Electronic Supplementary Information

Bifunctionality of Zn dust in Ullmann C−C cross-coupling by Ni/Pd dual catalysis: Theoretical insight

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1. Computational methods

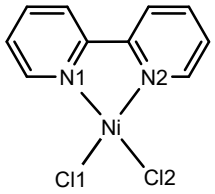
1.1 Heterogeneous calculations

The active species of Ni and Pd catalysts produced via the reduction by zinc powder was calculated by the Vienna Ab initio Simulation Package (VASP) program with the Perdew-Burke-Ernzerhof (PBE) functional.[S1] For zinc powder, we used 90 zinc atoms in 16.8 × 13.3 × 19.5 Å cells as the model. The lowest-layer zinc atoms are frozen in the three-layer zinc atom model. Taking into account of the large number of atoms in the system, the convergence threshold of geometric optimization and electronic structure iteration was set to 0.1 eV/Å and 10^{-4} eV, and the spin polarization was considered. The cut-off energy was 400 eV, and the k-point was set to 3 × 3 × 1 to ensure the result was more reliable.

1.2 Homogeneous calculations

All the structures involved in the homogeneous reaction were optimized by (U)M06[S2] method in the gas phase employed Gaussian 09 program. The LANL2DZ basis sets were used for valence electrons of Ni, Pd and Zn atoms with corresponding effective core potentials (ECPs) representing their core electrons and 6-31G(d, p) basis set is used for other atoms. Moreover, intrinsic reaction coordinates (IRC) and vibration frequency calculations were performed at the same level as geometric optimization. The IRC was performed to confirm that the transition state could connect the correct reactants and products.[S3] In addition, the translational entropy was corrected using the method developed by Whitesides et al.[S4] The single point calculation was performed at the SMD (1:1 NMP/DMF)/(U)M06/[6-311++G(d,p)/SDD(Ni, Pd, Zn)] level, considering the solvent effect using the SMD solvation model.[S5,S6] The combination of low-cost optimization in gas phase with high-cost single-point calculation in solution has been proved to be reasonable for evaluating the mechanism of organic reactions. The 3D visualization structures were generated by CYLview and VMD program.[S7]

Additionally, different methods were used to test the initial catalyst (bpy)$Ni^{II}Cl_2$ under the double-zeta basis sets and the triple-zeta basis sets, as shown in Table S1, the double-zeta basis sets and gas-phase optimization have little effect on the geometric structures, so the final gas-phase optimization was performed with the double-zeta basis sets and the M06 functional. Then the energy was refined by the single point calculation using the triple-zeta basis sets under solvation condition.



(bpy)$Ni^{II}Cl_2$

Table S1. Comparison of the DFT-optimized geometry of (bpy)$Ni^{II}Cl_2$.

	d (Ni-Cl1)	d (Ni-Cl2)	d (Ni-N1)	d (Ni-N2)	∠(N1-Ni-N2)	∠(Cl1-Ni-Cl2)
M06[a]	2.170	2.171	1.948	1.948	82.7	89.8
M06[b]	2.195	2.195	1.939	1.939	83.1	89.2
B3LYP[c]	2.231	2.232	1.955	1.955	82.7	89.3
B3LYP-D3[d]	2.233	2.234	1.956	1.956	82.6	89.3
B97XD[e]	2.215	2.215	1.950	1.950	82.6	89.5

[a] (U)M06/[6-31G(d,p)/Lanl2DZ(Ni,Pd,Zn)].

[b] SMD(1:1 NMP/DMF)/(U)M06/[6-311G(d)/SDD(Ni,Pd,Zn)].

[c] (U)B3LYP/[6-31G(d,p)/Lanl2DZ(Ni,Pd,Zn)].

[d] (U)B3LYP-D3/[6-31G(d,p)/Lanl2DZ(Ni,Pd,Zn)].

[e] (U) B97XD/[6-31G(d,p)/Lanl2DZ(Ni,Pd,Zn)].

1.3 Correction of translational entropy in solution

We evaluated the electronic energy (E_{sol}) with zero-point energy correction in solution. For each species, the E_{sol} is defined through equation (S1):

$$E_{sol} = E_{sol}^{pot} + E_{gas}^{v_0} \quad \text{(S1)}$$

the E_{sol}^{pot} is the potential energy including non-electrostatic energy in solution and $E_{gas}^{v_0}$ delegates the zero-point vibrational energy in the gas phase. In a bimolecular process, such as the coordination of Ni(II) center to the alkyne, the entropy change which can decreases considerably must be taken into consideration. In such case, Gibbs energy (G_{sol}^{o}) need be computed as follows:

$$G_{sol}^{o} = H_0 - T(S_r^o + S_v^o + S_t^o)$$

$$= E^T + P\Delta V - T(S_r^o + S_v^o + S_t^o)$$

$$= E_{sol} + E_{therm} - T(S_r^o + S_v^o + S_t^o) \quad \text{(S2)}$$

where ΔV is 0 in solution, E_{therm} is the thermal correction by translational, vibrational, and rotational movements, and S_r^o, S_v^o, and S_t^o are rotational, vibrational, and translational entropies, respectively. In general, the Sackur-Tetrode equation is used to evaluate translational entropy S_t^o. In solution, however, the usual Sackur-Tetrode equation cannot be directly applied to the evaluation of S_t^o, because the translation movement is suppressed very much in solution. In this context, the translational entropy was corrected with the method developed by Whitesides et al.,[S4] where the rotational entropy was evaluated in a normal manner. Thermal correction and entropy contributions of vibration movements to the Gibbs energy were evaluated with the frequencies calculated at 353.15 K and 1 atm.

2. Single-electron reduction

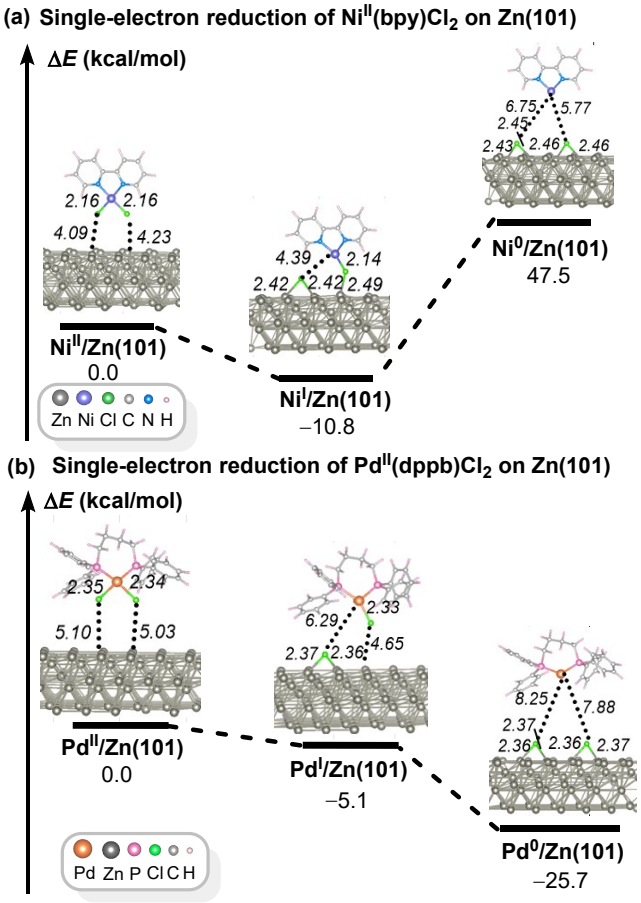


Fig. S1. Single-electron reduction process of Ni^{II}(bpy)Cl$_2$ on Zn(101) (a) and single-

electron reduction process of $Pd^{II}(dppb)Cl_2$ on Zn(101) (b). The bond distances are given in angstroms (Å).

As shown in Fig. S1, when **Ni^{II}** interacts with Zn(101) surface, nickel complexes with three oxidation states were located, namely $Ni^{II}(bpy)Cl_2$ (**Ni^{II}**), $Ni^{I}(bpy)Cl$ (**Ni^{I}**) and $Ni^{0}(bpy)$ (**Ni^{0}**). By comparison, **Ni^{I}**/Zn(101) is the most stable, whereas **Ni^{0}**/Zn(101) is the most unstable. It can be suggested from the non-monotonicity of energy changes that a double-electron reduction of **Ni^{II}** on the Zn(101) surface is inaccessible. **Ni^{II}** is more favorably reduced to **Ni^{I}** rather than **Ni^{0}** in the presence of zinc powder. In contrast, as shown in Fig. S1(b), the energy change of continuous single-electron reduction of **Pd^{II}** on the Zn(101) surface decreases monotonously. Unlike the single-electron reduction of **Ni^{II}** → **Ni^{I}**, **Pd^{II}** is more inclined to complete the double-electron reduction to form Pd(dppb) (**Pd^{0}**) on the Zn(101) surface. Therefore, it can be concluded that **Ni^{I}** and **Pd^{0}** would be the active species to participate the following reaction.

3. **Selective oxidative additions**

3.1 Gibbs energy profiles for oxidative additions by **Ni^{I}** and **Pd^{0}**.

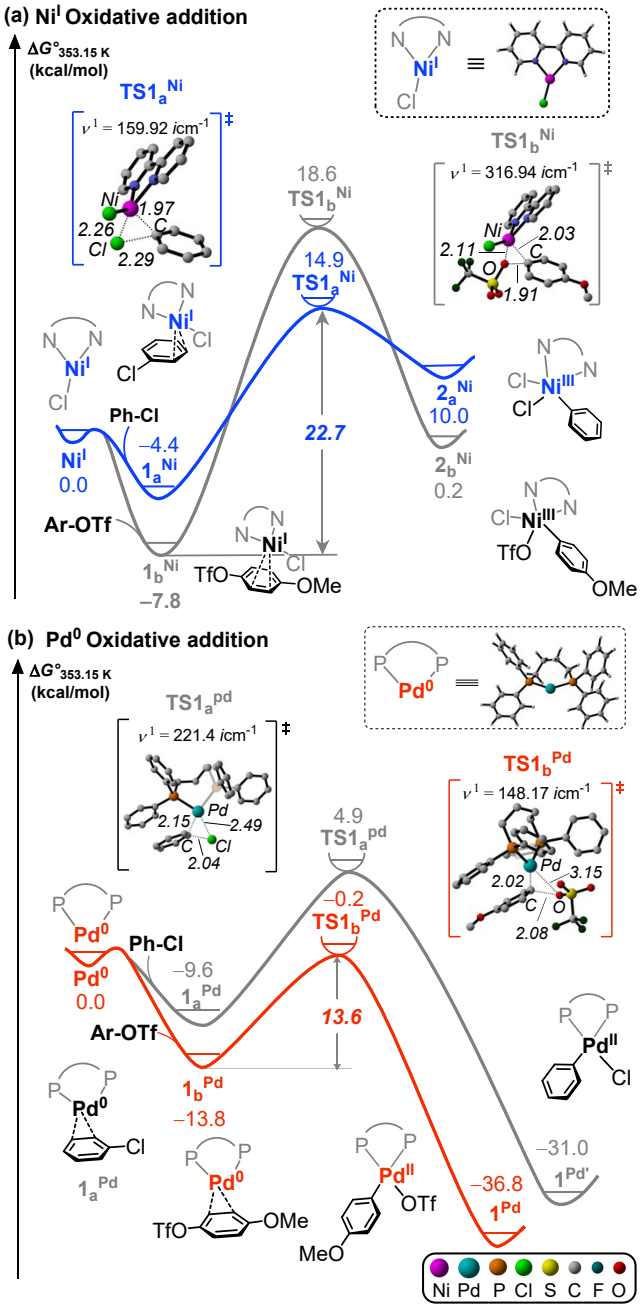


Fig. S2. Gibbs energy profiles (ΔG°, in kcal/mol) of oxidative additions of chlorobenzene and 4-methoxyphenyltriflate by Ni^{I}(bpy)Cl (a) and Pd^{0}(dppb) (b). The bond distances are given in angstroms (Å).

3.2 Gibbs energy profiles for oxidative additions by Ni^0(bpy).

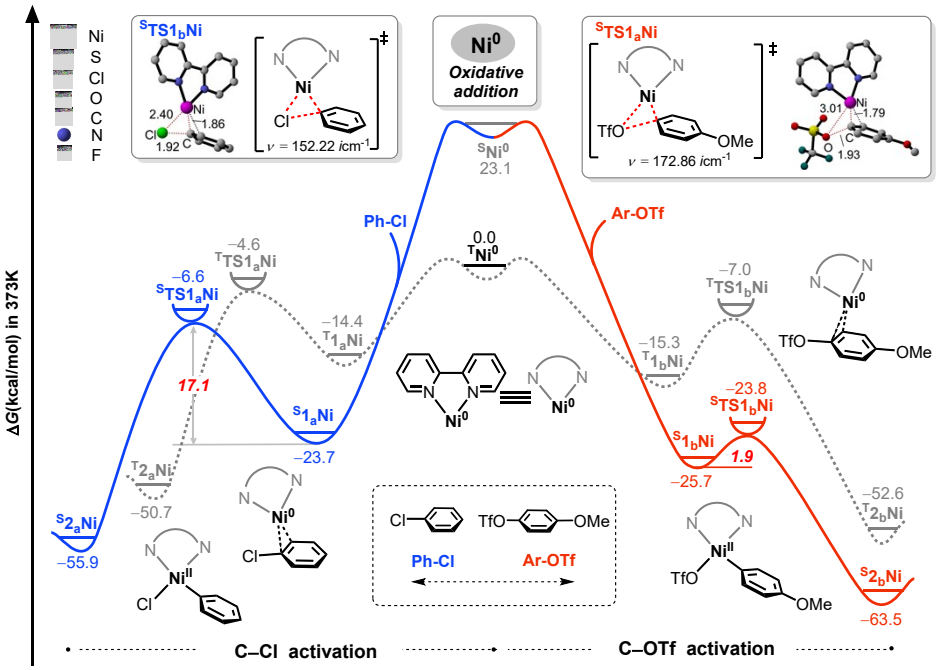


Fig. S3. Gibbs energy profiles (ΔG°, in kcal/mol) for oxidative additions of chlorobenzene and 4-methoxyphenyltriflate catalyzed by Ni^0(bpy).

3.3 Selected bond dissociation energies analysis

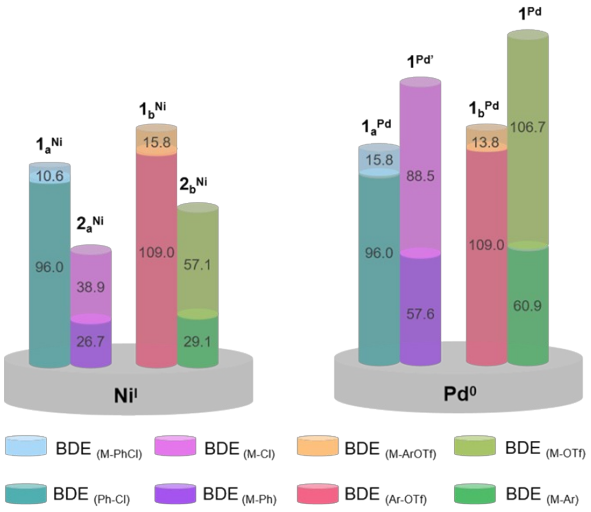


Fig. S4. Selected bond dissociation energies (in kcal/mol) of reaction intermediates involved in the oxidative additions of Ph-Cl and Ar-OTf to **Ni^I** and **Pd^0**.

The relevant bond dissociation energies (BDEs) were evaluated based on the reaction intermediates involved in the oxidative additions, as shown in Fig. S4. In the **Ni^I** case, $BDE_{(Ph\text{-}Cl)}$ and $BDE_{(Ar\text{-}OTf)}$ are much larger than the sum of $BDE_{(Ni\text{-}Ph)}$ and $BDE_{(Ni\text{-}Cl)}$ and

the sum of $BDE_{(Ni-Ar)}$ and $BDE_{(Ni-OTf)}$, respectively. Considering that the newly formed bonds are far less strong than the original bonds in the oxidative additions, so the weaker C−Cl bond of Ph-Cl is easier to be activated by **Ni^{I}** than the C−OTf bond activation of Ar-OTf. In the **Pd^{0}** case, on the contrary, $BDE_{(Ph-Cl)}$ and $BDE_{(Ar-OTf)}$ are much smaller than the sum of $BDE_{(Pd-Ph)}$ and $BDE_{(Pd-Cl)}$ and the sum of $BDE_{(Pd-Ar)}$ and $BDE_{(Pd-OTf)}$, respectively. Moreover, the Pd−OTf bond is stronger than the Pd−Cl bond, inducing the C−OTf bond of Ar-OTf is easier to be activated than C−Cl bond of Ph-Cl by **Pd^{0}**. In other words, the origin of such orthogonal reactivity results from the difference that the Ni−Cl and Ni−OTf bonds are too weak to reverse the selectivity determined by C−Cl bond of Ph-Cl and C−OTf bond of Ar-OTf, but the quite strong Pd−OTf bond can reverse it.

4. The transmetalation between Ni^{III} and Pd^{II} complexes

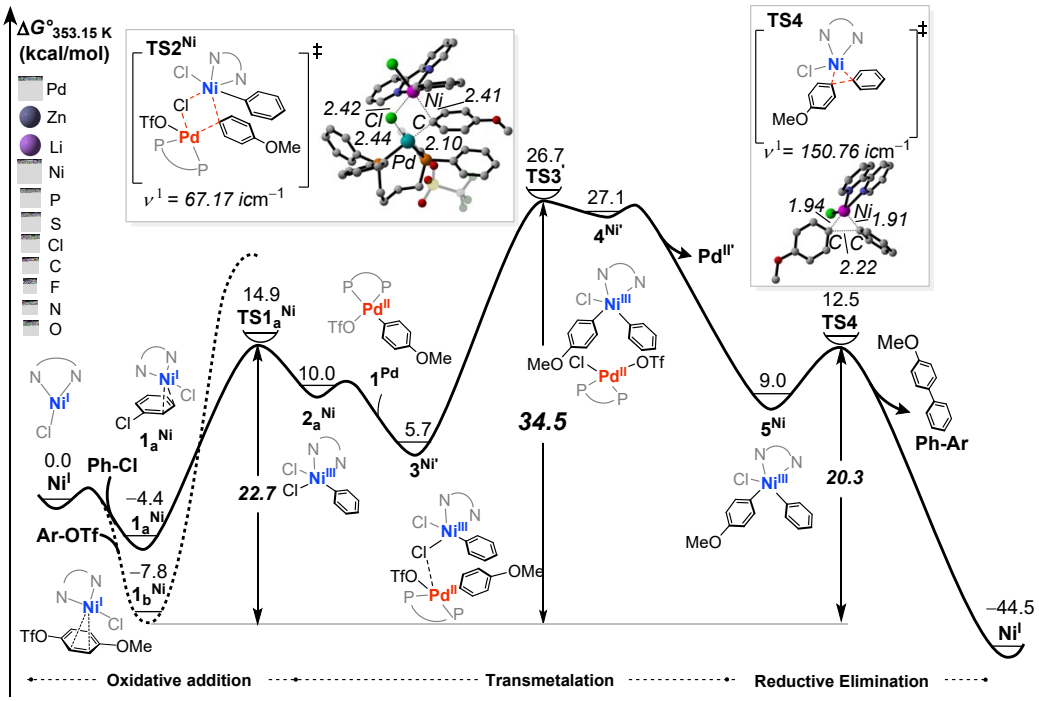


Fig. S5 Gibbs energy profiles (ΔG°, in kcal/mol) for the transmetalation.

It is that aryl migrates from the Pd^{II} center to the Ni^{III} center in **3$^{Ni'}$**, while the Cl group from Ni^{III} complex migrates to the Pd^{II} center simultaneously, and then the reductive elimination occurs from Ni^{III} center in **5^{Ni}**.

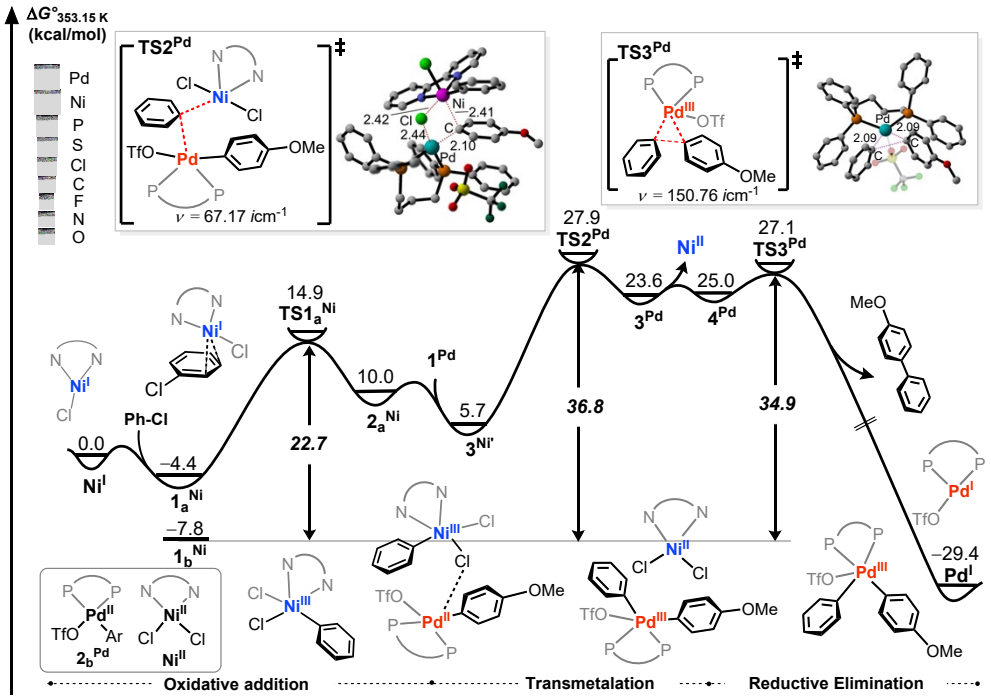


Fig. S6. Gibbs energy profiles (Δ*G*°, in kcal/mol) for transmetalation.

It is that phenyl radical migrates from the Ni^{III} center to the Pd^{II} center in $\mathbf{3}^{\mathbf{Ni'}}$, and then the reductive elimination occurs from Pd^{III} center in $\mathbf{4}^{\mathbf{Pd}}$.

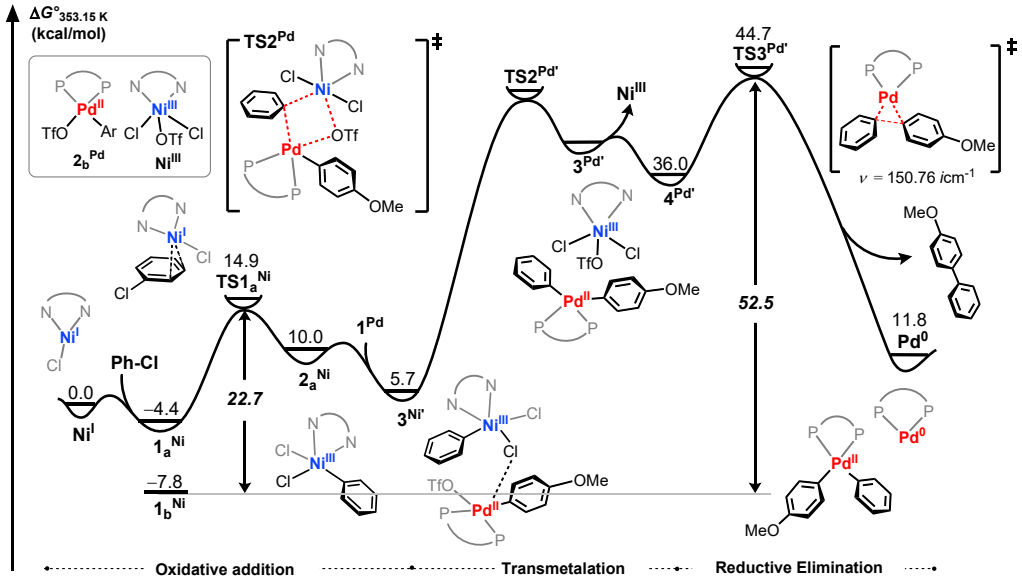


Fig. S7. Gibbs energy profiles (Δ*G*°, in kcal/mol) for transmetalation.

It is that phenyl in Ni^{III} complex migrates to the Pd^{II} center, while the OTf group in Pd^{II} complex migrates to the Ni^{III} center simultaneously, and then the reductive elimination occurs from Pd^{II} center in $\mathbf{4}^{\mathbf{Pd}}$'.

5. The relative stability of Zn^{II}&LiCl/Zn(101) (IV) and $ZnCl_2$·LiCl/Zn(101) (V)

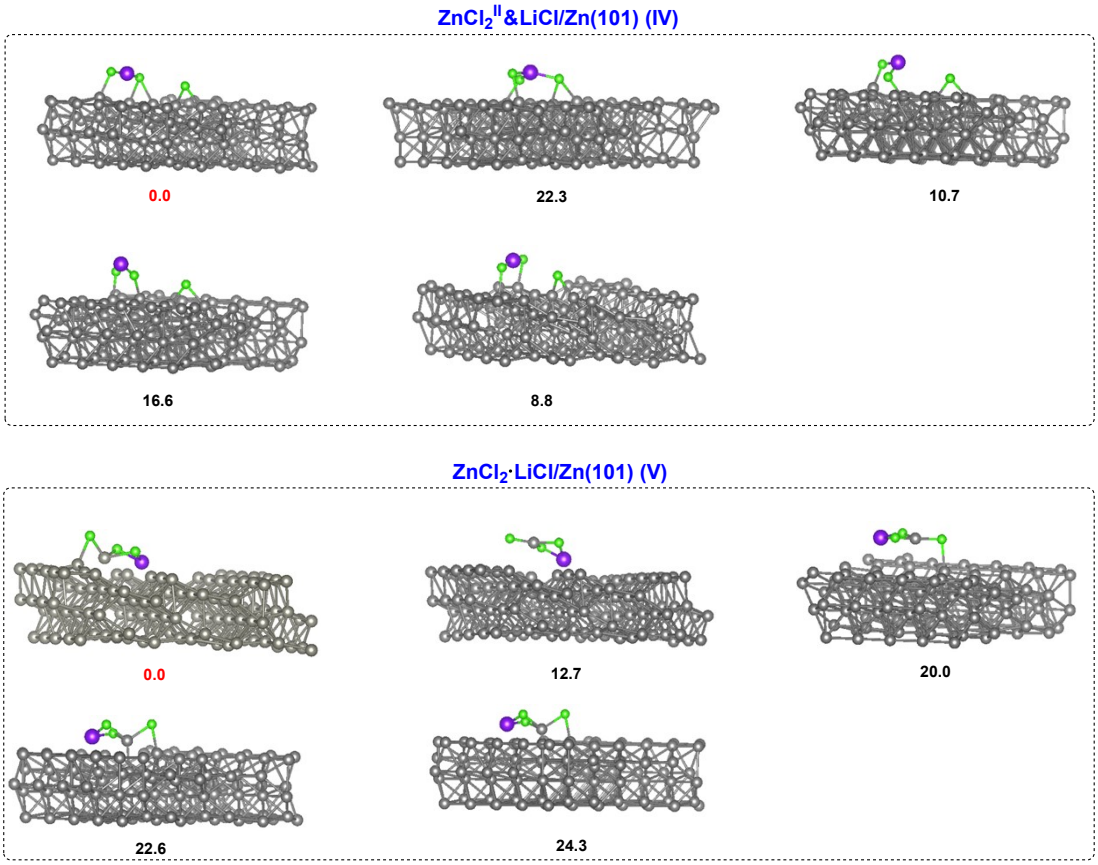


Fig. S8. Relative stability of $ZnCl_2$ LiCl/Zn(101) (IV) and $ZnCl_2$·LiCl/Zn(101) (V). The Gibbs free energies are given in kcal/mol.

6. The oxidative addition of substrate to Zn

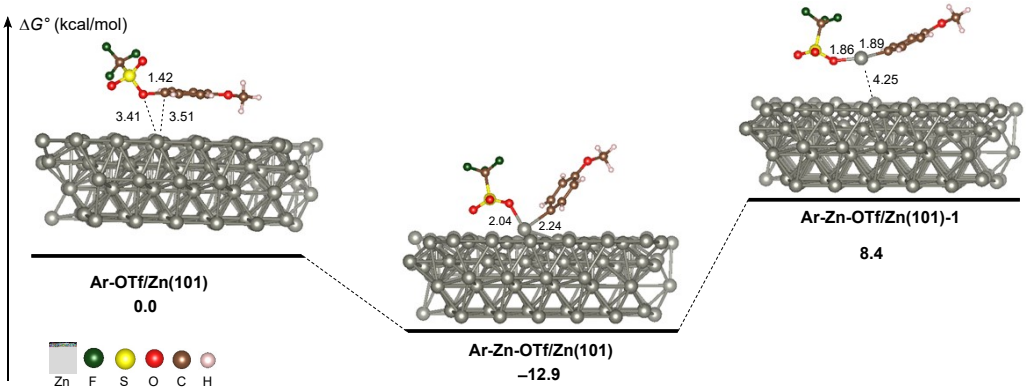


Fig. S9. Energy profile of oxidative addition of Ar-OTf by Zn on zinc surface. Gibbs free energies are given in kcal/mol.

7. The energy barrier of transmetalation involving other additives

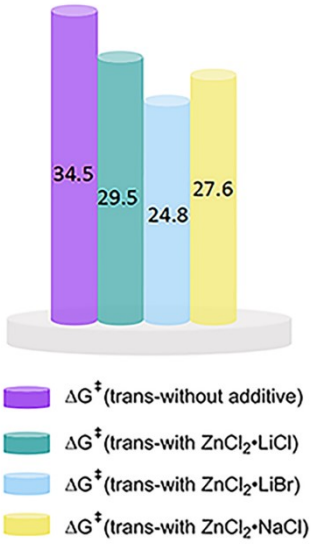


Fig. S10. The energy barrier of transmetalation involving other additives.

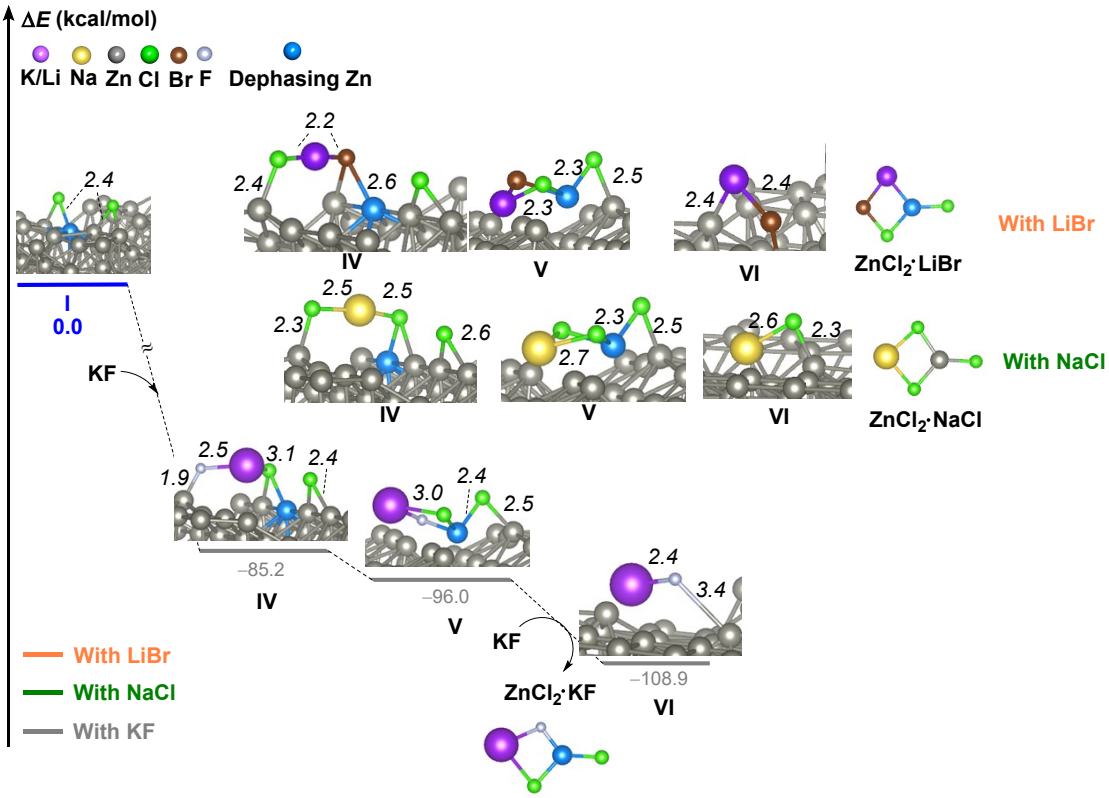


Fig. S11. Dissociation of $ZnCl_2$ in the absence and presence of additives. Selected bond distances are given in Å.

Coordinates of All Geometry Optimized Structures

Ph-Cl

G(Gibbs Free Energy) = -691.579328 hartree

E(electronic Energy) = -691.6341002 hartree

C	0.00000000	1.20385600	-1.56664900
C	0.00000000	1.21312100	-0.17576800
C	0.00000000	0.00000000	0.50098500
C	0.00000000	-1.21312100	-0.17576800
C	0.00000000	-1.20385600	-1.56664900
C	0.00000000	0.00000000	-2.26307700
H	0.00000000	2.14715400	-2.10727100
H	0.00000000	2.14455700	0.38273000
H	0.00000000	-2.14455700	0.38273000
H	0.00000000	-2.14715400	-2.10727100
H	0.00000000	0.00000000	-3.34994500
Cl	0.00000000	0.00000000	2.25179900

Ar-OTf

G(Gibbs Free Energy) = -1307.025979 hartree

E(electronic Energy) = -1307.1249029 hartree

C	-2.28153700	-1.25985200	-0.69360900
C	-0.97127500	-0.94761900	-1.00391600
C	-0.50166000	0.33294700	-0.73885000
C	-1.31250600	1.30382100	-0.18115200
C	-2.62945600	0.98705100	0.13868600
C	-3.11664200	-0.29580000	-0.11743000
H	-2.68989300	-2.24777700	-0.88612500
H	-0.30527400	-1.67919600	-1.45388400
H	-0.91610400	2.29650000	0.00924200
H	-3.26275500	1.74886300	0.58161300
O	-4.37768400	-0.70253700	0.15171900
C	-5.26004900	0.22585000	0.73687600
H	-4.89438600	0.57173800	1.71383000
H	-5.42133600	1.09695100	0.08648000
H	-6.20905000	-0.29468200	0.87593000
O	0.81170400	0.64048000	-1.14099800
S	1.96583500	0.87364000	-0.03600600
O	1.42792000	1.47996300	1.15821500
O	3.09302500	1.40088700	-0.75822500
C	2.37316400	-0.88060600	0.38712600
F	2.57868900	-1.56670300	-0.72192700
F	1.37742100	-1.42198400	1.06466000
F	3.46672100	-0.87972800	1.12359300

Ni^{I}

G(Gibbs Free Energy) = -1124.514016 hartree

E(electronic Energy) = -1124.6224425 hartree

C	0.56520500	1.36272700	-0.00001900
C	0.91985300	2.70894500	0.00055600
C	-0.08651100	3.66572700	0.00052100
C	-1.41577400	3.25819600	-0.00006300
C	-1.69088900	1.89744900	-0.00055300
N	-0.72403900	0.97871500	-0.00052800
H	0.16684200	4.72248100	0.00099000
H	1.96346000	3.01053600	0.00114100
H	-2.22761300	3.97864600	-0.00010300
H	-2.70722200	1.50654700	-0.00098400
C	1.52212000	0.24120600	0.00000800
C	2.90528900	0.39507400	-0.00079500
C	1.73057600	-2.06525500	0.00078400
C	3.71164400	-0.73421200	-0.00077100
H	3.34959800	1.38625100	-0.00155400
H	1.21261400	-3.02187800	0.00143400
H	4.79356300	-0.63418100	-0.00142900
C	3.11547900	-1.98983400	0.00005400
H	3.70887200	-2.89863700	0.00010400
N	0.94755300	-0.98140700	0.00074500
Ni	-1.03098000	-0.99761500	0.00021300
Cl	-2.97760000	-1.91399000	-0.00031800

1_a^{Ni}

G(Gibbs Free Energy) =-1816.089589 hartree

E(electronic Energy) =-1816.2734729 hartree

C	0.66730600	1.68008200	0.56368600
C	0.59458400	3.02274000	0.20112700
C	1.65277300	3.58518500	-0.49995600
C	2.75293300	2.79777700	-0.82318300
C	2.75156900	1.46680900	-0.42785500
N	1.73590600	0.92794400	0.24814000
H	1.61698800	4.63079700	-0.79413400
H	-0.27546200	3.62152000	0.45551800
H	3.59650800	3.20332800	-1.37297400
H	3.57324800	0.78888100	-0.65630700
C	-0.39511600	0.94818800	1.27865300
C	-1.59892300	1.52114700	1.67919400
C	-1.03924700	-1.10969900	2.11733900

C	-2.54396100	0.73134600	2.31728900
H	-1.80366600	2.56972000	1.48308600
H	-0.77034900	-2.15462300	2.26028200
H	-3.49466200	1.15698400	2.62572900
C	-2.26170700	-0.61101400	2.54140600
H	-2.97584400	-1.26515500	3.03138000
N	-0.12416100	-0.35478100	1.50104400
Ni	1.55173800	-1.02239300	0.67854000
C	-0.26115200	0.36527400	-2.35300300
C	-1.58062300	0.61727500	-1.98784700
C	-2.33527600	-0.41952100	-1.45271400
C	-1.80657200	-1.69285500	-1.27648700
C	-0.48053800	-1.92268300	-1.62865100
C	0.29397800	-0.89633000	-2.16528100
H	0.34068800	1.17142800	-2.76892900
H	-2.02409200	1.60223200	-2.11368100
H	-2.42430100	-2.48248200	-0.85642000
H	-0.03395400	-2.90133600	-1.46932700
H	1.33562900	-1.08845700	-2.41239300
Cl	-3.99747600	-0.10880100	-0.97984300
Cl	2.94737100	-2.52298200	-0.02942400

$TS1_a^{Ni}$

G(Gibbs Free Energy) =-1816.048819 hartree

E(electronic Energy) =-1816.2368637 hartree

C	-1.59085800	1.38536000	-0.00255100
C	-2.18515400	2.59268700	-0.36028200
C	-1.48332500	3.77254600	-0.15113800
C	-0.21642300	3.72082800	0.41376000
C	0.31031800	2.47926700	0.74861700
N	-0.36212600	1.34969700	0.53639300
H	-1.92772800	4.72555100	-0.42592800
H	-3.17826800	2.61826500	-0.79856400
H	0.35827600	4.62271800	0.59871800
H	1.28297000	2.35273500	1.22395500
C	-2.24379600	0.06822800	-0.16672700
C	-3.54997400	-0.09184200	-0.62348900
C	-1.99265500	-2.22260100	0.06773500
C	-4.07439100	-1.37289400	-0.72784700
H	-4.15567200	0.76950500	-0.88817400
H	-1.31518500	-3.02865200	0.34655800
H	-5.09264200	-1.51730000	-1.07923300
C	-3.28691800	-2.46132700	-0.37648900

H	-3.66167100	-3.47774200	-0.44279100
N	-1.48906700	-0.99270000	0.16821800
Ni	0.44615700	-0.50680100	0.89643000
C	1.51110200	-0.14774100	-3.05569900
C	0.92318400	-0.76367100	-1.95372400
C	1.55799400	-0.64553100	-0.72509200
C	2.80081000	-0.04498600	-0.57316600
C	3.36618600	0.56528200	-1.69049600
C	2.72510400	0.52100600	-2.92560100
H	1.01815600	-0.20506100	-4.02397200
H	-0.00756700	-1.31610900	-2.05028100
H	3.28383900	-0.03089000	0.40001900
H	4.32504600	1.06900700	-1.58921400
H	3.18294600	0.98956100	-3.79318800
Cl	1.34559700	-2.54521500	0.53285100
Cl	1.65006400	0.19181600	2.70849800

2_a^{Ni}

G(Gibbs Free Energy) =-1816.051659 hartree

E(electronic Energy) =-1816.2390933 hartree

C	1.57453900	1.38396200	0.09231500
C	2.17080900	2.58859100	0.45508800
C	1.46830900	3.77127300	0.27110200
C	0.19413800	3.72580500	-0.27695700
C	-0.33603400	2.49014600	-0.62299300
N	0.33856100	1.35594500	-0.43599400
H	1.91716000	4.72050200	0.55122000
H	3.17170700	2.60689800	0.87501200
H	-0.38527400	4.62823400	-0.44243200
H	-1.31267400	2.37618500	-1.09057200
C	2.23467500	0.07022600	0.24014700
C	3.52181700	-0.09889400	0.74400100
C	1.99434700	-2.21368000	-0.07021600
C	4.04261500	-1.38345400	0.83049500
H	4.11364500	0.75339600	1.06360800
H	1.32244100	-3.00530500	-0.40163400
H	5.04578400	-1.53781700	1.21912200
C	3.27192200	-2.46199300	0.41732000
H	3.64661000	-3.47922700	0.47021100
N	1.49835300	-0.98064300	-0.15399600
Ni	-0.44674000	-0.45331500	-0.89342000
C	-1.67987800	-0.46327400	3.08523600
C	-0.93763500	-0.73891400	1.93641800

C	-1.50240000	-0.43235300	0.71280000
C	-2.78709500	0.06133600	0.57032400
C	-3.51014600	0.33003500	1.73318800
C	-2.95889000	0.07365400	2.98430500
H	-1.25273900	-0.68387100	4.06139700
H	0.04960900	-1.18797100	2.01002000
H	-3.20812300	0.23150000	-0.41730900
H	-4.51850200	0.72967800	1.64917200
H	-3.53478300	0.27686700	3.88387700
Cl	-1.18630700	-2.52638400	-0.96512900
Cl	-1.51787500	0.37472600	-2.73495700

1_b^{Ni}

G(Gibbs Free Energy) = -2431.538913 hartree

E(electronic Energy) =-2431.7725024 hartree

C	-0.50928600	-2.23563800	-1.23388200
C	0.60402500	-1.41577700	-1.17618700
C	0.92951600	-0.80954500	0.03040000
C	0.18210800	-1.01318200	1.17561500
C	-0.93124200	-1.84516900	1.12053400
C	-1.29226700	-2.44198400	-0.09059700
H	-0.81395100	-2.71367300	-2.16125600
H	1.21897800	-1.22406200	-2.05319300
H	0.44736700	-0.50939300	2.10131800
H	-1.54417900	-1.96055800	2.00869700
O	-2.38801300	-3.20873700	-0.26203700
C	-3.23832500	-3.40163800	0.85751900
H	-2.71987900	-3.94845600	1.65694400
H	-3.60814300	-2.44555600	1.25583500
H	-4.07528400	-4.00431700	0.50073900
O	1.95796700	0.15724700	0.00007700
S	3.33192000	-0.03316600	0.81316800
O	3.14433300	-0.83333300	1.99858400
O	3.94993000	1.26925500	0.82365000
C	4.26696800	-1.06648000	-0.39988800
F	4.27251000	-0.46533000	-1.57638700
F	3.69013000	-2.24850400	-0.51132300
F	5.50223900	-1.20766200	0.03789400
C	-1.47669200	1.30925400	-1.61817700
C	-1.35702800	1.19357200	-3.00093000
C	-2.27707100	0.41599900	-3.69087700
C	-3.29004600	-0.22684800	-2.98841100
C	-3.34882900	-0.05652900	-1.61207700
N	-2.46821500	0.69453100	-0.94887700

H	-2.20129500	0.31132900	-4.76998600
H	-0.55601400	1.69822000	-3.53358200
H	-4.02312800	-0.84821100	-3.49287000
H	-4.11465500	-0.53176700	-1.00052900
C	-0.54658100	2.06837300	-0.76008700
C	0.57934700	2.73491000	-1.23427900
C	-0.03854500	2.66182400	1.41797500
C	1.42042100	3.36928100	-0.33188900
H	0.81086200	2.74108400	-2.29545700
H	-0.32946400	2.60171100	2.46521100
H	2.31873700	3.87210300	-0.67830100
C	1.10992800	3.33173200	1.02175300
H	1.75127300	3.80014200	1.76128600
N	-0.84923500	2.04190600	0.55426500
Ni	-2.42062500	0.91923900	1.04105000
Cl	-3.76990300	-0.02450700	2.46378800

$TS1_b^{Ni}$

G(Gibbs Free Energy) =-2431.481212 hartree

E(electronic Energy) =-2431.7123944 hartree

C	-2.52776900	-1.88235300	0.24936400
C	-3.88232000	-2.20238500	0.28393000
C	-4.70063900	-1.54659500	1.19519100
C	-4.15273200	-0.59839700	2.04895900
C	-2.79123300	-0.33416700	1.95857000
N	-2.01400800	-0.95991100	1.07770300
H	-5.76132000	-1.77965500	1.23749600
H	-4.29881700	-2.94717500	-0.38765700
H	-4.76285000	-0.07311100	2.77680400
H	-2.27474800	0.37447000	2.60660600
C	-1.55037400	-2.51264800	-0.66614400
C	-1.87312700	-3.54357400	-1.54448800
C	0.65869800	-2.53631000	-1.37523500
C	-0.87930000	-4.07441200	-2.35590300
H	-2.88520000	-3.93376400	-1.59327100
H	1.64382900	-2.08723900	-1.26981000
H	-1.11284900	-4.88047100	-3.04631400
C	0.41043500	-3.56705900	-2.27245500
H	1.21462400	-3.95591600	-2.88866200
N	-0.29729500	-2.02515700	-0.59697700
Ni	-0.02079400	-0.52215900	0.80345500
C	-1.66761200	1.93611100	-2.02720500
C	-0.76913800	0.95991500	-1.63527000
C	-0.16275400	1.10846100	-0.39349600

C	-0.23166900	2.26849600	0.35872900
C	-1.14204300	3.24141100	-0.05141400
C	-1.86708200	3.07472000	-1.23389800
H	-2.21429700	1.85564000	-2.96312000
H	-0.56892800	0.09225500	-2.25613700
H	0.36050400	2.38127700	1.26086600
H	-1.25704400	4.13202800	0.55873100
O	-2.76606800	3.96550700	-1.71166700
C	-2.95725500	5.15963400	-0.98972800
H	-3.33255900	4.96392400	0.02473600
H	-2.02919800	5.74342000	-0.92008500
H	-3.70208200	5.73768400	-1.53948600
O	1.51705500	0.20350700	-0.44848900
S	2.83805300	1.02690300	-0.36543900
O	2.78275700	2.09594100	0.60976800
O	3.35451700	1.27512500	-1.69765400
C	3.91250000	-0.29560700	0.34252100
F	3.92013500	-1.34525000	-0.48039800
F	3.47412200	-0.67999700	1.52245500
F	5.14442200	0.17072900	0.45214400
Cl	0.43645600	0.11180600	2.91581600

2_b^{Ni}

G(Gibbs Free Energy) =-2431.508793 hartree

E(electronic Energy) =-2431.7402024 hartree

C	-2.53716900	-2.06637600	-0.36739000
C	-3.69112100	-2.84294900	-0.43355300
C	-4.28474000	-3.26612100	0.74827900
C	-3.71817800	-2.90680200	1.96391800
C	-2.56667700	-2.13000000	1.95160600
N	-1.99772000	-1.72575700	0.81585300
H	-5.18467800	-3.87455600	0.71657800
H	-4.12139200	-3.12062300	-1.39074000
H	-4.15391500	-3.21905100	2.90747900
H	-2.06826600	-1.80073600	2.86274200
C	-1.81763100	-1.55934900	-1.55509800
C	-2.25897900	-1.75498100	-2.85935400
C	0.04833400	-0.39423800	-2.30099800
C	-1.50519500	-1.24301400	-3.90799800
H	-3.17834500	-2.29626500	-3.06025800
H	0.96890300	0.12600300	-2.02921700
H	-1.83369000	-1.38491200	-4.93415200
C	-0.33482100	-0.55463900	-3.62832900
H	0.28589700	-0.14360500	-4.41771900

N	-0.68191900	-0.88519500	-1.29810700
Ni	-0.21995900	-0.57900300	0.66243200
C	-2.62267300	2.76260900	0.28046100
C	-2.20198600	1.49840900	0.66448100
C	-0.83666500	1.26496500	0.73511100
C	0.10936100	2.25848100	0.59754600
C	-0.32442500	3.52564900	0.20205500
C	-1.68696000	3.77553200	0.03621700
H	-3.67856200	2.99592300	0.16851100
H	-2.92767600	0.71779900	0.87647900
H	1.16498500	2.07645200	0.79799300
H	0.41659900	4.30529000	0.05527200
O	-2.20716700	4.96873200	-0.33534800
C	-1.31375800	6.03553700	-0.55374600
H	-0.75011400	6.28466900	0.35585400
H	-0.60398800	5.81045400	-1.36207700
H	-1.92233700	6.89435000	-0.84248000
O	1.75743900	-0.81372100	0.21683100
S	2.89455500	0.13945900	-0.02815400
O	3.12503100	1.08910200	1.05412000
O	2.88602000	0.67538800	-1.39318100
C	4.32067300	-1.01556000	0.02450500
F	4.19405300	-1.94276400	-0.91800900
F	4.38942900	-1.61077400	1.20500300
F	5.44205800	-0.34096200	-0.18645600
Cl	-0.07028000	-0.10248500	2.80843400

Pd^0

G(Gibbs Free Energy) =-1892.0878 hartree

E(electronic Energy) =-1892.4824623 hartree

P	-2.03867500	-0.03684500	0.01641500
P	2.05675800	-0.07342800	0.00000900
C	-1.50484400	0.23207700	1.78283100
H	-2.38240100	0.44541600	2.41032500
H	-1.14594600	-0.75699500	2.10126100
C	-0.40333000	1.29379900	1.93963300
H	-0.76438900	2.10197700	2.59121400
H	-0.19518400	1.76624100	0.96649300
C	1.64209000	-0.34722100	1.80712800
H	2.56948800	-0.57788600	2.35115800
C	3.03987000	1.47677400	0.08015400
C	2.70510500	2.50703300	-0.80006700
C	4.06545100	1.68741400	1.00944200

H	1.89578700	2.34366300	-1.51248300
C	3.38474100	3.72118900	-0.76350100
C	4.74480000	2.89861800	1.04776800
H	4.34139300	0.89388800	1.70384300
H	3.11425200	4.51508900	-1.45563100
C	4.40486900	3.91663400	0.15966400
H	5.54136100	3.05114200	1.77255100
H	4.93687200	4.86470400	0.19149200
C	3.31204700	-1.40241200	-0.21125900
C	2.86848800	-2.72473700	-0.08470800
C	4.64557200	-1.17273400	-0.55455400
H	1.81912100	-2.92080800	0.14115000
C	3.74335400	-3.78752800	-0.26334500
C	5.51911700	-2.23956900	-0.74613500
H	5.00767600	-0.15350200	-0.67490900
H	3.38361400	-4.80820800	-0.15395500
C	5.07447700	-3.54717000	-0.59416900
H	6.55497500	-2.04391300	-1.01468300
H	5.75959900	-4.37868400	-0.74136200
C	-3.10349500	-1.52084600	0.23207800
C	-2.56544800	-2.76014900	-0.12175200
C	-4.38598200	-1.46721300	0.78484500
H	-1.56779700	-2.79221200	-0.56394800
C	-3.29239900	-3.92885500	0.07826900
C	-5.11574800	-2.63436900	0.97733500
H	-4.81704200	-0.50412800	1.05804800
H	-2.86544800	-4.88889300	-0.20280500
C	-4.56948600	-3.86572900	0.62553100
H	-6.11530400	-2.58406200	1.40356500
H	-5.14357900	-4.77736400	0.77497600
C	-3.27924700	1.28987200	-0.25745000
C	-3.49210100	2.34498400	0.63143300
C	-4.00969700	1.25949800	-1.45174600
H	-2.93338300	2.39806600	1.56397200
C	-4.41716400	3.34375500	0.33675300
C	-4.94221500	2.24578800	-1.73870300
H	-3.84159400	0.44690500	-2.15920900
H	-4.56890400	4.16130900	1.03804700
C	-5.14635700	3.29452800	-0.84427500
H	-5.50819800	2.20202200	-2.66640600
H	-5.87037800	4.07319200	-1.07221300
H	1.04445600	-1.26974900	1.82016100
Pd	0.00350500	-0.14369000	-1.07987700
C	0.91108300	0.78323600	2.53350700

H	0.72154100	0.43787500	3.56182700
H	1.59563700	1.63875700	2.62727100

1_a^{Pd}

G(Gibbs Free Energy) =-2583.668038 hartree

E(electronic Energy) =-2584.141877 hartree

P	2.16226700	-0.09390000	-0.61313900
P	-1.69049000	-0.16266200	-1.00102700
C	1.86501100	0.07019600	-2.43986000
H	2.80769000	0.24652800	-2.97589700
H	1.53135000	-0.92909100	-2.75472200
C	0.80882900	1.14045500	-2.74961300
H	1.26082900	1.93536200	-3.35721100
H	0.48950100	1.63635100	-1.81858100
C	-1.22581500	-0.47834200	-2.78503300
H	-2.13437900	-0.69449500	-3.36402400
C	-2.59410300	1.43041400	-1.11272700
C	-2.28779500	2.41531800	-0.17171900
C	-3.54568100	1.70706900	-2.10067500
H	-1.54194800	2.19613200	0.59400600
C	-2.92299400	3.65297000	-0.21093700
C	-4.17930400	2.94278300	-2.14196600
H	-3.80174900	0.94497200	-2.83687300
H	-2.67856200	4.41121100	0.52905500
C	-3.86765100	3.91647200	-1.19580100
H	-4.91904600	3.14825700	-2.91245000
H	-4.36452100	4.88343900	-1.22887700
C	-3.01595100	-1.42204000	-0.81135000
C	-2.64576600	-2.76855100	-0.92372500
C	-4.33465400	-1.11701200	-0.46839500
H	-1.61053100	-3.02627600	-1.15335200
C	-3.57630800	-3.78088600	-0.72954100
C	-5.26390100	-2.13256600	-0.26340300
H	-4.63726900	-0.07780400	-0.35421600
H	-3.27279000	-4.82077000	-0.82871600
C	-4.89141500	-3.46462700	-0.39916100
H	-6.28659200	-1.87764700	0.00550400
H	-5.62014500	-4.25575700	-0.23951200
C	3.46677700	-1.39087900	-0.60703700
C	3.04061300	-2.71366200	-0.45139800
C	4.82870500	-1.13428400	-0.78033800
H	1.97763000	-2.90999000	-0.29522500

C	3.95328300	-3.76136500	-0.48615600
C	5.74389600	-2.18139000	-0.80063600
H	5.17702800	-0.10812000	-0.89180900
H	3.60877200	-4.78625600	-0.36763600
C	5.30827400	-3.49498300	-0.65767600
H	6.80332900	-1.97045800	-0.92907800
H	6.02642200	-4.31157900	-0.67385900
C	3.07634000	1.44801200	-0.20628900
C	3.77225200	2.22378900	-1.13802600
C	3.04878600	1.86464500	1.12888700
H	3.80020800	1.92856300	-2.18607600
C	4.43609700	3.38034800	-0.74202700
C	3.71940300	3.01529200	1.52679800
H	2.48023500	1.28134000	1.85448300
H	4.97102600	3.97589400	-1.47849800
C	4.41392100	3.77555800	0.59141000
H	3.68952500	3.32554700	2.56888000
H	4.93176200	4.68092600	0.89955100
H	-0.65075100	-1.41548500	-2.76277100
Pd	0.12489300	-0.45097700	0.53701200
C	-0.43153300	0.62775900	-3.47886100
H	-0.13848400	0.25784200	-4.47326700
H	-1.10038800	1.48150800	-3.65853500
C	0.56980700	0.65750600	4.07701700
C	-0.79428900	0.92179600	3.83856500
C	-1.51714800	0.05028400	3.05978900
C	-0.94050200	-1.09466100	2.46003900
C	0.43908500	-1.32947200	2.69205000
C	1.17298600	-0.44786600	3.51910300
H	1.13852800	1.33121000	4.71370700
H	-1.28197100	1.78780000	4.27770900
H	-1.59234500	-1.86687200	2.05463600
H	0.87740900	-2.28440100	2.40792500
H	2.22277700	-0.65886600	3.71383200
Cl	-3.22116400	0.35093500	2.77552700

$TS1_a^{Pd}$

G(Gibbs Free Energy) =-2583.639368 hartree

E(electronic Energy) =-2584.1142353 hartree

P	-1.47264000	0.22846900	-1.11146700
P	2.05250700	0.08211800	-0.41800400
C	-0.97022200	0.11572300	-2.91817400
H	-1.79018000	-0.41079400	-3.42119900
H	-0.94361100	1.12683300	-3.34939100

C	0.34811700	-0.61945700	-3.17793800
H	0.28116500	-1.11900800	-4.15409400
H	0.46467700	-1.42504300	-2.43542100
C	1.90451500	1.09042300	-1.96662700
H	2.83177700	1.65745000	-2.13341300
C	3.53283100	-0.94381900	-0.77148800
C	3.37478200	-2.32978400	-0.82164400
C	4.79363300	-0.38738200	-1.00890900
H	2.39372400	-2.75953600	-0.61494800
C	4.46044300	-3.15006700	-1.11627400
C	5.87636000	-1.20640200	-1.30083600
H	4.92916100	0.69284600	-0.94937200
H	4.33030600	-4.22908300	-1.15069100
C	5.70866500	-2.58859500	-1.35734500
H	6.85562300	-0.76873500	-1.48136100
H	6.55833700	-3.22861800	-1.58399900
C	2.67519100	1.28585200	0.81698300
C	2.81161800	2.65578800	0.58551500
C	2.94199300	0.78589200	2.09875800
H	2.59528500	3.07417000	-0.39555500
C	3.21435100	3.50738200	1.61221100
C	3.35614300	1.63332100	3.11625600
H	2.81305000	-0.28035800	2.29403300
H	3.31352200	4.57337400	1.41867000
C	3.49047100	2.99954300	2.87528800
H	3.56598100	1.22969800	4.10399300
H	3.80578200	3.66583500	3.67476200
C	-1.45440100	2.03788800	-0.77980600
C	-0.80442200	2.50111100	0.36630700
C	-2.04436800	2.96769300	-1.64473200
H	-0.34466800	1.77838700	1.04268700
C	-0.72523100	3.86537400	0.63475800
C	-1.97259700	4.32807300	-1.37435800
H	-2.57737600	2.62187300	-2.53047700
H	-0.19977800	4.20833700	1.52321700
C	-1.30735000	4.77852000	-0.23577300
H	-2.43541300	5.04096300	-2.05303900
H	-1.24626300	5.84460400	-0.02914600
C	-3.26431300	-0.15891100	-1.18099200
C	-3.65288900	-1.38744600	-1.72853100
C	-4.23301000	0.63672800	-0.56550700
H	-2.90081300	-2.04713200	-2.16520800
C	-4.98294600	-1.78668300	-1.70781400
C	-5.56355800	0.23270000	-0.53618700

H	-3.94602500	1.57827600	-0.10067500
H	-5.26878300	-2.73918900	-2.14840700
C	-5.94453000	-0.97325200	-1.11451400
H	-6.30708300	0.86696000	-0.05856500
H	-6.98624200	-1.28470600	-1.09459800
H	1.10622900	1.82715400	-1.78663000
Pd	0.00829900	-0.96448000	0.37039400
C	1.59988900	0.25623000	-3.21008400
H	1.51985500	0.94688300	-4.06326200
H	2.46647200	-0.38640200	-3.42375600
C	-3.75879400	-1.87243800	1.98425900
C	-2.55995400	-2.33114100	1.46187700
C	-1.37114500	-1.69738300	1.84280200
C	-1.37134100	-0.70225800	2.82893900
C	-2.59160700	-0.24797300	3.32427400
C	-3.78661500	-0.82415300	2.90706500
H	-4.68899700	-2.32985400	1.65198700
H	-2.53369000	-3.14037000	0.73543400
H	-0.42803200	-0.28661800	3.18068300
H	-2.59869500	0.55157000	4.06277200
H	-4.73451900	-0.47443900	3.30810000
Cl	0.27301300	-2.91144900	1.90613300

1$^{Pd'}$

G(Gibbs Free Energy) =-2583.681562 hartree

E(electronic Energy) =-2584.160208 hartree

P	1.40597800	-0.36914700	-1.03906200
P	-2.06966400	0.00124600	-0.43709200
C	0.85186800	-0.27632900	-2.82515600
H	1.74845500	-0.05871800	-3.41643000
H	0.53796200	-1.28747700	-3.11650600
C	-0.25693000	0.74424800	-3.10463300
H	-0.03435500	1.27816900	-4.03745700
H	-0.26449800	1.51186400	-2.31467200
C	-2.06230100	-0.81154800	-2.10101700
H	-3.06317000	-1.21446400	-2.30881200
C	-3.42504200	1.21311300	-0.63756100
C	-3.13179400	2.57730300	-0.62306300
C	-4.73753300	0.78954100	-0.86716100
H	-2.11833300	2.90254100	-0.39266700
C	-4.14089900	3.50772000	-0.85199400
C	-5.74301400	1.72095600	-1.09035800
H	-4.97579900	-0.27432300	-0.85592900
H	-3.90918200	4.56971700	-0.83193900

C	-5.44285500	3.08091600	-1.08659000
H	-6.76366900	1.38728100	-1.26264900
H	-6.23124500	3.81022600	-1.25825000
C	-2.77030000	-1.29541800	0.65217600
C	-3.01417100	-2.60471700	0.22838200
C	-3.00564000	-0.95527100	1.99099800
H	-2.82998200	-2.89889000	-0.80257600
C	-3.49119200	-3.55736200	1.12459900
C	-3.48897600	-1.90821900	2.87801100
H	-2.78358800	0.05660100	2.33330400
H	-3.67694400	-4.57299300	0.78217700
C	-3.73144900	-3.21055700	2.44853200
H	-3.66899000	-1.63230300	3.91418300
H	-4.10519900	-3.95507000	3.14773100
C	1.47997300	-2.16431400	-0.70178000
C	0.70725100	-2.69553000	0.33268500
C	2.25028600	-3.02301300	-1.49487400
H	0.10748700	-2.02543500	0.95156400
C	0.69477300	-4.06791700	0.56654900
C	2.24157600	-4.39050500	-1.25586000
H	2.86711300	-2.61521700	-2.29565500
H	0.08262500	-4.47029300	1.37002200
C	1.46149400	-4.91324800	-0.22604500
H	2.84415800	-5.05251400	-1.87314300
H	1.45501600	-5.98509200	-0.04258900
C	3.14946000	0.16468900	-1.14747600
C	3.46908100	1.28667400	-1.91709500
C	4.14057600	-0.43276900	-0.36711400
H	2.69677800	1.78979600	-2.50047600
C	4.76403800	1.78936900	-1.92421600
C	5.43520900	0.07231800	-0.37558600
H	3.89626100	-1.28649300	0.26220500
H	5.00168000	2.66251800	-2.52706000
C	5.74999100	1.18015100	-1.15516300
H	6.19932800	-0.39839500	0.23803700
H	6.76311100	1.57476000	-1.15698000
H	-1.38068600	-1.67294600	-2.03386200
Pd	0.06608900	0.75035700	0.48546000
C	-1.64534300	0.12006800	-3.23581300
H	-1.68565500	-0.45479400	-4.17281100
H	-2.39128500	0.92077000	-3.33754700
C	1.79115600	1.20741800	1.47903800
C	2.23099200	0.34537900	2.48086300
C	3.39413100	0.63704300	3.19350300

C	4.11780700	1.79011800	2.91046600
C	3.66941100	2.65733100	1.91823300
C	2.50890700	2.36797500	1.20413000
H	1.66556700	-0.55552400	2.71996400
H	3.72989100	-0.04042200	3.97712900
H	5.02527400	2.01713000	3.46605200
H	4.22630600	3.56603400	1.69509200
H	2.16831900	3.05306300	0.42779900
Cl	-1.07887200	2.03996200	2.14977900

1_b^{Pd}

G(Gibbs Free Energy) =-3199.117482 hartree

E(electronic Energy) =-3199.6439712 hartree

P	-0.63856800	2.06936500	0.55101400
P	2.90336100	0.54646300	0.23194000
C	0.43359300	3.48092700	1.10600500
H	-0.16231200	4.39810900	1.20699900
H	0.75106100	3.21421200	2.12410200
C	1.64660900	3.68775700	0.18485000
H	1.67010300	4.72944300	-0.16332100
H	1.54125900	3.07351200	-0.72399900
C	3.20730300	1.97702100	1.38380600
H	4.21463800	1.89007700	1.81739400
C	4.30711400	0.60877200	-0.95167200
C	4.26631500	-0.29259900	-2.02230700
C	5.40877900	1.45971400	-0.82903800
H	3.41720100	-0.97084100	-2.11862300
C	5.30509800	-0.34251900	-2.94326100
C	6.44196700	1.41881200	-1.76114900
H	5.47559300	2.15555000	0.00559300
H	5.26282100	-1.05205100	-3.76656300
C	6.39209000	0.51836100	-2.81890500
H	7.29094100	2.09056700	-1.65549700
H	7.20004300	0.48691900	-3.54615700
C	3.42189300	-0.82728200	1.34830000
C	2.42473100	-1.48101500	2.07900800
C	4.74794100	-1.24633100	1.48942100
H	1.38543300	-1.17185400	1.94773700
C	2.74598300	-2.52283300	2.94334900
C	5.06816700	-2.29377400	2.34660400
H	5.53533200	-0.75483600	0.91882300
H	1.95804300	-3.02240400	3.50311300
C	4.06908400	-2.93292200	3.07606600
H	6.10342800	-2.61261600	2.44640400

H	4.32215600	-3.75263300	3.74463200
C	-1.77373300	1.83895800	1.97448100
C	-1.88585000	0.56753800	2.53801900
C	-2.55058900	2.88375300	2.48571300
H	-1.29504000	-0.25019400	2.12344600
C	-2.76238200	0.33874500	3.59472200
C	-3.41543700	2.65929800	3.54831400
H	-2.49201800	3.87420600	2.03423000
H	-2.85878400	-0.66024200	4.01296100
C	-3.52319400	1.38496900	4.10156600
H	-4.01791100	3.47572300	3.94017000
H	-4.21189000	1.20744400	4.92428500
C	-1.76172700	2.84338600	-0.67742400
C	-1.52370900	4.07921700	-1.28016800
C	-2.88023600	2.10064700	-1.07788300
H	-0.65910000	4.67474900	-0.99125700
C	-2.38700100	4.56477700	-2.26015000
C	-3.74430700	2.58971400	-2.04647200
H	-3.07724800	1.13328900	-0.61199400
H	-2.18864100	5.52964800	-2.72169900
C	-3.49769200	3.82437600	-2.64371400
H	-4.61279400	2.00397900	-2.33818500
H	-4.17132100	4.20605200	-3.40721700
H	2.51024000	1.77907400	2.21250800
Pd	0.59377300	0.25688900	-0.35171100
C	2.99877300	3.38720200	0.83018200
H	3.15984500	4.09489500	1.65794700
H	3.78163300	3.60728200	0.09075900
C	0.38290100	-1.59373900	-1.64926500
C	-0.92147700	-1.21135500	-1.25216600
C	-1.53467500	-1.96774800	-0.22423200
C	-0.91549600	-3.01937200	0.39424700
C	0.38129200	-3.40267800	-0.00934300
C	1.01729100	-2.69558100	-1.01066700
H	0.81550600	-1.23020900	-2.57981800
H	-1.53206500	-0.55029800	-1.86409300
H	-1.42683500	-3.55991900	1.18551100
H	0.86394100	-4.24095600	0.48247700
O	2.26444700	-2.95405500	-1.46895100
C	3.05243900	-3.88139000	-0.75529400
H	3.09442900	-3.62764500	0.31319300
H	2.67222900	-4.90581200	-0.87310800
H	4.05834000	-3.81881000	-1.17756800
O	-5.03701700	-1.95429800	1.07907700

S	-4.12543000	-2.39278800	0.05354800
O	-3.81389700	-3.78018200	-0.19184600
O	-2.79196400	-1.50519900	0.22858600
C	-4.74072600	-1.69858700	-1.54125500
F	-4.95587700	-0.40075600	-1.40814600
F	-5.86950200	-2.30525800	-1.85354000
F	-3.84530800	-1.90382800	-2.49078300

$TS1_b^{Pd}$

G(Gibbs Free Energy) =-3199.082381 hartree

E(electronic Energy) =-3199.6056655 hartree

C	-0.76588600	-2.93030700	-0.03875700
C	0.15287000	-3.92720900	0.21256600
C	1.48069800	-3.83717300	-0.25981600
C	1.88151900	-2.75598700	-1.02781800
C	0.96781800	-1.71343300	-1.28417400
C	-0.29061800	-1.78543900	-0.67997700
H	-1.78632000	-2.98312400	0.33452400
H	-0.12041700	-4.79865900	0.80377900
H	2.87641800	-2.69984000	-1.46107600
H	1.20548900	-0.93268400	-2.00466200
O	2.27856100	-4.88573700	0.07573400
C	3.57762700	-4.90619300	-0.46279800
H	4.16824100	-4.03659500	-0.13556900
H	4.05161600	-5.81987700	-0.09816900
H	3.55911600	-4.92571500	-1.56203400
O	-1.78303300	-1.23826000	-2.02399400
S	-1.55975500	-0.02982900	-2.89536200
O	-0.40661300	0.78017000	-2.46439400
O	-2.78660300	0.67116500	-3.24507700
C	-0.98615000	-0.78468000	-4.47153800
F	-1.92096300	-1.57770300	-4.97127700
F	0.11560100	-1.50189600	-4.26296200
F	-0.71045100	0.16771400	-5.35173900
P	-1.71391600	0.46919500	1.58509600
P	1.90655000	1.39001400	0.98302700
C	-1.16829400	1.52156300	3.00867000
H	-2.01328700	1.68247800	3.69061700
H	-0.45787100	0.89737900	3.56682300
C	-0.52301000	2.83847800	2.55322500
H	-1.14656100	3.68444900	2.86843100
H	-0.50537800	2.89124300	1.45238600
C	1.89988200	1.95937700	2.75137500
H	2.91417700	2.27325400	3.03288300

C	2.39217000	2.87296400	0.03683200
C	1.73382500	3.11124700	-1.17333400
C	3.36746100	3.77374800	0.48064100
H	0.96887700	2.41578400	-1.52413300
C	2.05444100	4.23475600	-1.93043400
C	3.68238200	4.89422800	-0.27709700
H	3.89053200	3.59462800	1.42022700
H	1.53792300	4.41303600	-2.87002300
C	3.02421100	5.12425100	-1.48332200
H	4.44099400	5.59059000	0.07259300
H	3.26979100	6.00339300	-2.07455500
C	3.37208000	0.28413600	0.99874000
C	3.23039200	-0.94475400	1.65551500
C	4.56673500	0.56059400	0.33254900
H	2.28013200	-1.19927100	2.12884200
C	4.26999200	-1.86416300	1.67169200
C	5.60303300	-0.36988100	0.33448800
H	4.68731100	1.50338700	-0.19802800
H	4.14091800	-2.81538400	2.18502600
C	5.46104400	-1.57778800	1.00782000
H	6.52733000	-0.14557100	-0.19290500
H	6.27401600	-2.30072600	1.01010100
C	-2.32173700	-1.03726600	2.43149800
C	-1.37181700	-1.86967100	3.03517700
C	-3.66193600	-1.42758600	2.43185700
H	-0.31581200	-1.59544900	2.99891700
C	-1.75472400	-3.05642200	3.64493400
C	-4.04258100	-2.62630600	3.02888900
H	-4.41079100	-0.79626200	1.95736600
H	-1.00546800	-3.69318100	4.10970400
C	-3.09348400	-3.43981100	3.63720100
H	-5.08839700	-2.92394900	3.01718000
H	-3.39453500	-4.37645800	4.10023400
C	-3.22294300	1.29128600	0.97229800
C	-3.83705600	2.35663200	1.63767200
C	-3.77611200	0.82224200	-0.22298500
H	-3.42767600	2.74053000	2.56957300
C	-4.98297700	2.94249600	1.11250400
C	-4.92143400	1.41006800	-0.74542500
H	-3.30487700	-0.00417200	-0.75413100
H	-5.45131700	3.77345900	1.63505200
C	-5.52498300	2.47111900	-0.07900400
H	-5.31778000	1.04713500	-1.68979600
H	-6.41525900	2.93874200	-0.49299100

H	1.69773900	1.05014200	3.33614700
Pd	0.12223100	0.00987100	0.14737700
C	0.89485500	3.06280200	3.07594400
H	0.86909700	3.19067900	4.16810400
H	1.26604200	4.01243200	2.66620300

1^{Pd}

G(Gibbs Free Energy) =-3199.135345 hartree

E(electronic Energy) =-3199.6619974 hartree

C	2.31728700	1.39436700	-1.02564100
C	3.51200500	2.10243000	-1.04952500
C	4.19165500	2.38035200	0.13811100
C	3.65465600	1.96991800	1.35760400
C	2.45973700	1.25023800	1.36902500
C	1.79252600	0.94962400	0.18762100
H	1.78458900	1.21281200	-1.95756500
H	3.93987900	2.45860900	-1.98393800
H	4.15749900	2.18293500	2.29691300
H	2.07133000	0.90291600	2.32675300
O	5.36861100	3.05140000	0.00428100
C	6.10368100	3.30649400	1.17168200
H	6.37824400	2.37527400	1.69157000
H	7.01499800	3.82300000	0.86238500
H	5.55158800	3.94876700	1.87339900
O	-0.79179100	1.34053300	-2.28646900
S	-1.48597100	2.18113400	-1.29940000
O	-1.01551300	1.94862800	0.11052000
O	-2.93822200	2.27393400	-1.41983300
C	-0.86966200	3.88159800	-1.62544900
F	-1.22864300	4.25224200	-2.84791700
F	0.45189900	3.92120400	-1.53699000
F	-1.38675900	4.72994700	-0.74855300
P	1.31474500	-1.85328900	0.18441600
P	-2.19661500	-0.95399500	0.96079300
C	0.56089300	-3.44689000	0.75062400
H	1.30117500	-4.23400900	0.55936600
H	0.44241900	-3.39839700	1.84070400
C	-0.77498300	-3.73891400	0.05417800
H	-0.70065500	-4.69013800	-0.48605500
H	-0.97660800	-2.98853500	-0.72570200
C	-2.17377400	-2.56894600	1.87637100
H	-3.10901900	-2.66641600	2.44371800
C	-3.49354600	-1.22137600	-0.29954600
C	-3.20917100	-0.99751600	-1.64674400

C	-4.77003800	-1.65779900	0.07362500
H	-2.23215900	-0.61524000	-1.94241400
C	-4.18836100	-1.21706900	-2.61163800
C	-5.74138700	-1.88271100	-0.89142700
H	-5.00833200	-1.80707000	1.12676400
H	-3.96393200	-1.02323100	-3.65717300
C	-5.44846200	-1.66366400	-2.23621400
H	-6.73190000	-2.22077000	-0.59612000
H	-6.21284500	-1.83234900	-2.99117900
C	-2.98161400	0.16839300	2.17328800
C	-2.83791900	-0.02806100	3.54953700
C	-3.67019500	1.29435500	1.70854700
H	-2.29532700	-0.89034200	3.93313200
C	-3.39094600	0.87610900	4.45038900
C	-4.22340700	2.19061700	2.61383000
H	-3.76187800	1.48070500	0.63887000
H	-3.27775900	0.71024600	5.51929200
C	-4.08752600	1.98442400	3.98333400
H	-4.75778700	3.06141800	2.24251600
H	-4.52047700	2.69150300	4.68707200
C	2.93834300	-1.83913500	1.01510900
C	3.00196500	-2.07618100	2.39078500
C	4.09575200	-1.45657200	0.33302100
H	2.10244300	-2.34240000	2.94571000
C	4.20627500	-1.94249900	3.07186000
C	5.29696600	-1.32021600	1.01666700
H	4.05094600	-1.23317300	-0.73096900
H	4.24515600	-2.12877700	4.14237900
C	5.35510900	-1.56344600	2.38532300
H	6.18835200	-1.00846200	0.47747400
H	6.29568000	-1.45195000	2.91948800
C	1.64823200	-2.21845600	-1.57395700
C	2.47679800	-3.29035100	-1.92635200
C	1.01838300	-1.47540200	-2.57488100
H	2.98275400	-3.86896800	-1.15379000
C	2.67723800	-3.60903800	-3.26248700
C	1.22023000	-1.80220800	-3.91315800
H	0.37451800	-0.63352600	-2.31448300
H	3.32692700	-4.43901400	-3.52951600
C	2.04695300	-2.86463400	-4.25691500
H	0.72874500	-1.21552700	-4.68490200
H	2.20485400	-3.11516400	-5.30325900
H	-1.36892700	-2.48167300	2.62068900
Pd	-0.00978000	-0.00331100	0.36369200

C	-1.96992800	-3.80139700	1.00009400
H	-1.86901200	-4.67595500	1.65939900
H	-2.87775700	-3.96881200	0.40493800

2^{Pd}

G(Gibbs Free Energy) =-4652.912226 hartree

E(electronic Energy) =-4653.4318118 hartree

C	-2.26204300	-1.96814700	0.70114600
C	-3.63151800	-2.01855300	0.89951800
C	-4.34020800	-0.84398000	1.17345200
C	-3.65448600	0.36659700	1.33006300
C	-2.27560000	0.39046200	1.18982200
C	-1.53761500	-0.76036900	0.84536300
H	-1.74231000	-2.88600300	0.42149300
H	-4.19027300	-2.94569500	0.79594400
H	-4.18000200	1.29108900	1.54972300
H	-1.75572700	1.33894000	1.31904500
O	-5.67695100	-0.97494000	1.25296900
C	-6.44897400	0.19554800	1.42316900
H	-6.28032300	0.90558300	0.60204400
H	-7.49272700	-0.12244400	1.41750900
H	-6.22951000	0.68871500	2.37921800
O	-0.06708200	2.44428600	-1.04111300
S	-0.44937700	3.87998200	-1.13868300
O	-1.44552200	4.15977000	-2.17585000
O	0.68740600	4.79669900	-1.03628500
C	-1.36825900	4.12873100	0.43369800
F	-0.63286500	3.73167700	1.47283100
F	-2.49698000	3.40830000	0.43068000
F	-1.69112100	5.40174900	0.60476100
P	-0.51200500	-0.62407700	-1.93401100
P	2.60002400	0.58433900	-0.52840300
C	0.36989100	0.19138900	-3.32744700
H	-0.24380800	0.03530200	-4.22376200
H	0.34015700	1.26563800	-3.10444500
C	1.79912300	-0.33309200	-3.50594200
H	1.88463900	-0.83030700	-4.47995400
H	2.02018200	-1.12416900	-2.77146300
C	2.84992700	1.53952900	-2.09337400
H	3.78015800	2.11019500	-1.97696400
C	3.80828600	-0.78614200	-0.56771700
C	3.47432600	-2.00105700	0.03458900
C	5.07575600	-0.63354100	-1.13886900
H	2.49904700	-2.11412500	0.50841100

C	4.38244500	-3.05434600	0.05124300
C	5.98097900	-1.68774700	-1.12696700
H	5.36366400	0.31999900	-1.58034100
H	4.10810000	-3.99263700	0.52809200
C	5.63327100	-2.89980600	-0.53600000
H	6.96338800	-1.56208300	-1.57577200
H	6.34433100	-3.72252600	-0.52791700
C	3.27553300	1.73749500	0.71596300
C	2.74271100	3.02785500	0.78594000
C	4.25068900	1.33760100	1.63253500
H	1.97234700	3.35785800	0.09247600
C	3.19323000	3.90974600	1.75981900
C	4.69618100	2.22742000	2.60319100
H	4.65554800	0.32770500	1.59908100
H	2.76808100	4.90985900	1.79979900
C	4.16787100	3.51243800	2.66942300
H	5.45512600	1.91066400	3.31478700
H	4.51481900	4.20366700	3.43413400
C	-2.25886900	-0.17002300	-2.21516300
C	-2.57306800	1.18009400	-2.40103100
C	-3.28508400	-1.11971500	-2.21421000
H	-1.80103100	1.94239100	-2.40623800
C	-3.89515300	1.57528100	-2.55816000
C	-4.60682100	-0.71846600	-2.37709900
H	-3.05762500	-2.17551100	-2.08246200
H	-4.10672600	2.63420800	-2.68648000
C	-4.91464300	0.62888700	-2.54171300
H	-5.39838900	-1.46469100	-2.36602700
H	-5.95072800	0.93766900	-2.66456600
C	-0.37766600	-2.40438700	-2.32880400
C	-0.79683600	-2.89440700	-3.57096200
C	0.20482000	-3.28082200	-1.41227600
H	-1.25805500	-2.22445200	-4.29596000
C	-0.64016400	-4.23956800	-3.88012500
C	0.35985400	-4.62808000	-1.72140200
H	0.53805900	-2.90302000	-0.44547000
H	-0.96945100	-4.61313500	-4.84663800
C	-0.06226900	-5.10712700	-2.95602600
H	0.81174300	-5.29623200	-0.99186200
H	0.05857700	-6.15920100	-3.20277900
H	2.03639000	2.27728400	-2.07849200
Pd	0.40091000	-0.19015100	0.15064200
C	2.87160500	0.74158500	-3.39434200
H	2.77354900	1.45192400	-4.22716300

H	3.85098900	0.25956400	-3.51629800
Zn	-0.45521100	-1.47524900	2.58453300
Cl	0.47616500	-3.69950800	2.39195800
Cl	-1.70378700	-1.85383700	4.54404700
Li	-0.70671700	-3.85581200	4.30977800
Cl	1.18554600	0.13725200	2.54573300

TS2

G(Gibbs Free Energy) =-4652.883826 hartree

E(electronic Energy) =-4653.401504 hartree

C	-2.81049500	-2.21312500	1.75473500
C	-4.15211800	-2.17638700	1.40281500
C	-4.81294500	-0.94706800	1.31712700
C	-4.11937200	0.23343000	1.56957200
C	-2.77208500	0.16752300	1.92551600
C	-2.07754000	-1.04445100	2.03185400
H	-2.32446700	-3.18840500	1.82837100
H	-4.72081000	-3.08296600	1.20387400
H	-4.60124900	1.20334600	1.48165300
H	-2.25568600	1.10881100	2.10880400
O	-6.12751100	-1.00752400	0.95921700
C	-6.85279700	0.19787000	0.95483700
H	-6.46699700	0.90413800	0.20426400
H	-7.88481700	-0.06027800	0.70615800
H	-6.83178500	0.68656800	1.93904100
O	-1.21471200	2.06462400	0.13386900
S	-0.86229200	3.27919100	-0.67330300
O	-2.00651300	3.97915700	-1.23991900
O	0.28002500	3.04157100	-1.58339800
C	-0.19812100	4.43757100	0.59083300
F	0.88468500	3.92774400	1.16791800
F	-1.11121700	4.67025500	1.51897000
F	0.13443900	5.58418200	0.01025600
P	-0.68496400	-0.40168000	-2.02933100
P	2.52033800	0.20890800	-1.00915200
C	0.01248600	-0.00910700	-3.68586200
H	-0.76397500	-0.27504300	-4.41407100
H	0.11443500	1.08341300	-3.73462400
C	1.33873000	-0.72166200	-3.97175200
H	1.28991600	-1.18549300	-4.96467000
H	1.48503400	-1.56324200	-3.27803900
C	2.69504100	1.03179000	-2.65926600
H	3.67829300	1.51937900	-2.64354300

C	3.32665100	-1.41235900	-1.07449300
C	2.79177100	-2.46578000	-0.33532800
C	4.51528500	-1.59636600	-1.79250700
H	1.89029600	-2.31866900	0.25540500
C	3.42046000	-3.70620700	-0.33135200
C	5.13734500	-2.83748300	-1.78881900
H	4.96642900	-0.76544200	-2.33384500
H	2.98831400	-4.51517500	0.25305400
C	4.58608300	-3.89343000	-1.06447100
H	6.05876700	-2.98149800	-2.34753500
H	5.07760200	-4.86337300	-1.06699300
C	3.58490800	1.25551000	0.02703800
C	3.37057400	2.63764100	0.02139400
C	4.55562400	0.69764100	0.86058300
H	2.57522200	3.07183600	-0.58425900
C	4.13822500	3.45370100	0.84040600
C	5.32350200	1.52466100	1.67081400
H	4.70294200	-0.38020700	0.88705500
H	3.95756800	4.52552800	0.84791800
C	5.11486200	2.89957900	1.66239000
H	6.07953000	1.09058800	2.32014400
H	5.70854700	3.54197500	2.30808800
C	-2.41836500	0.11218600	-2.15493900
C	-2.73219600	1.35960200	-2.70487900
C	-3.43902100	-0.73718400	-1.71929400
H	-1.94933800	2.05385000	-3.00317100
C	-4.05807800	1.74180500	-2.83772500
C	-4.76637300	-0.35494000	-1.87434600
H	-3.20520400	-1.69191800	-1.25130600
H	-4.29059600	2.72320600	-3.24176600
C	-5.07451400	0.88030900	-2.43374900
H	-5.55548400	-1.01434100	-1.51922900
H	-6.11465500	1.18053600	-2.54356500
C	-0.73344200	-2.22269600	-1.95695100
C	-1.00886900	-2.97317000	-3.10672800
C	-0.54890400	-2.87791900	-0.73998500
H	-1.17953600	-2.47843400	-4.06183900
C	-1.07397300	-4.35784900	-3.03537400
C	-0.61111000	-4.26608000	-0.67100400
H	-0.37248200	-2.30427100	0.17012800
H	-1.28602700	-4.93445300	-3.93232300
C	-0.86872600	-5.00518500	-1.81864400
H	-0.45186900	-4.75230400	0.28943200
H	-0.91600000	-6.09035000	-1.76846400

H	1.95278500	1.84220600	-2.63023100
Pd	0.38010200	0.43064300	-0.15439900
C	2.55569200	0.18700400	-3.91979900
H	2.53008500	0.88343000	-4.76999600
H	3.45270300	-0.43025900	-4.05837500
Zn	-0.24348200	-1.05435900	2.86255700
Cl	0.92568500	-3.29704200	2.53839000
Cl	0.19359400	-1.02646500	5.24881600
Li	1.18152600	-2.92752000	4.72299800
Cl	1.26619900	0.68980400	2.13061200

$Pd^{II'}$

G(Gibbs Free Energy) =-3313.516783 hartree

E(electronic Energy) =-3313.9309663 hartree

O	1.37838600	2.57354300	0.32893100
S	2.31815000	1.87646900	-0.54918000
O	1.69665600	0.68840200	-1.25898300
O	3.64075700	1.56199100	-0.01373900
C	2.62695600	3.01930700	-1.95599900
F	3.20815800	4.12077900	-1.49662100
F	1.49535100	3.34191100	-2.55176100
F	3.43523200	2.44208400	-2.83546900
Cl	-1.38621900	1.56309200	-1.88917500
P	1.00703200	-1.57117100	0.66782900
P	-2.27486700	-0.24745200	0.43914000
C	0.12261100	-3.04973400	1.36460300
H	0.82152000	-3.89019100	1.27389800
H	0.01231200	-2.86395200	2.44124500
C	-1.22988800	-3.37593600	0.72880000
H	-1.32789600	-4.46261100	0.61088400
H	-1.28834400	-2.96269100	-0.29042500
C	-2.37860800	-1.38850300	1.89505800
H	-3.28136100	-1.11051800	2.45536600
C	-3.58854900	-0.86370500	-0.65930300
C	-3.30688700	-1.20518600	-1.98271800
C	-4.87883200	-1.06021900	-0.15261400
H	-2.31193100	-1.01858400	-2.38203400
C	-4.30511600	-1.74150600	-2.78894800
C	-5.87385100	-1.58941300	-0.96442600
H	-5.11327600	-0.78802700	0.87623700
H	-4.08073700	-1.99990900	-3.82046300
C	-5.58520000	-1.93283900	-2.28246200
H	-6.87602700	-1.73224900	-0.56810200
H	-6.36478600	-2.34721000	-2.91710900

C	-2.81201200	1.33472700	1.15401200
C	-2.09232200	1.84858100	2.23650300
C	-3.87565400	2.06202600	0.61927400
H	-1.23012100	1.31013400	2.63020600
C	-2.45508100	3.06576300	2.79744300
C	-4.23513900	3.27819700	1.18675500
H	-4.40955500	1.68697000	-0.25063600
H	-1.88813300	3.46444800	3.63454100
C	-3.52983500	3.77858300	2.27550700
H	-5.06261300	3.84353800	0.76585200
H	-3.80888200	4.73483900	2.71090900
C	1.99503200	-0.99385100	2.08301900
C	1.85660600	0.31001700	2.55880000
C	2.87534700	-1.87837000	2.71873600
H	1.21734500	1.02093800	2.03556100
C	2.59071000	0.72407200	3.66679800
C	3.59857000	-1.46114100	3.82646300
H	3.00782300	-2.88963100	2.33512500
H	2.49631600	1.74801400	4.01793200
C	3.45418900	-0.15893400	4.30127700
H	4.28456600	-2.14838500	4.31556400
H	4.03013000	0.16902500	5.16330200
C	2.18850000	-2.30755300	-0.50697200
C	1.82980400	-3.44134000	-1.24286500
C	3.42951200	-1.70127100	-0.72593700
H	0.86004500	-3.91515600	-1.09415700
C	2.71033400	-3.97707700	-2.17467500
C	4.30687000	-2.24876200	-1.65336000
H	3.70461300	-0.79327000	-0.19105400
H	2.42600700	-4.86005500	-2.74176600
C	3.95132100	-3.38228900	-2.37700200
H	5.27107900	-1.77510500	-1.81780900
H	4.64101800	-3.80089500	-3.10600700
H	-1.52944500	-1.13961700	2.54753800
Pd	-0.21268400	0.07122600	-0.46448700
C	-2.40817900	-2.87482200	1.55520800
H	-2.44268700	-3.43416600	2.50142000
H	-3.34299100	-3.10616600	1.02784200

3^{Ni}

G(Gibbs Free Energy) =-3155.430997 hartree

E(electronic Energy) =-3155.71966 hartree

C	2.50250600	0.01744900	-1.41750200

C	2.95997600	-0.40259000	-2.66044700
C	2.03932000	-0.69550700	-3.65849500
C	0.68690600	-0.55605400	-3.39401000
C	0.29769700	-0.13553400	-2.12925900
N	1.18278000	0.13516500	-1.17264200
H	2.38125400	-1.03070900	-4.63354700
H	4.02465100	-0.49374600	-2.85204700
H	-0.06882700	-0.79048900	-4.13609100
H	-0.75320300	-0.02709500	-1.86218000
C	3.39069900	0.38534000	-0.29934900
C	4.77558800	0.24731400	-0.31465900
C	3.44410700	1.22734900	1.86790400
C	5.49692700	0.62343300	0.81059500
H	5.28458600	-0.16032500	-1.18258300
H	2.84179300	1.58924300	2.70052600
H	6.57853900	0.51892100	0.82093400
C	4.82784500	1.12166200	1.92150700
H	5.36122600	1.41450000	2.81997300
N	2.76310600	0.87645400	0.77951200
Ni	0.73126000	0.69829700	0.68536900
C	0.73305800	4.61723800	-0.81401000
C	1.15075200	3.47189200	-0.13271900
C	0.25781000	2.42404500	-0.03082200
C	-1.02871300	2.47495800	-0.53127500
C	-1.42799000	3.62660300	-1.20919800
C	-0.54778800	4.69435900	-1.35164700
H	1.41888300	5.45614100	-0.91324600
H	2.14277500	3.42240400	0.30909700
H	-1.72804500	1.65195800	-0.39559500
H	-2.43990800	3.67371100	-1.60893100
H	-0.86324100	5.59425600	-1.87395300
Cl	0.10892800	1.58682700	2.59665600
Cl	1.02162700	-1.56657900	1.46784100
C	-3.58655400	0.80634200	1.06370300
C	-2.66010900	-0.23393300	1.17968000
C	-2.33384900	-1.08413700	0.11518200
C	-3.01190200	-0.84515500	-1.09493300
C	-3.92675300	0.18911900	-1.24433200
C	-4.21223700	1.02775900	-0.16167100
H	-3.77563100	1.44834100	1.91995000
H	-2.16212800	-0.35209600	2.14338500
H	-2.81159400	-1.48365900	-1.95949300
H	-4.43841800	0.37466400	-2.18683300
Zn	-0.91940300	-2.50648300	0.38697200

Cl	-1.18755800	-4.66646500	1.44054400
Cl	0.01776500	-3.47081600	-1.74255700
Li	-0.25905000	-5.27632100	-0.47786000
O	-5.09130900	2.03687700	-0.40984200
C	-5.34049500	2.94548900	0.63383600
H	-6.03715600	3.68915000	0.24080700
H	-4.41866500	3.45058200	0.95933200
H	-5.79739500	2.45393700	1.50450100

TS3

G(Gibbs Free Energy) =-3155.42222 hartree

E(electronic Energy) =-3155.7113701 hartree

C	2.77150900	0.16448500	1.12804700
C	3.49410700	0.55602800	2.25115000
C	2.85200300	0.63982600	3.47805000
C	1.50972400	0.30224900	3.56010700
C	0.85091000	-0.06418200	2.39574100
N	1.45433800	-0.10456500	1.20867800
H	3.40319300	0.94386900	4.36368800
H	4.55700900	0.76217800	2.17117200
H	0.97007700	0.33036800	4.50072800
H	-0.19734000	-0.34707300	2.40012600
C	3.40083000	-0.07235200	-0.18469000
C	4.66864600	0.38856500	-0.52427000
C	3.13479000	-1.07263700	-2.24956800
C	5.16927500	0.08723900	-1.78390800
H	5.24353600	0.99796600	0.16670300
H	2.45616500	-1.62364200	-2.89924100
H	6.15132300	0.44664400	-2.07998800
C	4.39871400	-0.66434300	-2.65981400
H	4.75514000	-0.91639400	-3.65356900
N	2.65602700	-0.78447300	-1.04251000
Ni	0.51428800	-0.61932200	-0.54016100
C	1.08711400	-4.34184200	1.24448800
C	1.27961800	-3.15966300	0.52913300
C	0.16714200	-2.40805400	0.19035100
C	-1.12328000	-2.82999400	0.45461200
C	-1.29408900	-4.01186600	1.17601400
C	-0.19541600	-4.76423500	1.57531700
H	1.95337700	-4.93202500	1.53687500
H	2.28186200	-2.83767400	0.26161000
H	-1.98439300	-2.27134000	0.10293500
H	-2.30343800	-4.34757800	1.40455200
H	-0.33919300	-5.68938300	2.12827800

Cl	-0.07580500	-1.67952700	-2.42777800
Cl	1.09051800	1.68287800	-1.65686900
C	-3.75853500	-0.45639800	-1.11313500
C	-2.45552400	0.03208500	-1.15479800
C	-1.70072500	0.32273800	-0.00170500
C	-2.39466200	0.16871900	1.22230000
C	-3.69097700	-0.30714600	1.29919600
C	-4.37713200	-0.64108700	0.12456300
H	-4.27885800	-0.67550100	-2.04095300
H	-2.00191700	0.17444100	-2.13472200
H	-1.92173900	0.46754700	2.15945700
H	-4.21124800	-0.41554700	2.24816600
Zn	-0.64523800	2.09070900	-0.19971500
Cl	-1.99026900	3.97106600	-0.91037300
Cl	0.11262900	3.16073900	1.87685600
Li	-1.12253800	4.78464500	0.95708500
O	-5.63339800	-1.11038100	0.29228100
C	-6.37501200	-1.43632500	-0.86060900
H	-7.34571300	-1.79432500	-0.51250400
H	-5.88745000	-2.22885400	-1.44481100
H	-6.52549100	-0.56007700	-1.50588000

4^{Ni}

G(Gibbs Free Energy) =-3155.447916 hartree

E(electronic Energy) =-3155.7359449 hartree

C	-2.14788500	-2.15889100	0.72614500
C	-1.99980000	-3.39566100	1.34660500
C	-0.85824900	-3.64160700	2.09915700
C	0.09868400	-2.64637400	2.22292900
C	-0.11337800	-1.44630000	1.55635900
N	-1.19812900	-1.21058500	0.82209400
H	-0.72199400	-4.60536300	2.58224800
H	-2.75836600	-4.16477800	1.23805500
H	1.01072600	-2.78618200	2.79531100
H	0.62060900	-0.64329800	1.61241300
C	-3.34008300	-1.77735800	-0.05713400
C	-4.48843400	-2.56178500	-0.13853700
C	-4.29729900	-0.14958100	-1.40215500
C	-5.56738600	-2.10049900	-0.87868400
H	-4.54470400	-3.51635500	0.37533000
H	-4.14205700	0.80222200	-1.90606100
H	-6.47265300	-2.69744600	-0.95163500
C	-5.47642500	-0.87267900	-1.51997300
H	-6.29774900	-0.47744200	-2.10891700

N	-3.26313200	-0.59250800	-0.68655900
Ni	-1.50018300	0.43438500	-0.52545700
C	-3.31631700	2.58678000	2.52161400
C	-2.60445400	1.61496300	1.81844600
C	-2.24564900	1.85539500	0.49731800
C	-2.56743900	3.05393400	-0.12686800
C	-3.27940100	4.01844000	0.58612100
C	-3.65333500	3.78832700	1.90645100
H	-3.60885200	2.39922400	3.55323200
H	-2.33465500	0.67779700	2.30564400
H	-2.26873400	3.22454500	-1.15915300
H	-3.53467900	4.96013000	0.10366800
H	-4.20444300	4.54671600	2.45785900
Cl	-1.63387600	0.99744100	-2.77889400
Cl	1.51682700	-2.52485200	-1.23995000
C	2.46541500	1.38804200	-1.02824300
C	1.11425800	1.05401700	-1.18603100
C	0.18018600	1.29311600	-0.16749100
C	0.63535700	1.91119200	0.99922000
C	1.97603700	2.25863100	1.16932200
C	2.88391300	1.99444500	0.15944100
H	3.15655500	1.24149800	-1.85651800
H	0.79394800	0.60944800	-2.12551100
H	-0.05700500	2.12590900	1.81071300
H	2.32623100	2.71865500	2.09038900
Zn	2.98778600	-1.14171900	-0.37056200
Cl	5.19286900	-0.68146800	-1.01209100
Cl	3.31349700	-0.88388300	1.95412100
Li	4.95539900	0.48788300	1.01105000
O	4.22898400	2.26217500	0.40955500
C	4.92981800	2.93138500	-0.64497200
H	5.84466900	3.33687400	-0.20670200
H	4.31832600	3.75109500	-1.03586300
H	5.18995500	2.23550900	-1.45160200

5^{Ni}

G(Gibbs Free Energy) =-1701.669029 hartree

E(electronic Energy) =-1701.9669667 hartree

C	0.64309100	-1.45367300	3.32487800
C	0.46530800	-0.67917400	2.17890500
C	0.36117100	-1.29817300	0.93783900
C	0.42088200	-2.68504200	0.83630900
C	0.59854100	-3.45274500	1.98641200

C	0.70891300	-2.84000800	3.23108000
H	0.72364600	-0.96840900	4.29630800
H	0.38814600	0.40434800	2.27384200
H	0.31266000	-3.15971400	-0.13825500
H	0.64068000	-4.53756800	1.90692100
H	0.83989400	-3.44236400	4.12731300
C	2.86091600	0.98118000	-0.27410900
C	4.23753100	1.19053400	-0.24490000
C	5.07741700	0.20803000	-0.75101800
C	4.52539100	-0.95052800	-1.27933400
C	3.14242200	-1.08220800	-1.28979100
N	2.33845700	-0.14010200	-0.79825200
H	6.15460400	0.35183700	-0.73634800
H	4.65183600	2.11041300	0.15649200
H	5.14817700	-1.74050100	-1.68679500
H	2.63260400	-1.94400400	-1.71974100
C	1.87918000	1.95412800	0.24893300
C	2.23895500	3.09359200	0.96618500
C	-0.36757800	2.47076500	0.45935100
C	1.24179100	3.93972100	1.43009300
H	3.28182400	3.31166300	1.17531600
H	-1.39026200	2.16283600	0.24089900
H	1.50253900	4.83085300	1.99501500
C	-0.08687000	3.63016900	1.17063200
H	-0.89578000	4.26550100	1.51717700
N	0.58956500	1.65812900	0.01088500
Ni	0.28686800	-0.35095300	-0.71362800
C	-2.15418300	0.41237100	-1.52287300
C	-3.49955000	0.74904800	-1.54357800
C	-4.34423800	0.31949200	-0.51700800
C	-3.82455500	-0.44452400	0.52333700
C	-2.46299200	-0.76401700	0.54333700
C	-1.61327400	-0.33207100	-0.46513500
H	-1.52196400	0.73147800	-2.35180900
H	-3.92687000	1.32558900	-2.36088200
H	-4.46009000	-0.79996200	1.32990100
H	-2.08948200	-1.35641600	1.37494000
O	-5.64747100	0.69559300	-0.62653100
C	-6.53804100	0.24152400	0.35886800
H	-6.27217700	0.61911000	1.35755600
H	-7.52525800	0.62234800	0.08826100
H	-6.57736900	-0.85681200	0.39883800
Cl	0.23368100	-1.62028200	-2.62294300

TS4

G(Gibbs Free Energy) =-1701.66492 hartree

E(electronic Energy) =-1701.9629817 hartree

C	0.17598000	0.05791600	-3.62072900
C	-0.03811800	-0.32841100	-2.29973100
C	-0.11689000	0.63524300	-1.29829500
C	-0.02230300	1.98865600	-1.63157500
C	0.20189700	2.36722300	-2.95237400
C	0.30292200	1.40316800	-3.95107700
H	0.23457900	-0.70165200	-4.39825800
H	-0.15844200	-1.38351200	-2.06350200
H	-0.12547100	2.74116300	-0.84883200
H	0.29256700	3.42309900	-3.20031700
H	0.46729800	1.69999600	-4.98431400
C	3.09489200	-0.23764300	0.59464300
C	4.46938300	-0.03195400	0.70728800
C	4.94019000	1.24300800	0.98573000
C	4.03074300	2.27694600	1.15360100
C	2.67582100	1.99049900	1.04959900
N	2.22297000	0.76574200	0.77535600
H	6.00850000	1.42202500	1.07539800
H	5.16889800	-0.85347600	0.59004500
H	4.35531500	3.28873400	1.37502600
H	1.90266400	2.73904400	1.21933000
C	2.50402100	-1.55462900	0.27162700
C	3.29020100	-2.65247600	-0.08336300
C	0.58425900	-2.79604900	0.00348600
C	2.67902900	-3.85705900	-0.39135600
H	4.37069800	-2.56572000	-0.13430100
H	-0.50412000	-2.80847600	0.02418800
H	3.27811700	-4.72003800	-0.66959200
C	1.29421500	-3.93505900	-0.34928000
H	0.76631700	-4.85229700	-0.59042600
N	1.16288200	-1.63478900	0.31723100
Ni	0.17543500	0.40075800	0.57280800
C	-2.06921400	-1.03770500	0.89931500
C	-3.40613300	-1.35246600	1.10573300
C	-4.40553000	-0.54188000	0.57160300
C	-4.04766800	0.59836300	-0.14638500
C	-2.70376000	0.90500200	-0.34124500
C	-1.69390300	0.09249800	0.16251300
H	-1.32175500	-1.64844300	1.40252600
H	-3.69816100	-2.21402000	1.70175100
H	-4.80310900	1.26157100	-0.55814700

H	-2.45605600	1.80557300	-0.89715400
O	-5.68484100	-0.93722500	0.80856600
C	-6.71724700	-0.10955400	0.33811700
H	-6.70376400	-0.02101900	-0.75825600
H	-7.65604500	-0.57660200	0.64352600
H	-6.66158100	0.89893000	0.77299800
Cl	-0.35456300	2.04018800	2.08682200

Zn-Ar

G(Gibbs Free Energy) =-1339.356205 hartree

E(electronic Energy) =-1339.4266251 hartree

C	-2.66738000	0.97121500	0.00035600
C	-1.27423100	1.03255500	0.00033900
C	-0.48103200	-0.11783000	-0.00024800
C	-1.14301900	-1.35675800	-0.00076300
C	-2.52535300	-1.44045500	-0.00075100
C	-3.29467700	-0.27377700	-0.00014400
H	-3.24570900	1.89098700	0.00076200
H	-0.80777200	2.01882900	0.00066200
H	-0.56905300	-2.28423900	-0.00119700
H	-3.04252600	-2.39716400	-0.00116400
Zn	1.49221600	0.00134300	0.00000200
Cl	2.95909600	1.87712900	-0.00046000
Cl	3.20058800	-1.65372500	0.00059800
Li	4.47281700	0.20728600	0.00036500
O	-4.63965600	-0.45642000	-0.00028200
C	-5.45564200	0.68766100	0.00068400
H	-6.48862700	0.33375100	0.00100700
H	-5.29074100	1.30727000	-0.89265000
H	-5.28987300	1.30625000	0.89449700

$ZnCl_2 \cdot LiCl$

G(Gibbs Free Energy) =-1453.757468 hartree

E(electronic Energy) =-1453.7200586 hartree

Zn	-0.28278500	-0.00153700	-0.00217700
Cl	1.23905000	-1.75372300	0.00040800
Cl	1.23211400	1.75744000	0.00040300
Li	2.68620100	0.00481700	0.00588100
Cl	-2.44616700	-0.00185400	0.00199300

$^{S}Ni^{0}$

G(Gibbs Free Energy) =-664.213852 hartree

E(electronic Energy) =-664.3245165 hartree

C	-0.73247600	0.70292800	0.03045300
C	-1.50018500	1.82515200	-0.26464900
C	-2.88461300	1.73049200	-0.28063900
C	-3.46716100	0.49268900	-0.01029600
C	-2.65113600	-0.58012000	0.30070200
N	-1.30344400	-0.50052900	0.34781400
H	-3.49607700	2.59581200	-0.52014900
H	-1.00563300	2.75837700	-0.52338000
H	-4.54611200	0.36550500	-0.01165100
H	-3.07415500	-1.54568400	0.56800000
C	0.73253100	0.70285600	-0.02999000
C	1.50042400	1.82496900	0.26517100
C	2.65105600	-0.58020700	-0.30135200
C	2.88483000	1.73021900	0.28051800
H	1.00603800	2.75814200	0.52440900
H	3.07386700	-1.54577300	-0.56897400
H	3.49645500	2.59542700	0.52003600
C	3.46726600	0.49249400	0.00948700
H	4.54622300	0.36537300	0.01025500
N	1.30335800	-0.50051700	-0.34778500
Ni	-0.00011500	-1.83531000	0.00017200

$^{S}\mathbf{1}_{a}^{Ni}$

G(Gibbs Free Energy) =-1355.847287 hartree

E(electronic Energy) =-1356.037031 hartree

C	-3.08528500	-0.59045400	-1.91530100
C	-2.82407800	0.46680900	-1.08707000
C	-2.33204200	0.24374500	0.23987000
C	-2.17352400	-1.12155000	0.71173300
C	-2.55978800	-2.18089600	-0.17297400
C	-2.96719900	-1.93056500	-1.45445300
H	-3.41944200	-0.40093100	-2.93341800
H	-2.98484100	1.49182900	-1.41802800
H	-2.17233500	-1.31779600	1.78593400
H	-2.55252900	-3.20352100	0.20479800
H	-3.24293100	-2.75053400	-2.11359300
Cl	-2.70908400	1.56184900	1.43856800
C	2.03624200	0.93351000	-0.16853600
C	3.03687700	1.87620600	-0.38835200
C	2.68512600	3.21119400	-0.53461400
C	1.34520200	3.56994300	-0.45190000
C	0.40392400	2.57411500	-0.22811700
N	0.73648600	1.28746700	-0.09463200
H	3.45100800	3.96278200	-0.70634400

H	4.07988000	1.57648500	-0.43899800
H	1.02859700	4.60323100	-0.55581100
H	-0.65915100	2.79586500	-0.13849800
C	2.28611800	-0.51075800	0.00717900
C	3.54190100	-1.10181600	-0.10539200
C	1.30801100	-2.56043400	0.45034000
C	3.66315100	-2.47262800	0.07478100
H	4.41685800	-0.50162500	-0.33835600
H	0.38299500	-3.09399900	0.66106900
H	4.63494800	-2.95164700	-0.00918300
C	2.52585400	-3.21944500	0.35762500
H	2.57579500	-4.29425900	0.50263500
N	1.18451700	-1.24067900	0.28420000
Ni	-0.50980000	-0.21131000	0.27522300

$^{S}TS1_{a}^{Ni}$

G(Gibbs Free Energy) =-1355.823629 hartree

E(electronic Energy) =-1356.0136291 hartree

C	-3.79783700	-0.82646200	-0.23088900
C	-3.01337800	0.05826000	-0.93930300
C	-2.12748400	0.89637100	-0.22075500
C	-2.18125700	0.97019400	1.19591100
C	-2.96587400	0.02498600	1.87267200
C	-3.75731200	-0.87246900	1.17591300
H	-4.45239700	-1.50778800	-0.77231100
H	-3.02514300	0.09442700	-2.02594000
H	-1.70876000	1.79094200	1.72867800
H	-2.98788500	0.03703500	2.96091200
H	-4.38726800	-1.57705400	1.71252000
Cl	-1.50755900	2.49538500	-1.07450200
C	1.59643800	-1.41828500	-0.11249300
C	2.12003400	-2.69822000	0.06301800
C	1.29162500	-3.79707300	-0.10608200
C	-0.04427000	-3.58411200	-0.43579200
C	-0.49553800	-2.28175300	-0.58234800
N	0.29836900	-1.21309400	-0.43750400
H	1.67772800	-4.80360500	0.03114500
H	3.15857400	-2.82907600	0.35615100
H	-0.72949500	-4.41459000	-0.57872700
H	-1.53370400	-2.06191700	-0.83172500
C	2.37851200	-0.19215800	0.07686000
C	3.77186100	-0.14465700	0.03808700
C	2.26815400	2.09366200	0.43576800
C	4.41514000	1.06926000	0.21556900

H	4.34267900	-1.04889400	-0.15585700
H	1.62372700	2.95863800	0.58428100
H	5.49976600	1.12693300	0.18400600
C	3.64668600	2.21460300	0.41664900
H	4.10791300	3.18731700	0.55827000
N	1.63465700	0.92132900	0.27797800
Ni	-0.29005100	0.69984100	-0.05517400

$^{S}2_{a}^{Ni}$

G(Gibbs Free Energy) =-1355.885425 hartree

E(electronic Energy) =-1356.0769979 hartree

C	4.07800000	-0.01082700	-1.20225900
C	2.72452100	-0.34503200	-1.20307400
C	2.03351800	-0.49284100	0.00003500
C	2.72393100	-0.34466500	1.20343700
C	4.07742100	-0.01048200	1.20318800
C	4.75609600	0.16545100	0.00060600
H	4.60667800	0.10760700	-2.14696900
H	2.20518200	-0.49075500	-2.15032600
H	2.20413500	-0.49004000	2.15049300
H	4.60563600	0.10821800	2.14812400
H	5.81240500	0.42596000	0.00082100
Cl	0.50167400	-2.85033200	-0.00047500
C	-1.49442800	1.53333400	-0.00005600
C	-1.90703800	2.86165500	-0.00013500
C	-0.95566500	3.87088400	-0.00031300
C	0.38684800	3.52198900	-0.00041600
C	0.73085900	2.17769300	-0.00032600
N	-0.18205300	1.19716900	-0.00014000
H	-1.26152700	4.91352200	-0.00037600
H	-2.96486100	3.10572200	-0.00007900
H	1.16938800	4.27396700	-0.00057000
H	1.76958200	1.85631000	-0.00039600
C	-2.42850400	0.39662300	0.00009400
C	-3.81478500	0.51848800	0.00037700
C	-2.56902400	-1.91564600	0.00005200
C	-4.58674500	-0.63564200	0.00050100
H	-4.28991200	1.49488700	0.00052600
H	-1.99711400	-2.84418500	-0.00008500
H	-5.67128900	-0.56516100	0.00073000
C	-3.95787800	-1.87315200	0.00033600
H	-4.52783200	-2.79691300	0.00044000
N	-1.82827100	-0.80711200	-0.00006600
Ni	0.18216300	-0.71003100	-0.00018200

$^{S}\mathbf{1}_{b}^{Ni}$

G(Gibbs Free Energy) =-1971.294021 hartree

E(electronic Energy) =-1971.5293125 hartree

C	-2.14376700	-1.88804300	0.86660700
C	-2.62303100	-2.86436000	1.73473200
C	-1.97423600	-3.06890400	2.94473100
C	-0.87122000	-2.28629300	3.25638300
C	-0.45001400	-1.33327500	2.33768700
N	-1.06215800	-1.13879000	1.16645300
H	-2.33236700	-3.82633500	3.63689900
H	-3.50166400	-3.44927100	1.47818700
H	-0.33501300	-2.40898400	4.19222300
H	0.41986900	-0.70921400	2.52421400
C	-2.78749200	-1.55853000	-0.41987700
C	-3.82482100	-2.29852800	-0.98107600
C	-2.83779200	-0.05991300	-2.18042500
C	-4.37664100	-1.88325300	-2.18473200
H	-4.19174600	-3.19581100	-0.49110100
H	-2.40786400	0.84031900	-2.61595500
H	-5.18464700	-2.44931700	-2.64035900
C	-3.88010900	-0.73860900	-2.79619900
H	-4.28698000	-0.37582400	-3.73508100
N	-2.29819700	-0.45759000	-1.02553700
Ni	-0.63221300	0.25048500	-0.20617800
C	1.04026400	2.14550900	1.09354000
C	0.21352300	3.22068600	1.26239000
C	-0.67383800	3.61454100	0.21589500
C	-0.69398100	2.93542000	-0.97457200
C	0.08536900	1.74830800	-1.17208400
C	0.94262700	1.33038300	-0.07660600
H	1.78504300	1.88545000	1.84394800
H	0.26931100	3.79372400	2.18299900
H	-1.29834800	3.34074700	-1.78415800
H	0.35283800	1.45955800	-2.19185100
O	-1.49709400	4.70309800	0.31300200
C	-1.40585500	5.50272000	1.46033800
H	-0.39824300	5.92475600	1.59337600
H	-2.11348600	6.32418500	1.32464000
H	-1.67912200	4.95308500	2.37378700
O	2.21449400	0.71730500	-0.46997400
S	2.38815000	-0.82691500	-0.14220400
O	1.61217500	-1.67889300	-1.01990500
O	2.41718800	-1.06268400	1.28986200

C	4.13175800	-0.91469500	-0.73288500
F	4.89956300	-0.10889400	-0.02417300
F	4.19895000	-0.58954900	-2.00961500
F	4.53680800	-2.16432700	-0.57253400

$^{S}TS1_{b}^{Ni}$

G(Gibbs Free Energy) =-1971.279431 hartree

E(electronic Energy) =-1971.5137906 hartree

C	2.98087400	-0.76485700	-0.63827100
C	3.87016600	-1.69173600	-1.16970800
C	3.40511100	-2.61325200	-2.09994200
C	2.06911800	-2.58563000	-2.47233800
C	1.23966500	-1.62676700	-1.90418200
N	1.68602700	-0.73833300	-1.01381000
H	4.08203600	-3.35191400	-2.52053600
H	4.90979300	-1.70696400	-0.85572900
H	1.66091400	-3.29925400	-3.18031100
H	0.17774900	-1.57440500	-2.13840500
C	3.34614200	0.24768800	0.37197500
C	4.63353200	0.42640500	0.86950900
C	2.53953900	1.95866600	1.71093500
C	4.85788600	1.40956800	1.82342500
H	5.45349600	-0.19283900	0.51808600
H	1.66851500	2.54152400	2.00449800
H	5.85612100	1.56227500	2.22468500
C	3.79479600	2.19244400	2.25548300
H	3.92967500	2.97124700	2.99927500
N	2.31951200	1.01277700	0.79581200
Ni	0.58855200	0.57385100	-0.05197600
C	-1.57952500	1.38223700	-1.73886800
C	-1.95790200	2.70320800	-1.64255900
C	-1.97082700	3.36480700	-0.39097200
C	-1.60682100	2.69253100	0.75694200
C	-1.14585000	1.35365000	0.69142500
C	-1.10724400	0.73012000	-0.58924200
H	-1.60356500	0.85547700	-2.68969600
H	-2.24555500	3.23343200	-2.54622200
H	-1.74199100	3.19250800	1.71379900
H	-1.10870500	0.75120500	1.59987400
O	-2.37136700	4.65900100	-0.23291200
C	-2.87645700	5.33732400	-1.35271900
H	-3.74759400	4.82417700	-1.78619600
H	-3.18694700	6.32483100	-1.00427100

H	-2.11588700	5.46510700	-2.13747900
O	-1.84384000	-1.04824800	-0.77872700
S	-1.42789000	-2.11813500	0.21409800
O	-0.52961900	-1.62076200	1.25949900
O	-1.08701000	-3.37502400	-0.43865200
C	-3.01415100	-2.41818400	1.09132400
F	-3.94503300	-2.82834200	0.24346000
F	-3.42332100	-1.29528900	1.67075200
F	-2.83983100	-3.34350400	2.02438900

$^{S}2_{b}^{Ni}$

G(Gibbs Free Energy) =-1971.338375 hartree

E(electronic Energy) =-1971.5757308 hartree

C	2.91186400	-1.74211700	0.11133500
C	3.69625100	-2.86170000	0.36362300
C	3.08875000	-4.09835000	0.52615900
C	1.70828600	-4.18398900	0.42651300
C	0.98128900	-3.02881100	0.17658400
N	1.56113000	-1.83031700	0.02831800
H	3.68936000	-4.98204000	0.72333600
H	4.77583100	-2.76780600	0.42716000
H	1.18729100	-5.12907700	0.54002500
H	-0.10223200	-3.03934700	0.09741700
C	3.46606300	-0.39553800	-0.10382700
C	4.81742300	-0.07863300	-0.02582400
C	2.91524900	1.79385000	-0.63260600
C	5.20971000	1.23273400	-0.26580100
H	5.55602900	-0.83476800	0.22262100
H	2.11556900	2.49812200	-0.85582200
H	6.25992500	1.50566700	-0.20742100
C	4.24873000	2.18401500	-0.57561200
H	4.51511300	3.21865600	-0.76522100
N	2.54124600	0.53500100	-0.40058900
Ni	0.66399300	-0.16914600	-0.31731400
C	-1.84181200	-1.08268300	-1.28965200
C	-3.12799500	-1.62048000	-1.18665200
C	-3.63897700	-1.93876700	0.07026300
C	-2.86465200	-1.71650300	1.21181900
C	-1.58730900	-1.18658300	1.09388800
C	-1.05784500	-0.87608900	-0.16207100
H	-1.46550100	-0.80974800	-2.27549300
H	-3.71835100	-1.77191400	-2.08639000
H	-3.29620400	-1.95653200	2.18109700
H	-1.00323300	-0.99808600	1.99489700

O	-4.87532200	-2.46720100	0.28930100
C	-5.70529200	-2.65893000	-0.82553000
H	-5.27135500	-3.37169300	-1.54301300
H	-6.64654200	-3.06579000	-0.44929800
H	-5.90938500	-1.71437200	-1.35086200
O	-0.14769500	1.88924900	1.68034100
S	-0.34436700	2.48975700	0.36555600
O	-0.07203000	1.51377100	-0.77282300
O	0.25645300	3.78905200	0.08945700
C	-2.15591700	2.75603500	0.19091900
F	-2.54839400	3.65576500	1.08279900
F	-2.81598700	1.62821800	0.39565200
F	-2.43106600	3.20514700	-1.02540700

^{T}Ni0

G(Gibbs Free Energy) =-664.234759 hartree

E(electronic Energy) =-664.3444118 hartree

C	-0.71469500	0.70099600	0.00008900
C	-1.51100100	1.87251200	-0.00015100
C	-2.87811100	1.78972800	-0.00011000
C	-3.50181800	0.51914600	0.00012800
C	-2.69167700	-0.59082000	0.00012300
N	-1.34830100	-0.53358100	0.00009000
H	-3.47828400	2.69612800	-0.00027200
H	-1.02931700	2.84640000	-0.00044000
H	-4.58132600	0.41150600	0.00022800
H	-3.12069700	-1.59244000	0.00017200
C	0.71448600	0.70116000	0.00016600
C	1.51076100	1.87271000	0.00003800
C	2.69159100	-0.59062700	0.00018500
C	2.87787400	1.78990900	-0.00011700
H	1.02912800	2.84662500	0.00014300
H	3.12054400	-1.59227300	0.00036800
H	3.47801400	2.69633300	-0.00021700
C	3.50169600	0.51936600	-0.00011600
H	4.58121900	0.41188700	-0.00018000
N	1.34822100	-0.53327500	0.00037400
Ni	0.00023700	-1.88430900	-0.00015900

^{T}1$_{a}^{Ni}$

G(Gibbs Free Energy) =-1355.830665 hartree

E(electronic Energy) =-1356.017645 hartree

C	-3.35999000	1.03549200	1.07284300

C	-2.83842300	-0.22885900	1.26312800
C	-2.37220900	-0.95009100	0.14671200
C	-2.41378700	-0.39587600	-1.15326500
C	-2.96076700	0.89333800	-1.30728600
C	-3.43768200	1.59109300	-0.21526800
H	-3.71814700	1.59902100	1.93010400
H	-2.79460600	-0.68657800	2.24721300
H	-2.19036500	-1.01423300	-2.01966500
H	-3.02068900	1.32218400	-2.30418200
H	-3.87111000	2.57866600	-0.35066700
Cl	-2.03401300	-2.68240000	0.32446900
C	2.34812500	-0.13588200	0.02093900
C	3.70701900	-0.51154100	0.11967900
C	4.06557100	-1.83381300	0.07363300
C	3.06183200	-2.82109400	-0.07113300
C	1.75602800	-2.40290400	-0.16268700
N	1.38178300	-1.11100900	-0.12286200
H	5.11163400	-2.11983600	0.14942800
H	4.46824800	0.25610900	0.23357100
H	3.30320300	-3.87835800	-0.10919700
H	0.94407000	-3.12233100	-0.27288700
C	1.86245100	1.20422400	0.05381800
C	2.67815300	2.35042600	0.18642200
C	-0.03042300	2.58341000	-0.03763100
C	2.11841300	3.60177200	0.20885100
H	3.75555400	2.23324200	0.27107800
H	-1.11462700	2.63407500	-0.13405300
H	2.74798200	4.48190900	0.31326700
C	0.71571500	3.73171500	0.09209300
H	0.23037100	4.70251500	0.10049600
N	0.49219300	1.34565800	-0.05629500
Ni	-0.42111800	-0.40344900	-0.21648100

$^{T}TS1_{a}^{Ni}$

G(Gibbs Free Energy) =-1355.817272 hartree

E(electronic Energy) =-1356.0030793 hartree

C	3.67737800	0.25346000	-1.53370100
C	2.63131100	-0.64297100	-1.39229300
C	2.13482800	-0.88800500	-0.10503800
C	2.76094900	-0.36853100	1.03694900
C	3.81204800	0.53262700	0.86647100
C	4.26699300	0.84646100	-0.41002500
H	4.04085200	0.50060500	-2.52904500
H	2.16830000	-1.11985100	-2.25284500

H	2.42196600	-0.66102300	2.02892200
H	4.28856900	0.97195500	1.74061600
H	5.09895500	1.53443000	-0.53627300
Cl	1.24979800	-2.75861300	0.25201900
C	-2.42949000	0.20044600	-0.06728500
C	-3.82178100	0.11844300	-0.22462200
C	-4.43049100	-1.11636600	-0.28580600
C	-3.64500200	-2.27564100	-0.18203100
C	-2.28093600	-2.13034900	-0.03195600
N	-1.67434300	-0.93542900	0.01472400
H	-5.50844200	-1.18921000	-0.40428400
H	-4.41621300	1.02648900	-0.28174800
H	-4.08722000	-3.26592300	-0.22201900
H	-1.61915800	-2.99213500	0.04601600
C	-1.68393100	1.43430100	0.02311300
C	-2.21982300	2.71200000	-0.20214900
C	0.42312700	2.37549900	0.40436200
C	-1.41179500	3.82286100	-0.09970100
H	-3.26729100	2.81953300	-0.47152100
H	1.47299800	2.18316200	0.62965400
H	-1.82051700	4.81508300	-0.27130700
C	-0.04993400	3.65513300	0.20899700
H	0.62126000	4.50381900	0.29284800
N	-0.35878600	1.28597100	0.33334000
Ni	0.25680600	-0.56644700	0.26708900

$T2_a^{Ni}$

G(Gibbs Free Energy) =-1355.858617 hartree

E(electronic Energy) =-1356.0446843 hartree

C	-4.03579300	0.69969100	1.57472800
C	-2.68743800	0.50247100	1.27767500
C	-2.28276500	-0.37098900	0.25889100
C	-3.27944200	-1.02983400	-0.46884900
C	-4.62769700	-0.83469700	-0.18108300
C	-5.00921000	0.02917600	0.84231700
H	-4.32577600	1.37827200	2.37601500
H	-1.94065200	1.04736500	1.86297300
H	-2.99003200	-1.70183400	-1.27652700
H	-5.38799900	-1.35711800	-0.75992500
H	-6.06341000	0.18222600	1.06551100
Cl	-0.16202900	-1.75000700	-2.01197800
C	2.43908100	0.08669400	0.36482900
C	3.82180100	-0.00316800	0.50649500
C	4.38763600	-1.23832000	0.79146200

C	3.56712400	-2.35186500	0.91394200
C	2.19853100	-2.18045900	0.75173200
N	1.65264700	-0.99272400	0.50145700
H	5.46454800	-1.33057100	0.90409600
H	4.45367600	0.87082500	0.38060800
H	3.97411700	-3.33633300	1.12114400
H	1.50682500	-3.01902300	0.80868500
C	1.73390700	1.34114800	0.01947300
C	2.36252400	2.57846100	-0.09126800
C	-0.31099300	2.27406300	-0.56351300
C	1.60907600	3.68493700	-0.46064900
H	3.42481500	2.68242300	0.10767600
H	-1.37062000	2.08153900	-0.72455500
H	2.08364700	4.65805500	-0.55508100
C	0.25094900	3.53608500	-0.70764300
H	-0.36732000	4.37708100	-1.00436800
N	0.41516800	1.21546300	-0.20707100
Ni	-0.39306300	-0.66722600	-0.04052100

$^{T}1_{b}^{Ni}$

G(Gibbs Free Energy) =-1971.277379 hartree

E(electronic Energy) =-1971.5117651 hartree

C	2.21271400	1.95109700	-0.02621900
C	2.93233100	2.96891700	0.64895200
C	2.26943400	4.02674400	1.21430800
C	0.86077700	4.09916600	1.11985800
C	0.21035700	3.08434100	0.45030600
N	0.83575200	2.03808500	-0.10923000
H	2.82612300	4.80504500	1.73118500
H	4.01558900	2.90582300	0.71753100
H	0.29968900	4.92133100	1.55186800
H	-0.87612800	3.09110900	0.34843500
C	2.80449200	0.81304600	-0.64523100
C	4.19785900	0.55341300	-0.69818200
C	2.41720300	-1.18551800	-1.82357100
C	4.67284000	-0.57549600	-1.31395200
H	4.89144200	1.26427000	-0.25545500
H	1.67268800	-1.85580000	-2.25581700
H	5.74322100	-0.76362200	-1.35834700
C	3.75956300	-1.49134100	-1.89353800
H	4.09217600	-2.39986900	-2.38456200
N	1.92658700	-0.08439300	-1.23532400
Ni	0.08154200	0.45721100	-1.00932600
C	-0.03366000	-0.65838100	1.76155900

C	1.19364400	-1.31143300	1.74847500
C	1.31222100	-2.54517200	1.10306900
C	0.19283500	-3.13529000	0.49939900
C	-1.03181600	-2.49298500	0.51997500
C	-1.11967800	-1.26114000	1.15301300
H	-0.14602400	0.31664000	2.22997500
H	2.05420300	-0.82494100	2.19576100
H	0.31952600	-4.09826800	0.01307100
H	-1.91274400	-2.92693800	0.05396700
O	2.45651500	-3.24675900	1.00672900
C	3.63954800	-2.65812100	1.50734100
H	3.58223700	-2.50956800	2.59469500
H	4.44552200	-3.35974300	1.28539000
H	3.85237300	-1.70094400	1.01060700
O	-2.37856800	-0.61071300	1.20945600
S	-2.78666900	0.41417800	0.04505200
O	-1.95501700	0.22210400	-1.14693300
O	-3.01844900	1.72636200	0.59073900
C	-4.41452700	-0.34001900	-0.39109300
F	-5.19811100	-0.31385900	0.66391500
F	-4.22023400	-1.58336600	-0.78529000
F	-4.93558900	0.36966500	-1.36894300

$^{T}TS1_{b}^{Ni}$

G(Gibbs Free Energy) =-1971.262154 hartree

E(electronic Energy) =-1971.494216 hartree

C	-2.10277900	-2.60171500	0.01466700
C	-2.58807600	-3.88782400	0.27490300
C	-1.69839900	-4.93456600	0.42353200
C	-0.32830900	-4.68143200	0.31503100
C	0.08573200	-3.38577100	0.06801900
N	-0.76946500	-2.36363700	-0.08098800
H	-2.06272400	-5.93860500	0.62400800
H	-3.65652300	-4.06445800	0.35994700
H	0.40552800	-5.47345800	0.42526400
H	1.13975200	-3.12986700	-0.01422800
C	-2.95375400	-1.43083700	-0.16943100
C	-4.35190500	-1.46722000	-0.12803000
C	-3.00016000	0.85355600	-0.59407600
C	-5.07158200	-0.30507600	-0.32996700
H	-4.87015500	-2.40346700	0.05826100
H	-2.41603600	1.75395800	-0.77988800
H	-6.15787100	-0.32194800	-0.30133600
C	-4.38248600	0.88608200	-0.57444300

H	-4.90653600	1.82041100	-0.75006800
N	-2.29235700	-0.26555700	-0.39259900
Ni	-0.28662900	-0.42531000	-0.23515100
C	-0.04420700	1.92698600	1.51740800
C	-0.78422600	3.06729100	1.29822800
C	-0.85087700	3.63403500	0.00867200
C	-0.14673200	3.04458200	-1.04598000
C	0.60078000	1.89654900	-0.84232400
C	0.59154600	1.25037300	0.43588300
H	0.03551400	1.50501300	2.51641900
H	-1.31159500	3.52299400	2.13181200
H	-0.19415700	3.51832400	-2.02400800
H	1.18946900	1.47405600	-1.65395100
O	-1.56753800	4.74821100	-0.30284600
C	-2.26079700	5.39364100	0.73423800
H	-1.58227100	5.74123000	1.52667800
H	-2.75539900	6.25866000	0.28757900
H	-3.02366100	4.74100300	1.18495900
O	2.10928100	0.85372000	0.93286900
S	2.67234600	-0.47840900	0.39032700
O	1.84106300	-0.97172700	-0.72013500
O	3.06775800	-1.40652400	1.42792400
C	4.21529700	0.11962700	-0.41768200
F	5.00160700	0.68166400	0.47998500
F	3.91107500	0.99999600	-1.35606400
F	4.83049400	-0.91447900	-0.96522700

$^{T}2_{b}^{Ni}$

G(Gibbs Free Energy) =-1971.316216 hartree

E(electronic Energy) =-1971.5480835 hartree

C	-3.07660400	1.30114900	-0.30062100
C	-4.45429800	1.42358800	-0.45697900
C	-5.13127400	0.47779400	-1.21526300
C	-4.42120500	-0.56659000	-1.78918000
C	-3.04786300	-0.62184500	-1.58757400
N	-2.39442500	0.29569000	-0.87233500
H	-6.20709000	0.55511600	-1.34824800
H	-4.99680700	2.24211000	0.00591200
H	-4.91442500	-1.33502700	-2.37529600
H	-2.43789100	-1.43141600	-1.98147500
C	-2.26011100	2.23541400	0.50201200
C	-2.79838500	3.29217900	1.23234300
C	-0.12335900	2.76668700	1.20653800
C	-1.94666500	4.09911800	1.97382100

H	-3.86754900	3.48042600	1.23428000
H	0.93399400	2.51257800	1.14855900
H	-2.34748500	4.92598700	2.55412800
C	-0.58442800	3.83453300	1.96632700
H	0.11458200	4.43984200	2.53456100
N	-0.94032900	1.99061700	0.49608500
Ni	-0.27015200	0.22295400	-0.58211200
C	2.39515100	0.46125800	0.38914300
C	3.77045500	0.69272000	0.36027000
C	4.33277400	1.30362700	-0.76105100
C	3.51809500	1.67627300	-1.83570700
C	2.15582400	1.42992400	-1.78813700
C	1.56131600	0.80218500	-0.68209500
H	1.96755700	-0.01797600	1.27292100
H	4.38634100	0.39388000	1.20416400
H	3.98845300	2.15359600	-2.69269900
H	1.54548800	1.72982700	-2.64065700
O	5.65335800	1.58629000	-0.90031200
C	6.51727300	1.20932000	0.14213700
H	6.49985000	0.12346600	0.31302600
H	7.52279500	1.50512200	-0.16413100
H	6.26693200	1.71809800	1.08440800
O	-0.54233500	-1.40101700	1.59493300
S	-0.71088800	-2.37967800	0.51515900
O	-0.43138400	-1.74193400	-0.83508200
O	-1.89682000	-3.22108500	0.51205400
C	0.71763000	-3.52379800	0.67436900
F	0.64005000	-4.16484200	1.83186300
F	1.85339200	-2.84081100	0.63479500
F	0.70861300	-4.40622200	-0.31265600

3$^{Ni'}$

G(Gibbs Free Energy) =-5015.203873 hartree

E(electronic Energy) =-5015.9530427 hartree

C	3.99278500	0.22503200	2.40353300
C	4.68989200	1.04573100	3.28694900
C	4.09739700	1.37797700	4.49611100
C	2.83251900	0.88635500	4.79327900
C	2.20394700	0.07084300	3.86244600
N	2.77247700	-0.23937500	2.70097800
H	4.62470200	2.01160100	5.20420800
H	5.68200300	1.41208400	3.04332900
H	2.34198900	1.11665500	5.73366400
H	1.21867200	-0.36015300	4.03304600

C	4.52287100	-0.21147600	1.09904100
C	5.67803200	0.32090500	0.53381800
C	4.19415100	-1.57401500	-0.75058200
C	6.08669100	-0.12111300	-0.71601700
H	6.23347600	1.09531600	1.05432300
H	3.56613400	-2.32300700	-1.22781400
H	6.98255000	0.29057200	-1.17422100
C	5.33205700	-1.08177000	-1.37438200
H	5.60722800	-1.44851900	-2.35769700
N	3.80429700	-1.15451600	0.45540700
Ni	2.10714300	-1.70634400	1.42358100
C	0.97885000	-2.57894600	-0.98341700
C	0.89724900	-3.37684100	-2.12977600
C	1.47030400	-4.64285400	-2.14295900
C	2.11857100	-5.13071400	-1.01370200
C	2.22246400	-4.35140300	0.14045700
C	1.67238000	-3.08254200	0.10266100
H	0.50860900	-1.59573700	-0.99794700
H	0.36075000	-2.99015000	-2.99578300
H	2.55799500	-6.12653600	-1.01669300
H	2.73745100	-4.71588200	1.02276900
O	-0.80244100	-0.24691300	-2.38710600
S	-0.75292600	-0.34688700	-3.86598000
O	-1.43827300	0.75373400	-4.55490800
O	-0.98101200	-1.69528100	-4.39434200
C	1.03003400	-0.03984800	-4.23051200
F	1.80674500	-0.91084800	-3.58028800
F	1.39463600	1.18399800	-3.83620900
F	1.27303100	-0.14867000	-5.52829800
P	-1.91592600	2.24758300	-0.50300900
P	-2.98862800	-1.21719400	0.14756700
C	-3.17921500	2.06495900	-1.84813000
H	-3.10606700	2.97606600	-2.45559200
H	-2.80252600	1.25651000	-2.48802700
C	-4.63419800	1.85679700	-1.44145100
H	-5.20277000	1.71543400	-2.37207200
H	-5.02302600	2.77662400	-0.98300300
C	-4.32882800	-0.64293100	-0.98414500
H	-5.08952700	-1.43010100	-1.05061900
H	-3.89276400	-0.54957200	-1.98698900
Pd	-1.08722900	0.28815700	0.47407500
C	2.69330000	2.00907400	-0.53575600
C	1.49006600	1.30431600	-0.50272000
C	0.63410800	1.38530700	0.59437300

C	1.00209400	2.18996700	1.67398900
C	2.19943400	2.89716800	1.65518800
C	3.04731500	2.80960200	0.54923500
H	3.32210500	1.93579200	-1.42079700
H	1.20282300	0.71781800	-1.37556300
H	0.34758100	2.28248400	2.54235600
H	2.49948500	3.53310200	2.48631900
Cl	2.92416900	-3.17368900	2.98321800
C	-0.73066200	3.40567900	-1.28352600
C	-0.09065600	4.39056300	-0.52450300
C	-0.41509900	3.26735300	-2.63747600
C	0.85468700	5.22171200	-1.11033900
H	-0.32243600	4.50195800	0.53291600
C	0.53085000	4.10595600	-3.21846000
H	-0.88612800	2.49938000	-3.25071900
C	1.16663000	5.08134900	-2.46028800
H	1.35161000	5.97886900	-0.50732100
H	0.77284700	3.97845800	-4.27079800
H	1.90566500	5.73510000	-2.91918300
C	-2.73265000	3.27800800	0.77218300
C	-3.32903900	4.49621200	0.42750900
C	-2.78972100	2.84329200	2.09644900
C	-3.97964000	5.25541200	1.39132500
H	-3.27417300	4.85649700	-0.59940700
C	-3.44077100	3.60443200	3.06261600
H	-2.31697400	1.89540200	2.35844800
C	-4.03794300	4.80870000	2.70930700
H	-4.44226200	6.19967900	1.11458600
H	-3.48195800	3.25344900	4.09100800
H	-4.54908300	5.40436800	3.46187100
C	-2.58490700	-2.87993600	-0.49110600
C	-2.30085000	-3.93153200	0.38686300
C	-2.51358400	-3.09973700	-1.86944200
C	-1.98453300	-5.18975300	-0.11023200
H	-2.32738000	-3.76705000	1.46240800
C	-2.20526000	-4.36222800	-2.36083300
H	-2.64728500	-2.28582300	-2.57798400
C	-1.94789900	-5.40976800	-1.48391400
H	-1.76183800	-5.99960900	0.58033100
H	-2.14125200	-4.50801400	-3.43690000
H	-1.69671800	-6.39537900	-1.86999600
C	-3.93784600	-1.56348300	1.68131000
C	-5.07357200	-2.37997700	1.66253500
C	-3.54025500	-0.98488200	2.88701600

C	-5.80063000	-2.60185800	2.82428500
H	-5.38214700	-2.86107700	0.73491200
C	-4.26822100	-1.20665900	4.05260700
H	-2.63826100	-0.37351700	2.90876500
C	-5.40005800	-2.01175700	4.02072300
H	-6.68078100	-3.24004400	2.79880800
H	-3.94469500	-0.75497000	4.98743300
H	-5.96960200	-2.18750800	4.93031800
H	1.39084000	-5.25990600	-3.03562900
O	4.20749700	3.52786000	0.62585500
C	4.91140900	3.73455100	-0.57391200
H	5.70809200	4.44881700	-0.35232100
H	5.36488700	2.80558500	-0.95461800
H	4.25962500	4.14893100	-1.35656200
Cl	-0.12031900	-1.51315500	1.96589800
C	-4.91401500	0.69024000	-0.50377000
H	-5.99944100	0.59248200	-0.37902300
H	-4.53933900	0.93955100	0.50183500

TS3'

G(Gibbs Free Energy) =-5015.169948 hartree

E(electronic Energy) =-5015.9217627 hartree

C	-4.18038400	1.01298000	0.38408500
C	-4.78765400	2.02871800	1.12343500
C	-4.24505600	3.30511600	1.09736700
C	-3.11368200	3.54101200	0.32884300
C	-2.56051700	2.47565200	-0.36993600
N	-3.06229900	1.24054700	-0.32451000
H	-4.71578700	4.10917400	1.65836900
H	-5.69359400	1.83745300	1.68933800
H	-2.65254000	4.52335200	0.25571200
H	-1.68334300	2.60648500	-0.99975600
C	-4.78001500	-0.32937300	0.23635800
C	-5.94196700	-0.70827400	0.90808500
C	-4.79683300	-2.28298400	-0.98402400
C	-6.53523800	-1.92475100	0.60685100
H	-6.38922500	-0.05666900	1.65184100
H	-4.32310900	-2.86730900	-1.76846800
H	-7.44060400	-2.23499100	1.12169300
C	-5.96970900	-2.71719700	-0.38035700
H	-6.41878400	-3.65734000	-0.68429700
N	-4.18966300	-1.14418900	-0.65578000
Ni	-2.37203700	-0.33994900	-1.55112200
C	-2.05000000	-3.11397900	-2.28504800

C	-1.72092000	-4.19160200	-3.11164100
C	-1.27561100	-3.96640600	-4.40617000
C	-1.15218900	-2.66135400	-4.87318300
C	-1.47667500	-1.57726700	-4.05975000
C	-1.92392400	-1.82693900	-2.77166300
H	-2.33894000	-3.31065000	-1.25484100
H	-1.79368200	-5.20360200	-2.71530800
H	-0.80206200	-2.47300500	-5.88575500
H	-1.38979100	-0.56465400	-4.43800400
O	3.13475500	-1.90397800	-1.96875200
S	3.96713400	-1.41461600	-0.86074300
O	3.20231700	-0.68239700	0.18310100
O	5.24691700	-0.80256500	-1.20657100
C	4.44148200	-2.97626100	-0.00199100
F	5.25915000	-3.70029300	-0.75012800
F	3.36009600	-3.72084300	0.27148800
F	5.04732500	-2.71927700	1.16105800
P	0.92411000	0.25993700	2.29072700
P	1.87711900	2.55249700	-0.40020600
C	2.56079800	0.95770000	2.78699400
H	2.81810500	0.52294100	3.76070700
H	3.28147400	0.56497500	2.05835100
C	2.54358400	2.48902700	2.83602900
H	2.68087700	2.82198500	3.87271200
H	1.55008700	2.87177700	2.55291200
C	3.50661900	2.77792500	0.47134100
H	4.06951700	3.50339300	-0.12951100
H	3.97560500	1.79900500	0.27843200
Pd	0.37436500	0.66909600	0.03847800
C	0.21582000	-3.36242000	-0.07511300
C	0.17766900	-2.04775800	-0.49932600
C	-0.73461000	-1.11195300	0.04425400
C	-1.65901400	-1.58668700	0.99428900
C	-1.70660100	-2.92415600	1.34862300
C	-0.72850600	-3.80458500	0.86086600
H	0.97571400	-4.02165300	-0.48293000
H	0.91421000	-1.73649700	-1.24262700
H	-2.33974600	-0.89000500	1.48558100
H	-2.42008500	-3.30063100	2.07929500
Cl	-3.75655200	0.46228500	-3.19430800
C	1.01212300	-1.44119100	2.96788200
C	0.00036600	-1.97172800	3.77554800
C	2.13689700	-2.22143000	2.68766200
C	0.11744700	-3.25328800	4.29981900

H	-0.88769000	-1.38305400	3.99818700
C	2.25040300	-3.50371200	3.21489300
H	2.91922700	-1.82816700	2.04490500
C	1.24282100	-4.02203500	4.02043600
H	-0.67817000	-3.65415600	4.92368500
H	3.13431300	-4.09296800	2.98244800
H	1.33174800	-5.02605800	4.43000400
C	-0.20717800	1.12401400	3.44934000
C	0.01561400	1.08008600	4.83119400
C	-1.23783400	1.92113900	2.95431500
C	-0.78442900	1.81360100	5.69655300
H	0.81698300	0.46161100	5.23360100
C	-2.03702400	2.66058600	3.82250400
H	-1.39819200	1.96925500	1.87633200
C	-1.81271500	2.60650000	5.19220800
H	-0.60295900	1.77123000	6.76783100
H	-2.83260200	3.28380000	3.41996100
H	-2.43526000	3.18507500	5.87065700
C	2.56680500	2.46547500	-2.09498200
C	3.02899800	3.61693300	-2.74282500
C	2.78054200	1.21828200	-2.67805600
C	3.68150100	3.51328300	-3.96431800
H	2.87711100	4.59844400	-2.29434600
C	3.45559900	1.11554600	-3.88904000
H	2.42996000	0.31202600	-2.19294300
C	3.89917400	2.26154800	-4.53607300
H	4.03031200	4.41240500	-4.46726000
H	3.63451800	0.12699600	-4.30377500
H	4.42315400	2.18388300	-5.48595700
C	0.94965600	4.13820500	-0.38298400
C	0.92276200	4.98505100	0.72942600
C	0.14030600	4.45491700	-1.48422400
C	0.12685200	6.12713100	0.73615500
H	1.53187000	4.76625900	1.60267500
C	-0.65371700	5.59580000	-1.47583300
H	0.13494200	3.80106600	-2.35545800
C	-0.65996200	6.43896200	-0.36688300
H	0.13229900	6.77941100	1.60638100
H	-1.26722500	5.82679100	-2.34358400
H	-1.27299900	7.33731900	-0.36594000
H	-1.01485800	-4.80361800	-5.04915900
O	-0.76479700	-5.05251900	1.36300600
C	0.27897600	-5.93503100	1.00090700
H	0.10981700	-6.85551500	1.56260200

H	0.26073000	-6.15852400	-0.07431400
H	1.26122800	-5.51828300	1.26594900
Cl	-0.42812500	0.91374000	-2.25169900
C	3.58662800	3.14714600	1.94877100
H	4.59194200	2.87958300	2.30376800
H	3.51486000	4.23780700	2.06223500

4$^{Ni'}$

G(Gibbs Free Energy) =-5015.170495 hartree

E(electronic Energy) =-5015.923516 hartree

C	-4.39446800	0.15476200	0.59340800
C	-5.18778300	1.00431000	1.36659300
C	-4.89747200	2.35973500	1.40726100
C	-3.82724200	2.83867100	0.66540400
C	-3.08054400	1.93006100	-0.07320300
N	-3.33509200	0.61992800	-0.09053000
H	-5.51502600	3.03348800	1.99655600
H	-6.04713300	0.62008300	1.90635000
H	-3.56208700	3.89276900	0.63821300
H	-2.24785800	2.25727800	-0.69160900
C	-4.73950100	-1.26780700	0.38656000
C	-5.80358300	-1.88497200	1.04550300
C	-4.39915300	-3.13833500	-0.91210900
C	-6.16266800	-3.17653900	0.69117200
H	-6.35580800	-1.36395400	1.82107700
H	-3.82619100	-3.58960600	-1.71878200
H	-6.99025500	-3.67150500	1.19251700
C	-5.46569200	-3.80933900	-0.32717400
H	-5.73309200	-4.80463300	-0.66795500
N	-4.01977200	-1.91734200	-0.54210200
Ni	-2.37525900	-0.71947100	-1.45686100
C	-1.59114700	-3.37225900	-2.43043600
C	-1.20035900	-4.29426100	-3.40357400
C	-0.91883700	-3.86747500	-4.69400800
C	-1.02420200	-2.51503300	-5.00383900
C	-1.42170900	-1.59059400	-4.04056500
C	-1.72143000	-2.02811500	-2.75494400
H	-1.74266900	-3.72012300	-1.40942500
H	-1.09437200	-5.34383200	-3.13358800
H	-0.80192300	-2.16649600	-6.01039500
H	-1.51697600	-0.54255700	-4.30517300
O	3.37755600	-1.19046500	-2.05164800
S	4.16895200	-0.46674100	-1.04650000
O	3.36505300	0.04492300	0.09459800

O	5.17744200	0.46852500	-1.53567300
C	5.16284700	-1.81443600	-0.27137000
F	6.10419600	-2.24820800	-1.09340700
F	4.38116200	-2.85748500	0.05039800
F	5.74186200	-1.39732500	0.85725600
P	0.95591700	0.20980900	2.23881000
P	1.24733600	2.81481500	-0.28820000
C	2.36671600	1.27623600	2.77707900
H	2.74806700	0.84595700	3.71064900
H	3.14770700	1.13881000	2.01987300
C	1.96128700	2.74099900	2.95395600
H	2.05311500	3.02253500	4.01059400
H	0.89123300	2.86891600	2.72736400
C	2.77558100	3.37847300	0.60945800
H	3.13651600	4.24359500	0.03925100
H	3.46927900	2.55544900	0.37670300
Pd	0.19403000	0.64304100	0.03045800
C	1.06975800	-2.95917100	-0.40430300
C	0.41739800	-1.82587900	-0.86682600
C	-0.78284200	-1.32718600	-0.28099800
C	-1.28989100	-2.06770400	0.82510400
C	-0.73631800	-3.26402600	1.20678000
C	0.45598300	-3.71683600	0.59455900
H	2.01500900	-3.24037900	-0.85907100
H	0.86058000	-1.31941800	-1.72435300
H	-2.16703000	-1.70051100	1.35797100
H	-1.15041800	-3.86588600	2.01297700
Cl	-3.99399800	-0.04833900	-2.94850800
C	1.53863500	-1.42767600	2.81814400
C	0.75401000	-2.24644000	3.63749300
C	2.83812500	-1.83114400	2.49761800
C	1.26951400	-3.43327500	4.14462200
H	-0.26243000	-1.95232400	3.89176700
C	3.34910300	-3.02050000	3.00584400
H	3.44863700	-1.21122200	1.84720200
C	2.56888100	-3.82128900	3.83243100
H	0.65041800	-4.05879300	4.78352500
H	4.36458300	-3.30968100	2.74453200
H	2.96993200	-4.75039200	4.23140400
C	-0.32115800	0.66486700	3.47787700
C	-0.03122900	0.61250100	4.84752100
C	-1.55483100	1.16587900	3.06642300
C	-0.96308300	1.04238300	5.78161400
H	0.92825000	0.22496200	5.18726800

C	-2.48844500	1.60120000	4.00450300
H	-1.77563900	1.22399800	2.00057200
C	-2.19498500	1.53787600	5.36034000
H	-0.72706500	0.99470900	6.84197400
H	-3.44457800	1.99339700	3.66542900
H	-2.92306300	1.87829900	6.09283500
C	1.94051700	2.96643800	-1.97683300
C	2.19464600	4.23259100	-2.51816500
C	2.36183600	1.83100800	-2.66368500
C	2.84834900	4.34950700	-3.73750600
H	1.87699300	5.13172000	-1.99082700
C	3.03832700	1.95205200	-3.87184900
H	2.17345800	0.84033400	-2.26129600
C	3.27477300	3.20848500	-4.41316100
H	3.03330100	5.33570600	-4.15702100
H	3.38641300	1.05033300	-4.36848800
H	3.79983500	3.30430400	-5.36062500
C	-0.01117500	4.14999200	-0.18824500
C	-0.28106300	4.82659000	1.00666800
C	-0.79544500	4.44175700	-1.31357400
C	-1.28412900	5.78897100	1.06955100
H	0.29470400	4.61520400	1.90333300
C	-1.80346000	5.39645100	-1.24568500
H	-0.61657700	3.91421200	-2.24760900
C	-2.04622600	6.07944800	-0.05683100
H	-1.46428600	6.31534700	2.00396000
H	-2.39833600	5.60812000	-2.13067800
H	-2.82629300	6.83584500	-0.01010100
H	-0.60550500	-4.58089900	-5.45272300
O	0.91673600	-4.88445200	1.05629100
C	2.13461300	-5.38042600	0.52633400
H	2.32120900	-6.32783800	1.03469100
H	2.05383200	-5.55358700	-0.55401800
H	2.96116000	-4.68752400	0.72439000
Cl	-0.73689900	1.07348400	-2.17047200
C	2.76636600	3.70246100	2.09723800
H	3.81115900	3.71012500	2.43850900
H	2.39592400	4.72488300	2.25343200

TS2^{Pd}

C	4.85682800	-0.59616000	-0.95322200
C	6.17613600	-0.47807900	-0.52408700
C	6.63959500	-1.34045100	0.45980200
C	5.78668800	-2.30532100	0.98025200

C	4.48179100	-2.35703200	0.50780200
N	4.03792200	-1.51152900	-0.41676600
H	7.66505600	-1.26280800	0.81117400
H	6.83452000	0.27397500	-0.94706700
H	6.11952900	-3.00702000	1.73831500
H	3.75176400	-3.07723700	0.87502600
C	4.26200700	0.23011000	-2.02270900
C	4.96649100	1.21965300	-2.70396300
C	2.39935900	0.56899100	-3.35662400
C	4.34184100	1.89977500	-3.73966700
H	5.99013400	1.45664800	-2.43023800
H	1.37807300	0.26727900	-3.58065900
H	4.87385800	2.67825300	-4.28042200
C	3.04055800	1.56186100	-4.08516900
H	2.52092600	2.05466200	-4.90019600
N	2.98736300	-0.05682500	-2.33858400
Ni	2.11449100	-1.47454800	-1.14304000
C	-0.77241600	0.17912900	-2.37027400
C	-1.23975300	0.06482700	-3.67781900
C	-1.24705500	-1.17942200	-4.30732500
C	-0.81584300	-2.30774600	-3.62367400
C	-0.39722600	-2.21679800	-2.29169700
C	-0.37896100	-0.96730200	-1.68462900
H	-0.77050300	1.16379600	-1.91005300
H	-1.61711600	0.95986900	-4.16961600
H	-0.80182300	-3.28097500	-4.10981400
H	-0.09385700	-3.11465300	-1.76089900
O	-2.79908600	2.25968000	-0.32579900
S	-2.59731400	3.02559100	-1.57833100
O	-3.31270800	2.50162900	-2.74525600
O	-1.19729100	3.42365300	-1.80760000
C	-3.43434500	4.62015100	-1.21419100
F	-2.87429000	5.20301600	-0.14814000
F	-4.72013400	4.42542900	-0.94895000
F	-3.33277300	5.45115400	-2.24277600
P	-0.95289300	0.98815300	2.35600900
P	-2.59548400	-2.03671700	0.49033700
C	-3.74937300	0.51846600	2.20702700
H	-4.74673800	0.94939000	2.36514500
H	-3.64796500	0.44099200	1.11558500
C	-3.66298500	-0.86227600	2.86211400
H	-4.39724200	-0.94841500	3.67449600
H	-2.68532000	-1.00802100	3.34392300
C	-3.89158700	-1.97232800	1.85380800

H	-3.92692500	-2.95935600	2.32901400
H	-4.85170100	-1.82729600	1.34175300
Pd	-0.50043200	-0.54240700	0.43762300
C	2.44252900	2.60355500	-0.24560200
C	1.30713700	1.80088800	-0.29055400
C	1.24704500	0.59371300	0.41238900
C	2.31624000	0.26688000	1.25857700
C	3.44833800	1.06929700	1.32109900
C	3.53024300	2.22474600	0.54529300
H	2.44702100	3.52912500	-0.81488100
H	0.45935100	2.17511900	-0.86521700
H	2.27943700	-0.63590700	1.86491700
H	4.29400400	0.80342700	1.95372100
Cl	2.66583000	-3.16487500	-2.62331200
C	-0.08767400	2.60490500	2.38686800
C	1.08750000	2.81215500	3.11391300
C	-0.58095200	3.63449600	1.57817600
C	1.74496800	4.03612400	3.04377800
H	1.49922400	2.01679200	3.73208500
C	0.07769400	4.85481900	1.51175000
H	-1.46540700	3.47306400	0.96751200
C	1.24010100	5.05998100	2.24780000
H	2.66083600	4.18543000	3.61198000
H	-0.32324900	5.63332500	0.86721500
H	1.75632000	6.01685700	2.20051900
C	-0.43078500	0.16328600	3.91406900
C	-0.56871600	0.80160000	5.15178900
C	0.05996200	-1.14396700	3.87559000
C	-0.22938600	0.14063200	6.32560400
H	-0.93272200	1.82745100	5.19880800
C	0.39420600	-1.80681800	5.05291900
H	0.17628200	-1.65233000	2.91641800
C	0.24865200	-1.16638800	6.27798200
H	-0.34083000	0.64648000	7.28172500
H	0.76862100	-2.82707000	5.00549600
H	0.50816400	-1.68355100	7.19872300
C	-3.66320000	-1.92230200	-0.99100400
C	-4.46317400	-2.98572200	-1.42691500
C	-3.77718100	-0.67940800	-1.61556000
C	-5.32454200	-2.81135700	-2.50253600
H	-4.41462100	-3.95116100	-0.92567500
C	-4.64768100	-0.50488900	-2.68726800
H	-3.19576700	0.17343100	-1.26999400
C	-5.41111400	-1.57420400	-3.13829200

H	-5.93553300	-3.64449600	-2.84304400
H	-4.70025100	0.47726500	-3.15279100
H	-6.08639700	-1.44528100	-3.98130500
C	-2.04172300	-3.77759500	0.63283300
C	-1.65519500	-4.22679500	1.90089000
C	-1.86086500	-4.62336700	-0.46306000
C	-1.11318900	-5.49279700	2.07095700
H	-1.75850400	-3.57187000	2.76788300
C	-1.31382300	-5.89123700	-0.29203900
H	-2.14973700	-4.29281800	-1.45830300
C	-0.93938500	-6.32892700	0.97227900
H	-0.81824600	-5.82506900	3.06369500
H	-1.17824100	-6.53743600	-1.15571400
H	-0.50936500	-7.31899800	1.10163200
H	-1.59963300	-1.26711400	-5.33238500
O	4.69644800	2.91610000	0.63154200
C	4.76605200	4.15315700	-0.03686100
H	5.75011300	4.57211000	0.18361200
H	4.66159300	4.03354200	-1.12572300
H	3.99080300	4.84741700	0.31674700
Cl	1.10595400	-2.70231200	0.60277900
C	-2.70770000	1.51273300	2.67846800
H	-2.84435500	2.45592800	2.14107600
H	-2.78501700	1.71664800	3.75604200

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G(Gibbs Free Energy) =-5015.178194 hartree

E(electronic Energy) =-5015.9268832 hartree

C	-4.88964700	-1.26870900	-0.85753000
C	-6.05851200	-1.00402000	-1.56495700
C	-6.04138300	-1.11028600	-2.94928500
C	-4.87039000	-1.48868700	-3.59327200
C	-3.74487800	-1.74408500	-2.82032800
N	-3.76480200	-1.62063700	-1.49698500
H	-6.94223900	-0.90307200	-3.52067800
H	-6.96937800	-0.71880000	-1.04832600
H	-4.82386400	-1.58952000	-4.67273100
H	-2.79105900	-2.04482300	-3.25177500
C	-4.77809000	-1.18172500	0.61215600
C	-5.81809200	-0.75568800	1.43301200
C	-3.40005700	-1.51993900	2.44596000
C	-5.62114100	-0.72428100	2.80653100
H	-6.76438200	-0.43814500	1.00636700
H	-2.42024900	-1.83285500	2.80046500

H	-6.42197000	-0.39529600	3.46404600
C	-4.39569300	-1.11593600	3.32636000
H	-4.20064300	-1.10848700	4.39368900
N	-3.59040900	-1.54702800	1.12751300
Ni	-2.18535600	-2.02827400	-0.26896000
C	0.21721100	-0.88799900	2.91969100
C	-0.03761500	-1.76812400	3.96894800
C	-0.39651400	-3.09417400	3.72305000
C	-0.48263800	-3.53768000	2.41285000
C	-0.18570700	-2.66751500	1.35404900
C	0.15425800	-1.33533000	1.59896900
H	0.49742800	0.13566100	3.16015300
H	0.05368800	-1.40489700	4.99119600
H	-0.77696600	-4.55816500	2.17702100
H	-0.16253700	-3.09220700	0.35232000
O	1.42260000	1.97578900	1.32390900
S	1.76991000	2.58231000	2.63889100
O	3.20975500	2.58273600	2.91631000
O	0.88166600	2.20624800	3.74081000
C	1.35711500	4.34670600	2.32435800
F	0.06524400	4.46484500	2.01383900
F	2.06917600	4.81928500	1.30008900
F	1.60584100	5.08764000	3.39170900
P	1.39218500	1.61402300	-1.78092400
P	3.06049100	-0.91488000	0.39011200
C	2.67225900	2.92967400	-1.44423200
H	2.98051600	3.28276200	-2.43761500
H	2.13456700	3.75776800	-0.97075100
C	4.56965900	1.23277300	-0.82123600
H	5.63858900	1.39605300	-1.01042000
H	4.19747800	0.75067700	-1.73776700
C	4.45808100	0.29529000	0.38672900
H	5.36887100	-0.30063700	0.53505400
H	4.33981200	0.89328600	1.29883900
Pd	0.69982400	-0.03128700	0.07027400
C	-2.90447900	1.95009400	1.49824500
C	-1.64790700	1.35756100	1.38093900
C	-1.24277600	0.75954500	0.18667000
C	-2.09992300	0.83342000	-0.91436300
C	-3.35059400	1.43466800	-0.81095000
C	-3.77487900	1.96205500	0.40464000
H	-3.18718700	2.39263400	2.44985700
H	-0.98999800	1.38799800	2.24709400
H	-1.79553500	0.43472600	-1.87837500

H	-4.01962000	1.48566500	-1.66957300
Cl	-2.63859700	-4.27712400	-0.34600100
C	-0.00810800	2.69400500	-2.27101300
C	-0.68944500	2.54648000	-3.48017800
C	-0.47091200	3.63066500	-1.33845200
C	-1.79367100	3.34422400	-3.76717500
H	-0.35754800	1.80376100	-4.20369800
C	-1.57284600	4.42341900	-1.62742100
H	0.01329900	3.72105400	-0.36618800
C	-2.23424400	4.28644700	-2.84509800
H	-2.30968700	3.22688200	-4.71765200
H	-1.92134600	5.14368100	-0.89074200
H	-3.09718000	4.90889100	-3.07023000
C	1.99507600	0.91611100	-3.37628900
C	2.30067700	1.74263900	-4.46629600
C	2.22422500	-0.45507500	-3.49223200
C	2.82243500	1.20663400	-5.63589200
H	2.11709200	2.81500300	-4.40749700
C	2.75950800	-0.99246900	-4.65974200
H	1.98434700	-1.11511600	-2.66363700
C	3.05841400	-0.16319900	-5.73257000
H	3.05054700	1.86067600	-6.47442200
H	2.94040800	-2.06404400	-4.71595100
H	3.47500300	-0.57955600	-6.64692800
C	3.32037100	-1.69438900	2.03308800
C	3.30876300	-3.08006100	2.20396300
C	3.46431000	-0.86968000	3.15608700
C	3.45587300	-3.63341200	3.47117800
H	3.19196400	-3.73669300	1.34401600
C	3.61826700	-1.42893000	4.41871000
H	3.44668000	0.21675000	3.06466600
C	3.61434500	-2.81039100	4.58020100
H	3.44791000	-4.71465900	3.58801100
H	3.73294300	-0.77413700	5.27905000
H	3.73262500	-3.24537100	5.57001100
C	3.58561900	-2.19498800	-0.81614900
C	4.82875100	-2.17288000	-1.45507500
C	2.67556300	-3.20411400	-1.15259800
C	5.15140800	-3.13608700	-2.40581000
H	5.55586000	-1.39755100	-1.22580200
C	3.00016000	-4.16950700	-2.09763000
H	1.69010300	-3.22008000	-0.69270400
C	4.24022500	-4.13558100	-2.72858500
H	6.12088800	-3.10126200	-2.89721700

H	2.27490800	-4.94039300	-2.34570900
H	4.49488900	-4.88614000	-3.47329400
H	-0.60045900	-3.77144300	4.54931500
O	-5.04780300	2.44833900	0.43337100
C	-5.48519000	3.04619900	1.62775300
H	-6.50388500	3.39711100	1.44775900
H	-5.49554900	2.32926400	2.46366500
H	-4.85742500	3.90294700	1.91052800
Cl	-0.40483700	-1.77627600	-1.79244300
C	3.88368600	2.58868500	-0.58572000
H	3.59231000	2.65848600	0.46584700
H	4.61254300	3.39490400	-0.74151800

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G(Gibbs Free Energy) =-3430.464908 hartree

E(electronic Energy) =-3431.0725201 hartree

C	-1.16636600	-2.22498300	1.63612600
C	-1.67730300	-3.07243900	2.61763300
C	-2.28829800	-2.54919000	3.75399900
C	-2.38170700	-1.17252100	3.92018800
C	-1.87430200	-0.31077600	2.94516700
C	-1.26999400	-0.85062900	1.81783200
H	-0.69320300	-2.63293700	0.74236300
H	-1.60108800	-4.14940200	2.48122300
H	-2.85052100	-0.75660100	4.81020000
H	-1.95412100	0.76616900	3.08674400
O	-0.34970800	-3.59725700	-2.39205100
S	0.82353400	-2.77756000	-2.08537200
O	0.59309500	-1.73671600	-1.05066100
O	1.62026100	-2.30260400	-3.22418800
C	1.95420900	-3.91942800	-1.19518300
F	2.26794500	-4.96831300	-1.94034200
F	1.38497600	-4.34760600	-0.07027800
F	3.08369200	-3.28327300	-0.86595800
P	1.13202500	1.42140000	-1.31624800
P	-2.59806100	0.33072100	-0.62310500
C	0.83996200	0.93880500	-3.08783300
H	1.05757400	1.81800500	-3.70992600
H	1.56265200	0.15395000	-3.33594100
C	-1.69273100	1.39927400	-3.07513500
H	-2.00010300	1.86804100	-4.01929200
H	-1.35998000	2.23317400	-2.43663100
C	-2.88726100	0.71294400	-2.43011300
H	-3.79915200	1.31846600	-2.49604200

H	-3.09369700	-0.24082700	-2.93259300
Pd	-0.32840200	0.30879600	0.38601700
C	3.24247700	-0.67018300	2.50579200
C	2.25877500	-0.62658300	1.52722100
C	1.35825000	0.43871500	1.50065000
C	1.52899900	1.53958200	2.34742700
C	2.50723900	1.50029500	3.32491800
C	3.37290000	0.39880500	3.40121000
H	3.91578100	-1.52125300	2.54390900
H	2.17587100	-1.42792200	0.79440300
H	0.88363600	2.41441400	2.26354800
H	2.64600900	2.31434000	4.03207900
C	2.92549700	1.11724900	-1.07765200
C	3.68975700	1.99078900	-0.29575200
C	3.50357300	-0.07196000	-1.53441100
C	5.00881300	1.68714400	0.01667200
H	3.24980600	2.91285300	0.08109900
C	4.82516500	-0.36995400	-1.21746700
H	2.92958400	-0.79096000	-2.11860100
C	5.57928100	0.50355800	-0.44245900
H	5.58991000	2.37676300	0.62492200
H	5.25775900	-1.30065300	-1.57690700
H	6.61151400	0.26401800	-0.19610900
C	1.01474700	3.25401900	-1.32688700
C	1.84010400	4.03608600	-2.14292500
C	0.06210300	3.88628400	-0.52817400
C	1.70775500	5.41839800	-2.15642800
H	2.60127500	3.55952100	-2.75995900
C	-0.07565800	5.27095700	-0.54358800
H	-0.58863800	3.27820600	0.09961800
C	0.74876700	6.03771400	-1.35772900
H	2.35534700	6.01688300	-2.79271300
H	-0.83035200	5.74577600	0.07947600
H	0.64648400	7.12015400	-1.37275700
C	-3.49308800	-1.24534800	-0.40673900
C	-4.51377400	-1.43640900	0.52487800
C	-3.00156400	-2.33901200	-1.12729500
C	-5.05483300	-2.70466100	0.71045800
H	-4.87849900	-0.60040900	1.11911600
C	-3.54013100	-3.60349500	-0.93356400
H	-2.15689300	-2.23805800	-1.80970600
C	-4.57277600	-3.78675800	-0.01864000
H	-5.85143800	-2.84716600	1.43711500
H	-3.12600600	-4.44055300	-1.49014600

H	-4.99434500	-4.77723800	0.13688400
C	-3.61273000	1.61881100	0.20129800
C	-4.96035400	1.81444400	-0.12252500
C	-3.02437100	2.45542700	1.15123100
C	-5.69356600	2.82513000	0.48619300
H	-5.44504500	1.16241400	-0.84867400
C	-3.75322700	3.47454200	1.75630500
H	-1.97865000	2.29452300	1.41989700
C	-5.08953600	3.65972200	1.42295600
H	-6.74066300	2.96349300	0.22805000
H	-3.27705200	4.11948900	2.49115300
H	-5.66423100	4.45320800	1.89450000
H	-2.69446700	-3.21723000	4.51027400
O	4.32437000	0.47617900	4.35517100
C	5.29794700	-0.54273800	4.40334300
H	5.98678500	-0.27361700	5.20580500
H	4.84996300	-1.52025200	4.62748700
H	5.85185400	-0.61054900	3.45656000
C	-0.55965100	0.40049700	-3.31787200
H	-0.62673100	-0.00634100	-4.33544700
H	-0.67873500	-0.46419400	-2.65122800

Ni^{II}

G(Gibbs Free Energy) =-1584.704906 hartree

E(electronic Energy) =-1584.8169541 hartree

C	1.57450100	0.73466500	-0.00002100
C	2.72379300	1.51582700	0.00018300
C	2.59984600	2.89791100	0.00024500
C	1.33096400	3.45757600	0.00009200
C	0.22449500	2.61864400	-0.00009600
N	0.34180900	1.28692400	-0.00013300
H	3.48602900	3.52668700	0.00042200
H	3.70492000	1.05146400	0.00032200
H	1.18529800	4.53292300	0.00013900
H	-0.80056800	2.98537300	-0.00023000
C	1.57648700	-0.73038700	-0.00004300
C	2.72794400	-1.50837100	-0.00027600
C	0.23170300	-2.61806100	0.00015900
C	2.60781500	-2.89077800	-0.00025800
H	3.70778500	-1.04129200	-0.00049900
H	-0.79231700	-2.98766200	0.00030500
H	3.49572800	-3.51710800	-0.00044100
C	1.34046800	-3.45392600	-0.00002400
H	1.19776700	-4.52967200	-0.00000300

N	0.34532400	-1.28599200	0.00014700
Ni	-1.11919800	-0.00154600	0.00006000
Cl	-2.65758700	1.53034900	-0.00027300
Cl	-2.65330200	-1.53755700	0.00018100

TS3^{Pd}

G(Gibbs Free Energy) =-3430.462681 hartree

E(electronic Energy) =-3431.071409 hartree

C	-0.96983800	-2.25095100	1.68080100
C	-1.60875300	-3.10163200	2.58152000
C	-2.25333000	-2.58767100	3.70371700
C	-2.25732500	-1.21697200	3.93932800
C	-1.62085300	-0.35115500	3.04827500
C	-1.04462100	-0.88085000	1.90119000
H	-0.45368900	-2.64678600	0.80570700
H	-1.59479800	-4.17427900	2.39897400
H	-2.74256800	-0.81235800	4.82556300
H	-1.60388300	0.71893600	3.24945600
O	-0.15266900	-3.59175800	-2.49910800
S	0.95528700	-2.70313200	-2.14589400
O	0.64469900	-1.72368000	-1.07340900
O	1.72533400	-2.12887400	-3.25743300
C	2.15726100	-3.79775500	-1.28984700
F	2.53363600	-4.80369900	-2.06445200
F	1.61733300	-4.29279700	-0.17702200
F	3.24613200	-3.10416400	-0.93994200
P	1.04865700	1.52351400	-1.29785800
P	-2.60625300	0.22728000	-0.65707800
C	0.79318600	1.05202700	-3.07866700
H	0.95422600	1.95499900	-3.68401900
H	1.56839900	0.32132400	-3.33667200
C	-1.76996200	1.34338500	-3.09694700
H	-2.09644700	1.79040000	-4.04529300
H	-1.50250800	2.19786500	-2.45448500
C	-2.92470100	0.57731300	-2.46416900
H	-3.87385800	1.12045700	-2.54382000
H	-3.06032900	-0.38854900	-2.96801900
Pd	-0.35455900	0.34476200	0.34250600
C	3.21130100	-0.65929200	2.49461800
C	2.20235900	-0.62944000	1.54512800
C	1.27623400	0.42476800	1.52315300
C	1.45473000	1.51842200	2.38899700
C	2.45010800	1.49290400	3.34476400
C	3.34117800	0.40691500	3.39460600

H	3.90352000	-1.49578900	2.51172600
H	2.11738000	-1.43028700	0.81065100
H	0.79275000	2.38331900	2.32578000
H	2.59005400	2.30417900	4.05498200
C	2.84807000	1.29101400	-1.03313800
C	3.56746600	2.18309400	-0.23054900
C	3.47453400	0.12774300	-1.49221800
C	4.89252700	1.92315600	0.09762300
H	3.08916600	3.08553900	0.14737400
C	4.80094000	-0.12644200	-1.15917100
H	2.93286400	-0.60502200	-2.09032500
C	5.51242000	0.76663400	-0.36621600
H	5.44019100	2.62702800	0.72048000
H	5.26901500	-1.03968900	-1.51895900
H	6.54961100	0.56308000	-0.10839900
C	0.83974300	3.34633600	-1.27104800
C	1.63108700	4.18471000	-2.06452200
C	-0.14945700	3.91224900	-0.46675000
C	1.42938900	5.55864800	-2.05120900
H	2.41905800	3.75932500	-2.68534600
C	-0.35633000	5.28833900	-0.45619500
H	-0.77126500	3.25747000	0.14416600
C	0.43425400	6.11190200	-1.24841100
H	2.05046900	6.20215300	-2.66973500
H	-1.13820400	5.71244400	0.16977000
H	0.27709800	7.18784800	-1.24278700
C	-3.37138800	-1.41184200	-0.40323700
C	-4.34953000	-1.66172000	0.55985700
C	-2.82182000	-2.48030100	-1.12028200
C	-4.79157400	-2.96241800	0.78118100
H	-4.75937100	-0.84405700	1.15038300
C	-3.26635300	-3.77631300	-0.89659300
H	-2.00674700	-2.32977700	-1.82845300
C	-4.25721200	-4.01859600	0.05069400
H	-5.55452100	-3.14928400	1.53366400
H	-2.81265400	-4.59049300	-1.45623000
H	-4.60413300	-5.03386300	0.22984400
C	-3.72367900	1.42454100	0.17268300
C	-5.07687200	1.53374100	-0.16798600
C	-3.21270900	2.26492800	1.16350700
C	-5.89116000	2.46672800	0.46099300
H	-5.50195100	0.87142200	-0.92171700
C	-4.02395200	3.20582800	1.79056600
H	-2.16277800	2.16897600	1.44589000

C	-5.36418700	3.30763000	1.43804400
H	-6.94146300	2.53855100	0.18888300
H	-3.60867400	3.85569400	2.55740200
H	-6.00236600	4.04019800	1.92638800
H	-2.73711100	-3.26075100	4.40806500
O	4.30968100	0.49898100	4.32649200
C	5.30375200	-0.50235800	4.35443000
H	6.00025000	-0.22257700	5.14636600
H	4.87678800	-1.48814200	4.58180500
H	5.84192600	-0.55515000	3.39812300
C	-0.56740200	0.42505200	-3.32594200
H	-0.59320500	0.01780800	-4.34523200
H	-0.63661800	-0.44819700	-2.66391400

Pd^{I}

G(Gibbs Free Energy) =-2853.308238 hartree

E(electronic Energy) =-2853.7209229 hartree

O	1.73694800	-2.02929200	0.60650600
S	1.87544200	-2.28629300	-0.87472000
O	2.12961400	-1.06637300	-1.64385900
O	0.87933100	-3.21773300	-1.39659800
C	3.47676100	-3.18361300	-0.89968700
F	3.39346800	-4.30553400	-0.20038400
F	4.42824700	-2.41848700	-0.37146600
F	3.81045600	-3.47755400	-2.14810100
P	-2.25550000	-0.27508800	0.86027300
P	0.77793300	1.63308800	0.86768200
C	-2.86506600	0.39227000	2.47550900
H	-3.80542100	0.94721400	2.35689900
H	-3.09726600	-0.49373400	3.08035300
C	-1.42024600	2.53547000	2.44359800
H	-1.77355200	3.39944300	3.02115400
H	-1.94962000	2.60146400	1.48155300
C	0.08379700	2.70002500	2.21276700
H	0.33906900	3.74560000	1.99166700
H	0.64181700	2.43154300	3.12018200
Pd	0.03356100	-0.62256000	0.81913300
C	-3.17535900	-1.83521600	0.60759900
C	-4.53484700	-1.94421600	0.91625900
C	-2.49777200	-2.92752900	0.05982500
C	-5.20524000	-3.13975300	0.69448200
H	-5.07484000	-1.09034300	1.32550100
C	-3.17705900	-4.12062000	-0.16802600
H	-1.43792800	-2.85358500	-0.19773400

C	-4.52490100	-4.22829800	0.15338700
H	-6.26132000	-3.22308700	0.94007100
H	-2.64335900	-4.96558900	-0.59488600
H	-5.05166600	-5.16368700	-0.01995100
C	-2.87853200	0.79961000	-0.48259200
C	-3.92999200	1.70720800	-0.34216700
C	-2.26196300	0.65301600	-1.73031000
C	-4.35424900	2.46240500	-1.43099000
H	-4.42847100	1.83595500	0.61726800
C	-2.69774700	1.39713200	-2.81859700
H	-1.42993800	-0.04542400	-1.84301600
C	-3.74032500	2.30674000	-2.66855200
H	-5.17077100	3.17056700	-1.31085400
H	-2.20838300	1.27716900	-3.78185000
H	-4.07288000	2.89775600	-3.51864500
C	2.58589100	1.84600400	1.04885100
C	3.15256600	3.12606600	1.05137900
C	3.40834000	0.72338900	1.15468000
C	4.52598100	3.27869200	1.18029800
H	2.52032400	4.00605900	0.93298300
C	4.78626600	0.88327300	1.27309300
H	2.97694200	-0.27686600	1.12256600
C	5.34324700	2.15553500	1.29200100
H	4.96264300	4.27468600	1.18326900
H	5.42028900	0.00235800	1.33744900
H	6.42011500	2.27725500	1.38338400
C	0.40639200	2.51488800	-0.68851900
C	-0.41137500	3.64448900	-0.76379600
C	0.97706500	1.99607900	-1.85869400
C	-0.65095300	4.25420100	-1.99137900
H	-0.87006400	4.06105600	0.13117800
C	0.74556900	2.61931000	-3.07753200
H	1.59117700	1.09519000	-1.81343400
C	-0.06862900	3.74726900	-3.14705200
H	-1.29398000	5.13002600	-2.04086200
H	1.19997400	2.21578000	-3.97914200
H	-0.25201700	4.22938400	-4.10468200
C	-1.80271000	1.23654300	3.17596300
H	-2.15571000	1.47206900	4.18815900
H	-0.90866300	0.60934100	3.30786300

4$^{Pd'}$

G(Gibbs Free Energy) =-2469.277973 hartree

E(electronic Energy) =-2469.8671544 hartree

C	-1.98462400	-0.88303000	-1.87160100
C	-3.16579500	-1.43851500	-2.35048800
C	-3.83387900	-2.40726100	-1.60248700
C	-3.29076100	-2.83928300	-0.39450300
C	-2.10271200	-2.27073200	0.06695700
C	-1.44303800	-1.26860800	-0.63994400
H	-1.48933000	-0.11881500	-2.47453400
H	-3.59818800	-1.12897200	-3.30002200
H	-3.78470700	-3.60087400	0.20364900
H	-1.70216800	-2.61706300	1.02088200
O	-5.01033000	-2.86276500	-2.12889600
C	-5.74061300	-3.78037400	-1.36246300
H	-6.00552400	-3.36808800	-0.37573500
H	-6.65772600	-3.99545700	-1.91638800
H	-5.19109500	-4.72136000	-1.20845400
P	2.37763900	0.65528800	0.68456700
P	-1.43859100	1.35228500	1.05824900
C	2.65391200	1.98980300	1.96324600
H	2.96110900	1.51323600	2.90330300
H	3.49013900	2.62059300	1.64054400
C	0.37857300	2.06819100	3.07295900
H	0.52045800	2.39149300	4.11370700
H	0.59236400	0.98676000	3.06189100
C	-1.06795200	2.27020400	2.65208300
H	-1.75974500	1.90620400	3.42021700
C	-3.05783700	0.58031400	1.44186800
C	-4.11122200	0.58385300	0.52634400
C	-3.18430300	-0.17169800	2.61413800
H	-4.01796700	1.13140600	-0.40928900
C	-5.27379400	-0.13315800	0.78810300
C	-4.35082500	-0.87690100	2.88153100
H	-2.35317900	-0.22880900	3.31872300
H	-6.07898800	-0.13301700	0.05635400
C	-5.40091300	-0.85619800	1.96865000
H	-4.43594200	-1.45184000	3.80084900
H	-6.31269500	-1.41316000	2.17300600
C	-1.86022000	2.71274800	-0.09860400
C	-1.12283000	2.83563800	-1.27586200
C	-2.85686600	3.65536700	0.17895900
H	-0.34766500	2.10078000	-1.48754200
C	-1.36393800	3.88211400	-2.16040200
C	-3.10322300	4.69735900	-0.70568800
H	-3.45111500	3.56472400	1.08809900

H	-0.77435800	3.96739100	-3.07048700
C	-2.35517800	4.81299400	-1.87555100
H	-3.88167000	5.42348000	-0.48320600
H	-2.54897200	5.63171800	-2.56457900
C	3.05663600	1.45925300	-0.82359800
C	2.30175800	1.44644100	-1.99779300
C	4.30724100	2.08695800	-0.83497200
H	1.34536800	0.92213400	-1.99861300
C	2.76771800	2.07017600	-3.15130800
C	4.77808800	2.70422200	-1.98644600
H	4.92931000	2.07844600	0.05977900
H	2.16551700	2.05301300	-4.05682600
C	4.00474700	2.70292200	-3.14478300
H	5.75266800	3.18673700	-1.98206500
H	4.37317100	3.19015100	-4.04450600
C	3.64221300	-0.58998000	1.13381000
C	3.62498000	-1.11705200	2.42893500
C	4.50457700	-1.14707500	0.18852800
H	2.92677100	-0.72388400	3.16939600
C	4.47043000	-2.16149800	2.77943900
C	5.34370400	-2.19921900	0.53761700
H	4.50391700	-0.77546900	-0.83433500
H	4.44908000	-2.55866500	3.79170400
C	5.33364300	-2.70450900	1.83244600
H	6.00043500	-2.63248900	-0.21303300
H	5.99031000	-3.52813200	2.10246300
H	-1.28885900	3.33533900	2.50172600
Pd	0.17366900	-0.27611400	0.16142100
C	2.28969900	-4.01782900	-0.22225400
C	1.54213700	-2.93201000	0.22655300
C	1.16806100	-1.90011300	-0.64102700
C	1.53653300	-2.01176600	-1.98382000
C	2.28805000	-3.09509600	-2.43786500
C	2.67297600	-4.10051100	-1.55756800
H	2.57998300	-4.79931000	0.47902200
H	1.26449200	-2.88395700	1.28113700
H	1.23129400	-1.24940400	-2.70207400
H	2.56563400	-3.15500200	-3.48948600
H	3.25859100	-4.94691100	-1.91095900
C	1.37915700	2.79736300	2.17122100
H	0.92421000	3.01689600	1.19084300
H	1.61736100	3.77894200	2.60223400

TS3$^{Pd'}$

G(Gibbs Free Energy) =-2469.268543 hartree

E(electronic Energy) =-2469.8579447 hartree

C	-1.73697100	-1.13872400	-1.96416900
C	-2.98669500	-1.58008800	-2.37143900
C	-3.73176800	-2.42951100	-1.55141800
C	-3.20141400	-2.84407400	-0.33179800
C	-1.94680500	-2.38528100	0.06506500
C	-1.19308600	-1.51791900	-0.72685200
H	-1.17329200	-0.48053000	-2.62748800
H	-3.41445200	-1.27520000	-3.32427000
H	-3.75818500	-3.50432000	0.32790200
H	-1.55422200	-2.71901800	1.02607400
O	-4.96210500	-2.78614800	-2.02246600
C	-5.74656900	-3.61283500	-1.20591100
H	-5.95754100	-3.14270700	-0.23210700
H	-6.68873300	-3.77540800	-1.73475800
H	-5.26759600	-4.58687000	-1.02532400
P	2.38234100	0.66834400	0.72218000
P	-1.44750300	1.39936700	1.03422500
C	2.64878800	1.95976100	2.04779100
H	2.91685600	1.45377000	2.98469100
H	3.50358300	2.58783100	1.77092600
C	0.33414700	2.05740500	3.09027900
H	0.45879600	2.35128700	4.14213400
H	0.52072900	0.97134400	3.05527300
C	-1.09885200	2.30691200	2.63956700
H	-1.81775100	1.96247900	3.39225200
C	-3.07037100	0.61226300	1.36972700
C	-4.08901200	0.59888700	0.41479300
C	-3.23391100	-0.14013600	2.53809000
H	-3.96700200	1.14689900	-0.51781200
C	-5.25843400	-0.11950900	0.64028800
C	-4.40636000	-0.84832600	2.76886000
H	-2.42896900	-0.18600400	3.27330300
H	-6.03851500	-0.12580200	-0.11845900
C	-5.42563500	-0.83450800	1.82109300
H	-4.52193600	-1.41764400	3.68848000
H	-6.34514400	-1.38830800	1.99960300
C	-1.87192300	2.76224500	-0.12077300
C	-1.15913100	2.85851300	-1.31590700
C	-2.85305600	3.71939600	0.16232600
H	-0.39787800	2.10921800	-1.53166900
C	-1.40855000	3.89431400	-2.21123100
C	-3.10621100	4.75183700	-0.73141200

H	-3.43033800	3.64675300	1.08406000
H	-0.83974000	3.95994600	-3.13595100
C	-2.38192900	4.84149900	-1.91848000
H	-3.87157700	5.49024200	-0.50363700
H	-2.58065600	5.65251700	-2.61527300
C	3.15447100	1.48052400	-0.73633800
C	2.43717300	1.52515600	-1.93299900
C	4.43212200	2.04954700	-0.69628100
H	1.45541400	1.05089800	-1.96995100
C	2.96945800	2.14322600	-3.06071200
C	4.96777500	2.66392800	-1.82071300
H	5.02210400	1.99664100	0.21860500
H	2.39692100	2.17148500	-3.98500100
C	4.23371900	2.71646700	-3.00356500
H	5.96248500	3.10148200	-1.77683900
H	4.65353300	3.20048800	-3.88232900
C	3.57808700	-0.64501700	1.16923600
C	3.51852300	-1.19954400	2.45257800
C	4.41488500	-1.23438000	0.21996400
H	2.83686900	-0.78296800	3.19553700
C	4.30560600	-2.29271100	2.79014200
C	5.19506300	-2.33553000	0.55573500
H	4.44548400	-0.84331200	-0.79540500
H	4.25436800	-2.70640600	3.79480800
C	5.14974300	-2.86221500	1.84099700
H	5.83395300	-2.78920300	-0.19864500
H	5.76204000	-3.72232100	2.10160100
H	-1.28191800	3.37934600	2.48954500
Pd	0.18027800	-0.22138600	0.16319000
C	2.12763100	-3.99666500	-0.29866300
C	1.23300200	-3.01443900	0.11107100
C	0.84205700	-1.98121300	-0.75385400
C	1.37165800	-1.98535900	-2.05125400
C	2.26410300	-2.97034700	-2.46281100
C	2.64918900	-3.98327300	-1.58948400
H	2.42463300	-4.77619700	0.40147200
H	0.83676200	-3.04856300	1.12675400
H	1.06944900	-1.21743100	-2.76409100
H	2.65611000	-2.94718600	-3.47863400
H	3.34461500	-4.75524800	-1.91163600
C	1.37750900	2.78256400	2.23353600
H	0.95719000	3.02551000	1.24311700
H	1.61686600	3.75275200	2.68961100

Pd^0

G(Gibbs Free Energy) -1892.0878 hartree

E(electronic Energy) =-1892.4824623 hartree

P	2.00562600	-0.47137600	0.16120200
P	-2.07614600	-0.50385700	0.17816600
C	1.82816800	-0.47619000	2.01681600
H	2.08044600	-1.49764600	2.33541800
H	2.59835300	0.17511800	2.45380100
C	-0.55982300	-1.29139100	2.45285000
H	-0.59903200	-1.75401200	3.44993200
H	-0.17057600	-2.06235300	1.77068200
C	-1.97770000	-0.95321900	2.00210200
H	-2.62973200	-1.82427300	2.14391100
C	-3.79595500	-1.04326100	-0.21640900
C	-4.76118100	-0.20072100	-0.77239400
C	-4.10259000	-2.40102000	-0.06441200
H	-4.54013100	0.85464800	-0.91935100
C	-6.00894100	-0.69768500	-1.13825600
C	-5.34991100	-2.89504400	-0.42029100
H	-3.34703100	-3.08520100	0.32437800
H	-6.74978500	-0.02572900	-1.56611000
C	-6.31045000	-2.04188300	-0.95723100
H	-5.57101400	-3.95169800	-0.28706400
H	-7.28671800	-2.42733400	-1.24138900
C	-2.21678300	1.33379300	0.23254300
C	-1.33588000	2.09429400	-0.53941000
C	-3.13466600	1.99687100	1.05589900
H	-0.60940800	1.57858900	-1.17024300
C	-1.36022000	3.48495800	-0.48486100
C	-3.16584300	3.38486200	1.10632800
H	-3.84151100	1.42289200	1.65510600
H	-0.65392300	4.05749200	-1.08237300
C	-2.27478700	4.13091300	0.33831100
H	-3.88499800	3.88741400	1.74940400
H	-2.29548900	5.21746400	0.38498900
C	2.27205900	1.30807700	-0.23041100
C	2.43356700	1.63824800	-1.58218800
C	2.26149600	2.33938900	0.71091800
H	2.42092500	0.84275000	-2.32793900
C	2.59343400	2.95815900	-1.97981500
C	2.40989100	3.66609800	0.31204300
H	2.12723800	2.11973900	1.76835100
H	2.72352500	3.19393200	-3.03355900
C	2.57930100	3.97882000	-1.03078500

H	2.39214500	4.45693000	1.05865000
H	2.69725200	5.01472600	-1.34033100
C	3.70909100	-1.15409000	0.00307900
C	3.84980000	-2.46812200	-0.44644400
C	4.85143500	-0.42777700	0.35209900
H	2.95858900	-3.02610800	-0.73511400
C	5.10866000	-3.05374300	-0.53520900
C	6.10968700	-1.00950700	0.25660500
H	4.75391700	0.60368100	0.69094200
H	5.20724600	-4.07809000	-0.88720700
C	6.23908200	-2.32383600	-0.18488800
H	6.99398400	-0.43605700	0.52588700
H	7.22493600	-2.77682800	-0.26118700
H	-2.40603700	-0.13737600	2.60097600
Pd	-0.01904400	-1.11657000	-0.76012300
C	0.41632700	-0.10529000	2.48381300
H	0.02942100	0.71953000	1.86712100
H	0.46760600	0.29831200	3.50503300

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