Electronic Supplementary Information

Orthogonal Reactivity of Ni(I)/Pd(0) Dual Catalysts for Ullman C-C Cross-Coupling: Theoretical Insight

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1. Methods

1.1. 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 eqn (S1):

$$E_{sol} = E_{sol}^{pot} + E_{gas}^{v_0}$$

(S1)

where E_{sol}^{pot} is the potential energy including non-electrostatic energy in solution and $E_{gas}^{v_0}$ represents the zero-point vibrational energy in the gas phase. In a bimolecular process, such as the coordination of Ni center to the C=C bond of Ph-Br, the entropy change must be taken into consideration because the entropy considerably decreases. In this case, Gibbs energy (G_{sol}^{o}) must be evaluated as follows:

$$\begin{aligned} G_{sol}^{o} &= H_0 - T\left(S_r^o + S_v^o + S_t^o\right) \\ &= E^T + P\Delta V - T\left(S_r^o + S_v^o + S_t^o\right) \\ &= E_{sol} + E_{therm} - T\left(S_r^o + S_v^o + S_t^o\right) \end{aligned}$$

(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.[S1] In this context, the translational entropy was corrected with the method developed by Whitesides et al., 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 298.15 K and 1 atm.

1.2. Computational details for the reductive process of $Pd^{II}(dppp)Cl_2$ and $Ni^{II}(bpy)Br_2$ by Zn dust

The spin-polarized DFT calculations were carried out with the Dmol^3 code in the Materials Studio software package[S2,S3] at the generalized gradient approximation (GGA) level. The model of Zn with (3 × 8 ×1) supercell and perfect (101) surface presented by a three-layer slab were applied for the calculation. To avoid the interlayer interaction, a vacuum space of 15 Å was set along the z direction. The double numerical plus polarization (DNP) basis set[S4] and Perdew–Burke–Ernzerh (PBE) functional[S5] were adopted, which are the most common in materials and surface science. The size and quality of DNP basis set are comparable to that of the Gaussian 6-31G(d,p) basis set. The solvent effect of N,N-dimethylformamide (DMF) was evaluated by the conductor–like screening model (COSMO),[S6] where the dielectric constant was set as 37.219. The geometry optimizations was performed at γ points. The structure optimizations were based on the following points: (1) an energy tolerance of 2×10^{-5} Ha; (2) a maximum force tolerance of 4×10^{-3} Ha/Å; and (3) a maximum displacement tolerance of 5×10^{-3} Å. To accelerate convergence of the self-consistent electron density, we used a mixing of Fermi smearing of 0.005 Ha and Pulay.

References

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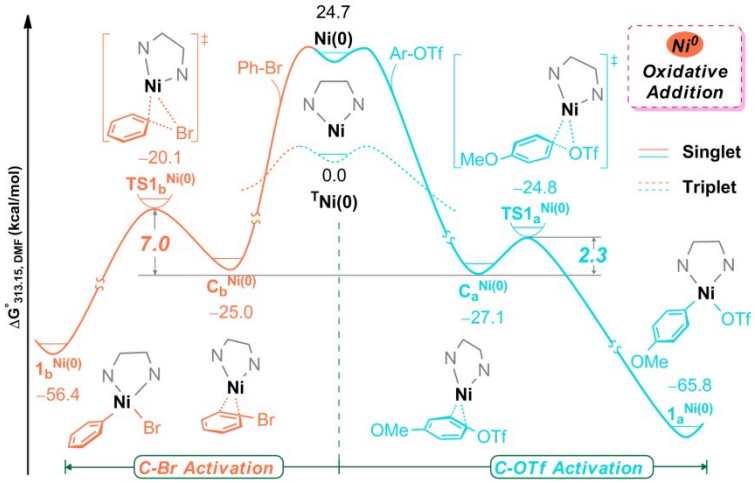

Fig. S1 Energy profiles ($\Delta G^{\circ}_{313.15}$) of oxidative additions of bromobenzene and 4-methoxyphenyltriflate catalyzed by **Ni⁰(bpy)**.

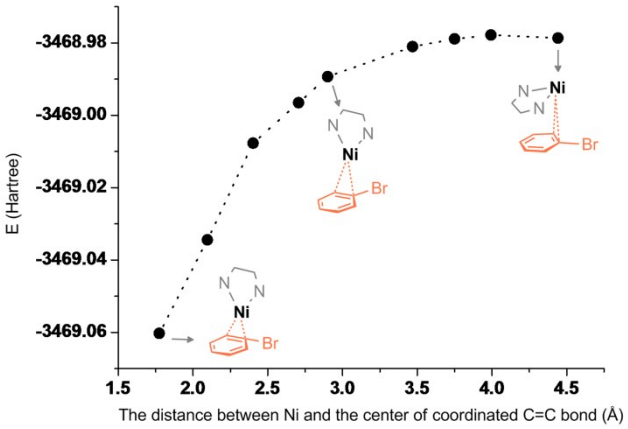

Fig. S2 Relaxed PES scan for the coordination of **Ph-Br** to **Ni⁰(bpy)**.

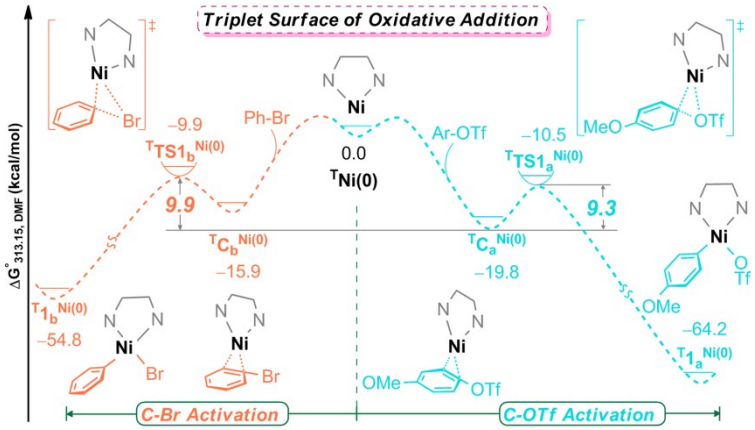

Fig. S3 The triplet energy profiles ($\Delta G^{\circ}_{313.15}$) of oxidative additions of bromobenzene and 4-methoxyphenyltriflate catalyzed by **Ni⁰(bpy)**.

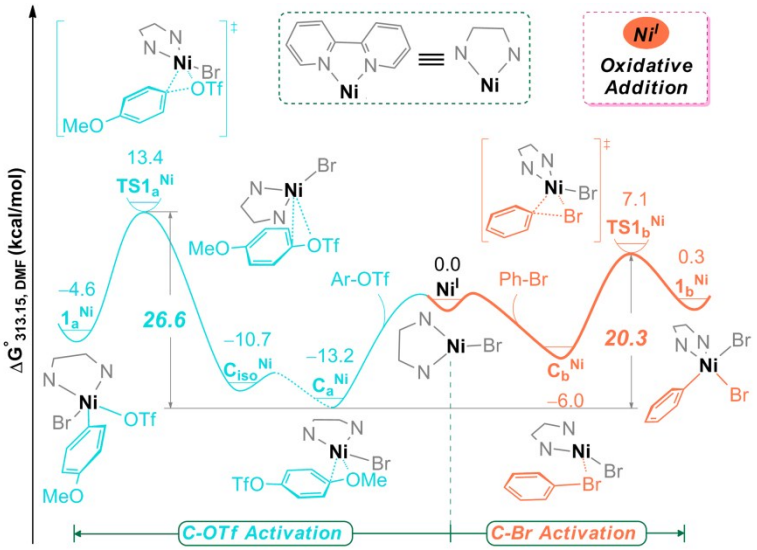

Fig. S4 Energy profiles ($\Delta G^{\circ}_{313.15}$) of oxidative additions of bromobenzene and 4-methoxyphenyltriflate catalyzed by **Ni^{I}(bpy)Br**.

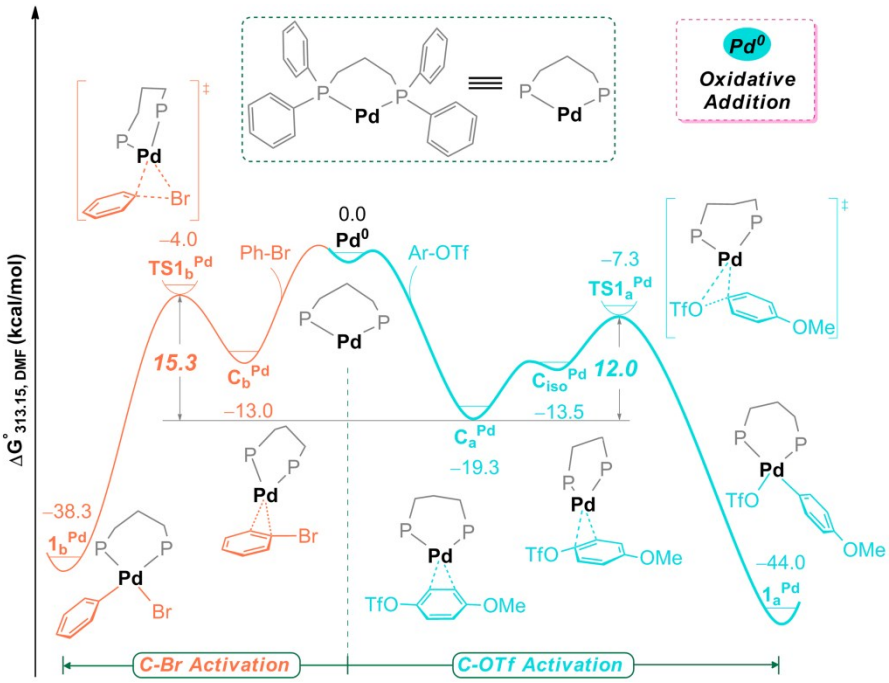

Fig. S5 Energy profiles ($\Delta G^{\circ}_{313.15}$) of oxidative additions of bromobenzene and 4-methoxyphenyltriflate catalyzed by **Pd^{0}(dppp)**.

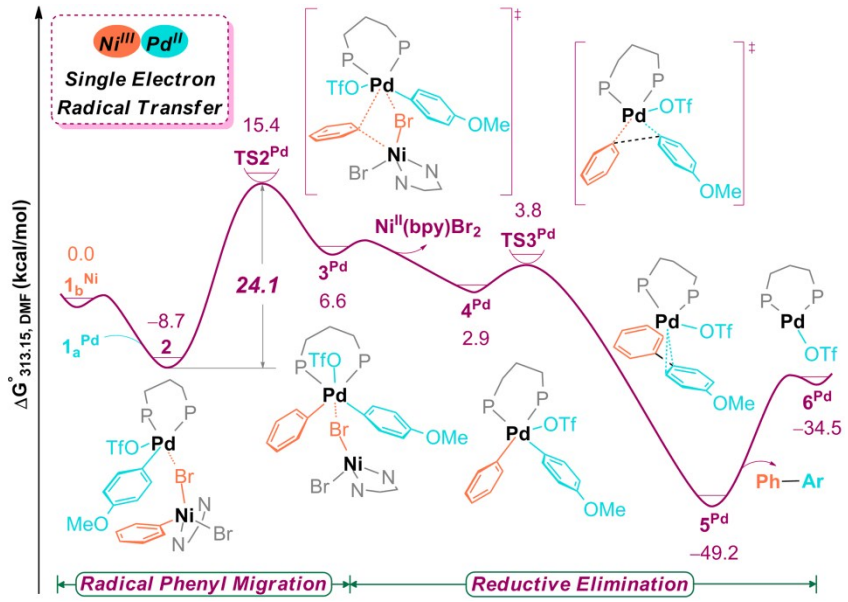

Fig. S6 Energy profiles ($\Delta G^{\circ}_{313.15}$) of single electron radical transfer mechanism of Ni/Pd dual catalysis.

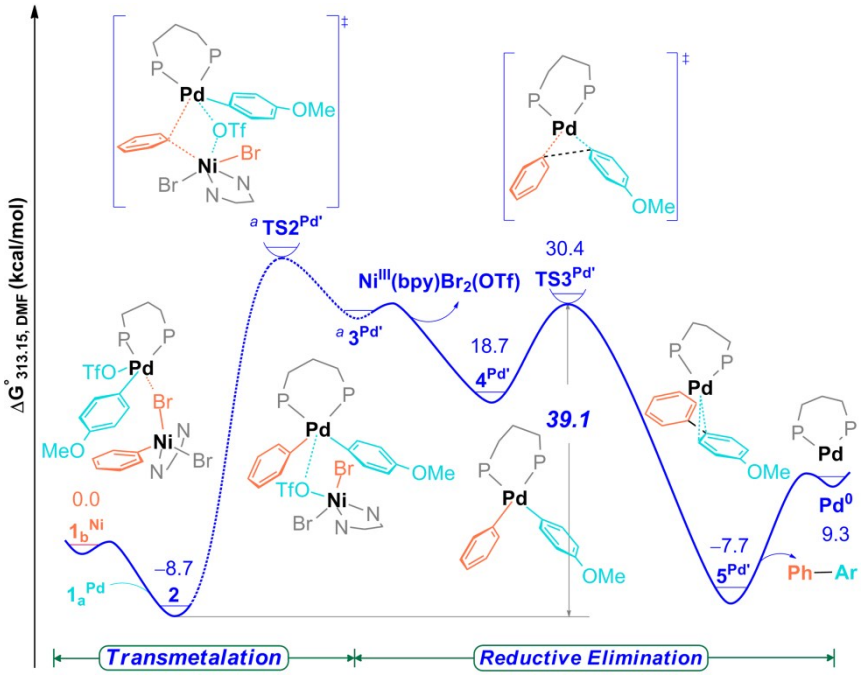

Fig. S7 Energy profiles ($\Delta G^{\circ}_{313.15}$) of the phenyl migration from Ni^{III} to Pd^{II} without alternation of the oxidation states and reductive elimination from Pd^{II} species.

[a] Proposed structure has not been located.

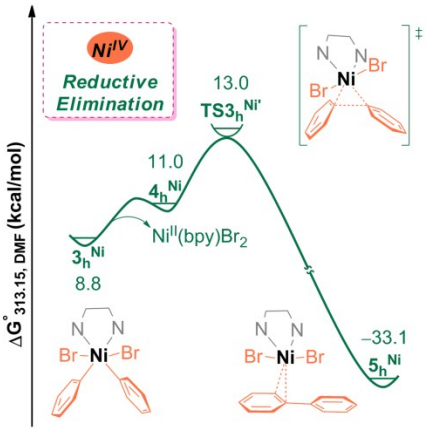

Fig. S8 Energy profiles ($\Delta G^{\circ}_{313.15}$) of dissociated reductive elimination in the homobimetallic disproportionation mechanism.

Coordinates of All Geometry Optimized Structures

Ph-Br	**HF =** −2803.0087635 hartree		
C	0.00000000	1.20541100	-2.16992500
C	0.00000000	1.21383900	-0.77807200
C	0.00000000	0.00000000	-0.10241000
C	0.00000000	-1.21383900	-0.77807200
C	0.00000000	-1.20541100	-2.16992500
C	0.00000000	0.00000000	-2.86622200
H	0.00000000	2.15055300	-2.70930300
H	0.00000000	2.14976700	-0.22393100
H	0.00000000	-2.14976700	-0.22393100
H	0.00000000	-2.15055300	-2.70930300
H	0.00000000	0.00000000	-3.95415600
Br	0.00000000	0.00000000	1.80023900

Ar-OTf	**HF =** −1307.122161 hartree		
C	1.43420400	1.04179000	-0.43204500
C	2.81157700	0.98038900	-0.24194900
C	3.43185200	-0.26147800	-0.08002000
C	2.66968900	-1.43705400	-0.10951400
C	1.30062900	-1.37761700	-0.29856800
C	0.70493500	-0.13282900	-0.45906400
H	0.92964200	1.99611800	-0.56419800
H	3.38489200	1.90261700	-0.22415000
H	3.17834200	-2.38994100	0.01706800
H	0.69272800	-2.27882600	-0.32777800
O	4.75782400	-0.43112400	0.10787900
C	5.57757300	0.72139100	0.14110400
H	5.29474000	1.38952100	0.96612900
H	6.59785200	0.36588900	0.29907200

H	5.52884000	1.27370300	-0.80737700
O	-0.68702800	-0.06977400	-0.70822600
S	-1.61420900	0.05805300	0.60332600
O	-1.45084200	1.35647100	1.22168300
O	-1.55167000	-1.15242800	1.39446200
C	-3.20836100	0.05881600	-0.32964100
F	-3.32706200	-1.06650600	-1.00043900
F	-3.23905600	1.08742100	-1.14937800
F	-4.17372100	0.15980200	0.56312900

Ph-Ar **HF =** −577.4035913 hartree

C	-0.50368300	1.28131900	-0.37082700
C	-1.88397700	1.36747500	-0.39007900
C	-2.66429700	0.25309400	-0.06470300
C	-2.03793800	-0.94588200	0.27704600
C	-0.64783900	-1.01417600	0.29197200
C	0.14944400	0.08714400	-0.02830900
H	0.08405300	2.15467100	-0.65199200
H	-2.38810000	2.29226600	-0.66480400
H	-2.61731700	-1.82598300	0.54376900
H	-0.17547400	-1.95062900	0.58773800
O	-4.00619200	0.43674200	-0.10762800
C	-4.83212400	-0.66846100	0.19429300
H	-4.65911400	-1.03387300	1.21631600
H	-5.86208400	-0.31459600	0.10926700
H	-4.67366200	-1.49323200	-0.51479500
C	3.67048100	-1.25824900	-0.35831600
C	2.28319500	-1.17570000	-0.38402500
C	1.62318400	0.00066800	-0.00539200
C	2.40217000	1.09352200	0.39648400
C	3.78975000	1.01383400	0.41789100
C	4.43124000	-0.16294300	0.04151100
H	4.16042700	-2.18168500	-0.66299300
H	1.70043100	-2.03055400	-0.72631800
H	1.91179000	2.01112400	0.72079300
H	4.37332100	1.87517400	0.73903300
H	5.51762200	-0.22648700	0.05974400

Ni^{II}(bpy)Br_2 **HF =** −5809.2800609 hartree

C	-1.71668500	-0.72999800	-0.11167900
C	-2.86971500	-1.50528100	-0.18856800
C	-2.74947000	-2.87312300	-0.39701700
C	-1.48626200	-3.43690500	-0.52627200
C	-0.38093200	-2.60289800	-0.43644400
N	-0.49945200	-1.29113200	-0.23427500
H	-3.64006900	-3.49372000	-0.45376600

H	-3.85199400	-1.05457000	-0.08022500
H	-1.35310000	-4.50215300	-0.68892900
H	0.63523500	-2.98627900	-0.52497500
C	-1.71703800	0.72913600	0.11199000
C	-2.87046100	1.50381000	0.18897500
C	-0.38221900	2.60276100	0.43654700
C	-2.75091100	2.87172100	0.39733800
H	-3.85252500	1.05260100	0.08072500
H	0.63374800	2.98669400	0.52496900
H	-3.64182600	3.49186300	0.45412200
C	-1.48798800	3.43617700	0.52645800
H	-1.35537300	4.50150100	0.68906100
N	-0.50007700	1.29092200	0.23441900
Ni	1.05077200	0.00028500	-0.00007400
Br	1.49277900	-0.44538100	2.25401900
Br	1.49210900	0.44609900	-2.25424500

Pd^0(dppp) **HF =** −1854.3302728 hartree

P	-1.92674800	-0.21614000	0.03880600
P	1.92679900	-0.21619700	0.03890600
C	-1.30314900	-0.36735200	1.78868100
H	-2.10419700	-0.06471100	2.48099900
H	-1.16566200	-1.44861000	1.94504000
C	-0.00003600	0.37818200	2.11357500
H	-0.00013000	0.58029200	3.19476900
H	-0.00011900	1.37073700	1.63331100
C	1.30328800	-0.36702800	1.78885300
H	2.10424700	-0.06388500	2.48105000
C	2.74517000	1.43017700	0.00006600
C	3.28238800	1.83870000	-1.22760200
C	2.84718200	2.29076500	1.09659200
H	3.19472100	1.18088000	-2.09501600
C	3.92147500	3.06551200	-1.35303700
C	3.47509600	3.52824600	0.96797300
H	2.43866900	2.00468000	2.06522000
H	4.34000200	3.36381600	-2.31266500
C	4.01550200	3.91640900	-0.25308800
H	3.54387700	4.18893800	1.83052600
H	4.50653500	4.88289700	-0.35041600
C	3.36598900	-1.36232700	0.12561400
C	3.24561200	-2.61380100	-0.48352900
C	4.54599000	-1.04779000	0.80712800
H	2.32854800	-2.85554500	-1.02561800
C	4.28162400	-3.54077900	-0.40861200
C	5.58514300	-1.96959500	0.87531800
H	4.65587600	-0.07210800	1.28309400

H	4.17683000	-4.51293400	-0.88729800
C	5.45340400	-3.21718900	0.26870200
H	6.50220000	-1.71455500	1.40393200
H	6.26877900	-3.93649700	0.32160500
C	-3.36558700	-1.36273000	0.12520300
C	-3.24423600	-2.61452100	-0.48311300
C	-4.54621000	-1.04830200	0.80567700
H	-2.32668400	-2.85618800	-1.02441700
C	-4.27990500	-3.54189000	-0.40841500
C	-5.58503800	-1.97050100	0.87361400
H	-4.65681300	-0.07241800	1.28106000
H	-4.17434800	-4.51428300	-0.88644900
C	-5.45233800	-3.21838700	0.26782300
H	-6.50259300	-1.71553100	1.40140000
H	-6.26745900	-3.93799800	0.32051900
C	-2.74557900	1.43000600	0.00054900
C	-2.84781500	2.29015100	1.09740000
C	-3.28295400	1.83883200	-1.22694900
H	-2.43919800	2.00382300	2.06591300
C	-3.47609600	3.52749700	0.96926600
C	-3.92240300	3.06550400	-1.35190400
H	-3.19513200	1.18136000	-2.09461200
H	-3.54504500	4.18784100	1.83207100
C	-4.01664700	3.91596100	-0.25163400
H	-4.34104400	3.36404200	-2.31140900
H	-4.50796600	4.88234200	-0.34858800
H	1.16616700	-1.44827700	1.94559600
Pd	-0.00000100	-0.50294700	-1.18391700

C_a^{Pd} **HF =** −3161.491503 hartree

P	2.87583900	0.51191600	-0.21971200
P	-0.28502200	2.15803500	-0.44227200
C	3.29034200	2.30934900	-0.40160300
H	4.27807900	2.49465600	0.04690700
H	3.41204100	2.47245600	-1.48386300
C	2.25375600	3.29262200	0.15138800
H	2.74511700	4.27190700	0.23721700
H	1.96696900	3.01999900	1.18013600
C	0.99463400	3.47879400	-0.70123600
H	0.54367700	4.45984800	-0.48913900
C	-0.77005100	2.45809500	1.30540000
C	-0.53469000	1.45166300	2.24707700
C	-1.31632800	3.67372700	1.73040900
H	-0.12172700	0.49632900	1.91043000
C	-0.82169400	1.66075300	3.59396100
C	-1.60925800	3.88102500	3.07340700

H	-1.51748000	4.46338000	1.00454100
H	-0.62661700	0.87215600	4.31905100
C	-1.35759300	2.87619500	4.00682700
H	-2.03270700	4.83054100	3.39645000
H	-1.58369200	3.04356600	5.05844600
C	-1.73019000	2.79079500	-1.37713900
C	-1.63796900	3.75660900	-2.38292300
C	-2.97159400	2.18587500	-1.13633200
H	-0.68876900	4.24637800	-2.59538800
C	-2.76211500	4.10650600	-3.12964700
C	-4.09192300	2.53780900	-1.87673000
H	-3.05987200	1.43016500	-0.35327300
H	-2.67395500	4.86167900	-3.90905400
C	-3.98835100	3.50007000	-2.88094200
H	-5.04473300	2.05204300	-1.67005100
H	-4.86269400	3.77451000	-3.46834400
C	4.25625300	-0.26303400	-1.14891900
C	4.13966500	-0.29450600	-2.54467100
C	5.35545700	-0.87993400	-0.54748700
H	3.26851300	0.16192300	-3.02170600
C	5.10416400	-0.92223700	-3.32333500
C	6.31343100	-1.52381400	-1.32742200
H	5.46217400	-0.86699500	0.53693900
H	5.00118900	-0.93853400	-4.40686000
C	6.19013600	-1.54759300	-2.71301100
H	7.16112500	-2.00955600	-0.84680400
H	6.93854300	-2.05535100	-3.31853400
C	3.24233300	0.12635800	1.53238100
C	3.68602600	1.06719000	2.46505400
C	2.97571600	-1.18107600	1.96490800
H	3.90954400	2.08804800	2.15834400
C	3.84666000	0.71398100	3.80353400
C	3.14843500	-1.53535800	3.29673900
H	2.64033200	-1.93044200	1.24416300
H	4.18965400	1.45873300	4.51960200
C	3.57569500	-0.58417100	4.22225700
H	2.94127700	-2.55588300	3.61534900
H	3.69931700	-0.85710600	5.26863700
H	1.26631900	3.47391100	-1.76816300
Pd	0.61803900	-0.01802300	-0.73860600
C	-1.01426900	-1.49598700	-1.08977000
C	0.23494500	-2.17592300	-1.23678500
C	0.68934900	-3.03134600	-0.19070200
C	-0.05268700	-3.20473900	0.96374500
C	-1.28479100	-2.54120200	1.11275700
C	-1.73997400	-1.73291000	0.10629300

H	-1.53786500	-1.10399800	-1.96135700
H	0.67621200	-2.25712600	-2.22896300
H	0.33322000	-3.85249200	1.74797300
H	-1.87040200	-2.65347300	2.02320800
O	1.87094800	-3.69085800	-0.24673400
C	2.65115400	-3.59883200	-1.42638200
H	3.57632800	-4.14253000	-1.21969500
H	2.13976100	-4.06849700	-2.27789400
H	2.89392900	-2.55437600	-1.67034800
O	-2.92842200	-0.99454300	0.34512000
S	-4.28947800	-1.36964800	-0.41436100
O	-4.04220200	-1.88081200	-1.74449500
O	-5.18843600	-0.26655500	-0.16472400
C	-4.89114000	-2.79147000	0.61394200
F	-4.77132200	-2.48316700	1.89047500
F	-4.18364200	-3.86897500	0.34038800
F	-6.15831600	-2.99777800	0.31512300

C_{iso}^{Pd} **HF =** −3161.4820922 hartree

C	1.52008100	-0.23470200	2.84172200
C	0.85208300	-1.32343500	3.32728800
C	-0.55887600	-1.41620100	3.17365200
C	-1.28041400	-0.37572200	2.63122500
C	-0.61720000	0.77696300	2.10080100
C	0.80753600	0.77661000	2.14027100
H	2.59474300	-0.11843700	2.97411800
H	1.37521200	-2.14058300	3.81977000
H	-2.36645400	-0.40789200	2.58623400
H	-1.16743700	1.71420600	2.00294400
O	-1.10171900	-2.58097400	3.61748800
C	-2.46798200	-2.80344700	3.33724300
H	-2.67400200	-2.70643700	2.25880600
H	-2.68909800	-3.82321000	3.66167800
H	-3.11577400	-2.10285500	3.88470800
O	1.47630600	2.05217900	2.16135000
S	2.01757900	2.88567300	0.91486000
O	1.60353300	2.35941000	-0.36815600
O	3.39780100	3.23358500	1.17388000
C	1.00988900	4.40514300	1.20605900
F	1.28148600	4.90531300	2.39332100
F	-0.27391800	4.09633900	1.13104600
F	1.31226800	5.27825600	0.26460000
P	-1.93259500	-0.01418100	-1.26167700
P	1.42991100	-1.26901100	-1.21881600
C	-1.67711700	-0.80555900	-2.92509500
H	-2.65280600	-1.12653100	-3.32031600

H	-1.33171600	0.00909300	-3.58035000
C	-0.67351500	-1.96242100	-2.99080300
H	-0.84378900	-2.48482700	-3.94273900
H	-0.87879000	-2.71257200	-2.20916700
C	0.80547900	-1.56324300	-2.93962500
H	1.40988800	-2.35040000	-3.41421400
C	1.46484500	-2.98896900	-0.55611100
C	2.36111700	-3.95235200	-1.03148900
C	0.56137000	-3.34444000	0.45037500
H	3.07933200	-3.69043300	-1.81025600
C	2.35251200	-5.24147500	-0.51030000
C	0.55157200	-4.63491100	0.97386800
H	-0.12745100	-2.58843000	0.83896600
H	3.05682700	-5.98189200	-0.88601300
C	1.44799200	-5.58417700	0.49349800
H	-0.15120800	-4.88994200	1.76568100
H	1.44781600	-6.59241600	0.90405500
C	3.21326300	-0.91010600	-1.46620100
C	3.95047400	-0.58992200	-0.31857400
C	3.85918400	-0.90255900	-2.70518500
H	3.44746800	-0.57748600	0.65192600
C	5.30286500	-0.28693700	-0.40256100
C	5.21376800	-0.58489800	-2.79176100
H	3.31210100	-1.14795000	-3.61465900
H	5.86353800	-0.04612800	0.49899700
C	5.93732500	-0.28045500	-1.64416100
H	5.70425200	-0.58016500	-3.76374800
H	6.99506000	-0.03376300	-1.71503100
C	-2.73388700	1.56726600	-1.73785100
C	-2.05292100	2.75341300	-1.45453400
C	-3.97432500	1.63075200	-2.38229500
H	-1.08511000	2.70203400	-0.95180400
C	-2.59810400	3.98629400	-1.80443900
C	-4.52012300	2.86100100	-2.73114200
H	-4.52177000	0.71359500	-2.60460900
H	-2.05772800	4.90220700	-1.56967400
C	-3.83342000	4.03962500	-2.44170000
H	-5.48716200	2.90338800	-3.22950600
H	-4.26681700	5.00062300	-2.71301300
C	-3.31614000	-0.95895600	-0.51817000
C	-3.58459500	-2.29304100	-0.83803100
C	-4.04515600	-0.35792800	0.51818200
H	-3.03990600	-2.79066800	-1.63993000
C	-4.56015200	-3.00683100	-0.14331300
C	-5.02346100	-1.06619600	1.20425200
H	-3.84276300	0.68165400	0.78602000

H	-4.75912700	-4.04381200	-0.40851900
C	-5.28103500	-2.39740900	0.87774900
H	-5.58442300	-0.57959600	2.00066100
H	-6.04409800	-2.95471200	1.41783700
H	0.96472100	-0.63862100	-3.51605800
Pd	0.00721800	0.10744800	0.10809900

$TS1_a^{Pd}$ **HF =** −3161.462374 hartree $\nu^{\ddagger} = -264.64\ icm^{-1}$

C	0.01864600	2.47842000	1.90181600
C	-1.18487600	2.97140400	2.33760000
C	-2.32912700	2.98983800	1.49566700
C	-2.25053900	2.51270600	0.20556200
C	-1.03519200	1.93041700	-0.25783600
C	0.07026800	1.87362000	0.62699200
H	0.90098000	2.49259100	2.53921100
H	-1.29106900	3.36234800	3.34839400
H	-3.08594500	2.59143100	-0.48638600
H	-0.89321900	1.78883900	-1.33078000
O	-3.43369900	3.53909300	2.06174100
C	-4.58294800	3.65903400	1.25033400
H	-4.92675300	2.67583900	0.89491100
H	-5.35765400	4.10884500	1.87552100
H	-4.39261600	4.30855500	0.38354300
O	1.75899500	2.44776900	-0.02208000
S	2.09295800	2.54613200	-1.49692000
O	1.28443500	1.67833300	-2.35118000
O	3.53609700	2.56917800	-1.71399700
C	1.54131800	4.25309700	-1.90966300
F	2.19659200	5.13230800	-1.16683600
F	0.24034800	4.38676100	-1.68849300
F	1.78829100	4.49462300	-3.18943800
P	-1.86682600	-1.81000900	-0.05987900
P	1.45473400	-1.62492500	0.88136200
C	-1.77165200	-3.28851300	1.07512200
H	-2.65734800	-3.27401600	1.72376200
H	-1.84698100	-4.19226500	0.45349400
C	-0.50294700	-3.34920400	1.92386300
H	-0.54268000	-4.27058100	2.51985600
H	-0.50479300	-2.52326300	2.65456900
C	0.79355300	-3.34025300	1.10282100
H	1.57004100	-3.95566300	1.57847500
C	2.31151600	-1.33047000	2.47432400
C	3.52506200	-1.95695800	2.77707400
C	1.72045500	-0.48784300	3.41886500
H	3.99683100	-2.61414900	2.04506000
C	4.13683000	-1.73940900	4.00572100

C	2.33125300	-0.27559300	4.65245400
H	0.77584300	0.00490400	3.17971300
H	5.08328200	-2.22644400	4.23321500
C	3.54020100	-0.89870200	4.94391700
H	1.86371000	0.38212600	5.38287100
H	4.02269500	-0.72825900	5.90453200
C	2.82147700	-1.80146100	-0.31791900
C	3.52310100	-0.63903000	-0.66011300
C	3.17948400	-3.01308100	-0.91520900
H	3.24640900	0.31403600	-0.20396300
C	4.56328800	-0.68560900	-1.57861300
C	4.22084300	-3.05685000	-1.84000100
H	2.65886000	-3.93473900	-0.66092400
H	5.08931700	0.23115000	-1.83813400
C	4.91272000	-1.89703500	-2.17233000
H	4.49223600	-4.00585600	-2.29877900
H	5.72368700	-1.93547800	-2.89720900
C	-1.83784000	-2.52519900	-1.74024100
C	-0.89525000	-2.04196300	-2.65279200
C	-2.70668200	-3.55088100	-2.13168300
H	-0.21394300	-1.24290100	-2.34979600
C	-0.81807000	-2.57702000	-3.93631500
C	-2.63201900	-4.08064700	-3.41398500
H	-3.45279900	-3.93130500	-1.43251800
H	-0.07877800	-2.19695300	-4.63863100
C	-1.68615600	-3.59501700	-4.31578500
H	-3.31253500	-4.87583900	-3.71217000
H	-1.62765200	-4.01412100	-5.31848200
C	-3.55972400	-1.16591800	0.18780400
C	-3.92261400	-0.77887300	1.48458900
C	-4.42659100	-0.89212200	-0.87191100
H	-3.23587800	-0.94916000	2.31742500
C	-5.14558300	-0.16310600	1.72010800
C	-5.64852300	-0.26666600	-0.63453600
H	-4.15203500	-1.17077100	-1.88901400
H	-5.41915300	0.12754000	2.73295800
C	-6.01387900	0.09106300	0.65931400
H	-6.32001900	-0.06458000	-1.46705500
H	-6.97088400	0.57630400	0.84261400
H	0.60837500	-3.76817100	0.10521300
Pd	-0.25669600	-0.09729000	0.31899900

1_a^{Pd} **HF =** −3161.5270993 hartree

C	2.45603600	1.11856400	-1.13564300
C	3.59110700	1.91974500	-1.07908700
C	4.02448600	2.44342700	0.14099000

C	3.30905400	2.16096400	1.30552300
C	2.17027500	1.35742300	1.23009300
C	1.72260300	0.83239700	0.01825300
H	2.15231900	0.71777800	-2.10366100
H	4.16434200	2.15038800	-1.97661400
H	3.62654300	2.55391600	2.26891300
H	1.63187500	1.13686300	2.15524700
O	5.15011400	3.20711100	0.09564800
C	5.62958200	3.73610700	1.31156400
H	5.88808600	2.93987300	2.02473800
H	6.53013600	4.30508500	1.06783700
H	4.89480700	4.40824300	1.77813100
O	-1.02200600	1.93709300	-2.25712700
S	-1.53333600	2.51605300	-1.01251200
O	-1.10263000	1.80066500	0.23237600
O	-2.94957200	2.88797800	-0.99294500
C	-0.63182500	4.10871900	-0.84025600
F	-0.91366400	4.89714200	-1.87100000
F	0.67529400	3.89502400	-0.80796500
F	-0.99444300	4.72063800	0.28060000
P	-2.18843500	-1.23187900	0.53540800
P	1.19822100	-2.02281500	-0.00645600
C	-2.11510200	-3.05791000	0.77964000
H	-2.99550900	-3.37546600	1.35591700
H	-2.22225500	-3.50366500	-0.22049500
C	-0.82085700	-3.54790100	1.42994900
H	-0.99042100	-4.56212700	1.81560000
H	-0.57032900	-2.93427700	2.30961300
C	0.35764600	-3.61345800	0.46151100
H	1.14587100	-4.26738700	0.85979100
C	2.68928700	-1.97998500	1.04162200
C	3.95008500	-1.66935300	0.52688400
C	2.53140500	-2.14384200	2.42136000
H	4.08220900	-1.52205500	-0.54412300
C	5.03851400	-1.53296600	1.38216200
C	3.62006800	-2.00095800	3.27380900
H	1.55157600	-2.36727200	2.84482900
H	6.01831800	-1.29585700	0.97196500
C	4.87489100	-1.69391600	2.75529200
H	3.48628200	-2.12863900	4.34615000
H	5.72664800	-1.58054700	3.42294400
C	1.73044300	-2.37686100	-1.71102500
C	1.13821200	-1.68612100	-2.77175800
C	2.63506900	-3.41050300	-1.97915200
H	0.42667100	-0.88420300	-2.56307100
C	1.45435500	-2.01719900	-4.08609500

C	2.95335200	-3.73354700	-3.29298900
H	3.09585300	-3.96563700	-1.16168300
H	0.98910600	-1.47533000	-4.90693100
C	2.36352100	-3.03759200	-4.34575500
H	3.66210500	-4.53393900	-3.49514900
H	2.61339700	-3.29420300	-5.37338000
C	-3.49592700	-1.04064000	-0.72323400
C	-3.14922300	-0.61608200	-2.00757000
C	-4.82825600	-1.35954900	-0.43699900
H	-2.11790400	-0.33957200	-2.22854700
C	-4.12386800	-0.51157000	-2.99673500
C	-5.79809900	-1.25588000	-1.42624600
H	-5.10904800	-1.68081600	0.56673200
H	-3.84819800	-0.17229700	-3.99348800
C	-5.44573700	-0.83191500	-2.70670400
H	-6.83310700	-1.50374900	-1.19834300
H	-6.20834300	-0.74549900	-3.47850700
C	-2.94993300	-0.58512900	2.06769700
C	-2.97089800	-1.31296800	3.26067600
C	-3.48414900	0.71062300	2.04867100
H	-2.56901100	-2.32409900	3.30624000
C	-3.51657700	-0.75646800	4.41483200
C	-4.03318500	1.25901100	3.20090200
H	-3.46321000	1.29137400	1.12631000
H	-3.52949400	-1.33562700	5.33615700
C	-4.04783500	0.52814500	4.38697600
H	-4.45168800	2.26337700	3.17274700
H	-4.47577400	0.96052000	5.28947800
H	0.02466400	-4.06090900	-0.48613200
Pd	-0.07441300	-0.15229500	0.11790000

C_b^{Pd} **HF =** −4657.3825799 hartree

P	1.40156200	0.78491100	-0.88519000
P	-2.00186600	-0.04947600	-0.67437600
C	0.78273200	1.05875700	-2.61420400
H	1.43992400	1.78209800	-3.12030600
H	0.87403000	0.10378800	-3.15453300
C	-0.66715100	1.54688000	-2.68448300
H	-0.82920200	1.94161500	-3.69752200
H	-0.80317200	2.40860800	-2.01137900
C	-1.74826200	0.49189700	-2.43209800
H	-2.71159400	0.82881200	-2.84476900
C	-2.80629900	1.38485600	0.13776100
C	-2.86350200	1.36490300	1.53720400
C	-3.30094700	2.50207900	-0.54041400
H	-2.45832800	0.50499400	2.07564900

C	-3.41006600	2.43071300	2.24205000
C	-3.83608300	3.57704300	0.16575200
H	-3.27144400	2.54581900	-1.62882100
H	-3.45000100	2.39889800	3.32941400
C	-3.89210200	3.54341600	1.55539300
H	-4.21236300	4.44357600	-0.37509300
H	-4.30885900	4.38544400	2.10489000
C	-3.37519100	-1.24701400	-0.91980200
C	-3.05138300	-2.60615200	-0.97824000
C	-4.70674800	-0.85593500	-1.08639500
H	-2.01166800	-2.91411000	-0.83725700
C	-4.03974800	-3.55876900	-1.20784900
C	-5.69679500	-1.80905400	-1.30263900
H	-4.97327500	0.20097200	-1.04270500
H	-3.77677800	-4.61415200	-1.25377900
C	-5.36434400	-3.16023900	-1.36524400
H	-6.73239900	-1.49603600	-1.42463400
H	-6.14068200	-3.90439500	-1.53378800
C	3.19820700	0.52074000	-1.11105100
C	3.74444000	0.00450100	-2.28988300
C	4.03492100	0.69327200	0.00042400
H	3.11892100	-0.14594600	-3.16902300
C	5.09640200	-0.32555100	-2.35663500
C	5.38331200	0.36723500	-0.06842500
H	3.62067500	1.09028800	0.92941600
H	5.50780200	-0.72218100	-3.28339500
C	5.91820700	-0.14640900	-1.24901500
H	6.02056100	0.51368300	0.80214300
H	6.97394000	-0.40531600	-1.30346100
C	1.31513700	2.48646300	-0.19591700
C	2.06906600	3.54407200	-0.71633400
C	0.42196400	2.73943400	0.84895400
H	2.77774800	3.36073100	-1.52550500
C	1.92604900	4.82821500	-0.20328200
C	0.27006500	4.02738600	1.35697000
H	-0.17558800	1.91667500	1.24993600
H	2.51827700	5.64468000	-0.61303800
C	1.02383100	5.07168700	0.83169800
H	-0.43916400	4.20971900	2.16349300
H	0.91113500	6.07930100	1.22798000
H	-1.49722500	-0.43425000	-2.97429700
Pd	0.02829000	-0.76186300	0.31066600
C	-0.43037600	-1.76604800	3.23226600
C	-0.06654700	-2.30727100	1.96840700
C	1.26484600	-2.06724500	1.51220400
C	2.21786500	-1.42770600	2.35024000

C	1.80967800	-0.90331400	3.55283300
C	0.47368400	-1.06265300	3.99423400
H	-1.43708200	-1.95289800	3.60559900
H	-0.67963300	-3.08850300	1.52050600
H	3.24687800	-1.32598700	2.00714000
H	2.52696400	-0.37438300	4.17824600
H	0.17626900	-0.66472600	4.96268300
Br	1.93512500	-3.19839300	0.08434700

$TS1_b^{Pd}$ **HF =** −4657.3741977 hartree $\nu^{\ddagger} = -147.04\ icm^{-1}$

P	-1.39294900	0.54064600	1.09413900
P	2.04933400	0.10786600	0.62567100
C	-0.66907700	0.91475500	2.76695500
H	-1.37758800	1.55110100	3.31718400
H	-0.59015600	-0.03343400	3.31968500
C	0.69846000	1.59812300	2.70808100
H	0.88882500	2.04099500	3.69608500
H	0.65776600	2.44970500	2.00969400
C	1.88927000	0.69498600	2.38027200
H	2.82969300	1.18629900	2.67326000
C	2.53133700	1.60896300	-0.31312700
C	2.44731400	1.53675900	-1.70869900
C	2.93759500	2.81001300	0.27463800
H	2.11323800	0.60614300	-2.17351500
C	2.76074800	2.63585500	-2.49938900
C	3.24133200	3.91617200	-0.51559800
H	3.02010000	2.89554800	1.35778200
H	2.69034500	2.56270100	-3.58316700
C	3.15298800	3.83186600	-1.90145800
H	3.54979900	4.84731900	-0.04362300
H	3.38780200	4.69848400	-2.51667200
C	3.62204700	-0.83396400	0.77052100
C	3.53008900	-2.21328100	0.98233800
C	4.88402200	-0.23514600	0.72201500
H	2.54523900	-2.68510900	1.01115300
C	4.67855700	-2.98123300	1.14816700
C	6.03279000	-1.00481000	0.87579200
H	4.97099400	0.83978100	0.55900900
H	4.59533300	-4.05396200	1.31385600
C	5.93160300	-2.37723000	1.09063100
H	7.01182400	-0.53066100	0.83038700
H	6.83186200	-2.97735000	1.21020400
C	-3.07554100	-0.04930500	1.50423700
C	-3.19903300	-1.14175500	2.37419500
C	-4.21479500	0.40333800	0.83188700
H	-2.31740800	-1.53874900	2.88091200

C	-4.43253500	-1.74566200	2.58568300
C	-5.44951000	-0.20617900	1.03945900
H	-4.13849000	1.23644200	0.13303000
H	-4.51118300	-2.58804500	3.27088100
C	-5.56327400	-1.27943600	1.91706800
H	-6.32645700	0.16035700	0.50807100
H	-6.52851500	-1.75608200	2.07738900
C	-1.62144600	2.23972100	0.44072500
C	-2.42650000	3.19672500	1.07049900
C	-0.87365400	2.61495600	-0.67866900
H	-3.01349800	2.92397900	1.94852000
C	-2.49175900	4.49497800	0.57798300
C	-0.93327000	3.91722600	-1.16943600
H	-0.22797400	1.87702300	-1.15906800
H	-3.12489300	5.23030100	1.07143800
C	-1.74427300	4.85668100	-0.54209800
H	-0.34193900	4.19436500	-2.04110700
H	-1.79501500	5.87519100	-0.92290400
H	1.83334000	-0.22897300	2.97824500
Pd	0.03489000	-0.91200900	-0.18622900
C	-1.53549600	-0.40130800	-3.68966900
C	-0.71435200	-1.14416100	-2.83837000
C	-1.27779000	-1.72660100	-1.69096100
C	-2.66880500	-1.72821400	-1.49710100
C	-3.46127800	-0.99254200	-2.36170800
C	-2.90188000	-0.31433600	-3.45298900
H	-1.09728300	0.08296900	-4.56137300
H	0.34607000	-1.27314700	-3.05013900
H	-3.10108900	-2.23727800	-0.63543100
H	-4.53437100	-0.94016900	-2.17983500
H	-3.54099000	0.24787900	-4.13066800
Br	-0.19026800	-3.36613100	-0.96031900

1_b^{Pd} **HF =** −4657.4390619 hartree

P	1.41400100	0.61829100	-0.98283300
P	-1.94159400	0.17629900	-0.78518000
C	0.79765100	1.05527900	-2.67067100
H	1.57253500	1.67647400	-3.14155900
H	0.73967100	0.12431800	-3.25366700
C	-0.54817700	1.77641300	-2.70186900
H	-0.65329300	2.24317900	-3.69041600
H	-0.54861300	2.60905400	-1.98073500
C	-1.75680500	0.86938100	-2.48578000
H	-2.68900900	1.38083800	-2.76408600
C	-2.52790700	1.56259100	0.25291100
C	-2.49577700	1.39500300	1.64416900

C	-2.94819800	2.78648600	-0.27414000
H	-2.16375900	0.44309000	2.06446700
C	-2.87482100	2.43259000	2.48749100
C	-3.31602800	3.82838100	0.57330500
H	-2.98937600	2.94374400	-1.35092100
H	-2.84733800	2.28983700	3.56613700
C	-3.27830900	3.65416700	1.95272700
H	-3.63429700	4.77926900	0.15041100
H	-3.56420200	4.47064200	2.61306700
C	-3.37788200	-0.92734100	-1.01416400
C	-3.17753200	-2.10817100	-1.73867200
C	-4.63927400	-0.64820900	-0.48882400
H	-2.18639800	-2.34007000	-2.13492500
C	-4.23132500	-2.98777700	-1.94910400
C	-5.69217300	-1.53711400	-0.69330400
H	-4.80467600	0.26628300	0.08030800
H	-4.06902500	-3.90194400	-2.51702900
C	-5.49069800	-2.70378700	-1.42309700
H	-6.67426100	-1.31349400	-0.28065100
H	-6.31491100	-3.39672000	-1.58144200
C	3.10717100	0.03633200	-1.32139800
C	3.29659300	-0.96042500	-2.28398600
C	4.19951800	0.48866800	-0.57812500
H	2.44886200	-1.34782200	-2.85058300
C	4.56388100	-1.48414700	-2.51076700
C	5.46627200	-0.04038600	-0.80458400
H	4.06207500	1.25411200	0.18493000
H	4.70207300	-2.25677500	-3.26461100
C	5.65032300	-1.02535500	-1.77032200
H	6.31220400	0.31907300	-0.22172000
H	6.64197500	-1.43797400	-1.94578600
C	1.57384200	2.24749900	-0.17419800
C	2.31747900	3.27865700	-0.76136300
C	0.86712800	2.50071500	1.00403200
H	2.88040400	3.09895700	-1.67774600
C	2.34941800	4.53798600	-0.17524700
C	0.89127700	3.76534100	1.58471800
H	0.28308600	1.70118800	1.46297400
H	2.93160600	5.33352200	-0.63589500
C	1.63290500	4.78336500	0.99506200
H	0.32427800	3.95054100	2.49547200
H	1.65421200	5.77344200	1.44638900
H	-1.68482700	-0.00665400	-3.14842300
Pd	0.03286900	-0.78192600	0.20773800
C	3.35722800	-1.36378700	2.93068800
C	2.22948700	-0.85803500	2.28054700

C	1.73135000	-1.47555900	1.13061100
C	2.38714800	-2.60981600	0.64369600
C	3.51079900	-3.11933900	1.29332000
C	4.00192900	-2.49475000	2.43832200
H	3.73164300	-0.86775400	3.82638900
H	1.73869000	0.03075500	2.68436400
H	2.02137400	-3.10749700	-0.25774500
H	4.00695200	-4.00670400	0.89945400
H	4.88234600	-2.88891900	2.94390400
Br	-1.29048600	-2.33415400	1.62548600

Ni^{I}(bpy)Br **HF =** −3237.6740201 hartree

C	-1.76304100	0.77726900	0.00002900
C	-2.89107200	1.59074900	0.00057400
C	-2.72731300	2.96999500	0.00048400
C	-1.44364500	3.50170800	-0.00012300
C	-0.36686300	2.62602200	-0.00053400
N	-0.51858900	1.29853200	-0.00045100
H	-3.59807900	3.62095100	0.00088900
H	-3.88779900	1.15876500	0.00118000
H	-1.27393500	4.57440100	-0.00022400
H	0.66097400	2.98612300	-0.00093000
C	-1.80955100	-0.69678000	-0.00000200
C	-2.98546100	-1.43918000	-0.00055100
C	-0.53097900	-2.63011400	0.00051200
C	-2.90763700	-2.82596100	-0.00049900
H	-3.95511300	-0.94878800	-0.00113000
H	0.47305600	-3.05212700	0.00093400
H	-3.81588500	-3.42338800	-0.00091700
C	-1.65960200	-3.43711200	0.00007800
H	-1.55533200	-4.51810100	0.00014000
N	-0.60059700	-1.29555300	0.00046000
Ni	0.95428300	-0.05218300	0.00001000
Br	3.21649900	-0.04506100	-0.00000200

C_a^{Ni} **HF =** −4544.8152299 hartree

C	2.66503900	-1.68200700	-0.80634500
C	3.24849400	-2.92340700	-0.57584900
C	4.45294100	-2.98623300	0.11337500
C	5.04957500	-1.80858100	0.54605100
C	4.40431500	-0.60861300	0.28320600
N	3.23883400	-0.54264200	-0.36707300
H	4.92106900	-3.94840200	0.30621700
H	2.76933900	-3.83548100	-0.92103000
H	5.99411600	-1.81298600	1.08229500
H	4.82606800	0.34414600	0.60269500

C	1.38435800	-1.49463400	-1.51602300
C	0.65600500	-2.52871400	-2.09628300
C	-0.22116700	0.05405700	-2.13740500
C	-0.55701700	-2.23717100	-2.70762700
H	1.02195100	-3.55156200	-2.07163400
H	-0.52677300	1.10082000	-2.11998700
H	-1.14269300	-3.03261400	-3.16197600
C	-1.01300700	-0.92437800	-2.72387600
H	-1.96686600	-0.65800700	-3.17103000
N	0.94954500	-0.21985700	-1.55680700
Ni	2.15759600	1.10282800	-0.65360600
C	-0.81615400	0.81397400	1.37304400
C	0.42092500	0.61650900	1.98094900
C	0.95044100	-0.67439400	2.06810300
C	0.22860600	-1.76513300	1.56710400
C	-0.99982800	-1.57047300	0.95999900
C	-1.49717700	-0.27649500	0.86545500
H	-1.23433700	1.81341100	1.26936100
H	0.96102200	1.47467600	2.37018400
H	0.66207900	-2.76024600	1.64971300
H	-1.56215400	-2.40211000	0.54094600
O	2.15698900	-0.96605400	2.60138400
Br	2.08464900	3.36551600	-0.50804000
C	2.89490800	0.09140900	3.18383600
H	2.34914100	0.53965300	4.02556700
H	3.82642500	-0.34964500	3.54628400
H	3.12895700	0.87293700	2.44506000
O	-2.69653000	-0.05512100	0.14844000
S	-4.06291500	-0.18901900	0.98803000
O	-4.17871000	0.88212800	1.95441300
O	-4.29589100	-1.56414500	1.37521600
C	-5.15379700	0.20015700	-0.45159500
F	-4.94198900	-0.67329800	-1.41332800
F	-4.90231200	1.41941100	-0.87703900
F	-6.39862900	0.11447200	-0.02563100

C_{iso}^{Ni} **HF =** −4544.8179248 hartree

C	-2.41820900	-0.40663700	-1.31661400
C	-3.71371100	0.09973500	-1.36389500
C	-4.66870000	-0.41399900	-0.49607100
C	-4.30676200	-1.41614200	0.39747100
C	-2.99097000	-1.86002200	0.39308600
N	-2.07038600	-1.36933000	-0.44013300
H	-5.68653200	-0.03146600	-0.51654600
H	-3.97657500	0.89321600	-2.05824800
H	-5.02478900	-1.84472100	1.09133000

H	-2.64693300	-2.63339800	1.07983200
C	-1.31708800	0.06493700	-2.17838400
C	-1.46825300	1.02870200	-3.17041500
C	0.94860700	-0.11364200	-2.62835600
C	-0.35542600	1.42693300	-3.89933500
H	-2.43990500	1.47244000	-3.37032400
H	1.88946600	-0.59954300	-2.37276200
H	-0.45392800	2.18330500	-4.67409500
C	0.87918500	0.85055500	-3.62316600
H	1.77544100	1.13724000	-4.16590400
N	-0.11877900	-0.49987300	-1.92250400
Ni	-0.10237600	-1.78028400	-0.41051800
C	-1.74450600	2.74760200	0.31768100
C	-0.44733700	2.37304800	0.01413900
C	0.13071400	1.33501700	0.73189200
C	-0.53976500	0.67426300	1.74534200
C	-1.84012200	1.06032200	2.05876400
C	-2.44930500	2.08989300	1.33597000
H	-2.24207700	3.54743300	-0.22668900
H	0.11421300	2.86024900	-0.78111800
H	-0.05847800	-0.14753000	2.27269400
H	-2.37155200	0.53482700	2.84714000
O	-3.71393800	2.51661300	1.54094600
C	-4.48269400	1.85744400	2.52957900
H	-4.59995100	0.78879700	2.29472600
H	-4.02990700	1.96420700	3.52492200
H	-5.46305900	2.33824400	2.52501900
O	1.40302500	0.87349000	0.32580600
S	2.67696100	1.38494800	1.15950100
O	2.82047300	0.63736900	2.39067500
O	2.75100900	2.83011400	1.15398200
C	3.89996300	0.72429900	-0.05850600
F	3.70150900	1.28440600	-1.23412100
F	3.76603800	-0.58416100	-0.15143300
F	5.10087300	1.02592700	0.39224800
Br	0.93370900	-3.28057700	0.94069700

$TS1_a^{Ni}$ **HF =** −4544.7708273 hartree $\nu^{\ddagger} = -417.39\ icm^{-1}$

C	2.59619400	1.74868100	0.06188600
C	3.96421300	1.95798700	-0.08141100
C	4.84443400	1.18676500	0.66739800
C	4.34290700	0.22635500	1.53675800
C	2.96548200	0.07772400	1.62960800
N	2.12106200	0.82199800	0.91556700
H	5.91673900	1.33449000	0.56629200
H	4.34679000	2.70408700	-0.77171200

H	5.00087900	-0.39875700	2.13312100
H	2.50889700	-0.65839200	2.29093600
C	1.56765900	2.48253000	-0.70543200
C	1.86019900	3.51354600	-1.59227700
C	-0.69989500	2.66057600	-1.17723300
C	0.82276800	4.12248100	-2.28667500
H	2.88352800	3.84494000	-1.74268500
H	-1.69852500	2.27285400	-0.98385800
H	1.03534200	4.92825000	-2.98479600
C	-0.48132500	3.69140900	-2.08008900
H	-1.31872800	4.14157900	-2.60470400
N	0.29713200	2.07189600	-0.51137800
Ni	0.09927500	0.56481900	0.82690300
C	1.77607800	-1.54494400	-2.16711100
C	0.76853500	-0.69261600	-1.76090400
C	0.15824400	-0.95695800	-0.53415400
C	0.32716100	-2.15493000	0.14886400
C	1.34947600	-3.00462400	-0.27396000
C	2.08853300	-2.69372800	-1.41858900
H	2.33598300	-1.35100200	-3.07981900
H	0.50465600	0.18458100	-2.34596600
H	-0.26478700	-2.39046400	1.02886800
H	1.54538700	-3.90799100	0.29727600
O	3.09410000	-3.44795400	-1.90738200
C	3.44349300	-4.62617900	-1.20573300
H	3.76133900	-4.39781800	-0.17909400
H	2.60704800	-5.33769800	-1.17888300
H	4.27790800	-5.07071800	-1.75179100
O	-1.55733100	-0.24397800	-0.53227500
S	-2.76813400	-1.18844500	-0.62531600
O	-2.87748600	-2.11519400	0.49148900
O	-2.95254400	-1.70525100	-1.97376700
C	-4.07738100	0.08371400	-0.36368100
F	-4.02938100	0.98460600	-1.33344400
F	-3.89239800	0.68611400	0.80022400
F	-5.25935000	-0.50869800	-0.37173200
Br	-0.61667900	0.00626000	2.98473500

1_a^{Ni} **HF =** −4544.798107 hartree

C	-3.12230700	-1.09855600	-0.14889800
C	-4.51042400	-1.04938300	-0.08862500
C	-5.12026800	-0.56820900	1.06266900
C	-4.33241600	-0.15790800	2.12956700
C	-2.95330500	-0.23587000	2.00185600
N	-2.36788300	-0.69121900	0.89162400
H	-6.20436600	-0.51894000	1.12333100

H	-5.11538700	-1.38237500	-0.92657500
H	-4.76977100	0.21848100	3.04937700
H	-2.27728800	0.05331300	2.80541900
C	-2.37630400	-1.60257400	-1.31772400
C	-2.98671200	-2.05277300	-2.48320500
C	-0.27085300	-2.06687000	-2.18113800
C	-2.19185100	-2.52392900	-3.52010300
H	-4.06702200	-2.03770500	-2.58952400
H	0.80223800	-2.02731800	-2.00919900
H	-2.65120800	-2.87694500	-4.43989400
C	-0.81150800	-2.53907500	-3.36841200
H	-0.15710700	-2.90338000	-4.15451600
N	-1.03666200	-1.60789900	-1.18698600
Ni	-0.34929700	-0.77376700	0.56059600
C	-0.41360200	2.66702900	-1.90711900
C	-0.48583000	1.34708700	-1.47902400
C	-0.51853800	1.12879800	-0.11347600
C	-0.58213000	2.13102200	0.83030500
C	-0.51426400	3.45148900	0.38092500
C	-0.42707200	3.72064300	-0.98707700
H	-0.35301900	2.89863500	-2.96875900
H	-0.46755000	0.54803300	-2.21327100
H	-0.63451000	1.92055900	1.89471600
H	-0.53124500	4.25133800	1.11644300
O	-0.36058500	4.96039900	-1.51732000
C	-0.37680600	6.06308800	-0.63116100
H	-1.29852600	6.08245300	-0.03363800
H	0.49220500	6.04729700	0.04092000
H	-0.33402800	6.95771900	-1.25561800
O	1.56023300	-1.02209000	-0.09979700
S	2.63093600	-0.06990300	-0.55237600
O	2.65997800	1.21125600	0.14817000
O	2.77433900	-0.03771500	-2.00814800
C	4.12270600	-0.95885200	0.05231000
F	4.17177300	-2.18254300	-0.45732200
F	4.09674200	-1.04442500	1.37569500
F	5.21299800	-0.29608500	-0.31383300
Br	0.34020900	-0.61347700	2.82158600

C_b^{Ni} **HF =** −6040.7083756 hartree

C	-1.59746100	-1.19108600	-0.89464200
C	-2.77743000	-1.91604000	-0.75483400
C	-2.72931200	-3.17148700	-0.16290300
C	-1.50890700	-3.66843000	0.27878200
C	-0.37595700	-2.88549900	0.10368600
N	-0.41588700	-1.68228200	-0.47290600

H	-3.63993600	-3.75429300	-0.04763200
H	-3.72407700	-1.51276300	-1.10492900
H	-1.42965400	-4.64420100	0.74955900
H	0.60686400	-3.22212200	0.43348900
C	-1.52300600	0.15430200	-1.49604400
C	-2.63454600	0.86605900	-1.93781100
C	-0.11209900	1.89032800	-2.09859500
C	-2.45571600	2.13499200	-2.47124700
H	-3.63250600	0.44457500	-1.85165800
H	0.91394100	2.25239100	-2.14250000
H	-3.31329700	2.70916300	-2.81328500
C	-1.17108800	2.66009000	-2.55625000
H	-0.98813600	3.64801200	-2.96904400
N	-0.27923000	0.66881500	-1.58022500
Ni	1.14295800	-0.44614900	-0.76190300
C	-2.80163600	0.94275200	1.76211500
C	-1.67146000	1.67413100	1.40722200
C	-0.41962100	1.16652800	1.72910400
C	-0.26667400	-0.03699500	2.40620800
C	-1.40698100	-0.75210200	2.76138300
C	-2.67180400	-0.26856300	2.43615300
H	-3.78771300	1.32445600	1.50284400
H	-1.76206500	2.61901300	0.87453500
H	0.72677000	-0.42361000	2.62822100
H	-1.30054900	-1.70240300	3.28198000
H	-3.55788000	-0.84021300	2.70527900
Br	1.12614000	2.14118700	1.20809200
Br	3.28795700	-1.08134200	-0.31139600

$TS1_b^{Ni}$ **HF =** −6040.6876734 hartree $\nu^{\ddagger} = -175.37\ icm^{-1}$

C	2.24600500	0.65596600	-0.45429900
C	3.35789700	1.49262400	-0.40736600
C	3.17638500	2.86194400	-0.55154600
C	1.89444200	3.36340700	-0.73892000
C	0.83573800	2.46638700	-0.77793100
N	1.00946800	1.15187800	-0.64100600
H	4.03258000	3.53089800	-0.51316900
H	4.35385200	1.08928500	-0.24901300
H	1.71204800	4.42803700	-0.85231600
H	-0.19269200	2.79601900	-0.92330400
C	2.31935500	-0.81096700	-0.29290600
C	3.51836400	-1.51410200	-0.21801700
C	1.10309200	-2.76953200	-0.05987200
C	3.48388100	-2.89334200	-0.05982700
H	4.47196400	-0.99900200	-0.29054200
H	0.11267000	-3.21706800	0.00906200

H	4.41116700	-3.45806600	-0.00293500
C	2.25623400	-3.53711700	0.02261500
H	2.18561100	-4.61362200	0.14755700
N	1.13176100	-1.44395600	-0.21591800
Ni	-0.52252600	-0.20879600	-0.46720700
C	0.30862300	0.88290000	3.34278800
C	0.02282200	-0.07470600	2.37575900
C	-0.95716000	0.21807400	1.42862800
C	-1.74482400	1.36486500	1.50915000
C	-1.43742900	2.31164300	2.48438800
C	-0.40969200	2.07818600	3.39417500
H	1.09788100	0.68839900	4.06729400
H	0.57810400	-1.00929600	2.33579100
H	-2.55016800	1.53399300	0.79634100
H	-2.01743500	3.23162800	2.53556600
H	-0.18106700	2.81703700	4.15933300
Br	-2.10403400	-1.59953000	0.65058500
Br	-1.84496000	0.58510800	-2.31116600

1_b^{Ni} **HF =** −6040.7003749 hartree

C	-1.99795000	-1.05918400	0.01904600
C	-3.05522600	-1.93522900	-0.20454800
C	-3.08872000	-2.66794100	-1.38266500
C	-2.07014100	-2.50906800	-2.31475100
C	-1.04404300	-1.62267500	-2.02571700
N	-1.01382100	-0.92705800	-0.88939200
H	-3.90745000	-3.35746100	-1.57112800
H	-3.84637800	-2.04502300	0.53170600
H	-2.06401900	-3.05994200	-3.25023100
H	-0.22070300	-1.45440000	-2.71825700
C	-1.87099600	-0.20987100	1.21623300
C	-2.79623100	-0.18029800	2.25463100
C	-0.56678400	1.40530200	2.25879100
C	-2.57761900	0.68178400	3.32139400
H	-3.67756800	-0.81487600	2.23491900
H	0.34274500	2.00254900	2.20207800
H	-3.28860600	0.72081500	4.14271700
C	-1.44839400	1.49129800	3.32780100
H	-1.24755700	2.17915700	4.14363300
N	-0.77814500	0.57305300	1.23980900
Ni	0.38961400	0.39353500	-0.41713800
C	2.15463600	-2.71960200	1.83388900
C	1.44891500	-1.55414400	1.52613100
C	1.45705500	-1.10172200	0.21708500
C	2.17254900	-1.75212400	-0.77865400
C	2.87001100	-2.91749800	-0.45854000

C	2.85954500	-3.40115200	0.84689200
H	2.15074800	-3.08881900	2.85853700
H	0.90979100	-1.02479500	2.31028400
H	2.19809500	-1.36193600	-1.79841900
H	3.42710200	-3.43887600	-1.23553900
H	3.40870100	-4.30702700	1.09662200
Br	2.27298200	1.66331600	0.05101800
Br	-0.76526700	2.07446700	-1.69850600

Ni^0(bpy) **HF =** −665.9916144 hartree

C	0.71332900	0.72170100	-0.00001100
C	1.51279900	1.89335900	-0.00020300
C	2.88047500	1.80501500	-0.00003700
C	3.49681000	0.52943500	0.00030700
C	2.67846300	-0.57835600	0.00036400
N	1.33458800	-0.52113100	0.00019100
H	3.48628500	2.70941000	-0.00013600
H	1.03538400	2.87121000	-0.00050300
H	4.57719600	0.41516800	0.00047700
H	3.10220300	-1.58343000	0.00057800
C	-0.71311500	0.72182500	0.00001800
C	-1.51248300	1.89354000	-0.00029600
C	-2.67840000	-0.57807400	0.00049100
C	-2.88016800	1.80532200	-0.00016100
H	-1.03498100	2.87135200	-0.00063200
H	-3.10220300	-1.58312100	0.00084200
H	-3.48590100	2.70976500	-0.00040600
C	-3.49663200	0.52978800	0.00028400
H	-4.57703000	0.41562000	0.00050000
N	-1.33450200	-0.52093900	0.00034600
Ni	-0.00028700	-1.92831500	-0.00032200

$C_a^{Ni(0)}$ **HF =** −1973.1633468 hartree

C	-2.28556800	-1.80797600	0.85304000
C	-2.84851000	-2.71225600	1.74743700
C	-2.21812000	-2.94092900	2.96397600
C	-1.04663800	-2.25516100	3.25549900
C	-0.54127200	-1.37226800	2.31009800
N	-1.13556700	-1.15308400	1.13203900
H	-2.64464900	-3.64222700	3.67703400
H	-3.77715200	-3.22384700	1.50936000
H	-0.52494400	-2.39784000	4.19765300
H	0.38185300	-0.82386500	2.48382800
C	-2.89656400	-1.45718100	-0.44338400
C	-3.99980400	-2.11047800	-0.98295600
C	-2.79568000	-0.02126800	-2.25775900

C	-4.50384200	-1.68669900	-2.20599600
H	-4.45992100	-2.94700900	-0.46401900
H	-2.28228800	0.81782800	-2.72525900
H	-5.36374200	-2.18669000	-2.64499300
C	-3.89559500	-0.62040300	-2.85658000
H	-4.26058600	-0.25500500	-3.81227900
N	-2.30166500	-0.42657600	-1.08324300
Ni	-0.62606100	0.20256200	-0.23757300
C	1.04791100	2.05547900	1.14774500
C	0.26005300	3.16018000	1.29929300
C	-0.58255900	3.59808100	0.22738800
C	-0.59492400	2.92776400	-0.96722700
C	0.13580900	1.70166200	-1.15028900
C	0.94688000	1.24234700	-0.02939600
H	1.75725700	1.76366700	1.92274500
H	0.31151600	3.72600600	2.22590000
H	-1.15502600	3.35676300	-1.79850600
H	0.44006800	1.43734300	-2.16893700
O	-1.35628300	4.72405700	0.31159500
C	-1.27297500	5.50659200	1.47969000
H	-0.25367900	5.88417100	1.64913800
H	-1.94385500	6.35651800	1.32919900
H	-1.60026000	4.95089800	2.37093200
O	2.24978300	0.64623800	-0.41171400
S	2.44328300	-0.90162700	-0.16052600
O	1.72385300	-1.72285000	-1.11842400
O	2.40547400	-1.23002300	1.25358100
C	4.21386300	-0.93639200	-0.67599600
F	4.93061500	-0.15703600	0.10935900
F	4.32621000	-0.54185600	-1.92928100
F	4.62715300	-2.18674800	-0.56237700

$TS1_a^{Ni(0)}$ **HF =** −1973.1561724 hartree $\nu^{\ddagger} = -314.68\ icm^{-1}$

C	-2.95516400	-1.18373500	0.55813200
C	-3.79328800	-2.13423300	1.13027300
C	-3.29388100	-2.95779600	2.13185400
C	-1.97340400	-2.81155800	2.53792000
C	-1.19645400	-1.83940900	1.92266200
N	-1.67210700	-1.04574700	0.95851400
H	-3.93433000	-3.70745500	2.58985100
H	-4.82442900	-2.23664900	0.80353600
H	-1.54619300	-3.43647100	3.31672500
H	-0.15411500	-1.68007800	2.19851600
C	-3.36355700	-0.25071200	-0.51025800
C	-4.63305200	-0.21894800	-1.07573300
C	-2.65819400	1.49021100	-1.87095700

C	-4.90340700	0.70924700	-2.07403100
H	-5.40671500	-0.90713400	-0.74667500
H	-1.83682500	2.14920200	-2.14836900
H	-5.89054600	0.74859000	-2.52786100
C	-3.90211500	1.58149500	-2.48086600
H	-4.07445300	2.32217800	-3.25625300
N	-2.39151200	0.59852000	-0.91221400
Ni	-0.67537800	0.35157400	0.01911000
C	1.23115900	1.44233100	1.80506900
C	1.28639400	2.81290600	1.74789800
C	1.20815000	3.49637700	0.50306300
C	1.06084000	2.78726000	-0.66531500
C	0.89513100	1.36943300	-0.64706300
C	0.98195800	0.69784200	0.62383300
H	1.33823600	0.91971400	2.75505000
H	1.39832700	3.37059100	2.67471500
H	1.10889200	3.32271600	-1.61329300
H	1.07131800	0.82504900	-1.57748400
O	1.31589500	4.85331200	0.39059000
C	1.56462800	5.60087600	1.55901600
H	2.50332100	5.29756500	2.04576200
H	1.64903900	6.64422900	1.24458500
H	0.74171200	5.51434200	2.28368000
O	2.04463900	-0.70766000	0.79901700
S	2.00004800	-1.89388200	-0.16189800
O	0.95588600	-1.79850400	-1.17622500
O	2.16258700	-3.15527100	0.54923000
C	3.57039200	-1.64384300	-1.08523900
F	4.59980000	-1.68097100	-0.25475500
F	3.54581200	-0.46889400	-1.69785900
F	3.70139300	-2.60338500	-1.98891100

$\mathbf{1_a^{Ni(0)}}$ **HF =** −1973.2254065 hartree

C	-3.03621300	1.62228300	0.10640500
C	-3.87238500	2.70591600	0.34036300
C	-3.32871600	3.97946700	0.43790800
C	-1.95906200	4.13490300	0.28794000
C	-1.17776800	3.01081600	0.06540300
N	-1.69117500	1.77464700	-0.01224100
H	-3.97152300	4.83680700	0.61980800
H	-4.94395900	2.55988900	0.43807800
H	-1.48689300	5.11120500	0.34180000
H	-0.10118400	3.08775300	-0.04893000
C	-3.52326300	0.24779100	-0.06814700
C	-4.85688200	-0.13193300	0.02605700
C	-2.88077100	-1.91805500	-0.58273300

C	-5.19214200	-1.46127300	-0.19807100
H	-5.62870600	0.59234600	0.26930000
H	-2.05761600	-2.58707400	-0.82495300
H	-6.22923900	-1.77972600	-0.12941400
C	-4.19141900	-2.37044800	-0.51328400
H	-4.41384800	-3.41643200	-0.70211800
N	-2.55392500	-0.64243700	-0.36108300
Ni	-0.72876600	0.14958800	-0.29859500
C	1.83441000	0.98119800	-1.24040100
C	3.11920700	1.52474200	-1.14468400
C	3.56594900	2.01328500	0.08257500
C	2.72191800	1.96029500	1.19564900
C	1.44505400	1.42712700	1.07613400
C	0.97457700	0.92765600	-0.14538000
H	1.51426600	0.58181800	-2.20516700
H	3.75646200	1.55350700	-2.02596800
H	3.09021200	2.34532700	2.14618700
H	0.80133900	1.40776000	1.95924800
O	4.79670500	2.55630800	0.29645300
C	5.67812800	2.62689900	-0.80119900
H	5.26735300	3.24736200	-1.61121600
H	6.59845700	3.08551800	-0.43107100
H	5.90893300	1.62823100	-1.20009500
O	0.18537100	-2.13680600	1.68486600
S	0.51364700	-2.53105400	0.31638400
O	0.08140700	-1.53149100	-0.73017400
O	0.18601700	-3.89369400	-0.09715800
C	2.35455000	-2.46962300	0.21641400
F	2.85009300	-3.49573000	0.89846700
F	2.82658700	-1.34902600	0.73224600
F	2.74017800	-2.56548700	-1.04863500

$C_b^{Ni(0)}$ **HF =** −3469.0602565 hartree

C	2.56056100	-1.23584000	2.27790300
C	2.49475300	-0.15324400	1.44445500
C	2.00064700	-0.30466800	0.10467400
C	1.65304300	-1.63512400	-0.38038400
C	1.83770800	-2.73831400	0.52106600
C	2.24196000	-2.54628300	1.81352500
H	2.88630100	-1.09774800	3.30856700
H	2.78904300	0.83769300	1.79238700
H	1.69415600	-1.85247500	-1.45254800
H	1.67756300	-3.74984800	0.14424200
H	2.36384800	-3.39534500	2.48438400
Br	2.76328100	1.00083300	-1.19824900
C	-2.14606700	1.15823900	0.23023500

C	-2.97326000	2.23802600	0.52235300
C	-2.39894800	3.47010800	0.80891300
C	-1.01518500	3.59440500	0.78964800
C	-0.25473700	2.47312400	0.48732500
N	-0.80060200	1.28266900	0.21984200
H	-3.02955200	4.32480200	1.04132600
H	-4.05409400	2.12649500	0.52793300
H	-0.52714500	4.54123700	1.00280000
H	0.83356700	2.51541200	0.43673200
C	-2.63859200	-0.19574400	-0.09268600
C	-3.98545200	-0.53995700	-0.14306400
C	-2.01542200	-2.35703200	-0.64977900
C	-4.33829400	-1.84479400	-0.46321500
H	-4.75646000	0.19704300	0.06468600
H	-1.19184600	-3.04447800	-0.83821700
H	-5.38622500	-2.13108800	-0.50794800
C	-3.33774500	-2.77299700	-0.72306400
H	-3.57068100	-3.80315600	-0.97714100
N	-1.66743000	-1.10279300	-0.34347600
Ni	0.16868200	-0.40772300	-0.12537500

TS1$_b^{Ni(0)}$ **HF =** −3469.0489922 hartree $\nu^{\ddagger} = -86.28\ icm^{-1}$

C	3.12727800	-1.46863900	2.06627100
C	2.57801300	-0.33053800	1.50641600
C	1.82208900	-0.47091400	0.33452200
C	1.71462700	-1.71517200	-0.33958100
C	2.32001000	-2.85233000	0.25152000
C	3.00107000	-2.72815100	1.44368800
H	3.65235600	-1.39423000	3.01813500
H	2.66145500	0.63780300	1.99885600
H	1.41684800	-1.77130200	-1.39184500
H	2.30305200	-3.80577400	-0.27566900
H	3.47369600	-3.59775600	1.89612700
Br	2.56302300	1.42460200	-1.33183000
C	-2.18625400	1.07366900	0.34139300
C	-2.98419600	2.15465900	0.69517900
C	-2.37614500	3.35643700	1.03773300
C	-0.99094700	3.45036000	1.00952200
C	-0.25439100	2.33142700	0.64406200
N	-0.83783000	1.17252600	0.32447600
H	-2.98399100	4.21248800	1.31994400
H	-4.06682700	2.06573800	0.70757900
H	-0.48014500	4.37446000	1.26401700
H	0.83222800	2.34723100	0.55791300
C	-2.70361400	-0.25107400	-0.04468400
C	-4.05309000	-0.56843900	-0.14308700

C	-2.09775000	-2.39991600	-0.67754200
C	-4.41541400	-1.85392200	-0.52618000
H	-4.81699100	0.17349700	0.07215800
H	-1.28059100	-3.09193000	-0.87432900
H	-5.46591300	-2.12102100	-0.60945300
C	-3.42462100	-2.78816500	-0.80049100
H	-3.66815500	-3.80217200	-1.10342400
N	-1.74421900	-1.16486000	-0.31002700
Ni	0.08327000	-0.49205400	-0.03069800

$1_b^{Ni(0)}$ **HF =** −3469.1191172 hartree

C	4.00656100	0.57040900	-1.20249900
C	2.67674500	0.14873700	-1.20063500
C	1.98705800	-0.05168900	0.00014700
C	2.67670800	0.14900300	1.20090300
C	4.00655700	0.57054300	1.20269200
C	4.67494600	0.78887100	0.00007100
H	4.52254900	0.73070700	-2.14946400
H	2.16836400	-0.01391500	-2.15402600
H	2.16836900	-0.01323700	2.15439500
H	4.52264600	0.73094000	2.14958500
H	5.71189000	1.12181100	0.00008900
Br	0.65916700	-2.64200700	-0.00018600
C	-1.66336600	1.71842200	-0.00018200
C	-2.16208800	3.01575300	-0.00020700
C	-1.27931400	4.08613500	-0.00009600
C	0.08328200	3.82717400	-0.00001000
C	0.51321400	2.50883600	-0.00002900
N	-0.33096000	1.46772800	-0.00008300
H	-1.65493900	5.10615500	-0.00008600
H	-3.23328700	3.19318000	-0.00029600
H	0.81588700	4.62882200	0.00006600
H	1.57255800	2.26726500	-0.00010500
C	-2.52077900	0.52551400	-0.00015000
C	-3.91089300	0.56956000	-0.00010900
C	-2.53997800	-1.78771700	0.00025400
C	-4.62280800	-0.62262100	0.00018000
H	-4.43940800	1.51818500	-0.00028200
H	-1.93844900	-2.69530000	0.00031100
H	-5.70988800	-0.60868000	0.00023700
C	-3.92725900	-1.82370000	0.00040800
H	-4.44299800	-2.77957800	0.00069500
N	-1.84826500	-0.64444700	-0.00005100
Ni	0.14746100	-0.41565900	0.00006900

2 **HF =** −9202.2713541 hartree

C	-3.86699700	1.15731200	1.56111200
C	-3.95406500	1.96359500	2.69203900
C	-3.13676000	3.08364700	2.78538100
C	-2.26609300	3.38023200	1.74353200
C	-2.21676400	2.51511200	0.65931700
N	-2.98194800	1.42652500	0.58241200
H	-3.19118000	3.72474200	3.66197600
H	-4.64979100	1.73000400	3.49243400
H	-1.62702400	4.26202800	1.75567800
H	-1.53662400	2.68551300	-0.17517400
C	-4.72569000	-0.01432000	1.31777600
C	-5.76101200	-0.39254300	2.16531200
C	-5.25913800	-1.72082400	-0.16488500
C	-6.55825900	-1.47541800	1.82099500
H	-5.95515600	0.15731200	3.08135100
H	-5.02633500	-2.21124100	-1.10793100
H	-7.37089100	-1.78302400	2.47399000
C	-6.31386500	-2.14489900	0.62985800
H	-6.92478600	-2.98432700	0.31220600
N	-4.47406700	-0.69555700	0.17834100
Ni	-2.92993300	0.02826900	-0.88861500
C	-2.36243600	-2.65214600	-1.28471600
C	-2.29551800	-3.89691000	-1.91076200
C	-2.64503200	-4.02154900	-3.25306600
C	-3.05913000	-2.90232800	-3.96911300
C	-3.13002300	-1.64808600	-3.35622100
C	-2.79991500	-1.55773600	-2.01491900
H	-2.08461100	-2.56052200	-0.23484500
H	-1.96119000	-4.76128200	-1.33657700
H	-3.32970200	-2.99392700	-5.02009900
H	-3.45282700	-0.77272500	-3.91504200
O	1.97650800	-1.99746200	-1.87419400
S	3.43325600	-2.13853500	-2.04559700
O	4.24895600	-1.45231500	-1.02443500
O	3.91648500	-1.98759700	-3.42429200
C	3.71040500	-3.91789500	-1.68409900
F	3.06191100	-4.67359100	-2.56501600
F	3.26389100	-4.22159700	-0.46586500
F	5.00444800	-4.21476300	-1.74339600
P	2.45419200	0.24944500	1.93026200
P	2.19223400	2.23491500	-0.86786200
C	4.17640100	0.72337100	1.47773500
H	4.80494400	0.48749700	2.34781400
H	4.48134900	0.06097500	0.65508200
C	4.34595900	2.18906100	1.08694100
H	5.40959800	2.44263500	1.19120400

H	3.82292600	2.83435700	1.80905200
C	3.95057400	2.51630200	-0.35043600
H	4.21307600	3.55516100	-0.59898600
H	4.53058900	1.87404300	-1.03096300
Pd	0.99754300	0.38849400	0.16744200
C	-0.53722000	-3.41151200	1.57130000
C	0.21167100	-2.40971500	0.94963300
C	-0.04358500	-1.06033900	1.18544800
C	-1.05371600	-0.72754600	2.09304100
C	-1.82045500	-1.71264600	2.70975700
C	-1.56974100	-3.06251000	2.44563800
H	-0.31490600	-4.45428100	1.35331700
H	0.99983000	-2.70119900	0.25191000
H	-1.25165500	0.31766100	2.33915300
H	-2.61746200	-1.45351000	3.40800800
Br	-4.31698000	1.35632800	-2.34696000
C	2.66112100	-1.35844200	2.75822200
C	1.97754400	-1.65368600	3.94088300
C	3.45218100	-2.33902600	2.15266900
C	2.10099500	-2.91006900	4.52285000
H	1.34261500	-0.90190300	4.40883200
C	3.57178500	-3.59447700	2.74053300
H	3.95302000	-2.13492000	1.20496500
C	2.90052400	-3.88101800	3.92525900
H	1.56997200	-3.13072900	5.44700200
H	4.18741800	-4.35420900	2.26244300
H	2.99649300	-4.86428600	4.38213200
C	2.02746600	1.43301000	3.25224200
C	2.83016800	1.53281600	4.39582400
C	0.95087400	2.30733100	3.09417400
C	2.55354800	2.49053500	5.36272100
H	3.67385000	0.85645000	4.53552100
C	0.67631100	3.26864500	4.06355000
H	0.33506300	2.24153000	2.19379000
C	1.47651800	3.35976800	5.19670900
H	3.18169300	2.56157100	6.24826200
H	-0.16063400	3.95261100	3.92930500
H	1.26404300	4.11181100	5.95391300
C	2.39081400	2.24298400	-2.68548000
C	2.71368900	3.41766400	-3.37503800
C	2.32801100	1.03281100	-3.37918100
C	2.95302200	3.37975700	-4.74347800
H	2.77162800	4.36795900	-2.84346400
C	2.58042100	0.99718500	-4.74826300
H	2.08699300	0.10946700	-2.85078000
C	2.88588900	2.16918700	-5.43126300

H	3.19717500	4.29763900	-5.27500300
H	2.54221000	0.04496500	-5.27404900
H	3.07738600	2.14238300	-6.50244400
C	1.30539700	3.79533400	-0.50378300
C	1.61724100	4.56424300	0.62113900
C	0.22661100	4.18335700	-1.30950000
C	0.86943400	5.69582000	0.93552300
H	2.45070100	4.28986100	1.26657600
C	-0.51762400	5.31554400	-0.99634800
H	-0.03132100	3.59950800	-2.19362700
C	-0.19897300	6.07436400	0.12828100
H	1.12845900	6.28310500	1.81470400
H	-1.34965100	5.60590000	-1.63523500
H	-0.78172600	6.96041600	0.37233000
H	-2.58977500	-4.99158000	-3.74341900
O	-2.37059300	-3.95421700	3.08712300
C	-2.17616400	-5.32330200	2.80694400
H	-2.92105600	-5.86785600	3.39204200
H	-2.32653100	-5.53907000	1.73846300
H	-1.17109400	-5.65763900	3.10234100
Br	-0.73678700	0.49668000	-1.67980600

TS2^{Ni} **HF =** −9202.2713541 hartree $\nu^{\ddagger} = -58.33\ icm^{-1}$

C	-3.86699700	1.15731200	1.56111200
C	-3.95406500	1.96359500	2.69203900
C	-3.13676000	3.08364700	2.78538100
C	-2.26609300	3.38023200	1.74353200
C	-2.21676400	2.51511200	0.65931700
N	-2.98194800	1.42652500	0.58241200
H	-3.19118000	3.72474200	3.66197600
H	-4.64979100	1.73000400	3.49243400
H	-1.62702400	4.26202800	1.75567800
H	-1.53662400	2.68551300	-0.17517400
C	-4.72569000	-0.01432000	1.31777600
C	-5.76101200	-0.39254300	2.16531200
C	-5.25913800	-1.72082400	-0.16488500
C	-6.55825900	-1.47541800	1.82099500
H	-5.95515600	0.15731200	3.08135100
H	-5.02633500	-2.21124100	-1.10793100
H	-7.37089100	-1.78302400	2.47399000
C	-6.31386500	-2.14489900	0.62985800
H	-6.92478600	-2.98432700	0.31220600
N	-4.47406700	-0.69555700	0.17834100
Ni	-2.92993300	0.02826900	-0.88861500
C	-2.36243600	-2.65214600	-1.28471600
C	-2.29551800	-3.89691000	-1.91076200

C	-2.64503200	-4.02154900	-3.25306600
C	-3.05913000	-2.90232800	-3.96911300
C	-3.13002300	-1.64808600	-3.35622100
C	-2.79991500	-1.55773600	-2.01491900
H	-2.08461100	-2.56052200	-0.23484500
H	-1.96119000	-4.76128200	-1.33657700
H	-3.32970200	-2.99392700	-5.02009900
H	-3.45282700	-0.77272500	-3.91504200
O	1.97650800	-1.99746200	-1.87419400
S	3.43325600	-2.13853500	-2.04559700
O	4.24895600	-1.45231500	-1.02443500
O	3.91648500	-1.98759700	-3.42429200
C	3.71040500	-3.91789500	-1.68409900
F	3.06191100	-4.67359100	-2.56501600
F	3.26389100	-4.22159700	-0.46586500
F	5.00444800	-4.21476300	-1.74339600
P	2.45419200	0.24944500	1.93026200
P	2.19223400	2.23491500	-0.86786200
C	4.17640100	0.72337100	1.47773500
H	4.80494400	0.48749700	2.34781400
H	4.48134900	0.06097500	0.65508200
C	4.34595900	2.18906100	1.08694100
H	5.40959800	2.44263500	1.19120400
H	3.82292600	2.83435700	1.80905200
C	3.95057400	2.51630200	-0.35043600
H	4.21307600	3.55516100	-0.59898600
H	4.53058900	1.87404300	-1.03096300
Pd	0.99754300	0.38849400	0.16744200
C	-0.53722000	-3.41151200	1.57130000
C	0.21167100	-2.40971500	0.94963300
C	-0.04358500	-1.06033900	1.18544800
C	-1.05371600	-0.72754600	2.09304100
C	-1.82045500	-1.71264600	2.70975700
C	-1.56974100	-3.06251000	2.44563800
H	-0.31490600	-4.45428100	1.35331700
H	0.99983000	-2.70119900	0.25191000
H	-1.25165500	0.31766100	2.33915300
H	-2.61746200	-1.45351000	3.40800800
Br	-4.31698000	1.35632800	-2.34696000
C	2.66112100	-1.35844200	2.75822200
C	1.97754400	-1.65368600	3.94088300
C	3.45218100	-2.33902600	2.15266900
C	2.10099500	-2.91006900	4.52285000
H	1.34261500	-0.90190300	4.40883200
C	3.57178500	-3.59447700	2.74053300
H	3.95302000	-2.13492000	1.20496500

C	2.90052400	-3.88101800	3.92525900
H	1.56997200	-3.13072900	5.44700200
H	4.18741800	-4.35420900	2.26244300
H	2.99649300	-4.86428600	4.38213200
C	2.02746600	1.43301000	3.25224200
C	2.83016800	1.53281600	4.39582400
C	0.95087400	2.30733100	3.09417400
C	2.55354800	2.49053500	5.36272100
H	3.67385000	0.85645000	4.53552100
C	0.67631100	3.26864500	4.06355000
H	0.33506300	2.24153000	2.19379000
C	1.47651800	3.35976800	5.19670900
H	3.18169300	2.56157100	6.24826200
H	-0.16063400	3.95261100	3.92930500
H	1.26404300	4.11181100	5.95391300
C	2.39081400	2.24298400	-2.68548000
C	2.71368900	3.41766400	-3.37503800
C	2.32801100	1.03281100	-3.37918100
C	2.95302200	3.37975700	-4.74347800
H	2.77162800	4.36795900	-2.84346400
C	2.58042100	0.99718500	-4.74826300
H	2.08699300	0.10946700	-2.85078000
C	2.88588900	2.16918700	-5.43126300
H	3.19717500	4.29763900	-5.27500300
H	2.54221000	0.04496500	-5.27404900
H	3.07738600	2.14238300	-6.50244400
C	1.30539700	3.79533400	-0.50378300
C	1.61724100	4.56424300	0.62113900
C	0.22661100	4.18335700	-1.30950000
C	0.86943400	5.69582000	0.93552300
H	2.45070100	4.28986100	1.26657600
C	-0.51762400	5.31554400	-0.99634800
H	-0.03132100	3.59950800	-2.19362700
C	-0.19897300	6.07436400	0.12828100
H	1.12845900	6.28310500	1.81470400
H	-1.34965100	5.60590000	-1.63523500
H	-0.78172600	6.96041600	0.37233000
H	-2.58977500	-4.99158000	-3.74341900
O	-2.37059300	-3.95421700	3.08712300
C	-2.17616400	-5.32330200	2.80694400
H	-2.92105600	-5.86785600	3.39204200
H	-2.32653100	-5.53907000	1.73846300
H	-1.17109400	-5.65763900	3.10234100
Br	-0.73678700	0.49668000	-1.67980600

3^{Ni} **HF =** −3815.0170452 hartree

C	-4.13565900	0.14139600	0.98280800
C	-4.85042900	1.05354100	1.75927000
C	-4.62794000	2.41228400	1.59610500
C	-3.69323400	2.82948800	0.65877300
C	-3.00597900	1.86385500	-0.06199700
N	-3.20208100	0.55146800	0.09991200
H	-5.19123100	3.13336700	2.18423200
H	-5.60301900	0.71218800	2.46304600
H	-3.48601500	3.88201000	0.47802400
H	-2.26568600	2.14445200	-0.80881200
C	-4.44258900	-1.30219000	0.99322800
C	-5.34882200	-1.87276300	1.88627700
C	-4.22945900	-3.29562600	-0.13963200
C	-5.69212300	-3.20891700	1.74078000
H	-5.79050300	-1.28653900	2.68632700
H	-3.78188500	-3.82263500	-0.97968200
H	-6.39444800	-3.67063000	2.43039800
C	-5.14663000	-3.92971900	0.68803900
H	-5.41447900	-4.96670100	0.50659400
N	-3.85006100	-2.02873500	0.02914700
Ni	-2.31461900	-0.91952400	-1.11773000
C	-1.51651700	-3.69490700	-1.68224800
C	-1.09185000	-4.76111900	-2.47717700
C	-0.77262000	-4.55297300	-3.81402300
C	-0.87665700	-3.26965400	-4.34481300
C	-1.30870800	-2.20700300	-3.55222000
C	-1.64939100	-2.41575500	-2.21550100
H	-1.68940800	-3.87317200	-0.62103500
H	-0.98922500	-5.75086900	-2.03248400
H	-0.62316500	-3.08604600	-5.38874500
H	-1.38124700	-1.21370400	-3.98920200
O	3.23497900	-1.44736500	-2.18934300
S	4.26778500	-0.75138600	-1.40490400
O	3.75083700	0.04085200	-0.27078100
O	5.31840600	-0.08934800	-2.18884500
C	5.17303400	-2.12414000	-0.57839200
F	5.81801200	-2.86457300	-1.47126800
F	4.32714200	-2.91602000	0.08573000
F	6.05281600	-1.64340800	0.29493600
P	1.31834100	0.60411900	2.23592500
P	1.30755500	2.80794900	-0.32283100
C	2.88496100	1.56863200	2.41470800
H	3.24245700	1.37075800	3.43378400
H	3.61291500	1.12818800	1.71917100
C	2.76573800	3.06479100	2.17589800
H	3.65496000	3.54917900	2.60142000

H	1.91414800	3.48041200	2.73336800
C	2.71772400	3.42470400	0.70018700
H	2.75774000	4.51350500	0.55244100
H	3.60462100	2.99789400	0.20735500
Pd	0.38303100	0.65943000	0.06554900
C	1.10079600	-3.01369800	0.22440300
C	0.47303700	-1.96259700	-0.42776500
C	-0.69010400	-1.31651800	0.08077100
C	-1.14912500	-1.78648200	1.34711300
C	-0.60013300	-2.88329700	1.96192100
C	0.52290700	-3.52343500	1.38983400
H	1.99292400	-3.45225200	-0.21127100
H	0.88223100	-1.66008600	-1.39254400
H	-1.98463600	-1.28770500	1.83787000
H	-0.98418000	-3.26709500	2.90583200
Br	-4.06117600	-0.52014700	-2.72234600
C	1.84525400	-0.95197200	3.02852400
C	1.15512500	-1.50807800	4.10888800
C	3.02436500	-1.55782200	2.58119300
C	1.65716400	-2.63452600	4.75262800
H	0.22368500	-1.06058400	4.45430500
C	3.53082600	-2.67331800	3.23829500
H	3.54993700	-1.15546600	1.71603300
C	2.84938400	-3.21213700	4.32594600
H	1.11417300	-3.05900300	5.59487600
H	4.46097500	-3.12078800	2.88960400
H	3.24394800	-4.08876500	4.83673000
C	0.20940700	1.41935500	3.43621200
C	0.64856100	1.69481200	4.73897500
C	-1.05564200	1.85584300	3.03956200
C	-0.16313500	2.39794500	5.61882400
H	1.62897300	1.35708900	5.07458400
C	-1.86715800	2.56401100	3.92299800
H	-1.39791000	1.65981000	2.02136500
C	-1.42146800	2.83672800	5.21034200
H	0.18866600	2.60790000	6.62673300
H	-2.84636600	2.91053400	3.59694400
H	-2.05320500	3.39450000	5.89865400
C	2.04161900	3.06573400	-1.97784800
C	2.24566900	4.36695800	-2.45098700
C	2.53954200	1.98493700	-2.70735600
C	2.91941100	4.57724500	-3.64910300
H	1.87348300	5.22333700	-1.88887900
C	3.22209000	2.19975400	-3.89956500
H	2.39559700	0.97016400	-2.34255200
C	3.40776600	3.49408300	-4.37504300

H	3.06565600	5.59201800	-4.01389000
H	3.61695600	1.34597300	-4.44769500
H	3.93749400	3.66124700	-5.31102400
C	-0.00470900	4.07105900	-0.17078500
C	-0.29095100	4.64758600	1.07161200
C	-0.76192500	4.45088000	-1.28574800
C	-1.29183000	5.60595000	1.19233800
H	0.26539800	4.35744800	1.96171700
C	-1.75945700	5.41239800	-1.16313500
H	-0.55664600	4.00727600	-2.25913600
C	-2.02075000	5.99829600	0.07356800
H	-1.49627300	6.04738300	2.16596600
H	-2.33104600	5.70814400	-2.04057500
H	-2.79717900	6.75521000	0.16621600
H	-0.43343600	-5.38033700	-4.43517300
O	0.95647000	-4.60467400	2.04163500
C	2.04831500	-5.33250600	1.49703400
H	2.22872900	-6.16161900	2.18375800
H	1.79790500	-5.72132300	0.50153800
H	2.94726600	-4.70634700	1.43612400
Br	-0.59028800	0.84672400	-2.21053100

4^{Ni} **HF =** −3237.6740201 hartree

C	-0.18532600	3.81997400	-1.84838100
C	-0.16318800	2.45315800	-1.57388000
C	-0.16298300	1.99800200	-0.25303600
C	-0.22374000	2.92076000	0.78960100
C	-0.25316600	4.28708700	0.51175900
C	-0.23101300	4.74087600	-0.80449500
H	-0.16809300	4.16365100	-2.88214100
H	-0.12275400	1.74253000	-2.40327200
H	-0.21689400	2.56843400	1.82076200
H	-0.28991300	5.00159400	1.33384000
H	-0.25104700	5.80855300	-1.01686800
C	2.85508200	-0.93713200	-0.69681700
C	4.22289300	-1.02970100	-0.93613900
C	4.97777500	0.13445400	-0.99533500
C	4.35297900	1.36142500	-0.81389400
C	2.98435600	1.37590600	-0.58337800
N	2.25746400	0.25937700	-0.53026900
H	6.04815200	0.07919400	-1.17747000
H	4.70182300	-1.99574300	-1.06755600
H	4.91028500	2.29303500	-0.84577100
H	2.43861100	2.30682200	-0.42607300
C	1.96484300	-2.10993100	-0.58003500
C	2.39830300	-3.42279400	-0.73648900

C	-0.19549100	-2.82614300	-0.13204400
C	1.48553700	-4.45754600	-0.57858600
H	3.43432600	-3.64357400	-0.97712100
H	-1.21565600	-2.52742300	0.11197400
H	1.80771000	-5.48922800	-0.69628500
C	0.16526500	-4.16008600	-0.26696700
H	-0.57704000	-4.94108700	-0.13027600
N	0.67869000	-1.83156300	-0.28802900
Ni	0.27961000	0.16317200	-0.01821300
C	-2.38562500	0.10029200	1.18496600
C	-3.73948400	-0.20463100	1.15343300
C	-4.36911800	-0.51205400	-0.05684900
C	-3.62730200	-0.51033100	-1.23780900
C	-2.26681500	-0.19539000	-1.19185800
C	-1.62720400	0.09405800	0.01192300
H	-1.90418400	0.32407500	2.13642400
H	-4.33677000	-0.21058700	2.06458000
H	-4.08908400	-0.74170900	-2.19482700
H	-1.70526300	-0.19503000	-2.12941800
O	-5.69761800	-0.79195300	0.01823900
C	-6.37065600	-1.09076300	-1.18493800
H	-5.95184600	-1.98412700	-1.67038400
H	-7.41261000	-1.28324000	-0.91834100
H	-6.32869700	-0.24834900	-1.89045700
Br	0.87977700	0.02192500	2.39903700

TS3^{Ni} **HF =** −3815.0163478 hartree $\nu^{\ddagger} = -151.51\ icm^{-1}$

C	-0.25532100	3.76900100	-1.87308900
C	-0.30020800	2.40589300	-1.59050300
C	-0.33810600	1.95581700	-0.26580000
C	-0.36657400	2.89310800	0.76955200
C	-0.33163900	4.25561300	0.48213100
C	-0.27365200	4.69970900	-0.83681900
H	-0.21085800	4.10309000	-2.90901500
H	-0.29230500	1.68863000	-2.41446600
H	-0.38415400	2.55163100	1.80396300
H	-0.34521800	4.97608300	1.29947400
H	-0.24635400	5.76549900	-1.05673000
C	2.88907200	-0.90623000	-0.68303300
C	4.25940100	-0.97796400	-0.91671400
C	4.99327100	0.19930800	-0.98685100
C	4.34688700	1.41799000	-0.82320200
C	2.97735900	1.40957200	-0.59573000
N	2.27226700	0.28088000	-0.53038700
H	6.06505300	0.16111300	-1.16548600
H	4.75590300	-1.93671200	-1.03715000

H	4.88823400	2.35859000	-0.86693100
H	2.41276500	2.33231800	-0.45141900
C	2.01459500	-2.09403100	-0.56509200
C	2.47019000	-3.40147700	-0.70590000
C	-0.14099700	-2.83857600	-0.14615000
C	1.56953100	-4.44813300	-0.55450200
H	3.51288500	-3.60942500	-0.92914400
H	-1.16986400	-2.55297800	0.08041600
H	1.90882700	-5.47581100	-0.65910500
C	0.23958300	-4.16878600	-0.26694500
H	-0.49297600	-4.96017600	-0.13717800
N	0.72163400	-1.83391000	-0.29368100
Ni	0.28383000	0.17019800	0.00143100
C	-2.39896400	0.25736000	1.14744500
C	-3.72512800	-0.14502000	1.12730300
C	-4.32430300	-0.55648700	-0.06833100
C	-3.57697900	-0.55787300	-1.24599000
C	-2.24453600	-0.14369400	-1.21272700
C	-1.63093300	0.25068400	-0.02260600
H	-1.94292800	0.55880700	2.08952600
H	-4.32572800	-0.14876200	2.03604000
H	-4.01361600	-0.87211500	-2.19099400
H	-1.67950900	-0.14659900	-2.14762400
O	-5.62783000	-0.92806300	0.01807200
C	-6.27960700	-1.31037500	-1.17378600
H	-5.81019400	-2.19627700	-1.62516900
H	-7.30957100	-1.55116700	-0.90024900
H	-6.28287700	-0.49336900	-1.90950700
Br	0.84694100	0.03386700	2.42053100

TS2^{Pd} **HF =** − 9202.2511787 hartree $\nu^{\ddagger} = -72.11\ icm^{-1}$

C	-4.26679000	-1.58239500	-1.21509600
C	-5.31930600	-1.44994400	-2.11853700
C	-5.11642100	-1.79873200	-3.44582000
C	-3.87283800	-2.27760900	-3.83859500
C	-2.86950600	-2.36564200	-2.88489400
N	-3.05938300	-2.01815100	-1.61188500
H	-5.92485000	-1.69857800	-4.16585300
H	-6.28717200	-1.07591200	-1.79801500
H	-3.67324000	-2.56977100	-4.86546500
H	-1.86665300	-2.70754000	-3.13821000
C	-4.39163700	-1.29316000	0.22449800
C	-5.58541200	-0.87675700	0.80893300
C	-3.36447700	-1.38387500	2.29268500
C	-5.64375100	-0.69436100	2.18247700
H	-6.46724600	-0.69488700	0.20191500

H	-2.46491800	-1.62919700	2.85283500
H	-6.56572200	-0.35857700	2.65064700
C	-4.51773600	-0.97366100	2.94489700
H	-4.52299100	-0.88205500	4.02690500
N	-3.28528500	-1.50437900	0.96638600
Ni	-1.60859400	-2.01216300	-0.13021300
C	-0.29542400	-0.99727000	2.43400700
C	0.10888900	-1.39974400	3.71122000
C	0.69954400	-2.64154100	3.89635200
C	0.95803200	-3.46214100	2.79893900
C	0.59523500	-3.05815400	1.52052300
C	-0.10117700	-1.85546200	1.35742700
H	-0.77711000	-0.03016200	2.33440200
H	-0.05565900	-0.71777300	4.54455000
H	1.45874400	-4.41986700	2.93336200
H	0.81051200	-3.69691400	0.66868300
O	0.82966100	1.99773400	2.25493500
S	0.35585700	2.42046100	3.58747200
O	1.42472400	2.68592200	4.55873100
O	-0.80165800	1.67252100	4.10366400
C	-0.36828600	4.07793700	3.25185700
F	-1.43611100	3.96076500	2.45789700
F	0.51548400	4.86507000	2.63983800
F	-0.75111100	4.66645900	4.37803800
P	1.31231200	2.04319300	-1.22867100
P	3.12736600	-0.30734900	0.38550800
C	2.50795900	3.06989300	-0.26846500
H	2.59495600	4.02891900	-0.79727200
H	2.02790800	3.26936700	0.69957000
C	3.87979000	2.45300800	-0.05337800
H	4.53248100	3.23491300	0.35899300
H	4.32909800	2.17017600	-1.01645800
C	3.88563400	1.28958200	0.92752400
H	4.90799900	1.06706000	1.26402900
H	3.30921300	1.57682800	1.81916600
Pd	0.74197700	-0.01492500	-0.20456900
C	-3.15624600	1.84951100	0.09452300
C	-1.91118500	1.28450300	0.35576200
C	-1.19129000	0.59556800	-0.62783200
C	-1.71785000	0.58837700	-1.93024600
C	-2.94616600	1.16199500	-2.21349400
C	-3.68340400	1.78115100	-1.19806600
H	-3.69081600	2.35136200	0.89881000
H	-1.48994500	1.42761600	1.35170700
H	-1.16647100	0.10972500	-2.74181900
H	-3.36650100	1.13085900	-3.21853400

Br	-2.15210100	-4.38861300	0.27514000
C	0.05161600	3.30853300	-1.61062700
C	-0.34972900	3.60701900	-2.91450700
C	-0.50050800	4.01787900	-0.54147100
C	-1.28301800	4.61453800	-3.14079500
H	0.06739200	3.05557200	-3.75673200
C	-1.43255500	5.02193300	-0.76958000
H	-0.20788300	3.77162400	0.47656800
C	-1.82435800	5.32341700	-2.07174300
H	-1.58732700	4.84579100	-4.15994500
H	-1.85280700	5.56343300	0.07688100
H	-2.55372400	6.11078500	-2.25339000
C	2.15953100	1.73263000	-2.81972000
C	2.87480900	2.75822100	-3.45219400
C	2.10980400	0.46939300	-3.41282500
C	3.53378000	2.51657600	-4.65082900
H	2.91546000	3.75565500	-3.01457800
C	2.77297100	0.22964500	-4.61387300
H	1.55890400	-0.33731800	-2.92843600
C	3.48484100	1.25073100	-5.23246300
H	4.08679200	3.31967400	-5.13382400
H	2.73292400	-0.76253500	-5.06009900
H	4.00454600	1.06338800	-6.17018700
C	3.58697500	-1.30125600	1.86223700
C	4.31287300	-2.49110600	1.76219500
C	3.26034500	-0.80583400	3.12962300
C	4.72115900	-3.16390200	2.90992300
H	4.57963500	-2.88911600	0.78380300
C	3.68301700	-1.47399100	4.27317200
H	2.66244700	0.10174400	3.23236300
C	4.41587000	-2.65205800	4.16757800
H	5.29125400	-4.08667000	2.81782600
H	3.42384900	-1.07543600	5.25300500
H	4.74514200	-3.17338600	5.06453700
C	4.23648100	-0.93992300	-0.92621700
C	5.46742400	-0.34924900	-1.23070100
C	3.83445100	-2.07206900	-1.64342000
C	6.26198900	-0.86587400	-2.24996600
H	5.82389800	0.51575300	-0.67511200
C	4.63908800	-2.60000000	-2.64640600
H	2.87198100	-2.53251600	-1.42177200
C	5.85095900	-1.99042200	-2.95876300
H	7.21252200	-0.38957000	-2.48267700
H	4.31360700	-3.48380700	-3.19187800
H	6.47741300	-2.39330400	-3.75221100
H	0.99619200	-2.96092300	4.89420200

O	-4.88602500	2.28254000	-1.56314900
C	-5.60439400	3.03662400	-0.60740600
H	-6.51627200	3.37407500	-1.10490200
H	-5.87542200	2.43004200	0.26835900
H	-5.02580700	3.91077600	-0.27570000
Br	0.27414600	-2.31353300	-1.62809600

3^{Pd} **HF =** −9202.2618929 hartree

C	4.64193600	-1.45234500	0.76452700
C	5.76425900	-1.42470200	1.58727700
C	5.65566600	-1.89480800	2.88926000
C	4.43661600	-2.38824000	3.33816800
C	3.36084300	-2.38024500	2.46195100
N	3.46440300	-1.91732600	1.21731600
H	6.52199200	-1.88021200	3.54585700
H	6.71541200	-1.04938900	1.22109900
H	4.31433800	-2.77103500	4.34705500
H	2.37391500	-2.73701400	2.75561100
C	4.64574400	-1.00275900	-0.64141900
C	5.76076800	-0.45028000	-1.26587900
C	3.42003800	-0.87255500	-2.60744900
C	5.68059500	-0.10815500	-2.60866300
H	6.68258000	-0.28693000	-0.71453800
H	2.45934200	-1.05050900	-3.09251800
H	6.54030000	0.32749400	-3.11184000
C	4.49629300	-0.33601200	-3.29957800
H	4.39887100	-0.09739600	-4.35452700
N	3.49076400	-1.17656500	-1.31091100
Ni	1.94106500	-1.81148200	-0.14903800
C	-0.05991700	-0.14520600	-2.93392900
C	0.09915200	-0.63747900	-4.22665700
C	0.03456100	-2.00817700	-4.46990200
C	-0.21467700	-2.87329000	-3.41146400
C	-0.38409500	-2.37899400	-2.11451800
C	-0.28405500	-1.01080200	-1.85856300
H	-0.07995600	0.93235600	-2.78826800
H	0.25238300	0.06446600	-5.04660800
H	-0.28389300	-3.94741800	-3.58169700
H	-0.60416300	-3.08460100	-1.31494200
O	-1.23749900	2.44424500	-1.38517400
S	-1.42683900	3.42712400	-2.47188700
O	-2.75117200	4.06168300	-2.49064200
O	-0.90540500	2.99855500	-3.77719800
C	-0.29945400	4.79456800	-1.97964000
F	0.93833300	4.33831600	-1.80019500
F	-0.70928300	5.34253300	-0.83604000

F	-0.27367300	5.73857700	-2.91301800
P	-1.45828200	1.34316100	1.90190000
P	-3.12867500	-0.44763400	-0.52768400
C	-2.79206500	2.50606700	1.35307300
H	-2.96157700	3.21219400	2.17745700
H	-2.38899800	3.07044700	0.50223000
C	-4.10364000	1.83263000	0.96932200
H	-4.87375400	2.61442700	0.91194700
H	-4.43108300	1.15707100	1.77407700
C	-4.10067100	1.11604200	-0.37827800
H	-5.12855100	0.88573300	-0.69373900
H	-3.67332500	1.78041000	-1.14193000
Pd	-0.73100800	-0.09782400	-0.03048200
C	3.00174700	2.07879600	-0.45037300
C	1.87322200	1.31047800	-0.70786900
C	1.29030900	0.48890900	0.26676400
C	1.88348500	0.49631400	1.54443400
C	3.02853600	1.22736400	1.81134600
C	3.60013500	2.02112800	0.81332600
H	3.40640700	2.70976800	-1.23861300
H	1.44608000	1.36714600	-1.70673500
H	1.44675400	-0.08799700	2.35579800
H	3.49306200	1.20718900	2.79727900
Br	2.35521900	-4.11710700	-0.80893300
C	-0.19634800	2.53146100	2.48646900
C	0.33719000	2.52740600	3.77698300
C	0.28077600	3.45541000	1.55139900
C	1.32149600	3.44764400	4.12764000
H	-0.01111500	1.80443600	4.51385100
C	1.26159100	4.37286700	1.90404200
H	-0.09933700	3.43130600	0.53191200
C	1.78412500	4.37170900	3.19536000
H	1.72944400	3.43930600	5.13692000
H	1.62577100	5.08019900	1.15908100
H	2.55636500	5.08689000	3.47313900
C	-2.20922100	0.63644900	3.41840500
C	-2.67230600	1.48444200	4.43547100
C	-2.43029300	-0.73776600	3.53389200
C	-3.32928900	0.96467700	5.54300000
H	-2.51585700	2.56113500	4.36772400
C	-3.09307900	-1.25735600	4.64397300
H	-2.08614000	-1.41330600	2.75283400
C	-3.54219800	-0.40888400	5.64812000
H	-3.68112300	1.63475500	6.32502600
H	-3.26025800	-2.33048100	4.71570900
H	-4.06102300	-0.81437100	6.51466500

C	-3.56526500	-0.93509800	-2.23691300
C	-4.26093600	-2.10958500	-2.53271100
C	-3.19087100	-0.07977700	-3.27903500
C	-4.57000100	-2.42512300	-3.85292900
H	-4.56713000	-2.78343200	-1.73376900
C	-3.50698100	-0.39489800	-4.59438500
H	-2.62641000	0.82719700	-3.06221700
C	-4.19386800	-1.57079300	-4.88465700
H	-5.11204800	-3.34299500	-4.07326400
H	-3.20183700	0.27656300	-5.39547400
H	-4.43657700	-1.82057700	-5.91587300
C	-3.98238400	-1.67529400	0.51975200
C	-5.20302100	-1.41157600	1.14787200
C	-3.39368500	-2.93529000	0.68289400
C	-5.80248300	-2.37479600	1.95380900
H	-5.69916400	-0.45229000	1.01445400
C	-3.99816500	-3.89929800	1.48073200
H	-2.45763800	-3.16700300	0.17553500
C	-5.19890100	-3.61582900	2.12748200
H	-6.74844700	-2.15276000	2.44385100
H	-3.53019700	-4.87501200	1.59721200
H	-5.66811200	-4.36696500	2.75984300
H	0.15963200	-2.39674100	-5.47920500
O	4.71262200	2.70227200	1.16031500
C	5.28974200	3.55400500	0.18927400
H	6.16361900	4.00973200	0.65947200
H	5.60620800	2.98772100	-0.69814500
H	4.58636600	4.34209900	-0.11501800
Br	-0.02491800	-2.27879200	1.28877000

4^{Pd} **HF =** −3392.9408191 hartree

C	-0.82793100	-2.40991200	1.90621900
C	-1.22131800	-3.28790700	2.91464400
C	-1.91096900	-2.81354200	4.02991700
C	-2.20057700	-1.45648400	4.14179400
C	-1.80516700	-0.56994500	3.13770800
C	-1.10040600	-1.04810900	2.03445500
H	-0.31081000	-2.78295300	1.01933800
H	-0.99755800	-4.35045400	2.82178900
H	-2.74079600	-1.08108600	5.01033000
H	-2.03995800	0.49194000	3.23433300
O	0.59498500	-1.77958700	-1.20560200
S	1.08356300	-2.68034200	-2.26778200
O	1.56702600	-1.99070300	-3.47540500
O	0.24376400	-3.86116900	-2.51223100
C	2.61004100	-3.38682800	-1.52438200

F	2.32355700	-3.96311800	-0.35888300
F	3.51454800	-2.43260100	-1.30472400
F	3.14789000	-4.29568100	-2.32892800
P	0.57203900	1.68694400	-1.08651600
P	-2.35583000	-0.15089000	-0.56352200
C	-0.01773500	1.27125500	-2.78216500
H	0.41256800	2.01068300	-3.47163100
H	0.41734800	0.29707900	-3.04780900
C	-1.53706600	1.21915500	-2.92832100
H	-1.77056700	1.28564600	-3.99916100
H	-2.00621800	2.10634500	-2.47116900
C	-2.16622800	-0.06648100	-2.39746200
H	-3.15902600	-0.22456500	-2.84054900
H	-1.54719100	-0.92605900	-2.69000600
Pd	-0.30043000	0.23092900	0.64039900
C	3.63644300	-0.46442600	2.04879500
C	2.49821700	-0.39527300	1.25702800
C	1.49434300	0.54082100	1.53526700
C	1.72101400	1.53751400	2.49719100
C	2.85520300	1.48291300	3.28621000
C	3.81716400	0.47927100	3.07086700
H	4.38182700	-1.23220300	1.85543800
H	2.36702900	-1.09690000	0.43303600
H	0.98935200	2.32898400	2.66419900
H	3.03262200	2.20804100	4.07837900
C	2.38792100	1.75059700	-1.27935200
C	3.13424800	2.74334700	-0.63572400
C	3.05060500	0.74168100	-1.98520000
C	4.52307100	2.73001000	-0.70266300
H	2.62872000	3.53503500	-0.08189600
C	4.44069500	0.73420300	-2.04887500
H	2.49232900	-0.05261800	-2.48179000
C	5.17896700	1.72517100	-1.40992500
H	5.09358400	3.50997100	-0.20179600
H	4.94720100	-0.05673000	-2.59976300
H	6.26604400	1.71571600	-1.46179800
C	0.07915200	3.43052300	-0.85014400
C	0.28611600	4.38738500	-1.85109400
C	-0.50072500	3.82471500	0.35721800
C	-0.09907700	5.70651500	-1.64886200
H	0.76199600	4.10949500	-2.79150100
C	-0.88515200	5.14698300	0.56171700
H	-0.64783700	3.08477300	1.14505900
C	-0.68845000	6.08665500	-0.44437100
H	0.06193400	6.44322200	-2.43338100
H	-1.33979000	5.43916400	1.50646000

H	-0.99077600	7.12062600	-0.29013600
C	-3.16511100	-1.77156500	-0.32762300
C	-4.24571900	-1.92240900	0.54621600
C	-2.63449000	-2.89916000	-0.96236400
C	-4.79739800	-3.18052100	0.76721800
H	-4.66433600	-1.05504000	1.05672400
C	-3.18863800	-4.15419100	-0.73790800
H	-1.76571000	-2.81478100	-1.61325300
C	-4.27144100	-4.29853900	0.12510500
H	-5.64160700	-3.28589100	1.44615200
H	-2.76299000	-5.02246800	-1.23882700
H	-4.70502800	-5.28173100	0.29891700
C	-3.65082400	1.08180200	-0.19092700
C	-4.83493900	1.15019500	-0.93511900
C	-3.45558900	1.98153000	0.85874600
C	-5.79174600	2.11366600	-0.64132100
H	-5.02088100	0.44003600	-1.74095800
C	-4.41252600	2.94888800	1.15242100
H	-2.54253400	1.92215100	1.45167200
C	-5.57907800	3.01686700	0.39890500
H	-6.70801900	2.16006600	-1.22646800
H	-4.24281300	3.64875200	1.96851100
H	-6.32910100	3.77321900	0.62180800
H	-2.23100600	-3.50504300	4.80762300
O	4.88839300	0.52026700	3.88167800
C	5.90663200	-0.44888500	3.69962800
H	6.65546800	-0.25227100	4.46911800
H	5.51118000	-1.46528600	3.82632600
H	6.36849800	-0.35573300	2.70793700

TS3^{Pd} **HF =** −3392.9387011 hartree $\nu^{\ddagger} = -147.67\ icm^{-1}$

C	-0.45490200	-2.39798900	2.13102300
C	-0.84432800	-3.29174600	3.12893000
C	-1.66041500	-2.86607100	4.17470300
C	-2.07133600	-1.53698100	4.22536900
C	-1.67519500	-0.64102300	3.22994400
C	-0.88571800	-1.06737000	2.15903800
H	0.18073800	-2.75207200	1.31552000
H	-0.50634700	-4.32743700	3.08749500
H	-2.70187500	-1.19039500	5.04431500
H	-1.99900600	0.40054300	3.29379100
O	0.78365100	-1.61055900	-1.46533900
S	1.34579800	-2.59691300	-2.40714000
O	1.90982900	-2.01445400	-3.63437300
O	0.53029900	-3.80475000	-2.59824700
C	2.82341700	-3.20864600	-1.49836900

F	2.46250700	-3.72165900	-0.32331200
F	3.67488100	-2.20695900	-1.27026600
F	3.45695800	-4.14716400	-2.19212800
P	0.37418000	1.71461900	-1.10340600
P	-2.36826100	-0.29182400	-0.56964100
C	-0.14407200	1.22964500	-2.80137100
H	0.25816200	1.96551400	-3.51144700
H	0.34632800	0.26911300	-3.01407000
C	-1.65746100	1.08318800	-2.96989900
H	-1.87631400	1.10885900	-4.04580100
H	-2.18427200	1.95369900	-2.54448300
C	-2.22988400	-0.22001000	-2.41362300
H	-3.22857900	-0.40597600	-2.83228600
H	-1.59505000	-1.06297300	-2.72013300
Pd	-0.36452600	0.23484700	0.62206900
C	3.69416200	-0.19150400	1.83477500
C	2.48057600	-0.25193300	1.19607800
C	1.34290000	0.49768400	1.63182600
C	1.52624100	1.37335800	2.74254700
C	2.72735400	1.45294700	3.39330900
C	3.83395400	0.68209000	2.93697700
H	4.53455000	-0.77886300	1.47252500
H	2.36922900	-0.89269800	0.32171400
H	0.68687900	1.97486000	3.09279500
H	2.88385600	2.10172500	4.25263200
C	2.19380000	1.89470200	-1.21129800
C	2.83272700	2.90765100	-0.48661800
C	2.96879600	0.95474200	-1.89929700
C	4.22075200	2.97966000	-0.45093000
H	2.24333300	3.64705500	0.05643100
C	4.35777600	1.03558800	-1.86537100
H	2.49712400	0.13797200	-2.44497600
C	4.98681700	2.04334800	-1.14041900
H	4.70529300	3.77492000	0.11288000
H	4.94914700	0.29673700	-2.40393900
H	6.07348400	2.10069700	-1.11267900
C	-0.22703200	3.42727800	-0.89084000
C	-0.19788800	4.35910100	-1.93419800
C	-0.69634000	3.82532800	0.36368600
C	-0.64791700	5.65751400	-1.72680800
H	0.18198900	4.07710000	-2.91587700
C	-1.14011600	5.12750700	0.57403600
H	-0.71236300	3.10084600	1.18021100
C	-1.12071000	6.04235000	-0.47397200
H	-0.62719300	6.37343900	-2.54612500
H	-1.50270900	5.42579700	1.55590900

H	-1.47371700	7.05952800	-0.31552000
C	-3.02002800	-1.97660400	-0.29503700
C	-4.10830600	-2.21973500	0.54748500
C	-2.33873000	-3.05821000	-0.86392000
C	-4.51635400	-3.52548800	0.80596100
H	-4.64077600	-1.38785000	1.00882500
C	-2.75615800	-4.35994900	-0.61080600
H	-1.46133700	-2.89347600	-1.48970900
C	-3.84568100	-4.59716600	0.22349300
H	-5.36597900	-3.70446200	1.46256200
H	-2.21888400	-5.19077100	-1.06619100
H	-4.16953400	-5.61697600	0.42350600
C	-3.76814400	0.82952700	-0.21361400
C	-4.98235100	0.74184000	-0.90555800
C	-3.61322000	1.81713100	0.76169900
C	-6.01310500	1.63177200	-0.63083300
H	-5.13175500	-0.03345500	-1.65768200
C	-4.64367900	2.71271900	1.03475200
H	-2.66975300	1.88405100	1.30478100
C	-5.84291300	2.62063200	0.33716700
H	-6.95310000	1.55574900	-1.17401800
H	-4.50514400	3.48286900	1.79155200
H	-6.64998500	3.32021000	0.54631200
H	-1.96604300	-3.56495000	4.95199300
O	4.96020600	0.87036200	3.60400200
C	6.14671200	0.19207800	3.18932900
H	6.93140600	0.52937000	3.86671900
H	6.01935700	-0.89259500	3.27616100
H	6.40048100	0.46353800	2.15802000

5^{Pd} **HF =** −3393.029194 hartree

C	0.58196200	1.68315400	2.49873700
C	1.78901100	2.36387100	2.65666900
C	2.87882900	1.73912700	3.24712800
C	2.76042400	0.42086500	3.69104100
C	1.56296200	-0.26359400	3.54841400
C	0.44573500	0.34934200	2.94530100
H	-0.26197900	2.19339700	2.02981500
H	1.87261100	3.38964800	2.30309600
H	3.60548500	-0.07283700	4.16780000
H	1.47603600	-1.27882200	3.93345400
O	-1.87623200	2.78916400	0.44495900
S	-1.04198700	3.41507900	-0.59518400
O	-0.53361300	2.49317300	-1.63055400
O	-0.05993800	4.39222000	-0.10322800
C	-2.25127300	4.43889600	-1.52970800

F	-2.81833800	5.33833000	-0.73209100
F	-3.21019800	3.67047300	-2.04536700
F	-1.64596700	5.07947600	-2.52467200
P	-0.89152800	-1.19541600	-1.20423600
P	2.27181800	0.04030600	-0.74420500
C	-0.46060700	-0.52245300	-2.86776100
H	-1.08420000	-1.04316500	-3.60839500
H	-0.75066600	0.53719300	-2.86405300
C	1.01679700	-0.65752700	-3.23038100
H	1.11002700	-0.48766300	-4.31175800
H	1.35765200	-1.69278000	-3.06612300
C	1.93953700	0.34190700	-2.53264900
H	2.90721900	0.40609800	-3.05107900
H	1.48990800	1.34652500	-2.56975800
Pd	0.30734900	-0.16816400	0.54975800
C	-3.28172900	-0.35312400	2.69807700
C	-2.06875000	0.31475400	2.78579600
C	-0.84357700	-0.37320900	2.80345300
C	-0.89138300	-1.78405200	2.72980800
C	-2.09360300	-2.45806500	2.62795000
C	-3.30159300	-1.74963200	2.61924700
H	-4.20414000	0.22141600	2.70584200
H	-2.07463000	1.40086800	2.85188300
H	0.03460200	-2.35883200	2.74217200
H	-2.12455000	-3.54371300	2.55574100
C	-2.70663000	-1.02983200	-1.15819900
C	-3.54820500	-2.08842900	-0.80534200
C	-3.25720200	0.23555600	-1.40406100
C	-4.92309400	-1.88967100	-0.72383400
H	-3.13152500	-3.07406600	-0.59864500
C	-4.63018700	0.42890300	-1.31776600
H	-2.60621700	1.07833500	-1.63924800
C	-5.46664500	-0.63398900	-0.98128000
H	-5.56980400	-2.72174700	-0.44904700
H	-5.04589500	1.41637900	-1.51108000
H	-6.54279500	-0.48265000	-0.91503000
C	-0.53513400	-2.97875600	-1.38191000
C	-1.06668400	-3.73372700	-2.43465300
C	0.35733300	-3.58306400	-0.49327800
C	-0.70838200	-5.06757500	-2.58945800
H	-1.77029700	-3.28153400	-3.13458000
C	0.72485200	-4.91601200	-0.65446800
H	0.78010900	-2.99276300	0.32106000
C	0.19074500	-5.65791000	-1.70245400
H	-1.12827600	-5.64859300	-3.40821900
H	1.43036700	-5.36891900	0.03992500

H	0.47457100	-6.70058400	-1.83213100
C	3.41102100	1.40758900	-0.34267800
C	4.72567300	1.20213800	0.08301300
C	2.90912900	2.71157200	-0.42637200
C	5.53064300	2.29023000	0.40939900
H	5.12816800	0.19218000	0.15736500
C	3.71786500	3.79368500	-0.10417000
H	1.87328000	2.88436300	-0.72374200
C	5.03017100	3.58569700	0.31703800
H	6.55514600	2.12236300	0.73700500
H	3.31239700	4.80242000	-0.17094200
H	5.66123800	4.43395900	0.57581900
C	3.28493700	-1.47488000	-0.65461300
C	3.90957800	-2.04341300	-1.76774500
C	3.41009100	-2.10061600	0.59221400
C	4.63340200	-3.22548100	-1.63724600
H	3.83331000	-1.57077300	-2.74622900
C	4.14637500	-3.27168200	0.72379000
H	2.91715000	-1.66131200	1.46337200
C	4.75277100	-3.83995200	-0.39451700
H	5.10880900	-3.66549800	-2.51179600
H	4.24074900	-3.74626100	1.69873000
H	5.31825400	-4.76461400	-0.29681700
H	3.81990600	2.27372500	3.36388400
O	-4.42296000	-2.49451400	2.54241400
C	-5.66937100	-1.83131600	2.64312200
H	-6.43488600	-2.60520300	2.55234600
H	-5.77193500	-1.32641800	3.61350100
H	-5.79807900	-1.10002700	1.83306900

6^{Pd} **HF =** −2815.5992709 hartree

O	0.82583400	3.50629000	-0.00002200
S	-0.62305600	3.45706600	0.22896100
O	-1.30400300	2.31689500	-0.46123300
O	-1.35536500	4.71692200	0.11926200
C	-0.77447800	3.00509300	2.01181300
F	-0.35617800	4.01177900	2.76573200
F	-0.04338000	1.92985600	2.29720300
F	-2.04306400	2.74123500	2.31160100
P	-1.50384800	-1.23022400	-0.78080600
P	1.90194800	-0.87351700	-0.70037400
C	-0.89233100	-2.79210100	-1.54563500
H	-1.65234600	-3.57311300	-1.39187500
H	-0.88037500	-2.58775200	-2.62747600
C	0.48294100	-3.28633000	-1.09266000
H	0.60298700	-4.31007600	-1.47120900

H	0.52517500	-3.37287800	0.00486000
C	1.67510500	-2.46719600	-1.59303300
H	2.59279200	-3.06165600	-1.47552400
C	2.39973000	-1.40999000	0.97894900
C	3.65877500	-1.97739700	1.20346400
C	1.50334400	-1.28337800	2.04474000
H	4.37010100	-2.07395300	0.38231200
C	4.01435400	-2.41006200	2.47530300
C	1.86012900	-1.72295300	3.31663700
H	0.51984900	-0.83911700	1.87807600
H	4.99727000	-2.84630400	2.64290900
C	3.11490600	-2.28400800	3.53197200
H	1.15641300	-1.61915800	4.14060900
H	3.39654200	-2.62129100	4.52769300
C	3.40111100	-0.11391200	-1.40991700
C	3.65532100	1.21962500	-1.06290900
C	4.27973500	-0.77978300	-2.26895300
H	2.95477600	1.75251800	-0.41395200
C	4.78169900	1.86859800	-1.55252000
C	5.40159100	-0.12176500	-2.76591800
H	4.09776300	-1.81485600	-2.55540500
H	4.97417800	2.90361400	-1.27677600
C	5.65517400	1.19822300	-2.40669000
H	6.08067700	-0.64645700	-3.43512800
H	6.53327900	1.70862100	-2.79748400
C	-3.06189800	-0.93136900	-1.68138400
C	-3.05952700	-0.00648500	-2.72938800
C	-4.23222900	-1.63521300	-1.38045900
H	-2.14747500	0.55030200	-2.95319500
C	-4.21464000	0.20837700	-3.47471500
C	-5.38581400	-1.41475800	-2.12453300
H	-4.24147800	-2.35490000	-0.56104900
H	-4.20838700	0.92970100	-4.28945800
C	-5.37681500	-0.49471800	-3.17078800
H	-6.29536200	-1.96329000	-1.88706800
H	-6.28265800	-0.32232400	-3.74885600
C	-1.99735800	-1.63558200	0.92573700
C	-1.96334400	-2.92491400	1.46139000
C	-2.33632200	-0.55663600	1.75360400
H	-1.70542100	-3.78003100	0.83763300
C	-2.25032500	-3.12904700	2.80923300
C	-2.62559300	-0.76367600	3.09563300
H	-2.35248400	0.45528600	1.34363600
H	-2.21551000	-4.13586000	3.22070400
C	-2.57562300	-2.05173700	3.62683300
H	-2.88003600	0.08427400	3.72903500

H	-2.79004400	-2.21478700	4.68123900
H	1.56444700	-2.23862600	-2.66387600
Pd	0.06758500	0.52015300	-0.71251700

2_h^{Ni} **HF =** −12081.4306075 hartree

C	-2.05751200	2.57177200	-0.22826800
C	-1.89713600	3.89644200	0.16441900
C	-1.87793700	4.20732600	1.51707900
C	-2.02392600	3.18687900	2.44685600
C	-2.15716200	1.88490700	1.98712300
N	-2.16597200	1.58397900	0.68660300
H	-1.76064400	5.23946800	1.83779900
H	-1.80766100	4.68519400	-0.57670100
H	-2.03314200	3.38573600	3.51464800
H	-2.26806100	1.04989700	2.67715600
C	-2.16078100	2.15205000	-1.63663300
C	-1.99288700	3.01276200	-2.71630900
C	-2.55357000	0.36186200	-3.05869200
C	-2.11458300	2.50725300	-4.00454100
H	-1.75861600	4.06205800	-2.56348000
H	-2.75981300	-0.70631600	-3.12617200
H	-1.98109000	3.16364800	-4.86079200
C	-2.40535800	1.16121100	-4.18375600
H	-2.50893000	0.72919700	-5.17473300
N	-2.43262000	0.84684900	-1.82435100
Ni	-2.48613400	-0.23381900	-0.09648100
C	-0.54112800	-1.64749100	3.27304100
C	-0.86047800	-1.21899200	1.98469700
C	-2.19244100	-1.15598200	1.59286800
C	-3.20831800	-1.58012700	2.43742300
C	-2.87736800	-2.01344300	3.72359100
C	-1.55170800	-2.04048100	4.14633000
H	0.50415200	-1.67758700	3.58493500
H	-0.07429600	-0.91636600	1.29216900
H	-4.24582000	-1.54950000	2.11156300
H	-3.67216300	-2.33107200	4.39727900
H	-1.30521900	-2.37795700	5.15114400
Br	-2.37460100	-2.37171400	-1.00423200
Br	-4.92490400	0.11241900	0.04955800
C	3.96592900	1.77642700	-0.46347900
C	4.94706400	2.55454200	-1.07118000
C	5.77578800	1.97530900	-2.02238300
C	5.61952500	0.63018600	-2.32877100
C	4.61696600	-0.08173300	-1.68504900
N	3.79904300	0.48161500	-0.79658500
H	6.54805400	2.56823400	-2.50578800

H	5.08029600	3.59642700	-0.79498500
H	6.26095500	0.13250800	-3.04990700
H	4.46576100	-1.14269800	-1.87543400
C	3.08831900	2.27101900	0.61381200
C	3.04566200	3.59713500	1.03532200
C	1.51769200	1.66416400	2.21172900
C	2.20952500	3.94316900	2.08811000
H	3.65086500	4.35647900	0.54869600
H	0.91690500	0.85833700	2.63745100
H	2.16332000	4.97401400	2.43026200
C	1.43919100	2.96102500	2.69866500
H	0.78293000	3.19060500	3.53328000
N	2.32031700	1.33523400	1.19982000
Ni	2.29306300	-0.47742600	0.26282300
C	1.89238000	-3.65566900	-2.50042400
C	2.18581800	-2.41363300	-1.93612900
C	2.00393200	-2.22148900	-0.57171500
C	1.49766600	-3.24313600	0.22551300
C	1.18440000	-4.47397200	-0.35291800
C	1.38888800	-4.68604300	-1.71241000
H	2.04011400	-3.80270500	-3.56946300
H	2.51206200	-1.60011800	-2.58172200
H	1.34468600	-3.10172800	1.29463000
H	0.78667100	-5.27070200	0.27446200
H	1.15155300	-5.65019700	-2.15824000
Br	0.59079700	0.33886100	-1.09010400
Br	3.83125300	-1.42194400	1.70170400

$TS2_h^{Ni}$ **HF =** −12081.4040545 hartree $\nu^{\ddagger} = -58.83\ icm^{-1}$

C	-2.71563600	2.29612600	0.83631100
C	-2.93115200	3.30663800	1.77008300
C	-2.68127200	3.04975600	3.11129500
C	-2.22372400	1.79325100	3.48981900
C	-2.02049600	0.84131000	2.50054500
N	-2.25163100	1.09109200	1.21227500
H	-2.85231800	3.82337900	3.85584100
H	-3.31242900	4.27587300	1.46166200
H	-2.02696500	1.54877400	4.53004900
H	-1.67174500	-0.16646500	2.73775000
C	-3.01819300	2.44232300	-0.60229700
C	-3.37482800	3.64576800	-1.20239400
C	-3.20350100	1.32159400	-2.63057100
C	-3.65626200	3.66199300	-2.56282600
H	-3.42424100	4.56334500	-0.62322900
H	-3.10022700	0.36223300	-3.13747100

H	-3.93385700	4.59427400	-3.04849200
C	-3.57490700	2.48315300	-3.29320900
H	-3.78745600	2.45883700	-4.35783900
N	-2.93637700	1.30889800	-1.32430300
Ni	-2.24632700	-0.31293100	-0.30654400
C	0.97801200	-3.40738300	3.49052900
C	0.55833300	-2.16911800	2.98953600
C	-0.35555600	-2.20078200	1.96303100
C	-0.90102700	-3.33203600	1.40108700
C	-0.47675100	-4.55530000	1.92855100
C	0.46028800	-4.58764700	2.96088800
H	1.70805200	-3.44199000	4.29798400
H	0.95517100	-1.24290300	3.40438800
H	-1.59637000	-3.28096800	0.56219100
H	-0.87365300	-5.48440900	1.52133100
H	0.79085000	-5.54528400	3.35872200
Br	-2.09795900	-2.04708000	-1.97745100
Br	-4.34490600	-1.15163500	0.60425300
C	3.36622500	2.44984100	-0.55014800
C	4.20196800	3.39982100	-1.12975100
C	5.01596200	3.02634100	-2.18990000
C	4.99083600	1.70978500	-2.62892000
C	4.12693100	0.82025400	-2.00576700
N	3.31539500	1.18501600	-1.01232100
H	5.67821000	3.75398600	-2.65202500
H	4.23728100	4.41546500	-0.74673000
H	5.63004200	1.36746900	-3.43727000
H	4.08536700	-0.22554900	-2.30366300
C	2.54171200	2.72237500	0.63955300
C	2.39669200	3.98334200	1.21154900
C	1.21898100	1.77368400	2.28889500
C	1.64085100	4.11726000	2.36762700
H	2.86402800	4.85486200	0.76253600
H	0.75773400	0.86039900	2.66618400
H	1.51969400	5.09406900	2.82904100
C	1.04701600	2.99291500	2.92741400
H	0.46127000	3.05454700	3.84003900
N	1.94588200	1.64505300	1.18084100
Ni	2.04906500	-0.07861400	0.07929100
C	2.02066500	-2.81343300	-3.14572100
C	2.04309000	-1.63860700	-2.39219100
C	2.03070700	-1.71794600	-1.00393700
C	1.95892200	-2.94870300	-0.36472300
C	1.91006800	-4.11581700	-1.12856000
C	1.95337900	-4.05314500	-2.51714600
H	2.03267200	-2.74636200	-4.23273000

H	2.02837800	-0.67922000	-2.90583200
H	1.95764800	-3.01735500	0.72012400
H	1.85104600	-5.07782800	-0.62025900
H	1.92847600	-4.96620000	-3.10919600
Br	0.09986000	0.62828700	-1.01025500
Br	3.86128500	-0.87488000	1.28124200

3_h^{Ni} **HF =** −12081.4367568 hartree

C	-2.85749800	2.12174500	0.35407400
C	-3.08350900	3.31215400	1.03967000
C	-2.81056700	3.36879900	2.40052300
C	-2.31656400	2.24034200	3.04392600
C	-2.11515800	1.08918900	2.29399100
N	-2.37550600	1.03754100	0.98849600
H	-2.98723200	4.28870800	2.95279600
H	-3.48137800	4.18329900	0.52725800
H	-2.09156500	2.24234900	4.10698600
H	-1.73972000	0.17009000	2.74719500
C	-3.14452300	1.93860100	-1.08367000
C	-3.56622700	2.96034900	-1.92842000
C	-3.20920500	0.40457500	-2.83006100
C	-3.81541300	2.67007700	-3.26414900
H	-3.69544400	3.97313500	-1.55768200
H	-3.03845800	-0.63224300	-3.12025100
H	-4.14444000	3.45720800	-3.93803500
C	-3.63764700	1.37265900	-3.72788500
H	-3.82191100	1.10966400	-4.76526800
N	-2.97218500	0.68667200	-1.54871900
Ni	-2.31448900	-0.65798400	-0.17128700
C	0.48157500	-0.87097600	4.13056900
C	1.26022200	-0.41427000	3.06152500
C	1.02655700	-0.88795300	1.77286300
C	0.03786500	-1.85373500	1.57224700
C	-0.72533700	-2.31457500	2.64426400
C	-0.51343400	-1.81939900	3.92932900
H	0.67483500	-0.47841300	5.12793600
H	2.05219000	0.30305800	3.26177500
H	-0.14394900	-2.28094100	0.58849300
H	-1.49114200	-3.06812100	2.45627200
H	-1.11082900	-2.17807100	4.76524200
Br	-2.01423400	-2.70836700	-1.41091000
Br	-4.47440000	-1.28670200	0.74163500
C	3.14035000	2.10512400	-1.24147900
C	3.92832000	2.82943300	-2.13263200
C	4.72085000	2.15046800	-3.04619300
C	4.71942200	0.76276600	-3.03527200

C	3.91541600	0.10846600	-2.11374800
N	3.12916400	0.75802200	-1.25260800
H	5.34259700	2.70210300	-3.74672200
H	3.94194900	3.91466100	-2.10439700
H	5.33601000	0.18648900	-3.71871200
H	3.90144100	-0.97730900	-2.05497000
C	2.30358700	2.74807300	-0.21500600
C	2.05414700	4.11818700	-0.19845000
C	0.99287400	2.44345400	1.66260500
C	1.25181000	4.65141900	0.79934400
H	2.46819500	4.76629300	-0.96485200
H	0.56960500	1.73901400	2.37601600
H	1.04692100	5.71862700	0.82480400
C	0.71190500	3.79923500	1.75195200
H	0.07560600	4.16750000	2.55219600
N	1.77440900	1.92743400	0.71343300
Ni	2.04255600	-0.11666000	0.29500300
C	2.21435600	-3.62959800	-2.00611700
C	2.00041800	-2.32621600	-1.55010800
C	2.32569500	-1.98516000	-0.23949100
C	2.83133900	-2.96171900	0.61764500
C	3.02872300	-4.26131100	0.15752800
C	2.72512500	-4.60172100	-1.15714900
H	1.95988900	-3.87330600	-3.03681700
H	1.57034000	-1.60147300	-2.23521200
H	3.07286600	-2.72674300	1.65038800
H	3.42386400	-5.00976500	0.84310100
H	2.88106500	-5.61826800	-1.51342700
Br	0.06834900	0.16411500	-0.95062700
Br	4.04596600	-0.14807600	1.43231100

$TS3_h^{Ni}$ **HF =** −12081.4305083 hartree $\nu^{\ddagger} = -214.69\ icm^{-1}$

C	-2.80602100	1.94534500	0.72893000
C	-3.06433700	2.99802800	1.60306700
C	-2.78062900	2.83783900	2.95305800
C	-2.24156200	1.63672600	3.39750200
C	-2.00921700	0.63379100	2.46625100
N	-2.28287800	0.78760900	1.17110200
H	-2.98373500	3.64565900	3.65192900
H	-3.49921400	3.92589500	1.24250200
H	-2.00737400	1.47011700	4.44526900
H	-1.59952400	-0.33386800	2.75987300
C	-3.11786500	1.99188400	-0.71335500
C	-3.52001300	3.14476400	-1.37980000
C	-3.26629100	0.75013500	-2.67216800
C	-3.80489600	3.07336100	-2.73735600

H	-3.60198400	4.09174600	-0.85392700
H	-3.13332900	-0.23303200	-3.12383800
H	-4.11732300	3.96515000	-3.27500300
C	-3.68190700	1.85776800	-3.39852800
H	-3.89613300	1.76361100	-4.45897800
N	-2.99381400	0.82206500	-1.36900100
Ni	-2.27860800	-0.72059600	-0.23964800
C	0.64537200	-1.70788400	3.82260200
C	1.44564300	-1.14850400	2.82201700
C	1.15453700	-1.37783300	1.47387300
C	0.08365400	-2.22641900	1.15822500
C	-0.69515000	-2.79522500	2.16039700
C	-0.42584500	-2.53189000	3.50305000
H	0.88083100	-1.49148800	4.86372000
H	2.29318400	-0.53346900	3.11185100
H	-0.13489000	-2.49094700	0.12620500
H	-1.51332500	-3.45646700	1.87425100
H	-1.03494100	-2.97662500	4.28734700
Br	-2.10852300	-2.55330100	-1.82237700
Br	-4.39475700	-1.46943000	0.68274200
C	2.72371400	2.33812600	-1.23507600
C	3.24573500	3.17446900	-2.21791400
C	3.96465600	2.61416600	-3.26562600
C	4.15000200	1.23811400	-3.30746300
C	3.59815800	0.46776700	-2.29255600
N	2.90305400	1.00826900	-1.29519600
H	4.37965800	3.25247700	-4.04162000
H	3.10127400	4.24995400	-2.17079200
H	4.70954100	0.76383800	-4.10845300
H	3.70612300	-0.61794800	-2.26921500
C	1.96932900	2.82343200	-0.06106700
C	1.69484700	4.16730700	0.17574300
C	0.93188200	2.21397700	1.92134600
C	1.01733300	4.52401500	1.33404300
H	2.00935300	4.93154900	-0.52906500
H	0.66027500	1.39139000	2.58551600
H	0.79904500	5.56949200	1.53717800
C	0.63578700	3.53475900	2.23145200
H	0.12338700	3.77669300	3.15836200
N	1.57366900	1.87664500	0.80684800
Ni	2.02383700	-0.07988500	0.25988800
C	2.65699000	-3.57006900	-1.88958000
C	2.07278800	-2.44028500	-1.31752700
C	2.52147900	-1.96507500	-0.08030600
C	3.50347400	-2.68886600	0.60276800
C	4.07324000	-3.81970500	0.02754600

C	3.66320900	-4.26143900	-1.22706500
H	2.30413200	-3.90716700	-2.86324200
H	1.26664600	-1.94218200	-1.84765900
H	3.82981500	-2.38056700	1.59118800
H	4.84023700	-4.36275600	0.57772600
H	4.11195600	-5.14646300	-1.67399800
Br	0.05167700	0.11726200	-1.04073800
Br	4.02906300	0.28922100	1.38382900

$Ni^{III}(bpy)Br_2(OTf)$ **HF =** − 6770.4712195 hartree

C	-2.35258100	1.44167200	-0.71990300
C	-3.46280700	1.98027400	-1.36009900
C	-4.27907600	1.14598000	-2.11320500
C	-3.97448400	-0.20526000	-2.20192900
C	-2.84764200	-0.67297200	-1.54188600
N	-2.05412300	0.12970100	-0.82833500
H	-5.14792200	1.55325500	-2.62395900
H	-3.69086200	3.03914700	-1.28309900
H	-4.59064900	-0.89088000	-2.77553000
H	-2.55777500	-1.72152300	-1.57247800
C	-1.43310100	2.23418900	0.12002800
C	-1.63403500	3.57273100	0.43910000
C	0.50617000	2.17184600	1.40062100
C	-0.72070100	4.21141300	1.26833900
H	-2.49495900	4.11398000	0.05913800
H	1.33588100	1.55981500	1.74786800
H	-0.86432100	5.25710900	1.52813400
C	0.36571500	3.50286600	1.76456800
H	1.09431700	3.96575100	2.42302600
N	-0.36659700	1.56426200	0.59428100
O	4.00062100	-1.24631100	0.10659900
S	2.78178400	-0.66750000	-0.44672200
O	1.70132400	-0.50830500	0.58983400
O	2.30301500	-1.17824800	-1.72981100
C	3.21323300	1.08459400	-0.79642700
F	4.19936100	1.13842800	-1.67899300
F	3.59387200	1.69676100	0.31790600
F	2.15688400	1.72336400	-1.29290700
Br	-0.43564100	-2.81955600	-0.30458800
Ni	-0.28175100	-0.39656900	0.08156600
Br	-1.18244700	-1.38954400	2.12163700

$4^{Pd'}$ **HF =** − 2431.7162449 hartree

C	-2.26684200	-1.15907300	-1.75623100
C	-3.49167200	-1.76520400	-2.04130000
C	-4.15599900	-2.47412600	-1.04646800

C	-3.59176100	-2.59015000	0.22046900
C	-2.37275000	-1.97087000	0.49033200
C	-1.68434600	-1.23457300	-0.48413200
H	-1.75765900	-0.61731700	-2.55792000
H	-3.94197400	-1.69484700	-3.03229800
H	-4.12439800	-3.15317500	0.98833400
H	-1.95906400	-2.05742300	1.49843200
O	-5.38198600	-3.04958800	-1.31224900
C	-5.27432200	-4.38195700	-1.77046400
H	-4.78601000	-5.02440300	-1.02074700
H	-6.28883400	-4.75017200	-1.95214300
H	-4.69709000	-4.43640100	-2.70707600
P	2.22883900	0.64215700	0.51278000
P	-1.12188400	1.59779700	0.83186500
C	2.14540200	2.20203300	1.50202200
H	3.14118600	2.41520700	1.91586000
H	1.93823000	3.00324800	0.77508300
C	1.06619800	2.18863700	2.59058900
H	1.38766600	2.83504400	3.41905800
H	0.95842200	1.17972300	3.02320900
C	-0.28832300	2.69032500	2.10007700
H	-0.97868100	2.81357100	2.94491800
C	-2.69478900	1.15393300	1.65536300
C	-3.91675800	1.20036300	0.98115200
C	-2.65259600	0.63493900	2.95347000
H	-3.96349800	1.58728100	-0.03693700
C	-5.07924600	0.75375200	1.60191300
C	-3.81496900	0.18984500	3.57335000
H	-1.70229700	0.56803500	3.48726800
H	-6.02710500	0.80089600	1.06846900
C	-5.03180500	0.25046200	2.89857700
H	-3.76976400	-0.20598200	4.58636400
H	-5.94222000	-0.09697300	3.38340800
C	-1.61596900	2.78295500	-0.47088300
C	-1.30015900	2.50582000	-1.80255600
C	-2.29214200	3.96959400	-0.16193100
H	-0.78372700	1.57470900	-2.04307800
C	-1.64439900	3.40203400	-2.81203000
C	-2.63779200	4.86229300	-1.16851800
H	-2.55774600	4.19291700	0.87231600
H	-1.39074600	3.17750700	-3.84632600
C	-2.31193800	4.57962500	-2.49439500
H	-3.16377900	5.78210700	-0.91992900
H	-2.58214200	5.28135500	-3.28126700
C	3.23895400	1.17949200	-0.91594800
C	2.60823000	1.39687800	-2.14337900

C	4.60513800	1.45040800	-0.79067500
H	1.54386200	1.17703800	-2.24392100
C	3.32966400	1.87868500	-3.23187300
C	5.32625500	1.92861600	-1.87894700
H	5.10855300	1.28223400	0.16222200
H	2.82981600	2.04165000	-4.18488500
C	4.68932800	2.14259700	-3.09968800
H	6.38977100	2.13559300	-1.77469000
H	5.25682600	2.51457900	-3.95072000
C	3.36787700	-0.43050800	1.46424700
C	3.69379700	-0.18811300	2.80163500
C	3.89141200	-1.56750900	0.83427300
H	3.30655100	0.68907800	3.31842200
C	4.52626000	-1.06387500	3.49526600
C	4.72511200	-2.43636400	1.52669100
H	3.63905900	-1.77507300	-0.20632700
H	4.77321700	-0.86022100	4.53559500
C	5.04302500	-2.18781500	2.86037000
H	5.12364000	-3.31514800	1.02200900
H	5.69384800	-2.87061400	3.40337600
H	-0.16507900	3.68330900	1.64483200
Pd	0.09060000	-0.29085300	-0.01059600
C	1.67217100	-4.32011900	-0.39394100
C	1.02033000	-3.16779100	0.04381500
C	0.95049900	-2.01457800	-0.75037100
C	1.53347500	-2.07863800	-2.02341300
C	2.18503500	-3.22963700	-2.47160200
C	2.26472100	-4.35451700	-1.65439700
H	1.71739000	-5.19643400	0.25382800
H	0.56106600	-3.16769600	1.03600000
H	1.49865800	-1.20775100	-2.68344100
H	2.63579000	-3.24405600	-3.46463100
H	2.77641400	-5.25196500	-1.99978800

TS3$^{Pd'}$ **HF =** − 2431.698607 hartree $\nu^{\ddagger} = -277.39\ icm^{-1}$

C	-2.06336500	-1.33971600	-1.81557800
C	-3.38943500	-1.69357100	-2.04240400
C	-4.12437300	-2.31124600	-1.03334000
C	-3.52621600	-2.57744200	0.19586100
C	-2.20324300	-2.21193500	0.41671400
C	-1.43632500	-1.58168200	-0.57942100
H	-1.50001500	-0.86973100	-2.62446200
H	-3.86897900	-1.49273700	-3.00089700
H	-4.11368500	-3.06372900	0.97512400
H	-1.75427100	-2.43017600	1.38756700
O	-5.44541000	-2.64037200	-1.24105900

C	-5.61289900	-3.92097000	-1.81750500
H	-5.19747600	-4.70678700	-1.16728700
H	-6.68748600	-4.08656700	-1.94080500
H	-5.12213800	-3.98343300	-2.80129800
P	2.28051200	0.64724600	0.43519300
P	-1.07332500	1.63622900	0.86750100
C	2.19925300	2.22763300	1.39443300
H	3.20289500	2.50807300	1.74471400
H	1.90615300	2.99944800	0.66441800
C	1.18665500	2.17604100	2.54771000
H	1.55363100	2.79991200	3.37508800
H	1.11528000	1.15354400	2.95633600
C	-0.20502300	2.67384200	2.16445800
H	-0.84806200	2.72433300	3.05349100
C	-2.64608900	1.18114000	1.68794200
C	-3.86969700	1.23951700	1.01564800
C	-2.60214600	0.60619700	2.96378200
H	-3.92010700	1.66681400	0.01368300
C	-5.02827900	0.75418300	1.61555500
C	-3.76078100	0.12660500	3.56427800
H	-1.65066300	0.52431200	3.49403300
H	-5.97527900	0.81017800	1.08107100
C	-4.97874400	0.20277200	2.89219100
H	-3.71212100	-0.30928400	4.56073600
H	-5.88601900	-0.17285700	3.36166900
C	-1.57639000	2.88393000	-0.37703800
C	-1.26802400	2.65361800	-1.71983800
C	-2.24555900	4.06246400	-0.02469700
H	-0.75390400	1.73059100	-1.99602600
C	-1.61250700	3.58649900	-2.69602400
C	-2.59100800	4.99230100	-0.99730300
H	-2.50525100	4.24962500	1.01832300
H	-1.36451800	3.39779300	-3.73893300
C	-2.27251000	4.75544600	-2.33415600
H	-3.11116800	5.90558300	-0.71407400
H	-2.54251900	5.48623500	-3.09428900
C	3.28569500	1.14547500	-1.01619200
C	2.67211200	1.19475500	-2.27044500
C	4.62944500	1.51628800	-0.89795100
H	1.62724000	0.89073100	-2.36419400
C	3.38554800	1.61605400	-3.39008100
C	5.34274700	1.93347200	-2.01553700
H	5.12226800	1.47259500	0.07450800
H	2.89893700	1.65002100	-4.36322200
C	4.72066800	1.98490100	-3.26201500
H	6.38839800	2.21944800	-1.91591900

H	5.28191600	2.31030600	-4.13608200
C	3.44296800	-0.40162300	1.38606600
C	3.96258900	-0.06281200	2.63832100
C	3.77620600	-1.64301800	0.82742800
H	3.71830300	0.89349400	3.09990300
C	4.80465300	-0.94381900	3.31391500
C	4.62139800	-2.51715900	1.49888300
H	3.35954500	-1.92941800	-0.14053400
H	5.20423300	-0.66627200	4.28780400
C	5.13735200	-2.16913900	2.74607100
H	4.86965600	-3.47802900	1.04985800
H	5.79531700	-2.85552700	3.27594000
H	-0.12976000	3.69772500	1.77092200
Pd	0.10580500	-0.29031900	-0.00750400
C	1.57091900	-4.30217900	-0.09344000
C	0.78212000	-3.20560700	0.23966100
C	0.43852700	-2.23009900	-0.71393500
C	0.90771600	-2.42329100	-2.02659400
C	1.70074700	-3.51672500	-2.35899100
C	2.04116500	-4.46591000	-1.39481200
H	1.82687500	-5.03177100	0.67538100
H	0.42644700	-3.10293600	1.26706000
H	0.64756600	-1.70270700	-2.80469500
H	2.05592900	-3.62954100	-3.38352900
H	2.65606900	-5.32488100	-1.65784500

5$^{Pd'}$ **HF =** −2431.7659992 hartree

C	0.00252200	0.02995700	-2.74353400
C	-0.92981000	1.06430000	-2.86980400
C	-2.30728200	0.78359000	-2.91489300
C	-2.74936000	-0.53386500	-2.82771300
C	-1.81563900	-1.54950500	-2.61421600
C	-0.44426100	-1.30210100	-2.55274100
H	1.06325000	0.24075900	-2.87673900
H	-0.60520800	2.09222600	-3.02920700
H	-3.80566100	-0.78224900	-2.88602200
H	-2.17272700	-2.57439400	-2.50837900
O	-3.11587300	1.86230400	-3.05400700
C	-4.51023900	1.63352300	-3.09696200
H	-4.86184500	1.14868200	-2.17384000
H	-4.98008000	2.61554400	-3.18975700
H	-4.78807100	1.01506300	-3.96172100
P	1.94886100	1.11815600	0.64133700
P	-1.59115500	0.34162200	1.33571100
C	1.45616200	1.82289600	2.29054500
H	2.34861200	2.15671500	2.84067600

H	0.88510800	2.73545100	2.05756700
C	0.61771800	0.86830800	3.15184200
H	0.81762100	1.09912400	4.20834400
H	0.97411600	-0.16512800	3.01307000
C	-0.90100300	0.94132900	2.96174100
H	-1.40423100	0.40835500	3.78344600
C	-1.87769200	-1.45689100	1.60119300
C	-2.79751800	-2.10871600	0.76779500
C	-1.12487800	-2.22497400	2.49399300
H	-3.38351300	-1.52693000	0.05304000
C	-2.96242100	-3.48656600	0.82909200
C	-1.28172400	-3.60947600	2.54769500
H	-0.40795200	-1.74903100	3.16195800
H	-3.68535500	-3.97357300	0.17608600
C	-2.19804300	-4.24441100	1.71660500
H	-0.68618100	-4.19088300	3.24971400
H	-2.32074000	-5.32501900	1.76034600
C	-3.30457800	1.00937000	1.45300300
C	-3.74986200	1.89424200	0.46852600
C	-4.16458500	0.67534100	2.50565600
H	-3.08834500	2.14581800	-0.36506400
C	-5.02754700	2.44770800	0.53963000
C	-5.44026400	1.22235900	2.57511600
H	-3.83672400	-0.02671600	3.27385200
H	-5.36328800	3.14021300	-0.23123900
C	-5.87201500	2.11222700	1.59258700
H	-6.10187100	0.95501300	3.39743900
H	-6.87109800	2.54088000	1.64804600
C	3.00260200	2.49300500	0.00498300
C	2.46345700	3.29701600	-1.00372300
C	4.27944300	2.78725800	0.49356100
H	1.47070600	3.05922400	-1.39571400
C	3.17688100	4.38078100	-1.50844100
C	4.99888000	3.86275400	-0.01746900
H	4.72130400	2.16655800	1.27432100
H	2.74347100	4.99969300	-2.29231300
C	4.44794100	4.66210800	-1.01695700
H	5.99485000	4.07880600	0.36595200
H	5.01363800	5.50248600	-1.41546300
C	3.18035100	-0.17449500	1.09888300
C	3.86607600	-0.21982700	2.31841000
C	3.43082200	-1.17667900	0.15395900
H	3.68503800	0.53604800	3.08252400
C	4.78626400	-1.23121700	2.57861700
C	4.35856200	-2.18177900	0.40808700
H	2.88168300	-1.17703200	-0.79215900

H	5.30854100	-1.25273400	3.53367200
C	5.03818200	-2.21114600	1.62254800
H	4.53691900	-2.95098300	-0.34238200
H	5.75748700	-3.00192500	1.82803100
H	-1.22137300	1.99252100	3.03321500
Pd	-0.07833200	0.60231200	-0.42845100
C	1.13879800	-4.38606800	-1.05205100
C	0.23088700	-3.37028600	-1.32847000
C	0.51890300	-2.39082800	-2.28930000
C	1.74459300	-2.45895100	-2.96219600
C	2.65214600	-3.47716700	-2.68734200
C	2.35349800	-4.44515800	-1.73143600
H	0.89565900	-5.13030300	-0.29442000
H	-0.70933200	-3.31790600	-0.77510000
H	1.98196700	-1.71638700	-3.72437500
H	3.59687000	-3.51733100	-3.22768900
H	3.06562400	-5.23991500	-1.51552900

4_h^{Ni} **HF =** −6272.1195786 hartree

C	2.46087400	3.30791300	1.12585300
C	1.49381300	2.30084600	1.06290800
C	1.56337100	1.32078300	0.07465900
C	2.62807600	1.34175300	-0.82709400
C	3.59660100	2.33898600	-0.74803900
C	3.51609300	3.33118300	0.22462900
H	2.37782000	4.06922400	1.90057300
H	0.69621800	2.29869900	1.80063200
H	2.72166700	0.57802000	-1.59406400
H	4.42112100	2.33271900	-1.45989600
H	4.27376000	4.11055200	0.28263400
C	-2.70160300	0.73554600	-0.02454000
C	-3.87163600	1.48410900	-0.12954600
C	-3.79128500	2.86658300	-0.19805400
C	-2.54055100	3.46761100	-0.17837500
C	-1.41844800	2.65805900	-0.07897800
N	-1.49352000	1.32973500	0.01877100
H	-4.69622700	3.46354400	-0.27775600
H	-4.84085800	0.99675200	-0.17339400
H	-2.42529000	4.54529600	-0.24727500
H	-0.41752400	3.08477600	-0.08277000
C	-2.70162900	-0.73552100	0.02444600
C	-3.87169300	-1.48402600	0.12951700
C	-1.41856800	-2.65809100	0.07880800
C	-3.79140900	-2.86650500	0.19801500
H	-4.84088800	-0.99662200	0.17342700
H	-0.41767300	-3.08486900	0.08255300

H	-4.69637500	-3.46342000	0.27777900
C	-2.54070700	-3.46759000	0.17825800
H	-2.42549100	-4.54528100	0.24714300
N	-1.49356900	-1.32976200	-0.01892900
Ni	0.12132600	-0.00001700	-0.00001300
C	1.49399800	-2.30079800	-1.06290500
C	2.46109200	-3.30783400	-1.12578700
C	3.51619500	-3.33113200	-0.22442700
C	3.59655800	-2.33898500	0.74830300
C	2.62799800	-1.34178100	0.82729200
C	1.56339200	-1.32079800	-0.07458200
H	0.69650600	-2.29860800	-1.80074100
H	2.37816600	-4.06909800	-1.90056800
H	4.42099400	-2.33273500	1.46025800
H	2.72147700	-0.57808200	1.59430700
H	4.27388900	-4.11047800	-0.28238100
Br	0.02941600	-0.26917600	2.30036300
Br	0.02967000	0.26913100	-2.30039700

$TS3_h^{Ni'}$ **HF =** −6272.11233 hartree $\nu^{\ddagger} = -215.90\ icm^{-1}$

C	2.82282200	3.00024400	0.98428000
C	1.95603700	1.90869200	1.04851700
C	1.78142700	1.07349000	-0.06104200
C	2.55568300	1.31575400	-1.20242300
C	3.42827400	2.39616100	-1.25225500
C	3.56063800	3.25463000	-0.16394200
H	2.91563500	3.64854600	1.85461200
H	1.41320700	1.72540600	1.97109100
H	2.48935300	0.65602100	-2.06203500
H	4.01674300	2.55886500	-2.15418100
H	4.24228400	4.10194100	-0.20751100
C	-2.70491400	0.73706100	0.05250300
C	-3.86198500	1.50933700	0.10265800
C	-3.74682300	2.89011100	0.19942600
C	-2.48421900	3.46806900	0.24249900
C	-1.37586500	2.63335800	0.18616700
N	-1.49200200	1.31198800	0.09696400
H	-4.64009700	3.50857200	0.23816800
H	-4.84424400	1.04679900	0.06642900
H	-2.35424900	4.54385900	0.31629600
H	-0.35693400	3.02336000	0.21423500
C	-2.70493200	-0.73704700	-0.05249900
C	-3.86202600	-1.50928300	-0.10271000
C	-1.37594300	-2.63339600	-0.18605200
C	-3.74691000	-2.89006200	-0.19944500
H	-4.84427200	-1.04671000	-0.06655200

H	-0.35702600	-3.02343700	-0.21405000
H	-4.64020500	-3.50849200	-0.23823000
C	-2.48432500	-3.46806800	-0.24242400
H	-2.35438900	-4.54386400	-0.31618300
N	-1.49203500	-1.31201800	-0.09688900
Ni	0.11840700	-0.00003500	0.00001700
C	1.95611600	-1.90866100	-1.04854700
C	2.82300900	-3.00013000	-0.98435900
C	3.56092300	-3.25443600	0.16381700
C	3.42853800	-2.39598000	1.25213800
C	2.55583700	-1.31566000	1.20235600
C	1.78149500	-1.07346900	0.06101700
H	1.41322000	-1.72542700	-1.97109300
H	2.91583500	-3.64842300	-1.85469600
H	4.01708200	-2.55862100	2.15402600
H	2.48949200	-0.65593400	2.06197300
H	4.24266200	-4.10167500	0.20734300
Br	-0.16235800	-0.21663400	2.31893600
Br	-0.16245300	0.21652300	-2.31890000

5_h^{Ni} **HF =** −6272.1872546 hartree

C	0.57266700	2.97705100	0.96216700
C	1.35278100	1.80677000	0.97179600
C	2.26359200	1.54906300	-0.07952100
C	2.35451000	2.47850400	-1.12281800
C	1.58487900	3.63125100	-1.11145500
C	0.68339300	3.88468400	-0.07352100
H	-0.09693200	3.17177800	1.79815200
H	1.39689200	1.21383400	1.88213400
H	3.06000500	2.30134300	-1.93349300
H	1.68759400	4.35021400	-1.92247700
H	0.08287600	4.79162600	-0.08040100
C	-3.04216400	-0.45006900	0.30273900
C	-4.40068400	-0.26221400	0.04543000
C	-5.04333200	0.82914200	0.61590400
C	-4.31625000	1.69477100	1.42167800
C	-2.96480800	1.42831900	1.61729600
N	-2.33880600	0.38777600	1.07519900
H	-6.09910300	1.00433200	0.42219900
H	-4.94556400	-0.93305400	-0.61387300
H	-4.77904200	2.56172900	1.88579100
H	-2.35625000	2.08360200	2.24155500
C	-2.30107000	-1.57207000	-0.31813300
C	-2.94136800	-2.74449100	-0.71870500
C	-0.27156900	-2.39628500	-1.12054100
C	-2.22022700	-3.74757100	-1.34711000

H	-4.00170600	-2.87335400	-0.52013300
H	0.79489400	-2.20982000	-1.23938400
H	-2.71630600	-4.66307500	-1.65932200
C	-0.85962300	-3.56750000	-1.56485600
H	-0.25444300	-4.32183700	-2.05846700
N	-0.97503500	-1.43315800	-0.51065900
Ni	-0.01829500	0.08411700	0.12448500
C	3.22832000	-0.44221700	-1.22151800
C	4.00397300	-1.59619500	-1.21612300
C	4.71257200	-1.95537800	-0.07170700
C	4.64084200	-1.15608200	1.06594800
C	3.84846900	-0.01389700	1.06782200
C	3.13314700	0.35396100	-0.07428800
H	2.66265900	-0.16614600	-2.11299700
H	4.05475500	-2.21726200	-2.10881600
H	5.20078400	-1.42691400	1.95929900
H	3.78701900	0.60508200	1.96249600
H	5.32448900	-2.85558600	-0.06899500
Br	0.66603900	-1.22375300	1.90858800
Br	-0.75751900	1.22857000	-1.72154700