295300
Ni -0.352914 -1.103231 -0.41713800
H -2.918897 -2.498989 0.28460200
H 1.699385 0.933409 -1.37470200
O -0.865198 -2.868867 -0.38453300
H -0.134500 -3.463734 -0.57465300
C 3.089862 0.047522 2.42648500
C 4.204056 0.705209 1.89395600
C 4.469829 0.587285 0.53306700
C 3.633476 -0.171540 -0.29015800
C 2.499858 -0.826241 0.22004800
C 2.258346 -0.700434 1.60308900
H 2.869901 0.125569 3.48623100
H 4.851177 1.295624 2.53287000
H 5.333144 1.085351 0.10379200
H 3.870909 -0.247877 -1.34510700
H 1.383167 -1.191519 2.01802300
C 1.556419 -1.635893 -0.61812200
C 1.925054 -1.792900 -2.09355100
H 1.535826 -2.631822 -0.16031700
H 1.218239 -2.470212 -2.57849700
H 1.884466 -0.845419 -2.64112200
H 2.933963 -2.205465 -2.24066600

Int-SW4-S

PBE SCF Energy: -1051.74309655 a.u.

C -3.301185 -1.017204 0.52773600
C -2.179907 0.962978 0.05525000
C -3.256654 1.721652 0.51535600
C -4.385149 1.064943 0.99325400
C -4.410722 -0.327700 1.00096100
H -3.221066 2.801882 0.50201300
H -5.232441 1.634860 1.35435000
H -5.271075 -0.873139 1.36610900
C -0.922813 1.513596 -0.48010300
C -0.646906 2.877546 -0.54745700
C 0.566377 3.306455 -1.07078400
H -1.369988 3.597819 -0.19159000
C 1.133425 1.009621 -1.42111400
C 1.470755 2.352092 -1.52019800
H 0.797224 4.363040 -1.12423700
H 2.430378 2.630025 -1.93477300

N -2.216536 -0.385125 0.06600100
N -0.029423 0.579161 -0.90904700
Ni -0.553824 -1.286280 -0.59376300
H 1.820870 0.246224 -1.74410900
H -3.231404 -2.097529 0.50394200
C 4.222574 0.668859 0.66117700
C 3.473096 1.346735 1.62156600
C 2.286433 0.781195 2.09053100
C 1.853500 -0.446103 1.59453000
C 2.588372 -1.133065 0.62021000
C 3.782223 -0.560293 0.16901800
H 5.148417 1.097490 0.29275600
H 3.810253 2.304278 2.00250700
H 1.695916 1.299762 2.83818300
H 0.917073 -0.871256 1.94135400
H 4.366438 -1.077894 -0.58590600
C 2.060847 -2.411885 0.00983500
C 1.092538 -2.164603 -1.17002800
H 2.913640 -3.024404 -0.31491300
H 1.611185 -1.607744 -1.96174300
H 0.836739 -3.136908 -1.61382800
O -1.275826 -2.909963 -0.13862800
H -0.682022 -3.629484 -0.37016000
H 1.534417 -2.988633 0.77730600

Int-W1-S

PBE SCF Energy: -742.316613102 a.u.
C -0.357816 1.181074 0.05685700
C -2.511590 0.369043 0.48051900
C -3.088301 1.564606 0.11212700
C -2.257571 2.622551 -0.31411300
C -0.891069 2.414347 -0.34948100
C 1.042268 0.832098 -0.01759200
C 2.557631 -0.960725 -0.02461200
C 3.634422 -0.110216 0.09951600
C 3.409685 1.282008 0.10389700
C 2.107168 1.742249 0.05704300
H -3.120174 -0.465256 0.81256300
H -4.163168 1.686176 0.17204600
H -2.681675 3.568459 -0.62807300
H -0.227968 3.186559 -0.72101600
H 2.688961 -2.033352 -0.09528400
H 4.636039 -0.517533 0.15496300
H 4.238569 1.975906 0.17080100
H 1.895933 2.802517 0.12318500
N -1.170477 0.144490 0.48651900
N 1.273205 -0.527171 -0.13649100
Ni -0.277910 -1.564608 -0.05216400
H -1.588858 -3.622023 -0.75736600
O -1.789082 -2.823725 -0.25350000
H -2.171581 -3.126086 0.58161400

Int-W1-T

PBE SCF Energy: -742.327090303 a.u.
C -0.349602 -1.206020 -0.00007500
C -2.570689 -0.415348 0.00096000
C -3.100135 -1.690849 0.00073400
C -2.193202 -2.782942 -0.00013300
C -0.840743 -2.539530 -0.00045300
C 1.031067 -0.836929 -0.00023200
C 2.573705 0.951684 -0.00094600
C 3.661924 0.103986 0.00058500
C 3.414985 -1.294670 0.00161200
C 2.119012 -1.749972 0.00113700
H -3.217075 0.457537 0.00165600
H -4.171808 -1.841110 0.00112300
H -2.563062 -3.802116 -0.00058900
H -0.144664 -3.369040 -0.00118900
H 2.707215 2.028669 -0.00185800
H 4.667206 0.504413 0.00098900
H 4.240420 -1.997454 0.00285200
H 1.923250 -2.814933 0.00208400
N -1.252437 -0.148378 0.00038600
N 1.291444 0.533542 -0.00136800
Ni -0.321060 1.607926 -0.00162400
H -2.155650 3.271946 0.78676900
O -1.605452 3.171021 -0.00038600
H -2.203511 3.239368 -0.75553000

Int-W2-S

PBE SCF Energy: -1358.73403339 a.u.
C 0.699518 0.607146 -0.18982800
C 2.698492 1.764802 -0.51492600
C 3.414477 0.586437 -0.32846100
C 2.779698 -0.643036 -0.09084800
C 1.364407 -0.638143 -0.04418800
C -0.711156 0.683491 -0.05664500
C -2.577296 2.094506 0.00720400

C -3.414507 0.985138 -0.05523800
C -2.916536 -0.327493 -0.05809900
C -1.510208 -0.487143 -0.04435200
H 4.495347 0.619240 -0.39713500
H -4.485302 1.145505 -0.08134100
N 1.344925 1.800333 -0.46175700
N -1.231668 1.956051 0.08292200
Ni 0.114163 3.266571 0.18833000
O 1.248958 4.797161 0.73235600
C 3.397944 3.061302 -0.80936900
H 2.880609 3.592267 -1.61354900
H 3.381118 3.710034 0.07171600
H 4.437277 2.901483 -1.09872500
C -3.112828 3.494193 0.03185100
H -2.585331 4.069342 0.80356700
H -2.913681 3.997088 -0.91929300
H -4.187841 3.517224 0.21618600
C 0.541397 -1.812537 0.06346400
C -0.818430 -1.744654 0.03427200
H 1.020517 -2.779462 0.13998300
H -1.396523 -2.657049 0.09507200
C 3.598846 -1.864748 0.08593800
C 4.622132 -2.170049 -0.82674900
C 3.411769 -2.721458 1.18344600
C 5.420242 -3.297883 -0.65584900
H 4.778649 -1.524156 -1.68344300
C 4.211021 -3.849008 1.35436100
H 2.648393 -2.487681 1.91624300
C 5.217363 -4.144178 0.43466100
H 6.198354 -3.519164 -1.37792900
H 4.052991 -4.492742 2.21249100
H 5.838879 -5.022213 0.56797900
C -3.864990 -1.465597 -0.09229600
C -3.748887 -2.487013 -1.04928800
C -4.938154 -1.520531 0.81159100
C -4.666955 -3.533241 -1.09184200
H -2.946073 -2.446973 -1.77612200
C -5.855105 -2.567567 0.76940500
H -5.041118 -0.742560 1.55977300
C -5.722610 -3.579846 -0.18141500
H -4.562400 -4.308085 -1.84308200
H -6.671481 -2.595258 1.48246400
H -6.436681 -4.394712 -0.21456500
H 1.576990 5.334067 -0.00163300
H 0.818413 5.410504 1.34029500

Int-W2-T

PBE SCF Energy: -1358.74586652 a.u.

C -0.708858 0.606155 0.00209300
C -2.714820 1.819331 0.08466100
C -3.448625 0.637994 0.06771500
C -2.812020 -0.621191 -0.01055200
C -1.402765 -0.640975 -0.02086600
C 0.702331 0.655276 -0.00556100
C 2.623289 2.009114 -0.06869000
C 3.435528 0.887006 -0.06042600
C 2.888984 -0.420229 0.00779200
C 1.483575 -0.537836 0.01304100
H -4.529950 0.690459 0.07755100
H 4.510406 1.016545 -0.06204900
N -1.370128 1.825665 0.03285000
N 1.275986 1.919035 -0.02779500
Ni -0.063922 3.335666 -0.01155700
O -0.778694 5.238283 -0.03006900
C -3.391112 3.159976 0.16364900
H -3.154806 3.643711 1.11687000
H -3.017670 3.822381 -0.62092400
H -4.474381 3.069800 0.07675800
C 3.190327 3.400385 -0.10519400
H 2.820519 3.933976 -0.98718600
H 2.854922 3.965725 0.77088600
H 4.280484 3.396534 -0.12670300
C -0.597726 -1.831759 -0.01501000
C 0.762317 -1.782957 -0.00496500
H -1.089810 -2.795299 -0.01223400
H 1.320750 -2.709496 -0.01737900
C -3.646386 -1.844066 -0.07118800
C -4.693667 -2.029430 0.84701300
C -3.458292 -2.819684 -1.06478700
C -5.510174 -3.155432 0.78608300
H -4.854859 -1.288807 1.62237100
C -4.276220 -3.945183 -1.12662500
H -2.679052 -2.681284 -1.80505500
C -5.304234 -4.120642 -0.20012000
H -6.305823 -3.281575 1.51204600
H -4.115807 -4.681738 -1.90618600
H -5.940206 -4.997144 -0.24884400
C 3.809214 -1.577375 0.06757500

C 3.675656 -2.581969 1.04235600
C 4.889492 -1.669662 -0.82780800
C 4.574272 -3.643695 1.10655000
H 2.874479 -2.514259 1.76891800
C 5.787749 -2.731248 -0.76351200
H 5.011714 -0.907382 -1.58924900
C 5.633845 -3.726208 0.20268800
H 4.453116 -4.402256 1.87208400
H 6.607124 -2.784281 -1.47203000
H 6.333614 -4.552524 0.25370900
H -0.682953 5.752265 0.78153500
H -0.493523 5.812649 -0.75159600

$Mn(H_2O)_6$-H

PBE SCF Energy: -562.699207391 a.u.

Mn 0.001571 -0.071712 -0.70000100
O 2.277753 2.342217 0.42110500
O -1.011924 -1.810081 0.57422900
O 3.161190 -0.214570 1.07298500
O -3.283923 -0.461471 1.15579000
H 1.933363 2.732172 1.23597200
H -1.196693 -2.591840 0.03869100
H 2.643899 -0.419709 1.86071500
H 2.904286 0.709158 0.85012000
H -3.197847 -0.084353 2.03888700
H -3.218234 0.309783 0.54930500
O -2.944562 1.715127 -0.55857400
O 1.899827 -1.583446 -0.90306700
H 1.463354 2.057021 -0.05639500
H -1.891842 -1.424359 0.81702800
H -3.106740 1.392478 -1.45603700
H -1.961651 1.756439 -0.52714700
H 2.329540 -1.374687 -1.74220600
H 2.472397 -1.171514 -0.20864300

$Mn(OCOOH)_2(H_2O)_4$-H

PBE SCF Energy: -938.599181079 a.u.

Mn -0.030741 0.714789 -0.02109000
O 1.829896 -0.288089 -0.55024100
O 1.175784 2.377665 -0.98489900
H 2.038465 1.963115 -1.12826400
H 1.346362 3.194076 -0.50019100
O -1.325397 2.467218 0.68046500
H -1.563365 3.161805 0.05497500
H -2.141079 1.974878 0.85912200
O -1.895390 -0.189372 0.55019000
O 0.521445 0.303925 2.09461200
H -0.201269 -0.195534 2.49366400
H 1.297803 -0.320879 1.99801000
O -0.487022 0.040781 -2.13828400
H -1.136925 -0.679623 -2.00379100
H 0.331409 -0.387578 -2.42235300
C -2.693785 -1.088734 0.13753200
O -3.755620 -1.458209 0.61388700
C 2.612102 -0.987010 0.16123800
O 2.551164 -1.192098 1.38921200
O -2.237456 -1.712919 -1.03571600
O 3.627146 -1.562694 -0.54407100
H -2.909965 -2.351810 -1.30491400
H 4.160772 -2.063397 0.08713200

$Mn^{2+}(H_2O)_4$-branacid-H

PBE SCF Energy: -1406.97086223 a.u.

Mn 0.029998 -1.927521 0.06709000
O -0.507807 -2.070535 -2.11140900
O -2.037423 -1.772521 0.47500900
O 2.135702 -1.565560 -0.33054800
O 0.614960 -2.008873 2.21028500
O 0.828150 -4.043135 -0.38462100
H -1.497019 -1.932517 -2.06199900
H -0.366129 -2.972655 -2.42172800
H 1.779312 -3.863292 -0.38784200
H 0.691344 -4.769363 0.23520100
H 1.580566 -1.734185 2.16867900
H 0.574194 -2.849040 2.67972800
O -0.000998 0.315028 -0.02003900
H 0.649100 0.736061 -0.59911900
H -0.823281 0.815466 -0.11414600
C -2.942745 -1.298984 -0.29280400
O -2.999671 -1.460421 -1.53027900
C -3.966273 -0.374453 0.38939900
H -4.122495 -0.762900 1.39781800
C -3.281547 0.981712 0.51179000
C -2.947116 1.510763 1.76207600
C -2.918487 1.701234 -0.63778100
C -2.269986 2.726361 1.86653200
H -3.209700 0.961753 2.65968000
C -2.241246 2.916486 -0.53508300

H -3.145374 1.290568 -1.61464700
C -1.912302 3.432009 0.71940400
H -2.014051 3.116157 2.84521000
H -1.956798 3.450435 -1.43432600
H -1.375661 4.369757 0.79968800
C -5.304646 -0.303911 -0.35295300
H -5.776073 -1.289329 -0.38492900
H -5.983515 0.387770 0.15179600
H -5.163064 0.031656 -1.38090400
C 2.973874 -0.986257 0.43846400
O 3.003575 -1.090487 1.68398600
C 3.952335 -0.018455 -0.25588400
H 4.188829 -0.458608 -1.22707300
C 3.152136 1.254034 -0.50540700
C 2.620450 1.519576 -1.77399100
C 2.844776 2.131940 0.54242100
C 1.805587 2.632843 -1.99174900
H 2.838633 0.844367 -2.59398000
C 2.033637 3.243636 0.32741400
H 3.218589 1.929131 1.53846900
C 1.507993 3.497880 -0.93936500
H 1.399842 2.816999 -2.97997600
H 1.796149 3.903303 1.15409400
H 0.867521 4.356296 -1.10275400
C 5.243215 0.203902 0.53632200
H 5.800781 -0.732003 0.62203600
H 5.877859 0.938807 0.03512900
H 5.030653 0.553534 1.54674100

$Mn^{2+}(H2O)_6$-H
PBE SCF Energy: -562.492842362 a.u.
Mn -0.047809 -0.021599 -0.16900900
O -1.059386 -1.487275 1.09553300
O -2.008241 -0.156801 -1.23576900
O 1.468479 0.148564 1.47526400
O 1.433260 1.386930 -1.02312900
O -1.116340 1.658582 0.81797700
H -2.083361 -0.506275 -2.13220200
H -2.525826 0.658270 -1.20830200
H -1.994421 -1.685847 0.96663700
H -0.820957 -1.744717 1.99337400
H -1.588052 1.533494 1.65055700
H -0.751340 2.551573 0.83695500
H 1.281750 0.463712 2.36715900
H 2.088235 -0.587076 1.55648100
H 2.046321 1.762580 -0.37889100
H 1.260084 2.062036 -1.68977600
O 1.422566 -1.568111 -0.79067200
H 1.149127 -2.483442 -0.92888500
H 2.010952 -1.339437 -1.52151000

$Mn^{2+}(OCOOH)_2(H_2O)_2$-linacid2-H-B
PBE SCF Energy: -1478.43538674 a.u.
Mn 0.217126 -0.714634 0.22486600
O -1.746681 -1.589501 0.35982300
O 2.228687 0.019042 0.01280500
O 0.764203 -1.028473 2.49057900
O 0.192290 -1.194687 -1.98562800
H 0.774227 -1.974684 -2.03394200
H -0.749479 -1.524725 -2.04035600
H 1.563384 -0.432201 2.47076100
H 1.105983 -1.898564 2.21833600
C 2.916449 0.699084 0.84089200
O 2.825278 0.625172 2.08986200
C 3.921538 1.679215 0.23087700
H 4.333531 2.300416 1.03032800
H 4.745103 1.089646 -0.18811500
C 3.289927 2.542834 -0.87025200
H 4.063974 3.158190 -1.34426000
H 2.891540 1.877425 -1.64242700
C -2.611142 -1.761778 -0.55980600
O -2.355731 -1.852260 -1.78665600
C -4.074671 -1.789222 -0.13189800
H -4.161217 -2.263947 0.84968100
H -4.638655 -2.377975 -0.85873400
C -4.647648 -0.356899 -0.06864400
H -5.738710 -0.418056 0.02093700
H -4.442459 0.146018 -1.02173200
C -1.125010 2.167808 -0.03744100
O -1.436226 3.293854 0.35461400
O -0.519975 1.253860 0.59659600
O -1.458359 1.811894 -1.34244800
H -1.900892 2.581704 -1.72100200
C 2.189338 -3.213520 -0.09868600
O 3.286552 -3.548595 0.34005600
O 2.004954 -3.265262 -1.49675900
O 1.151369 -2.822801 0.50593700
H 2.851782 -3.521836 -1.88257200

C 2.161794 3.440698 -0.35040400
H 1.443398 2.828420 0.20106100
H 2.575259 4.161646 0.36640400
C 1.424360 4.183459 -1.46746500
H 0.624593 4.808109 -1.06259300
H 2.105032 4.820499 -2.04229600
H 0.962448 3.471968 -2.15910200
C -4.094298 0.489475 1.08336700
H -3.003484 0.501279 1.03538200
H -4.355366 0.004843 2.03276500
C -4.630139 1.923439 1.07025600
H -4.254027 2.494984 1.92295300
H -4.313182 2.446802 0.16359900
H -5.724818 1.940397 1.10825100

$Mn^{2+}(OCOOH)_2(H_2O)_2$-linacid2-H
PBE SCF Energy: -1783.02919331 a.u.
Mn 0.143980 0.839020 -0.19292700
O 2.152535 0.498384 -0.85887300
O -1.896413 1.304051 0.32824100
O 0.653323 1.196974 2.06291000
O -0.362345 1.402429 -2.33198800
H -0.461289 2.369360 -2.26226600
H 0.530609 1.226854 -2.74137000
H -0.289859 1.106806 2.37547000
H 0.744458 2.139975 1.84051300
C -2.503794 1.154067 1.43412800
O -1.955655 0.961237 2.54631000
C -4.030866 1.260191 1.39642800
H -4.434904 0.773842 2.28709200
H -4.269772 2.327788 1.47652500
C -4.675018 0.693780 0.11798800
H -5.730897 0.980168 0.10057900
H -4.193108 1.162728 -0.74239300
C -4.564482 -0.812475 0.00989900
C -3.420320 -1.417470 -0.52671500
C -5.597824 -1.636942 0.47253100
C -3.318635 -2.805761 -0.60576900
H -2.593126 -0.801550 -0.85458100
C -5.497746 -3.026063 0.39849700
H -6.491963 -1.184739 0.89125700
C -4.356509 -3.615968 -0.14533200
H -2.424559 -3.246045 -1.03209200
H -6.311403 -3.645898 0.75989800
H -4.277275 -4.695765 -0.20874800
C 2.605956 0.284465 -2.02690100
O 2.068524 0.666098 -3.09555500
C 3.915978 -0.498154 -2.12427800
H 4.737211 0.195581 -1.91217800
H 4.034832 -0.823776 -3.15955600
C 4.001362 -1.714062 -1.17595200
H 4.816868 -2.352908 -1.53458500
H 3.083027 -2.301590 -1.25579500
C 4.258581 -1.385144 0.27967100
C 3.326865 -1.713748 1.26944900
C 5.451579 -0.762934 0.66741700
C 3.577383 -1.417793 2.60912100
H 2.397579 -2.191576 0.98126200
C 5.703808 -0.462146 2.00506500
H 6.192013 -0.509194 -0.08534600
C 4.763897 -0.787443 2.98370500
H 2.837595 -1.671219 3.36120200
H 6.633505 0.022726 2.28364500
H 4.955353 -0.553038 4.02516800
C 0.167755 -2.245809 -0.61755300
O 0.693807 -3.316256 -0.29701400
O -0.113929 -1.253866 0.11201300
O -0.194285 -2.074364 -1.95173100
H 0.077619 -2.880280 -2.40826100
C -0.296141 3.983731 -0.11438600
O -0.876090 4.761454 0.63892600
O -0.603843 4.059253 -1.48936500
O 0.568302 3.096321 0.13359900
H -1.304411 4.716608 -1.58411800

$OCOOH^-$
PBE SCF Energy: -264.403644006 a.u.
O -1.175417 -0.637515 0.00006500
C -0.148069 0.057713 -0.00012000
O 0.004797 1.297094 0.00000900
O 1.061369 -0.698355 -0.00005300
H 1.762423 -0.036071 0.00054600

$OCOOH^·$
PBE SCF Energy: -264.194617259 a.u.
O -0.874740 -0.947600 -0.00023000
C -0.046153 -0.003199 0.00009700
O -0.554183 1.138296 -0.00003900

O 1.244364 -0.259254 0.00017100
H 1.753400 0.567657 0.00020100

Styrene
PBE SCF Energy: -309.350746792 a.u.
C 0.406551 -1.281408 0.00000200
C -0.514526 -0.221376 -0.00008900
C -0.010035 1.091157 -0.00012100
C 1.359479 1.328588 -0.00003700
C 2.262444 0.262399 0.00007200
C 1.779553 -1.044524 0.00008500
H 0.038578 -2.302370 0.00001000
H -0.691103 1.934026 -0.00024100
H 1.726781 2.348817 -0.00006600
H 3.329824 0.451443 0.00013400
H 2.470203 -1.880325 0.00016100
C -1.954728 -0.530611 -0.00013400
C -2.971939 0.336339 0.00018800
H -2.188667 -1.593215 -0.00045000
H -3.997559 -0.013204 0.00010800
H -2.828851 1.411451 0.00054400

TS-A-S
PBE SCF Energy: -494.038697752 a.u.
C 1.514365 -0.434900 -0.02633500
O 1.530777 1.122164 -0.04629500
H 2.023270 1.442782 0.72136700
H 0.420886 1.604533 -0.19670200
O -0.663559 2.049393 -0.35039900
H -1.377516 1.427505 0.05139900
H -0.850765 2.143646 -1.29295700
O -1.670570 -1.957436 -0.12710400
H -0.763067 -1.708193 -0.40589700
H -2.114132 -2.237699 -0.93534000
O 0.688475 -0.831644 -0.84177700
O 2.306404 -0.894372 0.76401600
H -2.417205 0.505230 1.59647600
O -2.415423 0.495960 0.63277900
H -2.216495 -0.440920 0.36990200

TS-AS1-S
PBE SCF Energy: -1240.20618969 a.u.
C 0.994749 -0.010742 1.48505200
C 0.985338 -2.330358 1.32800100
C 2.186246 -2.425035 2.01507100
C 2.807753 -1.255421 2.44923900
C 2.204520 -0.035358 2.17810200
C 0.274084 1.217013 1.12181700
C -1.520104 2.051848 -0.11577000
C -1.253951 3.349356 0.29228700
C -0.181169 3.573820 1.15653700
C 0.586387 2.498231 1.58026000
H 0.469776 -3.210877 0.96935700
H 2.620523 -3.398114 2.20362300
H 3.750171 -1.293601 2.98078900
H 2.678642 0.887570 2.48179700
H -2.341278 1.799028 -0.77323500
H -1.874886 4.162598 -0.05914200
H 0.049125 4.574816 1.49952500
H 1.410868 2.650003 2.26272700
N 0.389022 -1.154685 1.06568600
N -0.772281 1.014256 0.28618600
Ni -1.032896 -0.810874 -0.25418500
C -3.863288 -0.551421 0.16306600
O -2.959194 -0.550255 -0.74460800
O -5.116009 -0.198230 -0.30168300
O -3.764200 -0.811219 1.35771900
H -5.023759 -0.021704 -1.24636400
H -1.131771 -2.225156 -0.67659400
C 3.653203 -0.524593 -1.16715200
C 2.391258 -1.008501 -1.48944200
C 1.360915 -0.137887 -1.89416900
C 1.661167 1.235768 -1.97053300
C 2.925690 1.718478 -1.65083900
C 3.931180 0.841546 -1.24268200
H 4.423309 -1.217211 -0.84630600
H 2.202685 -2.071811 -1.40990500
H 0.879609 1.928826 -2.26390800
H 3.123743 2.783038 -1.71059300
H 4.915316 1.215854 -0.98561100
C -0.002993 -0.584871 -2.18281600
C -0.479230 -1.898627 -2.06499400
H -0.647497 0.142416 -2.66654000
H -1.378324 -2.164419 -2.60917300
H 0.222342 -2.715637 -1.93398200

TS-AS2-S
PBE SCF Energy: -1240.2022347 a.u.

C 0.781825 1.806283 0.15927900
C -0.559228 1.852718 -1.73964300
C -0.507050 3.238639 -1.79997100
C 0.219462 3.922444 -0.82968500
C 0.869102 3.197395 0.16192000
C 1.439104 0.933516 1.14741400
C 1.735299 -1.265350 1.83505500
C 2.642897 -0.887785 2.81500900
C 2.939796 0.463963 2.96276100
C 2.334573 1.384195 2.11646100
H -1.114650 1.276041 -2.46576100
H -1.028688 3.762095 -2.59020300
H 0.277973 5.003619 -0.84132800
H 1.432470 3.711454 0.92789800
H 1.478173 -2.302943 1.67736700
H 3.101100 -1.640219 3.44296600
H 3.640568 0.797213 3.71807400
H 2.572741 2.435062 2.19895200
N 0.067634 1.148100 -0.78585000
N 1.133494 -0.380213 1.03014000
Ni 0.012671 -0.785116 -0.53806400
C 2.866798 -1.000408 -1.57127600
O 1.772686 -1.642096 -1.56597000
O 3.998847 -1.792381 -1.79562800
O 3.082579 0.201175 -1.40575300
H 3.675367 -2.695260 -1.90182300
H -0.856614 -0.923946 -1.68422300
C -0.730024 -2.527959 0.09643600
C -1.768578 -1.920591 -0.63547600
H -0.192236 -3.357923 -0.34980400
H -2.032660 -2.370381 -1.58791000
H -0.755208 -2.507999 1.18039100
C -2.869744 -1.119625 -0.03554400
C -4.053807 -0.941045 -0.76136000
C -2.768056 -0.530667 1.23486700
C -5.113658 -0.205380 -0.23213200
H -4.144278 -1.380702 -1.74919100
C -3.825354 0.198496 1.76512200
H -1.846991 -0.625867 1.79782900
C -5.004440 0.365596 1.03361100
H -6.022146 -0.079087 -0.81013900
H -3.728586 0.646471 2.74769600
H -5.825424 0.940242 1.44670500

TS-BA1-S

PBE SCF Energy: -1704.31690054 a.u.

C 2.271278 2.053990 -0.44935600
C 0.299854 0.829187 -0.37330800
C -0.503271 1.984286 -0.24793400
C 0.159973 3.242811 -0.17380500
C 1.535356 3.244598 -0.30655100
H 2.074879 4.182349 -0.27356200
C -0.328774 -0.462908 -0.46833000
C -1.734059 -0.580046 -0.46532600
C -2.279575 -1.889039 -0.61974400
C -0.006949 -2.731614 -0.84047500
C -1.401008 -2.929502 -0.85419700
H -1.781250 -3.932120 -1.00412500
N 1.667388 0.859788 -0.44914100
N 0.505642 -1.526480 -0.59856100
Ni 2.420489 -0.981103 -0.13199600
O 1.432099 -3.042334 1.87424900
C 4.287015 -1.056914 0.18371600
C 3.724936 -2.313714 0.71253100
H 4.708201 -0.386941 0.93869200
H 2.389468 -2.474055 1.16077300
H 3.923311 -3.217468 0.13213000
H 3.943440 -2.481811 1.76884500
C 0.639610 -2.199327 2.42339200
O 0.813665 -0.997923 2.61810700
O -0.544033 -2.787993 2.80593600
H -1.072870 -2.091344 3.21619500
C 5.134230 -1.131060 -1.07790900
H 5.229021 -0.140282 -1.53060500
H 4.625935 -1.761256 -1.81761400
C 6.542191 -1.693244 -0.81483900
H 7.134086 -1.737188 -1.73454600
H 7.079887 -1.066160 -0.09650000
H 6.486109 -2.703320 -0.39862200
C -1.928703 1.835703 -0.26337400
C -2.517647 0.613900 -0.36940300
H -2.544385 2.723426 -0.22099400
H -3.595702 0.539576 -0.41087900
C -0.561797 4.523083 0.02878100
C -1.439115 4.693509 1.10950000
C -0.337624 5.600816 -0.83887000
C -2.078504 5.913163 1.31383900
H -1.604294 3.874690 1.79986200

C -0.985330 6.816996 -0.63754800
H 0.333606 5.477599 -1.68107600
C -1.856752 6.976738 0.43916800
H -2.746574 6.033495 2.15877400
H -0.810241 7.638427 -1.32266000
H -2.358539 7.924368 0.59704900
C -3.736515 -2.156715 -0.53794800
C -4.471950 -1.756330 0.58676000
C -4.388215 -2.856028 -1.56222900
C -5.830201 -2.046662 0.68138100
H -3.971468 -1.234235 1.39397500
C -5.749173 -3.137242 -1.46951400
H -3.828447 -3.165451 -2.43745400
C -6.473266 -2.733848 -0.34812700
H -6.384812 -1.739457 1.56045700
H -6.243569 -3.669887 -2.27369000
H -7.531776 -2.955308 -0.27565800
C 3.759578 2.112096 -0.60179700
H 4.246789 1.591215 0.22278300
H 4.057254 1.608395 -1.52267700
H 4.111192 3.142790 -0.63306700
C 0.927685 -3.883522 -1.05562300
H 1.895082 -3.526067 -1.40760100
H 1.085971 -4.399295 -0.10599100
H 0.511290 -4.589915 -1.77590600

TS-BA2-S

PBE SCF Energy: -1704.31679176 a.u.

C 2.321151 0.985991 -1.07805800
C 0.145556 0.390706 -0.53203100
C -0.273395 1.727888 -0.37970600
C 0.711106 2.741134 -0.57031200
C 1.980244 2.345908 -0.94670900
H 2.739891 3.092387 -1.14146200
C -0.799659 -0.687342 -0.41060400
C -2.157359 -0.402403 -0.15346400
C -3.063381 -1.502025 -0.12608200
C -1.171042 -2.975773 -0.57529200
C -2.544203 -2.763933 -0.34653000
H -3.207523 -3.619234 -0.36515700
N 1.426429 0.034673 -0.81905900
N -0.309789 -1.953589 -0.58379400
Ni 1.670779 -1.938396 -0.34557700
O 3.521918 -0.256348 1.41283400
C 3.415749 -2.744895 0.42365200
C 2.295603 -3.650443 0.14509200
H 3.710372 -2.763703 1.47800200
H 3.178295 -1.363677 0.77288300
H 2.393518 -4.325232 -0.70923800
H 1.809723 -4.131819 0.99491600
C 2.561468 0.248699 2.09273000
O 1.486571 -0.262083 2.39942200
O 2.841860 1.538748 2.48654400
H 2.074006 1.841191 2.98899400
C 4.636998 -2.784861 -0.49357300
H 5.217408 -1.863714 -0.37721100
H 4.296914 -2.805256 -1.53505500
C 5.538114 -3.995640 -0.22221100
H 6.405607 -4.008542 -0.88903500
H 5.906272 -3.980924 0.80887300
H 4.986694 -4.929850 -0.36421900
C 3.702038 0.586955 -1.50015200
H 4.376357 0.651209 -0.64415000
H 3.705576 -0.441293 -1.85817300
H 4.067732 1.249584 -2.28724100
C -1.632929 1.974822 -0.00370700
C -2.532080 0.958013 0.09943700
H -1.944386 2.989328 0.20415300
H -3.551995 1.172372 0.38745000
C 0.425983 4.183780 -0.36803100
C -0.577034 4.845065 -1.08887500
C 1.199531 4.909686 0.54772300
C -0.799997 6.206320 -0.89647400
H -1.169434 4.296148 -1.81154900
C 0.968344 6.268816 0.74470700
H 1.968916 4.397138 1.11431600
C -0.030991 6.920300 0.02251100
H -1.572188 6.709589 -1.46677400
H 1.567155 6.817338 1.46259800
H -0.209101 7.978684 0.17383000
C -4.519706 -1.337549 0.10870100
C -5.291519 -0.483644 -0.69192800
C -5.150912 -2.075984 1.11881100
C -6.663376 -0.370055 -0.48297000
H -4.818123 0.076770 -1.48950700
C -6.521535 -1.952816 1.33251000
H -4.560735 -2.734828 1.74534900
C -7.281096 -1.100280 0.53225700

H -7.249846 0.286497 -1.11522000
H -6.994982 -2.521721 2.12432300
H -8.348254 -1.006718 0.69707100
C -0.659578 -4.362185 -0.82654600
H 0.166531 -4.338165 -1.53541400
H -0.283293 -4.800619 0.10152000
H -1.454755 -5.003502 -1.20840200

TS-BC1-S

PBE SCF Energy: -1627.91407597 a.u.
C -1.252757 1.548478 -0.09885300
C -1.075904 2.960880 -0.07409300
C 0.218447 3.437694 -0.12896700
C 1.332965 2.579912 -0.17987400
C -1.553924 -2.712273 -0.25400500
C -0.354615 -3.390457 -0.37833800
C 0.881817 -2.720370 -0.33212800
H 0.394384 4.505187 -0.11010200
H -0.355620 -4.468152 -0.47980200
N 1.183167 1.248263 -0.17663000
N 0.931322 -1.399167 -0.14082700
Ni 2.506535 -0.180886 0.09663000
C 4.287280 0.412022 -0.13374900
C 4.457516 -0.877443 0.58048100
H 5.266417 -0.841822 1.31128300
H 4.586065 -1.768819 -0.03293200
H 4.653346 1.275294 0.42134600
C 4.657864 0.444837 -1.60824900
H 4.179937 1.299617 -2.09841900
H 4.260907 -0.448683 -2.10418500
C 6.177341 0.519508 -1.84262000
H 6.414001 0.551744 -2.91045000
H 6.596363 1.415825 -1.37501500
H 6.680081 -0.349822 -1.40905800
C 2.706214 3.176743 -0.20377600
H 3.237891 2.927265 0.71626200
H 3.286611 2.780326 -1.03478400
H 2.653170 4.261091 -0.29445100
C 2.171703 -3.461100 -0.51151500
H 2.734313 -3.014500 -1.33618900
H 2.779933 -3.373776 0.39086300
H 1.993304 -4.512634 -0.73539400
C 3.371363 -1.196952 1.96976100
O 3.058107 -0.175035 2.59206600
O 3.289011 -2.398947 2.21256000
C -2.208957 3.914786 0.00938100
C -3.155338 3.822372 1.04003900
C -2.319265 4.955517 -0.92275500
C -4.189729 4.749448 1.13252000
H -3.068480 3.034737 1.77928400
C -3.360675 5.875726 -0.83360200
H -1.595512 5.031605 -1.72611000
C -4.297763 5.775594 0.19408200
H -4.908630 4.672226 1.93989100
H -3.440125 6.669491 -1.56731100
H -5.106408 6.493785 0.26459500
C -2.829704 -3.469042 -0.22978200
C -3.754369 -3.287626 0.80881700
C -3.106704 -4.413644 -1.22757100
C -4.928911 -4.034105 0.84590800
H -3.541950 -2.575180 1.59728700
C -4.287028 -5.151534 -1.19371400
H -2.402253 -4.556306 -2.03893600
C -5.200422 -4.964867 -0.15678500
H -5.629846 -3.890882 1.66006900
H -4.493308 -5.870770 -1.97785000
H -6.117509 -5.541815 -0.12911300
C -1.503871 -1.289802 -0.17516400
C -0.226826 -0.688991 -0.13078600
C -0.092077 0.743721 -0.12446400
C -2.534528 0.911444 -0.16024500
C -2.656159 -0.442283 -0.20454500
H -3.420078 1.529846 -0.20501800
H -3.636248 -0.891033 -0.28866100

TS-BC2-S

PBE SCF Energy: -1627.91343433 a.u.
C -1.913932 2.350257 -0.33436100
C -2.937138 1.562169 -0.81954400
C -2.761433 0.186781 -1.08772000
C 1.920062 0.455249 -0.22228700
C 3.164345 -0.232990 -0.35051300
C 3.127215 -1.540975 -0.79450200
C 1.912668 -2.220489 -1.01189100
H -3.916687 1.993242 -0.98629000
H 4.051853 -2.083084 -0.94889300
N -1.602435 -0.417432 -0.82447800
N 0.745389 -1.613098 -0.78709800

Ni -1.000219 -2.344300 -0.40661500
C -1.695972 -3.625630 1.22692100
C -0.424997 -3.879138 0.56595000
H -0.344348 -4.792587 -0.02105800
H 0.481172 -3.652435 1.12825800
H -2.322338 -4.515928 1.32278800
C -1.698012 -2.799341 2.50425000
H -2.684924 -2.348440 2.62318300
H -0.983196 -1.975016 2.40312300
C -1.347268 -3.639801 3.73882900
H -1.361895 -3.032040 4.64819800
H -2.063919 -4.457116 3.86953300
H -0.351112 -4.082452 3.64477100
C -3.886606 -0.581557 -1.71157400
H -3.551411 -1.556874 -2.05496000
H -4.689552 -0.740714 -0.99005600
H -4.286491 -0.009600 -2.55310500
C 1.924913 -3.640149 -1.49463500
H 2.149533 -4.326335 -0.67373200
H 0.955512 -3.910027 -1.90936100
H 2.698490 -3.769079 -2.25443600
C -3.030305 -3.083848 -0.00205100
O -3.918212 -2.473850 0.57974300
O -2.956244 -3.680841 -1.09024500
C -2.163384 3.773788 -0.00116100
C -2.808479 4.612562 -0.92022600
C -1.797590 4.291704 1.24977100
C -3.073759 5.941268 -0.59878800
H -3.086126 4.225225 -1.89375300
C -2.072247 5.617875 1.57218600
H -1.314817 3.648062 1.97584600
C -2.707515 6.447057 0.64793700
H -3.564180 6.581314 -1.32305700
H -1.792985 6.002156 2.54637700
H -2.916465 7.480662 0.89839100
C 4.466740 0.412171 -0.05481700
C 5.503654 0.372631 -0.99691000
C 4.695751 1.032921 1.18172400
C 6.738166 0.950858 -0.71282700
H 5.333435 -0.097138 -1.95876800
C 5.933882 1.601862 1.46683400
H 3.908024 1.052359 1.92576300
C 6.956730 1.566247 0.51927700
H 7.527847 0.922557 -1.45466200
H 6.100226 2.069896 2.43014000
H 7.918617 2.014030 0.74058500
C 0.744782 -0.284877 -0.46249500
C 1.795317 1.854940 0.04978000
C 0.579625 2.469233 0.05938000
H 2.690834 2.439242 0.20950000
H 0.522242 3.535783 0.22803900
C -0.537332 0.362432 -0.46530700
C -0.625587 1.746120 -0.21158300

TS-BC3-S

PBE SCF Energy: -1627.92089591 a.u.

C 1.556117 1.436384 -0.03468900
C 1.456033 2.853064 -0.14923200
C 0.211002 3.384005 -0.43236200
C -0.928889 2.573120 -0.58593600
C 1.652902 -2.839688 -0.04528300
C 0.443743 -3.467599 -0.28890500
C -0.741410 -2.737292 -0.49087600
H 0.104077 4.452928 -0.56558200
H 0.405622 -4.547417 -0.35410300
N -0.850094 1.244429 -0.44772400
N -0.742023 -1.402187 -0.45069300
Ni -2.269888 -0.096853 -0.34096400
C -3.934325 0.626407 0.16072400
C -4.176979 -0.818194 0.02118700
H -4.045839 -1.296192 -0.95196700
H -4.033396 -1.467947 0.87973100
H -4.433751 1.231566 -0.60037800
C -4.047959 1.226845 1.55318300
H -3.591832 0.542893 2.27752600
C -2.247276 3.194006 -0.93897500
H -2.798938 2.545529 -1.61800900
H -2.861255 3.330314 -0.04605800
H -2.100028 4.170608 -1.40102900
C -2.038059 -3.439813 -0.76720000
H -2.710343 -3.338397 0.08828700
H -2.536889 -2.988463 -1.62661800
H -1.879331 -4.500271 -0.96154400
C 2.624657 3.756310 -0.00480000
C 3.779198 3.577956 -0.78060400
C 2.567419 4.835300 0.88782600
C 4.852168 4.457050 -0.66094700
H 3.827472 2.761323 -1.49130400

C 3.645659 5.707788 1.01239900
H 1.680881 4.978537 1.49488500
C 4.790683 5.520900 0.23890100
H 5.734530 4.312721 -1.27360300
H 3.591358 6.531820 1.71438700
H 5.628874 6.201371 0.33431600
C 2.879838 -3.655192 0.13361500
C 4.020374 -3.429132 -0.65036200
C 2.895263 -4.700039 1.06778500
C 5.150336 -4.228196 -0.49884800
H 4.013588 -2.639228 -1.39220000
C 4.029990 -5.491964 1.22396100
H 2.020301 -4.879024 1.68208100
C 5.160142 -5.258453 0.44125600
H 6.021370 -4.048295 -1.11825400
H 4.031286 -6.289821 1.95758300
H 6.042217 -5.876723 0.56119900
C 1.658976 -1.415717 0.01044600
C 0.432316 -0.753820 -0.21387700
C 0.376865 0.684740 -0.22259300
C 2.763654 0.736599 0.29136000
C 2.812502 -0.622884 0.31636900
H 3.648883 1.308264 0.53345500
H 3.735319 -1.120608 0.58048200
C -5.492691 1.537830 1.97949600
H -5.967625 2.219402 1.26662000
H -6.090338 0.624003 2.01701500
H -5.524095 2.007196 2.96769100
H -3.457711 2.148306 1.59841800
C -6.123551 -0.978451 -0.24542200
O -6.432275 -0.364988 -1.23435700
O -6.558340 -1.658688 0.64902100

TS-BC4-S

PBE SCF Energy: -1627.91836376 a.u.

C 1.029383 1.682267 -0.08482600
C 0.521516 3.007015 -0.22265200
C -0.814685 3.152009 -0.55289400
C -1.659131 2.039694 -0.72582900
C 2.360449 -2.383263 -0.07124600
C 1.394191 -3.331831 -0.35259100
C 0.047940 -2.984709 -0.57124800
H -1.223324 4.142416 -0.70811800
H 1.677142 -4.373471 -0.43520900
N -1.200102 0.797991 -0.55430000
N -0.351366 -1.709274 -0.51117800
Ni -2.155980 -0.958235 -0.36039600
C -4.062755 -0.998828 0.45833000
C -3.479264 -2.257176 0.00683900
H -3.871539 -2.691489 -0.91474900
H -3.319236 -3.008251 0.78183200
H -4.165941 -0.180803 -0.26078700
C -3.996619 -0.624583 1.93048800
H -4.867059 -1.064790 2.42998400
C -3.091370 2.225704 -1.13640600
H -3.411998 1.396333 -1.76782600
H -3.745191 2.256460 -0.26190200
H -3.217998 3.161613 -1.68186900
C -0.960026 -4.048791 -0.88701600
H -1.468265 -4.368746 0.02694400
H -1.720409 -3.662306 -1.56372200
H -0.476921 -4.920894 -1.32948500
C 1.369618 4.213409 -0.05477600
C 2.550437 4.379665 -0.79251300
C 0.968546 5.230879 0.82175500
C 3.313628 5.535618 -0.65163100
H 2.859018 3.611101 -1.49128500
C 1.738381 6.382053 0.96769800
H 0.059232 5.109326 1.39915100
C 2.912468 6.537605 0.23170000
H 4.219091 5.654901 -1.23526200
H 1.421493 7.156272 1.65687900
H 3.509950 7.434906 0.34385700
C 3.767832 -2.807213 0.13306900
C 4.810570 -2.245624 -0.61803300
C 4.066392 -3.817673 1.05760300
C 6.120900 -2.682340 -0.44329900
H 4.590312 -1.480567 -1.35313500
C 5.379063 -4.246523 1.23695400
H 3.267954 -4.255179 1.64595200
C 6.409499 -3.680256 0.48735000
H 6.915497 -2.245788 -1.03722800
H 5.596463 -5.021492 1.96286600
H 7.430709 -4.016060 0.62554500
C 1.946838 -1.020605 -0.01146700
C 0.585606 -0.744112 -0.25906200
C 0.124047 0.619101 -0.28825700
C 2.377836 1.362438 0.27821100

C 2.813656 0.073584 0.31465200
H 3.055901 2.164287 0.53573100
H 3.834470 -0.137181 0.60202800
C -3.981616 0.881852 2.19408000
H -3.075150 1.339988 1.78864300
H -4.846421 1.365352 1.72884700
H -4.016441 1.098399 3.26529900
H -3.110618 -1.081132 2.38685200
C -6.025655 -1.196149 -0.10955600
O -6.685135 -1.128746 0.89087500
O -6.052249 -1.332872 -1.30374500

TS-BCA1-D

PBE SCF Energy: -1892.91362461 a.u.
C -1.697208 1.624024 0.03617800
C -1.372644 3.007618 0.12428900
C -0.053969 3.339681 0.38168700
C 0.939398 2.355081 0.53594600
C -2.488949 -2.573035 0.19325900
C -1.390543 -3.385917 0.42560800
C -0.089532 -2.861745 0.51055900
H 0.221553 4.380501 0.50080100
H -1.533906 -4.450002 0.56613200
N 0.656841 1.055813 0.40222700
N 0.139224 -1.552119 0.35813900
Ni 1.899845 -0.603220 -0.11764800
C 3.727932 0.265453 -0.83574400
C 4.584669 -0.915592 -1.30857700
H 5.216481 -1.260870 -0.48114900
H 5.278722 -0.676717 -2.12673600
H 4.403901 1.002113 -0.38289900
C 3.074051 0.981414 -2.04614600
H 2.257735 1.635752 -1.72484900
H 2.603758 0.234229 -2.69734700
C 4.053734 1.826046 -2.88189900
H 3.559693 2.289908 -3.74352700
H 4.483501 2.627902 -2.27127000
H 4.883309 1.222519 -3.26166100
C 2.343813 2.758247 0.88581400
H 2.826282 1.979077 1.47171200
H 2.941564 2.907879 -0.01675700
H 2.342326 3.695023 1.44620200
C 1.084605 -3.746273 0.80988300
H 1.569455 -3.411015 1.73200100
H 0.780796 -4.786945 0.92770100
H 1.817592 -3.647791 0.00730300
C 3.754507 -2.124594 -1.76544500
O 2.544257 -2.175772 -1.33293100
O 4.276942 -2.985745 -2.49495300
C -2.385218 4.084894 -0.01688500
C -3.528671 4.120880 0.79405200
C -2.182186 5.116259 -0.94414600
C -4.448056 5.159937 0.67493500
H -3.687279 3.341696 1.53035100
C -3.106370 6.151133 -1.06709800
H -1.302728 5.096184 -1.57771000
C -4.241948 6.175754 -0.25838200
H -5.323123 5.178048 1.31443600
H -2.939724 6.936673 -1.79527500
H -4.960267 6.981993 -0.35274500
C -3.842335 -3.178035 0.11049900
C -4.888834 -2.736450 0.93344800
C -4.079667 -4.243000 -0.76974500
C -6.141305 -3.341881 0.87197000
H -4.713670 -1.929203 1.63491600
C -5.334871 -4.843093 -0.83488900
H -3.278781 -4.589742 -1.41283100
C -6.369387 -4.394150 -0.01469100
H -6.937514 -2.994585 1.52042300
H -5.504702 -5.659608 -1.52737700
H -7.345797 -4.862215 -0.06416800
C -2.258780 -1.173943 0.07059900
C -0.924207 -0.720027 0.19540900
C -0.640826 0.696442 0.19610300
C -3.013678 1.123049 -0.23031500
C -3.282602 -0.210172 -0.20823700
H -3.805463 1.824909 -0.45437800
H -4.286279 -0.557159 -0.41305700
C 5.119431 -0.005218 2.19893900
O 6.056904 0.281892 1.47443900
O 5.290636 -0.208696 3.53761400
O 3.868853 -0.165072 1.88094300
H 3.610165 -0.034712 0.78323900
H 6.231399 -0.079123 3.71735800

TS-BCW1-D

PBE SCF Energy: -1704.41274969 a.u.
C 1.334898 1.595450 -0.06439700

C 1.079566 2.971735 -0.22524900
C -0.206199 3.346967 -0.65749900
C -1.206922 2.402924 -0.87528300
C 2.010237 -2.628828 -0.08454400
C 0.904723 -3.423177 -0.47062700
C -0.340614 -2.869078 -0.72268500
H -0.420091 4.389972 -0.85450200
H 1.040799 -4.487670 -0.61508100
N -1.003141 1.088343 -0.66748000
N -0.571986 -1.540420 -0.58737900
Ni -2.357802 -0.506504 -0.50990100
C -4.292685 0.566742 0.24018600
C -5.275336 -0.569480 0.53647700
H -5.918510 -0.749091 -0.33572900
H -5.960829 -0.375913 1.37090600
H -4.843874 1.409927 -0.20044100
C -3.616712 1.088643 1.52471400
H -2.763359 1.726893 1.27779500
H -3.192977 0.240057 2.07844600
C -4.549935 1.876842 2.45997000
H -4.026540 2.208835 3.36326500
H -4.938080 2.766053 1.95157000
H -5.407623 1.276885 2.77704000
C -2.554386 2.848323 -1.37596200
H -2.987271 2.095849 -2.03322700
H -3.248504 2.998169 -0.54604600
H -2.466058 3.793610 -1.91408100
C -1.475551 -3.722495 -1.21419000
H -2.335489 -3.616711 -0.55194900
H -1.794293 -3.376872 -2.20375700
H -1.178614 -4.769448 -1.28938600
C -4.577156 -1.906182 0.82624900
O -3.365742 -2.025329 0.39467600
O -5.188192 -2.802591 1.42160900
C 2.095384 4.025312 0.00827300
C 3.366687 3.974447 -0.58685000
C 1.778373 5.139820 0.80220500
C 4.292990 4.993885 -0.38080200
H 3.619738 3.140385 -1.23054700
C 2.705833 6.156986 1.01071500
H 0.801439 5.195861 1.26921400
C 3.968698 6.087792 0.42155500
H 5.266496 4.937351 -0.85499200
H 2.443698 7.002827 1.63656100
H 4.690759 6.880121 0.58268200
C 3.311402 -3.285322 0.16934600
C 4.504335 -2.826467 -0.41726800
C 3.374317 -4.438834 0.97131900
C 5.712151 -3.482046 -0.19382400
H 4.477133 -1.963994 -1.07251200
C 4.582129 -5.093798 1.19473500
H 2.466914 -4.810851 1.43385200
C 5.759080 -4.617029 0.61613700
H 6.617066 -3.111709 -0.66296500
H 4.605504 -5.975433 1.82586600
H 6.699820 -5.126990 0.78944700
C 1.804008 -1.236379 0.00331800
C 0.507053 -0.722012 -0.29787600
C 0.277053 0.674691 -0.33401400
C 2.580859 1.049403 0.39422000
C 2.801750 -0.291614 0.42617500
H 3.357211 1.724731 0.72855600
H 3.751480 -0.662989 0.78770900
O -3.597573 -0.255449 -2.21220300
H -4.113358 -1.064580 -2.31557600
H -3.922389 0.194992 -1.19066600

TS-BW1-S

PBE SCF Energy: -1515.80675969 a.u.

C -0.587136 1.671838 -0.06434800
C -1.836462 2.346706 -0.16743300
C -2.958600 1.577412 -0.41273600
C -2.890074 0.179636 -0.54437500
C 3.069890 -0.540918 0.03199600
C 2.951765 -1.908000 -0.14034700
C 1.703685 -2.522429 -0.35796600
H -3.921004 2.058908 -0.52923600
H 3.840937 -2.525700 -0.14096400
N -1.723365 -0.467243 -0.42046400
N 0.581014 -1.799718 -0.40663100
Ni -1.407291 -2.370098 -0.44263500
C -2.830922 -3.230861 0.48559200
C -1.858073 -4.277002 0.11896800
H -2.274539 -5.114519 -0.44586400
H -1.198350 -4.637172 0.90959200
H -3.794139 -3.304591 -0.02302200
C -2.955684 -2.784781 1.93018000
H -1.957932 -2.740085 2.38132900

C -4.135342 -0.600382 -0.84483100
H -3.916324 -1.415960 -1.53295400
H -4.539847 -1.041039 0.06930600
H -4.898129 0.048447 -1.27620400
C 1.608869 -4.009871 -0.53090200
H 1.246993 -4.463562 0.39739900
H 0.888610 -4.254278 -1.31330400
H 2.583028 -4.441107 -0.76251500
C -1.970477 3.819634 -0.04339300
C -1.229422 4.686962 -0.85874100
C -2.884494 4.362052 0.87018000
C -1.397186 6.065428 -0.75749900
H -0.536160 4.278780 -1.58475600
C -3.043670 5.741496 0.97616300
H -3.458863 3.698783 1.50676700
C -2.300858 6.596404 0.16277600
H -0.824867 6.724260 -1.40026300
H -3.746694 6.147672 1.69420000
H -2.426882 7.669883 0.24345900
C 4.413079 0.065449 0.20948700
C 4.852698 1.102859 -0.62533200
C 5.281383 -0.425951 1.19375800
C 6.129426 1.637455 -0.47527500
H 4.198636 1.477679 -1.40382700
C 6.554995 0.116165 1.34782300
H 4.949201 -1.223890 1.84798400
C 6.982529 1.148817 0.51403300
H 6.458623 2.433108 -1.13356300
H 7.211941 -0.267079 2.12009700
H 7.974549 1.568941 0.63295100
C 1.872290 0.230993 0.02593300
C 0.658440 -0.456016 -0.20233100
C -0.585749 0.268348 -0.22656900
C 0.651413 2.326286 0.23527000
C 1.824013 1.638829 0.28300000
H 0.643090 3.386836 0.44504100
H 2.739345 2.157437 0.53292500
C -3.857829 -3.704821 2.76989800
H -4.868508 -3.743222 2.35112800
H -3.464214 -4.725744 2.78312600
H -3.934201 -3.356884 3.80490100
H -3.350266 -1.762780 1.96581900
O -1.014317 -3.753869 -2.46447500
H -1.212925 -3.936100 -0.95327600
H -0.290943 -3.165037 -2.70489700

TS-BW2-S

PBE SCF Energy: -1515.80355281 a.u.

C -0.132859 1.779694 -0.01116900
C -1.182197 2.738965 -0.10545400
C -2.453414 2.268596 -0.37112100
C -2.716077 0.896847 -0.56275300
C 2.886960 -1.241236 -0.04123100
C 2.450287 -2.526190 -0.30300700
C 1.089278 -2.830402 -0.48098900
H -3.273536 2.968985 -0.46786000
H 3.172252 -3.327269 -0.39667500
N -1.737587 -0.008294 -0.48290500
N 0.152574 -1.876815 -0.39300600
Ni -1.766999 -2.078858 -0.39657300
C -3.437751 -3.003562 0.38090100
C -2.146186 -3.680318 0.57036400
H -2.012632 -4.634313 0.06303500
H -1.704331 -3.674962 1.56866000
H -4.179923 -3.638029 -0.11822900
C -4.063879 -2.261609 1.56082700
H -3.312855 -1.609708 2.01972500
C -4.113636 0.442922 -0.86297400
H -4.101029 -0.459861 -1.47521400
H -4.633358 0.220455 0.07403000
H -4.671735 1.235013 -1.36569100
C 0.681912 -4.240405 -0.78912900
H 0.390263 -4.759893 0.12705400
H -0.175447 -4.251645 -1.46032400
H 1.511006 -4.786496 -1.24086200
C -0.955562 4.197775 0.05221900
C -0.009419 4.873022 -0.73203300
C -1.727539 4.931277 0.96340800
C 0.161416 6.248942 -0.60392600
H 0.578946 4.320815 -1.45543300
C -1.549222 6.306177 1.09588800
H -2.458650 4.417888 1.57746300
C -0.604773 6.968671 0.31281000
H 0.890182 6.758880 -1.22334000
H -2.147033 6.858785 1.81150400
H -0.467832 8.039045 0.41429700
C 4.337957 -0.980192 0.12978200
C 5.001485 -0.027041 -0.65613300

C 5.077497 -1.726838 1.05724300
C 6.371405 0.176236 -0.51281800
H 4.445655 0.540926 -1.39287700
C 6.446103 -1.515625 1.20498600
H 4.573474 -2.463676 1.67221600
C 7.096718 -0.563903 0.42071300
H 6.872390 0.910027 -1.13356200
H 7.002994 -2.093563 1.93347200
H 8.162285 -0.401451 0.53419300
C 1.901819 -0.215250 0.02648400
C 0.554801 -0.584833 -0.18694200
C -0.471621 0.423560 -0.22054400
C 1.221739 2.104595 0.31838100
C 2.193485 1.153099 0.33236900
H 1.469149 3.127072 0.56841000
H 3.207288 1.425784 0.59073600
C -4.635003 -3.216938 2.61617600
H -5.403771 -3.862757 2.17941900
H -3.851249 -3.862390 3.02315700
H -5.088492 -2.669170 3.44764400
H -4.862088 -1.606824 1.19933500
O -3.284373 -2.157637 -2.26911000
H -3.360892 -3.082327 -2.53087600
H -3.367334 -2.350690 -0.76908200

TS-SA1-S-F

PBE SCF Energy: -1593.67005635 a.u.

C 1.7652900 0.9885880 0.77276100
C -0.4813140 0.8713830 0.24271100
C -0.5712280 2.2626020 0.20261200
C 0.5506350 3.0530790 0.45637300
C 1.7391470 2.3719990 0.75469700
H -1.5147760 2.7211820 -0.04851100
H 2.6551890 2.9071080 0.96632500
C -1.6189820 -0.0359320 -0.02513700
C -2.9322430 0.4014580 -0.09394700
C -3.9732760 -0.5061840 -0.31903900
H -3.1480150 1.4504440 0.04492600
C -2.2711680 -2.2447430 -0.36125000
C -3.6081310 -1.8440160 -0.44213600
H -4.3517810 -2.6106380 -0.60158900
N 0.6799690 0.2410970 0.51660600
N -1.2845460 -1.3474960 -0.17060900
Ni 0.6381380 -1.6632540 -0.02212500
O 2.7928820 -1.6406750 1.96408800
C 5.1332520 -0.0647220 -1.68476600
C 4.5456470 0.5901160 -2.76647400
C 3.2582680 0.2269020 -3.16520800
C 2.5656290 -0.7729200 -2.48744600
C 3.1425900 -1.4391740 -1.39508100
C 4.4391520 -1.0676020 -1.01022900
H 6.1334840 0.2055480 -1.36375500
H 5.0819590 1.3722090 -3.29181900
H 2.7887470 0.7294670 -4.00402700
H 1.5567220 -1.0231310 -2.79378900
H 4.8980270 -1.5614470 -0.16008100
C 2.3980830 -2.4559470 -0.58469100
C 1.1972990 -3.1424630 -1.07304700
H 3.0810690 -3.1050310 -0.03351000
H 2.2456290 -1.9035810 0.74340400
H 0.9226430 -3.0568050 -2.12454600
H 1.0416040 -4.1479500 -0.68532200
C 1.9960290 -1.9275630 2.92218300
O 0.8809060 -2.4472410 2.86172600
O 2.5191150 -1.5821660 4.14560200
H 1.8624100 -1.8432550 4.80443400
C 0.5247960 4.5833560 0.40504600
C 1.5203380 5.0613670 -0.67767400
H 2.5414010 4.7401910 -0.46095900
H 1.2423020 4.6710360 -1.66033200
H 1.5149760 6.1535310 -0.72819000
C 0.9499170 5.1404630 1.78317700
H 0.9400600 6.2334240 1.75822700
H 0.2614010 4.8095080 2.56516300
H 1.9573250 4.8212920 2.05854200
C -0.8709690 5.1336410 0.06470300
H -1.6147230 4.8421990 0.81122300
H -0.8338690 6.2251820 0.04303200
H -1.2132670 4.7956640 -0.91718800
C -5.4204130 -0.0120720 -0.40271500
C -5.8007770 0.6576810 0.93813800
H -5.1606770 1.5138520 1.16251800
H -6.8332160 1.0144100 0.89182700
H -5.7208100 -0.0535750 1.76440200
C -6.4106080 -1.1567210 -0.67771000
H -7.4235640 -0.7520150 -0.73766100
H -6.1962700 -1.6584580 -1.62504900
H -6.3987320 -1.9028410 0.12104200

C -5.5314220 1.0210320 -1.54822200
H -4.8871900 1.8869000 -1.38088300
H -5.2553550 0.5708930 -2.5054640
H -6.5614380 1.3799210 -1.62247700
C -1.9087880 -3.6948740 -0.49053500
H -1.3951500 -3.8716380 -1.43761100
H -1.2236260 -3.9877870 0.30524100
H -2.7999610 -4.3213660 -0.45221500
H 2.6679080 0.4397000 0.99832100

TS-SA1-S

PBE SCF Energy: -1240.20545852 a.u.

C 0.297180 1.938665 1.29260500
C 2.257950 0.725287 1.01823100
C 2.919216 1.526551 1.94683700
C 2.227254 2.564369 2.56204900
C 0.893116 2.772759 2.23233200
H 3.954395 1.342933 2.19730700
H 2.724912 3.194769 3.28848800
H 0.315732 3.566670 2.68743100
C 2.886455 -0.421369 0.32796300
C 4.232332 -0.763728 0.44423500
C 4.717322 -1.868094 -0.24691300
H 4.897607 -0.175715 1.06033000
C 2.516015 -2.209784 -1.11531600
C 3.844484 -2.605800 -1.04011700
H 5.761092 -2.144822 -0.16687900
H 4.178459 -3.472348 -1.59501400
N 0.958937 0.937529 0.69435400
N 2.042243 -1.144143 -0.45022500
Ni 0.227595 -0.487948 -0.55962500
H 1.797281 -2.746749 -1.71726200
H -0.728323 2.070004 0.97856800
O -1.782392 1.820232 -0.89480100
C -5.011407 -0.928007 0.83390100
C -4.629741 -1.593575 1.99785800
C -3.306652 -2.015912 2.13991500
C -2.379653 -1.775314 1.12945800
C -2.751340 -1.115303 -0.05237700
C -4.081189 -0.692372 -0.17782600
H -6.035428 -0.591899 0.71106000
H -5.351184 -1.778087 2.78581200
H -2.994809 -2.528633 3.04354900
H -1.349381 -2.090267 1.25871200
H -4.387539 -0.170599 -1.07857700
C -1.762652 -0.832086 -1.14330900
C -0.719722 -1.820192 -1.47865600
H -2.249530 -0.424095 -2.03089300
H -1.422664 0.526041 -0.90847500
H -0.743891 -2.784398 -0.96685500
H -0.477924 -1.919962 -2.53852700
C -1.203338 2.454318 -1.84591300
O -0.457461 2.008810 -2.71620100
O -1.499333 3.796062 -1.81825100
H -1.029998 4.192675 -2.56390600

TS-SA2-S-F

PBE SCF Energy: -1593.67692598 a.u.

C 2.1150460 1.5104620 0.30401700
C -0.1485320 1.1986680 -0.06721800
C -0.3673110 2.5743470 -0.02429900
C 0.6915900 3.4584580 0.18838000
C 1.9616730 2.8851980 0.34420900
H -1.3688590 2.9486110 -0.16519200
H 2.8392270 3.4981330 0.50006000
C -1.2046640 0.2012740 -0.35486600
C -2.5410880 0.5270420 -0.55427800
C -3.4553240 -0.4680750 -0.90769400
H -2.8630350 1.5486940 -0.42943600
C -1.5932270 -2.0317050 -0.87785900
C -2.9383220 -1.7504940 -1.10587600
H -3.5801380 -2.5605000 -1.42632100
N 1.0858440 0.6731770 0.10808300
N -0.7530540 -1.0693240 -0.45397100
Ni 1.0627290 -1.2372290 0.35546000
O -0.7141610 -3.0014590 1.93398400
C 5.8597840 -0.6071450 -0.82880300
C 5.7232230 -1.2247220 -2.07157000
C 4.6239770 -2.0561360 -2.29983300
C 3.6731340 -2.2609350 -1.30564800
C 3.7882200 -1.6404350 -0.04474700
C 4.9097630 -0.8159310 0.16855500
H 6.7117000 0.0349930 -0.63196600
H 6.4618630 -1.0655150 -2.84880300
H 4.5065070 -2.5457420 -3.26079800
H 2.8209850 -2.8993100 -1.50836300
H 5.0359130 -0.3392040 1.13585200
C 2.7697790 -1.7838820 1.01134300

C 1.8444000 -2.9244890 1.10202700
H 3.0700060 -1.3423550 1.96231300
H 0.4261030 -2.6872080 1.37948100
H 1.9450240 -3.7205380 0.36309800
H 1.7886450 -3.3531910 2.10342300
C -1.3299950 -2.0165910 2.47761700
O -0.8828470 -0.9194150 2.80201700
O -2.6596170 -2.3026380 2.68090600
H -3.0442500 -1.5223840 3.10134100
C 0.5125190 4.9784880 0.24322400
C 1.3412930 5.6199850 -0.89380000
H 2.4054770 5.3944260 -0.79752800
H 1.0035830 5.2625200 -1.87019100
H 1.2244090 6.7067840 -0.86761900
C 1.0200620 5.4952070 1.60952800
H 0.8985830 6.5804210 1.66094400
H 0.4525270 5.0478050 2.42978300
H 2.0774010 5.2695070 1.76356600
C -0.9577950 5.3992190 0.07647800
H -1.5897370 4.9835490 0.86592500
H -1.0312970 6.4877460 0.13176000
H -1.3614060 5.0901890 -0.89143800
C -4.9543850 -0.2034870 -1.07732200
C -5.3197940 1.2683760 -0.81881700
H -4.8208600 1.9400910 -1.52259400
H -6.3970220 1.4007370 -0.94239500
H -5.0631420 1.5775410 0.19801300
C -5.7201750 -1.0865490 -0.06397800
H -6.7946310 -0.9028320 -0.14849400
H -5.5448900 -2.1498080 -0.24098100
H -5.4104860 -0.8587590 0.95956600
C -5.3804150 -0.5706460 -2.51677600
H -4.8420670 0.0387670 -3.24757500
H -5.1901200 -1.6218010 -2.74337700
H -6.4512840 -0.3899290 -2.64274600
H 3.0847780 1.0477600 0.42543200
C -1.0438390 -3.4122960 -1.08938700
H 0.0153690 -3.3616840 -1.34116500
H -1.1414090 -3.9896040 -0.16844200
H -1.5839710 -3.9236070 -1.88768200

TS-SA2-S

PBE SCF Energy: -1240.21316472 a.u.

C -1.470673 1.474047 -1.58912200
C 0.330383 2.201761 -0.31179800
C 0.112347 3.519831 -0.70809000
C -0.937733 3.804873 -1.57375600
C -1.744706 2.764409 -2.02247600
H 0.754265 4.314199 -0.35469600
H -1.119165 4.823635 -1.89268200
H -2.573073 2.939917 -2.69589700
C 1.408548 1.773460 0.60259100
C 2.242794 2.655690 1.28611400
C 3.203740 2.147156 2.15315100
H 2.140606 3.723945 1.15708200
C 2.443328 -0.052071 1.59447800
C 3.302565 0.769915 2.31472800
H 3.858482 2.818468 2.69478300
H 4.031915 0.329573 2.98173100
N -0.459621 1.193210 -0.75430000
N 1.517906 0.430434 0.75204700
Ni 0.079392 -0.577896 -0.20034600
H 2.499972 -1.128246 1.66018900
H -2.073146 0.634619 -1.90259900
O 2.361742 -2.529543 -0.08751100
C -4.918666 -0.639642 0.09399100
C -4.913839 -0.532495 1.48402900
C -3.747043 -0.845605 2.18600500
C -2.602474 -1.252144 1.50868800
C -2.584907 -1.361207 0.10370400
C -3.772684 -1.051152 -0.58352200
H -5.818390 -0.407367 -0.46578700
H -5.804227 -0.213846 2.01389900
H -3.729312 -0.768033 3.26794400
H -1.701131 -1.472498 2.06926900
H -3.795345 -1.141173 -1.66523300
C -1.370213 -1.734383 -0.64790100
C -0.293032 -2.556153 -0.08109700
H -1.546983 -1.860336 -1.71723000
H 1.108448 -2.180118 -0.09508700
H -0.441903 -2.955682 0.92328900
H 0.043608 -3.344132 -0.75540500
C 2.986518 -2.096902 -1.12208800
O 2.529653 -1.502642 -2.09553300
O 4.329532 -2.369111 -1.04964800
H 4.721471 -2.023310 -1.86234600

TS-SAC2-D

PBE SCF Energy: -1164.4138104 a.u.

C -0.881709 2.270806 -1.09650900
C 1.234997 1.858578 -0.22569800
C 1.477344 3.225577 -0.09890400
C 0.496072 4.128610 -0.49560700
C -0.704306 3.645937 -1.00776200
H 2.410771 3.585440 0.31083600
H 0.668230 5.193696 -0.40188200
H -1.492601 4.314246 -1.32794700
C 2.203463 0.803817 0.15218600
C 3.531784 1.053328 0.49787000
C 4.366828 -0.017613 0.79691700
H 3.916500 2.063365 0.51982400
C 2.528229 -1.487480 0.37307800
C 3.860079 -1.312488 0.72723400
H 5.400892 0.157944 1.06669000
H 4.480937 -2.173797 0.93623300
N 0.060120 1.398195 -0.71589800
N 1.714088 -0.456988 0.10763500
Ni -0.225135 -0.572328 -0.45991900
H 2.081593 -2.467462 0.27176300
H -1.799702 1.838355 -1.47136700
C -1.276781 -2.268820 0.36577400
C -0.358599 -2.392385 -1.42165900
O -1.029051 -1.816316 -2.29456500
O 0.473076 -3.286237 -1.39785600
C -1.992712 -1.008145 0.72391500
C -1.620258 -0.201008 1.82613500
C -3.071876 -0.558523 -0.07874700
C -2.275715 0.999934 2.08926400
H -0.817891 -0.521350 2.47778500
C -3.719819 0.638871 0.19355400
H -3.370899 -1.161756 -0.92723500
C -3.321443 1.430861 1.27496500
H -1.962478 1.602516 2.93467100
H -4.537991 0.960957 -0.44135400
H -3.826816 2.366899 1.48226800
H -1.983220 -2.949865 -0.10565200
C -0.478402 -2.981923 1.44011700
H -1.134374 -3.363613 2.23100100
H 0.052521 -3.823477 0.99465600
H 0.263600 -2.332530 1.90783100

TS-SAC2-Q

PBE SCF Energy: -1164.35616824 a.u.

C 3.204151 -1.707394 -0.78322300
C 2.748042 0.528161 -0.14212400
C 4.107855 0.854561 -0.38243100
C 4.987891 -0.106271 -0.81534800
C 4.530939 -1.435644 -1.02520800
H 4.451381 1.868612 -0.22393800
H 6.025367 0.148877 -0.99669400
H 5.196263 -2.217934 -1.36466800
C 1.745179 1.440711 0.30355100
C 1.958872 2.812432 0.59796600
C 0.918820 3.601177 1.02427300
H 2.949427 3.234553 0.48940700
C -0.540148 1.704503 0.86489400
C -0.376843 3.037452 1.16506000
H 1.087498 4.647147 1.25227000
H -1.220465 3.627418 1.49701200
N 2.323297 -0.778007 -0.35591600
N 0.468528 0.911825 0.44850400
Ni 0.388932 -1.029197 -0.01197800
H -1.507417 1.224643 0.94655000
H 2.796095 -2.702316 -0.92585700
C -2.838459 1.484559 -2.09440400
C -4.010683 1.767678 -1.39098500
C -4.438859 0.884466 -0.40110500
C -3.702598 -0.261595 -0.10503300
C -2.505438 -0.548213 -0.78320500
C -2.103295 0.343308 -1.79682300
H -2.496771 2.155193 -2.87516900
H -4.584656 2.659040 -1.61705700
H -5.353628 1.086568 0.14576300
H -4.048362 -0.924261 0.67629500
H -1.189321 0.141969 -2.34815500
C -1.651009 -1.709746 -0.42788000
C -2.361384 -3.023477 -0.08363100
H -1.008399 -1.945759 -1.29807600
H -1.636483 -3.800471 0.17137000
H -3.049863 -2.921033 0.75534400
H -2.941076 -3.376151 -0.94468600
C -1.052342 -1.488264 1.76335400
O 0.099927 -1.864481 1.89353400
O -2.053251 -1.147486 2.28413600

TS-SAC3-D

PBE SCF Energy: -1164.3984262 a.u.

C 1.516129 2.497243 -0.17610200
C 2.762316 0.538143 -0.05228000
C 3.948720 1.266344 0.03225700
C 3.894574 2.656074 0.00834800
C 2.657674 3.285635 -0.09746400
H 4.901847 0.763885 0.12027800
H 4.806552 3.236522 0.07351200
H 2.572352 4.364170 -0.11758400
C 2.692742 -0.942803 -0.03748500
C 3.810527 -1.776309 -0.01684600
C 3.629392 -3.155423 -0.01415500
H 4.808844 -1.361895 -0.00884000
C 1.269548 -2.778963 -0.05464700
C 2.335787 -3.669158 -0.03381000
H 4.487012 -3.816495 0.00057300
H 2.150518 -4.735238 -0.03352800
N 1.564318 1.158472 -0.15416800
N 1.437898 -1.449890 -0.05646200
Ni -0.017463 -0.073608 -0.13717700
H 0.242616 -3.119799 -0.07011000
H 0.525640 2.928065 -0.25511700
C -2.043022 2.505220 -0.93813800
C -2.136766 3.146454 0.29946000
C -2.161246 2.361015 1.45932700
C -2.111806 0.975824 1.39763300
C -2.046630 0.283433 0.14157400
C -1.978338 1.116617 -1.02890400
H -2.013425 3.092270 -1.85071000
H -2.175972 4.227405 0.36202100
H -2.216969 2.841638 2.43123300
H -2.142630 0.397622 2.31253400
H -1.967072 0.640813 -2.00287100
C -2.047477 -1.155533 0.04761200
C -1.992259 -2.039434 1.27220000
H -1.904886 -1.609613 -0.92617200
H -1.108245 -1.867374 1.90030900
H -2.873787 -1.891377 1.90720300
H -1.986435 -3.092605 0.98020700
C -4.295824 -1.248263 -0.53240200
O -4.285691 -0.996291 -1.69094400
O -4.821400 -1.515427 0.49536300

TS-SC1-S-F

PBE SCF Energy: -1517.2738233 a.u.

C 0.5959900 1.0312350 -0.1488220
C 1.1511620 2.3035190 -0.16735800
C 0.3407840 3.4434550 -0.24396400
C -1.0376360 3.2231910 -0.29666600
C -1.5349010 1.9269500 -0.29691800
C 1.3746440 -0.2168470 0.01607200
C 2.7355450 -0.2451390 0.27690100
C 3.3762070 -1.4615720 0.54614900
C 2.5659420 -2.5944060 0.59158800
C 1.1963120 -2.5165310 0.32120200
H 2.2252670 2.4094870 -0.12171200
H -1.7431590 4.0394730 -0.34453400
H -2.5972750 1.7369340 -0.34441100
H 3.2961690 0.6777630 0.28993900
H 2.9743740 -3.5615730 0.84516000
N -0.7473910 0.8479540 -0.22962600
N 0.6273260 -1.3475030 -0.02152000
Ni -1.2376770 -0.9604280 -0.62398600
C -3.1279690 -0.9423860 -0.90328400
H -3.4836800 -0.3014520 -1.70946800
C -2.7055050 -2.2898140 -1.34459700
H -3.2599550 -2.6303650 -2.21862900
C -1.2489920 -2.3418110 -2.45563900
O -1.1540500 -1.3348590 -3.16110000
O -0.7602000 -3.4656250 -2.48198200
H -2.7004430 -3.0938160 -0.60996600
C -3.8152380 -0.7071740 0.38034000
C -4.7098200 0.3717950 0.50968700
C -3.5791730 -1.4951330 1.52543800
C -5.3277120 0.6609500 1.72437200
H -4.9280300 0.9828420 -0.36053500
C -4.1972100 -1.2075250 2.73720900
H -2.8956030 -2.3337790 1.46453200
C -5.0736390 -0.1252170 2.84738900
H -6.0126560 1.4992760 1.79149200
H -3.9938840 -1.8297570 3.60209600
H -5.5540480 0.0968990 3.79331900
C 0.3009080 -3.7118210 0.46046500
H -0.4446660 -3.5130850 1.23617000
H -0.2296520 -3.8995970 -0.47371000
H 0.8691960 -4.5981660 0.74264500
C 0.9758720 4.8368300 -0.26399300
C 1.8921340 4.9501080 -1.50461900

H 2.3557830 5.9397650 -1.53105700
H 2.6913180 4.2058010 -1.48984100
H 1.3181140 4.8157710 -2.42519300
C -0.0800610 5.9535950 -0.32877800
H -0.6880170 5.8847510 -1.23465600
H -0.7450640 5.9324930 0.53866300
H 0.4209590 6.9242710 -0.33911700
C 1.8149460 5.0280620 1.02090400
H 2.2650860 6.0242880 1.02126100
H 1.1884480 4.9352580 1.9119700
H 2.6231110 4.2970940 1.09506000
C 4.8850480 -1.4920530 0.80802600
C 5.6178880 -0.9332170 -0.43373400
H 5.3278300 0.0976870 -0.64828600
H 6.6976310 -0.9484130 -0.26281500
H 5.4024570 -1.5389380 -1.31789000
C 5.2030130 -0.6102340 2.03803700
H 4.6858540 -0.9818920 2.92657300
H 6.2783050 -0.6274550 2.23499400
H 4.9090520 0.4300580 1.88250400
C 5.3992790 -2.9159190 1.08060600
H 4.9395170 -3.3493450 1.97261500
H 5.2115360 -3.5821750 0.23453900
H 6.4786100 -2.8847450 1.24651400

TS-SC1-S-iso

PBE SCF Energy: -1163.8178702 a.u.

C 0.444787 -2.032401 -1.17339000
C -1.684757 -1.713734 -0.28579100
C -2.015634 -3.041937 -0.53829700
C -1.075611 -3.878666 -1.12995900
C 0.174205 -3.364599 -1.45651700
H -2.993678 -3.421740 -0.27886900
H 0.935702 -3.977145 -1.92028400
C -2.603076 -0.727643 0.31632900
C -3.919711 -0.990390 0.68787800
C -4.685831 0.036563 1.22929900
H -4.345398 -1.974769 0.55506000
C -2.805286 1.492635 0.98453400
C -4.123016 1.300594 1.37914700
H -4.687963 2.126127 1.79065100
N -0.455777 -1.222299 -0.59879500
N -2.062348 0.502829 0.47286000
Ni -0.209990 0.614047 -0.14286800
H -2.320818 2.456352 1.06916900
C 4.531782 -1.298446 0.19633600
C 3.603846 -0.514606 -0.48622700
C 2.638322 0.239341 0.20355200
C 2.648708 0.186552 1.61068800
C 3.577851 -0.591243 2.29262100
C 4.523288 -1.342199 1.58966800
H 5.265422 -1.870378 -0.36109300
H 3.628644 -0.476647 -1.57083500
H 1.911631 0.752647 2.16967100
H 3.563782 -0.616735 3.37677100
H 5.245136 -1.949876 2.12312900
C 1.625478 1.012094 -0.54004700
C 1.107504 2.308904 0.02281200
H 1.794559 1.028329 -1.61677900
H 0.196284 2.082914 0.70105400
H 1.778406 2.790628 0.73618700
C 0.509013 3.212810 -1.07838300
O -0.471290 2.649478 -1.65497700
O 1.012281 4.324219 -1.29929800
H 1.405640 -1.595045 -1.39675700
H -1.319232 -4.914062 -1.33194200
H -5.710649 -0.148986 1.52540200

TS-SC1-S

PBE SCF Energy: -1163.81398376 a.u.

C 0.978671 1.946557 -0.29501800
C 0.941316 3.327310 -0.47718500
C -0.134792 3.897957 -1.14688700
C -1.146998 3.072072 -1.62441900
C -1.051317 1.704762 -1.40581400
C 2.078294 1.226434 0.37534300
C 3.142033 1.854180 1.01970000
C 4.119632 1.075189 1.62904500
C 4.006346 -0.309601 1.57943400
C 2.918108 -0.870492 0.92058600
H 1.744837 3.950472 -0.11114500
H -0.176619 4.969432 -1.29689400
H -2.000290 3.470575 -2.15668700
H -1.816595 1.025957 -1.74856300
H 3.206070 2.932431 1.05599400
H 4.952573 1.545893 2.13632200
H 4.743199 -0.953410 2.04126200
H 2.778043 -1.940331 0.84504400

N -0.020499 1.149912 -0.75112500
N 1.974587 -0.123919 0.32816600
Ni 0.247905 -0.728153 -0.48509800
C -1.499179 -1.481474 -0.70150400
H -1.853624 -1.523814 -1.73209300
C -0.666948 -2.631853 -0.29604100
C 0.997969 -2.760812 -1.00620700
O 1.068648 -2.375653 -2.18090200
O 1.715362 -3.447534 -0.28303900
H -0.628603 -2.878130 0.76255300
C -2.470613 -0.861985 0.22464900
C -3.657629 -0.300553 -0.27715600
C -2.239104 -0.763630 1.61065200
C -4.567882 0.340843 0.56078400
H -3.868547 -0.374244 -1.33937400
C -3.147529 -0.125792 2.44763600
H -1.327831 -1.175104 2.02969400
C -4.317919 0.433859 1.92866900
H -5.474712 0.764915 0.14346100
H -2.941447 -0.060901 3.51054300
H -5.024011 0.931643 2.58333700
H -0.899232 -3.531377 -0.86608200

TS-SC1-T

PBE SCF Energy: -1163.76924339 a.u.

C -1.342357 0.775113 -1.09689400
C -2.157915 1.904526 -1.15894000
C -1.582774 3.140464 -1.43169800
C -0.207005 3.221692 -1.63063200
C 0.542044 2.054651 -1.55221300
C -1.827386 -0.590567 -0.79489200
C -3.162867 -0.905628 -0.54940400
C -3.510600 -2.215067 -0.24023500
C -2.512370 -3.185074 -0.18695900
C -1.204135 -2.804817 -0.45169300
H -3.222637 1.829438 -0.98875500
H -2.200925 4.028382 -1.48000700
H 0.279281 4.165887 -1.83813800
H 1.616548 2.051778 -1.68913200
H -3.923995 -0.139287 -0.58939900
H -4.543491 -2.472505 -0.04148700
H -2.736949 -4.215916 0.05332900
H -0.390519 -3.518504 -0.42226600
N -0.009524 0.863260 -1.29682500
N -0.861426 -1.541598 -0.74991400
Ni 0.957343 -0.876631 -1.02118300
C 1.535503 -1.027311 1.98148900
H 1.158618 -2.043924 1.90104900
C 2.877769 -0.833321 1.93944300
H 3.555255 -1.676672 1.91238500
C 3.735915 -0.400709 -0.40841400
O 2.859710 -0.571056 -1.29537200
O 4.915333 -0.139483 -0.42343700
H 3.329019 0.131850 2.13078100
C 0.512289 0.007880 2.11196300
C -0.820125 -0.360761 2.37789600
C 0.791052 1.380394 1.95571200
C -1.825698 0.593000 2.49087300
H -1.064853 -1.413328 2.47751000
C -0.214930 2.332142 2.06450300
H 1.797333 1.696806 1.70778500
C -1.530420 1.947542 2.33508100
H -2.845031 0.277302 2.68405700
H 0.021975 3.380066 1.91699600
H -2.314865 2.692080 2.40612600

TS-SC2-S

PBE SCF Energy: -1163.80572348 a.u.

C 2.240508 1.124246 0.39550500
C 2.985288 2.191747 0.89312700
C 2.458396 3.476552 0.82140300
C 1.201012 3.659998 0.25696600
C 0.512215 2.550633 -0.21994100
C 2.689718 -0.281201 0.42516700
C 3.926830 -0.696735 0.91307100
C 4.254002 -2.046996 0.88739800
C 3.334940 -2.952808 0.36814300
C 2.119322 -2.476827 -0.10224700
H 3.958652 2.029289 1.33368000
H 3.022720 4.317934 1.20383200
H 0.752091 4.641766 0.18451800
H -0.470565 2.633677 -0.66374300
H 4.630290 0.023740 1.30522400
H 5.211909 -2.382849 1.26406200
H 3.547050 -4.012642 0.32367500
H 1.377102 -3.143123 -0.51519800
N 1.018529 1.310270 -0.15821100
N 1.794680 -1.173693 -0.07340500

Ni 0.178670 -0.418224 -0.73241000
C -1.973338 -0.966883 -1.07813400
C -0.875530 -1.957397 -0.99463400
H -0.661110 -2.489664 -1.92199600
C -1.450784 0.560225 -1.94766100
O -2.120899 1.537313 -1.63305400
O -0.660945 0.321358 -2.87735000
H -0.884690 -2.620362 -0.12878300
C -2.795027 -0.674474 0.13950700
C -4.149109 -0.344741 -0.00055900
C -2.256199 -0.702766 1.43375400
C -4.940706 -0.056302 1.10904800
H -4.584368 -0.309345 -0.99360300
C -3.043551 -0.415838 2.54644200
H -1.207439 -0.943839 1.57312500
C -4.391043 -0.089556 2.39028300
H -5.986867 0.195467 0.97269400
H -2.602593 -0.443670 3.53697700
H -5.003764 0.136406 3.25568800
H -2.620547 -1.153190 -1.93794200

TS-SC2-T

PBE SCF Energy: -1163.77024289 a.u.

C 1.851997 1.419665 0.33302600
C 2.028930 2.803899 0.30792600
C 1.038039 3.623947 0.83686300
C -0.108564 3.045054 1.37775800
C -0.218931 1.661465 1.36784800
C 2.825634 0.442530 -0.20230900
C 4.048375 0.794698 -0.77661000
C 4.894353 -0.202155 -1.24648600
C 4.498612 -1.534045 -1.13673800
C 3.266985 -1.813499 -0.56266700
H 2.921257 3.240887 -0.11807900
H 1.159977 4.699936 0.82470500
H -0.903672 3.648914 1.79482900
H -1.086163 1.150409 1.76583100
H 4.339967 1.832551 -0.85688100
H 5.846716 0.056876 -1.69207300
H 5.126618 -2.341623 -1.48922600
H 2.906774 -2.830071 -0.46324600
N 0.734818 0.867970 0.86200400
N 2.447033 -0.856613 -0.10090300
Ni 0.612921 -1.123807 0.63849900
C -0.410961 -1.696362 -1.27074000
H 0.037171 -0.859978 -1.79843400
H 0.087786 -2.653595 -1.40511300
C -1.762394 -1.692797 -0.96836400
H -2.263100 -2.641844 -0.81391300
C -2.639277 -0.525976 -1.07219000
C -2.140202 0.778976 -1.25820500
C -4.037148 -0.684111 -0.99085400
C -2.998996 1.869096 -1.35559000
H -1.071149 0.942470 -1.30396400
C -4.893642 0.405678 -1.09250600
H -4.445139 -1.676625 -0.83312500
C -4.381322 1.693020 -1.27447300
H -2.585638 2.863364 -1.48795900
H -5.965760 0.253665 -1.02665300
H -5.048706 2.544068 -1.34862800
C -2.007604 -1.771284 1.53960500
O -0.852631 -1.574805 1.96522600
O -3.099240 -1.993832 1.99908400

TS-SC3-S-F

PBE SCF Energy: -1517.27661678 a.u.

C -0.8149710 2.10963100 -0.52676000
C 1.1066320 0.85317900 -0.22890100
C 1.8810610 2.00612800 -0.22743100
C 1.2956900 3.26927800 -0.38258100
C -0.0928600 3.29572300 -0.53199400
H 2.9510950 1.92356700 -0.10472100
H -0.6348490 4.22204700 -0.65319400
C 1.6496660 -0.51474600 -0.05963100
C 2.9981990 -0.78337600 0.11861200
C 3.4427850 -2.10071900 0.28586300
H 3.707223 0.0313230 0.13014400
C 1.1172990 -2.7737970 0.07882500
C 2.4652780 -3.0930640 0.26401700
H 2.7254190 -4.1336270 0.39045800
N -0.2401760 0.90922100 -0.38349900
N 0.7164430 -1.5004090 -0.08350900
Ni -1.1311430 -0.79427700 -0.4012010
C -4.9962660 2.19292900 0.99932300
C -4.3773580 1.40747500 0.02890600
C -3.6899230 0.22815200 0.36839900
C -3.6595570 -0.13671700 1.72841000
C -4.2849030 0.64155500 2.69669500

C -4.9553700 1.81442700 2.34055300
H -5.5171710 3.09797400 0.70560200
H -4.4274390 1.70580800 -1.01379000
H -3.1270060 -1.03232400 2.02601200
H -4.2450090 0.33607100 3.73688900
H -5.4388220 2.4211820 3.09768200
C -2.9863680 -0.5413140 -0.67783900
C -2.8265190 -2.00382800 -0.5760810
H -3.2251980 -0.1942400 -1.68566100
H -2.2826630 -2.5250010 -1.36208500
H -2.8441510 -2.4950380 0.3897020
C 2.1701690 4.52666500 -0.38365100
C 1.3382250 5.81000800 -0.54962500
H 2.0039700 6.67605200 -0.54115600
H 0.7933080 5.81993500 -1.49718100
H 0.6204640 5.9351120 0.26543200
C 3.1756160 4.43619500 -1.55525400
H 3.8058050 5.32941800 -1.57008100
H 3.8303180 3.56644800 -1.46501100
H 2.6517670 4.37018100 -2.51250600
C 2.9394730 4.6094740 0.95519200
H 3.5669210 5.5046910 0.96441200
H 2.2465020 4.66796600 1.79865300
H 3.5894840 3.74511000 1.10785000
C 4.9345360 -2.3899530 0.48050700
C 5.7069190 -1.89077900 -0.76263000
H 5.5852200 -0.81586700 -0.91276100
H 6.7743270 -2.09330100 -0.63995600
H 5.3625650 -2.40222100 -1.66539300
C 5.2170610 -3.8910570 0.66305000
H 6.2901490 -4.0425390 0.80061900
H 4.7090190 -4.2940610 1.54308400
H 4.9095850 -4.47055900 -0.21134400
C 5.4338560 -1.6393360 1.73668300
H 5.3082790 -0.5585430 1.64286400
H 4.8929200 -1.96953200 2.62742300
H 6.4978540 -1.8403430 1.88801300
C -4.5656400 -2.6225590 -1.28083000
O -4.5841200 -2.4364930 -2.47044100
O -5.209840 -3.03030800 -0.34955600
H -1.891211 2.11025900 -0.63088600
C 0.066155 -3.84504700 0.04942600
H -0.7383110 -3.6045950 0.74649100
H -0.3798250 -3.9086200 -0.94645600
H 0.4859590 -4.81741200 0.3060100

TS-SC3-S

PBE SCF Energy: -1163.81133112 a.u.

C 0.501741 2.287682 -0.89433500
C 2.436537 1.163911 -0.25005400
C 3.188639 2.328508 -0.38409700
C 2.560474 3.501442 -0.79010600
C 1.193406 3.482557 -1.04757200
H 4.248847 2.325754 -0.17371600
H 0.664221 4.372788 -1.36078300
C 2.985725 -0.139640 0.18388700
C 4.324262 -0.366302 0.49781900
C 4.719425 -1.637521 0.90190200
H 5.050944 0.431143 0.42981200
C 2.452624 -2.354331 0.65121500
C 3.769381 -2.651042 0.98181400
H 4.035492 -3.652617 1.29260100
N 1.103757 1.152755 -0.51018300
N 2.066232 -1.131914 0.26191300
Ni 0.247276 -0.559816 -0.26811100
H 1.673525 -3.104463 0.69423700
C -3.787676 2.461359 0.25544100
C -3.082741 1.511981 -0.48117700
C -2.401412 0.453454 0.14741100
C -2.468979 0.380913 1.55217500
C -3.181039 1.322657 2.28755700
C -3.842639 2.372413 1.64594000
H -4.300289 3.267477 -0.25842700
H -3.057360 1.584495 -1.56412000
H -1.946959 -0.414911 2.06997600
H -3.216588 1.241698 3.36877100
H -4.393540 3.107003 2.22209800
C -1.602759 -0.486171 -0.66469100
C -1.366307 -1.879711 -0.23173800
H -1.804105 -0.390154 -1.73368200
H -0.729772 -2.514621 -0.85034100
H -1.402739 -2.141464 0.81983400
C -2.981335 -2.781213 -0.86996200
O -2.961891 -2.810917 -2.07485000
O -3.633543 -3.090780 0.09469500
H -0.563227 2.220996 -1.06947300
H 3.131887 4.414672 -0.89943300
H 5.755513 -1.830950 1.15028300

TS-SC3-T

PBE SCF Energy: -1163.78232444 a.u.

C -2.787878 -2.266004 0.83627400
C -2.993054 -0.103388 -0.00513100
C -4.351263 -0.085401 0.31696400
C -4.926611 -1.201683 0.91056400
C -4.131740 -2.317568 1.17274500
H -4.955496 0.785819 0.10648400
H -5.979402 -1.201512 1.16388800
H -4.540898 -3.208522 1.63035200
C -2.279634 1.016545 -0.65279700
C -2.881457 2.225720 -1.00583300
C -2.119518 3.210160 -1.62316900
H -3.928942 2.400488 -0.80416800
C -0.237099 1.743579 -1.49205600
C -0.770449 2.966220 -1.87421200
H -2.572732 4.152667 -1.90417700
H -0.141165 3.704581 -2.35326400
N -2.224816 -1.189707 0.26219100
N -0.964606 0.789898 -0.89414500
Ni -0.295190 -0.973498 -0.15561900
H 0.805706 1.509180 -1.65377600
H -2.123264 -3.099786 1.02590200
C 1.834742 -1.496816 -0.93580600
C 1.649753 -1.138392 0.44080600
H 1.530780 -2.486413 -1.26404900
H 1.616573 -1.967606 1.14948900
C 2.091345 0.128327 1.01767900
C 2.733418 1.131415 0.26074200
C 1.871911 0.393401 2.38826000
C 3.097854 2.345558 0.83628600
H 2.969114 0.948262 -0.78075800
C 2.241166 1.602747 2.96067500
H 1.388553 -0.366066 2.99526900
C 2.851359 2.596656 2.18659300
H 3.589433 3.097369 0.22749800
H 2.053565 1.776550 4.01510900
H 3.137165 3.542687 2.63181100
H 1.827203 -0.740928 -1.71411800
C 3.877739 -1.916087 -1.31528500
O 3.946975 -2.045351 -2.50851900
O 4.464474 -1.929659 -0.27026800

TS-SC4-S

PBE SCF Energy: -1163.80600309 a.u.

C 0.567219 2.302289 -1.01845800
C 2.454149 1.152074 -0.29651300
C 3.239663 2.293806 -0.43781900
C 2.649160 3.469751 -0.89003100
C 1.289540 3.477866 -1.18445400
H 4.293039 2.274256 -0.19667400
H 0.791453 4.372570 -1.53349300
C 2.955120 -0.153551 0.18587000
C 4.282399 -0.412815 0.51804900
C 4.637302 -1.680981 0.96572000
H 5.032729 0.359925 0.42782400
C 2.351249 -2.340242 0.72096400
C 3.656363 -2.661733 1.07030900
H 3.889233 -3.660698 1.41407700
N 1.131896 1.166198 -0.59090700
N 2.004045 -1.118069 0.28886000
Ni 0.246869 -0.585675 -0.25404200
H 1.550074 -3.062944 0.77987000
C -3.500154 2.254629 0.70150200
C -2.898498 1.298987 -0.10953900
C -2.434170 0.079447 0.41372700
C -2.622932 -0.154226 1.78398200
C -3.231583 0.799953 2.59849800
C -3.669145 2.012034 2.06653000
H -3.842767 3.188278 0.26839800
H -2.792467 1.488825 -1.17329300
H -2.292259 -1.088127 2.22171100
H -3.362477 0.593720 3.65551800
H -4.138370 2.754054 2.70239700
C -1.826216 -0.921253 -0.50401900
C -0.949997 -2.011440 -0.01017000
H -1.487146 -0.468699 -1.45290100
H -0.822997 -2.838614 -0.70924000
H -1.126539 -2.368453 1.00459100
C -3.187987 -1.817605 -1.51109400
O -2.671600 -2.443665 -2.41113100
O -4.270862 -1.572630 -1.03404900
H 3.244696 4.366687 -1.00562500
H 5.665549 -1.897028 1.22724700
H -0.494878 2.256654 -1.21975700

TS-SC4-T

PBE SCF Energy: -1163.77707527 a.u.

C -1.080428 2.422549 -0.90991200
C -2.478142 0.785759 -0.02777300
C -3.380249 1.754688 0.40900600
C -3.103830 3.096506 0.16680100
C -1.932294 3.440789 -0.50086200
H -4.278690 1.474457 0.94057800
H -1.676450 4.473028 -0.69930900
C -2.645716 -0.669634 0.20525700
C -3.775027 -1.246526 0.78589200
C -3.809420 -2.624742 0.97223500
H -4.616687 -0.638328 1.08613800
C -1.633717 -2.751460 -0.00554400
C -2.720242 -3.394984 0.57446900
H -2.708621 -4.468788 0.70581800
N -1.347248 1.129707 -0.68577600
N -1.598418 -1.427517 -0.18605600
Ni -0.088314 -0.395653 -1.10202100
H -0.759217 -3.295390 -0.34133600
C 2.017417 1.996264 2.05075100
C 1.845108 0.678492 1.64587800
C 2.060790 0.291770 0.30763900
C 2.485420 1.283430 -0.59956900
C 2.656474 2.604101 -0.18928700
C 2.420391 2.973067 1.13454500
H 1.831704 2.267682 3.08464700
H 1.521418 -0.070355 2.36103600
H 2.671089 1.016921 -1.63243000
H 2.974483 3.349459 -0.91076600
H 2.547833 4.002225 1.44992600
C 1.862333 -1.120195 -0.10498700
C 1.535733 -1.470523 -1.49706900
H 1.382046 -1.723753 0.66117700
H 1.396478 -2.538084 -1.66833600
H 2.202171 -1.043329 -2.24639900
C 3.712791 -1.786510 0.26772900
O 4.428500 -1.523392 -0.66634800
O 3.696299 -2.304158 1.36027000
H -3.792474 3.861521 0.50329900
H -4.677888 -3.089544 1.42222300
H -0.147485 2.628579 -1.41943600

TS-SCA1-S

PBE SCF Energy: -1428.65791727 a.u.

C 0.114670 2.122009 1.11453100
C -1.941282 1.626255 0.13169600
C -2.408932 2.909759 0.39256400
C -1.571759 3.817455 1.03314900
C -0.291567 3.418591 1.40090500
H -3.408818 3.199137 0.10201500
H 0.389845 4.092093 1.90243200
C -2.716031 0.564821 -0.52953100
C -4.029188 0.686797 -0.97195300
C -4.647061 -0.406790 -1.56904600
H -4.564829 1.617601 -0.85188400
C -2.632727 -1.654617 -1.24900500
C -3.941086 -1.597209 -1.70898100
H -4.386254 -2.470296 -2.16594200
N -0.688107 1.251006 0.49140600
N -2.037068 -0.599120 -0.67711200
Ni -0.253114 -0.561990 0.00454700
H -2.042030 -2.556005 -1.33598600
C 3.962002 2.326390 -0.46072600
C 3.421960 1.125014 -0.00614500
C 2.380648 0.495366 -0.70221100
C 1.900527 1.096715 -1.87431700
C 2.442944 2.293195 -2.33219800
C 3.473228 2.915620 -1.62538700
H 4.764716 2.799073 0.09356500
H 3.803927 0.671099 0.90213800
H 1.086919 0.636478 -2.42262200
H 2.057889 2.744115 -3.23970200
H 3.891548 3.849856 -1.98165600
C 1.781348 -0.748169 -0.12493200
C 1.185598 -1.809631 -1.01572900
H 2.485145 -1.254057 0.54378900
H 0.133001 -2.109104 -0.69137100
H 1.129807 -1.551128 -2.06997900
C 1.838640 -3.270644 -0.83719000
O 2.310917 -3.505219 0.28903900
O 1.761470 -3.971809 -1.85730100
H 1.095049 1.762989 1.38693900
H -1.918692 4.821417 1.24227100
H -5.668572 -0.328162 -1.91859600
C 0.138837 -1.255457 2.76023500
O -0.661223 -1.741131 1.93180600
O 1.107523 -0.478893 2.49958700
O -0.002597 -1.556172 4.07604100

H 1.186621 -0.514245 1.05641700
H -0.765174 -2.145368 4.15307500

TS-SCA2-S

PBE SCF Energy: -1428.70031573 a.u.
C 1.683930 1.753736 -0.14376000
C 2.124671 3.020071 0.22482700
C 1.203660 3.942984 0.70867100
C -0.134522 3.578414 0.79833800
C -0.510267 2.294940 0.42314600
C 2.536885 0.702108 -0.71630400
C 3.907736 0.802270 -0.93022000
C 4.580624 -0.273024 -1.50201200
C 3.869666 -1.418642 -1.84385500
C 2.502921 -1.458384 -1.59829800
H 3.167568 3.286180 0.12873600
H 1.528555 4.933912 0.99979100
H -0.887671 4.269832 1.15124900
H -1.545547 1.985223 0.46004800
H 4.443735 1.699939 -0.65627200
H 5.647504 -0.213562 -1.67653100
H 4.357632 -2.274016 -2.29105900
H 1.885456 -2.315902 -1.82558000
N 0.379501 1.397473 -0.02318200
N 1.858672 -0.421238 -1.04996500
Ni 0.002766 -0.416692 -0.54622100
C -1.770167 -0.803319 0.52558200
H -2.599338 -0.126187 0.74365200
C -2.308681 -2.128417 -0.02320200
C -1.296325 -2.841180 -0.90868800
O -0.236230 -2.127883 -1.21727100
O -1.463655 -3.980708 -1.31413200
H -2.630504 -2.804970 0.77198900
C -0.941118 -0.894078 1.78973400
C -1.090132 0.086224 2.78355500
C -0.030022 -1.936710 2.03047100
C -0.337550 0.049532 3.95384500
H -1.807715 0.885476 2.63779100
C 0.718536 -1.978427 3.20448300
H 0.112590 -2.712304 1.28919000
C 0.576412 -0.981601 4.16892400
H -0.472141 0.822718 4.70207100
H 1.417181 -2.792431 3.36237500
H 1.162882 -1.013052 5.07988100
H -3.182120 -1.933042 -0.65143700
O -2.331897 0.507207 -1.74761400
H -1.721747 -0.054315 -0.62433700
C -3.254159 1.343607 -1.45696600
O -3.577572 1.757427 -0.33908500
O -3.919001 1.795332 -2.56620000
H -4.586704 2.418617 -2.25055200

TS-SCA2-T

PBE SCF Energy: -1428.69324906 a.u.
C 1.905226 0.563168 -1.11760400
C 3.255146 0.454285 -1.45083400
C 3.734459 -0.756546 -1.93873700
C 2.859627 -1.828313 -2.08518000
C 1.529895 -1.648937 -1.72669300
C 1.275942 1.804777 -0.60401800
C 1.993634 2.967712 -0.32607100
C 1.322863 4.079316 0.16924500
C -0.050636 4.005556 0.37586200
C -0.699407 2.814982 0.07565600
H 3.926123 1.293624 -1.33917200
H 4.780124 -0.857802 -2.20182100
H 3.194873 -2.784776 -2.46357400
H 0.791077 -2.436172 -1.79978300
H 3.062184 3.007685 -0.47978500
H 1.868128 4.987349 0.39474000
H -0.612149 4.844476 0.76443200
H -1.761506 2.703646 0.24007000
N 1.072466 -0.485631 -1.25415100
N -0.058284 1.743489 -0.40300000
Ni -0.915809 -0.147897 -0.68908700
C -1.166176 -0.812169 1.51619400
H -1.620966 -0.369878 2.41306300
C -1.804416 -2.190021 1.31261800
H -2.891704 -2.077799 1.39881600
C -1.574780 -2.841347 -0.05962500
O -1.403148 -2.032245 -1.05733700
O -1.594335 -4.069136 -0.16728500
H -1.506804 -2.911157 2.08095300
C 0.308193 -0.785631 1.78918200
C 0.900596 0.380729 2.30770100
C 1.149037 -1.884513 1.55136300
C 2.267996 0.459490 2.54164400
H 0.272771 1.243085 2.50796900

C 2.522103 -1.806282 1.77999900
H 0.736273 -2.805664 1.15826700
C 3.093566 -0.634088 2.27000600
H 2.693604 1.379237 2.92843100
H 3.147219 -2.666914 1.56742000
H 4.162238 -0.572137 2.44070300
C -3.542280 0.864105 -0.24516400
O -2.792342 0.586199 -1.20141700
O -4.777937 1.323135 -0.45710600
O -3.218864 0.761443 0.98723100
H -4.919536 1.377073 -1.41329000
H -2.169084 0.189432 1.05109900

TS-SCA3-D

PBE SCF Energy: -1428.82029572 a.u.
C 2.693632 2.836366 -0.12441500
C 2.017359 3.929840 0.39978700
C 0.649811 3.818911 0.65320500
C 0.019753 2.614346 0.37824900
C 4.435114 -0.900762 -1.75498500
C 3.530182 -1.938626 -1.98355300
C 2.193029 -1.732162 -1.67675000
H 0.081411 4.647108 1.05663300
H 3.853276 -2.888695 -2.38954900
N 0.665430 1.550121 -0.12277400
N 1.738109 -0.574261 -1.17326800
Ni -0.138893 -0.292591 -0.48394600
C -1.854762 -0.581701 0.88181900
C -2.605948 -1.789054 0.32518400
H -3.581183 -1.449777 -0.03845300
H -2.817785 -2.556441 1.08361900
H -2.551228 0.078310 1.40588400
C -1.936766 -2.513652 -0.85894400
O -0.901230 -1.952748 -1.37809500
O -2.428095 -3.583008 -1.25318800
C 3.969550 0.298654 -1.23071900
C 2.608152 0.436825 -0.94642500
C 1.992084 1.654527 -0.37962000
C -3.863883 1.448345 -0.76929400
O -4.593894 0.909699 0.04798400
O -4.344673 2.378813 -1.64442000
O -2.593037 1.264766 -0.95705000
H -2.110748 0.496738 -0.24248800
H -5.288828 2.469141 -1.45824300
H 1.433056 -2.489965 -1.82262200
H -1.039139 2.474913 0.54902600
H 3.752188 2.904750 -0.33469700
H 4.659157 1.109832 -1.04133900
H 2.545900 4.853181 0.60303700
H 5.487464 -1.025198 -1.97936200
C -0.713447 -0.862610 1.79510300
C -0.013005 -2.092852 1.81507000
C -0.276814 0.120254 2.71874300
C 1.082052 -2.297129 2.65254000
H -0.313347 -2.885182 1.14156100
C 0.815144 -0.084581 3.54986700
H -0.802145 1.069438 2.75058800
C 1.516712 -1.295606 3.52099400
H 1.601113 -3.250361 2.62298000
H 1.123030 0.702974 4.23103600
H 2.371777 -1.455395 4.16818900

TS-SCW1-S

PBE SCF Energy: -1240.17872268 a.u.
C 0.668413 -1.694506 1.11571600
C -1.598643 -1.670596 0.61673100
C -1.785848 -2.878714 1.27941000
C -0.697269 -3.503696 1.87780100
C 0.551465 -2.901697 1.79234800
H -2.767380 -3.328228 1.32762000
H 1.430351 -3.349287 2.23616300
C -2.670419 -0.925303 -0.06081500
C -4.006540 -1.306900 -0.13279000
C -4.901769 -0.491164 -0.81879700
H -4.346917 -2.220053 0.33423100
C -3.095959 1.002969 -1.30243000
C -4.442804 0.679952 -1.41358000
H -5.109836 1.337478 -1.95449400
N -0.374393 -1.081956 0.54074100
N -2.241661 0.215263 -0.64242600
Ni -0.375327 0.613655 -0.42428400
H -2.657469 1.893595 -1.73340500
C 3.362750 -1.276246 -2.37470300
C 2.500792 -0.287604 -1.91190900
C 2.633515 0.248401 -0.62104000
C 3.672667 -0.234444 0.18585900
C 4.536480 -1.229855 -0.27484700
C 4.385490 -1.756880 -1.55444100

H 3.233189 -1.677362 -3.37377600
H 1.699584 0.068596 -2.55130300
H 3.808917 0.156875 1.18664800
H 5.327511 -1.591798 0.37259000
H 5.053592 -2.532689 -1.91030200
C 1.693244 1.335558 -0.15975400
C 1.641115 1.691001 1.33133100
H 2.058965 2.259595 -0.64544400
H 1.340324 0.838777 1.94415100
H 2.642406 1.964917 1.68356100
C 0.722528 2.883485 1.73413800
O 0.154754 3.552246 0.81632400
O 0.640221 3.089492 2.95943500
H 1.624714 -1.207386 1.01841800
H -0.826398 -4.444547 2.39761900
H -5.945765 -0.770281 -0.88595200
O -0.432518 2.202018 -1.40525000
H 0.731747 1.740213 -0.97405500
H -0.390906 2.893473 -0.69397800

TS-SCW2-S

PBE SCF Energy: -1240.19507522 a.u.

C -1.911643 0.064011 -0.84422100
C -3.284852 -0.016449 -0.63634700
C -3.883607 -1.267776 -0.56064700
C -3.096385 -2.407959 -0.69703400
C -1.731370 -2.260809 -0.90194300
C -1.139839 1.306909 -0.94215900
C -1.658437 2.590834 -0.81634800
C -0.799358 3.678395 -0.92319000
C 0.555534 3.455941 -1.15135500
C 1.013506 2.149646 -1.25884100
H -3.875116 0.882238 -0.52850600
H -4.950145 -1.350969 -0.39406400
H -3.524401 -3.399839 -0.64444200
H -1.065702 -3.105334 -1.00552200
H -2.711955 2.739343 -0.62715700
H -1.183490 4.685760 -0.82383200
H 1.255462 4.275886 -1.23897800
H 2.054435 1.902143 -1.41076000
N -1.154367 -1.054208 -0.97480500
N 0.182948 1.104339 -1.16239500
Ni 0.724746 -0.725822 -1.03422500
C 1.452541 -1.477396 1.45475700
H 1.359769 -2.458237 1.92681100
C 2.890361 -1.021272 1.31363400
C 3.284746 -0.221298 0.05696100
O 2.528102 -0.299022 -1.01883000
O 4.322405 0.432104 0.04671000
H 3.256278 -0.421915 2.16118400
C 0.455765 -0.541134 1.93878000
C -0.832406 -0.985613 2.34491600
C 0.669709 0.861584 1.99879300
C -1.823693 -0.104470 2.74794500
H -1.046524 -2.050358 2.31125700
C -0.330543 1.741592 2.40453900
H 1.628708 1.268330 1.69762400
C -1.590177 1.277192 2.78303400
H -2.796268 -0.494194 3.03379700
H -0.122284 2.807298 2.41600700
H -2.369294 1.965375 3.09005200
H 3.543721 -1.901897 1.27717800
O 1.180748 -2.751704 -1.00715100
H 1.283861 -2.500551 -0.00820800
H 2.080865 -2.853560 -1.34722300

TS-SCW2-T

PBE SCF Energy: -1240.20094637 a.u.

C -1.342461 1.070542 -1.01442200
C -1.947325 2.323059 -1.10799100
C -1.165627 3.428093 -1.42723100
C 0.198237 3.260342 -1.64513000
C 0.733982 1.983879 -1.52877300
C -2.069997 -0.180064 -0.68293100
C -3.432726 -0.232884 -0.39537000
C -4.010348 -1.458425 -0.08096600
C -3.218719 -2.602691 -0.06554900
C -1.867536 -2.475560 -0.36490400
H -3.007061 2.442263 -0.93417500
H -1.619344 4.408613 -1.50201200
H 0.838116 4.096337 -1.89424600
H 1.786941 1.774021 -1.66536100
H -4.036299 0.663288 -0.40479700
H -5.066668 -1.515665 0.15100200
H -3.631761 -3.573159 0.17520200
H -1.186453 -3.316745 -0.36405600
N -0.019254 0.924206 -1.22203300
N -1.313763 -1.296499 -0.66347100

Ni 0.723022 -0.993103 -0.91030300
C 1.522156 -1.206237 1.36833900
H 1.404013 -2.023977 2.08961000
C 3.007330 -0.903514 1.16636200
H 3.556905 -1.852356 1.15566000
C 3.385323 -0.212280 -0.15803300
O 2.606936 -0.419546 -1.17550300
O 4.413786 0.464807 -0.21278800
H 3.437824 -0.311952 1.98121200
C 0.653680 -0.078789 1.82208200
C -0.628067 -0.344964 2.34206800
C 1.042663 1.269212 1.73388400
C -1.488934 0.679098 2.71727100
H -0.955440 -1.376682 2.42525700
C 0.178723 2.297980 2.10614000
H 2.020511 1.523733 1.34255300
C -1.094655 2.013983 2.59491800
H -2.475589 0.436885 3.09783700
H 0.503207 3.328126 2.00453400
H -1.768775 2.815195 2.87537300
O 1.136623 -2.982494 -0.56938700
H 1.254779 -2.224770 0.39583900
H 2.038656 -3.167043 -0.85958000

TS-SCW3-D

PBE SCF Energy: -1240.32184352 a.u.
C -1.496414 1.040209 -1.00235100
C -2.086054 2.315981 -1.10605200
C -1.321794 3.400363 -1.48393300
C 0.051846 3.210019 -1.75708600
C 0.575879 1.941388 -1.63755700
C -2.190852 -0.163051 -0.60500700
C -3.556778 -0.233628 -0.26169900
C -4.110763 -1.439623 0.11326800
C -3.295273 -2.592331 0.14476000
C -1.966488 -2.463209 -0.20405500
H -3.136984 2.446621 -0.88208000
H -1.768527 4.384366 -1.56348900
H 0.688088 4.036335 -2.04784400
H 1.622598 1.726608 -1.81494900
H -4.168007 0.659235 -0.28547600
H -5.158641 -1.499363 0.38304700
H -3.691946 -3.556687 0.43526800
H -1.280945 -3.302252 -0.19450200
N -0.161146 0.867106 -1.28493700
N -1.412096 -1.293492 -0.57682300
Ni 0.560225 -0.946435 -0.84222200
C 1.655626 -1.227367 1.29864200
H 1.574525 -2.021496 2.05091500
C 3.121133 -0.987299 0.94200000
H 3.630615 -1.957462 0.88696300
C 3.376741 -0.323862 -0.42993600
O 2.477233 -0.487066 -1.33888400
O 4.437207 0.292237 -0.60351500
H 3.665160 -0.402449 1.69337500
C 0.889462 -0.050580 1.80051600
C -0.367788 -0.235511 2.41327900
C 1.356254 1.273684 1.69646700
C -1.113714 0.834103 2.89017700
H -0.765142 -1.242970 2.48934400
C 0.607361 2.348391 2.17427300
H 2.308984 1.471775 1.22003800
C -0.631886 2.142032 2.77705400
H -2.080522 0.650207 3.34829400
H 0.996926 3.356044 2.06834400
H -1.214292 2.979079 3.14572500
O 1.074676 -3.012414 -0.58530000
H 1.273561 -2.221221 0.33139300
H 1.939020 -3.101784 -1.00478700

TS-SW1-S

PBE SCF Energy: -1051.69697498 a.u.
C -0.964370 1.500081 -1.41409600
C 1.035766 1.675354 -0.23464800
C 0.944235 3.065548 -0.24077000
C -0.140200 3.676456 -0.85941500
C -1.107563 2.879184 -1.46445200
H 1.711545 3.665059 0.22865400
H -0.224674 4.755865 -0.87132000
H -1.965043 3.310164 -1.96399200
C 2.159744 0.916828 0.34825300
C 3.273102 1.486473 0.96550600
C 4.277936 0.650109 1.44033200
H 3.361420 2.558792 1.07213100
C 3.020179 -1.223656 0.64054700
C 4.155583 -0.726981 1.27024700
H 5.149163 1.070541 1.92735500
H 4.924256 -1.406894 1.61366000

N 0.074476 0.902627 -0.80822800
N 2.041562 -0.421301 0.20704400
Ni 0.308661 -0.979879 -0.61451600
H 2.875078 -2.275679 0.43710800
H -1.697871 0.840425 -1.85237900
O 1.751666 -2.614430 -1.66826900
H 1.271555 -3.045098 -2.38529100
C -4.497768 0.246041 0.39003000
C -4.239534 0.487992 1.73810500
C -3.070946 -0.023826 2.30896500
C -2.174413 -0.760020 1.54288500
C -2.415561 -1.013858 0.17818800
C -3.600059 -0.496225 -0.37538700
H -5.401838 0.632756 -0.06814700
H -4.935786 1.064145 2.33678400
H -2.856257 0.157980 3.35675200
H -1.261790 -1.127926 1.99803000
H -3.816050 -0.681041 -1.42321900
C -1.454275 -1.738130 -0.67727600
C -0.557583 -2.803501 -0.15271600
H -1.843221 -1.927202 -1.67959100
H 0.616616 -2.668646 -0.63360500
H -0.571878 -2.974230 0.92321600
H -0.668953 -3.753472 -0.68103800

TS-SW2-S

PBE SCF Energy: -1051.68779586 a.u.

C -0.129147 2.412789 0.75633000
C -1.947100 1.301049 -0.16820400
C -2.523818 2.509067 -0.56108300
C -1.857798 3.697055 -0.28044400
C -0.634963 3.652064 0.38436900
H -3.470692 2.528700 -1.08222800
H -2.287392 4.644391 -0.58170400
H -0.082450 4.553735 0.61314100
C -2.525777 -0.031735 -0.43486000
C -3.751438 -0.239704 -1.06425600
C -4.205296 -1.536904 -1.26998600
H -4.347756 0.601327 -1.38892400
C -2.207894 -2.330715 -0.21871900
C -3.419183 -2.601360 -0.83830900
H -5.156082 -1.711428 -1.75760400
H -3.731832 -3.627974 -0.97566400
N -0.767831 1.267525 0.49126000
N -1.760866 -1.078420 -0.01759100
Ni -0.134639 -0.634557 0.86678800
H -1.561217 -3.121754 0.13164400
H 0.814085 2.314860 1.27882500
C 4.945853 0.298958 -0.76431500
C 4.441555 0.461204 -2.05491400
C 3.139859 0.040623 -2.33161700
C 2.354709 -0.530433 -1.33301400
C 2.847264 -0.705348 -0.02797800
C 4.159814 -0.277857 0.23127500
H 5.956452 0.618437 -0.53236600
H 5.051740 0.908237 -2.83158300
H 2.731437 0.161905 -3.32947900
H 1.338378 -0.833108 -1.56106200
H 4.567421 -0.401580 1.23003300
C 2.015317 -1.275544 1.07370900
C 0.895227 -2.221615 0.77587200
H 2.639899 -1.619502 1.90378400
H 0.882168 -2.695393 -0.20934000
H 0.702327 -2.949434 1.56803900
O 0.718953 0.084658 2.98160000
H 0.600192 1.040079 2.98066900
H 1.489364 -0.374476 1.86213700