-- Supporting Information --

Insights into the Capture of CO_2 by Nickel Hydride Complexes

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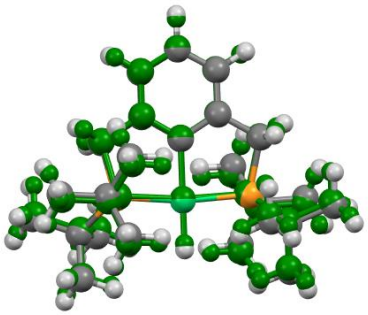
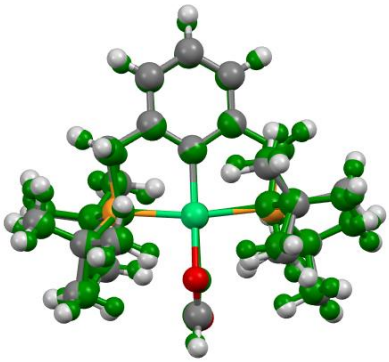
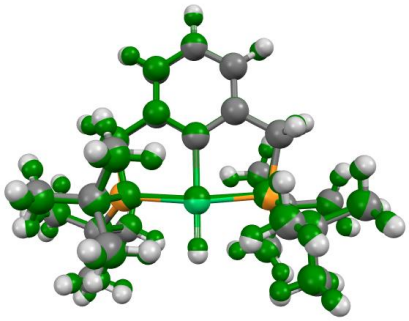
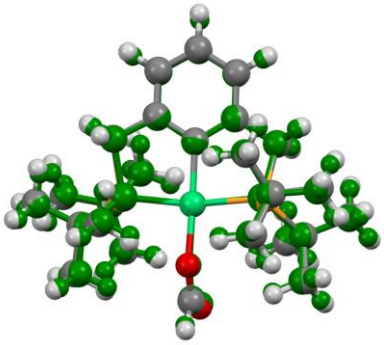
Table S1. The matched DFT optimized structure with the reported X-ray crystal structure. All non-hydrogen atoms are used to calculate the RMSD (in Å), X-ray crystal structures are presented in green.

 **I, [Ni^{II}]-H** **RMSD = 0.1680** CSD entry: SURZIP B3LYP-D3(BJ)/BS1 Optimized	 **I, [Ni^{II}]-(O)-formate** **RMSD = 0.1240** CSD entry: UMAPAA
 **I, [Ni^{II}]-H** **RMSD = 0.0921** CSD entry: SURZIP SMD(THF)-B3LYP-D3(BJ)/BS2 Optimized	 **I, [Ni^{II}]-(O)-formate** **RMSD = 0.0886** CSD entry: UMAPAA SMD(THF)-B3LYP-D3(BJ)/BS2 Optimized

$$\text{L-M-H} \longrightarrow \text{L-M}^{+} + \text{H}^{-} \quad \Delta G_{(soln,\ H^-)}$$

$$\Delta G_{(soln,\ H^-)} = (E_{(soln,\ H^-)} - E_{(gas,\ H^-)}) + (E_{(soln,\ L\text{-}M^+)} - E_{(gas,\ L\text{-}M^+)}) - (E_{(soln,\ L\text{-}M\text{-}H)} - E_{(gas,\ L\text{-}M\text{-}H)}) + (G_{(gas,\ H^-)} + G_{(gas,\ L\text{-}M^+)}) - G_{(gas,\ L\text{-}M\text{-}H)}$$

Scheme S1. Equation used to calculate the hydricity.

$$\Delta G^{\ddagger}_{(RDS)} = APT_{(M+)}\,(29.02) + \%V_{Bur(M+)}\,(-0.22) + 29.71 \qquad \text{Eq. 1b}$$
$$R^2 = 0.8269$$

$$\Delta G^{\ddagger}_{(RDS)} = APT_{(M+)}\,(-17.17) + \%V_{Bur(M+)}\,(0.65) + \Delta G_{(H^-)}\,(0.87) - 79.49 \qquad \text{Eq. 2b}$$
$$R^2 = 0.9578$$

Scheme S2. The multi-parameter models for the $\Delta G^{\ddagger}$ of RDS for TM–H complexes **I** to **VII**. In Eq. 1b and 2b, APT is APT charge of Ni atom in the axially vacant $[TM]^+$, $\%V_{Bur}$ is the percentages of buried volume in axially vacant $[TM]^+$.

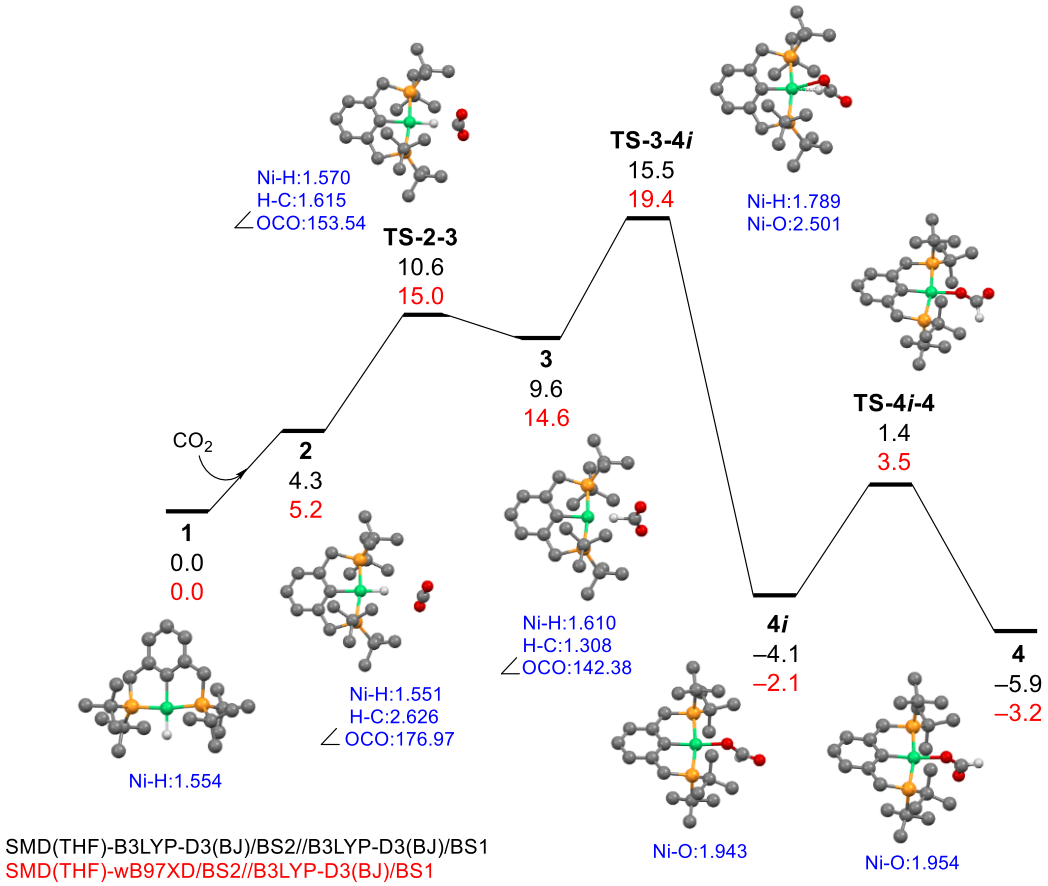


Figure S1. Free energy diagram for CO_2 insertion into **I**, ^{tBu2}(PCP)Ni–H.
Selected atom distances are given in Å, selected bond angles are given in degrees, and $\Delta G°/\Delta G^{\ddagger}$ are in kcal mol^{-1}. Hydrogen atoms except the hydride are omitted for clarity. Color code: green, Ni; yellow, P; gray, C; red, O; white, H. The red values are from SMD(THF)-wB97XD/BS2//B3LYP-D3(BJ)/BS1 computations, and the black values are from SMD(THF)-B3LYP-D3(BJ)/BS2//B3LYP-D3(BJ)/BS1 computations.

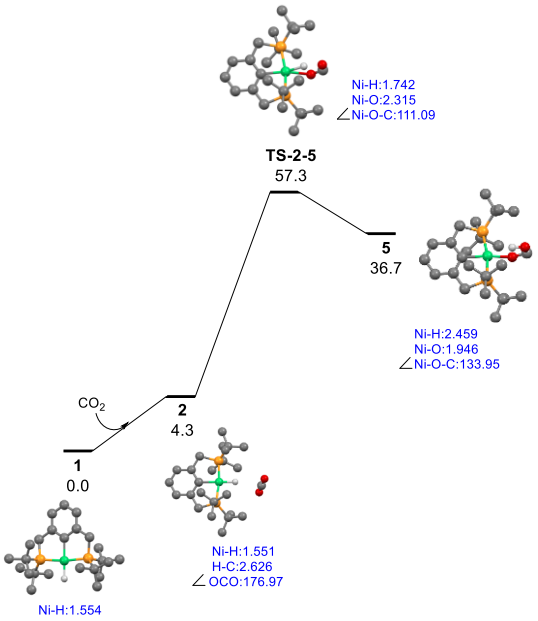


Figure S2. Free energy diagram for proton transfer from the Ni–H to the CO_2.
Selected atom distances are given in Å, selected bond angles are given in degrees, and $\Delta G°/\Delta G^{‡}$ are in kcal mol^{-1}. Hydrogen atoms except the hydride are omitted for clarity. Color code: green, Ni; yellow, P; gray, C; red, O; white, H.

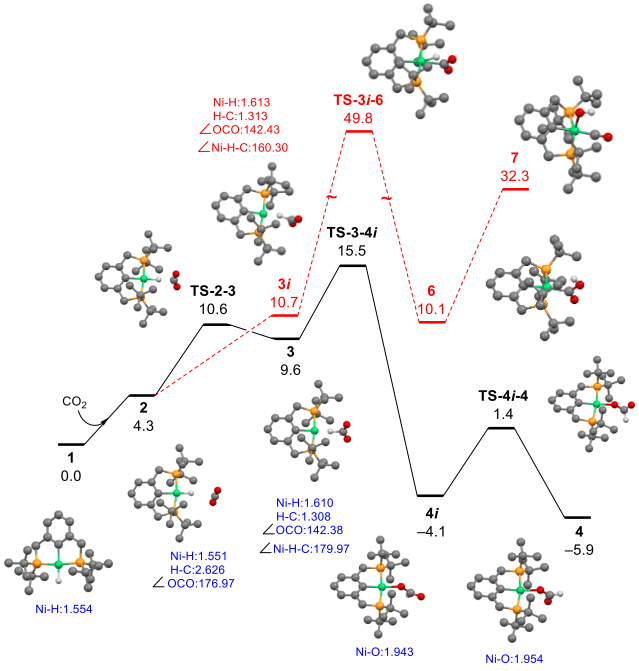


Figure S3. Free energy diagram for formate pathway and CO pathway with **I**, ^{tBu2}(PCP)Ni–H.

Selected atom distances are given in Å, selected bond angles are given in degrees, and $\Delta G°/\Delta G^{‡}$ are in kcal mol^{-1}. Hydrogen atoms except the hydride are omitted for clarity. Color code: green, Ni; yellow, P; gray, C; red, O; white, H. The red dashed line represents the CO pathway, and the black solid line represents the formate pathway.

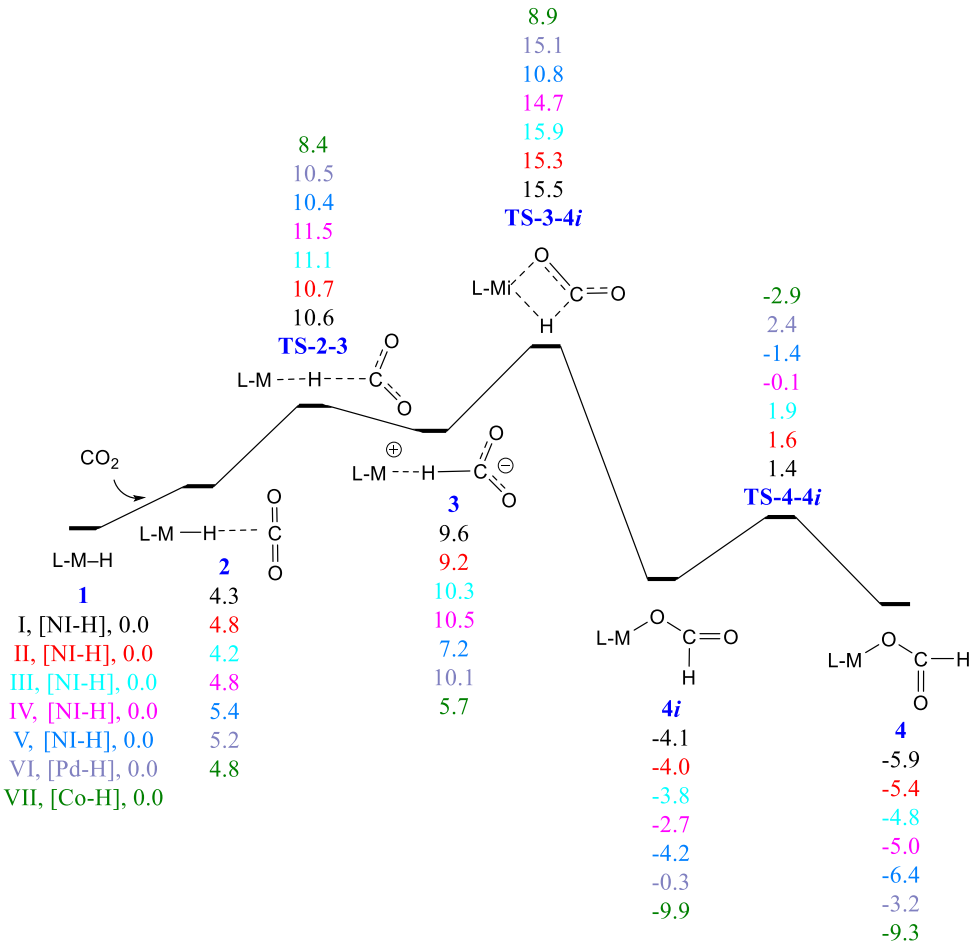


Figure S4. Free energy diagram for CO_2 insertion into TM–H.
$\Delta G°/\Delta G^{‡}$ are in kcal mol^{-1}.

Table S2. The AIM (Atoms-In-Molecules) analysis of the optimized structure **3**, M-(H)-formate. The orange balls represent the BCP (bond critical point), the yellow balls represent RCP (ring critical point), the green balls represent CCP (cage critical point), and the bond paths are shown in orange. Atom color codes: C, gray; H, white; O, red; N, blue; P, orange; Ni, Ni, lime; Co, ochre; Pd, tan. The electron densities of bond critical points [$\rho_{(BCP)}$] are given in a.u.

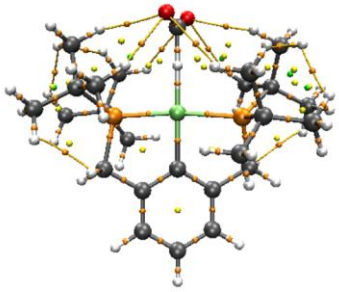
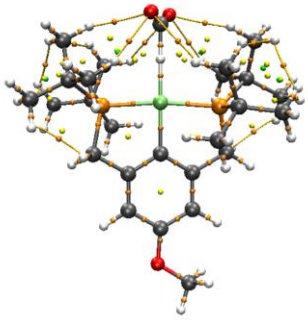
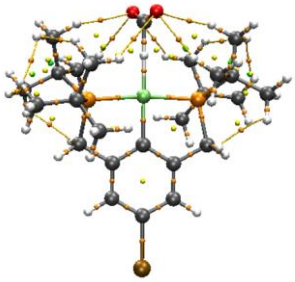
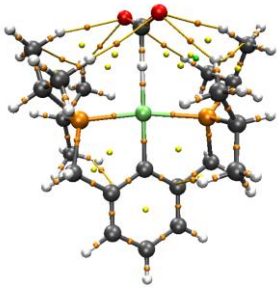
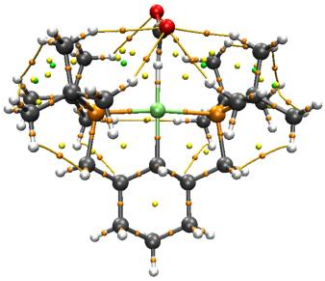
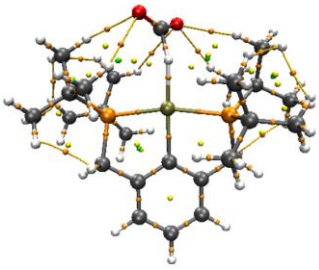
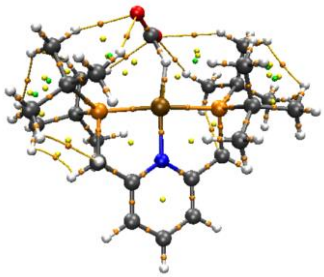
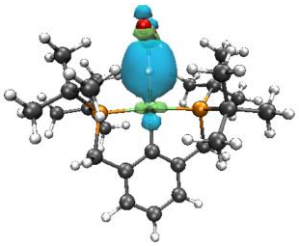
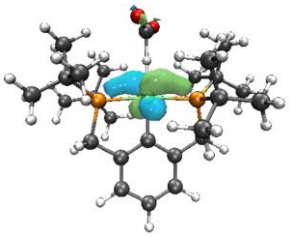
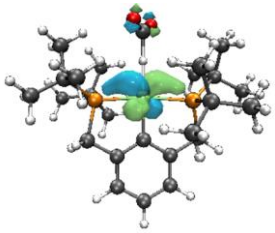
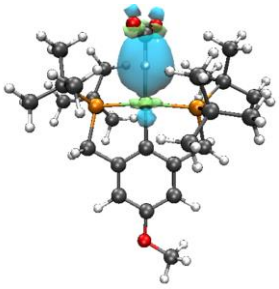
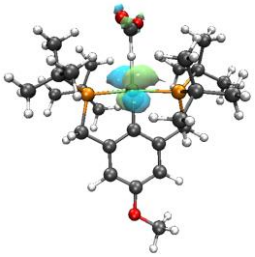
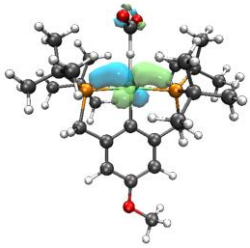
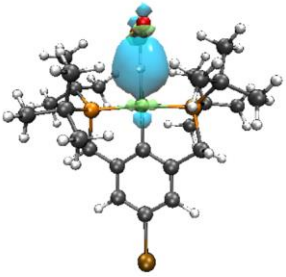
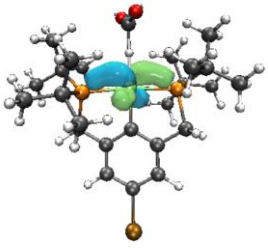
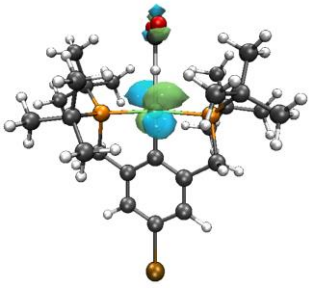
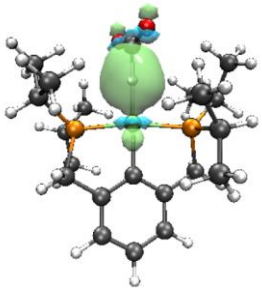
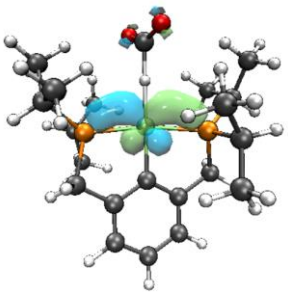
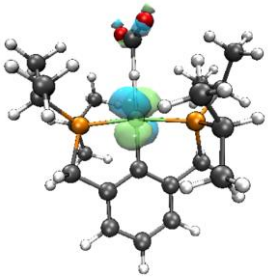
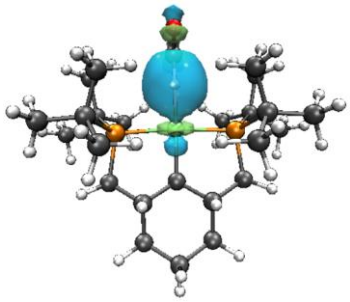
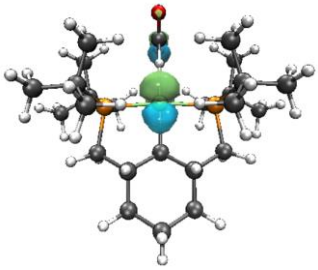
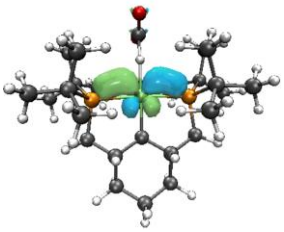
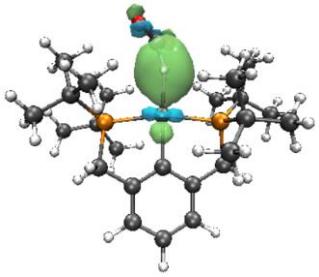
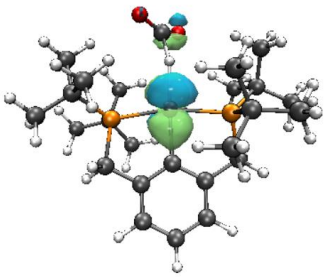
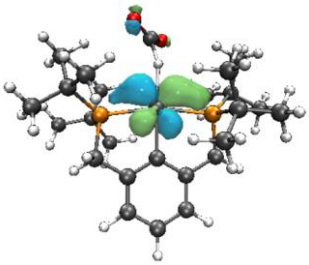
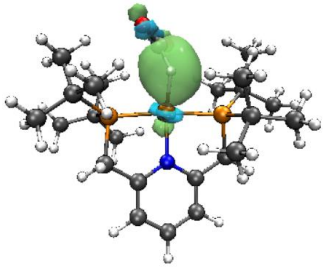
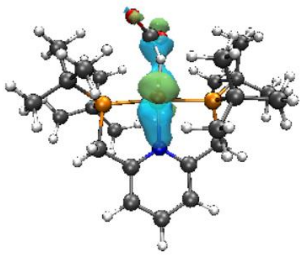
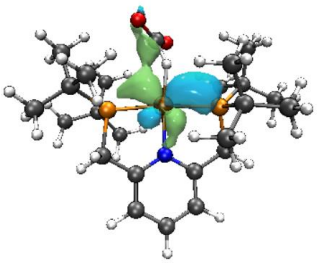
I, Ni-(H)-formate  $\rho_{(BCP,\ Ni\text{-}H)}$ = 0.0786 $\rho_{(BCP,\ C\text{-}H)}$ = 0.1527	**II, Ni-(H)-formate**  $\rho_{(BCP,\ Ni\text{-}H)}$ = 0.0782 $\rho_{(BCP,\ C\text{-}H)}$ = 0.1549	**III, Ni-(H)-formate**  $\rho_{(BCP,\ Ni\text{-}H)}$ = 0.0801 $\rho_{(BCP,\ C\text{-}H)}$ = 0.1473
IV, Ni-(H)-formate  $\rho_{(BCP,\ Ni\text{-}H)}$ = 0.0800 $\rho_{(BCP,\ C\text{-}H)}$ = 0.1464	**V, Ni-(H)-formate**  $\rho_{(BCP,\ Ni\text{-}H)}$ = 0.0730 $\rho_{(BCP,\ C\text{-}H)}$ = 0.1673	**VI, Pd-(H)-formate**  $\rho_{(BCP,\ Pd\text{-}H)}$ = 0.0706 $\rho_{(BCP,\ C\text{-}H)}$ = 0.1565
VII, Co-(H)-formate  $\rho_{(BCP,\ Co\text{-}H)}$ = 0.0698 $\rho_{(BCP,\ C\text{-}H)}$ = 0.1838		

Table S3. The first three NAdOs (natural adaptive orbitals, isovalue = 0.05) with their eigenvalues of M-H-C interaction in structure **3**, **TM-(H)-formate.**

Structure	Orbital 1	Orbital 2	Orbital 3
I	0.381  55.4%(H, 1s) + 10.2% (C, 2p) +3.6%(C, 2s) + 18.2% (Ni, 3d)+ 4.1% (Ni, 3p)+ 5.8% (Ni, 3s)	0.012 	0.012 
II	0.373  55.3%(H, 1s) + 10.3% (C, 2p) +3.6%(C, 2s) + 18.2% (Ni, 3d)+ 4.1% (Ni, 3p)+ 5.8% (Ni, 3s)	0.012 	0.012 
III	0.392  55.5%(H, 1s) + 9.7% (C, 2p) +3.5%(C, 2s) + 18.5% (Ni, 3d)+ 4.2% (Ni, 3p)+ 5.8% (Ni, 3s)	0.012 	0.012 
IV	0.392  57.6%(H, 1s) + 9.7% (C, 2p) +3.7%(C, 2s) + 18.3% (Ni, 3d)+ 2.7% (Ni, 3p)+ 5.4% (Ni, 3s)	0.12 	0.12 

V	0.351  53.6%(H, 1s) + 11.4% (C, 2p) +4.1%(C, 2s) + 17.2% (Ni, 3d)+ 6.0% (Ni, 3p)+ 5.2% (Ni, 3s)	0.012 	0.011 
VI	0.374  49.0%(H, 1s) + 9.8% (C, 2p) +4.6%(C, 2s) + 20.1% (Pd, 4d)+ 6.2% (Pd, 4p)+ 6.3% (Pd, 4s)	0.013 	0.012 
VII	0.326  52.1%(H, 1s) + 13.5% (C, 2p) +6.1%(C, 2s) + 15.9% (Co, 3d)+ 4.2% (Co, 3p)+ 4.3% (Co, 3s)	0.012 	0.012 

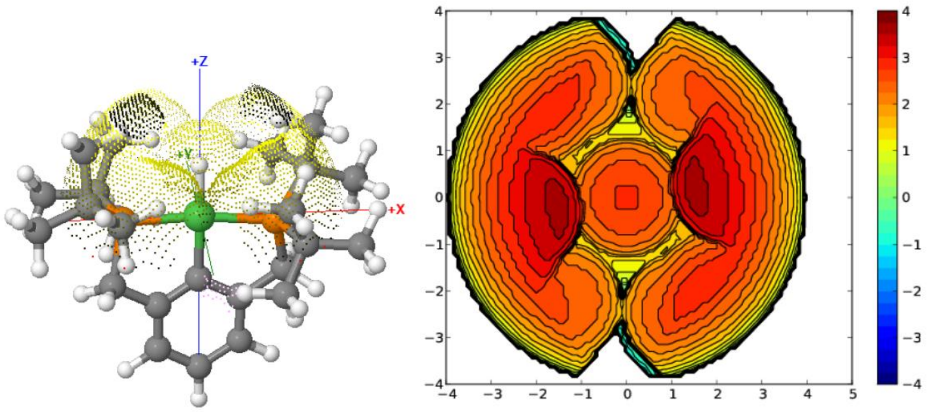
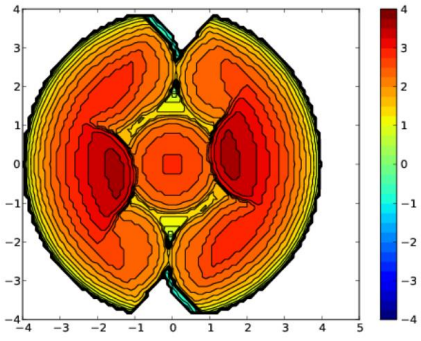
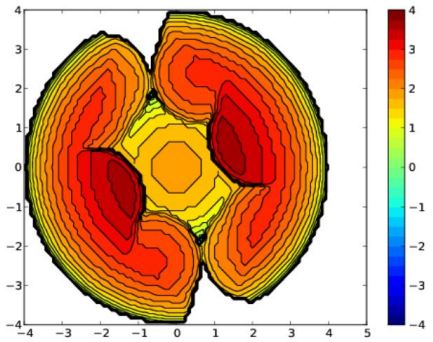
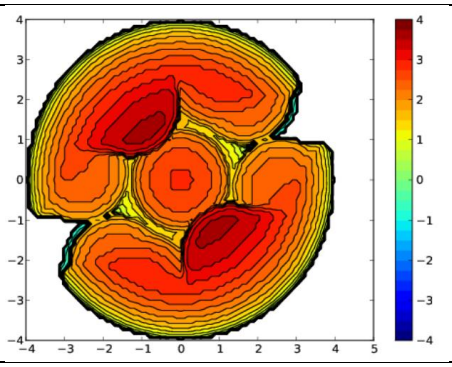
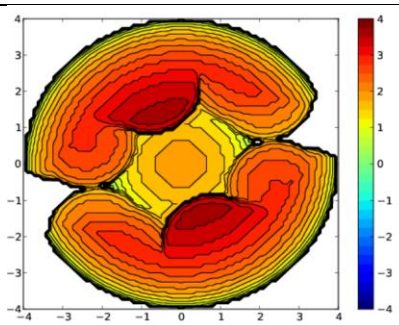


Figure S5. The representations of 3D and 2D steric maps of **TM–H**.
Details on the calculation of percentage buried volume ($\%V_{Bur}$) and the generation of steric map via SambVca (version 2.1): (1) Ni atom was coordinated to the center of the sphere, (2) $C_{tBu}/C_{tBu}/C_{tBu}/C_{tBu}$ atoms were defined as the positive z axis, (3) $C_{Me}/C_{Me}/C_{Me}/C_{Me}/C_{Me}/C_{Me}$ atoms of the coordinated pyridyl unit were defined as xz-plane, (4) Atomic Bondi radii were scaled by 1.17, (5) Sphere radius was set to 4.0 Å, (6) Mesh spacing for numerical integration was set to 0.10, (7) H atoms were included in the calculations.

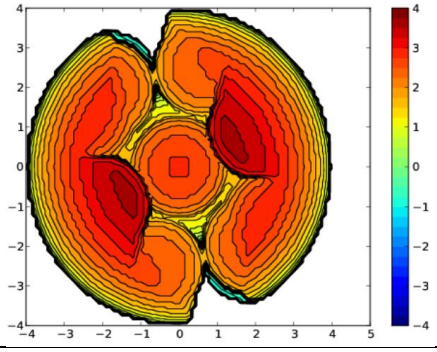
Table S4. The steric map of optimized **TM–H** and [**TM**]$^+$.

I, [Ni^{II}]-H **%V Buried = 82.9** 	**I, [Ni^{II}]$^+$** **%V Buried = 81.4** 
II, [Ni^{II}]-H **%V Buried = 82.9**	**II, [Ni^{II}]$^+$** **%V Buried = 81.4**

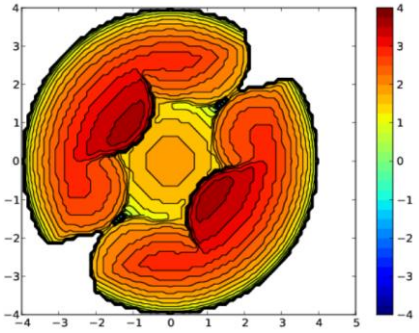




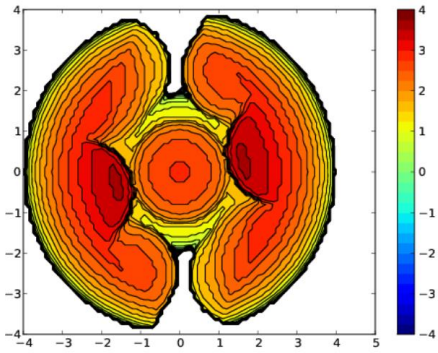
III, [Ni^{II}]-H
%V Buried = 82.9



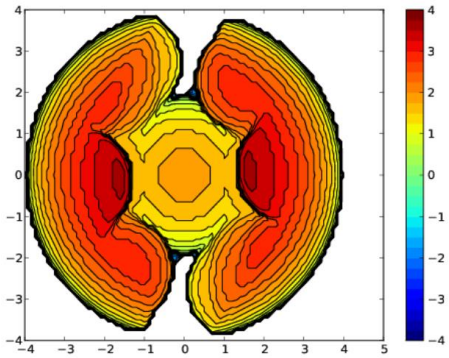
III, [Ni^{II}]$^{+}$
%V Buried = 81.4



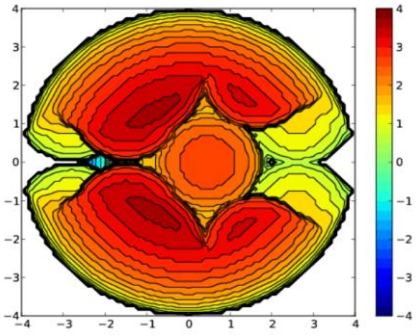
IV, [Ni^{II}]-H
%V Buried =79.2



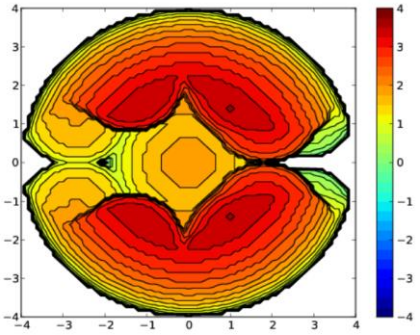
IV, [Ni^{II}]$^{+}$
%V Buried = 77.4



V, [Ni^{II}]-H
%V Buried = 84.5

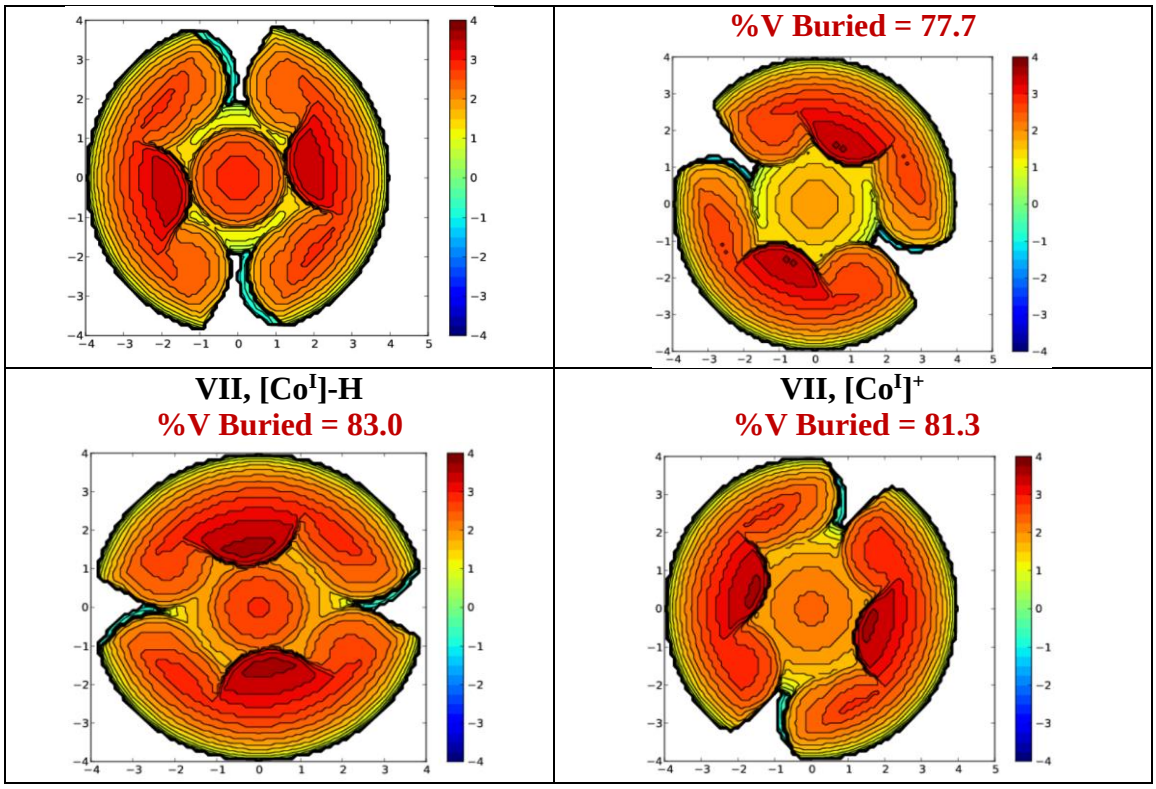


V, [Ni^{II}]$^{+}$
%V Buried = 83.4



VI, [Pd^{II}]-H
%V Buried = 79.3

VI, [Pd^{II}]$^{+}$



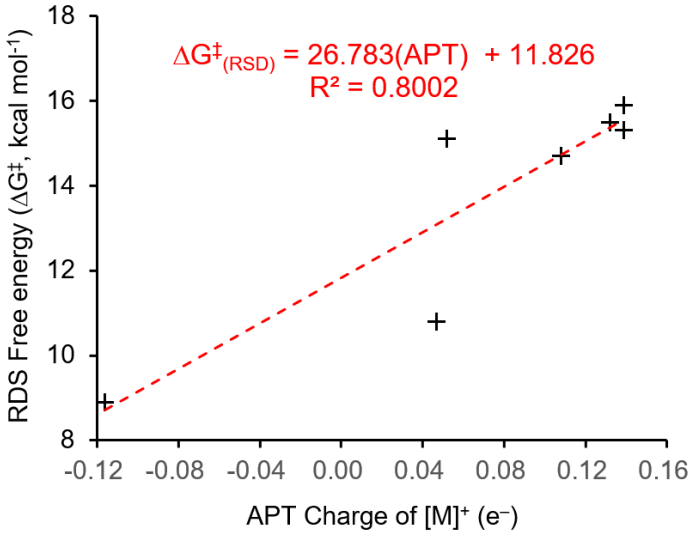


Figure S6. The linear fitting between the $\Delta G^{\ddagger}$ of RDS for **TM–H** complexes **I** to **VII** and the APT charges of TM atoms in the related $[TM]^{+}$.

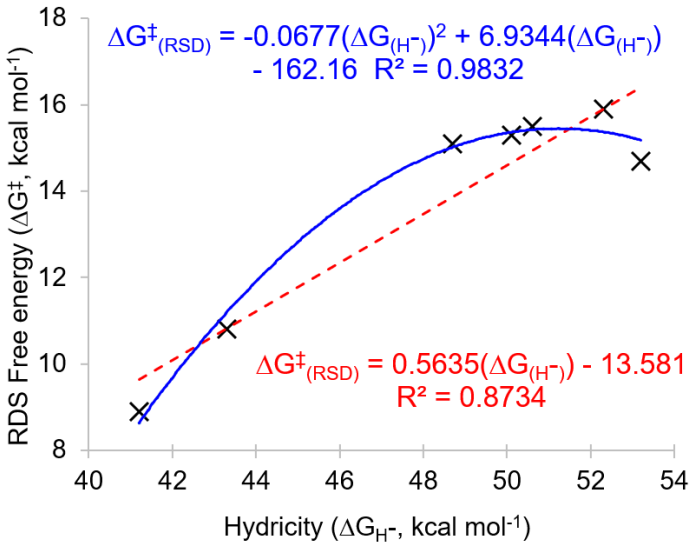


Figure S7. The fitting between the $\Delta G^{\ddagger}$ of RDS for **TM–H** complexes **I** to **VII** and the computed hydricities.
The blue line represents the second-order polynomial fitting, and the red line represents the linear fitting.

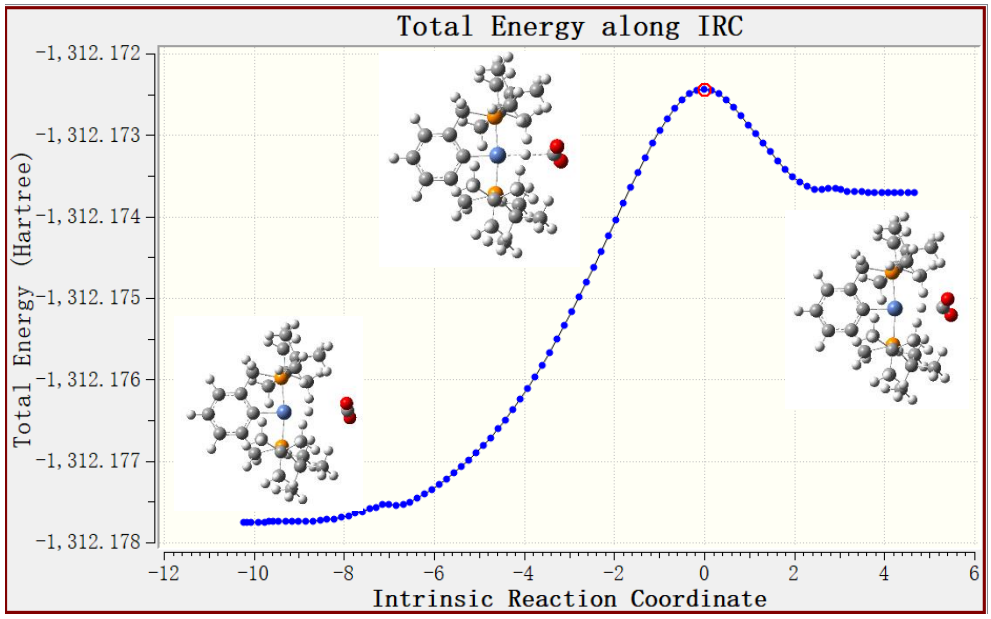


Figure S8. IRC plots for **TS-2-3**.

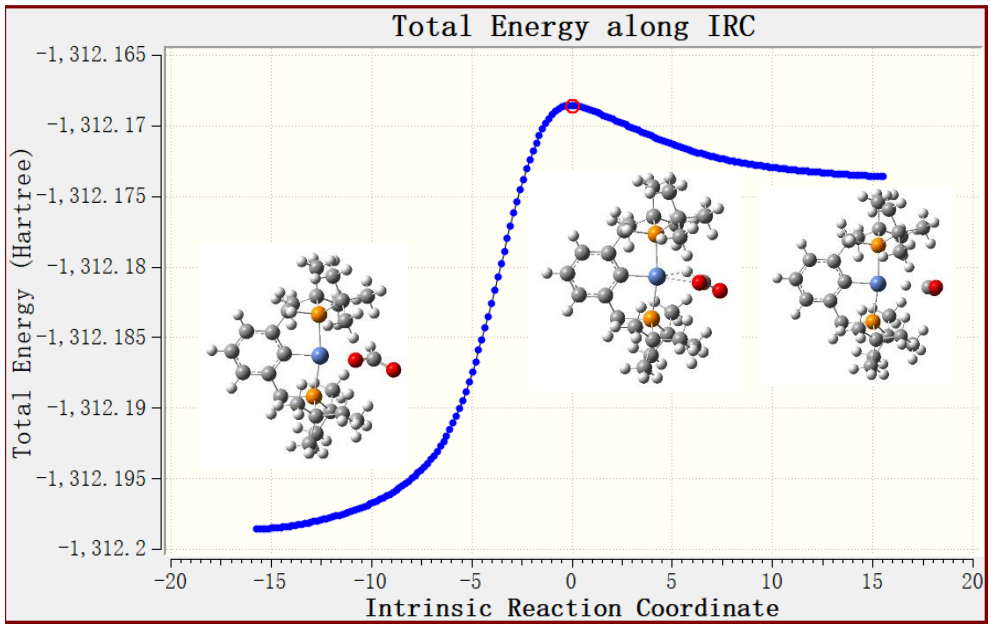


Figure S9. IRC plots for **TS-3-4i**.

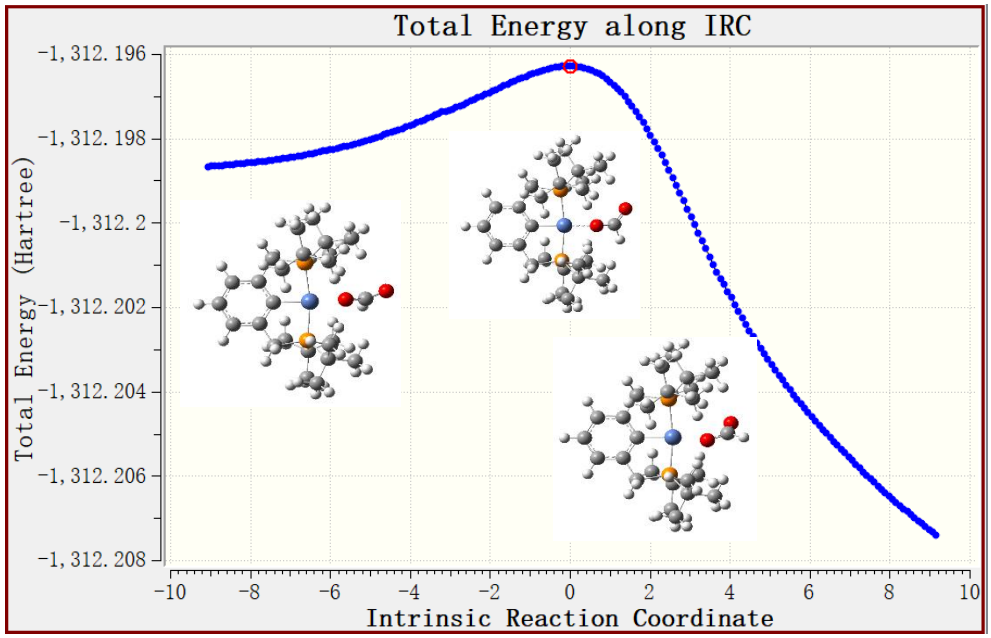


Figure S10. IRC plots for **TS-4i-4**.

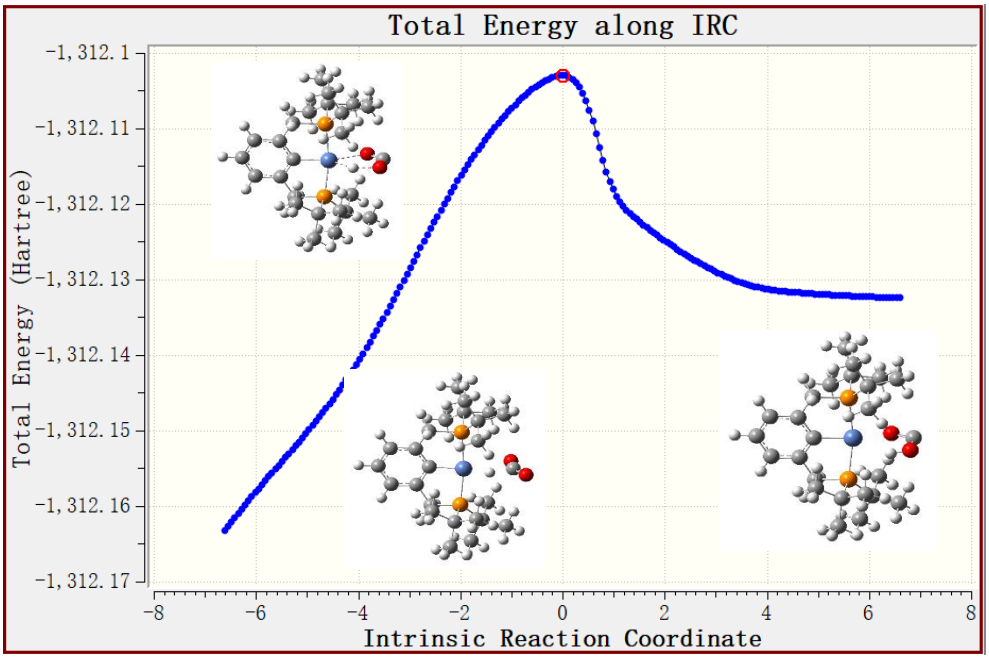


Figure S11. IRC plots for **TS-2-5**.

Table S5. DFT computed energies for species in **Chart 2** at 1 atm and 298.15 K. Energies are given in Hartrees.

Species	**E**(gas, B3LYP-D3(BJ)/BS1)	**G**(gas, B3LYP-D3(BJ)/BS1)	**E**(soln, SMD-B3LYP-D3(BJ)/BS2//B3LYP-D3(BJ)/BS1)
CO_2	-188.580762	-188.589853	-188.6727491
H^-	-0.461817	-0.471816	-0.640209
I, ^{tBu2}(PCP)Ni-H			
Ni-H,1	-1123.586868	-1123.016969	-3132.804606
Ni^+	-1122.803073	-1122.241500	-3132.065402
Ni-H + CO_2, 2	-1312.178776	-1311.604758	-3321.483774
Ni-(H)-formate, 3	-1312.173709	-1311.594479	-3321.480418
Ni-(O)-formate-isomer, 4i	-1312.199612	-1311.617444	-3321.505249
Ni-(O)-formate, 4	-1312.209734	-1311.627061	-3321.508558
Ni-(O)-hydroxyl, 5	-1312.133166	-1311.550291	-3321.440964
TS-2-3	-1312.172436	-1311.595445	-3321.476692
TS-3-4	-1312.168592	-1311.586299	-3321.474447
TS-4i-4	-1312.196289	-1311.613462	-3321.497111
TS-2-5	-1312.102943	-1311.527472	-3321.400638
Ni-(H)-formate-isomer, 3i	-1312.171706	-1311.592604	-3321.478616
TS-3i-6	-1312.104423	-1311.527661	-3321.413899
Ni-carboxylic acid, 6	-1312.176186	-1311.592516	-3321.484143
Ni-carbonyl, 7	-1312.135290	-1311.553514	-3321.446832
II, ^{tBu2}(*p*-MeO-PCP)Ni-H			

Ni-H	-1238.113514	-1237.514733	-3247.381892
Ni^+	-1237.331990	-1236.741655	-3246.643402
Ni-H + CO_2	-1426.705498	-1426.101645	-3436.061119
Ni-(H)-formate	-1426.700760	-1426.092707	-3436.058276
Ni-(O)-formate-isomer	-1426.726728	-1426.115124	-3436.082998
Ni-(O)-formate	-1426.736760	-1426.124144	-3436.086171
TS-2-3	-1426.699337	-1426.093004	-3436.054244
TS-3-4	-1426.695673	-1426.083743	-3436.052254
TS-4i-4	-1426.723374	-1426.110958	-3436.074789
III, ^{tBu2}(*p*-I-PCP)Ni-H			
Ni-H	-1134.380989	-1133.825648	-3430.009043
Ni^+	-1133.590997	-1133.043491	-3429.267600
Ni-H + CO_2	-1322.972813	-1322.413425	-3618.688213
Ni-(H)-formate	-1322.966368	-1322.401863	-3618.683688
Ni-(O)-formate-isomer	-1322.992463	-1322.425046	-3618.709042
Ni-(O)-formate	-1323.002723	-1322.434086	-3618.711789
TS-2-3	-1322.965691	-1322.402848	-3618.680708
TS-3-4	-1322.960981	-1322.393385	-3618.677800
TS-4i-4	-1322.990236	-1322.421622	-3618.701129
IV, ^{iPr2}(PCP)Ni-H			
Ni-H	-966.312419	-965.853026	-2975.473016
Ni^+	-965.525459	-965.073856	-2974.730284
Ni-H + CO_2	-1154.904581	-1154.441660	-3164.150734
Ni-(H)-formate	-1154.899530	-1154.430698	-3164.147560
Ni-(O)-formate-isomer	-1154.926243	-1154.463383	-3164.172687
Ni-(O)-formate	-1154.935887	-1154.453301	-3164.175886
TS-2-3	-1154.898904	-1154.431500	-3164.144532
TS-3-4	-1154.896520	-1154.423700	-3164.144851
TS-4i-4	-1154.925120	-1154.453157	-3164.167562
V, ^{tBu2}(PCyP)Ni-H			
Ni-H	-1127.209894	-1126.570965	-3136.423356
Ni^+	-1126.439528	-1125.808043	-3135.696733
Ni-H + CO_2	-1315.801791	-1315.157312	-3325.102211
Ni-(H)-formate	-1315.800916	-1315.150876	-3325.104876
Ni-(O)-formate-isomer	-1315.825145	-1315.172046	-3325.126089
Ni-(O)-formate	-1315.837804	-1315.183979	-3325.130271
TS-2-3	-1315.797641	-1315.150422	-3325.096915
TS-3-4	-1315.797942	-1315.145909	-3325.101131
TS-4i-4	-1315.823756	-1315.171094	-3325.121183
VI, ^{tBu2}(PCP)Pd-H			
Pd-H	-1081.042887	-1080.475067	-1752.397053
Pd^+	-1080.265952	-1079.704116	-1751.663330
Pd-H + CO_2	-1269.635512	-1269.062382	-1941.075876
Pd-(H)-formate	-1269.628678	-1269.049801	-1941.073837
Pd-(O)-formate-isomer	-1269.646459	-1269.067870	-1941.090198

Pd-(O)-formate	-1269.659888	-1269.079002	-1941.096981
TS-2-3	-1269.628128	-1269.053249	-1941.069278
TS-3-4	-1269.624038	-1269.042718	-1941.068291
TS-4i-4	-1269.646369	-1269.065735	-1941.087887
VII, ^{tBu2}(PNP)Co-H			
Co-H	-1115.976217	-1115.408356	-3023.874194
Co^{+}	-1115.213024	-1114.650186	-3023.153317
Co-H + CO_2	-1304.568979	-1303.996349	-3212.553180
Co-(H)-formate	-1304.571538	-1303.991872	-3212.558812
Co-(O)-formate-isomer	-1304.598259	-1304.017690	-3212.584472
Co-(O)-formate	-1304.608801	-1304.025703	-3212.586129
TS-2-3	-1304.565959	-1303.991926	-3212.548758
TS-3-4	-1304.570286	-1303.988559	-3212.555760
TS-4i-4	-1304.595249	-1304.013451	-3212.574651

Table S6. Cartesian coordinates of optimized species.

```
3
CO2          el energy= -188.580762132
C             0.169569        0.067934       -0.021409
O             0.169407        0.208296       -1.179089
O             0.169732       -0.072427        1.136272

71
1,Ni-H     el energy= -1123.58686785
Ni            0.000000        0.000000        0.219178
H             0.000000        0.000000        1.773663
C             0.000000        0.000000       -1.739477
C             1.198136        0.171310       -2.475506
C             2.487752        0.386304       -1.703269
C             1.197445        0.165666       -3.875765
H             2.129514        0.298793       -4.425261
C             0.000000        0.000000       -4.575765
H             0.000000        0.000000       -5.664208
C            -1.197445       -0.165666       -3.875765
H            -2.129514       -0.298793       -4.425261
C            -1.198136       -0.171310       -2.475506
C            -2.487752       -0.386304       -1.703269
P             2.160095       -0.143588        0.066085
P            -2.160095        0.143588        0.066085
C             3.185200        1.051275        1.124609
C             2.379082        2.367971        1.103681
```

C	4.601102	1.311952	0.583181
C	3.253657	0.547924	2.575169
C	2.773920	-1.939057	0.166026
C	4.300359	-2.082248	0.078327
C	2.251384	-2.566923	1.471987
C	2.121253	-2.686942	-1.015603
C	-2.773920	1.939057	0.166026
C	-2.121253	2.686942	-1.015603
C	-2.251384	2.566923	1.471987
C	-4.300359	2.082248	0.078327
C	-3.185200	-1.051275	1.124609
C	-4.601102	-1.311952	0.583181
C	-2.379082	-2.367971	1.103681
C	-3.253657	-0.547924	2.575169
H	3.348042	-0.130005	-2.150129
H	2.746275	1.453478	-1.680541
H	-2.746275	-1.453478	-1.680541
H	-3.348042	0.130005	-2.150129
H	2.896594	3.124477	1.710545
H	2.271789	2.772083	0.089220
H	1.375691	2.212570	1.515177
H	5.225603	0.414253	0.596850
H	4.584466	1.698071	-0.442457
H	5.095245	2.068398	1.209600
H	3.909327	-0.324290	2.675571
H	3.660841	1.340884	3.218354
H	2.257019	0.283376	2.946861
H	4.565233	-3.147573	0.017317
H	4.710472	-1.589718	-0.812092
H	4.802282	-1.671374	0.960801
H	2.702939	-2.118983	2.361987
H	1.166038	-2.445286	1.552526
H	2.487245	-3.640652	1.479604
H	2.468957	-2.321409	-1.987592
H	1.031013	-2.588120	-0.997535
H	2.377081	-3.753480	-0.944420
H	-2.377081	3.753480	-0.944420
H	-1.031013	2.588120	-0.997535
H	-2.468957	2.321409	-1.987592
H	-2.702939	2.118983	2.361987
H	-2.487245	3.640652	1.479604
H	-1.166038	2.445286	1.552526
H	-4.565233	3.147573	0.017317
H	-4.710472	1.589718	-0.812092
H	-4.802282	1.671374	0.960801

H	-5.095245	-2.068398	1.209600
H	-5.225603	-0.414253	0.596850
H	-4.584466	-1.698071	-0.442457
H	-1.375691	-2.212570	1.515177
H	-2.896594	-3.124477	1.710545
H	-2.271789	-2.772083	0.089220
H	-3.660841	-1.340884	3.218354
H	-2.257019	-0.283376	2.946861
H	-3.909327	0.324290	2.675571

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1,Ni+ el energy= -1122.80307291

Ni	0.000000	0.000000	-0.041785
C	0.000000	0.000000	-1.925698
C	0.680328	1.016179	-2.627781
C	1.402937	2.104166	-1.863765
C	0.676229	1.001967	-4.027906
H	1.206827	1.780732	-4.572639
C	0.000000	0.000000	-4.724566
H	0.000000	0.000000	-5.811543
C	-0.676229	-1.001967	-4.027906
H	-1.206827	-1.780732	-4.572639
C	-0.680328	-1.016179	-2.627781
C	-1.402937	-2.104166	-1.863765
P	1.698066	1.456173	-0.145906
P	-1.698066	-1.456173	-0.145906
C	1.542994	2.940263	1.019691
C	0.030204	3.245450	1.082342
C	2.295341	4.179070	0.502762
C	2.030749	2.566822	2.429749
C	3.398016	0.623386	-0.145379
C	4.557321	1.631498	-0.173951
C	3.492485	-0.279825	1.100100
C	3.461486	-0.273397	-1.398915
C	-3.398016	-0.623386	-0.145379
C	-3.461486	0.273397	-1.398915
C	-3.492485	0.279825	1.100100
C	-4.557321	-1.631498	-0.173951
C	-1.542994	-2.940263	1.019691
C	-2.295341	-4.179070	0.502762
C	-0.030204	-3.245450	1.082342
C	-2.030749	-2.566822	2.429749
H	2.329547	2.420256	-2.356934
H	0.771507	2.996855	-1.773662
H	-0.771507	-2.996855	-1.773662

H	-2.329547	-2.420256	-2.356934
H	-0.136527	4.129492	1.711310
H	-0.399415	3.457455	0.095937
H	-0.532178	2.412102	1.523852
H	3.375266	4.018933	0.447026
H	1.943814	4.492182	-0.486780
H	2.120011	5.016863	1.190725
H	3.115627	2.428586	2.469955
H	1.777224	3.376910	3.125653
H	1.551948	1.651581	2.802132
H	5.504828	1.087039	-0.280000
H	4.481361	2.324112	-1.020826
H	4.619724	2.217770	0.748266
H	3.462607	0.283320	2.037176
H	2.681082	-1.019083	1.114645
H	4.441443	-0.830933	1.075687
H	3.440801	0.302392	-2.329954
H	2.636554	-0.993220	-1.429680
H	4.403876	-0.835689	-1.377109
H	-4.403876	0.835689	-1.377109
H	-2.636554	0.993220	-1.429680
H	-3.440801	-0.302392	-2.329954
H	-3.462607	-0.283320	2.037176
H	-4.441443	0.830933	1.075687
H	-2.681082	1.019083	1.114645
H	-5.504828	-1.087039	-0.280000
H	-4.481361	-2.324112	-1.020826
H	-4.619724	-2.217770	0.748266
H	-2.120011	-5.016863	1.190725
H	-3.375266	-4.018933	0.447026
H	-1.943814	-4.492182	-0.486780
H	0.532178	-2.412102	1.523852
H	0.136527	-4.129492	1.711310
H	0.399415	-3.457455	0.095937
H	-1.777224	-3.376910	3.125653
H	-1.551948	-1.651581	2.802132
H	-3.115627	-2.428586	2.469955

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1,Ni-H+CO2 el energy= -1312.17877646

Ni	0.009243	0.061799	-0.001883
H	0.014529	1.612022	0.033646
C	0.010475	-1.899907	-0.033710
C	-1.165426	-2.641583	0.236586
C	-2.423945	-1.878996	0.605029

C	-1.167520	-4.041394	0.200198
H	-2.083868	-4.593378	0.409906
C	0.007456	-4.737392	-0.092283
H	0.005810	-5.825524	-0.116671
C	1.185459	-4.032650	-0.349613
H	2.101900	-4.577626	-0.576517
C	1.187278	-2.632612	-0.325135
C	2.457094	-1.858542	-0.626719
P	-2.159961	-0.094858	0.092711
P	2.177847	-0.101042	-0.038665
C	-3.049958	0.914668	1.432341
C	-2.089807	0.876286	2.640717
C	-4.414425	0.335410	1.845048
C	-3.213060	2.377191	0.990885
C	-2.981219	0.049418	-1.614253
C	-4.512423	-0.060486	-1.580049
C	-2.554732	1.381197	-2.258026
C	-2.403325	-1.098036	-2.469339
C	2.916185	-0.038618	1.712129
C	2.298810	-1.221716	2.487125
C	2.462580	1.265864	2.394733
C	4.447289	-0.151660	1.746204
C	3.130041	0.971906	-1.279920
C	4.519283	0.422816	-1.647398
C	2.238417	0.981854	-2.540102
C	3.253957	2.409214	-0.749064
H	-3.334636	-2.313992	0.172041
H	-2.566371	-1.887167	1.693806
H	2.632908	-1.815647	-1.709825
H	3.353116	-2.316235	-0.186383
H	-2.527453	1.442164	3.475278
H	-1.906087	-0.146810	2.992326
H	-1.124663	1.324491	2.380746
H	-5.141188	0.355793	1.027940
H	-4.334412	-0.697405	2.202189
H	-4.826442	0.935161	2.669155
H	-3.953906	2.484808	0.190699
H	-3.562314	2.976856	1.843332
H	-2.261626	2.799588	0.653089
H	-4.899727	-0.092013	-2.608508
H	-4.850325	-0.972937	-1.073423
H	-4.974195	0.799688	-1.083748
H	-2.949525	2.249842	-1.722188
H	-1.464955	1.470971	-2.285449
H	-2.933311	1.425749	-3.289128

H	-2.695497	-2.086338	-2.098795
H	-1.309059	-1.065398	-2.494031
H	-2.778734	-0.997847	-3.497424
H	2.637562	-1.175706	3.531693
H	1.204829	-1.180951	2.473346
H	2.596974	-2.192950	2.078311
H	2.905950	2.154466	1.935914
H	2.765851	1.247949	3.451217
H	1.373924	1.372937	2.344929
H	4.784731	-0.234047	2.789292
H	4.808266	-1.039587	1.212602
H	4.932952	0.730195	1.315166
H	4.463738	-0.591144	-2.059512
H	4.969148	1.064709	-2.418320
H	5.202522	0.404749	-0.793782
H	1.254372	1.405418	-2.320720
H	2.713565	1.594327	-3.319343
H	2.095319	-0.025594	-2.950623
H	3.565066	3.077515	-1.563925
H	2.297891	2.770153	-0.355686
H	4.004008	2.486401	0.046132
C	-0.123240	3.999735	-1.051378
O	-0.320965	4.414166	0.020437
O	0.072469	3.642907	-2.144936

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1,Ni-(H)-formate el energy= -1312.17370872

Ni	0.000047	0.091741	0.000142
H	0.000100	1.701639	-0.000024
C	0.000117	-1.840827	0.000238
C	-1.176702	-2.572164	0.282219
C	-2.439169	-1.815836	0.629326
C	-1.174811	-3.972498	0.273385
H	-2.093211	-4.517117	0.490296
C	0.000157	-4.673777	0.000313
H	0.000172	-5.761817	0.000316
C	1.175109	-3.972472	-0.272756
H	2.093527	-4.517076	-0.489631
C	1.176968	-2.572136	-0.281641
C	2.439461	-1.815815	-0.628681
P	-2.206846	-0.044489	0.088013
P	2.206964	-0.044274	-0.088017
C	-3.161832	0.965651	1.383987
C	-2.203424	1.051220	2.592136
C	-4.476055	0.280931	1.805105

C	-3.470468	2.391097	0.897442
C	-2.947676	0.074475	-1.652512
C	-4.472640	-0.108898	-1.680235
C	-2.556871	1.434742	-2.262708
C	-2.282282	-1.038928	-2.487761
C	2.947696	0.075306	1.652567
C	2.281724	-1.037413	2.488270
C	2.557467	1.436047	2.262024
C	4.472582	-0.108716	1.680564
C	3.161892	0.965469	-1.384320
C	4.476086	0.280700	-1.805411
C	2.203341	1.050789	-2.592399
C	3.470521	2.391054	-0.898215
H	-3.342653	-2.270893	0.203501
H	-2.580329	-1.802766	1.717458
H	2.580944	-1.803166	-1.716772
H	3.342846	-2.270671	-0.202427
H	-2.724469	1.528987	3.433703
H	-1.870503	0.060309	2.928739
H	-1.325274	1.657372	2.347276
H	-5.172995	0.162601	0.969549
H	-4.311071	-0.704311	2.253858
H	-4.970634	0.904266	2.562830
H	-4.203653	2.399592	0.083998
H	-3.901948	2.959040	1.733319
H	-2.570819	2.923185	0.580593
H	-4.817289	-0.124693	-2.723736
H	-4.784188	-1.053661	-1.217453
H	-4.995017	0.710467	-1.175973
H	-3.045726	2.274853	-1.762200
H	-1.477191	1.609890	-2.214930
H	-2.860833	1.454396	-3.318628
H	-2.520973	-2.042507	-2.119109
H	-1.191809	-0.938206	-2.491671
H	-2.640328	-0.964193	-3.523794
H	2.639707	-0.962346	3.524303
H	1.191296	-0.936198	2.492036
H	2.519986	-2.041281	2.120126
H	3.046770	2.275675	1.761127
H	2.861371	1.456099	3.317955
H	1.477885	1.611724	2.214082
H	4.817032	-0.124667	2.724129
H	4.783840	-1.053587	1.217814
H	4.995389	0.710453	1.176433
H	4.311169	-0.704779	-2.253664

H	4.970417	0.903752	-2.563528
H	5.173225	0.162868	-0.969951
H	1.325163	1.656916	-2.347542
H	2.724272	1.528472	-3.434079
H	1.870428	0.059816	-2.928815
H	3.902221	2.958668	-1.734206
H	2.570822	2.923272	-0.581761
H	4.203543	2.399800	-0.084638
C	-0.000546	3.009340	0.000125
O	-0.203362	3.400849	1.132175
O	0.201863	3.401255	-1.131857

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1,Ni-(0)-formate-isomer el energy= -1312.19961162

Ni	0.019566	-0.144145	0.012060
P	-2.219596	-0.068374	0.098512
P	2.225581	0.145100	-0.052815
O	0.095003	-2.048289	0.393277
O	-0.590468	-4.143777	-0.019924
C	-3.086215	-1.056834	1.472325
C	-2.089538	-1.032859	2.651583
C	-3.333753	-2.521362	1.072739
C	-4.416967	-0.411410	1.903190
C	-3.037294	-0.277894	-1.600424
C	-2.554861	-1.607401	-2.209552
C	-4.571964	-0.234298	-1.547149
C	-2.526807	0.871793	-2.492574
C	-2.494457	1.713819	0.560070
C	-1.279182	2.489924	0.105089
C	-1.353080	3.881892	-0.022883
C	-0.224208	4.620362	-0.377627
C	0.984148	3.960123	-0.597443
C	1.062733	2.566407	-0.484250
C	-0.072153	1.789137	-0.142634
C	2.385532	1.872028	-0.727894
C	3.250201	-0.923708	-1.235765
C	2.389635	-1.038507	-2.512367
C	4.606262	-0.295062	-1.603351
C	3.466806	-2.326173	-0.642174
C	2.923370	0.194138	1.710912
C	2.147587	1.311746	2.440326
C	2.613278	-1.144756	2.410912
C	4.428607	0.492530	1.774012
C	-0.099182	-3.079237	-0.366073
H	-1.171910	-1.562781	2.380002

H	-2.544024	-1.532220	3.518648
H	-1.830760	-0.010014	2.957580
H	-4.059229	-2.609620	0.256150
H	-3.760765	-3.047012	1.938881
H	-2.415609	-3.047154	0.794895
H	-4.837797	-0.996174	2.732937
H	-5.158535	-0.402661	1.098735
H	-4.290352	0.615915	2.262106
H	-1.469442	-1.593153	-2.355576
H	-3.025469	-1.749611	-3.192489
H	-2.795113	-2.476574	-1.591159
H	-4.941027	0.681452	-1.068973
H	-4.990443	-1.093872	-1.014783
H	-4.970811	-0.254766	-2.571243
H	-2.894288	0.714127	-3.516155
H	-1.432486	0.905012	-2.520410
H	-2.880016	1.852596	-2.156397
H	-3.435630	2.118015	0.166181
H	-2.571512	1.752206	1.654327
H	-2.297130	4.391556	0.167349
H	-0.283896	5.702493	-0.473449
H	1.873944	4.530817	-0.861799
H	3.233666	2.417537	-0.294290
H	2.587099	1.790233	-1.803702
H	2.188349	-0.060096	-2.966035
H	1.428327	-1.517798	-2.303988
H	2.921746	-1.646437	-3.256911
H	4.494219	0.689650	-2.071304
H	5.116273	-0.945302	-2.328147
H	5.265237	-0.186995	-0.737508
H	3.835221	-3.000857	-1.427152
H	2.540658	-2.743721	-0.238260
H	4.216614	-2.312522	0.156238
H	2.310146	2.299451	1.995321
H	2.485636	1.350200	3.484920
H	1.069538	1.119278	2.433262
H	2.790301	-1.033091	3.489639
H	3.255518	-1.954825	2.054054
H	1.575138	-1.454838	2.254517
H	4.728199	0.627550	2.822865
H	4.695139	1.410494	1.235326
H	5.025273	-0.331342	1.368947
H	0.229740	-2.952665	-1.426227

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1,Ni-(0)-formate el energy= -1312.20973375

Ni	-0.017168	-0.172096	0.105042
P	-2.253816	-0.069356	0.107649
P	2.211499	0.087142	-0.030996
O	0.038524	-2.032106	0.700592
O	0.143637	-3.120124	-1.282423
C	-3.183926	-1.023135	1.462435
C	-2.258784	-0.957841	2.697578
C	-3.380027	-2.496655	1.071416
C	-4.546636	-0.396511	1.809786
C	-3.009118	-0.286196	-1.621592
C	-2.649608	-1.677895	-2.173045
C	-4.532326	-0.084680	-1.645683
C	-2.336935	0.773622	-2.519636
C	-2.532200	1.718298	0.541423
C	-1.293870	2.477481	0.122668
C	-1.347031	3.871900	0.007391
C	-0.204787	4.597357	-0.329029
C	0.993348	3.919280	-0.549619
C	1.049391	2.523505	-0.449437
C	-0.095161	1.759357	-0.115005
C	2.355733	1.813000	-0.714313
C	3.244800	-0.948703	-1.244271
C	2.356726	-1.096175	-2.498935
C	4.566661	-0.259630	-1.633515
C	3.551642	-2.343505	-0.675464
C	2.956057	0.161150	1.715324
C	2.172716	1.262241	2.461264
C	2.698737	-1.180455	2.429773
C	4.454936	0.494868	1.741080
C	0.097439	-3.072559	-0.054438
H	-1.315936	-1.474835	2.498127
H	-2.758601	-1.441918	3.548618
H	-2.034354	0.075605	2.992502
H	-4.117206	-2.614037	0.270219
H	-3.751422	-3.052247	1.944045
H	-2.440579	-2.957106	0.755243
H	-5.002854	-0.970593	2.628679
H	-5.243740	-0.413457	0.967150
H	-4.452291	0.639679	2.152837
H	-1.577195	-1.886072	-2.106758
H	-2.949089	-1.727829	-3.229611
H	-3.174089	-2.481098	-1.647091
H	-4.836748	0.874920	-1.209733
H	-5.058573	-0.886708	-1.117562

H	-4.880463	-0.097353	-2.688108
H	-2.705333	0.645499	-3.546777
H	-1.248260	0.657037	-2.527464
H	-2.559568	1.798991	-2.205581
H	-3.451341	2.125392	0.101274
H	-2.657205	1.772028	1.630681
H	-2.286244	4.392528	0.192222
H	-0.246874	5.681284	-0.413732
H	1.893248	4.477234	-0.806952
H	3.220606	2.353467	-0.308934
H	2.525085	1.721745	-1.794411
H	2.078150	-0.121870	-2.921745
H	1.446116	-1.659631	-2.273623
H	2.919401	-1.639449	-3.271425
H	4.406464	0.716659	-2.103603
H	5.087828	-0.890954	-2.366810
H	5.238440	-0.121528	-0.781604
H	3.987134	-2.964003	-1.470671
H	2.651191	-2.849910	-0.321320
H	4.279476	-2.298112	0.142247
H	2.302206	2.252073	2.010262
H	2.532435	1.311332	3.498429
H	1.098951	1.045764	2.478563
H	2.937852	-1.069377	3.496881
H	3.326068	-1.984470	2.033453
H	1.655063	-1.494572	2.331504
H	4.776013	0.642548	2.782008
H	4.687687	1.415548	1.191871
H	5.060651	-0.316967	1.325426
H	0.105768	-4.019426	0.532279

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1,Ni-(0)-hydroxyl el energy= -1312.13316571

Ni	0.033219	-0.238258	0.000464
P	-2.206556	-0.038972	-0.065580
P	2.254102	-0.024079	0.149656
O	0.189463	-2.123679	-0.527937
O	-0.384699	-3.062938	1.364042
C	3.563023	-2.493038	0.713271
C	-1.117949	2.441480	-0.322793
C	-2.335538	1.676351	-0.788355
C	-3.152500	-1.134769	-1.301444
C	-2.193361	-1.305501	-2.501170
C	-3.097321	0.108981	1.617456
C	-4.618942	0.273423	1.469456

C	3.016151	0.065102	-1.592292
C	2.301125	1.215619	-2.331401
C	3.268543	-1.116087	1.331964
C	4.587054	-0.441183	1.757374
C	2.388527	-1.314780	2.584295
C	0.019780	1.706086	0.085447
C	0.018245	-3.220912	0.075703
C	-2.529119	1.346421	2.341593
C	-4.459325	-0.492903	-1.804384
C	2.713994	-1.246816	-2.343837
C	0.011045	4.545515	0.094758
C	-1.122552	3.841291	-0.312546
C	1.153506	3.844875	0.483497
C	1.161347	2.444622	0.477916
C	2.411648	1.689107	0.868534
C	4.528479	0.335868	-1.588010
C	-3.449770	-2.517462	-0.697078
C	-2.793710	-1.123567	2.488247
H	-0.474431	-2.089458	1.536659
H	2.660813	-2.968678	0.315398
H	4.308110	-2.427912	-0.086907
H	-3.278982	2.175186	-0.532964
H	2.474350	1.576373	1.958998
H	3.330347	2.199376	0.552243
H	-2.694693	-1.905521	-3.273303
H	-1.929393	-0.341987	-2.956790
H	-5.210133	-0.382865	-1.018283
H	-4.290643	0.490725	-2.257087
H	-4.889666	-1.139252	-2.582052
H	-4.190288	-2.462260	0.108940
H	-3.866026	-3.166819	-1.479681
H	-2.548372	-3.003073	-0.312065
H	-5.051179	0.497035	2.454810
H	-5.097876	-0.639599	1.102523
H	-3.004233	-2.073805	1.990826
H	-1.743921	-1.130126	2.801002
H	-3.402913	-1.076484	3.401571
H	-1.438459	1.302916	2.422772
H	-2.950793	1.380108	3.355923
H	2.681839	1.257553	-3.361236
H	1.218565	1.057355	-2.370386
H	2.475037	2.191374	-1.865878
H	2.989138	-1.120736	-3.400396
H	1.655347	-1.513812	-2.282328
H	2.034888	-0.364206	3.004223

H	4.868311	0.494464	-2.621158
H	4.790516	1.234000	-1.014958
H	5.095349	-0.509755	-1.185928
H	4.417096	0.505929	2.281640
H	5.255037	-0.248297	0.914100
H	1.522494	-1.943053	2.364662
H	2.979526	-1.819040	3.361345
H	3.974143	-3.151672	1.490810
H	3.286126	-2.091730	-1.951265
H	-4.885555	1.099158	0.799395
H	-2.786630	2.284298	1.839535
H	5.115979	-1.108290	2.452321
H	-1.272234	-1.813610	-2.206357
H	-2.323784	1.563228	-1.880317
H	-2.013103	4.382875	-0.630032
H	2.045659	4.390019	0.790140
H	0.006726	5.633503	0.102509

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1,TS-2-3 el energy= -1312.17243620

Ni	0.000002	0.092666	-0.000082
H	0.000079	1.662417	-0.000034
C	-0.000080	-1.856984	-0.000147
C	1.173460	-2.591888	-0.291040
C	2.432612	-1.829330	-0.644223
C	1.173182	-3.992178	-0.283416
H	2.088953	-4.538427	-0.508456
C	-0.000199	-4.693276	-0.000245
H	-0.000244	-5.781486	-0.000283
C	-1.173520	-3.992100	0.282979
H	-2.089336	-4.538287	0.507987
C	-1.173681	-2.591810	0.290702
C	-2.432758	-1.829170	0.643970
P	2.189649	-0.059096	-0.091059
P	-2.189668	-0.058921	0.090913
C	3.146846	0.961246	-1.377549
C	2.191100	1.052759	-2.586836
C	4.465758	0.292691	-1.808212
C	3.443348	2.383107	-0.875000
C	2.947653	0.043960	1.645358
C	4.474774	-0.121046	1.661817
C	2.543204	1.389141	2.278852
C	2.303456	-1.088574	2.471774
C	-2.947705	0.044287	-1.645483
C	-2.303627	-1.088261	-2.471974

C	-2.543148	1.389464	-2.278913
C	-4.474840	-0.120583	-1.661917
C	-3.146764	0.961407	1.377491
C	-4.465721	0.292922	1.808128
C	-2.190990	1.052758	2.586768
C	-3.443166	2.383325	0.875047
H	3.341655	-2.281638	-0.226504
H	2.567764	-1.810176	-1.733415
H	-2.567869	-1.810074	1.733168
H	-3.341854	-2.281376	0.226256
H	2.699619	1.565253	-3.415602
H	1.884860	0.061854	-2.946923
H	1.292300	1.622155	-2.330786
H	5.165668	0.173958	-0.975412
H	4.305887	-0.691412	-2.261250
H	4.954146	0.923542	-2.564102
H	4.189034	2.389845	-0.073011
H	3.848699	2.976397	-1.706321
H	2.542211	2.891318	-0.524771
H	4.826308	-0.151443	2.702845
H	4.794174	-1.053706	1.180403
H	4.985397	0.712805	1.169168
H	3.009535	2.244570	1.782299
H	1.459325	1.538184	2.242541
H	2.859566	1.402156	3.331352
H	2.556096	-2.083817	2.090509
H	1.211664	-1.005828	2.480037
H	2.665404	-1.019948	3.507068
H	-2.665586	-1.019542	-3.507258
H	-1.211827	-1.005618	-2.480250
H	-2.556353	-2.083503	-2.090763
H	-3.009405	2.244908	-1.782317
H	-2.859507	1.402558	-3.331414
H	-1.459256	1.538409	-2.242593
H	-4.826401	-0.150888	-2.702938
H	-4.794310	-1.053243	-1.180550
H	-4.985378	0.713284	-1.169207
H	-4.305916	-0.691223	2.261096
H	-4.954049	0.923759	2.564069
H	-5.165655	0.174299	0.975332
H	-1.292152	1.622108	2.330748
H	-2.699459	1.565227	3.415581
H	-1.884821	0.061803	2.946775
H	-3.848494	2.976576	1.706406
H	-2.541988	2.891504	0.524880

H	-4.188833	2.390175	0.073042
C	0.000243	3.277243	0.000247
O	0.124226	3.549967	-1.152142
O	-0.123672	3.549605	1.152730

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1,TS-3-4 el energy= -1312.16859221

Ni	0.043420	-0.096422	0.081916
H	0.316967	-1.734321	-0.584701
C	0.014200	1.829575	0.091754
C	-1.157018	2.534899	-0.268261
C	-2.362161	1.756788	-0.731996
C	-1.195149	3.934128	-0.238797
H	-2.113778	4.452162	-0.511531
C	-0.064176	4.665598	0.123169
H	-0.096972	5.752746	0.143615
C	1.113506	3.990956	0.442031
H	2.008195	4.553860	0.705536
C	1.158381	2.591347	0.425297
C	2.448934	1.875578	0.744519
P	-2.209868	0.020540	-0.077326
P	2.267244	0.130565	0.125726
C	-3.143933	-1.028431	-1.368408
C	-2.129101	-1.283037	-2.504111
C	-4.365971	-0.276326	-1.932606
C	-3.606095	-2.381977	-0.802952
C	-3.072826	0.045491	1.616208
C	-4.566651	0.394114	1.515987
C	-2.893294	-1.313318	2.320790
C	-2.350807	1.120335	2.455040
C	2.950586	0.137789	-1.652136
C	2.288099	1.320996	-2.387265
C	2.522373	-1.162208	-2.359650
C	4.477554	0.292468	-1.723275
C	3.321080	-0.888035	1.337260
C	4.710070	-0.266286	1.576932
C	2.539924	-0.891982	2.669776
C	3.471253	-2.336521	0.844695
H	-3.310896	2.234431	-0.459819
H	-2.350875	1.679735	-1.826887
H	2.609417	1.822330	1.828325
H	3.326246	2.380485	0.320563
H	-2.652968	-1.731544	-3.359803
H	-1.654403	-0.356553	-2.854703
H	-1.351740	-1.981290	-2.180589

H	-5.087053	-0.003526	-1.156009
H	-4.086833	0.633413	-2.474616
H	-4.881218	-0.934060	-2.645990
H	-4.419723	-2.263924	-0.079485
H	-3.993143	-2.988822	-1.633587
H	-2.786356	-2.942869	-0.346393
H	-4.979399	0.488632	2.530128
H	-4.743758	1.346440	1.001276
H	-5.137116	-0.387463	1.003924
H	-3.475151	-2.107433	1.845659
H	-1.846268	-1.629228	2.334474
H	-3.248463	-1.218124	3.356761
H	-2.447853	2.125596	2.031667
H	-1.282463	0.898955	2.550191
H	-2.790948	1.131309	3.461625
H	2.593500	1.292758	-3.442314
H	1.196085	1.262903	-2.342180
H	2.586467	2.291658	-1.976885
H	2.904585	-2.060697	-1.866062
H	2.908398	-1.154671	-3.388380
H	1.431665	-1.246424	-2.407605
H	4.775782	0.432395	-2.771652
H	4.834978	1.163471	-1.160691
H	4.996994	-0.596781	-1.352558
H	4.647448	0.776613	1.908316
H	5.209114	-0.831331	2.376322
H	5.354270	-0.307416	0.695622
H	1.557115	-1.351847	2.543811
H	3.111793	-1.472634	3.407030
H	2.414920	0.118397	3.079202
H	3.990623	-2.922531	1.615339
H	2.498117	-2.805230	0.675840
H	4.067327	-2.402061	-0.072350
C	-0.106659	-2.552960	0.180051
O	-0.567809	-3.525225	-0.405049
O	0.026911	-2.233237	1.381518

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1,TS-4i-4 el energy= -1312.19628880

Ni	-0.000916	-0.018186	-0.079909
P	-2.224965	0.199017	0.002582
P	2.244946	0.140452	-0.188210
O	-0.019005	-1.926529	0.335259
O	0.861713	-3.697421	-0.754903
C	-3.157619	-0.732955	1.370532

C	-2.180132	-0.741839	2.566275
C	-3.446813	-2.186939	0.968740
C	-4.469855	-0.038345	1.777542
C	-3.036997	0.037925	-1.706221
C	-2.638789	-1.318557	-2.316158
C	-4.566134	0.181372	-1.672383
C	-2.441075	1.151795	-2.591716
C	-2.407290	1.989912	0.466575
C	-1.145643	2.689237	0.014541
C	-1.131048	4.085102	-0.093581
C	0.036939	4.753050	-0.458840
C	1.192882	4.016301	-0.714778
C	1.181746	2.619097	-0.621590
C	0.008517	1.913702	-0.259489
C	2.441858	1.842694	-0.917531
C	3.305131	-0.951557	-1.330115
C	2.409014	-1.238447	-2.553695
C	4.584103	-0.224850	-1.792020
C	3.691023	-2.283590	-0.667176
C	2.939550	0.236381	1.576170
C	2.185742	1.378968	2.287811
C	2.613232	-1.083040	2.304863
C	4.448321	0.521066	1.626631
C	-0.072993	-2.997364	-0.387929
H	-1.272720	-1.297800	2.312144
H	-2.664384	-1.224975	3.426533
H	-1.893670	0.271801	2.875692
H	-4.181713	-2.257007	0.159405
H	-3.861486	-2.721398	1.834854
H	-2.532730	-2.701595	0.664802
H	-4.923932	-0.597805	2.607460
H	-5.198912	-0.009130	0.962485
H	-4.308394	0.987024	2.127464
H	-1.549583	-1.415937	-2.379568
H	-3.046757	-1.392287	-3.333811
H	-3.019477	-2.168004	-1.741952
H	-4.881596	1.119142	-1.198644
H	-5.047005	-0.649367	-1.146103
H	-4.952988	0.186269	-2.701179
H	-2.820415	1.027451	-3.615423
H	-1.347747	1.102558	-2.620183
H	-2.718816	2.154413	-2.249897
H	-3.320240	2.447026	0.063736
H	-2.491701	2.034054	1.560112
H	-2.037039	4.651515	0.119868

H	0.047861	5.838098	-0.538074
H	2.112877	4.529161	-0.993392
H	3.347366	2.355322	-0.568807
H	2.556095	1.710472	-2.001163
H	2.019818	-0.317689	-3.009051
H	1.570243	-1.882631	-2.277148
H	2.999072	-1.762699	-3.318392
H	4.371603	0.674657	-2.379687
H	5.156870	-0.906158	-2.436302
H	5.231176	0.058606	-0.956264
H	4.179370	-2.916295	-1.422191
H	2.811557	-2.825808	-0.309251
H	4.408905	-2.139077	0.147733
H	2.358382	2.354681	1.820979
H	2.532175	1.433666	3.329242
H	1.104801	1.202469	2.293340
H	2.823605	-0.960955	3.376822
H	3.214979	-1.918525	1.938588
H	1.561886	-1.359989	2.178354
H	4.758619	0.646441	2.673732
H	4.713047	1.442990	1.093673
H	5.036537	-0.300951	1.207288
H	-1.107399	-3.313654	-0.668267

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1,TS-2-5 el energy= -1312.10294254

Ni	-0.016344	-0.246896	-0.085801
P	-2.219701	-0.031313	-0.103655
P	2.200251	-0.048726	0.126316
O	0.249332	-2.236934	-1.238939
O	-0.191448	-3.169954	0.700932
C	3.476385	-2.483892	0.877904
C	-1.172575	2.454332	-0.451615
C	-2.423799	1.687749	-0.811103
C	-3.285711	-1.107135	-1.258445
C	-2.479302	-1.233974	-2.569630
C	-2.938806	0.076792	1.660795
C	-4.460305	0.296322	1.678289
C	3.134726	0.040896	-1.538063
C	2.446446	1.150788	-2.360544
C	3.130056	-1.090131	1.425620
C	4.412219	-0.402770	1.934007
C	2.155780	-1.251078	2.611598
C	-0.021562	1.718458	-0.085760
C	0.093000	-3.198185	-0.499471

C	-2.253869	1.266696	2.364052
C	-4.647159	-0.466631	-1.591770
C	2.999488	-1.279551	-2.318486
C	-0.022753	4.555765	-0.078357
C	-1.169881	3.854419	-0.453164
C	1.116030	3.852866	0.317891
C	1.114924	2.452534	0.323844
C	2.325783	1.688326	0.803859
C	4.625077	0.383003	-1.376869
C	-3.506786	-2.505234	-0.657310
C	-2.592692	-1.200496	2.447985
H	-0.256806	-1.707227	0.833224
H	2.608178	-2.977313	0.430391
H	4.277444	-2.441165	0.132223
H	-3.339549	2.182790	-0.463211
H	2.307558	1.604285	1.898500
H	3.272217	2.178186	0.543850
H	-3.058568	-1.835408	-3.284269
H	-2.300652	-0.257126	-3.036561
H	-5.302032	-0.378924	-0.722014
H	-4.538050	0.527205	-2.040020
H	-5.160632	-1.100890	-2.328090
H	-4.205136	-2.476513	0.186737
H	-3.944459	-3.161687	-1.422123
H	-2.574722	-2.963252	-0.314752
H	-4.779651	0.502778	2.709349
H	-5.006163	-0.590154	1.340500
H	-2.994772	-2.107148	1.987841
H	-1.510066	-1.327337	2.536256
H	-3.015374	-1.119134	3.459378
H	-1.164430	1.165640	2.355561
H	-2.593066	1.295479	3.409003
H	2.910236	1.186336	-3.356153
H	1.376705	0.952800	-2.484160
H	2.547816	2.140684	-1.904101
H	3.478917	-1.155125	-3.299984
H	1.954625	-1.554760	-2.471054
H	1.802904	-0.284799	2.994389
H	5.055254	0.574890	-2.369928
H	4.793041	1.279940	-0.769203
H	5.187927	-0.445524	-0.934877
H	4.205725	0.568462	2.396800
H	5.154122	-0.253259	1.145920
H	1.283582	-1.844881	2.328923
H	2.674347	-1.763545	3.433926

H	3.828886	-3.117279	1.703764
H	3.493341	-2.115546	-1.815020
H	-4.768153	1.149828	1.062535
H	-2.500090	2.228511	1.902500
H	4.871565	-1.038911	2.703581
H	-1.514258	-1.718268	-2.409464
H	-2.518475	1.577816	-1.899178
H	-2.067092	4.399345	-0.745503
H	2.006541	4.396428	0.632518
H	-0.020473	5.643863	-0.082754

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1,Ni-(H)-formate-isomer el energy= -1312.17170586

Ni	-0.000416	-0.019632	-0.255830
H	0.087843	-1.626818	-0.358179
C	-0.063491	1.897247	-0.032751
C	-1.299003	2.583451	0.052499
C	-2.567300	1.831757	-0.284829
C	-1.350185	3.936054	0.408159
H	-2.312921	4.439787	0.487931
C	-0.173089	4.642595	0.660552
H	-0.215720	5.690506	0.950245
C	1.058717	4.003406	0.519932
H	1.980408	4.560717	0.684480
C	1.117777	2.651037	0.158227
C	2.455353	1.997899	-0.109472
P	-2.210917	0.016312	-0.057051
P	2.204939	0.147796	-0.146707
C	-3.273803	-0.863610	-1.360957
C	-2.475707	-0.726618	-2.676370
C	-4.657066	-0.207844	-1.532031
C	-3.455336	-2.355951	-1.032142
C	-2.746848	-0.371941	1.722075
C	-4.269870	-0.335181	1.922033
C	-2.185803	-1.751356	2.113831
C	-2.099414	0.696896	2.625898
C	3.239072	-0.449858	-1.625228
C	2.345965	-0.162922	-2.852098
C	3.514700	-1.961134	-1.557433
C	4.577446	0.299789	-1.761643
C	2.852448	-0.472687	1.525405
C	4.367855	-0.282773	1.692723
C	2.105967	0.346157	2.598133
C	2.478662	-1.955838	1.708583
H	-3.438033	2.168241	0.291627

H	-2.814473	1.980731	-1.343923
H	3.234595	2.296627	0.602677
H	2.811966	2.303559	-1.100459
H	-3.076384	-1.128378	-3.504418
H	-2.246993	0.321133	-2.912199
H	-1.535233	-1.285075	-2.636551
H	-5.253721	-0.240511	-0.615501
H	-4.584934	0.836158	-1.856049
H	-5.212526	-0.752053	-2.308444
H	-4.147464	-2.506681	-0.196336
H	-3.884983	-2.860915	-1.908104
H	-2.515366	-2.857500	-0.789335
H	-4.496488	-0.468719	2.989229
H	-4.704530	0.623294	1.612054
H	-4.778079	-1.136888	1.377723
H	-2.639502	-2.567938	1.547277
H	-1.106017	-1.811022	1.946303
H	-2.382127	-1.930181	3.180363
H	-2.501356	1.699380	2.444690
H	-1.016190	0.747800	2.483490
H	-2.297286	0.438386	3.675136
H	2.904356	-0.397223	-3.769335
H	1.446918	-0.787647	-2.827827
H	2.042646	0.890992	-2.906008
H	4.203007	-2.218607	-0.745238
H	3.989658	-2.270994	-2.498682
H	2.595208	-2.541864	-1.455561
H	5.111930	-0.092926	-2.637625
H	4.444606	1.375057	-1.921070
H	5.225916	0.161818	-0.890757
H	4.677706	0.756856	1.529767
H	4.657601	-0.556062	2.717091
H	4.937104	-0.922178	1.010329
H	1.023180	0.208757	2.515237
H	2.417154	-0.000361	3.593087
H	2.312515	1.420042	2.535298
H	2.746968	-2.268525	2.727422
H	1.407311	-2.130345	1.570828
H	3.008745	-2.610924	1.012197
C	0.015324	-2.839309	-0.856002
O	-0.274417	-3.591172	0.050158
O	0.263554	-2.814818	-2.047075

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1,Ni-carboxylic acid el energy= -1312.17618615

Ni	-0.006358	-0.276533	0.008943
H	-0.398751	-2.550524	1.515828
C	-0.004665	1.746926	0.039430
C	-1.146009	2.486961	-0.345161
C	-2.401691	1.724901	-0.713291
C	-1.120463	3.886122	-0.405491
H	-2.011793	4.436902	-0.705680
C	0.050039	4.579929	-0.094088
H	0.071592	5.666643	-0.147509
C	1.193545	3.874093	0.286496
H	2.105424	4.416010	0.536521
C	1.164084	2.476033	0.359532
C	2.379382	1.699470	0.815396
P	-2.207569	-0.021987	-0.073220
P	2.197440	-0.052558	0.171093
C	-3.242991	-1.065972	-1.280357
C	-2.395494	-1.146997	-2.570389
C	-4.603951	-0.434131	-1.627805
C	-3.451322	-2.486496	-0.727467
C	-2.964573	0.025737	1.679801
C	-4.498459	0.114095	1.688606
C	-2.508569	-1.226930	2.450919
C	-2.391434	1.259089	2.407222
C	2.983578	-0.021330	-1.575779
C	1.846594	0.377200	-2.542337
C	3.482706	-1.417562	-1.983996
C	4.129266	0.996762	-1.693847
C	3.191140	-1.086671	1.427837
C	4.628992	-0.563255	1.581500
C	2.433646	-0.947782	2.766999
C	3.216654	-2.587296	1.080712
H	-3.319027	2.201333	-0.342476
H	-2.505800	1.656656	-1.804001
H	2.397125	1.639684	1.910429
H	3.324391	2.164071	0.515710
H	-2.953647	-1.719934	-3.324152
H	-2.198961	-0.154498	-2.995552
H	-1.438499	-1.646506	-2.400732
H	-5.283737	-0.389220	-0.773596
H	-4.496782	0.578228	-2.033564
H	-5.088506	-1.045295	-2.402159
H	-4.129977	-2.494710	0.133459
H	-3.905774	-3.112767	-1.507552
H	-2.508887	-2.958051	-0.432811
H	-4.845001	0.259683	2.721564

H	-4.864244	0.961818	1.097377
H	-4.968875	-0.799220	1.311506
H	-2.767471	-2.161281	1.943619
H	-1.422448	-1.197758	2.605451
H	-2.978597	-1.240008	3.444102
H	-2.729145	2.200817	1.962526
H	-1.297359	1.263329	2.395777
H	-2.731299	1.239673	3.452389
H	2.253473	0.438369	-3.562243
H	1.053905	-0.378807	-2.532034
H	1.408362	1.346765	-2.286254
H	4.391487	-1.704264	-1.443938
H	3.732979	-1.397603	-3.053997
H	2.712564	-2.180904	-1.836783
H	4.574729	0.915218	-2.695107
H	3.772975	2.026521	-1.579917
H	4.926937	0.822920	-0.962372
H	4.659557	0.502773	1.836246
H	5.136290	-1.111955	2.387808
H	5.212204	-0.713479	0.666185
H	1.392761	-1.276938	2.662766
H	2.915338	-1.585288	3.520550
H	2.428374	0.075425	3.156925
H	3.696052	-3.124660	1.911501
H	2.211632	-2.998061	0.955676
H	3.790578	-2.803522	0.178806
C	0.068855	-2.188412	-0.299781
O	-0.185791	-3.086500	0.738468
O	0.331403	-2.687233	-1.376763

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1,TS-3i-6 el energy= -1312.10442277

Ni	-0.055370	-0.004629	0.230834
H	0.203356	-1.600027	-0.255973
C	-0.125905	1.911306	-0.273844
C	0.975412	2.771021	-0.064249
C	2.253081	2.176916	0.485062
C	0.901460	4.136633	-0.367644
H	1.761896	4.782299	-0.193616
C	-0.274974	4.676162	-0.889794
H	-0.334574	5.738426	-1.118155
C	-1.370182	3.844356	-1.132979
H	-2.279762	4.259565	-1.566056
C	-1.291271	2.477638	-0.840709
C	-2.433924	1.548418	-1.178630

P	2.140297	0.321685	0.286749
P	-2.255023	0.035303	-0.092772
C	3.188784	-0.345822	1.726706
C	2.344195	-0.109836	2.998723
C	4.528065	0.397913	1.892876
C	3.446963	-1.853045	1.556989
C	2.909715	-0.049717	-1.417234
C	4.427886	0.185501	-1.461885
C	2.600328	-1.505112	-1.814700
C	2.227309	0.880229	-2.441113
C	-3.177077	0.492704	1.523393
C	-2.147572	1.216560	2.418709
C	-3.659321	-0.765823	2.264399
C	-4.369691	1.431145	1.271812
C	-3.105153	-1.345178	-1.091612
C	-4.551328	-0.966047	-1.452288
C	-2.266111	-1.511362	-2.377963
C	-3.082068	-2.702006	-0.362998
H	3.152355	2.586958	0.006858
H	2.350503	2.381281	1.558905
H	-2.340824	1.210462	-2.217732
H	-3.417643	2.020478	-1.092346
H	2.913276	-0.465920	3.868713
H	2.135232	0.955087	3.161475
H	1.393300	-0.645643	2.969219
H	5.209173	0.244444	1.052875
H	4.388537	1.476369	2.028768
H	5.027547	0.018500	2.795277
H	4.167866	-2.050851	0.755231
H	3.875649	-2.250275	2.487309
H	2.530431	-2.412069	1.343797
H	4.773529	0.095620	-2.501180
H	4.706398	1.185553	-1.108713
H	4.974844	-0.555990	-0.871426
H	2.991187	-2.236203	-1.102335
H	1.522170	-1.673491	-1.901375
H	3.052326	-1.711198	-2.795009
H	2.444460	1.938044	-2.259069
H	1.139749	0.760520	-2.430989
H	2.597413	0.626489	-3.444256
H	-2.647231	1.526844	3.347897
H	-1.323150	0.545458	2.678396
H	-1.736868	2.108123	1.935175
H	-4.503399	-1.244045	1.755957
H	-4.007212	-0.467387	3.263177

H	-2.852504	-1.492138	2.397371
H	-4.896822	1.592197	2.222306
H	-4.047251	2.413533	0.909980
H	-5.092709	1.018425	0.559276
H	-4.613087	-0.001714	-1.970825
H	-4.972953	-1.729787	-2.120867
H	-5.190929	-0.919833	-0.563987
H	-1.224028	-1.753135	-2.139053
H	-2.676561	-2.344537	-2.964041
H	-2.277126	-0.623515	-3.019109
H	-3.500380	-3.461478	-1.038722
H	-2.064210	-3.008428	-0.108470
H	-3.685153	-2.706064	0.546167
C	-0.106896	-1.802097	1.140769
O	0.214963	-2.831350	0.415231
O	-0.429414	-1.745413	2.313341

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1,Ni-carbonyl el energy= -1312.13529022

Ni	-0.114849	0.029367	0.609651
H	-0.081870	0.126266	3.166606
C	-0.105406	1.866327	-0.066901
C	1.035777	2.657300	0.177783
C	2.250188	1.977111	0.755606
C	1.052544	4.012276	-0.164720
H	1.942383	4.608847	0.033353
C	-0.062462	4.602666	-0.766438
H	-0.048795	5.659174	-1.025873
C	-1.182495	3.824075	-1.052172
H	-2.044646	4.271123	-1.545992
C	-1.200563	2.462334	-0.717123
C	-2.365339	1.585438	-1.102358
P	2.125874	0.182410	0.269049
P	-2.255506	0.053427	-0.048334
C	3.339205	-0.692316	1.462671
C	2.624329	-0.834982	2.824440
C	4.611541	0.152699	1.676473
C	3.722757	-2.098121	0.971675
C	2.724755	0.021173	-1.538402
C	4.227328	0.289514	-1.721428
C	2.364058	-1.389995	-2.041873
C	1.941130	1.031328	-2.399707
C	-3.389630	0.390796	1.437707
C	-2.950572	1.757216	2.008656
C	-3.122502	-0.673628	2.518441

C	-4.881813	0.425039	1.074735
C	-2.923951	-1.330363	-1.178567
C	-4.154939	-0.888915	-1.993946
C	-1.778095	-1.667170	-2.154198
C	-3.273466	-2.592466	-0.372254
H	3.193682	2.448023	0.454245
H	2.180202	1.967626	1.849437
H	-2.274518	1.276201	-2.152234
H	-3.339291	2.080566	-1.002639
H	3.372262	-1.080738	3.591446
H	2.082944	0.071541	3.111087
H	1.895255	-1.651052	2.801217
H	5.153067	0.358101	0.749394
H	4.381873	1.108469	2.158924
H	5.291372	-0.395709	2.343751
H	4.365863	-2.078076	0.086044
H	4.278267	-2.612093	1.768507
H	2.838600	-2.705376	0.745571
H	4.469893	0.268157	-2.793474
H	4.513314	1.277765	-1.341264
H	4.852412	-0.462980	-1.231573
H	2.918675	-2.181634	-1.531450
H	1.293363	-1.583607	-1.912906
H	2.594119	-1.461592	-3.114101
H	2.164877	2.069347	-2.136734
H	0.861159	0.891463	-2.299438
H	2.218263	0.876787	-3.452327
H	-3.548824	1.955558	2.910192
H	-1.886252	1.731096	2.285712
H	-3.128809	2.579833	1.306867
H	-3.353044	-1.691756	2.188793
H	-3.749206	-0.457145	3.394632
H	-2.075988	-0.624265	2.832332
H	-5.452633	0.753837	1.954285
H	-5.095698	1.133565	0.264920
H	-5.267284	-0.558773	0.785046
H	-3.939202	-0.027131	-2.634569
H	-4.462518	-1.714605	-2.651110
H	-5.008647	-0.636212	-1.360293
H	-0.914510	-2.084029	-1.627103
H	-2.127938	-2.409274	-2.885456
H	-1.432668	-0.786863	-2.710045
H	-3.508470	-3.410517	-1.067610
H	-2.442626	-2.925418	0.257759
H	-4.150135	-2.442320	0.265884

C	-0.082573	-1.701489	1.041944
O	0.016996	0.839209	2.520692
O	-0.046592	-2.812446	1.340081

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2,Ni-H	el energy= -1238.11351418		
Ni	0.037177	0.024550	0.254367
H	0.097177	-0.039857	1.806875
C	-0.039086	0.102063	-1.698719
C	1.133803	0.264092	-2.481375
C	2.457996	0.417068	-1.754657
C	1.084427	0.305534	-3.873930
H	1.981381	0.430944	-4.477764
C	-0.145897	0.196589	-4.537462
O	-0.088483	0.253372	-5.904535
C	-1.324020	0.041859	-3.799325
H	-2.284319	-0.049697	-4.299497
C	-1.260427	-0.008203	-2.397761
C	-2.530552	-0.211912	-1.590925
P	2.184055	-0.170475	0.005902
P	-2.121192	0.230731	0.186009
C	3.285464	0.954492	1.064864
C	2.516095	2.291644	1.128497
C	4.684721	1.199144	0.474856
C	3.399236	0.392560	2.490922
C	2.750610	-1.984368	0.012888
C	4.267634	-2.164164	-0.142514
C	2.262776	-2.647814	1.314544
C	2.030965	-2.668076	-1.168802
C	-2.683465	2.035413	0.384947
C	-2.058149	2.817160	-0.789545
C	-2.093529	2.592846	1.694078
C	-4.207717	2.219949	0.365483
C	-3.140865	-0.982008	1.230281
C	-4.582896	-1.181760	0.733877
C	-2.373007	-2.317154	1.122119
C	-3.140692	-0.541101	2.702731
H	3.286038	-0.101954	-2.255396
H	2.742297	1.476497	-1.703706
H	-2.827758	-1.269079	-1.606195
H	-3.385650	0.354675	-1.984222
H	3.078627	3.009524	1.742220
H	2.378911	2.738558	0.135828
H	1.526165	2.146100	1.574700
H	5.284818	0.285928	0.429859

H	4.636849	1.623607	-0.534487
H	5.224235	1.918750	1.107252
H	4.034675	-0.499371	2.530352
H	3.853380	1.148895	3.146682
H	2.411682	0.138855	2.893206
H	4.500344	-3.232905	-0.254162
H	4.655081	-1.648595	-1.030008
H	4.815544	-1.800750	0.733352
H	2.761429	-2.246211	2.201529
H	1.185330	-2.500341	1.443471
H	2.468597	-3.726941	1.272722
H	2.352564	-2.276257	-2.139608
H	0.945737	-2.538202	-1.104430
H	2.257118	-3.743460	-1.146826
H	-2.281710	3.885817	-0.662820
H	-0.971363	2.688995	-0.820956
H	-2.454817	2.503257	-1.760975
H	-2.520596	2.116866	2.581609
H	-2.301419	3.670533	1.757484
H	-1.009370	2.441734	1.724980
H	-4.446937	3.293089	0.362382
H	-4.665502	1.778197	-0.528385
H	-4.684763	1.781814	1.248582
H	-5.073351	-1.953090	1.344887
H	-5.181772	-0.270010	0.811950
H	-4.615798	-1.521084	-0.307798
H	-1.350782	-2.205837	1.500162
H	-2.887993	-3.085523	1.716138
H	-2.315155	-2.679426	0.088003
H	-3.544531	-1.350863	3.326831
H	-2.123804	-0.318575	3.046102
H	-3.768204	0.342316	2.865992
C	-1.304000	0.151878	-6.618280
H	-1.040240	0.221417	-7.677368
H	-1.805690	-0.809575	-6.431154
H	-1.995008	0.969023	-6.361412

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2,Ni+	el energy= -1237.33199012		
Ni	0.007117	0.046686	-0.002926
C	0.252525	1.910810	-0.048326
C	-0.813337	2.759222	-0.429418
C	-2.147651	2.156387	-0.811832
C	-0.626645	4.137439	-0.452784
H	-1.433153	4.809364	-0.736357

C	0.614535	4.699435	-0.110012
O	0.682153	6.047253	-0.172137
C	1.674609	3.862788	0.263857
H	2.641965	4.276661	0.530814
C	1.494189	2.473829	0.298688
C	2.635057	1.570925	0.715486
P	-2.194346	0.442924	-0.091801
P	2.235650	-0.131332	0.082354
C	-3.150696	-0.627243	-1.326672
C	-2.181906	-0.837117	-2.511144
C	-4.435576	0.054086	-1.829655
C	-3.478342	-1.996578	-0.707670
C	-2.991140	0.578325	1.620122
C	-4.508968	0.809496	1.558347
C	-2.668069	-0.707755	2.405809
C	-2.316604	1.765736	2.337747
C	3.034776	-0.290731	-1.626825
C	2.688021	0.993384	-2.408205
C	2.387358	-1.486870	-2.352069
C	4.560742	-0.457368	-1.561302
C	2.890905	-1.348137	1.377012
C	4.309603	-0.995684	1.857638
C	1.905496	-1.242668	2.561670
C	2.852997	-2.784601	0.828693
H	-2.995416	2.770797	-0.487638
H	-2.225354	2.057194	-1.901566
H	2.698509	1.510010	1.809050
H	3.608295	1.930343	0.360900
H	-2.686276	-1.417242	-3.294745
H	-1.853172	0.107627	-2.960372
H	-1.286825	-1.395381	-2.206815
H	-5.162358	0.217371	-1.029555
H	-4.231161	1.018176	-2.308787
H	-4.910704	-0.589329	-2.582151
H	-4.236189	-1.925154	0.078677
H	-3.875867	-2.659427	-1.487076
H	-2.587948	-2.481499	-0.286174
H	-4.887563	0.985620	2.573826
H	-4.768669	1.688124	0.955546
H	-5.044330	-0.056620	1.156716
H	-3.119749	-1.600672	1.964275
H	-1.583984	-0.866480	2.474750
H	-3.054183	-0.613212	3.428978
H	-2.536934	2.726087	1.860300
H	-1.228009	1.652932	2.379986

H	-2.695868	1.811430	3.366787
H	3.064962	0.889276	-3.433832
H	1.607235	1.163154	-2.457283
H	3.149182	1.886889	-1.974611
H	2.593102	-2.443116	-1.862603
H	2.782377	-1.546945	-3.374449
H	1.299088	-1.362465	-2.424757
H	4.969155	-0.437785	-2.580303
H	5.040724	0.353825	-1.000595
H	4.854521	-1.410516	-1.110596
H	4.606631	-1.701896	2.644422
H	5.050914	-1.063551	1.057137
H	4.361295	0.010762	2.288109
H	0.896155	-1.568191	2.277771
H	2.247737	-1.891720	3.378126
H	1.831151	-0.223526	2.959646
H	3.071154	-3.487959	1.642674
H	1.865720	-3.044961	0.424855
H	3.599509	-2.948893	0.045406
C	1.911200	6.682405	0.161673
H	1.732736	7.753055	0.044017
H	2.198513	6.469941	1.200535
H	2.717090	6.368139	-0.515705

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2,Ni-(H)-formate el energy= -1426.70076022

Ni	-0.228378	-0.403922	0.002110
H	-0.916788	-1.860064	0.023764
C	0.594931	1.340015	-0.025755
C	1.968013	1.510905	0.242275
C	2.796545	0.296507	0.596584
C	2.574409	2.776147	0.218960
H	3.636153	2.863058	0.431022
C	1.804765	3.909087	-0.062209
C	0.435613	3.767646	-0.325248
H	-0.139712	4.664090	-0.547164
C	-0.156352	2.506148	-0.315095
C	-1.622801	2.357393	-0.652418
P	1.827888	-1.215182	0.084123
P	-2.164364	0.662827	-0.086757
C	2.274711	-2.517668	1.394183
C	1.381918	-2.170177	2.605707
C	3.758764	-2.453334	1.802476
C	1.941389	-3.945235	0.930312
C	2.437027	-1.660920	-1.654970

C	3.894287	-2.145623	-1.684819
C	1.499805	-2.732848	-2.245061
C	2.304408	-0.381564	-2.506822
C	-2.876660	0.894238	1.654798
C	-1.796841	1.631590	2.473717
C	-3.097364	-0.494547	2.285563
C	-4.178767	1.708953	1.677751
C	-3.465581	0.140278	-1.369411
C	-4.366705	1.313345	-1.799599
C	-2.641529	-0.359375	-2.576373
C	-4.347344	-1.013336	-0.863900
H	3.802610	0.320431	0.157848
H	2.931761	0.240228	1.684103
H	-1.759144	2.390905	-1.740639
H	-2.242751	3.160764	-0.234784
H	1.655026	-2.815339	3.452581
H	1.508293	-1.128289	2.929102
H	0.326837	-2.344652	2.371377
H	4.433018	-2.656192	0.964608
H	4.033578	-1.485396	2.235019
H	3.946025	-3.216850	2.570157
H	2.593125	-4.277228	0.115237
H	2.097105	-4.631389	1.774344
H	0.897692	-4.046628	0.624920
H	4.207266	-2.291682	-2.728209
H	4.581356	-1.418224	-1.234582
H	4.019862	-3.102882	-1.168779
H	1.588752	-3.695118	-1.733742
H	0.448558	-2.431431	-2.192271
H	1.757945	-2.892674	-3.301292
H	2.948055	0.430524	-2.151199
H	1.274602	-0.009503	-2.511337
H	2.593241	-0.615281	-3.540830
H	-2.147139	1.730523	3.510393
H	-0.852136	1.077871	2.479741
H	-1.589499	2.636433	2.089708
H	-3.900745	-1.053671	1.798330
H	-3.373299	-0.368722	3.341910
H	-2.195056	-1.113038	2.239682
H	-4.478560	1.884629	2.720433
H	-4.061127	2.689830	1.200383
H	-5.002579	1.182545	1.185099
H	-3.801154	2.130918	-2.259065
H	-5.081905	0.950765	-2.550844
H	-4.944457	1.724828	-0.966082

H	-2.100730	-1.276723	-2.322248
H	-3.321574	-0.583622	-3.410186
H	-1.923012	0.392808	-2.928488
H	-4.986466	-1.352171	-1.691036
H	-3.756557	-1.874270	-0.543434
H	-5.007471	-0.700726	-0.048056
C	-1.467383	-3.039789	0.045126
O	-1.438877	-3.467963	1.182338
O	-1.829227	-3.325558	-1.079465
O	2.288491	5.184905	-0.105381
C	3.668482	5.376947	0.143362
H	3.947321	5.043495	1.153895
H	4.289257	4.845552	-0.593172
H	3.843864	6.452459	0.055942

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2,Ni-H+CO2 el energy= -1426.70549755

Ni	-0.226154	-0.377594	-0.005831
H	-0.892300	-1.777319	0.047892
C	0.608415	1.394405	-0.055258
C	1.983741	1.574053	0.205921
C	2.806288	0.355555	0.579142
C	2.592954	2.838177	0.165682
H	3.655180	2.931257	0.374733
C	1.820782	3.966617	-0.128329
C	0.448686	3.825491	-0.378156
H	-0.125254	4.722660	-0.602873
C	-0.142451	2.563426	-0.345514
C	-1.622854	2.405492	-0.637228
P	1.804772	-1.154082	0.093919
P	-2.116135	0.698223	-0.041012
C	2.188143	-2.423781	1.453200
C	1.339024	-1.961444	2.656817
C	3.670618	-2.472611	1.862702
C	1.713521	-3.824089	1.035682
C	2.485473	-1.660029	-1.606224
C	3.918132	-2.210935	-1.564877
C	1.532765	-2.694176	-2.233296
C	2.448506	-0.389209	-2.480970
C	-2.798140	0.964445	1.713954
C	-1.726182	1.768790	2.479254
C	-2.945706	-0.406146	2.401584
C	-4.130891	1.726143	1.755646
C	-3.445785	0.134812	-1.270875
C	-4.468496	1.225645	-1.632854

C	-2.654310	-0.259222	-2.536440
C	-4.170059	-1.109505	-0.732265
H	3.810374	0.359019	0.133738
H	2.952119	0.316912	1.666836
H	-1.804372	2.438787	-1.719552
H	-2.233984	3.203918	-0.195889
H	1.497539	-2.645734	3.502342
H	1.608095	-0.951286	2.990675
H	0.274143	-1.961334	2.399986
H	4.317625	-2.815735	1.050318
H	4.038878	-1.497526	2.200864
H	3.790354	-3.175243	2.699732
H	2.336549	-4.248638	0.240423
H	1.777673	-4.501734	1.898810
H	0.671967	-3.808393	0.700112
H	4.282339	-2.360749	-2.591356
H	4.611653	-1.522164	-1.066804
H	3.970063	-3.179086	-1.055543
H	1.520387	-3.639351	-1.681697
H	0.508471	-2.311756	-2.267385
H	1.856613	-2.912632	-3.260884
H	3.133634	0.386833	-2.123297
H	1.444055	0.045658	-2.509842
H	2.744226	-0.655050	-3.505591
H	-2.043333	1.873960	3.526342
H	-0.755940	1.262158	2.457337
H	-1.582032	2.773609	2.068142
H	-3.732816	-1.017788	1.950961
H	-3.202819	-0.256277	3.459835
H	-2.010217	-0.972472	2.345195
H	-4.392041	1.949001	2.800092
H	-4.078183	2.681453	1.218930
H	-4.952256	1.138217	1.332611
H	-3.987020	2.117470	-2.049806
H	-5.155271	0.837022	-2.398398
H	-5.072290	1.536103	-0.775543
H	-1.945465	-1.063664	-2.321054
H	-3.352358	-0.609924	-3.309676
H	-2.096003	0.588665	-2.952737
H	-4.745536	-1.580004	-1.541529
H	-3.457694	-1.845873	-0.345764
H	-4.873157	-0.856662	0.069418
C	-1.771327	-4.000177	-1.027913
O	-1.738666	-4.469894	0.038859
O	-1.826895	-3.585213	-2.117045

O	2.306769	5.244880	-0.192446
C	3.686348	5.436511	0.047945
H	3.969894	5.117317	1.062225
H	4.304676	4.892292	-0.681840
H	3.865667	6.510303	-0.056003

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2,Ni-(0)-formate-isomer el energy= -1426.72672840

Ni	0.206885	-0.472679	0.028422
P	-1.968565	-1.003990	0.111821
P	2.248876	0.409836	-0.038247
O	0.796622	-2.292866	0.373483
O	0.706049	-4.484447	-0.096663
C	-2.533478	-2.225032	1.455573
C	-1.577693	-1.962786	2.639761
C	-2.375928	-3.690919	1.017220
C	-3.988135	-1.975983	1.897196
C	-2.706714	-1.380549	-1.594979
C	-1.885103	-2.513538	-2.237399
C	-4.195964	-1.754534	-1.546912
C	-2.529458	-0.112669	-2.454942
C	-2.713640	0.625210	0.619264
C	-1.750777	1.710227	0.191880
C	-2.210296	3.033562	0.116476
C	-1.322216	4.060884	-0.213418
C	0.022025	3.754112	-0.457199
C	0.468582	2.435319	-0.392276
C	-0.407678	1.363212	-0.076331
C	1.926545	2.133089	-0.663828
C	3.511289	-0.307074	-1.256855
C	2.698422	-0.620980	-2.531298
C	4.639115	0.677251	-1.615039
C	4.110717	-1.611312	-0.703721
C	2.931043	0.601505	1.722217
C	1.892274	1.449524	2.487105
C	3.003304	-0.788380	2.386559
C	4.300415	1.293864	1.784442
C	0.887778	-3.317497	-0.412937
H	-0.551425	-2.216580	2.358735
H	-1.877669	-2.589306	3.491395
H	-1.605215	-0.916427	2.973262
H	-3.052452	-3.951040	0.195294
H	-2.642207	-4.335145	1.867477
H	-1.350329	-3.940767	0.730208
H	-4.232480	-2.674201	2.709823

H	-4.706684	-2.147494	1.090104
H	-4.143491	-0.962422	2.283096
H	-0.843710	-2.203728	-2.375927
H	-2.301326	-2.749567	-3.226820
H	-1.881919	-3.432247	-1.644459
H	-4.797284	-0.984416	-1.047973
H	-4.365733	-2.707987	-1.037526
H	-4.577310	-1.856560	-2.572828
H	-2.847602	-0.336146	-3.482808
H	-1.484778	0.214532	-2.479860
H	-3.131433	0.727648	-2.092334
H	-3.729043	0.772104	0.229083
H	-2.797615	0.613001	1.713604
H	-3.253878	3.246409	0.329860
H	0.699686	4.570052	-0.700194
H	2.600803	2.877605	-0.221764
H	2.124541	2.136524	-1.743230
H	2.231888	0.276220	-2.956736
H	1.907033	-1.349657	-2.331019
H	3.366764	-1.041603	-3.295186
H	4.256231	1.604781	-2.055747
H	5.298282	0.209180	-2.359822
H	5.254200	0.940505	-0.750219
H	4.638548	-2.140016	-1.509339
H	3.339423	-2.276106	-0.305702
H	4.839055	-1.413355	0.090164
H	1.777650	2.455759	2.069428
H	2.221085	1.550713	3.530501
H	0.905720	0.974236	2.480174
H	3.163016	-0.660253	3.466207
H	3.832528	-1.387489	1.999853
H	2.083533	-1.361362	2.231810
H	4.567096	1.477092	2.834881
H	4.301524	2.263601	1.271144
H	5.091446	0.672778	1.351665
H	1.165471	-3.078522	-1.468524
O	-1.660645	5.379920	-0.313427
C	-3.009341	5.734637	-0.072435
H	-3.689576	5.243247	-0.783826
H	-3.317668	5.479145	0.952182
H	-3.065200	6.818077	-0.207538

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1,Ni-(O)-formate el energy= -1426.73676049

Ni	0.173401	-0.510271	0.118930

P	-2.005901	-1.012247	0.118618
P	2.247472	0.348833	-0.017336
O	0.726844	-2.300906	0.672892
O	1.154135	-3.262337	-1.331954
C	-2.641527	-2.210323	1.449361
C	-1.769126	-1.920618	2.690482
C	-2.427256	-3.672775	1.027426
C	-4.123520	-1.987205	1.801591
C	-2.675483	-1.393946	-1.617831
C	-1.938912	-2.615833	-2.196489
C	-4.193618	-1.629580	-1.643047
C	-2.331508	-0.168610	-2.490481
C	-2.761598	0.623102	0.583675
C	-1.768890	1.695583	0.196017
C	-2.208973	3.026432	0.127170
C	-1.302237	4.043456	-0.180351
C	0.038334	3.716589	-0.416068
C	0.463774	2.390431	-0.358778
C	-0.427466	1.328985	-0.053170
C	1.911623	2.069892	-0.644665
C	3.511992	-0.325441	-1.267422
C	2.683810	-0.670804	-2.524195
C	4.590759	0.711145	-1.635757
C	4.195441	-1.600741	-0.748549
C	2.965005	0.571807	1.727649
C	1.923576	1.401221	2.508588
C	3.085066	-0.809066	2.402319
C	4.319560	1.294791	1.758375
C	1.081181	-3.263129	-0.104204
H	-0.720908	-2.155470	2.485209
H	-2.116629	-2.541204	3.528693
H	-1.836149	-0.871713	3.007808
H	-3.102654	-3.969687	0.218177
H	-2.634513	-4.327361	1.885743
H	-1.396924	-3.851429	0.709619
H	-4.406155	-2.682228	2.604960
H	-4.789297	-2.174417	0.954292
H	-4.315454	-0.972554	2.167702
H	-0.851198	-2.513943	-2.130373
H	-2.214161	-2.726943	-3.254995
H	-2.213478	-3.545116	-1.688615
H	-4.754674	-0.803532	-1.188580
H	-4.471184	-2.557653	-1.132414
H	-4.527056	-1.718923	-2.686555
H	-2.651848	-0.372863	-3.521441

H	-1.254433	0.027332	-2.496262
H	-2.833633	0.745240	-2.154816
H	-3.752126	0.776565	0.136287
H	-2.907219	0.619058	1.671668
H	-3.252725	3.251460	0.327138
H	0.730818	4.522673	-0.650089
H	2.600308	2.813311	-0.223978
H	2.086819	2.061199	-1.727440
H	2.144311	0.202441	-2.914014
H	1.965439	-1.468909	-2.313621
H	3.364523	-1.015459	-3.315633
H	4.164970	1.623187	-2.067707
H	5.253210	0.271739	-2.394717
H	5.212169	0.996259	-0.782124
H	4.786017	-2.043158	-1.562625
H	3.471170	-2.351621	-0.425823
H	4.882710	-1.387477	0.077586
H	1.782643	2.403659	2.089918
H	2.265980	1.511845	3.546914
H	0.945872	0.907244	2.518083
H	3.304320	-0.668140	3.470190
H	3.896238	-1.406383	1.975215
H	2.160585	-1.386271	2.303551
H	4.600557	1.494955	2.802148
H	4.290682	2.258684	1.235419
H	5.116180	0.686857	1.317289
H	1.344182	-4.186619	0.460568
O	-1.618860	5.369221	-0.269265
C	-2.964572	5.741313	-0.040393
H	-3.643633	5.268841	-0.765705
H	-3.289518	5.478208	0.977247
H	-3.002844	6.827076	-0.162951

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2,TS-2-3	el energy= -1426.69933708		
Ni	0.008061	0.106217	0.007448
H	-0.001400	1.675510	0.011763
C	0.018544	-1.840671	0.003088
C	1.187136	-2.574046	-0.288742
C	2.446195	-1.810649	-0.640996
C	1.204432	-3.977459	-0.290207
H	2.127142	-4.502254	-0.521323
C	0.030655	-4.683481	-0.008497
C	-1.148736	-3.982562	0.278001
H	-2.045886	-4.557604	0.498803

C	-1.151138	-2.588852	0.289822
C	-2.414367	-1.834191	0.644789
P	2.196594	-0.041020	-0.087111
P	-2.179509	-0.062443	0.091977
C	3.147842	0.982052	-1.376314
C	2.189242	1.068744	-2.583615
C	4.469047	0.320209	-1.810121
C	3.437928	2.405672	-0.875036
C	2.962394	0.061727	1.646481
C	4.490331	-0.095657	1.656805
C	2.552970	1.403589	2.283871
C	2.327889	-1.075733	2.473694
C	-2.935065	0.034414	-1.646588
C	-2.285683	-1.097518	-2.469761
C	-2.533882	1.379706	-2.281805
C	-4.461362	-0.136506	-1.665023
C	-3.148831	0.951117	1.374706
C	-4.464931	0.274407	1.801347
C	-2.199208	1.050058	2.588266
C	-3.451721	2.370759	0.869679
H	3.355525	-2.260482	-0.220659
H	2.582780	-1.793206	-1.730032
H	-2.544912	-1.816621	1.734433
H	-3.321314	-2.292477	0.229604
H	2.692942	1.585189	-3.412901
H	1.888145	0.076353	-2.943941
H	1.287496	1.632235	-2.324966
H	5.172056	0.206205	-0.979321
H	4.313061	-0.665365	-2.261453
H	4.951930	0.952603	-2.568302
H	4.184678	2.416682	-0.074134
H	3.838908	3.000809	-1.707189
H	2.534375	2.908898	-0.523851
H	4.846058	-0.126938	2.696414
H	4.812447	-1.025639	1.171823
H	4.995409	0.741666	1.164422
H	3.012899	2.262437	1.787115
H	1.468051	1.546348	2.251002
H	2.872620	1.416783	3.335405
H	2.583616	-2.068837	2.088629
H	1.235883	-0.998903	2.487284
H	2.695134	-1.007678	3.507193
H	-2.645001	-1.031073	-3.506149
H	-1.194161	-1.012021	-2.474242
H	-2.537256	-2.092874	-2.087924

H	-3.001692	2.235139	-1.786463
H	-2.850069	1.390689	-3.334417
H	-1.450174	1.530369	-2.245432
H	-4.811495	-0.169713	-2.706459
H	-4.777560	-1.069791	-1.182749
H	-4.975807	0.695805	-1.173943
H	-4.300224	-0.709263	2.253798
H	-4.958960	0.901554	2.556699
H	-5.162175	0.152126	0.966880
H	-1.301264	1.622211	2.335301
H	-2.714072	1.562888	3.412930
H	-1.891022	0.061474	2.952886
H	-3.863755	2.962861	1.698565
H	-2.551887	2.883312	0.522237
H	-4.193947	2.372335	0.064469
C	-0.008383	3.299181	0.012772
O	0.119339	3.570264	-1.139128
O	-0.138347	3.567246	1.165080
O	-0.069291	-6.046655	0.012746
C	1.097316	-6.797312	-0.263070
H	1.479802	-6.594335	-1.274532
H	1.893598	-6.590847	0.467664
H	0.804407	-7.848322	-0.191477

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2,TS-3-4i el energy= -1426.69567297

Ni	0.008185	-0.020929	-0.028426
P	-2.236955	0.195535	0.123997
P	2.237985	0.115465	-0.090336
O	-0.086624	-2.167669	-1.321813
O	-0.757738	-3.414868	0.469100
C	-3.227359	-0.814458	1.404013
C	-2.234300	-1.116837	2.547178
C	-3.744204	-2.144308	0.829708
C	-4.419747	-0.010853	1.960803
C	-3.085833	0.262702	-1.575922
C	-2.957691	-1.099959	-2.284382
C	-4.564569	0.672867	-1.484676
C	-2.314620	1.309983	-2.405844
C	-2.319972	1.935156	0.782644
C	-1.079866	2.661885	0.327794
C	-1.062861	4.054900	0.307426
C	0.102141	4.746529	-0.048089
C	1.255141	4.025277	-0.367623
C	1.229325	2.622164	-0.355148

C	0.061358	1.902400	-0.030462
C	2.492043	1.861407	-0.681755
C	3.232556	-0.926368	-1.332090
C	2.433925	-0.873517	-2.653254
C	4.644302	-0.361832	-1.580118
C	3.326034	-2.388368	-0.866346
C	2.943304	0.066315	1.678088
C	2.334220	1.261756	2.439451
C	2.475172	-1.227540	2.371207
C	4.475817	0.162015	1.732036
C	-0.244769	-2.470130	-0.118658
H	-1.487744	-1.849833	2.228272
H	-2.784994	-1.541533	3.398181
H	-1.719962	-0.213638	2.902515
H	-4.545516	-1.987519	0.099861
H	-4.164821	-2.736207	1.654799
H	-2.946210	-2.739385	0.377922
H	-4.968638	-0.647265	2.668436
H	-5.122434	0.295429	1.179790
H	-4.105123	0.884263	2.507573
H	-1.925261	-1.461387	-2.289296
H	-3.297965	-0.985762	-3.323450
H	-3.578061	-1.870003	-1.818372
H	-4.705328	1.630178	-0.967975
H	-5.170315	-0.085818	-0.978848
H	-4.966280	0.787622	-2.501180
H	-2.750436	1.345696	-3.413788
H	-1.256542	1.043237	-2.498400
H	-2.369906	2.316086	-1.976915
H	-3.245502	2.453985	0.507028
H	-2.315893	1.855872	1.877315
H	-1.943592	4.633589	0.577422
O	0.013530	6.107942	-0.038033
H	2.178234	4.535283	-0.627200
H	3.387240	2.323170	-0.245721
H	2.654909	1.821634	-1.765777
H	2.342711	0.148818	-3.041546
H	1.435892	-1.297392	-2.521153
H	2.971942	-1.461776	-3.409747
H	4.623857	0.687916	-1.894904
H	5.108826	-0.935610	-2.393995
H	5.296289	-0.444782	-0.707453
H	3.811823	-2.982047	-1.652957
H	2.334888	-2.816694	-0.695857
H	3.928691	-2.495214	0.042526

H	2.665238	2.227109	2.041376
H	2.649191	1.204808	3.490540
H	1.240426	1.245825	2.404532
H	2.876352	-1.252071	3.393868
H	2.814728	-2.131749	1.857338
H	1.382925	-1.270349	2.434576
H	4.792102	0.277414	2.778124
H	4.859462	1.025502	1.175132
H	4.956410	-0.741715	1.344169
H	0.213145	-1.668198	0.642132
C	1.170155	6.847135	-0.384223
H	0.884912	7.900506	-0.320905
H	1.998083	6.651610	0.313320
H	1.502601	6.620182	-1.407874

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2,TS-4i-4 el energy= -1426.72337444

Ni	-1.063388	1.172688	-0.014633
P	-3.291173	1.299197	0.093614
P	1.171502	1.435865	-0.131903
O	-0.999931	-0.742743	0.367448
O	-0.037551	-2.451638	-0.752349
C	-4.166732	0.302653	1.453402
C	-3.176286	0.313931	2.638457
C	-4.394891	-1.154832	1.025288
C	-5.503434	0.929792	1.889152
C	-4.118109	1.134238	-1.607977
C	-3.662844	-0.189099	-2.250088
C	-5.651846	1.202397	-1.552508
C	-3.588662	2.292898	-2.478017
C	-3.544685	3.072969	0.590095
C	-2.314796	3.828040	0.138878
C	-2.371266	5.228143	0.063625
C	-1.232692	5.950728	-0.300806
C	-0.046083	5.262833	-0.582785
C	-0.001498	3.871441	-0.517213
C	-1.139880	3.103042	-0.159726
C	1.288855	3.156221	-0.836598
C	2.279332	0.411284	-1.290838
C	1.396597	0.101228	-2.518724
C	3.522750	1.202594	-1.743398
C	2.726028	-0.911592	-0.648038
C	1.866807	1.538450	1.632328
C	1.066867	2.636921	2.362767
C	1.600748	0.195740	2.342909

C	3.361875	1.888136	1.683946
C	-1.003543	-1.800096	-0.376782
H	-2.248964	-0.197882	2.364437
H	-3.629806	-0.205259	3.494495
H	-2.929805	1.333078	2.963854
H	-5.136770	-1.242023	0.223978
H	-4.772777	-1.725309	1.885266
H	-3.462223	-1.620172	0.698967
H	-5.922588	0.334038	2.712202
H	-6.242886	0.943617	1.083150
H	-5.382792	1.953939	2.258945
H	-2.570915	-0.233423	-2.324914
H	-4.077200	-0.261429	-3.265279
H	-3.997152	-1.067090	-1.690080
H	-6.005923	2.113768	-1.055039
H	-6.085282	0.338754	-1.037992
H	-6.052129	1.209669	-2.576158
H	-3.975196	2.170302	-3.499269
H	-2.494821	2.298152	-2.519906
H	-3.910697	3.273822	-2.112516
H	-4.478473	3.498520	0.200155
H	-3.622182	3.097826	1.684798
H	-3.301347	5.735630	0.302998
H	0.832385	5.843466	-0.856620
H	2.173748	3.703555	-0.488571
H	1.396137	3.045918	-1.923328
H	0.963511	1.009303	-2.959642
H	0.589781	-0.586902	-2.253202
H	2.010820	-0.381768	-3.291567
H	3.267643	2.099322	-2.318136
H	4.125317	0.557621	-2.397850
H	4.157462	1.504138	-0.904561
H	3.239076	-1.511420	-1.413466
H	1.872449	-1.497117	-0.295517
H	3.439838	-0.747570	0.166765
H	1.198421	3.626198	1.911318
H	1.412898	2.689477	3.404480
H	-0.005669	2.415643	2.365931
H	1.810667	0.311114	3.415720
H	2.235888	-0.607864	1.961905
H	0.561660	-0.124313	2.216644
H	3.668747	2.012496	2.732195
H	3.584857	2.828128	1.163636
H	3.984718	1.098666	1.252359
H	-2.022153	-2.155614	-0.668787

O	-1.173153	7.310896	-0.403309
C	-2.351306	8.044796	-0.128031
H	-3.166512	7.772635	-0.814863
H	-2.690066	7.892190	0.907460
H	-2.092311	9.097049	-0.272583

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3,Ni-H el energy= -1134.38098892

Ni	0.000000	0.000000	0.230705
H	0.000000	0.000000	1.783739
C	0.000000	0.000000	-1.724964
C	1.197442	0.166693	-2.461319
C	2.488970	0.378796	-1.691089
C	1.206441	0.162215	-3.862215
H	2.134541	0.291146	-4.413580
C	0.000000	0.000000	-4.544967
I	0.000000	0.000000	-6.670697
C	-1.206441	-0.162215	-3.862215
H	-2.134541	-0.291146	-4.413580
C	-1.197442	-0.166693	-2.461319
C	-2.488970	-0.378796	-1.691089
P	2.162044	-0.145834	0.081623
P	-2.162044	0.145834	0.081623
C	3.186009	1.054656	1.134139
C	2.379314	2.370921	1.108047
C	4.602136	1.312975	0.592166
C	3.253913	0.555360	2.586252
C	2.775023	-1.940944	0.185585
C	4.301301	-2.083142	0.095825
C	2.255039	-2.563946	1.495019
C	2.120142	-2.692754	-0.992348
C	-2.775023	1.940944	0.185585
C	-2.120142	2.692754	-0.992348
C	-2.255039	2.563946	1.495019
C	-4.301301	2.083142	0.095825
C	-3.186009	-1.054656	1.134139
C	-4.602136	-1.312975	0.592166
C	-2.379314	-2.370921	1.108047
C	-3.253913	-0.555360	2.586252
H	3.346451	-0.139960	-2.139518
H	2.747578	1.445744	-1.673038
H	-2.747578	-1.445744	-1.673038
H	-3.346451	0.139960	-2.139518
H	2.895864	3.128969	1.713557
H	2.273841	2.772883	0.092527

H	1.375305	2.217123	1.518729
H	5.226522	0.415312	0.609548
H	4.586698	1.695808	-0.434707
H	5.095747	2.071536	1.216199
H	3.909424	-0.316629	2.689092
H	3.661300	1.350262	3.226658
H	2.257403	0.292249	2.959345
H	4.566790	-3.148356	0.038253
H	4.710054	-1.593655	-0.796819
H	4.803818	-1.668665	0.976132
H	2.707145	-2.111601	2.382484
H	1.169484	-2.444803	1.576801
H	2.493141	-3.637005	1.506520
H	2.467640	-2.332646	-1.966539
H	1.029791	-2.594521	-0.972773
H	2.375278	-3.759004	-0.917466
H	-2.375278	3.759004	-0.917466
H	-1.029791	2.594521	-0.972773
H	-2.467640	2.332646	-1.966539
H	-2.707145	2.111601	2.382484
H	-2.493141	3.637005	1.506520
H	-1.169484	2.444803	1.576801
H	-4.566790	3.148356	0.038253
H	-4.710054	1.593655	-0.796819
H	-4.803818	1.668665	0.976132
H	-5.095747	-2.071536	1.216199
H	-5.226522	-0.415312	0.609548
H	-4.586698	-1.695808	-0.434707
H	-1.375305	-2.217123	1.518729
H	-2.895864	-3.128969	1.713557
H	-2.273841	-2.772883	0.092527
H	-3.661300	-1.350262	3.226658
H	-2.257403	-0.292249	2.959345
H	-3.909424	0.316629	2.689092

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3,Ni+ el energy= -1133.59099658

Ni	0.000000	0.000000	0.036100
C	0.000000	0.000000	1.917768
C	0.085145	1.217241	2.623812
C	0.184046	2.522185	1.863803
C	0.079742	1.211369	4.023667
H	0.137498	2.150305	4.567691
C	0.000000	0.000000	4.714779
I	0.000000	0.000000	6.822823

C	-0.079742	-1.211369	4.023667
H	-0.137498	-2.150305	4.567691
C	-0.085145	-1.217241	2.623812
C	-0.184046	-2.522185	1.863803
P	-0.437702	2.195022	0.141403
P	0.437702	-2.195022	0.141403
C	0.608281	3.268117	-1.015485
C	1.987805	2.575486	-1.068451
C	0.775052	4.706999	-0.496140
C	0.003741	3.276071	-2.429872
C	-2.289603	2.585545	0.132532
C	-2.581748	4.093759	0.162853
C	-2.912871	1.934241	-1.117728
C	-2.897553	1.915350	1.381974
C	2.289603	-2.585545	0.132532
C	2.897553	-1.915350	1.381974
C	2.912871	-1.934241	-1.117728
C	2.581748	-4.093759	0.162853
C	-0.608281	-3.268117	-1.015485
C	-0.775052	-4.706999	-0.496140
C	-1.987805	-2.575486	-1.068451
C	-0.003741	-3.276071	-2.429872
H	-0.357264	3.337960	2.356574
H	1.230895	2.839520	1.781915
H	-1.230895	-2.839520	1.781915
H	0.357264	-3.337960	2.356574
H	2.668193	3.168642	-1.692992
H	2.450518	2.477912	-0.079069
H	1.919939	1.572579	-1.510387
H	-0.174755	5.245995	-0.447844
H	1.237277	4.737014	0.496971
H	1.434579	5.259077	-1.178824
H	-0.934464	3.837628	-2.476489
H	0.708395	3.757237	-3.120265
H	-0.182078	2.260892	-2.804666
H	-3.664054	4.248283	0.263246
H	-2.100140	4.590708	1.013645
H	-2.264550	4.595914	-0.756488
H	-2.537396	2.361584	-2.051809
H	-2.728430	0.852122	-1.133384
H	-4.000068	2.083785	-1.099095
H	-2.532663	2.355562	2.315779
H	-2.690560	0.840156	1.412224
H	-3.986255	2.051553	1.354957
H	3.986255	-2.051553	1.354957

H	2.690560	-0.840156	1.412224
H	2.532663	-2.355562	2.315779
H	2.537396	-2.361584	-2.051809
H	4.000068	-2.083785	-1.099095
H	2.728430	-0.852122	-1.133384
H	3.664054	-4.248283	0.263246
H	2.100140	-4.590708	1.013645
H	2.264550	-4.595914	-0.756488
H	-1.434579	-5.259077	-1.178824
H	0.174755	-5.245995	-0.447844
H	-1.237277	-4.737014	0.496971
H	-1.919939	-1.572579	-1.510387
H	-2.668193	-3.168642	-1.692992
H	-2.450518	-2.477912	-0.079069
H	-0.708395	-3.757237	-3.120265
H	0.182078	-2.260892	-2.804666
H	0.934464	-3.837628	-2.476489

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3,Ni-H+CO2 el energy= -1322.97281298

Ni	1.169186	-0.010570	0.001137
P	1.019102	2.161353	-0.089041
P	1.009502	-2.181556	0.033212
O	4.752605	-0.110904	2.151245
O	5.525872	0.371832	0.004779
C	2.015631	3.052693	-1.436764
C	1.967376	2.093977	-2.645898
C	3.481386	3.216171	-1.005803
C	1.431854	4.417456	-1.841728
C	1.175104	2.978138	1.618458
C	2.512807	2.551268	2.249956
C	1.063738	4.509202	1.588061
C	0.035042	2.396067	2.480535
C	-0.770094	2.428449	-0.588191
C	-1.530905	1.166887	-0.226037
C	-2.931363	1.179782	-0.190405
C	-3.611215	-0.005040	0.094379
C	-2.924639	-1.194116	0.343055
C	-1.523949	-1.187727	0.315240
C	-0.789746	-0.010538	0.033915
C	-0.753829	-2.462374	0.607692
C	2.069815	-3.135560	1.282175
C	2.069109	-2.245666	2.543688
C	1.517090	-4.525562	1.641326
C	3.511364	-3.259238	0.762720

C	1.082317	-2.913267	-1.719171
C	-0.092323	-2.286858	-2.499963
C	2.394137	-2.462619	-2.389697
C	0.962527	-4.443807	-1.760560
C	5.112575	0.129512	1.067748
H	2.417979	1.128379	-2.391661
H	2.526387	2.532972	-3.484198
H	0.941571	1.910980	-2.990053
H	3.594504	3.958733	-0.207954
H	4.074467	3.564150	-1.863209
H	3.907201	2.265908	-0.669170
H	2.026351	4.832258	-2.668066
H	1.456351	5.141888	-1.022741
H	0.397222	4.337750	-2.193517
H	2.603266	1.461450	2.275341
H	2.565667	2.928248	3.281084
H	3.376383	2.947952	1.707273
H	0.147190	4.848074	1.089660
H	1.919802	4.971911	1.085763
H	1.040336	4.894187	2.617460
H	0.142651	2.767748	3.509021
H	0.069456	1.301669	2.502110
H	-0.956640	2.689365	2.119886
H	-1.204365	3.335009	-0.146848
H	-0.786751	2.575913	-1.675869
H	-3.484311	2.094085	-0.391030
I	-5.735925	0.000400	0.144954
H	-3.472278	-2.107474	0.561724
H	-1.211606	-3.352128	0.155855
H	-0.720299	-2.646599	1.689411
H	1.058165	-2.101287	2.945153
H	2.497200	-1.262275	2.329946
H	2.673080	-2.723165	3.327918
H	0.501479	-4.471533	2.049576
H	2.155119	-4.978769	2.413298
H	1.502630	-5.205356	0.784909
H	4.172010	-3.573091	1.582558
H	3.876958	-2.302285	0.376106
H	3.594591	-4.007256	-0.033709
H	-1.068202	-2.584510	-2.101743
H	-0.039583	-2.619448	-3.545973
H	-0.047088	-1.193081	-2.480296
H	2.382710	-2.761973	-3.447232
H	3.276990	-2.912171	-1.925923
H	2.506119	-1.374641	-2.335381

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H            0.887264       -4.775834       -2.805784
H            0.068369       -4.803482       -1.236598
H            1.838486       -4.935696       -1.324572
H            2.718164       -0.016360       -0.034780

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3,Ni-(H)-formate    el energy= -1322.96636770
Ni           1.198485       -0.000331       -0.000279
P            1.064189        2.207666       -0.085440
P            1.063287       -2.207994        0.085201
O            4.508451       -0.200864        1.133815
O            4.510006        0.202252       -1.131945
C            2.068139        3.163178       -1.385029
C            2.150140        2.205112       -2.593639
C            3.494763        3.471493       -0.901403
C            1.381765        4.477478       -1.802923
C            1.185065        2.947301        1.655196
C            2.546405        2.555846        2.262533
C            1.001899        4.472301        1.683557
C            0.072898        2.281367        2.491735
C           -0.710243        2.441146       -0.621745
C           -1.464990        1.176457       -0.277601
C           -2.865817        1.184135       -0.271141
C           -3.552339        0.000609       -0.000827
C           -2.866373       -1.183197        0.269667
C           -1.465543       -1.176076        0.276556
C           -0.732559        0.000061       -0.000368
C           -0.711408       -2.441120        0.620780
C            2.066727       -3.163115        1.385437
C            2.148025       -2.204851        2.593937
C            1.380344       -4.477454        1.803209
C            3.493624       -3.471249        0.902518
C            1.184987       -2.947826       -1.655256
C            0.072938       -2.282229       -2.492223
C            2.546453       -2.556109       -2.262144
C            1.002210       -4.472877       -1.683489
C            4.125444        0.000129        0.000568
H            2.754368        1.325277       -2.350265
H            2.628063        2.725436       -3.435403
H            1.158210        1.874606       -2.929656
H            3.505174        4.204257       -0.087665
H            4.060727        3.903222       -1.738353
H            4.027587        2.571800       -0.585941
H            2.003243        4.973013       -2.561410
H            1.265106        5.173434       -0.966369
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H	0.395747	4.312976	-2.250127
H	2.719336	1.475764	2.217108
H	2.569203	2.862460	3.317520
H	3.385928	3.042181	1.758601
H	0.056387	4.784587	1.222895
H	1.820515	4.994797	1.178240
H	0.987904	4.816224	2.727211
H	0.150823	2.636678	3.528310
H	0.172140	1.190685	2.493590
H	-0.931597	2.523436	2.127598
H	-1.165860	3.342371	-0.192520
H	-0.701675	2.583341	-1.709586
H	-3.411866	2.099458	-0.484109
I	-5.673820	0.001035	-0.001138
H	-3.412855	-2.098314	0.482414
H	-1.167134	-3.342089	0.191131
H	-0.703359	-2.583587	1.708585
H	1.155910	-1.874300	2.929350
H	2.752400	-1.325064	2.350762
H	2.625478	-2.725035	3.436056
H	0.394067	-4.313023	2.249868
H	2.001498	-4.972755	2.562117
H	1.264230	-5.173575	0.966725
H	4.059201	-3.903023	1.739705
H	4.026512	-2.571452	0.587445
H	3.504519	-4.203892	0.088675
H	-0.931619	-2.524542	-2.128415
H	0.151306	-2.637566	-3.528754
H	0.171904	-1.191519	-2.494084
H	2.569788	-2.863009	-3.317034
H	3.385922	-3.042035	-1.757720
H	2.718987	-1.475950	-2.216952
H	0.988598	-4.816936	-2.727103
H	0.056648	-4.785344	-1.223050
H	1.820823	-4.995094	-1.177877
H	2.803710	-0.002173	-0.000866

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3,TS-2-3	el energy= -1322.96569093		
Ni	1.201059	0.000055	-0.000012
P	1.053363	2.193623	-0.089956
P	1.053977	-2.193547	0.089861
O	4.634254	-0.139555	1.150872
O	4.635020	0.141018	-1.148712
C	2.064666	3.150275	-1.383224

C	2.151171	2.193530	-2.592106
C	3.488520	3.449922	-0.887758
C	1.390891	4.467903	-1.809927
C	1.161375	2.949197	1.646488
C	2.510598	2.547246	2.273071
C	0.992935	4.475943	1.664428
C	0.033816	2.301059	2.476653
C	-0.720506	2.435034	-0.635880
C	-1.480104	1.173114	-0.285948
C	-2.880968	1.181841	-0.280721
C	-3.566112	-0.000684	-0.001281
C	-2.880747	-1.182989	0.278549
C	-1.479890	-1.173815	0.284549
C	-0.744585	-0.000236	-0.000509
C	-0.720074	-2.435470	0.634957
C	2.064952	-3.149896	1.383607
C	2.150618	-2.193122	2.592527
C	1.391350	-4.467712	1.810004
C	3.489123	-3.449134	0.888808
C	1.163008	-2.949098	-1.646530
C	0.035637	-2.301308	-2.477221
C	2.512396	-2.546740	-2.272491
C	0.995037	-4.475895	-1.664537
C	4.350690	0.000656	0.000975
H	2.725588	1.297017	-2.339179
H	2.656991	2.703085	-3.424161
H	1.159093	1.884388	-2.946587
H	3.497433	4.193150	-0.083591
H	4.074246	3.860597	-1.721695
H	4.003132	2.549518	-0.545190
H	2.018069	4.957851	-2.567648
H	1.274052	5.167054	-0.976261
H	0.405655	4.306980	-2.260091
H	2.661999	1.463658	2.238018
H	2.528233	2.864882	3.324977
H	3.362534	3.014785	1.771737
H	0.057187	4.794149	1.188299
H	1.823317	4.988576	1.168134
H	0.966971	4.826302	2.705829
H	0.106717	2.660435	3.512346
H	0.118695	1.209314	2.483027
H	-0.963998	2.554003	2.102089
H	-1.174193	3.340972	-0.213943
H	-0.707171	2.571440	-1.724687
H	-3.428824	2.094508	-0.500889

I	-5.689117	-0.001024	-0.001876
H	-3.428433	-2.095828	0.498425
H	-1.173284	-3.341596	0.212911
H	-0.707199	-2.571748	1.723787
H	1.158284	-1.884274	2.946547
H	2.724891	-1.296442	2.339869
H	2.656198	-2.702532	3.424817
H	0.405869	-4.307057	2.259726
H	2.018324	-4.957490	2.568004
H	1.275075	-5.166893	0.976284
H	4.074573	-3.859655	1.723014
H	4.003641	-2.548575	0.546503
H	3.498630	-4.192341	0.084629
H	-0.962274	-2.554555	-2.103119
H	0.109130	-2.660668	-3.512878
H	0.120183	-1.209538	-2.483561
H	2.530619	-2.864377	-3.324387
H	3.364246	-3.014008	-1.770757
H	2.663439	-1.463105	-2.237373
H	0.969678	-4.826270	-2.705948
H	0.059158	-4.794378	-1.188854
H	1.825336	-4.988274	-1.167841
H	2.772478	0.000282	0.000412

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3,Ni-(0)-formate-isomer el energy= -1322.99246259

Ni	1.237074	0.087191	0.027927
P	1.120097	-2.149538	0.159075
P	0.995605	2.301146	-0.060092
O	3.161932	0.121849	0.271978
O	5.207985	-0.608403	-0.284305
C	2.183082	-3.013332	1.476758
C	2.261445	-1.997258	2.636934
C	3.610571	-3.297952	0.979176
C	1.542889	-4.323015	1.974862
C	1.187074	-2.998662	-1.535780
C	2.479779	-2.558167	-2.247359
C	1.112573	-4.530726	-1.451510
C	-0.012325	-2.475015	-2.351727
C	-0.631917	-2.375235	0.750375
C	-1.409750	-1.147065	0.333102
C	-2.808967	-1.199383	0.311251
C	-3.531190	-0.050699	-0.008503
C	-2.877782	1.145805	-0.297379
C	-1.477248	1.184296	-0.285774

C	-0.701419	0.038165	0.015380
C	-0.776206	2.487963	-0.603515
C	1.987956	3.277021	-1.345850
C	1.983906	2.388141	-2.608100
C	1.359983	4.639131	-1.691068
C	3.436762	3.473949	-0.867912
C	1.096329	3.032667	1.687155
C	0.022575	2.295501	2.515809
C	2.479007	2.706195	2.287599
C	0.834801	4.545125	1.741562
C	4.130259	-0.102659	-0.559526
H	2.789097	-1.095311	2.313536
H	2.811454	-2.448224	3.474544
H	1.268058	-1.712735	3.009832
H	3.626503	-4.038815	0.171868
H	4.187343	-3.721277	1.813875
H	4.133455	-2.395792	0.648554
H	2.176525	-4.742699	2.768363
H	1.462261	-5.076937	1.186143
H	0.546522	-4.169255	2.403806
H	2.480135	-1.475263	-2.411633
H	2.539166	-3.047904	-3.229302
H	3.385731	-2.809929	-1.689287
H	0.225000	-4.870459	-0.903624
H	1.998229	-4.960570	-0.973882
H	1.051222	-4.946370	-2.467130
H	0.062357	-2.862550	-3.377146
H	-0.022187	-1.380777	-2.397804
H	-0.974375	-2.799879	-1.940853
H	-1.086170	-3.310689	0.400840
H	-0.596206	-2.434216	1.845620
H	-3.325967	-2.124592	0.552141
I	-5.651050	-0.121663	-0.042584
H	-3.448043	2.040699	-0.532774
H	-1.270357	3.353676	-0.144682
H	-0.774979	2.668472	-1.685910
H	0.968958	2.197683	-2.978561
H	2.460316	1.421727	-2.417245
H	2.540400	2.892185	-3.410013
H	0.339379	4.540187	-2.077850
H	1.961238	5.120360	-2.475237
H	1.334431	5.316828	-0.833407
H	4.055220	3.810591	-1.711154
H	3.865416	2.547200	-0.477435
H	3.501542	4.240091	-0.087803

H	-0.993692	2.475528	2.148330
H	0.074235	2.651058	3.553836
H	0.189569	1.213104	2.514095
H	2.455919	2.909302	3.367151
H	3.272102	3.321579	1.853719
H	2.753487	1.657937	2.132185
H	0.787253	4.867110	2.791275
H	-0.116204	4.822394	1.269804
H	1.637321	5.115462	1.262615
H	3.930528	0.212714	-1.612212

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3,Ni-(0)-formate el energy= -1323.00272269

Ni	1.298387	0.097651	0.155003
P	1.195141	-2.158690	0.177598
P	1.003458	2.302873	-0.037932
O	3.181702	0.294826	0.631522
O	4.156676	-0.225581	-1.342559
C	2.314800	-3.103145	1.387860
C	2.485150	-2.158966	2.598164
C	3.693007	-3.374159	0.760385
C	1.698208	-4.429443	1.869214
C	1.109236	-2.969133	-1.543854
C	2.421649	-2.715364	-2.307597
C	0.821329	-4.477748	-1.483139
C	-0.032284	-2.264977	-2.306827
C	-0.516232	-2.372811	0.889802
C	-1.324155	-1.166437	0.468710
C	-2.723335	-1.232900	0.480267
C	-3.462727	-0.112196	0.104929
C	-2.827783	1.068059	-0.279130
C	-1.428083	1.120122	-0.292964
C	-0.636922	0.006571	0.076603
C	-0.732820	2.396796	-0.708957
C	2.052689	3.223442	-1.320962
C	2.198459	2.238695	-2.502285
C	1.382020	4.517048	-1.819459
C	3.445800	3.548965	-0.756304
C	0.951969	3.160196	1.654614
C	-0.163034	2.458767	2.458742
C	2.291393	2.922031	2.379993
C	0.651616	4.664373	1.572826
C	4.180388	0.075628	-0.150700
H	2.981515	-1.229703	2.305571
H	3.089989	-2.663660	3.364725

H	1.521387	-1.902830	3.057948
H	3.647401	-4.180691	0.020698
H	4.390842	-3.689952	1.548314
H	4.111750	-2.489841	0.271715
H	2.385157	-4.899741	2.586954
H	1.536072	-5.140146	1.054130
H	0.743352	-4.278548	2.385045
H	2.729172	-1.666871	-2.264198
H	2.278303	-3.001968	-3.359018
H	3.249657	-3.312815	-1.915771
H	-0.080416	-4.713961	-0.905098
H	1.661384	-5.036982	-1.058809
H	0.663487	-4.852530	-2.504132
H	-0.069940	-2.671667	-3.326667
H	0.137194	-1.185420	-2.373682
H	-1.012735	-2.420836	-1.845143
H	-0.987723	-3.320080	0.601177
H	-0.407177	-2.393794	1.982002
H	-3.225958	-2.147849	0.782854
I	-5.582517	-0.202033	0.124402
H	-3.411675	1.938841	-0.565688
H	-1.268910	3.297970	-0.386341
H	-0.655620	2.450115	-1.802364
H	1.223418	1.936935	-2.907052
H	2.750245	1.337026	-2.217795
H	2.748314	2.736404	-3.313541
H	0.411049	4.325991	-2.289967
H	2.026796	4.978265	-2.580617
H	1.235758	5.251384	-1.022073
H	4.104050	3.859372	-1.578986
H	3.900074	2.683261	-0.268026
H	3.407460	4.373507	-0.035509
H	-1.154376	2.592213	2.012556
H	-0.188135	2.885239	3.470894
H	0.020124	1.382247	2.543383
H	2.187712	3.228717	3.430183
H	3.105549	3.507824	1.943642
H	2.586646	1.869006	2.345124
H	0.522258	5.063729	2.588630
H	-0.270233	4.876322	1.017091
H	1.471384	5.219795	1.105854
H	5.158231	0.190283	0.369165

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3,TS-3-4i el energy= -1322.96098092

Ni	0.004014	-0.004659	-0.041856
P	-2.243759	0.201021	0.118092
P	2.237461	0.127932	-0.097484
O	-0.094278	-2.135362	-1.341011
O	-0.739124	-3.405444	0.444464
C	-3.220280	-0.809413	1.407506
C	-2.219220	-1.105314	2.545488
C	-3.734640	-2.142791	0.838893
C	-4.412453	-0.008932	1.969255
C	-3.102017	0.267228	-1.576646
C	-2.973506	-1.095209	-2.285302
C	-4.581495	0.672706	-1.476911
C	-2.338350	1.317078	-2.410251
C	-2.325026	1.941825	0.776713
C	-1.087398	2.669877	0.316341
C	-1.076614	4.070197	0.298768
C	0.091163	4.742098	-0.059549
C	1.247893	4.035813	-0.383960
C	1.225777	2.635115	-0.374302
C	0.052389	1.917484	-0.047140
C	2.487049	1.871554	-0.700555
C	3.237303	-0.918218	-1.330186
C	2.446214	-0.873428	-2.656110
C	4.649381	-0.352094	-1.573207
C	3.330485	-2.377252	-0.854857
C	2.932260	0.091514	1.674964
C	2.315264	1.289412	2.425866
C	2.463845	-1.200110	2.372303
C	4.464188	0.192062	1.736155
C	-0.243714	-2.451334	-0.140795
H	-1.469532	-1.834334	2.224562
H	-2.763444	-1.532666	3.399153
H	-1.708826	-0.199077	2.898819
H	-4.541655	-1.991753	0.114278
H	-4.146746	-2.734840	1.667997
H	-2.937122	-2.735253	0.382890
H	-4.955196	-0.646153	2.680695
H	-5.120201	0.293154	1.191356
H	-4.098554	0.888182	2.513319
H	-1.938963	-1.449597	-2.301427
H	-3.326162	-0.983885	-3.320387
H	-3.583717	-1.868585	-1.811543
H	-4.723289	1.628803	-0.958345
H	-5.182784	-0.088744	-0.969999
H	-4.987887	0.787980	-2.491350

H	-2.774804	1.346987	-3.417869
H	-1.278472	1.057531	-2.503841
H	-2.401349	2.324592	-1.985487
H	-3.252244	2.459898	0.505637
H	-2.315020	1.863227	1.871295
H	-1.969623	4.625541	0.572903
I	0.113683	6.861712	-0.088910
H	2.161637	4.564607	-0.642006
H	3.383581	2.338510	-0.274198
H	2.641599	1.823431	-1.785239
H	2.360757	0.145754	-3.053739
H	1.446220	-1.293596	-2.527698
H	2.987520	-1.468886	-3.404370
H	4.629004	0.695433	-1.895230
H	5.119063	-0.930160	-2.380903
H	5.296808	-0.428485	-0.696626
H	3.819036	-2.975011	-1.636435
H	2.339875	-2.806683	-0.683843
H	3.930736	-2.477934	0.056194
H	2.644409	2.253766	2.024064
H	2.625838	1.240550	3.478476
H	1.221462	1.268041	2.388404
H	2.858133	-1.216594	3.397662
H	2.810687	-2.106135	1.866649
H	1.371321	-1.246845	2.428902
H	4.774183	0.311514	2.783529
H	4.848773	1.055041	1.179270
H	4.949184	-0.711489	1.353683
H	0.206097	-1.646314	0.627241

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3,TS-4i-4 el energy= -1322.99023550

Ni	1.276012	0.101156	-0.026011
P	1.181790	-2.149665	0.153654
P	0.988433	2.313036	-0.088316
O	3.218125	0.288915	0.049542
O	4.881777	-1.045641	-0.704885
C	2.250858	-3.010794	1.473341
C	2.451166	-1.933076	2.560387
C	3.627574	-3.426521	0.932914
C	1.549389	-4.241922	2.078730
C	1.177153	-3.048659	-1.516394
C	2.465203	-2.675454	-2.272395
C	1.049344	-4.573765	-1.378797
C	-0.025452	-2.511612	-2.318728

C	-0.553951	-2.340857	0.806756
C	-1.351254	-1.146391	0.343789
C	-2.749472	-1.219525	0.319611
C	-3.486894	-0.093797	-0.043723
C	-2.848803	1.101226	-0.370086
C	-1.449102	1.160158	-0.353693
C	-0.658651	0.034747	-0.014128
C	-0.763597	2.465110	-0.695376
C	2.006115	3.332785	-1.319470
C	2.099315	2.453487	-2.584857
C	1.338586	4.670042	-1.688605
C	3.420213	3.585892	-0.769876
C	1.010244	3.026942	1.670261
C	-0.118773	2.318587	2.447669
C	2.352848	2.660688	2.333728
C	0.784029	4.545340	1.720845
C	4.210319	-0.023127	-0.720644
H	3.014501	-1.086331	2.155806
H	3.012063	-2.364817	3.401029
H	1.496511	-1.559697	2.956494
H	3.553527	-4.255286	0.219502
H	4.236760	-3.781434	1.776815
H	4.153058	-2.593086	0.456484
H	2.215456	-4.686677	2.830901
H	1.339707	-5.012253	1.329830
H	0.610902	-3.992376	2.585238
H	2.509155	-1.595537	-2.452310
H	2.469315	-3.181930	-3.247910
H	3.376444	-2.949749	-1.737130
H	0.155799	-4.862837	-0.811537
H	1.923657	-5.020125	-0.896171
H	0.960938	-5.020172	-2.379265
H	0.008380	-2.939025	-3.330401
H	0.002684	-1.420221	-2.406755
H	-0.987269	-2.784908	-1.871519
H	-1.013830	-3.298252	0.532722
H	-0.482677	-2.327891	1.901557
H	-3.253130	-2.143339	0.591787
I	-5.605183	-0.196229	-0.084139
H	-3.429701	1.980445	-0.636285
H	-1.287188	3.337554	-0.284295
H	-0.723734	2.606705	-1.782987
H	1.111293	2.230462	-3.006994
H	2.599587	1.504745	-2.373981
H	2.675041	2.984880	-3.355011

H	0.345208	4.530798	-2.129877
H	1.959354	5.181774	-2.437455
H	1.239061	5.339966	-0.830272
H	4.061443	3.963952	-1.578034
H	3.862791	2.667516	-0.376213
H	3.415387	4.340930	0.024043
H	-1.112546	2.535835	2.041330
H	-0.097532	2.665414	3.489789
H	0.011637	1.231655	2.443592
H	2.304230	2.913532	3.401975
H	3.194108	3.207929	1.900112
H	2.569446	1.592082	2.236931
H	0.700358	4.864337	2.769221
H	-0.140971	4.844214	1.212058
H	1.617183	5.099490	1.277003
H	4.486265	0.774881	-1.452912

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4,Ni-H el energy= -966.312418964

Ni	0.000000	0.000000	0.338288
H	0.000000	0.000000	1.886182
C	0.000000	0.000000	-1.624243
C	1.131939	0.433381	-2.358590
C	2.341014	0.910709	-1.572730
C	1.131629	0.428428	-3.758522
H	2.010413	0.764098	-4.309107
C	0.000000	0.000000	-4.457178
H	0.000000	0.000000	-5.545624
C	-1.131629	-0.428428	-3.758522
H	-2.010413	-0.764098	-4.309107
C	-1.131939	-0.433381	-2.358590
C	-2.341014	-0.910709	-1.572730
P	2.141400	0.219083	0.157076
P	-2.141400	-0.219083	0.157076
C	3.107647	1.403502	1.238967
C	3.399416	0.820977	2.627186
C	2.302395	2.706915	1.362280
C	3.076014	-1.412839	0.161250
C	2.580382	-2.289156	1.323875
C	2.893978	-2.162108	-1.167891
C	-3.076014	1.412839	0.161250
C	-2.893978	2.162108	-1.167891
C	-2.580382	2.289156	1.323875
C	-3.107647	-1.403502	1.238967
C	-2.302395	-2.706915	1.362280

C	-3.399416	-0.820977	2.627186
H	3.298080	0.634201	-2.035834
H	2.341898	2.006074	-1.481586
H	-2.341898	-2.006074	-1.481586
H	-3.298080	-0.634201	-2.035834
H	2.468104	0.510470	3.117235
H	4.071772	-0.043044	2.580528
H	3.878427	1.581093	3.258777
H	1.337833	2.506122	1.844584
H	2.851287	3.437063	1.972029
H	2.101604	3.168813	0.388250
H	2.689586	-1.804258	2.297840
H	1.515383	-2.514311	1.192165
H	3.137832	-3.235627	1.345598
H	3.311204	-1.617800	-2.021091
H	1.832053	-2.336625	-1.374259
H	3.397754	-3.136368	-1.111113
H	-3.397754	3.136368	-1.111113
H	-1.832053	2.336625	-1.374259
H	-3.311204	1.617800	-2.021091
H	-2.689586	1.804258	2.297840
H	-3.137832	3.235627	1.345598
H	-1.515383	2.514311	1.192165
H	-1.337833	-2.506122	1.844584
H	-2.851287	-3.437063	1.972029
H	-2.101604	-3.168813	0.388250
H	-3.878427	-1.581093	3.258777
H	-2.468104	-0.510470	3.117235
H	-4.071772	0.043044	2.580528
H	4.059911	1.606438	0.724266
H	4.143223	-1.179983	0.300105
H	-4.143223	1.179983	0.300105
H	-4.059911	-1.606438	0.724266

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4,Ni+ el energy= -965.525459103

Ni	0.000000	0.000000	-0.033348
C	0.000000	0.000000	-1.921144
C	-0.383876	1.162402	-2.622370
C	-0.785739	2.400525	-1.851665
C	-0.374707	1.149760	-4.022369
H	-0.660677	2.047383	-4.567224
C	0.000000	0.000000	-4.718272
H	0.000000	0.000000	-5.805211
C	0.374707	-1.149760	-4.022369

H	0.660677	-2.047383	-4.567224
C	0.383876	-1.162402	-2.622370
C	0.785739	-2.400525	-1.851665
P	-0.020933	2.234225	-0.167317
P	0.020933	-2.234225	-0.167317
C	-1.096261	3.238027	0.987981
C	-0.421779	3.518815	2.337485
C	-2.439504	2.514547	1.178807
C	1.685369	3.005218	-0.226720
C	2.553767	2.403998	0.892429
C	2.355077	2.796000	-1.593259
C	-1.685369	-3.005218	-0.226720
C	-2.355077	-2.796000	-1.593259
C	-2.553767	-2.403998	0.892429
C	1.096261	-3.238027	0.987981
C	2.439504	-2.514547	1.178807
C	0.421779	-3.518815	2.337485
H	-0.490979	3.327920	-2.356396
H	-1.873883	2.442026	-1.712698
H	1.873883	-2.442026	-1.712698
H	0.490979	-3.327920	-2.356396
H	-0.170448	2.588123	2.863328
H	0.491753	4.113022	2.232278
H	-1.109788	4.081962	2.979468
H	-2.298497	1.562036	1.706844
H	-3.114132	3.133151	1.782821
H	-2.946655	2.302401	0.230578
H	2.110036	2.516637	1.886797
H	2.717560	1.333322	0.711398
H	3.534812	2.894088	0.907389
H	1.806828	3.274618	-2.410801
H	2.452569	1.730127	-1.829356
H	3.362007	3.230157	-1.569892
H	-3.362007	-3.230157	-1.569892
H	-2.452569	-1.730127	-1.829356
H	-1.806828	-3.274618	-2.410801
H	-2.110036	-2.516637	1.886797
H	-3.534812	-2.894088	0.907389
H	-2.717560	-1.333322	0.711398
H	2.298497	-1.562036	1.706844
H	3.114132	-3.133151	1.782821
H	2.946655	-2.302401	0.230578
H	1.109788	-4.081962	2.979468
H	0.170448	-2.588123	2.863328
H	-0.491753	-4.113022	2.232278

H	-1.269555	4.194513	0.472029
H	1.549593	4.082340	-0.051644
H	-1.549593	-4.082340	-0.051644
H	1.269555	-4.194513	0.472029

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4,Ni-H+CO2 el energy= -1154.90458105

Ni	-0.001519	-0.110716	-0.014124
P	-2.146026	0.077791	-0.241310
P	2.142723	0.067535	0.227284
C	-2.600198	-1.114814	2.246723
C	-0.000195	1.853248	-0.000238
C	1.129288	2.583868	0.444802
C	2.332976	1.794506	0.926240
C	-2.273877	-1.180522	-2.702712
C	-3.561410	-2.322984	-0.853236
C	-2.333246	1.809568	-0.928222
C	3.112677	-0.991041	1.433418
C	3.574092	-2.328269	0.843374
C	2.237474	-1.214954	2.677008
C	3.087172	0.066609	-1.396118
C	2.871675	1.380699	-2.162674
C	-3.078578	0.069255	1.389591
C	-2.875712	1.385812	2.155318
C	-3.127904	-0.975450	-1.441428
C	0.005215	4.686266	0.009200
C	2.628226	-1.123320	-2.255881
C	1.131548	3.983754	0.444867
C	-1.126868	2.591207	-0.440469
C	-1.123789	3.991059	-0.431169
H	-4.251954	-2.203859	-0.010691
H	4.000432	-0.402817	1.714040
H	4.156301	-0.037795	-1.155106
H	-4.147780	-0.048454	1.155170
H	3.292961	2.257083	0.658215
H	2.327359	1.695911	2.021509
H	-2.327359	1.718971	-2.024091
H	-3.291718	2.273219	-0.656947
H	2.724456	-2.914466	0.477174
H	4.083310	-2.919104	1.616733
H	1.336304	-1.778773	2.406618
H	2.790704	-1.782664	3.437223
H	1.913622	-0.271247	3.133000
H	1.565918	-1.014128	-2.504731
H	3.203696	-1.154764	-3.191204

H	3.256781	2.252675	-1.624191
H	1.805479	1.552260	-2.348956
H	3.385943	1.327987	-3.131644
H	-3.382909	1.325357	3.127571
H	-1.810926	1.572257	2.334966
H	-2.701940	-2.078773	1.741498
H	-3.170738	-1.153979	3.184802
H	-1.538321	-0.991607	2.490983
H	-1.361092	-1.734766	-2.452099
H	-1.971009	-0.230297	-3.159433
H	-4.074795	-2.916123	-1.621987
H	-2.696968	-2.898583	-0.504887
H	-0.002560	-1.650795	-0.035961
H	-2.834336	-1.751000	-3.455510
H	4.277151	-2.193193	0.013630
H	-3.276921	2.252605	1.620217
H	2.741266	-2.086026	-1.750190
H	-4.027312	-0.394744	-1.699850
H	2.008892	4.530997	0.789555
H	0.007351	5.774665	0.012772
H	-1.998873	4.543930	-0.772591
C	-0.004505	-4.100129	0.076141
O	-0.866512	-4.107821	0.862783
O	0.857496	-4.176086	-0.706825

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4,Ni-(H)-formate el energy= -1154.89952994

Ni	-0.000078	-0.177776	-0.000295
P	-2.167233	0.007665	-0.245441
P	2.167234	0.005289	0.245196
C	-2.513298	-0.965766	2.335447
C	0.000874	1.754116	0.000275
C	1.105897	2.477845	0.507851
C	2.286434	1.689137	1.040750
C	-2.256254	-1.452615	-2.603699
C	-3.592149	-2.422379	-0.679178
C	-2.284821	1.692057	-1.040076
C	3.124109	-1.139823	1.374695
C	3.589399	-2.426498	0.678254
C	2.253797	-1.456274	2.602756
C	3.095187	0.091472	-1.382938
C	3.024934	1.485113	-2.023026
C	-3.094535	0.093999	1.383074
C	-3.022942	1.487295	2.023750
C	-3.125760	-1.135847	-1.375148

C	0.002285	4.575953	0.001141
C	2.513412	-0.967384	-2.335987
C	1.102923	3.877626	0.502777
C	-1.103437	2.479262	-0.506827
C	-1.099059	3.879034	-0.500903
H	-4.285235	-2.217223	0.144829
H	4.009849	-0.568309	1.695022
H	4.145817	-0.145502	-1.159779
H	-4.145440	-0.142012	1.160194
H	3.251238	2.181603	0.863305
H	2.201607	1.533082	2.125549
H	-2.200254	1.536509	-2.124968
H	-3.249107	2.185404	-0.862261
H	2.745446	-2.997313	0.277518
H	4.114459	-3.062104	1.403276
H	1.376077	-2.047258	2.316711
H	2.832394	-2.038025	3.332158
H	1.899115	-0.548357	3.107062
H	1.502400	-0.671351	-2.643441
H	3.136005	-1.043055	-3.237556
H	3.505896	2.256491	-1.411848
H	1.985947	1.789646	-2.190650
H	3.533791	1.462464	-2.995733
H	-3.531586	1.464645	2.996569
H	-1.983661	1.790880	2.191255
H	-2.424485	-1.957621	1.884159
H	-3.135693	-1.041416	3.237154
H	-1.501981	-0.670629	2.642768
H	-1.379025	-2.044630	-2.318271
H	-1.900843	-0.544826	-3.107720
H	-4.118192	-3.057039	-1.404315
H	-2.748644	-2.994306	-0.279086
H	-0.000842	-1.782367	-0.000698
H	-2.835730	-2.033436	-3.333143
H	4.283043	-2.221657	-0.145363
H	-3.503406	2.259345	1.413026
H	2.423738	-1.959392	-1.885215
H	-4.011005	-0.563218	-1.694851
H	1.960051	4.425502	0.892437
H	0.002832	5.663993	0.001468
H	-1.955649	4.428007	-0.890205
C	-0.001603	-3.106677	-0.001203
O	-0.677669	-3.493117	0.929048
O	0.674064	-3.493207	-0.931696

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4,Ni-(0)-formate-isomer el energy= -1154.92624289

Ni	0.009868	-0.236002	-0.053286
P	2.089542	0.502173	0.229537
P	-2.167433	-0.551729	-0.208093
C	3.049683	-0.476993	-2.209437
C	-0.471478	1.645079	-0.080032
C	-1.735189	2.078181	-0.556054
C	-2.729792	1.028209	-1.012416
C	2.287928	-0.807326	2.654769
C	4.047998	-1.466608	0.962697
C	1.763824	2.191559	0.941157
C	-2.928098	-1.944193	-1.195427
C	-2.737671	-3.296183	-0.490523
C	-2.324213	-1.969205	-2.607701
C	-2.964123	-0.639512	1.492616
C	-3.223567	0.748409	2.094916
C	3.103967	0.777472	-1.322053
C	2.601106	2.000160	-2.104305
C	3.187120	-0.318843	1.506152
C	-1.158555	4.396083	-0.139772
C	-2.054923	-1.462683	2.422636
C	-2.070011	3.436857	-0.583163
C	0.427665	2.637634	0.385689
C	0.086397	3.994625	0.346794
H	4.725791	-1.133086	0.167786
H	-4.004616	-1.720915	-1.267140
H	-3.926202	-1.157673	1.363151
H	4.140109	0.956465	-0.996757
H	-3.769444	1.291608	-0.779100
H	-2.674301	0.875607	-2.098707
H	1.711209	2.066658	2.032076
H	2.575162	2.903983	0.742473
H	-1.677687	-3.481790	-0.288649
H	-3.115773	-4.104319	-1.130104
H	-1.244064	-2.149467	-2.562847
H	-2.777289	-2.778855	-3.194302
H	-2.490055	-1.032140	-3.151883
H	-1.120382	-0.920162	2.608944
H	-2.555526	-1.628703	3.385886
H	-3.932473	1.338480	1.504109
H	-2.294367	1.322975	2.175438
H	-3.642223	0.634010	3.103531
H	3.174808	2.099728	-3.035195
H	1.542821	1.887648	-2.367771

H	3.331881	-1.393782	-1.684768
H	3.719765	-0.354082	-3.070658
H	2.031429	-0.619047	-2.592477
H	1.626159	-1.598870	2.287536
H	1.668026	-0.002432	3.071973
H	4.669765	-1.861082	1.777814
H	3.432208	-2.289782	0.582913
H	2.905184	-1.208525	3.469377
H	-3.281501	-3.344000	0.459502
H	2.705714	2.934729	-1.543561
H	-1.777983	-2.433155	2.001284
H	3.849889	0.483279	1.869528
H	-3.047469	3.746568	-0.951199
H	-1.420197	5.451812	-0.166499
H	0.795225	4.740990	0.703624
O	0.504098	-2.107792	0.138767
O	1.979617	-3.642820	-0.576652
C	1.086117	-2.829317	-0.766019
H	0.706891	-2.673199	-1.806838

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4,Ni-(O)-formate el energy= -1154.93588671

Ni	-0.014431	-0.288663	0.159327
P	2.097558	0.431257	0.234171
P	-2.176785	-0.554201	-0.169373
C	2.896153	-0.325361	-2.374158
C	-0.422625	1.600813	-0.004078
C	-1.650388	2.056851	-0.544404
C	-2.623480	1.017719	-1.063224
C	2.701625	-0.873890	2.608186
C	4.167418	-1.498532	0.629873
C	1.803515	2.085723	1.047367
C	-2.762454	-1.933934	-1.288755
C	-2.849396	-3.286308	-0.568402
C	-1.822300	-2.013812	-2.504501
C	-3.218227	-0.601039	1.390511
C	-3.378263	0.801229	1.997880
C	2.952717	0.851645	-1.388903
C	2.361739	2.107088	-2.049105
C	3.390642	-0.373428	1.327477
C	-1.057657	4.359495	-0.070831
C	-2.568873	-1.545633	2.416485
C	-1.960251	3.421215	-0.575464
C	0.476574	2.570850	0.501391
C	0.158299	3.933596	0.466435

H	4.783325	-1.117008	-0.192243
H	-3.770468	-1.643787	-1.626063
H	-4.209765	-0.985413	1.105594
H	4.000893	1.057064	-1.118836
H	-3.674904	1.305234	-0.933655
H	-2.471549	0.831157	-2.135172
H	1.748895	1.907061	2.130066
H	2.623435	2.797167	0.879552
H	-1.887369	-3.548942	-0.117106
H	-3.115711	-4.070795	-1.288793
H	-0.802532	-2.276767	-2.200688
H	-2.183725	-2.781274	-3.201905
H	-1.775105	-1.065683	-3.054234
H	-1.583383	-1.165623	2.708445
H	-3.199160	-1.607068	3.313843
H	-3.908481	1.492765	1.335123
H	-2.401455	1.242564	2.226351
H	-3.947369	0.729275	2.934135
H	2.894937	2.299221	-2.989705
H	1.300998	1.965485	-2.282978
H	3.302757	-1.251746	-1.966570
H	3.455315	-0.062750	-3.282843
H	1.859297	-0.541520	-2.650259
H	1.953907	-1.637279	2.368851
H	2.190397	-0.064493	3.144506
H	4.839994	-1.981209	1.351555
H	3.496680	-2.260642	0.220994
H	3.445540	-1.306072	3.290715
H	-3.611906	-3.285422	0.218787
H	2.446845	3.002352	-1.425698
H	-2.416967	-2.556415	2.030320
H	4.098021	0.430136	1.588169
H	-2.910765	3.752546	-0.992181
H	-1.301671	5.419535	-0.096217
H	0.864437	4.665296	0.857508
O	0.219427	-2.161060	0.692042
O	1.413947	-2.747466	-1.132506
C	0.892061	-2.975843	-0.041555
H	0.980424	-3.988549	0.414032

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4,TS-2-3 el energy= -1154.89890440

Ni	-0.000164	-0.177918	-0.000294
P	2.166377	0.008123	0.137315
P	-2.166354	0.011913	-0.137439

C	2.471572	-1.049330	-2.424401
C	0.001406	1.769341	0.001176
C	-1.131826	2.499239	-0.431833
C	-2.344053	1.712158	-0.892678
C	2.372460	-1.398942	2.516566
C	3.634011	-2.403621	0.563603
C	2.346908	1.707183	0.894593
C	-3.189011	-1.097595	-1.247295
C	-3.637386	-2.397229	-0.566161
C	-2.375303	-1.391879	-2.518379
C	-3.024735	0.076561	1.530347
C	-2.839335	1.437996	2.216523
C	3.025016	0.073267	-1.530313
C	2.841252	1.435619	-2.215119
C	3.187060	-1.104244	1.246148
C	0.003709	4.595884	0.003014
C	-2.472610	-1.047616	2.423272
C	-1.128293	3.899006	-0.426254
C	1.135856	2.496816	0.435045
C	1.134591	3.896596	0.431318
H	4.292825	-2.214844	-0.291684
H	-4.082936	-0.512663	-1.515732
H	-4.097098	-0.087370	1.345340
H	4.097171	-0.092130	-1.345394
H	-3.297383	2.194880	-0.639345
H	-2.336785	1.576372	-1.983695
H	2.339757	1.570069	1.985447
H	3.300940	2.188682	0.641570
H	-2.782165	-2.982980	-0.213435
H	-4.194594	-3.013691	-1.283884
H	-1.481904	-1.979290	-2.276395
H	-2.981848	-1.965958	-3.231218
H	-2.045976	-0.474668	-3.022668
H	-1.416430	-0.858176	2.650556
H	-3.028144	-1.080426	3.370270
H	-3.289602	2.261587	1.652483
H	-1.776528	1.668237	2.350066
H	-3.310657	1.411923	3.207979
H	3.312428	1.409952	-3.206654
H	1.778717	1.667318	-2.348307
H	2.519964	-2.036949	-1.959387
H	3.026681	-1.081389	-3.371675
H	1.415446	-0.858767	-2.650986
H	1.478506	-1.985090	2.273600
H	2.043947	-0.481875	3.021652

H	4.190120	-3.021694	1.280793
H	2.778173	-2.987830	0.209810
H	-0.001592	-1.746933	-0.002011
H	2.978050	-1.974433	3.229079
H	-4.295600	-2.208658	0.289633
H	3.292602	2.258084	-1.650300
H	-2.521597	-2.034611	1.956981
H	4.081657	-0.520847	1.515682
H	-2.007638	4.449139	-0.759911
H	0.004594	5.684071	0.003738
H	2.014852	4.444858	0.765638
C	-0.002468	-3.324287	-0.002514
O	0.622119	-3.610889	-0.977506
O	-0.627367	-3.610982	0.972256

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4,TS-3-4i el energy= -1154.89652029

Ni	0.080721	-0.002373	0.077286
P	0.042985	-2.199589	-0.111344
P	-0.067342	2.204683	-0.135268
C	-2.629937	-2.342781	0.775212
C	-0.043493	-0.033288	-1.844319
C	-0.465568	1.101578	-2.575042
C	-0.889207	2.329415	-1.802182
C	2.398175	-2.784584	1.284142
C	0.240466	-3.557644	2.365315
C	0.841305	-2.387694	-1.780819
C	-1.152381	3.277528	0.955641
C	-0.463579	3.801835	2.222261
C	-2.440957	2.508245	1.292550
C	1.599010	3.047906	-0.268684
C	2.244139	2.833836	-1.645327
C	-1.677511	-2.944443	-0.270646
C	-2.271434	-2.775336	-1.676867
C	0.984612	-3.334152	1.039808
C	-0.042851	-0.047450	-4.669308
C	2.513803	2.508920	0.845640
C	-0.463135	1.088124	-3.974638
C	0.389786	-1.172336	-2.565025
C	0.383720	-1.173994	-3.964791
H	-0.700043	-4.100202	2.219135
H	-1.401437	4.136674	0.310775
H	1.421878	4.123020	-0.117562
H	-1.544790	-4.019433	-0.072599
H	-0.652298	3.267444	-2.320513

H	-1.972597	2.329117	-1.618948
H	1.928393	-2.374567	-1.624485
H	0.597298	-3.336035	-2.276510
H	-0.164333	2.983117	2.883835
H	-1.165585	4.446876	2.767240
H	-2.220633	1.632318	1.912378
H	-3.127695	3.163447	1.844396
H	-2.965644	2.162878	0.392326
H	2.792683	1.471010	0.622845
H	3.433681	3.106285	0.896466
H	1.662331	3.279258	-2.459621
H	2.360118	1.765855	-1.862713
H	3.241727	3.292420	-1.654946
H	-3.269444	-3.232489	-1.698244
H	-2.378789	-1.716621	-1.935255
H	-2.239510	-2.387991	1.792951
H	-3.591851	-2.871698	0.736251
H	-2.806441	-1.283471	0.559663
H	2.358424	-1.837975	1.834757
H	2.949128	-2.610287	0.352000
H	0.866815	-4.153821	3.041569
H	0.008467	-2.605877	2.854739
H	2.975638	-3.500690	1.882941
H	0.423397	4.402975	1.989501
H	-1.669365	-3.251892	-2.457298
H	2.042225	2.499557	1.832644
H	1.061589	-4.293860	0.503717
H	-0.787526	1.971066	-4.523689
H	-0.044164	-0.052722	-5.757164
H	0.714870	-2.059670	-4.505364
O	-0.987081	-0.305488	2.503142
O	0.722338	0.978159	3.315976
C	0.136064	0.222738	2.550492
H	0.865832	-0.104829	1.622579

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4,TS-4i-4 el energy= -1154.92511976

Ni	-0.045763	0.100843	0.062921
P	0.011060	-2.136249	-0.079792
P	-0.021124	2.284246	-0.223483
C	-2.502287	-2.564674	1.052394
C	-0.023189	0.055133	-1.875951
C	-0.388077	1.189028	-2.646275
C	-0.766156	2.462885	-1.916616
C	2.304263	-2.315458	1.463139

C	0.476287	-3.930412	2.148059
C	0.766752	-2.326845	-1.771393
C	-1.027525	3.391314	0.896091
C	-0.335865	3.641806	2.243648
C	-2.410658	2.754713	1.105044
C	1.713090	2.997957	-0.291937
C	2.371935	2.777281	-1.661404
C	-1.662446	-2.973015	-0.169028
C	-2.398849	-2.613083	-1.467712
C	1.145059	-3.201149	0.976855
C	-0.022775	-0.027915	-4.711703
C	2.563366	2.352466	0.816572
C	-0.384851	1.143211	-4.045230
C	0.354689	-1.116335	-2.576896
C	0.347375	-1.154593	-3.976045
H	-0.349853	-4.573204	1.820788
H	-1.141113	4.347840	0.361270
H	1.621609	4.079107	-0.107688
H	-1.480621	-4.057834	-0.147105
H	-0.445775	3.371763	-2.442052
H	-1.854353	2.537089	-1.783852
H	1.855841	-2.345855	-1.619093
H	0.495580	-3.278102	-2.249215
H	-0.131908	2.690925	2.746124
H	-0.991281	4.242997	2.887603
H	-2.304341	1.792053	1.616778
H	-3.036504	3.409357	1.725470
H	-2.942099	2.582952	0.161154
H	2.692062	1.282276	0.615941
H	3.555956	2.821335	0.846529
H	1.842129	3.288121	-2.472455
H	2.414845	1.710889	-1.909438
H	3.399597	3.163073	-1.636545
H	-3.391512	-3.082784	-1.467285
H	-2.534757	-1.528661	-1.552918
H	-1.995855	-2.753592	2.003002
H	-3.454246	-3.112027	1.053789
H	-2.728732	-1.491888	1.007768
H	1.926608	-1.574995	2.175571
H	2.791275	-1.781913	0.635258
H	1.220638	-4.575173	2.634827
H	0.112389	-3.216755	2.892184
H	3.065305	-2.932252	1.959563
H	0.607074	4.188268	2.129095
H	-1.866310	-2.949371	-2.363403

H	2.108919	2.436613	1.807214
H	1.529183	-3.954514	0.270580
H	-0.666930	2.027340	-4.615811
H	-0.024657	-0.061112	-5.799181
H	0.636090	-2.069099	-4.492911
O	-0.006835	0.296503	1.993233
O	-0.251476	-1.196768	3.662407
C	-0.668209	-0.318051	2.919143
H	-1.721040	0.040300	3.046404

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5,Ni-H el energy= -1127.20989380

Ni	7.585196	5.743055	0.795373
P	5.682730	6.489004	0.062163
H	6.964971	5.170026	2.100308
C	8.414801	6.652031	-0.774069
H	8.640212	7.629708	-0.293309
P	9.573529	5.004652	1.258927
C	7.484462	6.934977	-1.968154
H	7.305002	5.978448	-2.481497
C	8.145753	7.878762	-2.989044
H	7.486584	8.047351	-3.854671
H	8.299241	8.860305	-2.511874
C	9.497988	7.324177	-3.462587
H	9.980038	8.032589	-4.150783
H	9.323153	6.401974	-4.039000
C	10.432888	7.005657	-2.285801
H	10.706350	7.941362	-1.771640
H	11.369724	6.565178	-2.660696
C	9.750900	6.069750	-1.271295
H	9.526540	5.130322	-1.798392
C	6.134977	7.472586	-1.468689
H	5.351874	7.468665	-2.238196
H	6.262693	8.515353	-1.149718
C	10.660908	5.744990	-0.077136
H	11.066899	6.681707	0.326762
H	11.519421	5.113834	-0.341698
C	4.493789	5.124431	-0.528206
C	5.199584	4.419376	-1.704365
H	5.276085	5.063141	-2.587255
H	4.622695	3.528639	-1.989816
H	6.209929	4.096393	-1.425699
C	3.127911	5.644276	-0.999656
H	3.224745	6.430767	-1.758373
H	2.532652	6.038893	-0.169668

H	2.555932	4.819677	-1.449337
C	4.312071	4.090182	0.598334
H	5.282492	3.731930	0.956536
H	3.734478	3.236021	0.216346
H	3.774359	4.499094	1.458160
C	4.816318	7.748354	1.194883
C	5.968802	8.587408	1.786425
H	6.548258	9.104162	1.011533
H	6.656962	7.950696	2.352878
H	5.558267	9.351057	2.462470
C	3.834339	8.678750	0.463351
H	4.318096	9.228707	-0.351779
H	3.441675	9.421908	1.172320
H	2.979858	8.138550	0.046027
C	4.104402	7.028063	2.351111
H	3.197631	6.511927	2.016496
H	3.801285	7.764751	3.108812
H	4.768630	6.298072	2.827710
C	10.317763	5.650517	2.886418
C	11.854726	5.619268	2.929600
H	12.301277	6.182607	2.102459
H	12.252418	4.600950	2.898424
H	12.201150	6.081180	3.865405
C	9.737001	4.881216	4.083667
H	8.644446	4.821961	4.020103
H	10.000533	5.402356	5.015157
H	10.140483	3.864841	4.152846
C	9.835095	7.113911	2.973808
H	10.182557	7.718514	2.127059
H	10.221395	7.574133	3.894515
H	8.740757	7.157772	2.992028
C	9.754890	3.117041	1.090994
C	8.671205	2.427505	1.940649
H	8.825646	2.573254	3.013289
H	8.689230	1.346013	1.742733
H	7.678481	2.817837	1.694692
C	9.471439	2.788701	-0.389037
H	10.258399	3.160943	-1.053789
H	8.515410	3.216028	-0.714895
H	9.418145	1.698060	-0.512973
C	11.145405	2.585066	1.467167
H	11.341414	2.677976	2.540427
H	11.946347	3.102706	0.924824
H	11.211309	1.516956	1.213908

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5,Ni+ el energy= -1126.43952841

Ni	0.000053	0.110206	0.042509
P	2.242244	0.163659	0.021942
C	0.000037	1.981373	-0.455549
H	-0.000001	1.828958	-1.550366
P	-2.242138	0.163661	0.022019
C	1.265394	2.729665	-0.016127
H	1.226750	2.833759	1.076331
C	1.265136	4.152813	-0.615495
H	2.163121	4.690176	-0.281341
H	1.331781	4.074698	-1.711576
C	0.000053	4.925743	-0.226724
H	0.000037	5.913778	-0.703248
H	0.000094	5.102239	0.859127
C	-1.265064	4.152821	-0.615401
H	-1.331790	4.074709	-1.711479
H	-2.163021	4.690188	-0.281181
C	-1.265289	2.729668	-0.016041
H	-1.226577	2.833753	1.076415
C	2.535217	1.951997	-0.389412
H	3.431174	2.353384	0.097528
H	2.701560	2.016941	-1.471281
C	-2.535140	1.952012	-0.389255
H	-2.701566	2.016991	-1.471109
H	-3.431061	2.353383	0.097765
C	2.970299	-0.178132	1.738515
C	2.477827	0.957552	2.658208
H	2.920588	1.925247	2.398915
H	2.766670	0.729652	3.692278
H	1.385015	1.055969	2.631320
C	4.504974	-0.228082	1.761867
H	4.953541	0.677168	1.335340
H	4.897326	-1.095477	1.221951
H	4.849348	-0.307380	2.801669
C	2.376071	-1.503288	2.256164
H	1.278164	-1.467409	2.271974
H	2.714593	-1.675886	3.286096
H	2.680490	-2.367333	1.659562
C	3.065373	-0.827929	-1.370307
C	2.164738	-0.623556	-2.607174
H	2.073049	0.430892	-2.893106
H	1.155108	-1.016533	-2.439019
H	2.597794	-1.158365	-3.462359
C	4.487711	-0.334725	-1.689031

H	4.505511	0.726236	-1.962603
H	4.878251	-0.898678	-2.546594
H	5.178597	-0.483452	-0.855371
C	3.085009	-2.325324	-1.019919
H	3.787116	-2.552424	-0.211627
H	3.403390	-2.898707	-1.900159
H	2.091741	-2.692275	-0.729619
C	-3.065346	-0.827882	-1.370211
C	-4.487759	-0.334765	-1.688729
H	-4.505672	0.726212	-1.962231
H	-5.178528	-0.483597	-0.854989
H	-4.878364	-0.898693	-2.546278
C	-3.084829	-2.325302	-1.019916
H	-2.091492	-2.692209	-0.729798
H	-3.403315	-2.898650	-1.900142
H	-3.786792	-2.552497	-0.211525
C	-2.164865	-0.623354	-2.607164
H	-2.073291	0.431121	-2.893034
H	-2.597976	-1.158139	-3.462337
H	-1.155185	-1.016263	-2.439151
C	-2.970101	-0.178198	1.738614
C	-2.375920	-1.503425	2.256133
H	-2.680428	-2.367409	1.659486
H	-2.714388	-1.676077	3.286073
H	-1.278009	-1.467614	2.271877
C	-2.477504	0.957400	2.658348
H	-2.920229	1.925137	2.399147
H	-1.384688	1.055758	2.631391
H	-2.766290	0.729449	3.692422
C	-4.504777	-0.228063	1.762051
H	-4.897207	-1.095385	1.222073
H	-4.953317	0.677251	1.335632
H	-4.849099	-0.307439	2.801864

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5,Ni-H+CO2 el energy= -1315.80179121

Ni	-0.000130	-0.108038	-0.052948
P	2.171131	0.041382	0.014348
C	-0.000092	1.845948	-0.466923
H	0.000145	1.766271	-1.576451
P	-2.171395	0.041648	0.014941
C	1.259045	2.634610	-0.061989
H	1.226260	2.770320	1.029256
C	1.272772	4.040284	-0.690585
H	2.161800	4.605446	-0.370659

H	1.341398	3.934615	-1.785442
C	-0.000088	4.820965	-0.330880
H	0.000077	5.800625	-0.828848
H	-0.000407	5.023237	0.751890
C	-1.272770	4.040305	-0.691284
H	-1.340812	3.934540	-1.786167
H	-2.161962	4.605497	-0.371869
C	-1.259304	2.634740	-0.062484
H	-1.226717	2.770718	1.028726
C	2.520631	1.832482	-0.408660
H	3.430824	2.223611	0.064708
H	2.682332	1.874385	-1.493679
C	-2.520810	1.832514	-0.409110
H	-2.682281	1.873819	-1.494189
H	-3.431114	2.223874	0.063873
C	2.895529	-0.236378	1.753501
C	2.306909	0.873150	2.648386
H	2.698219	1.863057	2.390196
H	2.573335	0.671645	3.695273
H	1.213341	0.905953	2.575114
C	4.428650	-0.164825	1.810983
H	4.814934	0.765616	1.376617
H	4.897852	-1.007060	1.292059
H	4.758733	-0.201855	2.859293
C	2.403014	-1.590808	2.297218
H	1.313389	-1.667493	2.224678
H	2.697533	-1.686113	3.352227
H	2.829882	-2.439213	1.755503
C	3.119738	-0.942946	-1.308737
C	2.227246	-0.855584	-2.564888
H	2.065562	0.181494	-2.884246
H	1.249522	-1.310899	-2.382562
H	2.709690	-1.389817	-3.395873
C	4.510798	-0.373208	-1.635931
H	4.458952	0.664018	-1.985101
H	4.964312	-0.967252	-2.442465
H	5.189571	-0.408243	-0.778932
C	3.245127	-2.417941	-0.894454
H	4.011176	-2.561663	-0.124316
H	3.535447	-3.021957	-1.765512
H	2.298000	-2.805641	-0.507641
C	-3.120342	-0.943446	-1.307362
C	-4.511524	-0.374052	-1.634521
H	-4.459910	0.663172	-1.983736
H	-5.190244	-0.409196	-0.777487

H	-4.964953	-0.968239	-2.440995
C	-3.245232	-2.418273	-0.892270
H	-2.297746	-2.805475	-0.505812
H	-3.535852	-3.022810	-1.762870
H	-4.010820	-2.561804	-0.121653
C	-2.228174	-0.856648	-2.563800
H	-2.066858	0.180252	-2.883905
H	-2.710688	-1.391570	-3.394302
H	-1.250294	-1.311612	-2.381434
C	-2.895410	-0.235040	1.754410
C	-2.402055	-1.588889	2.298874
H	-2.828057	-2.437879	1.757401
H	-2.696761	-1.683944	3.353853
H	-1.312353	-1.664749	2.226625
C	-2.307269	0.875275	2.648617
H	-2.699248	1.864819	2.390040
H	-1.213738	0.908721	2.575156
H	-2.573374	0.674086	3.695647
C	-4.428548	-0.164205	1.812122
H	-4.897458	-1.007078	1.293976
H	-4.815350	0.765697	1.377057
H	-4.758408	-0.200535	2.860522
H	0.000043	-1.647842	0.131926
C	-0.000484	-3.974826	-1.112428
O	0.000246	-3.556661	-2.202461
O	-0.001158	-4.451808	-0.048988

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5,Ni-(H)-formate el energy= -1315.80091636

Ni	-0.000211	-0.126816	-0.024059
P	2.219368	-0.012424	-0.020569
C	-0.000221	1.790882	-0.471105
H	-0.000766	1.712428	-1.577140
P	-2.219492	-0.011925	-0.018349
C	1.258718	2.562064	-0.038888
H	1.228373	2.657514	1.055710
C	1.266721	3.988606	-0.620523
H	2.161995	4.532874	-0.285040
H	1.330421	3.920635	-1.718401
C	0.000191	4.759778	-0.228149
H	0.000065	5.755427	-0.692154
H	0.000731	4.922900	0.860837
C	-1.266882	3.988863	-0.619292
H	-1.331667	3.920896	-1.717107
H	-2.161713	4.533326	-0.282944

C	-1.258587	2.562332	-0.037640
H	-1.227110	2.657808	1.056922
C	2.517445	1.783249	-0.428270
H	3.432170	2.180448	0.029032
H	2.648764	1.844757	-1.515573
C	-2.517905	1.783771	-0.425666
H	-2.650426	1.845305	-1.512827
H	-3.432052	2.181094	0.032677
C	2.979594	-0.307849	1.694862
C	2.380052	0.761780	2.629726
H	2.736033	1.769928	2.390279
H	2.677353	0.540459	3.663823
H	1.283844	0.761814	2.586957
C	4.511307	-0.190713	1.712036
H	4.858904	0.765478	1.301254
H	4.990243	-1.000126	1.152231
H	4.869028	-0.253741	2.749546
C	2.540239	-1.690502	2.210717
H	1.452286	-1.801827	2.216396
H	2.904667	-1.819239	3.239786
H	2.941415	-2.512077	1.612608
C	3.134737	-0.958642	-1.398361
C	2.173134	-0.913624	-2.605704
H	1.885585	0.111775	-2.872183
H	1.267920	-1.492449	-2.396193
H	2.670359	-1.356519	-3.480204
C	4.475178	-0.299117	-1.772556
H	4.353211	0.730733	-2.124543
H	4.932390	-0.870890	-2.592057
H	5.185133	-0.292190	-0.939810
C	3.380637	-2.431234	-1.030293
H	4.105074	-2.540261	-0.216553
H	3.796223	-2.944945	-1.908489
H	2.456059	-2.948222	-0.763815
C	-3.136223	-0.958207	-1.395164
C	-4.477003	-0.298596	-1.767951
H	-4.355334	0.731287	-2.119946
H	-5.186090	-0.291735	-0.934459
H	-4.935066	-0.870271	-2.587044
C	-3.381782	-2.430793	-1.026859
H	-2.456869	-2.947801	-0.761581
H	-3.798435	-2.944434	-1.904586
H	-4.105242	-2.539878	-0.212260
C	-2.175814	-0.913246	-2.603458
H	-1.888368	0.112129	-2.870160

H	-2.673959	-1.356018	-3.477498
H	-1.270471	-1.492231	-2.394893
C	-2.977799	-0.307463	1.697897
C	-2.538066	-1.690204	2.213209
H	-2.939847	-2.511708	1.615408
H	-2.901546	-1.819005	3.242603
H	-1.450101	-1.801549	2.217872
C	-2.377138	0.762037	2.632198
H	-2.733177	1.770251	2.393123
H	-1.280974	0.761872	2.588352
H	-2.673463	0.540745	3.666581
C	-4.509496	-0.190134	1.716692
H	-4.989110	-0.999427	1.157286
H	-4.857401	0.766139	1.306364
H	-4.866137	-0.253227	2.754568
H	-0.002216	-1.725087	0.310078
C	0.000140	-2.972536	0.046457
O	-0.000565	-3.171236	-1.162114
O	0.001996	-3.585986	1.096514

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5,Ni-(O)-formate-isomer el energy= -1315.82514537

Ni	-0.026785	-0.182035	-0.067278
P	2.202496	0.083187	-0.033269
C	-0.116713	1.765150	-0.388084
H	-0.096593	1.705907	-1.497566
P	-2.254755	-0.119448	-0.049361
C	1.101903	2.595963	0.057170
H	1.082420	2.655334	1.154643
C	1.040923	4.038780	-0.479617
H	1.906582	4.614031	-0.118808
H	1.118390	4.008005	-1.578410
C	-0.264192	4.737117	-0.083214
H	-0.303123	5.748086	-0.511216
H	-0.293033	4.859319	1.010824
C	-1.480280	3.918933	-0.530787
H	-1.509444	3.877654	-1.631576
H	-2.410614	4.409905	-0.208257
C	-1.420864	2.480843	0.015835
H	-1.434451	2.552433	1.112327
C	2.396425	1.902294	-0.378033
H	3.295239	2.336157	0.077781
H	2.504160	2.011444	-1.464380
C	-2.633337	1.659866	-0.436930
H	-2.730605	1.739167	-1.527214

H	-3.579607	2.007493	-0.003784
C	3.021521	-0.210094	1.656625
C	2.440199	0.836733	2.627583
H	2.779498	1.852491	2.396603
H	2.769751	0.599881	3.648696
H	1.343266	0.826814	2.615962
C	4.551137	-0.069181	1.626357
H	4.868261	0.895816	1.211985
H	5.025427	-0.866002	1.045913
H	4.941733	-0.132291	2.652160
C	2.618494	-1.602914	2.172589
H	1.536660	-1.655690	2.331900
H	3.110665	-1.787687	3.137991
H	2.890852	-2.413853	1.493243
C	3.146318	-0.777204	-1.447942
C	2.165852	-0.746003	-2.639765
H	1.842950	0.273118	-2.890593
H	1.281689	-1.349299	-2.414821
H	2.660424	-1.165522	-3.527084
C	4.443379	-0.038416	-1.827193
H	4.264898	0.998530	-2.132534
H	4.905328	-0.554131	-2.680659
H	5.174468	-0.032195	-1.013241
C	3.467194	-2.246894	-1.127860
H	4.201078	-2.342459	-0.319795
H	3.915338	-2.704226	-2.021950
H	2.578002	-2.831237	-0.871751
C	-3.064493	-1.114197	-1.453820
C	-4.452724	-0.583973	-1.852075
H	-4.422698	0.466842	-2.161963
H	-5.185753	-0.679297	-1.045976
H	-4.824520	-1.165861	-2.707265
C	-3.149095	-2.606620	-1.093324
H	-2.173955	-2.986981	-0.777035
H	-3.461650	-3.172234	-1.982314
H	-3.886306	-2.802849	-0.307083
C	-2.094653	-0.963738	-2.646156
H	-1.922944	0.086222	-2.915889
H	-2.522175	-1.465805	-3.525425
H	-1.130228	-1.426270	-2.416553
C	-3.065298	-0.464652	1.636473
C	-2.508997	-1.784350	2.198058
H	-2.730109	-2.645245	1.562446
H	-2.949135	-1.972477	3.187506
H	-1.422183	-1.727023	2.313346

C -2.627811 0.666492 2.588271
H -3.073595 1.630853 2.321710
H -1.536972 0.779730 2.600452
H -2.953504 0.420650 3.608396
C -4.599869 -0.509296 1.582873
H -4.965955 -1.375539 1.023173
H -5.023824 0.396628 1.132436
H -4.997461 -0.586996 2.604932
O 0.094437 -2.115109 -0.297718
O 0.975356 -4.142064 0.077078
C 0.338901 -3.156120 0.427209
H -0.089075 -3.126727 1.457403

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5,Ni-(0)-formate el energy= -1315.83780414
Ni -0.006184 -0.191682 0.105423
P 2.234087 0.064936 0.026215
C -0.100435 1.716410 -0.419412
H -0.086307 1.643953 -1.525394
P -2.259188 -0.168571 -0.015989
C 1.109545 2.564203 0.021134
H 1.076554 2.640567 1.117855
C 1.045702 3.998095 -0.537183
H 1.912455 4.580006 -0.189361
H 1.117145 3.950861 -1.635808
C -0.258019 4.698986 -0.141356
H -0.305977 5.701925 -0.587269
H -0.275596 4.840971 0.950550
C -1.474473 3.867135 -0.560731
H -1.520146 3.813831 -1.660453
H -2.403199 4.355740 -0.229682
C -1.399775 2.433793 -0.002355
H -1.395384 2.512049 1.094722
C 2.411904 1.872853 -0.383005
H 3.302551 2.330695 0.064972
H 2.526059 1.948326 -1.471110
C -2.615690 1.611607 -0.430144
H -2.716664 1.675959 -1.520260
H -3.557209 1.974240 0.000665
C 3.110354 -0.167284 1.700781
C 2.447958 0.835875 2.667353
H 2.683245 1.875201 2.412889
H 2.816858 0.651167 3.685651
H 1.356928 0.720368 2.676521
C 4.621234 0.105245 1.645719

H	4.854592	1.085290	1.211941
H	5.151669	-0.660379	1.070452
H	5.030390	0.089879	2.666168
C	2.850093	-1.586192	2.241495
H	1.780804	-1.812156	2.266508
H	3.257632	-1.657367	3.260276
H	3.338189	-2.355671	1.636674
C	3.158972	-0.806930	-1.397276
C	2.162229	-0.797287	-2.575747
H	1.824018	0.216822	-2.825156
H	1.289587	-1.414970	-2.343059
H	2.654244	-1.211186	-3.467516
C	4.449549	-0.072021	-1.805451
H	4.262450	0.955735	-2.133860
H	4.904377	-0.605326	-2.652065
H	5.189045	-0.041958	-0.999850
C	3.498650	-2.267279	-1.057865
H	4.262890	-2.341676	-0.276891
H	3.902660	-2.751728	-1.957992
H	2.613437	-2.832198	-0.757128
C	-3.061847	-1.130070	-1.455874
C	-4.413767	-0.532415	-1.888854
H	-4.328168	0.509647	-2.214292
H	-5.167449	-0.580342	-1.097388
H	-4.794744	-1.108896	-2.743582
C	-3.254702	-2.618120	-1.121663
H	-2.321517	-3.088566	-0.803798
H	-3.589316	-3.140838	-2.028827
H	-4.021698	-2.772170	-0.355175
C	-2.049516	-1.015870	-2.615399
H	-1.813758	0.028105	-2.859400
H	-2.479062	-1.477724	-3.515858
H	-1.121997	-1.539872	-2.365779
C	-3.138015	-0.492128	1.641973
C	-2.742168	-1.876935	2.188820
H	-3.136423	-2.692290	1.575705
H	-3.159109	-1.991011	3.199866
H	-1.655868	-1.990824	2.234047
C	-2.601578	0.573352	2.619909
H	-2.938516	1.582934	2.360042
H	-1.504821	0.571584	2.649783
H	-2.968494	0.350374	3.631239
C	-4.667695	-0.377749	1.558201
H	-5.104907	-1.193686	0.973764
H	-4.993239	0.573238	1.119164

H	-5.092206	-0.436506	2.570771
O	0.082073	-2.016764	0.815748
O	0.157445	-3.113428	-1.159560
C	0.143109	-3.060958	0.072848
H	0.186374	-4.005273	0.661354

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5,TS-2-3 el energy= -1315.79764107

Ni	0.001259	-0.400184	-0.017875
P	2.196238	-0.264009	-0.002049
C	-0.000106	1.538702	-0.464716
H	-0.000013	1.466921	-1.573234
P	-2.194077	-0.267194	-0.002694
C	1.257806	2.319727	-0.045340
H	1.229453	2.430183	1.048435
C	1.268120	3.738505	-0.644156
H	2.159800	4.292948	-0.314207
H	1.334121	3.656505	-1.741142
C	-0.002209	4.512208	-0.265079
H	-0.002862	5.502104	-0.741887
H	-0.002465	4.690345	0.821767
C	-1.271321	3.736668	-0.644454
H	-1.336836	3.654432	-1.741451
H	-2.163904	4.289874	-0.314869
C	-1.259137	2.317971	-0.045475
H	-1.231037	2.428592	1.048291
C	2.514699	1.530063	-0.422988
H	3.432773	1.925135	0.030445
H	2.647340	1.580625	-1.511088
C	-2.514873	1.526556	-0.423284
H	-2.647456	1.577171	-1.511391
H	-3.433571	1.920239	0.030084
C	2.959559	-0.545545	1.716460
C	2.363403	0.536512	2.639462
H	2.725409	1.539693	2.389354
H	2.656539	0.325194	3.677084
H	1.267631	0.542753	2.591321
C	4.491537	-0.434792	1.738801
H	4.843130	0.515773	1.318715
H	4.970988	-1.251132	1.189303
H	4.846380	-0.487366	2.778094
C	2.510103	-1.918782	2.248171
H	1.420530	-2.012889	2.238202
H	2.862496	-2.037229	3.282775
H	2.913397	-2.750014	1.664140

C	3.130137	-1.221011	-1.361585
C	2.176624	-1.195106	-2.575305
H	1.904675	-0.172820	-2.867212
H	1.256642	-1.746563	-2.356909
H	2.667761	-1.669265	-3.436954
C	4.471142	-0.567671	-1.743371
H	4.347564	0.456007	-2.111770
H	4.934686	-1.151087	-2.551455
H	5.176714	-0.544252	-0.907245
C	3.378869	-2.686475	-0.971445
H	4.113910	-2.781976	-0.165665
H	3.776744	-3.223720	-1.843829
H	2.458037	-3.191557	-0.672402
C	-3.126397	-1.225114	-1.362657
C	-4.468163	-0.573498	-1.744710
H	-4.345934	0.450585	-2.112422
H	-5.174171	-0.551643	-0.908908
H	-4.930453	-1.157107	-2.553373
C	-3.373304	-2.690951	-0.972759
H	-2.451827	-3.194921	-0.673781
H	-3.770518	-3.228560	-1.845221
H	-4.108224	-2.787487	-0.166996
C	-2.172602	-1.197777	-2.576121
H	-1.902044	-0.175077	-2.867882
H	-2.662835	-1.672567	-3.437937
H	-1.251881	-1.747923	-2.357533
C	-2.957628	-0.549837	1.715563
C	-2.506877	-1.922637	2.247244
H	-2.909990	-2.754263	1.663634
H	-2.858513	-2.041151	3.282098
H	-1.417250	-2.015948	2.236661
C	-2.362786	0.532726	2.638831
H	-2.725864	1.535548	2.388837
H	-1.267014	0.540193	2.590812
H	-2.655813	0.320919	3.676382
C	-4.489720	-0.440701	1.737510
H	-4.968144	-1.257438	1.187704
H	-4.842225	0.509571	1.317528
H	-4.844800	-0.493883	2.776693
H	0.003223	-1.943975	0.259370
C	0.003721	-3.630484	0.042202
O	0.003740	-3.752834	-1.140622
O	0.003866	-4.007721	1.166001

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5,TS-3-4i el energy= -1315.79794206

Ni	0.007674	-0.458776	-0.038954
P	2.251484	-0.318093	-0.010065
C	0.013948	1.457330	-0.487588
H	0.057473	1.374923	-1.590985
P	-2.240362	-0.324804	-0.020858
C	1.247411	2.237706	0.003737
H	1.171522	2.317581	1.097808
C	1.268212	3.670441	-0.565718
H	2.144801	4.214104	-0.183490
H	1.387374	3.608905	-1.659277
C	-0.017781	4.435768	-0.236618
H	-0.000417	5.430335	-0.702509
H	-0.073816	4.600359	0.850598
C	-1.254284	3.651813	-0.689324
H	-1.265466	3.578513	-1.788480
H	-2.171538	4.184655	-0.398281
C	-1.258530	2.230051	-0.096642
H	-1.250967	2.338984	0.996012
C	2.534343	1.490699	-0.345300
H	3.415662	1.889400	0.171469
H	2.722471	1.591400	-1.420694
C	-2.509949	1.452286	-0.500413
H	-2.610548	1.477205	-1.592494
H	-3.431872	1.874107	-0.081369
C	3.031812	-0.648991	1.695990
C	2.402385	0.375806	2.661396
H	2.728490	1.400365	2.450402
H	2.705887	0.135182	3.689449
H	1.306607	0.345018	2.615868
C	4.559889	-0.483596	1.704821
H	4.880254	0.475644	1.280709
H	5.058024	-1.287830	1.154254
H	4.922023	-0.523645	2.741880
C	2.663164	-2.058904	2.194617
H	1.583544	-2.175717	2.322835
H	3.137467	-2.223707	3.172228
H	3.003438	-2.850420	1.522032
C	3.192247	-1.182128	-1.425534
C	2.286145	-1.011367	-2.664134
H	2.098188	0.044450	-2.898778
H	1.330157	-1.517232	-2.509685
H	2.786300	-1.456922	-3.535457
C	4.565632	-0.545012	-1.708575
H	4.495772	0.522318	-1.945581

H	5.006526	-1.043256	-2.583249
H	5.265347	-0.664034	-0.876999
C	3.370449	-2.684013	-1.148011
H	4.071401	-2.869243	-0.326346
H	3.789293	-3.160573	-2.045604
H	2.412019	-3.162804	-0.932481
C	-3.184968	-1.308117	-1.354679
C	-4.531275	-0.653883	-1.720596
H	-4.412367	0.370391	-2.090516
H	-5.234391	-0.634710	-0.883450
H	-4.994858	-1.238706	-2.527242
C	-3.428328	-2.767544	-0.931314
H	-2.516677	-3.277558	-0.610377
H	-3.829403	-3.317543	-1.794208
H	-4.170082	-2.840181	-0.128143
C	-2.261678	-1.293433	-2.591791
H	-2.008710	-0.272775	-2.908153
H	-2.782073	-1.777576	-3.430184
H	-1.337341	-1.840885	-2.388015
C	-3.021900	-0.524441	1.705399
C	-2.614022	-1.881312	2.306963
H	-2.933975	-2.734472	1.706362
H	-3.069950	-1.976006	3.302785
H	-1.529989	-1.963924	2.421654
C	-2.431700	0.584206	2.599318
H	-2.791408	1.580553	2.319501
H	-1.335328	0.586882	2.564022
H	-2.735399	0.401853	3.639233
C	-4.553279	-0.394121	1.694538
H	-5.031963	-1.240030	1.191983
H	-4.890240	0.531606	1.212143
H	-4.920564	-0.378701	2.730493
O	0.134432	-2.723556	-1.015715
O	-0.550830	-3.915899	0.803258
C	-0.124796	-2.946036	0.192240
H	0.080055	-2.012035	0.902572

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5,TS-4i-4 el energy= -1315.82375589

Ni	-0.889012	1.740216	-0.028135
P	1.362100	1.860145	-0.032584
C	-0.863813	3.676134	-0.411199
H	-0.844418	3.621688	-1.519750
P	-3.111851	1.930904	-0.051505
C	0.397127	4.432905	0.046334

H	0.372538	4.488662	1.143931
C	0.425302	5.878739	-0.485325
H	1.322870	6.398741	-0.118752
H	0.505924	5.846993	-1.583874
C	-0.836508	6.653478	-0.091835
H	-0.814323	7.665265	-0.519167
H	-0.861098	6.776344	1.002187
C	-2.097152	5.908551	-0.543106
H	-2.127869	5.872056	-1.644034
H	-2.998002	6.451273	-0.219916
C	-2.122939	4.467945	-0.000488
H	-2.125941	4.536719	1.096435
C	1.648461	3.666520	-0.384522
H	2.571043	4.052009	0.067197
H	1.759024	3.766226	-1.471123
C	-3.387226	3.725869	-0.446332
H	-3.483101	3.808193	-1.536447
H	-4.307023	4.135609	-0.010619
C	2.179352	1.533246	1.651308
C	1.635208	2.596030	2.626672
H	2.006031	3.601098	2.397109
H	1.960044	2.346193	3.646192
H	0.538355	2.621230	2.618514
C	3.712412	1.626799	1.613713
H	4.056939	2.587269	1.210688
H	4.158895	0.824220	1.019512
H	4.106792	1.538048	2.636167
C	1.732544	0.152185	2.163168
H	0.647565	0.130179	2.307643
H	2.209460	-0.044369	3.133970
H	1.988396	-0.664649	1.485246
C	2.266327	0.968569	-1.457016
C	1.259366	1.000326	-2.626084
H	0.937966	2.020361	-2.875225
H	0.371641	0.409019	-2.379911
H	1.726942	0.569053	-3.522345
C	3.566055	1.683930	-1.871846
H	3.396926	2.709162	-2.218096
H	4.019668	1.130061	-2.705567
H	4.300524	1.715194	-1.060994
C	2.577129	-0.499414	-1.127638
H	3.344154	-0.592699	-0.350415
H	2.978005	-0.979067	-2.032630
H	1.687113	-1.058501	-0.819194
C	-3.958019	0.977375	-1.464004

C	-5.302193	1.595440	-1.887461
H	-5.197929	2.636089	-2.214587
H	-6.047464	1.564291	-1.087269
H	-5.704732	1.025185	-2.736597
C	-4.152195	-0.503316	-1.098073
H	-3.218475	-0.940299	-0.734715
H	-4.466956	-1.055163	-1.994996
H	-4.931599	-0.640982	-0.340577
C	-2.961502	1.058633	-2.640201
H	-2.720887	2.094138	-2.912949
H	-3.401615	0.575758	-3.523987
H	-2.028443	0.543913	-2.391279
C	-3.948565	1.624319	1.627969
C	-3.508165	0.257170	2.181755
H	-3.852491	-0.577199	1.566308
H	-3.926553	0.128902	3.190158
H	-2.418707	0.192650	2.241381
C	-3.421201	2.709839	2.587954
H	-3.782036	3.710150	2.324794
H	-2.324630	2.729592	2.604540
H	-3.771045	2.487833	3.605426
C	-5.481642	1.707353	1.568285
H	-5.914013	0.880497	0.996135
H	-5.828829	2.650230	1.127756
H	-5.889343	1.649264	2.587662
O	-1.076514	-0.198639	0.079529
O	0.116204	-2.114145	0.059066
C	-0.712839	-1.345843	0.534249
H	-1.262903	-1.659910	1.456589

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6, Pd-H el energy= -1081.04288702

H	0.000000	0.000000	2.239116
C	0.000000	0.000000	-1.513399
C	-0.254203	1.184821	-2.241447
C	-0.574791	2.461118	-1.484617
C	-0.246402	1.182974	-3.642431
H	-0.443492	2.103520	-4.192033
C	0.000000	0.000000	-4.342382
H	0.000000	0.000000	-5.430691
C	0.246402	-1.182974	-3.642431
H	0.443492	-2.103520	-4.192033
C	0.254203	-1.184821	-2.241447
C	0.574791	-2.461118	-1.484617
P	-0.003725	2.287135	0.295043

P	0.003725	-2.287135	0.295043
C	-1.259055	3.298946	1.296255
C	-2.526075	2.418346	1.345821
C	-1.610141	4.657575	0.665558
C	-0.746160	3.491683	2.732495
C	1.746376	3.026914	0.327801
C	1.780627	4.551475	0.145094
C	2.425623	2.631505	1.652622
C	2.522366	2.357226	-0.825665
C	-1.746376	-3.026914	0.327801
C	-2.522366	-2.357226	-0.825665
C	-2.425623	-2.631505	1.652622
C	-1.780627	-4.551475	0.145094
C	1.259055	-3.298946	1.296255
C	1.610141	-4.657575	0.665558
C	2.526075	-2.418346	1.345821
C	0.746160	-3.491683	2.732495
H	-0.156669	3.355708	-1.965503
H	-1.662207	2.611712	-1.448121
H	1.662207	-2.611712	-1.448121
H	0.156669	-3.355708	-1.965503
H	-3.303009	2.932409	1.929184
H	-2.935012	2.224032	0.346475
H	-2.311192	1.452741	1.816482
H	-0.754799	5.337897	0.631803
H	-1.998545	4.548891	-0.353584
H	-2.394445	5.142146	1.264346
H	0.086290	4.202665	2.778994
H	-1.555952	3.891997	3.358479
H	-0.419354	2.539092	3.165761
H	2.824193	4.883765	0.050130
H	1.250529	4.871669	-0.760439
H	1.347625	5.077731	1.002335
H	1.956982	3.104340	2.520844
H	2.385649	1.546890	1.800651
H	3.478894	2.945211	1.627825
H	2.125342	2.626105	-1.810231
H	2.494645	1.265602	-0.745049
H	3.570614	2.684519	-0.782550
H	-3.570614	-2.684519	-0.782550
H	-2.494645	-1.265602	-0.745049
H	-2.125342	-2.626105	-1.810231
H	-1.956982	-3.104340	2.520844
H	-3.478894	-2.945211	1.627825
H	-2.385649	-1.546890	1.800651

H	-2.824193	-4.883765	0.050130
H	-1.250529	-4.871669	-0.760439
H	-1.347625	-5.077731	1.002335
H	2.394445	-5.142146	1.264346
H	0.754799	-5.337897	0.631803
H	1.998545	-4.548891	-0.353584
H	2.311192	-1.452741	1.816482
H	3.303009	-2.932409	1.929184
H	2.935012	-2.224032	0.346475
H	1.555952	-3.891997	3.358479
H	0.419354	-2.539092	3.165761
H	-0.086290	-4.202665	2.778994
Pd	0.000000	0.000000	0.587703

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6, Pd+ el energy= -1080.26595234

C	0.000000	0.000000	-1.479709
C	0.129596	1.219946	-2.171539
C	0.251346	2.530272	-1.428791
C	0.133409	1.199607	-3.572732
H	0.240296	2.136248	-4.116335
C	0.000000	0.000000	-4.270017
H	0.000000	0.000000	-5.356826
C	-0.133409	-1.199607	-3.572732
H	-0.240296	-2.136248	-4.116335
C	-0.129596	-1.219946	-2.171539
C	-0.251346	-2.530272	-1.428791
P	0.862319	2.185279	0.295795
P	-0.862319	-2.185279	0.295795
C	0.066889	3.502513	1.400169
C	-1.414237	3.087375	1.534980
C	0.148289	4.911973	0.786870
C	0.714181	3.487365	2.795482
C	2.754306	2.241300	0.237212
C	3.305645	3.670029	0.106476
C	3.299155	1.562292	1.509002
C	3.193623	1.406948	-0.983446
C	-2.754306	-2.241300	0.237212
C	-3.193623	-1.406948	-0.983446
C	-3.299155	-1.562292	1.509002
C	-3.305645	-3.670029	0.106476
C	-0.066889	-3.502513	1.400169
C	-0.148289	-4.911973	0.786870
C	1.414237	-3.087375	1.534980
C	-0.714181	-3.487365	2.795482

H	0.888676	3.247828	-1.958589
H	-0.735551	2.999071	-1.326957
H	0.735551	-2.999071	-1.326957
H	-0.888676	-3.247828	-1.958589
H	-1.944943	3.834927	2.138632
H	-1.924600	3.023342	0.566629
H	-1.518519	2.116001	2.035066
H	1.177674	5.263019	0.678818
H	-0.337301	4.964409	-0.194146
H	-0.374176	5.617996	1.445896
H	1.740770	3.866406	2.780509
H	0.135675	4.133837	3.467819
H	0.723380	2.480982	3.233862
H	4.393825	3.623007	-0.031518
H	2.888995	4.196551	-0.760658
H	3.116553	4.271593	1.001042
H	3.035625	2.100404	2.423991
H	2.930526	0.532052	1.595219
H	4.394621	1.520438	1.453688
H	2.882420	1.854136	-1.933223
H	2.799133	0.385858	-0.944584
H	4.289620	1.347913	-0.987478
H	-4.289620	-1.347913	-0.987478
H	-2.799133	-0.385858	-0.944584
H	-2.882420	-1.854136	-1.933223
H	-3.035625	-2.100404	2.423991
H	-4.394621	-1.520438	1.453688
H	-2.930526	-0.532052	1.595219
H	-4.393825	-3.623007	-0.031518
H	-2.888995	-4.196551	-0.760658
H	-3.116553	-4.271593	1.001042
H	0.374176	-5.617996	1.445896
H	-1.177674	-5.263019	0.678818
H	0.337301	-4.964409	-0.194146
H	1.518519	-2.116001	2.035066
H	1.944943	-3.834927	2.138632
H	1.924600	-3.023342	0.566629
H	-0.135675	-4.133837	3.467819
H	-0.723380	-2.480982	3.233862
H	-1.740770	-3.866406	2.780509
Pd	0.000000	0.000000	0.537232

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6,Pd-H+CO2 el energy= -1269.63551232

H	0.047899	1.839523	0.167934

C	0.012374	-1.906706	-0.022123
C	1.188776	-2.634496	-0.314472
C	2.471144	-1.881869	-0.616022
C	1.175550	-4.034812	-0.360508
H	2.090406	-4.582404	-0.587235
C	-0.009687	-4.735507	-0.129915
H	-0.018471	-5.822892	-0.173099
C	-1.183059	-4.036365	0.159269
H	-2.105551	-4.585450	0.348318
C	-1.173348	-2.636909	0.222668
C	-2.436089	-1.889487	0.606823
P	2.312416	-0.111549	-0.016075
P	-2.266709	-0.082722	0.131176
C	3.297698	0.897733	-1.284818
C	2.405686	0.925427	-2.544506
C	4.662280	0.285542	-1.645954
C	3.476223	2.338224	-0.779089
C	3.087253	-0.103549	1.719052
C	4.610784	-0.296356	1.722082
C	2.715584	1.216094	2.421214
C	2.422602	-1.261817	2.492438
C	-3.059222	0.049634	-1.590789
C	-2.430729	-1.068471	-2.448346
C	-2.666425	1.402999	-2.212710
C	-4.586530	-0.111889	-1.585187
C	-3.246241	0.840070	1.471152
C	-4.579990	0.165573	1.838123
C	-2.319280	0.841938	2.705510
C	-3.489926	2.296172	1.045336
H	3.358951	-2.376069	-0.199020
H	2.630192	-1.832243	-1.701298
H	-2.561887	-1.911315	1.697595
H	-3.343489	-2.342085	0.184795
H	2.902834	1.517207	-3.325831
H	2.230882	-0.078914	-2.949716
H	1.436014	1.382993	-2.330038
H	5.355969	0.276077	-0.801040
H	4.566940	-0.740455	-2.019669
H	5.123475	0.882587	-2.445442
H	4.196443	2.396159	0.044843
H	3.856244	2.967499	-1.595697
H	2.522325	2.759125	-0.443285
H	4.961040	-0.415955	2.757170
H	4.916713	-1.191229	1.166141
H	5.133423	0.567931	1.298807

H	3.180672	2.086299	1.948108
H	1.631206	1.370143	2.411467
H	3.057056	1.179805	3.465461
H	2.679458	-2.243394	2.080053
H	1.331025	-1.174071	2.482305
H	2.765836	-1.233181	3.536025
H	-2.779805	-0.958140	-3.484582
H	-1.337261	-1.010447	-2.441516
H	-2.711661	-2.069103	-2.103057
H	-3.059651	2.254409	-1.648816
H	-3.066661	1.463208	-3.234719
H	-1.577124	1.501980	-2.263042
H	-4.952875	-0.145457	-2.621082
H	-4.901476	-1.041659	-1.095625
H	-5.087340	0.725741	-1.088600
H	-4.441128	-0.865285	2.182807
H	-5.050479	0.723975	2.659776
H	-5.286165	0.152253	1.003357
H	-1.376024	1.352738	2.483475
H	-2.818390	1.364507	3.533697
H	-2.081562	-0.173188	3.047628
H	-3.892637	2.860479	1.898267
H	-2.562830	2.783352	0.728214
H	-4.220758	2.369976	0.232050
C	-0.383264	3.960043	-1.273733
O	0.311676	3.603548	-2.140392
O	-1.088744	4.377875	-0.444406
Pd	0.025901	0.192624	0.066073

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6,Pd-(H)-formate el energy= -1269.62867829

H	0.152854	2.012693	0.170810
C	0.000931	-1.858506	0.004691
C	1.165395	-2.591355	-0.313989
C	2.441743	-1.859337	-0.670365
C	1.131488	-3.991787	-0.333569
H	2.034203	-4.550090	-0.578674
C	-0.052254	-4.674980	-0.053952
H	-0.073163	-5.762364	-0.077447
C	-1.208985	-3.959480	0.257419
H	-2.132203	-4.492691	0.480925
C	-1.188996	-2.559401	0.297905
C	-2.432601	-1.794080	0.694236
P	2.338034	-0.099052	-0.047871
P	-2.299878	-0.023159	0.104233

C	3.292662	0.923399	-1.326606
C	2.341682	1.037216	-2.539004
C	4.608490	0.250692	-1.757983
C	3.571797	2.339682	-0.796369
C	3.125367	-0.100889	1.676794
C	4.651986	-0.270805	1.651832
C	2.739192	1.211431	2.386757
C	2.493326	-1.274278	2.453330
C	-3.037720	0.005584	-1.641625
C	-2.329335	-1.102129	-2.447832
C	-2.706501	1.363506	-2.292154
C	-4.553182	-0.250162	-1.657172
C	-3.314149	0.975853	1.363700
C	-4.562347	0.209292	1.840278
C	-2.351447	1.209911	2.548009
C	-3.736099	2.345586	0.805488
H	3.339365	-2.374535	-0.305033
H	2.542012	-1.795685	-1.761608
H	-2.497531	-1.742864	1.789001
H	-3.354062	-2.279797	0.348859
H	2.871630	1.543854	-3.357700
H	2.020219	0.056183	-2.912271
H	1.458083	1.633496	-2.288555
H	5.322251	0.153811	-0.934811
H	4.445114	-0.744068	-2.188117
H	5.081439	0.867042	-2.534848
H	4.287537	2.339703	0.033015
H	4.008026	2.938976	-1.607074
H	2.650854	2.841738	-0.485742
H	5.021967	-0.372812	2.681575
H	4.958165	-1.169722	1.102327
H	5.155567	0.593572	1.207283
H	3.150190	2.095419	1.890952
H	1.650557	1.329591	2.430500
H	3.125462	1.192848	3.415288
H	2.763040	-2.249296	2.033039
H	1.400355	-1.206610	2.465422
H	2.852792	-1.243845	3.491001
H	-2.688034	-1.063560	-3.485533
H	-1.243344	-0.962034	-2.453662
H	-2.534176	-2.104507	-2.056564
H	-3.222680	2.197782	-1.810158
H	-3.019800	1.341299	-3.345210
H	-1.632458	1.577751	-2.261354
H	-4.899698	-0.307045	-2.698498

H	-4.815712	-1.199106	-1.172631
H	-5.114496	0.552416	-1.168979
H	-4.311224	-0.728005	2.348644
H	-5.105687	0.834878	2.561689
H	-5.250241	-0.020606	1.020061
H	-1.531684	1.872452	2.250096
H	-2.900645	1.691109	3.369330
H	-1.928852	0.272512	2.933698
H	-4.200191	2.920974	1.618677
H	-2.879125	2.924670	0.451648
H	-4.479024	2.256391	0.006045
C	-0.154833	3.215055	-0.219492
O	0.274453	3.413208	-1.342270
O	-0.760769	3.770690	0.677950
Pd	0.033381	0.202395	0.059970

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6,Pd-(0)-formate-isomer el energy= -1269.64645852

P	-2.343812	-0.037083	0.109851
P	2.294875	0.128398	-0.069019
O	0.215004	-2.297671	0.529001
O	0.939611	-4.149245	-0.518995
C	-3.220912	-1.057751	1.444935
C	-2.229314	-1.097063	2.628984
C	-3.437100	-2.499333	0.955088
C	-4.552447	-0.439046	1.903809
C	-3.186934	-0.122090	-1.589901
C	-2.771727	-1.431438	-2.285407
C	-4.717742	-0.018926	-1.510572
C	-2.640108	1.054409	-2.424231
C	-2.508895	1.740085	0.654167
C	-1.291182	2.504052	0.176721
C	-1.337657	3.900345	0.081711
C	-0.207229	4.621683	-0.302190
C	0.977933	3.944378	-0.589858
C	1.037763	2.547136	-0.512633
C	-0.103378	1.801225	-0.135368
C	2.330053	1.830343	-0.839833
C	3.333647	-0.952725	-1.231659
C	2.419765	-1.256609	-2.437909
C	4.596340	-0.220406	-1.724517
C	3.725507	-2.280368	-0.559717
C	3.046098	0.301046	1.662476
C	2.285737	1.448223	2.359524
C	2.779818	-1.002470	2.442586

C	4.547740	0.624874	1.648507
C	0.142210	-3.234782	-0.362258
H	-1.308793	-1.617779	2.345724
H	-2.694989	-1.634681	3.466829
H	-1.966813	-0.093001	2.986490
H	-4.188895	-2.561704	0.160805
H	-3.793972	-3.112565	1.793973
H	-2.500835	-2.938784	0.596806
H	-4.968514	-1.049800	2.717179
H	-5.297910	-0.403414	1.104237
H	-4.421663	0.576945	2.294264
H	-1.681895	-1.497706	-2.375643
H	-3.200476	-1.455825	-3.296889
H	-3.119537	-2.322078	-1.754423
H	-5.043600	0.879092	-0.971281
H	-5.165023	-0.893030	-1.026723
H	-5.130009	0.040466	-2.527579
H	-3.032318	0.969862	-3.447038
H	-1.546411	1.041323	-2.472507
H	-2.944820	2.028581	-2.027723
H	-3.450791	2.196604	0.324203
H	-2.534701	1.725446	1.751912
H	-2.261327	4.426266	0.320485
H	-0.247580	5.706618	-0.370326
H	1.865377	4.505396	-0.880287
H	3.214364	2.407978	-0.541973
H	2.409384	1.674862	-1.923947
H	2.027248	-0.344983	-2.906907
H	1.576475	-1.887995	-2.145539
H	2.998672	-1.799555	-3.197522
H	4.359420	0.694934	-2.278997
H	5.143793	-0.883743	-2.408308
H	5.274886	0.041792	-0.907542
H	4.192105	-2.927216	-1.315770
H	2.861023	-2.820762	-0.160085
H	4.463129	-2.128165	0.235996
H	2.431187	2.414399	1.864160
H	2.654685	1.537251	3.390521
H	1.208980	1.251282	2.394996
H	3.023902	-0.839789	3.501769
H	3.390937	-1.833836	2.082404
H	1.733307	-1.314047	2.363893
H	4.888347	0.806423	2.677597
H	4.772103	1.526634	1.064632
H	5.142121	-0.202722	1.248921

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H          -0.753347       -3.174977       -1.031403
Pd         -0.017696       -0.222626        0.050652

74
6,Pd-(0)-formate    el energy= -1269.65988781
P          -2.332475       -0.064111        0.105694
P           2.310730        0.145154       -0.055828
O           0.102269       -2.378266        0.622654
O           0.020974       -3.043117       -1.539646
C          -3.214504       -1.020678        1.487050
C          -2.229051       -1.006490        2.676312
C          -3.440417       -2.482226        1.067069
C          -4.546932       -0.377973        1.910157
C          -3.164984       -0.226543       -1.591956
C          -2.855236       -1.611600       -2.189243
C          -4.682911        0.005790       -1.539084
C          -2.511019        0.842375       -2.492635
C          -2.520573        1.731628        0.578464
C          -1.297535        2.494523        0.117905
C          -1.359544        3.888453       -0.002264
C          -0.228376        4.621463       -0.359597
C           0.974052        3.956191       -0.595390
C           1.050162        2.561040       -0.494941
C          -0.091324        1.801202       -0.144761
C           2.364483        1.866182       -0.775578
C           3.339810       -0.901239       -1.253133
C           2.453556       -1.079076       -2.505441
C           4.661944       -0.224663       -1.657703
C           3.619253       -2.282141       -0.635401
C           3.058409        0.272955        1.683495
C           2.284733        1.398044        2.402492
C           2.794767       -1.050230        2.430182
C           4.558640        0.601348        1.691736
C           0.069891       -3.245192       -0.324535
H          -1.314928       -1.553961        2.425720
H          -2.704470       -1.491070        3.540930
H          -1.953974        0.012213        2.978530
H          -4.208825       -2.575395        0.292639
H          -3.780559       -3.056455        1.940222
H          -2.513213       -2.937535        0.706392
H          -4.975466       -0.957911        2.739643
H          -5.282946       -0.366710        1.100995
H          -4.415993        0.650380        2.266006
H          -1.785079       -1.842389       -2.166690
H          -3.193981       -1.628282       -3.234911
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H	-3.379126	-2.415797	-1.664085
H	-4.946016	0.961802	-1.069156
H	-5.199902	-0.796802	-1.002710
H	-5.080284	0.022722	-2.563578
H	-2.919208	0.740355	-3.507419
H	-1.425236	0.709310	-2.544494
H	-2.707967	1.864179	-2.150629
H	-3.454250	2.167906	0.201784
H	-2.582766	1.759700	1.674352
H	-2.298535	4.403343	0.197682
H	-0.281974	5.704473	-0.446882
H	1.863609	4.524009	-0.865740
H	3.225354	2.440900	-0.410339
H	2.505775	1.748061	-1.857547
H	2.184441	-0.116409	-2.959344
H	1.534269	-1.628317	-2.276462
H	3.018693	-1.648109	-3.257226
H	4.498314	0.747062	-2.137963
H	5.177711	-0.864659	-2.387189
H	5.339082	-0.077327	-0.811729
H	3.993361	-2.957568	-1.416455
H	2.714153	-2.726681	-0.211238
H	4.382873	-2.228518	0.148954
H	2.429578	2.376671	1.931911
H	2.642813	1.464606	3.439076
H	1.208782	1.194083	2.421029
H	3.024913	-0.912959	3.496003
H	3.422617	-1.865170	2.058661
H	1.750981	-1.368097	2.334842
H	4.885781	0.780674	2.725636
H	4.790084	1.504111	1.112559
H	5.159755	-0.224637	1.298115
H	0.092645	-4.294692	0.051214
Pd	0.003513	-0.233348	0.056144

74

6,TS-2-3	el energy= -1269.62812757		
H	0.054774	1.891388	0.073999
C	0.002063	-1.872604	0.001489
C	1.171646	-2.601925	-0.306500
C	2.440409	-1.856861	-0.667274
C	1.154860	-4.002804	-0.314512
H	2.063308	-4.555529	-0.552361
C	-0.023438	-4.695547	-0.032515
H	-0.033442	-5.783446	-0.046210

C	-1.188792	-3.988541	0.268026
H	-2.106954	-4.530245	0.493540
C	-1.179650	-2.587937	0.294833
C	-2.431976	-1.828347	0.680123
P	2.314611	-0.088803	-0.064220
P	-2.293449	-0.053249	0.099030
C	3.296521	0.915950	-1.338661
C	2.357160	1.037091	-2.558515
C	4.607463	0.229385	-1.762882
C	3.592548	2.329014	-0.810367
C	3.092557	-0.075722	1.666225
C	4.617032	-0.265235	1.656869
C	2.717486	1.248748	2.359000
C	2.440677	-1.231674	2.452801
C	-3.052217	-0.017405	-1.639082
C	-2.367125	-1.139477	-2.446068
C	-2.702508	1.331036	-2.298762
C	-4.571726	-0.245663	-1.646507
C	-3.299774	0.936259	1.370696
C	-4.574967	0.199705	1.821147
C	-2.347646	1.116019	2.572600
C	-3.672116	2.328285	0.834698
H	3.344997	-2.355925	-0.295714
H	2.542644	-1.803389	-1.759161
H	-2.514207	-1.784238	1.774239
H	-3.349079	-2.312015	0.319215
H	2.887963	1.555845	-3.369081
H	2.044504	0.057141	-2.941396
H	1.463542	1.617096	-2.308901
H	5.311392	0.118084	-0.933096
H	4.434543	-0.760938	-2.198844
H	5.097139	0.842758	-2.532017
H	4.320788	2.320742	0.007863
H	4.018768	2.931132	-1.624476
H	2.681413	2.833249	-0.476262
H	4.977690	-0.357366	2.690979
H	4.916003	-1.175822	1.122881
H	5.136143	0.585919	1.204427
H	3.161690	2.119920	1.868891
H	1.631060	1.390510	2.371776
H	3.077255	1.228568	3.397221
H	2.695579	-2.214647	2.042217
H	1.348964	-1.147146	2.458968
H	2.797748	-1.196386	3.491322
H	-2.724826	-1.094576	-3.484026

H	-1.278416	-1.022819	-2.449553
H	-2.592783	-2.136878	-2.053786
H	-3.189518	2.178194	-1.807758
H	-3.034819	1.316876	-3.346177
H	-1.622225	1.512764	-2.284013
H	-4.923820	-0.310925	-2.685598
H	-4.849474	-1.182420	-1.147326
H	-5.116675	0.574111	-1.167744
H	-4.355348	-0.764065	2.293258
H	-5.096651	0.816027	2.566481
H	-5.270382	0.023500	0.994605
H	-1.484679	1.729945	2.294618
H	-2.884775	1.621014	3.387632
H	-1.980928	0.156230	2.959257
H	-4.120972	2.910887	1.651210
H	-2.794349	2.880467	0.489491
H	-4.409838	2.277059	0.027073
C	-0.110973	3.420061	-0.214454
O	0.329437	3.574940	-1.314234
O	-0.609663	3.844204	0.784524
Pd	0.016803	0.204448	0.030831

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6,TS-3-4i el energy= -1269.62403797

H	-0.281090	-2.168701	0.804984
C	-0.084147	1.748233	0.051840
C	1.079325	2.483602	0.369299
C	2.341331	1.763168	0.775898
C	1.057497	3.883772	0.340395
H	1.964071	4.437248	0.580905
C	-0.112449	4.571257	0.019787
H	-0.122262	5.658754	0.004839
C	-1.270342	3.854324	-0.276821
H	-2.188789	4.384517	-0.525041
C	-1.266112	2.453430	-0.268908
C	-2.526164	1.701188	-0.627744
P	2.299249	0.011141	0.135212
P	-2.371352	-0.054647	-0.023023
C	3.375724	-0.954464	1.374353
C	2.443987	-1.279818	2.561652
C	4.567581	-0.108599	1.865063
C	3.898630	-2.274678	0.782956
C	3.042591	0.066879	-1.608729
C	4.526199	0.469033	-1.609441
C	2.853323	-1.308122	-2.280433

C	2.233530	1.110756	-2.405423
C	-3.158064	-0.078457	1.705867
C	-2.558930	1.112285	2.482251
C	-2.746835	-1.376508	2.426154
C	-4.689161	0.048689	1.680049
C	-3.300617	-1.084980	-1.315269
C	-4.677843	-0.493957	-1.666714
C	-2.401731	-1.076167	-2.571619
C	-3.444365	-2.537175	-0.830820
H	3.247379	2.300731	0.470701
H	2.377549	1.681032	1.870039
H	-2.636697	1.648616	-1.718134
H	-3.429798	2.192097	-0.245175
H	3.044199	-1.696194	3.382754
H	1.928147	-0.389257	2.945273
H	1.700052	-2.028199	2.272050
H	5.224810	0.206333	1.048296
H	4.252078	0.784693	2.414908
H	5.166776	-0.719018	2.554324
H	4.652781	-2.105690	0.006960
H	4.382414	-2.843145	1.589615
H	3.090757	-2.897314	0.388263
H	4.871624	0.563208	-2.648382
H	4.696089	1.436016	-1.119278
H	5.156967	-0.280958	-1.122333
H	3.500007	-2.074590	-1.845795
H	1.821209	-1.666007	-2.202144
H	3.113888	-1.218003	-3.344436
H	2.322098	2.121232	-1.992019
H	1.169661	0.852776	-2.435990
H	2.612027	1.131461	-3.436497
H	-2.910815	1.066152	3.521886
H	-1.464346	1.079250	2.487948
H	-2.863060	2.079732	2.068228
H	-3.094935	-2.276025	1.910040
H	-3.180638	-1.379316	3.435644
H	-1.658139	-1.446940	2.523307
H	-5.057710	0.170028	2.708104
H	-5.024913	0.920651	1.105392
H	-5.167197	-0.844337	1.264828
H	-4.608789	0.544837	-2.010732
H	-5.109640	-1.080189	-2.489489
H	-5.382309	-0.531855	-0.831937
H	-1.441114	-1.554808	-2.361499
H	-2.909150	-1.639873	-3.366876

H	-2.225403	-0.061975	-2.952277
H	-3.879564	-3.139422	-1.640019
H	-2.467913	-2.967747	-0.589027
H	-4.110358	-2.622255	0.035181
C	0.280442	-2.893844	0.053447
O	1.013222	-3.701530	0.618534
O	0.004321	-2.673438	-1.150823
Pd	-0.045793	-0.285920	0.073621

74

6,TS-4i-4 el energy= -1269.64636887

P	-2.354489	-0.056854	0.096572
P	2.299390	0.064949	-0.030101
O	0.112673	-2.402888	0.585855
O	1.028701	-4.057256	-0.641935
C	-3.252304	-1.038061	1.446969
C	-2.283413	-1.035231	2.650324
C	-3.450972	-2.495387	0.998867
C	-4.594671	-0.410122	1.859040
C	-3.166657	-0.188863	-1.614381
C	-2.740914	-1.518485	-2.264044
C	-4.698422	-0.081396	-1.567038
C	-2.600432	0.963265	-2.469688
C	-2.523048	1.733933	0.591088
C	-1.285206	2.479450	0.137515
C	-1.316450	3.875559	0.032743
C	-0.170092	4.585687	-0.322509
C	1.016438	3.896872	-0.573338
C	1.062994	2.499516	-0.488471
C	-0.094193	1.765427	-0.137895
C	2.355933	1.773532	-0.786202
C	3.372855	-0.994750	-1.182967
C	2.478558	-1.310621	-2.400879
C	4.629320	-0.236742	-1.653207
C	3.780626	-2.317956	-0.513091
C	3.013644	0.222361	1.718947
C	2.226043	1.350927	2.416168
C	2.746252	-1.096166	2.473832
C	4.511241	0.563860	1.740278
C	0.106981	-3.309453	-0.337719
H	-1.357768	-1.563672	2.400504
H	-2.763730	-1.547181	3.495921
H	-2.029813	-0.019633	2.980552
H	-4.182936	-2.586683	0.188958
H	-3.826200	-3.082547	1.848429

H	-2.501939	-2.937518	0.680045
H	-5.022739	-0.994436	2.685470
H	-5.325308	-0.406838	1.045175
H	-4.476458	0.619666	2.216040
H	-1.649847	-1.591399	-2.329964
H	-3.149255	-1.570037	-3.282886
H	-3.102632	-2.392445	-1.715048
H	-5.033136	0.831310	-1.058600
H	-5.156005	-0.941777	-1.068349
H	-5.091067	-0.049290	-2.592987
H	-2.972272	0.851769	-3.497444
H	-1.505966	0.946177	-2.495934
H	-2.910587	1.948658	-2.106205
H	-3.450035	2.187811	0.218169
H	-2.586322	1.748464	1.687195
H	-2.242258	4.409797	0.242820
H	-0.199431	5.670513	-0.397262
H	1.916454	4.448248	-0.842522
H	3.237187	2.343659	-0.465964
H	2.457897	1.624293	-1.869153
H	2.058189	-0.405630	-2.859068
H	1.659643	-1.979057	-2.121460
H	3.081906	-1.820745	-3.164411
H	4.386109	0.669887	-2.218791
H	5.204274	-0.892846	-2.321109
H	5.285390	0.044151	-0.823896
H	4.281534	-2.944565	-1.264472
H	2.914565	-2.881635	-0.150194
H	4.493972	-2.157390	0.302777
H	2.362936	2.323913	1.931637
H	2.578877	1.435903	3.453153
H	1.152055	1.136623	2.434740
H	2.946802	-0.941825	3.543356
H	3.389593	-1.908764	2.127079
H	1.710620	-1.430525	2.351709
H	4.830563	0.726126	2.779390
H	4.735048	1.481431	1.181319
H	5.123090	-0.247032	1.333071
H	-0.863767	-3.407967	-0.888393
Pd	-0.028614	-0.264069	0.060871

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7,Co-H	el energy= -1115.97621720		
H	0.000000	0.000000	1.936055
C	-0.254474	1.145082	-2.260116

C	-0.578756	2.385560	-1.462752
C	-0.248103	1.170044	-3.652530
H	-0.454124	2.106363	-4.165133
C	0.000000	0.000000	-4.370285
H	0.000000	0.000000	-5.457302
C	0.248103	-1.170044	-3.652530
H	0.454124	-2.106363	-4.165133
C	0.254474	-1.145082	-2.260116
C	0.578756	-2.385560	-1.462752
P	0.034404	2.145412	0.300454
P	-0.034404	-2.145412	0.300454
C	-1.215111	3.144089	1.331241
C	-2.469185	2.246386	1.393598
C	-1.597650	4.512229	0.743810
C	-0.673805	3.310755	2.761034
C	1.761973	2.954905	0.302204
C	1.775009	4.481968	0.154322
C	2.482962	2.533737	1.597206
C	2.517540	2.319605	-0.883567
C	-1.761973	-2.954905	0.302204
C	-2.517540	-2.319605	-0.883567
C	-2.482962	-2.533737	1.597206
C	-1.775009	-4.481968	0.154322
C	1.215111	-3.144089	1.331241
C	1.597650	-4.512229	0.743810
C	2.469185	-2.246386	1.393598
C	0.673805	-3.310755	2.761034
H	-0.212785	3.288454	-1.968154
H	-1.669906	2.485012	-1.392356
H	1.669906	-2.485012	-1.392356
H	0.212785	-3.288454	-1.968154
H	-3.229969	2.722201	2.029671
H	-2.915907	2.091169	0.403197
H	-2.217565	1.263317	1.806134
H	-0.751867	5.204219	0.706394
H	-2.007934	4.424085	-0.269393
H	-2.374981	4.974241	1.369803
H	0.153882	4.027577	2.805644
H	-1.472457	3.689588	3.414737
H	-0.329050	2.350988	3.163429
H	2.810656	4.834118	0.038244
H	1.213918	4.816343	-0.727649
H	1.358630	4.982558	1.034981
H	2.036258	2.984543	2.488608
H	2.446366	1.445640	1.719151

H	3.535236	2.850612	1.553007
H	2.100850	2.616875	-1.852962
H	2.490365	1.225423	-0.823996
H	3.567693	2.643455	-0.859314
H	-3.567693	-2.643455	-0.859314
H	-2.490365	-1.225423	-0.823996
H	-2.100850	-2.616875	-1.852962
H	-2.036258	-2.984543	2.488608
H	-3.535236	-2.850612	1.553007
H	-2.446366	-1.445640	1.719151
H	-2.810656	-4.834118	0.038244
H	-1.213918	-4.816343	-0.727649
H	-1.358630	-4.982558	1.034981
H	2.374981	-4.974241	1.369803
H	0.751867	-5.204219	0.706394
H	2.007934	-4.424085	-0.269393
H	2.217565	-1.263317	1.806134
H	3.229969	-2.722201	2.029671
H	2.915907	-2.091169	0.403197
H	1.472457	-3.689588	3.414737
H	0.329050	-2.350988	3.163429
H	-0.153882	-4.027577	2.805644
N	0.000000	0.000000	-1.550823
Co	0.000000	0.000000	0.389464

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7,Co+	el energy= -1115.21302423		
C	0.121961	1.168594	-2.184248
C	0.223069	2.443117	-1.385880
C	0.132105	1.191203	-3.577482
H	0.234362	2.141971	-4.092355
C	0.000000	0.000000	-4.287113
H	0.000000	0.000000	-5.373875
C	-0.132105	-1.191203	-3.577482
H	-0.234362	-2.141971	-4.092355
C	-0.121961	-1.168594	-2.184248
C	-0.223069	-2.443117	-1.385880
P	0.842078	2.071865	0.340126
P	-0.842078	-2.071865	0.340126
C	0.056834	3.431135	1.408158
C	-1.419755	3.014346	1.580600
C	0.118482	4.829435	0.768981
C	0.725638	3.453331	2.793882
C	2.734184	2.190129	0.233225
C	3.266541	3.617362	0.041269

C	3.322749	1.559622	1.511002
C	3.156326	1.317127	-0.966746
C	-2.734184	-2.190129	0.233225
C	-3.156326	-1.317127	-0.966746
C	-3.322749	-1.559622	1.511002
C	-3.266541	-3.617362	0.041269
C	-0.056834	-3.431135	1.408158
C	-0.118482	-4.829435	0.768981
C	1.419755	-3.014346	1.580600
C	-0.725638	-3.453331	2.793882
H	0.823927	3.189801	-1.917045
H	-0.781390	2.869145	-1.269291
H	0.781390	-2.869145	-1.269291
H	-0.823927	-3.189801	-1.917045
H	-1.941999	3.770433	2.181585
H	-1.949565	2.933299	0.623516
H	-1.510215	2.050038	2.095468
H	1.143377	5.181059	0.626420
H	-0.393257	4.864541	-0.199700
H	-0.388020	5.547514	1.427600
H	1.747176	3.844246	2.753587
H	0.150681	4.107251	3.462304
H	0.754814	2.456593	3.252841
H	4.351665	3.580860	-0.123974
H	2.820444	4.113204	-0.829644
H	3.093299	4.244712	0.921194
H	3.083939	2.130922	2.412566
H	2.957924	0.533720	1.647123
H	4.416575	1.519158	1.425608
H	2.827871	1.733423	-1.925765
H	2.764217	0.296869	-0.880793
H	4.251969	1.256852	-0.993856
H	-4.251969	-1.256852	-0.993856
H	-2.764217	-0.296869	-0.880793
H	-2.827871	-1.733423	-1.925765
H	-3.083939	-2.130922	2.412566
H	-4.416575	-1.519158	1.425608
H	-2.957924	-0.533720	1.647123
H	-4.351665	-3.580860	-0.123974
H	-2.820444	-4.113204	-0.829644
H	-3.093299	-4.244712	0.921194
H	0.388020	-5.547514	1.427600
H	-1.143377	-5.181059	0.626420
H	0.393257	-4.864541	-0.199700
H	1.510215	-2.050038	2.095468

H	1.941999	-3.770433	2.181585
H	1.949565	-2.933299	0.623516
H	-0.150681	-4.107251	3.462304
H	-0.754814	-2.456593	3.252841
H	-1.747176	-3.844246	2.753587
Co	0.000000	0.000000	0.420786
N	0.000000	0.000000	-1.495345

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7,Co-H+CO2 el energy= -1304.56897935

H	-0.023860	1.590881	-0.008343
C	-1.147324	-2.603022	0.354212
C	-2.387570	-1.807109	0.680372
C	-1.165309	-3.995463	0.388278
H	-2.092598	-4.505511	0.636894
C	-0.000625	-4.715017	0.123534
H	0.005540	-5.801548	0.156332
C	1.154539	-3.999696	-0.190686
H	2.084547	-4.513480	-0.420640
C	1.120979	-2.608084	-0.236206
C	2.336435	-1.818644	-0.653390
P	-2.164045	-0.052419	0.043037
P	2.135581	-0.037583	-0.082029
C	-3.172624	0.977840	1.285016
C	-2.281835	1.049662	2.543196
C	-4.537847	0.383135	1.668254
C	-3.354104	2.401494	0.731711
C	-2.979730	-0.075729	-1.682013
C	-4.504142	-0.248729	-1.688405
C	-2.583796	1.221769	-2.413061
C	-2.328453	-1.255946	-2.432693
C	3.064719	0.009873	1.583420
C	2.458512	-1.132921	2.424315
C	2.725010	1.338529	2.284566
C	4.585056	-0.174422	1.492656
C	3.062344	0.937151	-1.432473
C	4.379569	0.295715	-1.900750
C	2.071915	0.995411	-2.614564
C	3.324581	2.375370	-0.957182
H	-3.290328	-2.321126	0.326087
H	-2.480643	-1.724669	1.770946
H	2.368446	-1.783350	-1.750235
H	3.261634	-2.310819	-0.328051
H	-2.768059	1.682477	3.299862
H	-2.124896	0.060597	2.992328

H	-1.302048	1.473215	2.306808
H	-5.228655	0.333978	0.822336
H	-4.442611	-0.625847	2.087028
H	-5.004882	1.011821	2.440333
H	-4.098596	2.435230	-0.071772
H	-3.701958	3.068514	1.532989
H	-2.410560	2.798646	0.341585
H	-4.857227	-0.380193	-2.721830
H	-4.822939	-1.130550	-1.118082
H	-5.017548	0.627810	-1.279229
H	-3.053102	2.107398	-1.973869
H	-1.498519	1.366447	-2.378468
H	-2.899878	1.163123	-3.464790
H	-2.601450	-2.226989	-2.003023
H	-1.235629	-1.173485	-2.417711
H	-2.664400	-1.248675	-3.479269
H	2.855855	-1.080273	3.447828
H	1.366595	-1.047255	2.471337
H	2.703958	-2.123258	2.023201
H	3.155742	2.203305	1.770028
H	3.126591	1.327927	3.308354
H	1.641729	1.484670	2.336606
H	5.008943	-0.258243	2.504200
H	4.859210	-1.085459	0.945613
H	5.072542	0.676714	1.005519
H	4.231213	-0.719355	-2.287353
H	4.804449	0.895028	-2.719072
H	5.128754	0.247979	-1.105435
H	1.131991	1.464583	-2.305184
H	2.513111	1.579065	-3.435739
H	1.835941	-0.002595	-3.005716
H	3.691434	2.976842	-1.801161
H	2.407456	2.845443	-0.588736
H	4.085926	2.417339	-0.170364
C	0.162651	3.906504	0.960447
O	0.028426	3.582872	2.073863
O	0.302739	4.312795	-0.124018
N	-0.014075	-1.895694	0.048941
Co	-0.014411	0.050080	0.021224

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7,Co-(H)-formate el energy= -1304.57153757

H	0.288718	1.745409	0.352048
C	-1.138510	-2.474652	0.252679
C	-2.328900	-1.672117	0.692994

C	-1.206104	-3.866391	0.204717
H	-2.146836	-4.356162	0.440640
C	-0.071777	-4.605545	-0.118925
H	-0.102808	-5.691602	-0.153633
C	1.106515	-3.913629	-0.386399
H	2.022165	-4.442003	-0.637669
C	1.119367	-2.520272	-0.350537
C	2.381330	-1.768403	-0.679462
P	-2.183580	0.100059	0.106498
P	2.237920	-0.001970	-0.084941
C	-3.230692	1.022296	1.409244
C	-2.267669	1.252931	2.593514
C	-4.453358	0.214058	1.883656
C	-3.706708	2.389949	0.888421
C	-3.015797	0.097104	-1.605604
C	-4.512040	-0.245926	-1.582082
C	-2.789421	1.472505	-2.263658
C	-2.262214	-0.958510	-2.440837
C	3.036255	0.003074	1.643430
C	2.354758	-1.138307	2.426193
C	2.666741	1.334115	2.328337
C	4.556834	-0.202187	1.662812
C	3.273547	0.938591	-1.374754
C	4.613386	0.257441	-1.706265
C	2.392855	0.985049	-2.642657
C	3.523904	2.382001	-0.905118
H	-3.265160	-2.168943	0.413457
H	-2.313886	-1.617347	1.789169
H	2.488168	-1.719178	-1.770108
H	3.262981	-2.300126	-0.301754
H	-2.822783	1.706975	3.427082
H	-1.828545	0.314763	2.959748
H	-1.461189	1.932447	2.301219
H	-5.139953	-0.029616	1.066828
H	-4.173876	-0.719448	2.385009
H	-5.010856	0.816268	2.614443
H	-4.471560	2.288601	0.110747
H	-4.162530	2.939742	1.724132
H	-2.876317	2.994553	0.514835
H	-4.885109	-0.320049	-2.613659
H	-4.712137	-1.207976	-1.092989
H	-5.102317	0.524886	-1.076751
H	-3.351143	2.268308	-1.767034
H	-1.732826	1.758990	-2.254189
H	-3.128599	1.428885	-3.308675

H	-2.406982	-1.977262	-2.061277
H	-1.186255	-0.750203	-2.459802
H	-2.636754	-0.932110	-3.473478
H	2.683904	-1.103470	3.473916
H	1.263892	-1.032367	2.404004
H	2.611285	-2.128854	2.031233
H	3.112932	2.199782	1.829588
H	3.028991	1.322585	3.366086
H	1.581258	1.481217	2.342127
H	4.898899	-0.306622	2.702484
H	4.860534	-1.109308	1.124857
H	5.090320	0.649548	1.228669
H	4.481951	-0.769196	-2.068328
H	5.106213	0.821845	-2.510245
H	5.299244	0.232754	-0.855371
H	1.463793	1.528473	-2.446730
H	2.944511	1.507019	-3.437657
H	2.151387	-0.017766	-3.019846
H	4.014861	2.938645	-1.715520
H	2.585230	2.895919	-0.679269
H	4.185096	2.424361	-0.032421
C	-0.134309	2.795561	-0.158169
O	-0.685572	3.465506	0.706778
O	0.163952	2.918104	-1.344304
N	0.005802	-1.791057	-0.042615
Co	0.045628	0.156867	0.021270

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7,Co-(O)-formate-isomer el energy= -1304.59825933

P	-2.199471	-0.159177	0.058123
P	2.217916	0.071005	-0.005947
O	0.316206	-2.027410	0.490666
O	0.444275	-4.220822	0.044899
C	-3.184268	-1.152200	1.355464
C	-2.223052	-1.288076	2.556474
C	-3.508383	-2.561338	0.829855
C	-4.482673	-0.467799	1.818320
C	-3.079309	-0.139580	-1.636490
C	-2.735190	-1.443613	-2.379759
C	-4.601412	0.047757	-1.568831
C	-2.460713	1.027461	-2.433251
C	-2.396710	1.600885	0.670805
C	-1.230643	2.427375	0.201715
C	-1.331101	3.814284	0.112439
C	-0.224482	4.566917	-0.273418

C	0.959458	3.890851	-0.560946
C	1.008273	2.501134	-0.473813
C	2.276231	1.758077	-0.809911
C	3.242484	-1.018487	-1.177118
C	2.317069	-1.304085	-2.378932
C	4.527459	-0.340874	-1.685076
C	3.587302	-2.354832	-0.493808
C	3.057803	0.295535	1.685479
C	2.313989	1.464611	2.364690
C	2.801709	-0.977462	2.517787
C	4.558589	0.611254	1.631617
C	-0.023594	-3.105657	-0.138501
H	-1.302746	-1.804332	2.267752
H	-2.720614	-1.857475	3.354547
H	-1.945360	-0.310968	2.973596
H	-4.251041	-2.541692	0.024705
H	-3.929207	-3.161178	1.648760
H	-2.615958	-3.080528	0.468236
H	-4.953669	-1.084305	2.597133
H	-5.209203	-0.348880	1.009644
H	-4.297426	0.519123	2.257704
H	-1.649831	-1.562815	-2.470533
H	-3.162439	-1.411723	-3.392224
H	-3.130742	-2.332484	-1.879506
H	-4.883106	0.944992	-1.003578
H	-5.103166	-0.813723	-1.116851
H	-5.001981	0.162604	-2.586461
H	-2.833650	0.993858	-3.466403
H	-1.367670	0.953025	-2.460249
H	-2.726092	2.006158	-2.017729
H	-3.349348	2.076440	0.407809
H	-2.363335	1.535789	1.766121
H	-2.275356	4.291523	0.360679
H	-0.281193	5.650160	-0.343284
H	1.852845	4.430235	-0.864100
H	3.159259	2.360458	-0.564404
H	2.305507	1.578132	-1.892642
H	2.010106	-0.385485	-2.895963
H	1.413088	-1.832076	-2.064451
H	2.851610	-1.931143	-3.106303
H	4.319869	0.589063	-2.228584
H	5.038621	-1.018067	-2.384084
H	5.228439	-0.112318	-0.877472
H	3.999283	-3.042545	-1.245738
H	2.708974	-2.831622	-0.047174

H	4.352274	-2.225318	0.280054
H	2.474992	2.420883	1.852474
H	2.680843	1.573811	3.394643
H	1.234993	1.274814	2.402139
H	3.078927	-0.786389	3.564446
H	3.392499	-1.827522	2.166376
H	1.749123	-1.274638	2.475295
H	4.923246	0.838015	2.644047
H	4.777847	1.483001	1.001204
H	5.141051	-0.237412	1.258955
H	-0.812229	-2.960750	-0.916373
N	-0.077645	1.758089	-0.098782
Co	0.022768	-0.179473	0.076850

74

7,Co-(0)-formate el energy= -1304.60880069

P	-2.203969	-0.193600	0.096424
P	2.213952	0.073386	0.038121
O	0.267779	-2.002949	0.846815
O	-0.403832	-3.207097	-0.950165
C	-3.273656	-1.182345	1.324828
C	-2.405503	-1.316889	2.594785
C	-3.559169	-2.586343	0.761577
C	-4.600496	-0.499029	1.700251
C	-2.972440	-0.165230	-1.652446
C	-2.743144	-1.528485	-2.332584
C	-4.464738	0.194760	-1.685649
C	-2.176447	0.894509	-2.443017
C	-2.429133	1.564828	0.710477
C	-1.257237	2.400338	0.275276
C	-1.364920	3.787816	0.192195
C	-0.263814	4.549328	-0.191029
C	0.920673	3.880878	-0.494596
C	0.976330	2.491532	-0.412236
C	2.232913	1.750562	-0.786120
C	3.166378	-1.022026	-1.189256
C	2.164666	-1.322102	-2.325999
C	4.419770	-0.354376	-1.781068
C	3.553519	-2.347402	-0.509841
C	3.162684	0.324523	1.669715
C	2.446542	1.493129	2.379087
C	2.975119	-0.939944	2.532578
C	4.653276	0.655072	1.518527
C	-0.002954	-3.083979	0.208946
H	-1.463678	-1.829389	2.381564

H	-2.963869	-1.883546	3.354002
H	-2.161295	-0.338615	3.029988
H	-4.331879	-2.557239	-0.014571
H	-3.930913	-3.231433	1.570231
H	-2.667380	-3.054079	0.333021
H	-5.135002	-1.128164	2.426565
H	-5.260446	-0.356744	0.840050
H	-4.443184	0.477359	2.173508
H	-1.719678	-1.887667	-2.190542
H	-2.947101	-1.429222	-3.408615
H	-3.413894	-2.299368	-1.942270
H	-4.684756	1.136869	-1.167523
H	-5.083347	-0.593260	-1.244177
H	-4.786654	0.313129	-2.730443
H	-2.515518	0.886340	-3.488161
H	-1.103628	0.672475	-2.426465
H	-2.321954	1.909378	-2.055122
H	-3.374289	2.040695	0.422582
H	-2.428502	1.492749	1.806018
H	-2.313418	4.257352	0.438785
H	-0.327004	5.632656	-0.254330
H	1.806748	4.425513	-0.809649
H	3.124308	2.354891	-0.579851
H	2.220779	1.560477	-1.867278
H	1.820042	-0.405106	-2.822184
H	1.284314	-1.863370	-1.964775
H	2.664630	-1.937537	-3.088145
H	4.178865	0.566161	-2.326108
H	4.888507	-1.041953	-2.499552
H	5.167835	-0.112394	-1.020707
H	3.881210	-3.065083	-1.274559
H	2.707077	-2.786798	0.026230
H	4.381903	-2.216416	0.195549
H	2.568912	2.444880	1.848401
H	2.868904	1.617624	3.385900
H	1.372840	1.293873	2.477614
H	3.302031	-0.729508	3.561029
H	3.569257	-1.781061	2.163203
H	1.926896	-1.256383	2.549830
H	5.079115	0.899803	2.502588
H	4.822721	1.519721	0.863820
H	5.220725	-0.192445	1.120197
H	0.163942	-3.995731	0.828126
N	-0.096790	1.741017	-0.018047
Co	0.031392	-0.188268	0.221487

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7,TS-2-3 el energy= -1304.56595942

H	-0.000015	1.645187	0.000078
C	-1.135940	-2.563943	0.281690
C	-2.366862	-1.775767	0.647343
C	-1.162782	-3.957040	0.274453
H	-2.094664	-4.468116	0.502016
C	0.000094	-4.674357	-0.000169
H	0.000114	-5.761416	-0.000209
C	1.162944	-3.956977	-0.274736
H	2.094845	-4.468003	-0.502336
C	1.136053	-2.563881	-0.281870
C	2.366947	-1.775634	-0.647461
P	-2.166250	-0.001259	0.067424
P	2.166268	-0.001176	-0.067411
C	-3.187589	0.960908	1.358143
C	-2.250743	1.091147	2.577812
C	-4.488047	0.255161	1.782098
C	-3.520778	2.372666	0.848021
C	-2.992347	0.033529	-1.649146
C	-4.510718	-0.187970	-1.651142
C	-2.639874	1.377605	-2.316832
C	-2.311115	-1.089042	-2.459102
C	2.992362	0.033517	1.649162
C	2.311174	-1.089141	2.459034
C	2.639835	1.377530	2.316947
C	4.510742	-0.187921	1.651144
C	3.187569	0.961125	-1.358059
C	4.488061	0.255466	-1.782058
C	2.250723	1.091408	-2.577723
C	3.520692	2.372861	-0.847834
H	-3.277420	-2.277182	0.296408
H	-2.435925	-1.728506	1.741807
H	2.436013	-1.728290	-1.741921
H	3.277522	-2.277041	-0.296558
H	-2.775254	1.621142	3.386135
H	-1.943516	0.111975	2.968009
H	-1.348850	1.653066	2.318118
H	-5.184517	0.122164	0.948970
H	-4.301493	-0.728068	2.228734
H	-4.996093	0.864211	2.543494
H	-4.257710	2.355197	0.037962
H	-3.950622	2.960169	1.671474
H	-2.628174	2.900895	0.503120

H	-4.872021	-0.259916	-2.687414
H	-4.792606	-1.118073	-1.141080
H	-5.048498	0.639079	-1.176091
H	-3.137500	2.225415	-1.836648
H	-1.560650	1.561283	-2.281228
H	-2.957740	1.358454	-3.369298
H	-2.544698	-2.087087	-2.069304
H	-1.221588	-0.968600	-2.453486
H	-2.661032	-1.047685	-3.500178
H	2.661088	-1.047849	3.500113
H	1.221642	-0.968741	2.453427
H	2.544794	-2.087148	2.069161
H	3.137434	2.225394	1.836832
H	2.957693	1.358310	3.369415
H	1.560604	1.561170	2.281349
H	4.872046	-0.259931	2.687411
H	4.792668	-1.117974	1.141013
H	5.048489	0.639186	1.176156
H	4.301551	-0.727740	-2.228762
H	4.996081	0.864591	-2.543412
H	5.184534	0.122443	-0.948938
H	1.348804	1.653269	-2.317995
H	2.775215	1.621482	-3.386006
H	1.943542	0.112249	-2.967990
H	3.950506	2.960446	-1.671245
H	2.628063	2.901022	-0.502892
H	4.257626	2.355369	-0.037778
C	-0.000075	3.404042	0.000102
O	-0.223217	3.630367	1.140067
O	0.223051	3.630420	-1.139855
N	0.000043	-1.855011	-0.000064
Co	0.000008	0.093166	0.000010

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7,TS-3-4i el energy= -1304.57028629

H	-0.204697	-1.778768	0.799672
C	1.031045	2.468875	0.326429
C	2.253485	1.716353	0.764104
C	1.041929	3.860946	0.291208
H	1.962500	4.383111	0.537621
C	-0.117355	4.561545	-0.032720
H	-0.129292	5.647922	-0.058432
C	-1.263503	3.821465	-0.310656
H	-2.199909	4.312091	-0.562846
C	-1.222320	2.429434	-0.285711

C	-2.455779	1.637988	-0.625791
P	2.203511	-0.035237	0.122427
P	-2.259149	-0.121066	-0.038467
C	3.295791	-0.948128	1.395314
C	2.369801	-1.251951	2.592968
C	4.486913	-0.095605	1.873795
C	3.821904	-2.280748	0.833533
C	3.025696	0.047633	-1.591679
C	4.497247	0.484650	-1.567844
C	2.884126	-1.326502	-2.277695
C	2.201987	1.070027	-2.402407
C	-3.056391	-0.132700	1.694733
C	-2.387523	1.020365	2.471902
C	-2.688480	-1.451999	2.400527
C	-4.579207	0.059582	1.709301
C	-3.277037	-1.087871	-1.324831
C	-4.667096	-0.486867	-1.599283
C	-2.448175	-1.049547	-2.627727
C	-3.414321	-2.553630	-0.878299
H	3.167651	2.266968	0.515095
H	2.224089	1.623205	1.857886
H	-2.557654	1.589328	-1.716931
H	-3.356345	2.136531	-0.248037
H	2.973906	-1.654878	3.418537
H	1.857424	-0.354033	2.963687
H	1.619348	-1.999388	2.320341
H	5.148582	0.203011	1.055024
H	4.169468	0.809474	2.404013
H	5.083235	-0.689686	2.580109
H	4.580803	-2.126277	0.058897
H	4.299347	-2.838140	1.651888
H	3.014479	-2.905232	0.440420
H	4.858151	0.600798	-2.599868
H	4.639965	1.448306	-1.061979
H	5.137646	-0.257521	-1.080763
H	3.531832	-2.082527	-1.825658
H	1.855205	-1.697508	-2.229368
H	3.176715	-1.228085	-3.333111
H	2.278387	2.087114	-1.999536
H	1.142714	0.790160	-2.427062
H	2.577477	1.091946	-3.434779
H	-2.707506	0.978514	3.522205
H	-1.295385	0.933315	2.439523
H	-2.664836	2.006202	2.080196
H	-3.091848	-2.331005	1.888710

H	-3.097619	-1.442384	3.420605
H	-1.602528	-1.573936	2.469898
H	-4.918416	0.200469	2.745491
H	-4.895787	0.941034	1.137747
H	-5.104008	-0.815024	1.311769
H	-4.614011	0.567168	-1.897881
H	-5.128692	-1.035384	-2.432335
H	-5.341528	-0.564666	-0.743294
H	-1.458720	-1.484168	-2.469216
H	-2.976308	-1.632378	-3.395677
H	-2.334556	-0.030048	-3.018984
H	-3.888612	-3.131140	-1.684015
H	-2.434201	-2.998698	-0.683217
H	-4.045183	-2.656268	0.011872
C	0.232656	-2.597845	0.040983
O	0.814825	-3.502232	0.633344
O	-0.014472	-2.372714	-1.166538
Co	-0.035671	-0.204033	0.029395
N	-0.082718	1.733285	0.019469

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7,TS-4i-4 el energy= -1304.59524855

P	-2.242644	-0.110841	0.092473
P	2.201802	0.002275	-0.042757
O	0.021239	-2.082141	0.510579
O	1.002733	-3.752601	-0.654496
C	-3.219144	-1.020035	1.451704
C	-2.263812	-1.050279	2.664391
C	-3.503332	-2.470233	1.028301
C	-4.535323	-0.329375	1.849006
C	-3.098049	-0.229581	-1.605894
C	-2.715622	-1.581130	-2.238962
C	-4.623371	-0.063744	-1.576586
C	-2.479605	0.886815	-2.472517
C	-2.443091	1.679989	0.580531
C	-1.235218	2.459086	0.132834
C	-1.301053	3.847526	0.035689
C	-0.165437	4.576750	-0.306625
C	1.011190	3.872715	-0.547315
C	1.023361	2.481367	-0.462026
C	2.281661	1.720923	-0.774485
C	3.354915	-0.962818	-1.215420
C	2.486079	-1.302300	-2.445054
C	4.580242	-0.145190	-1.666360
C	3.826251	-2.276685	-0.569272

C	2.956216	0.172425	1.696924
C	2.129928	1.264930	2.407030
C	2.722915	-1.158645	2.441076
C	4.440793	0.558963	1.732468
C	0.030185	-3.135342	-0.233426
H	-1.343923	-1.585493	2.411498
H	-2.760215	-1.558378	3.503767
H	-1.993003	-0.041867	3.004289
H	-4.236239	-2.529801	0.216216
H	-3.916956	-3.021279	1.884667
H	-2.586860	-2.978263	0.715369
H	-5.002127	-0.892890	2.669468
H	-5.255134	-0.289704	1.026506
H	-4.375909	0.693026	2.210931
H	-1.627018	-1.695616	-2.283462
H	-3.109580	-1.630178	-3.264081
H	-3.120128	-2.433879	-1.685825
H	-4.928380	0.867793	-1.083113
H	-5.117974	-0.898054	-1.068838
H	-5.009758	-0.031641	-2.605606
H	-2.837894	0.780402	-3.505870
H	-1.385611	0.820299	-2.479402
H	-2.759144	1.889092	-2.127124
H	-3.369216	2.153720	0.232907
H	-2.475410	1.691006	1.677732
H	-2.243878	4.344419	0.248310
H	-0.195493	5.660926	-0.378825
H	1.928550	4.389150	-0.816778
H	3.168171	2.299248	-0.488111
H	2.337411	1.577427	-1.861495
H	2.038817	-0.407914	-2.899779
H	1.688359	-1.998464	-2.173373
H	3.114619	-1.782784	-3.208568
H	4.304587	0.749255	-2.236966
H	5.196529	-0.771062	-2.326973
H	5.210639	0.166728	-0.828267
H	4.359356	-2.866965	-1.328620
H	2.977835	-2.875518	-0.224457
H	4.526979	-2.098169	0.253921
H	2.259403	2.253398	1.949378
H	2.454106	1.338068	3.454615
H	1.061210	1.020166	2.391488
H	2.940616	-1.019403	3.509886
H	3.369989	-1.957838	2.069799
H	1.687488	-1.497279	2.328765

H	4.753458	0.720747	2.774423
H	4.639731	1.488788	1.183681
H	5.079846	-0.227140	1.318523
H	-0.986949	-3.532210	-0.483735
N	-0.088080	1.759257	-0.126433
Co	-0.027631	-0.185948	0.056752

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1,Ni-H (SMD-BS2-Opt) el energy= -3132.80740836

Ni	0.000000	0.000000	0.393645
H	0.000000	0.000000	1.939878
C	0.000000	0.000000	-1.565085
C	0.764932	0.933245	-2.297358
C	1.560839	1.962840	-1.530518
C	0.767513	0.927427	-3.692562
H	1.363679	1.651411	-4.238021
C	0.000000	0.000000	-4.390102
H	0.000000	0.000000	-5.473693
C	-0.767513	-0.927427	-3.692562
H	-1.363679	-1.651411	-4.238021
C	-0.764932	-0.933245	-2.297358
C	-1.560839	-1.962840	-1.530518
P	1.640500	1.416141	0.236919
P	-1.640500	-1.416141	0.236919
C	1.491432	3.011757	1.222652
C	0.000000	3.381351	1.151488
C	2.316635	4.173971	0.657408
C	1.868153	2.778571	2.688076
C	3.329687	0.603694	0.421489
C	4.498625	1.585608	0.320616
C	3.395303	-0.149878	1.756556
C	3.442942	-0.432080	-0.708827
C	-3.329687	-0.603694	0.421489
C	-3.442942	0.432080	-0.708827
C	-3.395303	0.149878	1.756556
C	-4.498625	-1.585608	0.320616
C	-1.491432	-3.011757	1.222652
C	-2.316635	-4.173971	0.657408
C	0.000000	-3.381351	1.151488
C	-1.868153	-2.778571	2.688076
H	2.549329	2.139459	-1.958296
H	1.039989	2.922405	-1.552910
H	-1.039989	-2.922405	-1.552910
H	-2.549329	-2.139459	-1.958296
H	-0.163876	4.317113	1.693324

H	-0.340014	3.528379	0.124742
H	-0.618894	2.607167	1.605392
H	3.386923	3.987427	0.705224
H	2.055089	4.399143	-0.376510
H	2.111102	5.071423	1.248374
H	2.939423	2.622741	2.810595
H	1.592857	3.661410	3.272057
H	1.340917	1.920525	3.106126
H	5.437318	1.023590	0.309272
H	4.458993	2.178829	-0.594144
H	4.532774	2.264585	1.171597
H	3.344220	0.515960	2.615580
H	2.583616	-0.872075	1.841392
H	4.343720	-0.692298	1.810699
H	3.459828	0.029211	-1.695898
H	2.619865	-1.146262	-0.681970
H	4.378309	-0.984122	-0.583085
H	-4.378309	0.984122	-0.583085
H	-2.619865	1.146262	-0.681970
H	-3.459828	-0.029211	-1.695898
H	-3.344220	-0.515960	2.615580
H	-4.343720	0.692298	1.810699
H	-2.583616	0.872075	1.841392
H	-5.437318	-1.023590	0.309272
H	-4.458993	-2.178829	-0.594144
H	-4.532774	-2.264585	1.171597
H	-2.111102	-5.071423	1.248374
H	-3.386923	-3.987427	0.705224
H	-2.055089	-4.399143	-0.376510
H	0.618894	-2.607167	1.605392
H	0.163876	-4.317113	1.693324
H	0.340014	-3.528379	0.124742
H	-1.592857	-3.661410	3.272057
H	-1.340917	-1.920525	3.106126
H	-2.939423	-2.622741	2.810595

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1,Ni-(0)-formate (SMD-BS2-Opt) el energy= -3321.51193555

Ni	0.012768	-0.200556	0.059444
P	-2.219814	-0.014588	0.092275
P	2.234400	0.010026	-0.035210
O	0.050246	-2.087619	0.558583
O	-0.079080	-3.285350	-1.353569
C	-3.146055	-0.940010	1.445178
C	-2.206952	-0.921531	2.663498

C	-3.414329	-2.393986	1.045643
C	-4.471081	-0.270503	1.833301
C	-3.037552	-0.176180	-1.596222
C	-2.745594	-1.558891	-2.189410
C	-4.548920	0.064688	-1.563107
C	-2.381033	0.876940	-2.503166
C	-2.419384	1.754251	0.549762
C	-1.170603	2.479011	0.127016
C	-1.179500	3.869290	0.017432
C	-0.023888	4.555543	-0.333107
C	1.145064	3.844027	-0.570772
C	1.159563	2.452877	-0.470806
C	-0.001934	1.728961	-0.126234
C	2.434572	1.698167	-0.732294
C	3.207268	-1.081034	-1.218610
C	2.310341	-1.229996	-2.459124
C	4.542289	-0.457593	-1.647917
C	3.470939	-2.464406	-0.616626
C	2.993264	0.075340	1.685535
C	2.331939	1.255637	2.415038
C	2.642347	-1.208484	2.449607
C	4.509941	0.279210	1.679355
C	-0.012038	-3.158139	-0.132595
H	-1.290001	-1.471527	2.459873
H	-2.715614	-1.390845	3.510283
H	-1.941322	0.094874	2.961129
H	-4.179986	-2.466052	0.274605
H	-3.776181	-2.939261	1.921939
H	-2.515380	-2.894058	0.690517
H	-4.919759	-0.838980	2.653248
H	-5.186477	-0.254573	1.014437
H	-4.330501	0.751309	2.185340
H	-1.682041	-1.791345	-2.182248
H	-3.098415	-1.576354	-3.224865
H	-3.259628	-2.354994	-1.654592
H	-4.808357	1.019198	-1.103297
H	-5.074065	-0.729492	-1.034633
H	-4.924966	0.080947	-2.590285
H	-2.791175	0.767065	-3.510521
H	-1.300976	0.742148	-2.560040
H	-2.579315	1.895727	-2.171777
H	-3.325740	2.199152	0.137243
H	-2.515951	1.795484	1.636641
H	-2.095529	4.415888	0.212816
H	-0.032949	5.635625	-0.415483

H	2.055073	4.371342	-0.835114
H	3.313052	2.212041	-0.339338
H	2.589840	1.590262	-1.807367
H	2.056078	-0.263244	-2.898416
H	1.388624	-1.760195	-2.223823
H	2.851237	-1.803096	-3.217933
H	4.409190	0.503530	-2.144006
H	5.021344	-1.130210	-2.365312
H	5.229444	-0.321085	-0.816257
H	3.864707	-3.120122	-1.397998
H	2.565621	-2.922930	-0.225003
H	4.210964	-2.420875	0.181741
H	2.568496	2.214601	1.954775
H	2.701965	1.277954	3.443501
H	1.247244	1.152982	2.446243
H	2.985512	-1.106371	3.483056
H	3.123178	-2.087898	2.026099
H	1.568264	-1.387056	2.457627
H	4.850345	0.435431	2.707249
H	4.806330	1.153580	1.098190
H	5.035582	-0.590944	1.289274
H	0.002894	-4.071249	0.499976

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1,TS-2-3 (SMD-BS2-Opt) el energy= -3321.47989815

Ni	-0.000020	0.107128	0.000048
H	-0.000111	1.682687	0.000136
C	0.000029	-1.841297	-0.000026
C	-1.172184	-2.571661	0.282468
C	-2.428846	-1.807303	0.612020
C	-1.170113	-3.966566	0.277424
H	-2.083621	-4.509490	0.494745
C	0.000121	-4.664600	-0.000066
H	0.000158	-5.748029	-0.000076
C	1.170307	-3.966482	-0.277548
H	2.083850	-4.509340	-0.494888
C	1.172285	-2.571577	-0.282558
C	2.428881	-1.807125	-0.612138
P	-2.183820	-0.061847	0.059919
P	2.183804	-0.061712	-0.059916
C	-3.118964	0.960627	1.333267
C	-2.182443	1.029067	2.551368
C	-4.449515	0.327440	1.759779
C	-3.380561	2.382717	0.830218
C	-2.960296	0.027453	-1.651557

C	-4.483313	-0.121302	-1.641176
C	-2.562892	1.350543	-2.318209
C	-2.353007	-1.118121	-2.476810
C	2.960368	0.027504	1.651521
C	2.353107	-1.118102	2.476749
C	2.563013	1.350567	2.318253
C	4.483384	-0.121256	1.641061
C	3.118851	0.960876	-1.333254
C	4.449350	0.327703	-1.759954
C	2.182206	1.029444	-2.551253
C	3.380540	2.382916	-0.830109
H	-3.324378	-2.259637	0.183022
H	-2.576297	-1.789793	1.693916
H	2.576249	-1.789537	-1.694045
H	3.324469	-2.259439	-0.183234
H	-2.683603	1.570208	3.358762
H	-1.924681	0.037026	2.926813
H	-1.258071	1.552861	2.310577
H	-5.153554	0.243865	0.934667
H	-4.314862	-0.661828	2.195933
H	-4.909129	0.960980	2.523900
H	-4.142900	2.405511	0.052842
H	-3.738089	2.992963	1.664003
H	-2.480710	2.853803	0.440902
H	-4.842324	-0.172285	-2.673296
H	-4.802299	-1.034604	-1.136649
H	-4.973950	0.725798	-1.164523
H	-2.992521	2.215665	-1.818416
H	-1.480917	1.476487	-2.335371
H	-2.923743	1.348879	-3.350740
H	-2.625566	-2.099460	-2.089588
H	-1.265412	-1.057185	-2.511258
H	-2.731564	-1.045553	-3.499894
H	2.731703	-1.045579	3.499822
H	1.265512	-1.057160	2.511241
H	2.625644	-2.099425	2.089474
H	2.992639	2.215703	1.818483
H	2.923911	1.348848	3.350768
H	1.481043	1.476534	2.335473
H	4.842441	-0.172308	2.673162
H	4.802350	-1.034522	1.136459
H	4.973999	0.725880	1.164448
H	4.314638	-0.661506	-2.196222
H	4.908917	0.961327	-2.524034
H	5.153457	0.244007	-0.934912

H	1.257873	1.553246	-2.310319
H	2.683295	1.570635	-3.358658
H	1.924374	0.037440	-2.926747
H	3.738018	2.993213	-1.663878
H	2.480741	2.854005	-0.440680
H	4.142954	2.405616	-0.052803
C	0.000080	3.363416	0.000494
O	0.108820	3.626078	1.147753
O	-0.108586	3.626561	-1.146661

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1,TS-3-4 (SMD-BS2-Opt) el energy= -3321.47977818

Ni	-0.012769	-0.174896	0.024466
H	-0.035600	-1.759997	0.837242
C	-0.078765	1.743917	0.004831
C	1.057200	2.507203	0.339230
C	2.329030	1.799951	0.714252
C	1.005967	3.900728	0.345760
H	1.896229	4.465472	0.598623
C	-0.173428	4.565043	0.035736
H	-0.208707	5.647497	0.043744
C	-1.309403	3.829832	-0.276405
H	-2.238500	4.338859	-0.506877
C	-1.269070	2.435985	-0.293386
C	-2.507658	1.651304	-0.621887
P	2.212797	0.074419	0.096511
P	-2.245143	-0.070452	-0.039607
C	3.201240	-0.928901	1.347542
C	2.293730	-1.098739	2.577854
C	4.483623	-0.208784	1.788506
C	3.560369	-2.312254	0.797222
C	3.017755	0.107467	-1.607240
C	4.518040	0.408349	-1.555630
C	2.783881	-1.222230	-2.334216
C	2.313086	1.213983	-2.408217
C	-2.999732	-0.145700	1.682849
C	-2.424173	1.036238	2.478494
C	-2.565167	-1.441690	2.378689
C	-4.527356	-0.045003	1.681176
C	-3.171354	-1.117632	-1.300034
C	-4.548093	-0.535449	-1.649152
C	-2.298077	-1.107066	-2.566333
C	-3.340271	-2.561126	-0.816545
H	3.217664	2.317912	0.352635
H	2.415624	1.748427	1.801553

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H          -2.653294        1.613057       -1.702800
H          -3.408007        2.098115       -0.198834
H           2.877044       -1.551959        3.383709
H           1.907475       -0.146226        2.945454
H           1.449749       -1.752681        2.369192
H           5.173723       -0.036978        0.966460
H           4.274981        0.747573        2.267324
H           4.994783       -0.836640        2.523529
H           4.320818       -2.251516        0.020094
H           3.966049       -2.918919        1.611332
H           2.695011       -2.837274        0.395721
H           4.882033        0.540594       -2.578534
H           4.743044        1.323471       -1.006768
H           5.081436       -0.410752       -1.112023
H           3.317269       -2.048283       -1.868918
H           1.728907       -1.484220       -2.361451
H           3.152043       -1.124504       -3.359483
H           2.472285        2.204378       -1.983256
H           1.239184        1.041430       -2.476047
H           2.721887        1.215587       -3.421891
H          -2.779805        0.962488        3.509464
H          -1.334630        1.021691        2.493968
H          -2.746564        1.999171        2.083292
H          -2.894989       -2.334576        1.852265
H          -3.001108       -1.464050        3.381153
H          -1.482249       -1.492486        2.483849
H          -4.873776        0.048681        2.714236
H          -4.881978        0.829498        1.134040
H          -4.993948       -0.933035        1.258183
H          -4.481876        0.484108       -2.028107
H          -4.987469       -1.148968       -2.440740
H          -5.234848       -0.545094       -0.806922
H          -1.333650       -1.575055       -2.381182
H          -2.814380       -1.667572       -3.350586
H          -2.132248       -0.095602       -2.941828
H          -3.753157       -3.156749       -1.635361
H          -2.394502       -3.013942       -0.526821
H          -4.033628       -2.629070        0.020752
C           0.074180       -2.727576        0.183528
O           0.066817       -3.743348        0.874492
O           0.171006       -2.544176       -1.043041

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1,TS-4i-4 (SMD-BS2-Opt)   el energy= -3321.50124094
Ni          0.026572       -0.172664       -0.017138
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P	-2.219052	-0.084375	0.068849
P	2.232745	0.128843	-0.023840
O	0.255596	-2.119359	0.123897
O	0.585180	-3.788599	-1.341721
C	-3.094573	-0.997954	1.470182
C	-2.114904	-0.927294	2.653713
C	-3.358020	-2.468332	1.142200
C	-4.422163	-0.341422	1.874162
C	-3.056226	-0.313394	-1.600251
C	-2.653212	-1.667411	-2.195042
C	-4.581222	-0.200965	-1.537949
C	-2.509203	0.787419	-2.522835
C	-2.488667	1.683304	0.492955
C	-1.266421	2.454448	0.081664
C	-1.334924	3.842159	-0.038328
C	-0.202125	4.578692	-0.358575
C	1.004071	3.919227	-0.554284
C	1.078722	2.530514	-0.447704
C	-0.060299	1.755419	-0.136029
C	2.395843	1.838226	-0.671538
C	3.286154	-0.905962	-1.186664
C	2.430307	-1.084090	-2.452155
C	4.600481	-0.210732	-1.567944
C	3.593441	-2.284570	-0.594775
C	2.907452	0.175022	1.731121
C	2.195804	1.328516	2.455472
C	2.539287	-1.132047	2.446025
C	4.418723	0.406587	1.798441
C	-0.100460	-3.147626	-0.549618
H	-1.186665	-1.450646	2.425064
H	-2.572998	-1.400782	3.526445
H	-1.869861	0.100915	2.926200
H	-4.073935	-2.589360	0.330400
H	-3.778702	-2.953132	2.027567
H	-2.444057	-2.996523	0.883509
H	-4.830313	-0.887491	2.729459
H	-5.161810	-0.378629	1.077344
H	-4.301357	0.696530	2.180620
H	-1.573773	-1.734962	-2.327354
H	-3.117123	-1.773025	-3.179588
H	-2.975363	-2.508322	-1.584517
H	-4.905865	0.734845	-1.081252
H	-5.030842	-1.027108	-0.989764
H	-4.979247	-0.225990	-2.556552
H	-2.907273	0.625688	-3.528069

H	-1.420955	0.760663	-2.581453
H	-2.808390	1.784923	-2.202663
H	-3.406772	2.082546	0.060494
H	-2.602060	1.742955	1.576694
H	-2.280394	4.346682	0.127381
H	-0.257458	5.656699	-0.449007
H	1.897612	4.485082	-0.793717
H	3.234266	2.378860	-0.229414
H	2.600779	1.765326	-1.741045
H	2.109263	-0.128584	-2.872179
H	1.554404	-1.695556	-2.245977
H	3.026914	-1.595049	-3.213362
H	4.436539	0.741231	-2.072675
H	5.142462	-0.858316	-2.263131
H	5.246286	-0.035817	-0.710316
H	4.068526	-2.896689	-1.366932
H	2.684963	-2.793004	-0.281713
H	4.286148	-2.218993	0.243644
H	2.437606	2.300767	2.026714
H	2.521056	1.333696	3.499202
H	1.112811	1.209639	2.437361
H	2.838016	-1.055998	3.495375
H	3.041143	-1.996601	2.017488
H	1.465980	-1.315646	2.407156
H	4.711392	0.534604	2.844739
H	4.718105	1.307118	1.260253
H	4.980342	-0.437103	1.401323
H	-1.129981	-3.509628	-0.354018