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Supporting Information

Halide Abstraction Competes with Oxidative Addition in the Reactions of Aryl Halides with $[\text{Ni}(\text{PMe}_n\text{Ph}_{(3-n)})_4]$

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COMPUTATIONAL DETAILS

Calculations were performed using Gaussian09 (Rev. D01)¹ at the B3LYP level of theory^{2,3,4} with Grimme's D3 dispersion correction.⁵ This correction renders B3LYP appropriate for studying organometallic chemistry.⁶ For optimizations and frequency calculations, the 6-31G(d) basis set^{7,8,9} was used for H, C, N, O, P, and Cl atoms, and the LANL2DZdp basis set/ECP¹⁰ used for Br and I, and LANL2LTZ(f)^{11,12,13} for Ni. The potential energies were refined using the same basis set for Br, I and Ni, and increasing the basis set for H, C, N, O, P and Cl, using 6-311+G(d,p).¹⁴ The solvent is experimentally significant, so all calculations were carried out in solvent (using the SMD method for implicit solvation), unless otherwise stated. Unless otherwise stated all calculations were carried out on THF. Toluene and *n*-hexane were used in specific cases (see the manuscript text for discussion of solvent effects).

The nature of each stationary point was verified using frequency analyses, and IRC calculations were used to verify that transition states linked the relevant minima. Free energy corrections were computed at 298 K and 1 atm. All energies quoted are Gibbs free energies in solution, in kcal mol⁻¹. Enthalpies are given in the schemes, in brackets, in kcal mol⁻¹.

In the case of open-shell singlet structures, where S^2 is not zero, we corrected the energy by applying the Yamaguchi's equation,^{15,16,17,18} in the form:¹⁹

$$E_{singlet} = \frac{2E_{OSS} - E_{triplet}\langle S^2 \rangle_{OSS}}{2 - \langle S^2 \rangle_{OSS}}$$

where E_{OSS} is the energy of open-shell singlet calculation, $E_{triplet}$ is the energy of the triplet state at the open-shell singlet geometry and $\langle S^2 \rangle_{OSS}$ is the S^2 value of the open-shell singlet calculation.

PEt₃ has a number of possible conformations, so the ligands were truncated to PMe₃, which has similar properties (Tolman electronic parameter = 2064.1 cm⁻¹ for PMe₃, 2061.7 cm⁻¹ for PEt₃; cone angle = 118° for PMe₃, 132° for PEt₃).²⁰ Tolman determined that both ligands undergo fast ligand exchange at a Ni⁰ centre in benzene or toluene solution, although PEt₃ has a slightly greater propensity for dissociation.²¹

BENCHMARK OF FUNCTIONALS

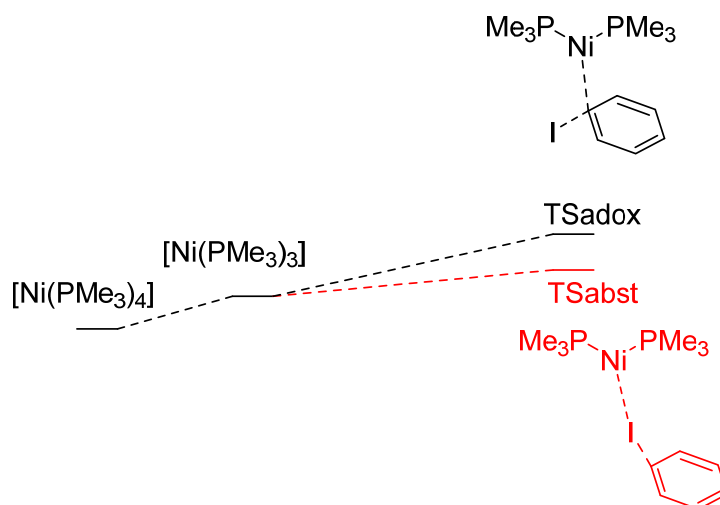


Table S1. Comparison of four different functionals on the key step of Ni(0) oxidation with PhI. Free energies in kcal/mol.

Method*	$\text{Ni}(\text{PMe}_3)_4$	$\text{Ni}(\text{PMe}_3)_3$	TSadox	TSabst
B3LYP-D3	0.0	7.8	16.2	10.0
TPSSH-D3	0.0	13.4	16.2	14.8
ω B97X-D	0.0	10.1	21.5	11.4
PBE1PBE-D3	0.0	12.2	19.4	11.4

* Single point energies on B3LYP-D3 geometries using the LANL2DZdp basis set/ECP for I, LANL2LTZ(f) for Ni and 6-311+G(d,p) for the rest of atoms, with free energy corrections from B3LYP-D3 calculations.

The evaluation of different functionals in the key step with PhI and PMe_3 as ligand shows minor differences among all of them. The open-shell single electronic structure for the halogen abstraction transition state was found to be the most stable electronic structure in all the cases (using the wavefunction stability evaluation of g09). We selected B3LYP-D3 as the functional because the dissociation energy of the phosphine was the most consistent with experimental data and the evaluation of the product ratio provides a full agreement with the experimental observations.

PHOSPHINE DISSOCIATION POTENTIAL ENERGY RELAXED SCAN FROM Ni(PMe₃)₄

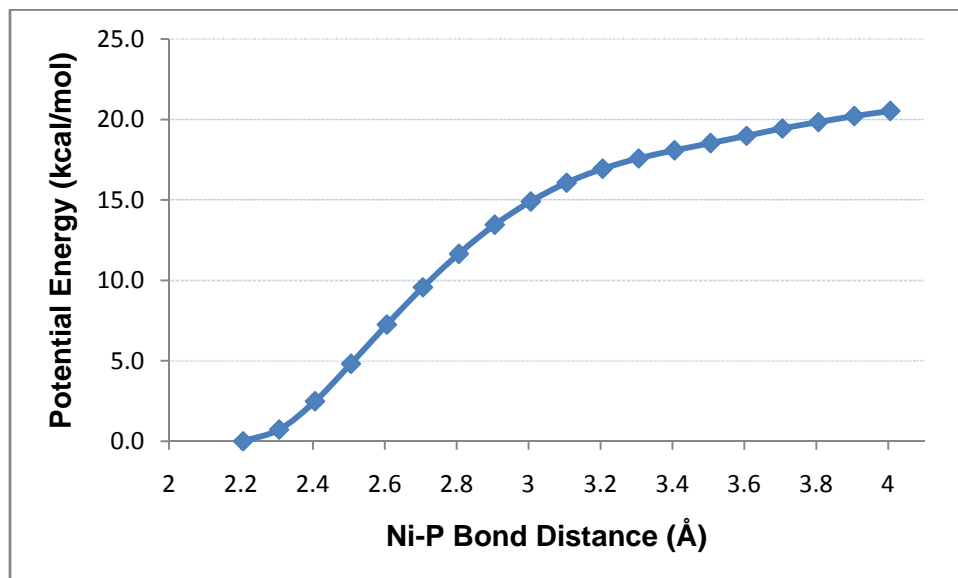


Figure S1. Potential energy relaxed scan for the phosphine dissociation in Ni(PMe₃)₄ complex.

According to the scan, there is no activation barrier for the phosphine dissociation in Ni(PMe₃)₄ complex.

ALTERNATIVE MECHANISMS

(A) Outer-sphere electron transfer from $[\text{Ni}(\text{PMe}_3)_4]$ to ArX

Electron transfer from $[\text{Ni}(\text{PMe}_3)_4]$ to ArX could in theory occur *via* an outer sphere mechanism, to form $[\text{Ni}(\text{PMe}_3)_4]^+$ and the radical anion of ArX; the latter would then spontaneously dissociate X^- to form an aryl radical. This was explored using Marcus-Hush theory, where the barrier to electron transfer can be estimated using equations S1-S3. This assumes that the major energetic barrier is the rearrangement of the products immediately following the electron transfer event. This has been successfully used to describe the reactions of aryl halides with 'super electron donors'.²²

$$\Delta G^\ddagger \approx (\lambda_i/4) \cdot (1 + \Delta G/\lambda_i)^2 \quad (\text{S1})$$

$$\lambda_i = (1/2) \cdot (\lambda_i(\text{NiP4}^+) + \lambda_i(\text{ArX})) \quad (\text{S2})$$

$$\lambda_i (\text{species}) = (E_N(\text{R}_C) - E_N(\text{R}_N)) + (E_C(\text{R}_N) - E_C(\text{R}_C)) \quad (\text{S3})$$

- λ_i is the internal reorganisation energy; $\lambda_i(\text{NiP4}^+)$ is the internal reorganisation energy of $[\text{Ni}(\text{PMe}_3)_4]^+$; and $\lambda_i(\text{ArX})$ is the internal reorganisation energy of ArX radical anion
- ΔG is the free energy change of the reaction
- $E_N(\text{R}_N)$ and $E_C(\text{R}_C)$ are the energies of the neutral and charged species in their respective geometries; $E_C(\text{R}_N)$ and $E_N(\text{R}_C)$ are the single point energies of the neutral and charged geometries as charged and neutral species, respectively.

While the initial result with $[\text{Ni}(\text{PMe}_3)]_4$ and PhI in THF was sensible ($\Delta G^\ddagger = 15.6 \text{ kcal mol}^{-1}$), barriers for PhBr and in toluene and hexane were far too high to account for the Ni^{I} products observed, albeit in reduced quantities, in these reactions (see Table S2). The major contributor to these energies was the very large value of ΔG for this process in non-polar solvents.

Table S2. Calculated energies for outer-sphere electron transfer from $[\text{Ni}(\text{PMe}_3)_4]$ to ArX.

Solvent	Aryl Halide	ΔG (kcal/mol)	λ_i (kcal/mol)	ΔG^\ddagger (kcal/mol)
THF	PhI	1.2	59.9	15.6
THF	PhBr	11.8	63.6	22.3
Toluene	PhI	29.8	56.8	33.0
Hexane	PhI	38.3	61.6	40.5

(B) Inner-sphere electron transfer from $[\text{Ni}(\text{PMe}_3)_3]$ to ArX

Inner-sphere electron transfer from $[\text{Ni}(\text{PMe}_3)_3]$ to ArX could occur *via* complex $[\text{Ni}(\text{PMe}_3)_3(\text{XAr})]$, with a concomitant change in multiplicity from singlet to triplet. This cannot be described by a simple transition state, and instead requires the geometry at which the singlet and triplet have the same energy to be located, termed the minimum energy crossing point (MECP).

The software tool published by Harvey was used, and the MECP could be located for a number of examples. However, the energies of MECPs for aryl bromides were too high to compete with oxidative addition to $[\text{Ni}(\text{PMe}_3)_2]$ (see Table S3). Energies are quoted as a range, because these structures typically have imaginary frequencies when either or both of the singlet and triplet frequency calculations are performed; there is a small discrepancy in their free energies, because the MECP calculation seeks the geometry at which the *potential energy E* is the same for both singlet and triplet.

Table S3. Calculated minimum energy crossing points for inner-sphere electron transfer from $[\text{Ni}(\text{PMe}_3)_4]$ to ArX.

Solvent	Aryl Halide	MECP G_{rel} (kcal/mol)
THF	PhI	15.0 – 15.2
THF	PhBr	22.5 – 22.6
Toluene	PhI	16.5 – 16.8
Toluene	PhBr	23.9 – 24.6
Hexane	PhI	16.7 – 17.1
Hexane	PhBr	24.7 – 26.0

(C) Oxidative Addition Pathway from $[\text{Ni}(\text{PMe}_3)_2]$

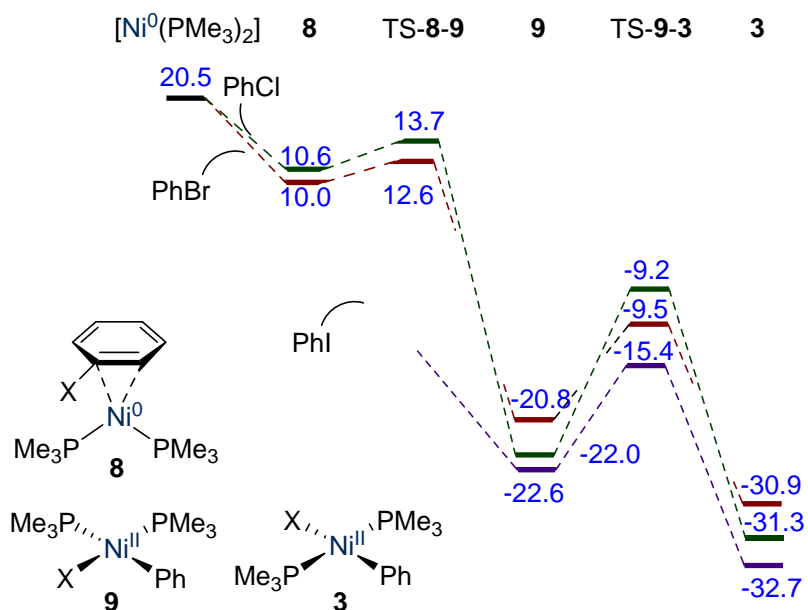


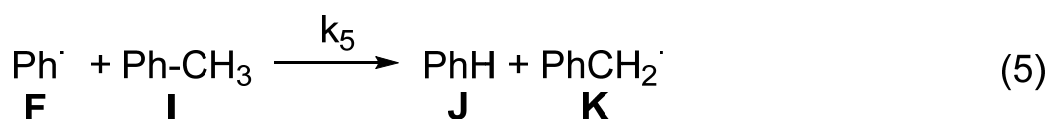
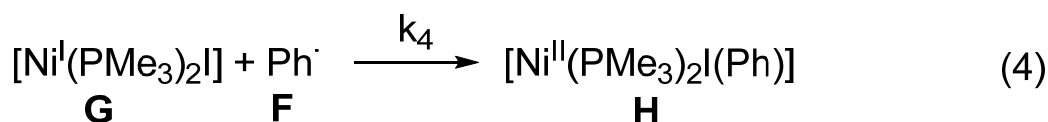
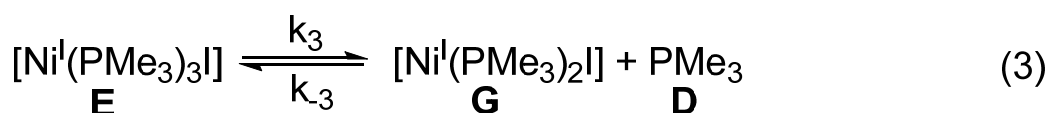
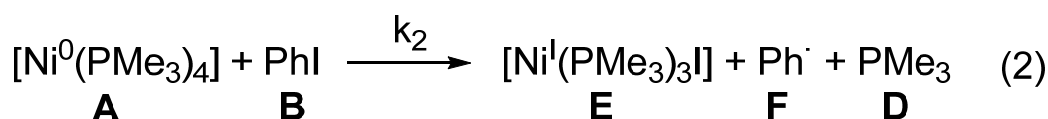
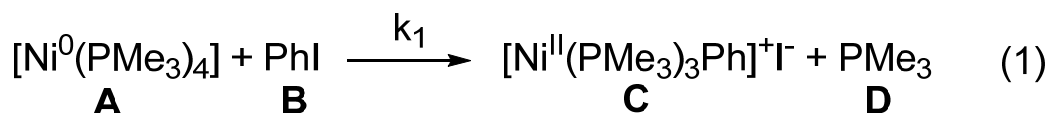
Figure S2. Oxidative addition of PhI (purple), PhBr (brown), and PhCl (green) to $[\text{Ni}(\text{PMe}_3)_2]$. Energies are in kcal mol⁻¹.

The dissociation energy of the second phosphine is always higher than the oxidative addition transition state from $[\text{Ni}(\text{PMe}_3)_3]$, so this mechanism is unfavourable in the three cases. We could not find the barrier for PhI oxidative addition, due to the high reactivity of this species with $\text{Ni}(\text{P})_2$, which forms the $\text{Ni}(\text{II})$ product **9** directly.

MICROKINETIC MODEL

(A) Reaction between $[\text{Ni}(\text{PMe}_3)_4]$ to PhI in toluene

We used the COPASI program package to run the reactions used in the microkinetic model, with the following equations:



The activation energies and the associated kinetic constants are in Table 4

Table S4. Calculated activation free energies and kinetic constants of kinetic model of the reaction between $[\text{Ni}(\text{PMe}_3)_4]$ and PhI in toluene.

Reaction	ΔG^\ddagger (kcal/mol)	Kinetic constant ($\text{M}^{-1}\cdot\text{s}$)
1	16.7	3.514
2	9.4	7.932e+5
3	10.0	2.784e+5
3(k_3)	3.7	1.18e+10
4 ¹	3.7	1.18e+10
5	10.6	1.046e+5

The reactions 3 and 4 are barrierless. For this reason, we considered them as diffusion-controlled, with the rate constant given by the equation $k_{\text{diff}} = 8k_bT/(3\eta) \cdot 1000 \cdot N_a$, in $\text{M}^{-1}\cdot\text{s}$.²³ The viscosity of toluene at 298 K is $0.560 \text{ mPa}\cdot\text{s}$.²⁴ The diffusion rate constant would correspond to an associated activation free energy of 3.7 kcal/mol, calculated from Eyring equation.

The conditions used to analyze the time course of the reaction were 0.01s in 20 steps, obtaining the results in Table S5. The initial concentrations were taken from the experiments (0.005 M for species

A and B and solvent concentration calculated from the density at 25°C (12.2 M for THF). The numbers represent the concentration of labelled species in mol per litre (Table S5).

Table S5. Concentrations of different species in solution during reaction time in mol/L for the reaction between $[\text{Ni}(\text{PMe}_3)_4]$ and PhI in toluene.

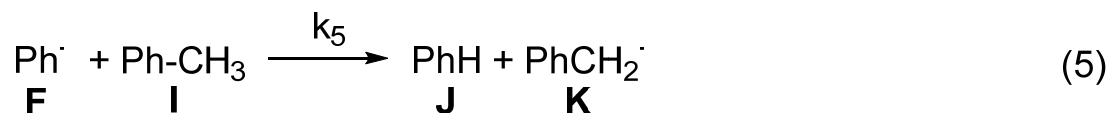
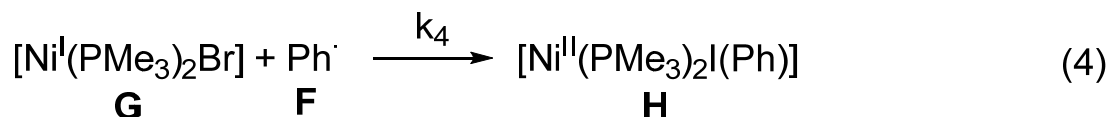
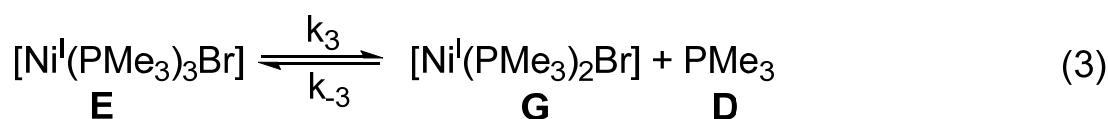
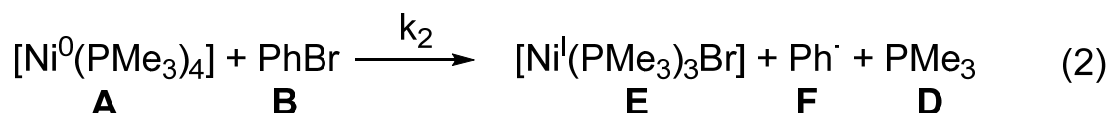
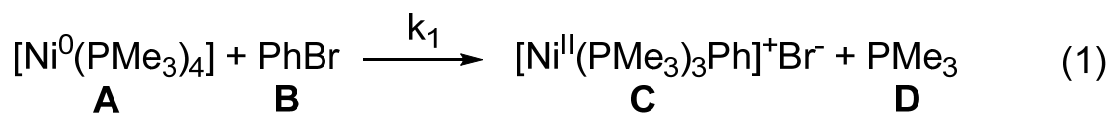
Time (s)	A	B	C	D	E	F	G	H	I	J	K
0	0.005	0	0	0	0	0	0	0	0	9.39	0
0.0005	1.68E-03	1.68E-03	1.47E-08	3.88E-03	2.76E-03	1.89E-06	1.68E-05	5.44E-04	9.39E+00	2.78E-03	2.78E-03
0.001	1.01E-03	1.01E-03	1.77E-08	4.67E-03	3.32E-03	6.83E-07	1.68E-05	6.57E-04	9.39E+00	3.34E-03	3.34E-03
0.0015	7.20E-04	7.20E-04	1.90E-08	5.00E-03	3.56E-03	3.49E-07	1.68E-05	7.05E-04	9.39E+00	3.58E-03	3.58E-03
0.002	5.60E-04	5.60E-04	1.97E-08	5.19E-03	3.69E-03	2.11E-07	1.68E-05	7.32E-04	9.39E+00	3.71E-03	3.71E-03
0.0025	4.58E-04	4.58E-04	2.01E-08	5.31E-03	3.78E-03	1.41E-07	1.68E-05	7.49E-04	9.39E+00	3.79E-03	3.79E-03
0.003	3.88E-04	3.88E-04	2.04E-08	5.39E-03	3.83E-03	1.01E-07	1.68E-05	7.61E-04	9.39E+00	3.85E-03	3.85E-03
0.0035	3.36E-04	3.36E-04	2.07E-08	5.45E-03	3.88E-03	7.60E-08	1.68E-05	7.69E-04	9.39E+00	3.89E-03	3.89E-03
0.004	2.96E-04	2.96E-04	2.08E-08	5.50E-03	3.91E-03	5.91E-08	1.68E-05	7.76E-04	9.39E+00	3.93E-03	3.93E-03
0.0045	2.65E-04	2.65E-04	2.10E-08	5.53E-03	3.94E-03	4.74E-08	1.68E-05	7.81E-04	9.39E+00	3.95E-03	3.95E-03
0.005	2.40E-04	2.40E-04	2.11E-08	5.56E-03	3.96E-03	3.88E-08	1.68E-05	7.86E-04	9.39E+00	3.97E-03	3.97E-03
0.0055	2.19E-04	2.19E-04	2.12E-08	5.59E-03	3.97E-03	3.23E-08	1.68E-05	7.89E-04	9.39E+00	3.99E-03	3.99E-03
0.006	2.02E-04	2.02E-04	2.13E-08	5.61E-03	3.99E-03	2.74E-08	1.68E-05	7.92E-04	9.39E+00	4.01E-03	4.01E-03
0.0065	1.87E-04	1.87E-04	2.13E-08	5.62E-03	4.00E-03	2.35E-08	1.68E-05	7.95E-04	9.39E+00	4.02E-03	4.02E-03
0.007	1.74E-04	1.74E-04	2.14E-08	5.64E-03	4.01E-03	2.03E-08	1.68E-05	7.97E-04	9.39E+00	4.03E-03	4.03E-03
0.0075	1.63E-04	1.63E-04	2.14E-08	5.65E-03	4.02E-03	1.78E-08	1.68E-05	7.99E-04	9.39E+00	4.04E-03	4.04E-03
0.008	1.53E-04	1.53E-04	2.15E-08	5.66E-03	4.03E-03	1.57E-08	1.68E-05	8.00E-04	9.39E+00	4.05E-03	4.05E-03
0.0085	1.44E-04	1.44E-04	2.15E-08	5.67E-03	4.04E-03	1.40E-08	1.68E-05	8.02E-04	9.39E+00	4.05E-03	4.05E-03
0.009	1.36E-04	1.36E-04	2.15E-08	5.68E-03	4.04E-03	1.25E-08	1.68E-05	8.03E-04	9.39E+00	4.06E-03	4.06E-03
0.0095	1.29E-04	1.29E-04	2.16E-08	5.69E-03	4.05E-03	1.12E-08	1.68E-05	8.04E-04	9.39E+00	4.07E-03	4.07E-03
0.01	1.23E-04	1.23E-04	2.16E-08	5.70E-03	4.05E-03	1.02E-08	1.68E-05	8.05E-04	9.39E+00	4.07E-03	4.07E-03

The ratio of Ni(I) vs Ni(II) (83:17 in this case) was obtained using the following formula:

$$\frac{[\text{Ni}(I)]}{[\text{Ni}(II)]} = \frac{[\text{Ph}I]}{[[\text{Ni}(II)(\text{PMe}_3)_3\text{Ph}]^+I^-] + [\text{Ni}(II)(\text{PMe}_3)_2(\text{Ph})I]}$$

(B) Reaction between [Ni(PMe₃)₄] to PhBr in THF

We ran the same microkinetic model for the reaction between Ni complex and PhBr in THF. The reactions were:



The activation energies and the associated kinetic constants are in Table S6:

Table S6. Calculated activation free energies and kinetic constants of kinetic model of the reaction between [Ni(PMe₃)₄] and PhBr in THF.

Reaction	ΔG^\ddagger (kcal/mol)	Kinetic constant (M ⁻¹ ·s)
1	15.0	62.015
2	16.3	6.904
3	6.0	2.471e+8
3(k ₋₃)	3.6	1.45e+10
4 ¹	3.6	1.45e+10
5	9.5	6.700e+5

The reactions 3 and 4 are also barrierless. We applied the same methodology that above, using the experimental value of 0.456 mPa·s for the viscosity of THF.²⁵ The associated activation free energy was calculated from Eyring equation and is 3.6 kcal/mol.

Table S7. Concentrations of different species in solution along reaction time in mol/L for the reaction between $[\text{Ni}(\text{PMe}_3)_4]$ and PhBr in THF.

Time (s)	A	B	C	D	E	F	G	H	I	J	K	
0	0.005	0.005	0	0	0	0	0	0	0	12.22	0	0
9	1.22E-03	1.22E-03	3.40E-03	4.10E-03	5.94E-05	8.72E-13	2.47E-04	7.23E-05	1.22E+01	3.06E-04	3.06E-04	
18	6.94E-04	6.94E-04	3.87E-03	4.66E-03	7.36E-05	2.75E-13	2.69E-04	8.88E-05	1.22E+01	3.43E-04	3.43E-04	
27	4.85E-04	4.85E-04	4.06E-03	4.89E-03	7.95E-05	1.33E-13	2.77E-04	9.56E-05	1.22E+01	3.57E-04	3.57E-04	
36	3.73E-04	3.73E-04	4.16E-03	5.01E-03	8.27E-05	7.83E-14	2.81E-04	9.93E-05	1.22E+01	3.64E-04	3.64E-04	
45	3.03E-04	3.03E-04	4.23E-03	5.08E-03	8.47E-05	5.15E-14	2.84E-04	1.02E-04	1.22E+01	3.69E-04	3.69E-04	
54	2.55E-04	2.55E-04	4.27E-03	5.13E-03	8.61E-05	3.64E-14	2.86E-04	1.03E-04	1.22E+01	3.72E-04	3.72E-04	
63	2.20E-04	2.20E-04	4.30E-03	5.17E-03	8.72E-05	2.71E-14	2.87E-04	1.04E-04	1.22E+01	3.74E-04	3.74E-04	
72	1.94E-04	1.94E-04	4.32E-03	5.20E-03	8.79E-05	2.10E-14	2.88E-04	1.05E-04	1.22E+01	3.76E-04	3.76E-04	
81	1.73E-04	1.73E-04	4.34E-03	5.22E-03	8.85E-05	1.67E-14	2.89E-04	1.06E-04	1.22E+01	3.78E-04	3.78E-04	
90	1.56E-04	1.56E-04	4.36E-03	5.24E-03	8.90E-05	1.36E-14	2.90E-04	1.07E-04	1.22E+01	3.79E-04	3.79E-04	
99	1.42E-04	1.42E-04	4.37E-03	5.25E-03	8.94E-05	1.13E-14	2.90E-04	1.07E-04	1.22E+01	3.80E-04	3.80E-04	
108	1.31E-04	1.31E-04	4.38E-03	5.27E-03	8.98E-05	9.53E-15	2.91E-04	1.07E-04	1.22E+01	3.80E-04	3.80E-04	
117	1.21E-04	1.21E-04	4.39E-03	5.28E-03	9.01E-05	8.15E-15	2.91E-04	1.08E-04	1.22E+01	3.81E-04	3.81E-04	
126	1.13E-04	1.13E-04	4.40E-03	5.29E-03	9.03E-05	7.05E-15	2.91E-04	1.08E-04	1.22E+01	3.81E-04	3.81E-04	
135	1.05E-04	1.05E-04	4.40E-03	5.29E-03	9.05E-05	6.16E-15	2.91E-04	1.08E-04	1.22E+01	3.82E-04	3.82E-04	
144	9.88E-05	9.88E-05	4.41E-03	5.30E-03	9.07E-05	5.43E-15	2.92E-04	1.09E-04	1.22E+01	3.82E-04	3.82E-04	
153	9.31E-05	9.31E-05	4.42E-03	5.31E-03	9.09E-05	4.82E-15	2.92E-04	1.09E-04	1.22E+01	3.83E-04	3.83E-04	
162	8.80E-05	8.80E-05	4.42E-03	5.31E-03	9.11E-05	4.30E-15	2.92E-04	1.09E-04	1.22E+01	3.83E-04	3.83E-04	
171	8.34E-05	8.34E-05	4.42E-03	5.32E-03	9.12E-05	3.87E-15	2.92E-04	1.09E-04	1.22E+01	3.83E-04	3.83E-04	
180	7.93E-05	7.93E-05	4.43E-03	5.32E-03	9.13E-05	3.50E-15	2.92E-04	1.09E-04	1.22E+01	3.84E-04	3.84E-04	

The conditions that are used to analyze the time course of the reaction were 180 s in 20 steps, obtaining the Table S7. The initial concentrations were taken from the experiments (0.005 M for species A and B and solvent concentration calculated from the density at 25°C (12.2 M for THF). The numbers represent the concentration of labelled species in mol per litre.

The ratio of Ni(I) vs Ni(II) (8:92 in this case) was obtained using the following formula:

$$\frac{[\text{Ni}(I)]}{[\text{Ni}(II)]} = \frac{[\text{PhH}]}{[[\text{Ni}(II)(\text{PMe}_3)_3\text{Ph}]^+\text{Br}^-] + [\text{Ni}(II)(\text{PMe}_3)_2(\text{Ph})\text{Br}]}$$

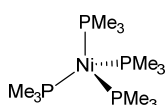
COORDINATES AND ENERGIES FOR MINIMA AND TRANSITION STATES

Energies are given in Hartrees and correspond to the potential energy with the large basis set (first line) and to the free energy correction (second line). The energies used to compute all the profiles were calculated by the sum of $E + G_{\text{corr}}$. In the case of open-shell singlet structures, the values of the potential energy at triplet electronic structure and the S^2 of the open-shell singlet are also provided.

Coordinates are Cartesian coordinates in Å.

In Tetrahydrofuran

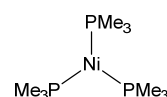
Ni(PMe₃)₄



E	=	-2014.13817957
G _{corr}	=	0.403583
Ni		2.97381100 7.49675000 11.85409900
P		1.37271500 8.84467500 11.13266300
P		2.20232100 6.27155600 13.51844500
C		0.89366400 10.25111400 12.25430200
C		-0.32028500 8.16982600 10.75440800
C		1.64237000 9.81235900 9.56509700
C		2.55471800 6.82320300 15.26175000
C		0.36359500 6.01879000 13.68224400
C		2.73487100 4.49313900 13.67924800
H		0.06919600 10.85075300 11.84660400
H		1.76215600 10.90192100 12.40339800
H		-0.99638400 8.94063300 10.36095200
H		-0.76101600 7.74569400 11.66173000
H		1.69654200 9.12553800 8.71509500
H		2.59494300 10.35007200 9.62310200
H		2.17994800 7.84212700 15.40599100
H		3.63677800 6.83117300 15.43343700
H		-0.12463500 6.98511600 13.85086800
H		0.11165200 5.34883700 14.51507000
H		2.35690800 3.92165300 12.82559900
H		2.36069900 4.03111600 14.60259900
P		4.57490600 8.84467500 12.57553600
P		3.74530100 6.27155500 10.18975400
C		5.05395800 10.25111300 11.45389700
C		6.26790600 8.16982500 12.95379100
C		4.30525200 9.81235900 14.14310200
C		3.39290300 6.82320300 8.44644900
C		5.58402600 6.01879000 10.02595500
C		3.21275000 4.49313900 10.02895100
H		5.87842600 10.85075200 11.86159500
H		4.18546600 10.90192100 11.30480100
H		6.94400500 8.94063200 13.34724800
H		6.70863700 7.74569400 12.04646900

H		4.25107900 9.12553800 14.99310400
H		3.35267900 10.35007200 14.08509700
H		3.76767300 7.84212700 8.30220800
H		2.31084300 6.83117300 8.27476200
H		6.07225600 6.98511600 9.85733000
H		5.83596900 5.34883700 9.19312900
H		3.59071400 3.92165300 10.88260000
H		3.58692200 4.03111600 9.10560000
H		0.59726200 9.85542400 13.23208300
H		-0.23262500 7.36424900 10.01614700
H		0.83498600 10.53369400 9.38176000
H		3.86048500 6.16419300 7.70282700
H		5.97907600 5.59522600 10.95569700
H		2.11850700 4.43465200 10.03648300
H		3.82911400 4.43465200 13.67171600
H		-0.03145400 5.59522600 12.75250200
H		2.08713600 6.16419300 16.00537200
H		5.11263600 10.53369400 14.32643800
H		5.35036000 9.85542400 10.47611600
H		6.18024600 7.36424900 13.69205200

Ni(PMe₃)₃



E	=	-1552.92475226
G _{corr}	=	0.291517
Ni		2.96964300 7.43814400 11.73948900
P		1.78588200 9.17165100 11.21717900
P		2.68132400 6.67241600 13.74450700
C		1.79598400 10.58439200 12.42628900
C		-0.04181500 8.86861400 11.07777300
C		2.06963900 10.11393500 9.63767100
C		3.57495300 7.68797300 15.01798000
C		0.97902400 6.63470300 14.49173100
C		3.25422900 4.96917000 14.22969100
H		1.15551600 11.41351500 12.09851300
H		2.82005700 10.95505800 12.54912700
H		-0.59829000 9.79323900 10.87757200
H		-0.40559000 8.42471400 12.01072500
H		1.96570000 9.43010700 8.78771700
H		3.09258400 10.50757700 9.63084000

H	3.22238500	8.72419700	14.96670900
H	4.64846300	7.68635400	14.79843400
H	0.55792400	7.64612100	14.49004800
H	0.98845100	6.25528300	15.52202300
H	2.72224900	4.22273200	13.62852200
H	3.08263200	4.75512200	15.29300900
P	4.45383700	6.54153700	10.44821300
C	4.60327800	7.07980900	8.67297700
C	6.21303400	6.77898100	10.99831900
C	4.42707200	4.69818700	10.21154500
H	4.80172900	8.15715900	8.64422400
H	3.65177000	6.90058000	8.15895700
H	6.43056300	7.85029900	11.07367200
H	6.92678200	6.32004700	10.30218900
H	4.50401700	4.20697500	11.18799600
H	5.24597500	4.35075900	9.56835400
H	1.44614000	10.22958800	13.40207200
H	-0.23565700	8.15585000	10.26833200
H	1.36788200	10.94931000	9.51041000
H	5.40333300	6.55470500	8.13409900
H	6.34660700	6.33642200	11.99147800
H	3.47314100	4.40221900	9.76000300
H	4.32488100	4.87366400	14.01640900
H	0.32692000	5.99561100	13.88540800
H	3.41884200	7.30404700	16.03434000

Ni(PMe₃)₂

		Me ₃ P—Ni—PMe ₃		
E	=	-1091.70993065		
G _{corr}	=	0.185935		
Ni		2.97940200	7.45613300	11.84238900
P		1.82760700	9.14688900	11.21331900
P		4.14634600	5.79697500	12.52380600
C		1.88491500	10.63783100	12.31406000
C		-0.00276200	8.91183500	11.03663200
C		2.24526000	9.90515700	9.57415300
C		5.40931900	6.15031900	13.83403500
C		3.23801200	4.37491100	13.29076200
C		5.18415800	4.91079900	11.26996800
H		1.26026200	11.45018600	11.92222000
H		2.91861800	10.99001700	12.39950100
H		-0.49668400	9.83947600	10.72147200
H		-0.42422300	8.58776900	11.99427500
H		2.14679100	9.15199800	8.78486600
H		3.28488800	10.25016200	9.58631900
H		4.91251800	6.56083300	14.71975700
H		6.12164400	6.89689400	13.46665300
H		2.65731000	4.73180200	14.14814100
H		3.92965900	3.59271500	13.62725900
H		4.54245400	4.51572800	10.47505300
H		5.74143700	4.08265400	11.72527000
H		1.53426800	10.36600100	13.31554000
H		-0.20289600	8.13003700	10.29592800

H	1.58780900	10.75335400	9.34658600
H	5.89276500	5.61284900	10.81737700
H	2.54108800	3.94792700	12.56145500
H	5.95561300	5.24216700	14.11834500

Ni(PMe₃)

		PMe ₃ Ni		
E	=	-630.471631181		
G _{corr}	=	0.081831		
Ni		3.06794400	7.21941500	11.85670300
P		4.21742000	5.68285000	12.55093100
C		5.63580600	6.13312300	13.65447800
C		3.35958800	4.39542600	13.56937000
C		5.06362100	4.63561000	11.27789100
H		5.25920200	6.65545900	14.54008500
H		6.31509500	6.80683700	13.12206300
H		2.90370800	4.86361200	14.44790400
H		4.06244000	3.61987800	13.89765000
H		4.31558300	4.19467400	10.61075800
H		5.64465900	3.83317600	11.74898300
H		5.73209000	5.25981700	10.67574400
H		2.56361100	3.93212800	12.97710200
H		6.18841900	5.23976400	13.97105400

PMe₃

		Me P Me		
E	=	-461.173291179		
G _{corr}	=	0.084310		
P		1.68046600	-0.11497800	-0.01298200
C		2.55738000	0.74229000	-1.41387900
H		2.39880900	0.18731300	-2.34576300
H		2.14691600	1.74954600	-1.54897100
H		3.63703800	0.82342500	-1.23338400
C		2.37105300	0.85390800	1.41780600
H		1.97873600	1.87728700	1.39604500
H		2.05802300	0.39463300	2.36254700
H		3.46755700	0.89693200	1.39420500
C		2.73435100	-1.64354700	0.11651900
H		2.46686700	-2.20396100	1.01978800
H		2.55202200	-2.29355600	-0.74702300
H		3.80469200	-1.40360800	0.15536100

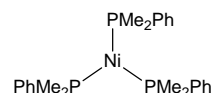
Ni(PMe₂Ph)₄

		PMe ₂ Ph Ni / \ / \ PhMe ₂ P PMe ₂ Ph PMe ₂ Ph		
E	=	-2781.32169362		

G_{corr}	=	0.601644	
Ni	-0.49706400	0.85226400	-0.02368300
P	0.01251600	0.52395400	-2.15370000
P	-1.49145900	-0.97581000	0.70533100
P	1.42367600	1.04561800	1.05462400
P	-1.80334900	2.60498900	0.24991400
C	1.44599200	1.50065700	-2.82277500
C	1.58777700	2.82186900	-2.36496000
H	0.87764400	3.20673000	-1.64199200
C	2.63543100	3.63129200	-2.80649600
H	2.71366800	4.65272600	-2.44247100
C	3.58266900	3.12311500	-3.70047800
H	4.40850900	3.74499500	-4.03692100
C	3.46370500	1.80709300	-4.15414400
H	4.19855600	1.40170300	-4.84581900
C	2.40074000	1.00476600	-3.72544200
H	2.33039800	-0.01259800	-4.09841600
C	-1.25265400	0.87681700	-3.47378900
H	-2.14416600	0.27210800	-3.27470100
H	-0.87875100	0.64356400	-4.47868900
H	-1.53122900	1.93466600	-3.43637800
C	0.45981000	-1.21197800	-2.63527700
H	-0.37075600	-1.86256600	-2.34484200
H	1.35010000	-1.52974500	-2.08220500
H	0.63660500	-1.33981400	-3.70983400
C	-2.50142700	-1.91250700	-0.54081700
C	-2.31480100	-3.26828100	-0.85570700
H	-1.57269000	-3.85922200	-0.32841100
C	-3.07014800	-3.88223000	-1.86133600
H	-2.90079400	-4.93073300	-2.09493400
C	-4.03654600	-3.15737200	-2.56063700
H	-4.62264800	-3.63567300	-3.34112900
C	-4.23998400	-1.80810100	-2.25135500
H	-4.98763600	-1.23121700	-2.79067800
C	-3.47235500	-1.19386600	-1.26174200
H	-3.61022300	-0.13670100	-1.05729600
C	-2.75428100	-0.82552000	2.06837600
H	-3.51881900	-0.09823100	1.77663000
H	-2.25326300	-0.45766700	2.97021900
H	-3.23954100	-1.78240600	2.29665000
C	-0.43652600	-2.32011200	1.43071300
H	0.12415400	-1.89283200	2.26718100
H	0.28595900	-2.66586800	0.68385200
H	-1.01630100	-3.17576000	1.79752000
C	1.44013600	0.45618400	2.81741300
C	0.30475800	0.73595300	3.59775500
H	-0.52847300	1.25974500	3.13913100
C	0.22032500	0.32062800	4.92731500
H	-0.66813800	0.55082500	5.51070500
C	1.26816400	-0.40728100	5.50010800
H	1.20116200	-0.74593800	6.53083900
C	2.39923900	-0.70153700	4.73529000
H	3.21762700	-1.26989600	5.17095000
C	2.48802200	-0.26730000	3.40832700
H	3.38110100	-0.50650400	2.83910300

C	2.87279200	0.14066400	0.32591400
H	2.67036100	-0.93561000	0.32112100
H	3.81634100	0.32944400	0.85153700
H	2.98546300	0.47259700	-0.71091700
C	2.22105300	2.71353100	1.30194400
H	1.56058100	3.34809800	1.90097300
H	2.36848500	3.18911900	0.32705200
H	3.18804700	2.62963300	1.81337100
C	-1.27360600	4.17381100	-0.58110800
C	-1.68428800	4.47886500	-1.89111400
H	-2.41726800	3.85324000	-2.39192000
C	-1.15463300	5.57511400	-2.57544900
H	-1.48480700	5.78616900	-3.58968800
C	-0.20459800	6.39671000	-1.96340500
H	0.21126500	7.24728800	-2.49691000
C	0.20256300	6.11578200	-0.65577600
H	0.93473800	6.75183500	-0.16397400
C	-0.32601500	5.01744000	0.02559000
H	0.01588100	4.81218700	1.03524600
C	-2.13437100	3.22646400	1.97428100
H	-2.63347800	2.42605600	2.53154900
H	-2.77333900	4.11784700	1.98271800
H	-1.19547800	3.45594400	2.48616600
C	-3.57308600	2.49774500	-0.32230300
H	-4.07770900	1.73805200	0.28448000
H	-3.61967100	2.17864900	-1.36763600
H	-4.10777600	3.44907700	-0.21241800

Ni(PMe₂Ph)₃



E	=	-2128.30803416	
G_{corr}	=	0.439835	
Ni	4.19121200	6.76005000	4.08091800
P	5.21356600	6.50865700	2.18812400
P	3.70034400	4.96200500	5.16838900
P	3.31464100	8.64088100	4.66770700
C	6.68591700	7.57572700	1.85295000
C	6.49986900	8.95486200	1.64500700
H	5.49876400	9.37361800	1.63613700
C	7.59107200	9.80313500	1.45629400
H	7.41970500	10.86406400	1.29357800
C	8.89359000	9.29463600	1.48605800
H	9.74396400	9.95655200	1.34369600
C	9.09260500	7.92948300	1.70288900
H	10.10067900	7.52261500	1.72875300
C	7.99902900	7.07694100	1.88293000
H	8.17977200	6.01839900	2.04575100
C	4.12410700	6.89228000	0.73193300
H	3.25517000	6.22592500	0.77775400
H	4.64020300	6.75115700	-0.22508300
H	3.76255500	7.92237500	0.80240100

C	5.81532500	4.82768500	1.67522000
H	4.94587500	4.16063700	1.66110100
H	6.52223500	4.43315300	2.41211200
H	6.28582100	4.82312800	0.68440700
C	2.50137300	4.12490600	4.04086200
C	2.73753100	2.88131400	3.43361500
H	3.62787700	2.31038700	3.68055900
C	1.83537700	2.36088600	2.49967600
H	2.03598600	1.39666800	2.03877000
C	0.68182700	3.07127400	2.16035900
H	-0.01761400	2.66506000	1.43438200
C	0.43354400	4.31049900	2.76076700
H	-0.46152100	4.87194800	2.50382100
C	1.33703100	4.83351600	3.68571200
H	1.14903700	5.80738000	4.13095800
C	2.74468600	4.98610600	6.76604500
H	1.86803700	5.63111800	6.64512000
H	3.37865000	5.41874900	7.54881800
H	2.41552000	3.98804300	7.08093200
C	4.93349100	3.63721800	5.56454500
H	5.61014300	4.02794900	6.33300400
H	5.53219200	3.41112200	4.67655600
H	4.46763000	2.71773700	5.93874700
C	3.70642200	10.14398700	3.65906700
C	3.04912200	10.35546900	2.43268700
H	2.24552000	9.69080800	2.12557300
C	3.42355200	11.40147100	1.58756400
H	2.89956600	11.54712800	0.64595700
C	4.46988600	12.25759600	1.94755400
H	4.76493200	13.06996900	1.28863800
C	5.13203600	12.05764900	3.16120800
H	5.94820600	12.71491500	3.45114400
C	4.75423800	11.01173200	4.00775800
H	5.29363000	10.86913900	4.94007700
C	3.64599800	9.24085100	6.39382600
H	3.21338400	8.50797000	7.08415100
H	3.20760800	10.22661600	6.58971000
H	4.72283900	9.27883200	6.58541300
C	1.45496100	8.69570800	4.67491100
H	1.09255400	7.96880000	5.40985300
H	1.06069200	8.40972200	3.69546300
H	1.07622300	9.68997700	4.93916500

Ni(PMe₂Ph)₂



E	=	-1475.29545173	
G _{corr}	=	0.28227	
Ni	2.92241100	7.11859900	5.19863800
P	3.47235300	5.05218800	5.30225500
P	2.40999600	9.18799300	5.00635800
C	2.11340800	3.83268800	5.01141200
C	2.32833800	2.44477700	5.01571100
H	3.32405800	2.04670600	5.19499900

C	1.27041100	1.56232400	4.79070400
H	1.44994400	0.49012600	4.79674500
C	-0.01768100	2.05566300	4.55728500
H	-0.84021400	1.36703600	4.38190200
C	-0.24309100	3.43400300	4.54980300
H	-1.24185700	3.82310600	4.36866100
C	0.81737400	4.31589400	4.77552800
H	0.65178300	5.39162200	4.77119100
C	4.21624900	4.43587200	6.88614000
H	3.49925300	4.56974200	7.70273900
H	5.10810500	5.03064700	7.11204500
H	4.49844100	3.37864200	6.82494500
C	4.76298600	4.49912500	4.08951200
H	5.66612400	5.10065000	4.24023900
H	4.40248200	4.67022500	3.07013300
H	5.01517600	3.43931400	4.20944800
C	3.83168800	10.35892800	4.84879700
C	3.65586400	11.74603700	4.71739000
H	2.65526400	12.17093400	4.70650000
C	4.75923800	12.59286600	4.59918200
H	4.61005900	13.66494600	4.49808800
C	6.05430600	12.06388800	4.61090400
H	6.91236200	12.72481400	4.51901000
C	6.24110700	10.68584400	4.74103300
H	7.24509300	10.26925700	4.75062900
C	5.13512600	9.83966600	4.85908900
H	5.26999500	8.76438200	4.96032200
C	1.41358700	9.95775500	6.36900800
H	0.47799100	9.39765500	6.47613900
H	1.17894100	11.00892900	6.16680900
H	1.96654800	9.88717000	7.31131800
C	1.37048500	9.64012100	3.53769000
H	0.43129400	9.07790900	3.58412100
H	1.89456300	9.35605500	2.61936600
H	1.14435600	10.71207600	3.50680400

Ni(PMe₂Ph)



E	=	-822.264490723	
G _{corr}	=	0.130288	
Ni	3.64952100	7.12531700	5.00244100
P	3.41747500	5.11515900	5.25861700
C	2.50041500	4.21075400	3.92761400
C	2.24237300	2.83206200	4.00590600
H	2.58070100	2.26020700	4.86635100
C	1.55079100	2.18047800	2.98316600
H	1.35592300	1.11348400	3.05667000
C	1.10918500	2.89760500	1.86640400
H	0.57117600	2.38864500	1.07077800
C	1.36195300	4.26833000	1.77702400
H	1.02235200	4.83123900	0.91130500
C	2.05274500	4.91888500	2.80286100

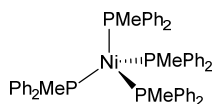
H	2.25421400	5.98640500	2.74311300
C	2.51599100	4.58407600	6.79081300
H	1.50187400	4.99570400	6.77850700
H	3.04140400	4.98493300	7.66408300
H	2.46104400	3.49294700	6.87634200
C	4.97271200	4.11402600	5.40575700
H	5.55908800	4.49693900	6.24767900
H	5.56528100	4.22584500	4.49240400
H	4.75977500	3.05136700	5.56956000

PMe₂Ph



E	=	-652.964031445	
G _{corr}	=	0.132457	
P	-1.30905200	-0.28950500	-0.03156300
C	-0.53198400	0.56311500	-1.48545100
C	-1.37168700	1.16607600	-2.43429200
C	0.85804100	0.63792200	-1.67860600
C	-0.84085600	1.82725300	-3.54607400
H	-2.45046600	1.11860000	-2.30335400
C	1.39128300	1.29448000	-2.78824400
H	1.53357900	0.18124100	-0.95957900
C	0.54176800	1.89158400	-3.72535300
H	-1.50740400	2.28884400	-4.27021800
H	2.46912700	1.34100900	-2.92329400
H	0.95767700	2.40268700	-4.58987700
C	-0.37379700	-1.90028000	-0.01465200
H	0.71302900	-1.75927200	0.00532400
H	-0.66727200	-2.47036700	0.87465000
H	-0.63735500	-2.49165700	-0.89839400
C	-0.44285900	0.57133100	1.37596200
H	-0.77915700	1.61227200	1.43393200
H	-0.70926800	0.07564300	2.31680100
H	0.64819800	0.55826200	1.26825500

Ni(PMePh₂)₄

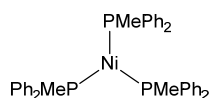


E	=	-3548.5036579	
G _{corr}	=	0.801946	
Ni	9.59031000	10.54489800	4.13449400
P	9.87146800	10.62134100	1.92237500
C	8.65761800	9.75601500	0.81128400
C	7.52397300	10.41534300	0.30694100
H	7.39665700	11.48197600	0.46109400
C	6.54045100	9.71644600	-0.39894900
H	5.67123900	10.24924900	-0.77695700
C	6.67334100	8.34394900	-0.62267500
H	5.90719900	7.80005300	-1.16891100

C	7.80715500	7.67943900	-0.14481600
H	7.93011500	6.61357300	-0.32113000
C	8.78660800	8.37778900	0.56176000
H	9.65572900	7.84194500	0.92929300
C	11.45461400	9.91898400	1.25612800
C	11.99216300	8.79464100	1.90215900
H	11.47276900	8.37774000	2.75750000
C	13.19301600	8.22396800	1.47436100
H	13.58519900	7.35070600	1.98908300
C	13.88904600	8.78522000	0.40025000
H	14.83204400	8.35480700	0.07299600
C	13.36400500	9.90448100	-0.25229200
H	13.89823600	10.34717500	-1.08947700
C	12.15250700	10.46113800	0.16566500
H	11.76819500	11.33019100	-0.35832100
C	9.87591400	12.32571300	1.18371100
H	9.86814100	12.32920600	0.08887700
H	10.76620600	12.85065800	1.54408300
H	8.99973600	12.86941800	1.54666400
P	7.81248900	11.83305100	4.60153700
C	6.88495300	11.55674000	6.18703700
C	7.19289300	12.27375300	7.35741600
H	7.92532000	13.07396800	7.32413600
C	6.56370500	11.97935300	8.56869200
H	6.81621100	12.55309200	9.45726000
C	5.60997500	10.95958800	8.63816400
H	5.12125600	10.72846600	9.58112400
C	5.28340200	10.24876700	7.48082200
H	4.53801400	9.45812100	7.51504600
C	5.91044800	10.54639600	6.26830500
H	5.63723200	9.97716700	5.38682800
C	8.02798800	13.67866900	4.61893600
C	7.02729700	14.57342300	5.03608000
H	6.09018700	14.19366700	5.43490000
C	7.23122300	15.95188400	4.95652200
H	6.45167800	16.63312600	5.28888200
C	8.43425700	16.45814100	4.45006800
H	8.59039500	17.53230500	4.38983200
C	9.43076800	15.57788100	4.02533200
H	10.37000400	15.95608300	3.62978700
C	9.22413000	14.19833200	4.11366200
H	9.99025800	13.50553100	3.78634700
C	6.39111700	11.77595200	3.39594600
H	5.53313300	12.35332200	3.75680000
H	6.08146600	10.74645900	3.20907100
H	6.73454400	12.20670800	2.45231900
P	9.09892300	8.55186700	5.01251600
C	10.06402400	7.05019800	4.49069000
C	11.24938400	6.68408200	5.15014200
H	11.55819300	7.20679500	6.04895900
C	12.05244000	5.64844000	4.66490800
H	12.96562400	5.38580600	5.19356100
C	11.68416900	4.95173200	3.51131900
H	12.30995100	4.14830900	3.13180100
C	10.49682600	5.29246000	2.85611000

H	10.19120500	4.75110900	1.96406000	P	9.90260700	10.75027500	1.79241700
C	9.69638400	6.32742500	3.34157400	C	8.66182700	9.90016100	0.71748400
H	8.78020600	6.57759800	2.81638900	C	7.48228000	10.57100500	0.34924700
C	7.37130700	7.92378600	4.75649200	H	7.36049700	11.62453800	0.58287400
C	6.74620800	8.22139100	3.53554100	C	6.44941500	9.89400100	-0.30294400
H	7.28528100	8.79667500	2.79217900	H	5.54456100	10.43042600	-0.57788100
C	5.43729900	7.80930800	3.27552100	C	6.57503600	8.53276600	-0.59668600
H	4.97962200	8.04980500	2.31949200	H	5.76898000	8.00456500	-1.09915400
C	4.72093300	7.10699600	4.24827500	C	7.74619100	7.85739700	-0.24124900
H	3.69593500	6.79894400	4.05855400	H	7.85512300	6.79936000	-0.46658000
C	5.33204700	6.80239200	5.46829200	C	8.77969100	8.53376500	0.41010100
H	4.78276400	6.25509400	6.23054800	H	9.67773100	7.99322900	0.69208600
C	6.64900800	7.19792200	5.71667700	C	11.47935000	9.87655900	1.37160200
H	7.09813700	6.94726200	6.67200100	C	12.21113600	9.29576800	2.41582700
C	9.26291100	8.44852400	6.86142800	H	11.83158100	9.37301600	3.43045100
H	9.16184800	7.43125400	7.25372100	C	13.39747300	8.60295200	2.15802000
H	8.49656500	9.09003600	7.30794900	H	13.94583800	8.14913100	2.97869200
H	10.23912900	8.84253600	7.15600500	C	13.86204700	8.48097900	0.84716000
P	11.56535900	11.16998300	4.99441200	H	14.78091200	7.93737400	0.64209100
C	11.61672700	11.87597000	6.71185900	C	13.13851600	9.05455500	-0.20481400
C	10.46879900	11.75001400	7.50153000	H	13.49469800	8.95733600	-1.22747500
H	9.58387300	11.30399300	7.06262700	C	11.95593300	9.74794900	0.05585500
C	10.45666300	12.18307400	8.83048600	H	11.39354100	10.17560400	-0.77049200
H	9.55089000	12.07542300	9.42177800	C	10.16056100	12.36692800	0.90612000
C	11.60269700	12.75465100	9.38569700	H	10.40528300	12.24007300	-0.15405300
H	11.59926300	13.09771700	10.41721900	H	10.97971400	12.90273100	1.39839900
C	12.75882400	12.88587300	8.60726400	H	9.25685400	12.97720400	0.99710400
H	13.65445800	13.33032000	9.03463200	P	7.44597800	11.91802300	4.42499000
C	12.76776100	12.44598000	7.28269100	C	6.76683200	11.55555900	6.10786900
H	13.67120000	12.55640500	6.68876800	C	7.35127200	12.11038900	7.25913200
C	12.60161700	12.39813600	4.06076600	H	8.12332900	12.86931100	7.16089400
C	12.51110800	13.78019000	4.30693300	C	6.95253600	11.69920800	8.53249300
H	11.89436100	14.14454900	5.12211700	H	7.41520400	12.14345700	9.41053200
C	13.21153500	14.69886700	3.52269400	C	5.96432000	10.72094600	8.68038800
H	13.12771500	15.76143900	3.73811700	H	5.65685700	10.39839200	9.67174300
C	14.02209200	14.25612000	2.47320400	C	5.37617500	10.16114100	7.54278100
H	14.56551800	14.97067100	1.86037800	H	4.61072800	9.39559400	7.64282300
C	14.13448900	12.88573200	2.22729800	C	5.77390300	10.57321900	6.26901500
H	14.76585300	12.52374800	1.41976400	H	5.31953500	10.10683400	5.40008900
C	13.43555800	11.96676600	3.01414800	C	7.83900700	13.72130500	4.54925900
H	13.54045600	10.90950000	2.79758600	C	6.91053600	14.67693800	4.99371900
C	12.84305600	9.83482700	5.26077300	H	5.92093800	14.36242800	5.31610700
H	13.81909900	10.25909200	5.52054100	C	7.25247000	16.02923900	5.03573800
H	12.94299000	9.21083600	4.37131400	H	6.52564200	16.76115200	5.37935600
H	12.50602700	9.20455500	6.08760400	C	8.52942300	16.44295400	4.63891600

Ni(PMePh₂)₃

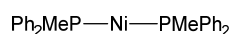


E	=	-1858.88033969
G _{corr}	=	0.588582
Ni		8.95690100 10.55166600 3.71532900

P	9.90260700	10.75027500	1.79241700
C	8.66182700	9.90016100	0.71748400
C	7.48228000	10.57100500	0.34924700
H	7.36049700	11.62453800	0.58287400
C	6.44941500	9.89400100	-0.30294400
H	5.54456100	10.43042600	-0.57788100
C	6.57503600	8.53276600	-0.59668600
H	5.76898000	8.00456500	-1.09915400
C	7.74619100	7.85739700	-0.24124900
H	7.85512300	6.79936000	-0.46658000
C	8.77969100	8.53376500	0.41010100
H	9.67773100	7.99322900	0.69208600
C	11.47935000	9.87655900	1.37160200
C	12.21113600	9.29576800	2.41582700
H	11.83158100	9.37301600	3.43045100
C	13.39747300	8.60295200	2.15802000
H	13.94583800	8.14913100	2.97869200
C	13.86204700	8.48097900	0.84716000
H	14.78091200	7.93737400	0.64209100
C	13.13851600	9.05455500	-0.20481400
H	13.49469800	8.95733600	-1.22747500
C	11.95593300	9.74794900	0.05585500
H	11.39354100	10.17560400	-0.77049200
C	10.16056100	12.36692800	0.90612000
H	10.40528300	12.24007300	-0.15405300
H	10.97971400	12.90273100	1.39839900
H	9.25685400	12.97720400	0.99710400
P	7.44597800	11.91802300	4.42499000
C	6.76683200	11.55555900	6.10786900
C	7.35127200	12.11038900	7.25913200
H	8.12332900	12.86931100	7.16089400
C	6.95253600	11.69920800	8.53249300
H	7.41520400	12.14345700	9.41053200
C	5.96432000	10.72094600	8.68038800
H	5.65685700	10.39839200	9.67174300
C	5.37617500	10.16114100	7.54278100
H	4.61072800	9.39559400	7.64282300
C	5.77390300	10.57321900	6.26901500
H	5.31953500	10.10683400	5.40008900
C	7.83900700	13.72130500	4.54925900
C	6.91053600	14.67693800	4.99371900
H	5.92093800	14.36242800	5.31610700
C	7.25247000	16.02923900	5.03573800
H	6.52564200	16.76115200	5.37935600
C	8.52942300	16.44295400	4.63891600
H	8.79381700	17.49682700	4.67261600
C	9.46252400	15.49972100	4.20289500
H	10.45694300	15.81534500	3.89715400
C	9.11674800	14.14576000	4.15891800
H	9.83290000	13.40115500	3.81757500
C	5.89616100	11.95461400	3.39852100
H	5.08737300	12.51462400	3.88039200
H	5.56254600	10.93203700	3.20148800
H	6.13782000	12.42280100	2.43985500
P	8.94024800	8.69131700	4.83412000

C	10.10321700	7.31188900	4.41387100
C	11.28554100	7.09996000	5.14207000
H	11.48730900	7.67734800	6.04026500
C	12.22549700	6.15492900	4.71960900
H	13.13459900	6.00577600	5.29738100
C	12.00066700	5.40602300	3.56232700
H	12.73358000	4.67497400	3.23132900
C	10.82420900	5.60488900	2.83266600
H	10.63631000	5.02475200	1.93237100
C	9.88734900	6.54852500	3.25349800
H	8.98219900	6.69858400	2.67199000
C	7.29046700	7.87855700	4.60966700
C	6.58159900	8.14374200	3.42548800
H	7.02261100	8.79272700	2.67453500
C	5.31334600	7.59783400	3.21473300
H	4.78420800	7.81024400	2.28928600
C	4.72760900	6.79189400	4.19519100
H	3.73591000	6.37475000	4.03957700
C	5.42237200	6.52489200	5.37869100
H	4.97176200	5.89936600	6.14533100
C	6.69741300	7.05902500	5.58190700
H	7.22117200	6.84029300	6.50786700
C	9.10770000	8.78321200	6.67987500
H	9.21766700	7.80301200	7.15535800
H	8.22106600	9.28307900	7.07873700
H	9.97866000	9.39785100	6.92725200

Ni(PMePh₂)₂



$$E = -1858.88033969$$

$$G_{\text{corr}} = 0.378772$$

Ni	-1.41586700	1.01000500	-0.08372400
P	-0.81611000	2.12220600	-1.80758100
C	-0.98230400	3.95372700	-1.63782700
C	-0.13827000	4.88889500	-2.25671500
H	0.68689900	4.55915400	-2.88069700
C	-0.34634200	6.25947000	-2.07586900
H	0.31677900	6.97276700	-2.55888100
C	-1.40037900	6.71223300	-1.27878100
H	-1.55958500	7.77837900	-1.13957500
C	-2.24431400	5.78901700	-0.65378100
H	-3.06092100	6.13381700	-0.02466000
C	-2.03092500	4.42109400	-0.82679300
H	-2.67032400	3.69751600	-0.32430600
C	-1.77848200	1.74749400	-3.34441400
C	-2.49248400	0.54034900	-3.39614000
H	-2.48598400	-0.11209800	-2.52493100
C	-3.20412300	0.18436200	-4.54468500
H	-3.75252000	-0.75384400	-4.57229500
C	-3.21602500	1.03761400	-5.65086500
H	-3.77473700	0.76655600	-6.54298100
C	-2.51245700	2.24569200	-5.60583500
H	-2.52325400	2.91437600	-6.46293300

C	-1.79628400	2.59812300	-4.46043300
H	-1.25764900	3.54188800	-4.43366800
C	0.91831900	1.88965600	-2.41947500
H	1.10625600	2.40968700	-3.36447600
H	1.07329600	0.81703000	-2.57483000
H	1.62747400	2.23525500	-1.66000100
P	-1.95177400	-0.18643300	1.60445500
C	-1.47310700	0.54269700	3.23203500
C	-2.19297600	0.36951500	4.42430000
H	-3.10710200	-0.21642000	4.43700000
C	-1.74285300	0.95040300	5.61383600
H	-2.31071900	0.80920600	6.53002300
C	-0.56882300	1.70716100	5.62787600
H	-0.22096000	2.15642100	6.55442200
C	0.15204700	1.89196400	4.44404200
H	1.06115700	2.48782900	4.44513300
C	-0.30222100	1.32045000	3.25529400
H	0.24186600	1.47969800	2.32611100
C	-1.14655700	-1.85454600	1.63149400
C	-0.66773100	-2.37221900	0.41779700
H	-0.75350700	-1.76657400	-0.48237600
C	-0.08517000	-3.64104700	0.36645900
H	0.28097300	-4.03043200	-0.58014200
C	0.03375100	-4.40189000	1.53215300
H	0.49304000	-5.38640000	1.49665800
C	-0.43439100	-3.89149400	2.74729100
H	-0.33871900	-4.47849300	3.65730800
C	-1.02240500	-2.62606600	2.79727300
H	-1.37613200	-2.23689100	3.74847700
C	-3.73027700	-0.65480000	1.83537800
H	-3.88189600	-1.35099100	2.66685800
H	-4.06875600	-1.13597800	0.91195800
H	-4.33073000	0.24665000	1.99621500

Ni(PMePh₂)



$$E = -844.755968904$$

$$G_{\text{corr}} = 0.178995$$

Ni	9.31802800	9.48396300	3.82312600
P	9.72794500	10.33446600	2.02123500
C	8.42705100	10.05837000	0.73423500
C	7.94132500	11.06150900	-0.11810100
H	8.31932700	12.07672600	-0.04968100
C	6.95838200	10.76881400	-1.06938600
H	6.58988100	11.55719200	-1.72090700
C	6.45325900	9.47247100	-1.18429300
H	5.69007500	9.24760500	-1.92475200
C	6.92830900	8.46587800	-0.33665000
H	6.53529300	7.45547100	-0.41527900
C	7.90023900	8.75998000	0.61876400
H	8.25500800	7.98338200	1.29309200
C	11.26492300	9.74579400	1.16536100

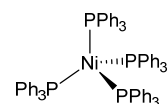
C	12.23804500	9.06480600	1.91103100
H	12.05139900	8.86885000	2.96491300
C	13.42679200	8.64118700	1.31102300
H	14.17296300	8.11468700	1.90070400
C	13.65071500	8.88889900	-0.04533100
H	14.57196500	8.55529400	-0.51590600
C	12.68391500	9.56301600	-0.79862300
H	12.85300700	9.75423800	-1.85534100
C	11.49832500	9.98957200	-0.19765400
H	10.75046900	10.50554800	-0.79465300
C	9.99733500	12.16858900	1.98247300
H	10.28291100	12.52489200	0.98698300
H	10.80643000	12.39927600	2.68235700
H	9.09249300	12.68575700	2.31715400

PMePh₂



E	=	-844.755968904	
G _{corr}	=	0.18076	
P	-1.19882300	-0.44166600	0.01868500
C	-0.58479000	0.57761700	-1.40342600
C	-1.47307300	0.88000500	-2.44556800
C	0.74095200	1.03645900	-1.49012200
C	-1.04780700	1.61868600	-3.55421100
H	-2.50452300	0.53933200	-2.39059700
C	1.16584100	1.77564100	-2.59375900
H	1.43995200	0.82193600	-0.68572200
C	0.27155500	2.06731000	-3.62953000
H	-1.74831300	1.84574300	-4.35376400
H	2.19379100	2.12549900	-2.64718800
H	0.60313200	2.64495300	-4.48856200
C	-0.11094700	-1.94065500	-0.16172500
H	0.95659900	-1.69504300	-0.15159400
H	-0.32582500	-2.65911500	0.63622400
H	-0.35467700	-2.41836200	-1.11669300
C	-0.41203600	0.43923800	1.44440300
C	-0.68192000	1.80931500	1.61881300
C	0.37817000	-0.21224400	2.40447600
C	-0.16435100	2.50833900	2.70825600
H	-1.29061100	2.33641400	0.88747400
C	0.89057200	0.48787900	3.50132300
H	0.60612700	-1.26938100	2.30535400
C	0.62499100	1.84896900	3.65600200
H	-0.37697400	3.56885400	2.81787500
H	1.50352000	-0.03450100	4.23175200
H	1.02759600	2.39243100	4.50672700

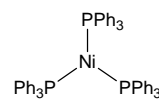
Ni(PPh₃)₄



E	=	-4315.67341777	
G _{corr}	=	1.003185	
Ni	9.57524700	10.55790800	4.18916900
P	9.74169400	10.45242400	1.90715400
C	8.53392100	9.40000600	0.95056500
C	7.20132900	9.82337500	0.79988600
H	6.89640200	10.78685300	1.18440400
C	6.25769000	9.02256900	0.15706600
H	5.23780900	9.38327400	0.05198800
C	6.62110800	7.76800900	-0.34081200
H	5.88574300	7.13831900	-0.83494300
C	7.94071300	7.33516500	-0.20063300
H	8.24142800	6.36431300	-0.58689500
C	8.88900800	8.14462200	0.43205600
H	9.90641300	7.78320700	0.52467500
C	11.31920400	9.80690200	1.15607700
C	12.01138800	8.80919800	1.85456500
H	11.63893000	8.48367200	2.81665400
C	13.18271600	8.25121600	1.33802400
H	13.69565400	7.47460600	1.89848700
C	13.69371800	8.70529500	0.12048500
H	14.61294100	8.28491400	-0.27949400
C	13.01786800	9.70955000	-0.58044200
H	13.41079600	10.07142800	-1.52749400
C	11.83410600	10.24965300	-0.07302000
H	11.31931900	11.02273100	-0.63442700
P	7.90869500	12.08454900	4.60375300
C	6.97656700	11.91024700	6.22232200
C	6.88228000	12.93310200	7.18269500
H	7.31152800	13.90944800	6.99003300
C	6.25293900	12.71091800	8.41127100
H	6.20299300	13.51871200	9.13745000
C	5.69101900	11.46719100	8.70628200
H	5.20030800	11.29806500	9.66121000
C	5.77500000	10.44155000	7.76225400
H	5.35677800	9.46056600	7.97308000
C	6.42212000	10.66020000	6.54598900
H	6.51146000	9.83628500	5.85189400
C	8.32641100	13.90442000	4.67465900
C	7.34002800	14.90812400	4.64396400
H	6.29121900	14.63589600	4.57576000
C	7.69125200	16.25713400	4.69820000
H	6.91390600	17.01658900	4.66932800
C	9.03637500	16.63238700	4.78842300
H	9.30839800	17.68423300	4.82330300
C	10.02332200	15.64725600	4.83195300
H	11.07418100	15.91689600	4.89522900
C	9.66225200	14.29892500	4.77700300
H	10.43170300	13.54238500	4.79555600

P	9.10187700	8.45462600	4.94328600	H	15.34521500	7.95533000	4.20773800
C	9.97374500	7.02050600	4.13351700	H	15.14255800	6.71773000	6.36374200
C	11.29676700	6.69449900	4.48063700	C	9.42454400	8.14170800	6.74553100
H	11.78736300	7.22239400	5.28677400	C	9.81648700	6.91297100	7.30148200
C	11.99370800	5.69473800	3.80103500	C	9.25062700	9.23622200	7.60303200
H	13.01383200	5.46341200	4.09634500	C	10.05284500	6.79781600	8.67384600
C	11.38744000	5.00530500	2.74726100	H	9.95408600	6.04395800	6.66655900
H	11.93141100	4.23191500	2.21113600	C	9.47351700	9.12357200	8.97579100
C	10.07393500	5.31864000	2.39286200	H	8.96115300	10.18715200	7.17898200
H	9.58689700	4.79020600	1.57700700	C	9.88614500	7.90244800	9.51498000
C	9.37210600	6.31123100	3.08184400	H	10.36998200	5.84266000	9.08503900
H	8.35406600	6.53522500	2.78507200	H	9.34460200	9.99467800	9.61259800
C	7.35442200	7.82605500	4.79261100	H	10.07844000	7.81088800	10.58091500
C	6.56590400	8.35981700	3.76640200	C	6.48936900	12.19593500	3.38722700
H	6.97809400	9.14523600	3.14652200	C	6.61037100	13.02592700	2.25580600
C	5.26033200	7.91190500	3.55412700	C	5.32206000	11.42690900	3.51417200
H	4.67316800	8.34023900	2.74676800	C	5.60321100	13.08143200	1.29112500
C	4.71535900	6.93488700	4.38907000	H	7.49205900	13.64053000	2.12127300
H	3.69509800	6.59157500	4.23789500	C	4.31812100	11.47405100	2.54302800
C	5.48825400	6.40381100	5.42733500	H	5.17790400	10.78253500	4.37190800
H	5.06929500	5.64623500	6.08514700	C	4.45220500	12.30056100	1.42550500
C	6.80075000	6.83822300	5.62322200	H	5.72903500	13.73136000	0.42922900
H	7.38609000	6.40840700	6.42979600	H	3.42636100	10.86521600	2.66981000
P	11.56165600	11.11721200	5.21215000	H	3.66982700	12.33878100	0.67203500
C	11.52704000	11.88361800	6.91666400	C	9.59224400	12.08407300	1.03130000
C	10.32341100	12.37309000	7.42892500	C	10.12815600	13.19390900	1.69870100
H	9.42534600	12.28275000	6.83693400	C	8.99379900	12.28302700	-0.22298500
C	10.25259300	12.95785500	8.69588900	C	10.05685300	14.47352900	1.14776400
H	9.29559600	13.31534500	9.06655500	H	10.58464800	13.04774900	2.66746700
C	11.40401800	13.06460100	9.47616200	C	8.90993300	13.56457300	-0.77411100
H	11.35749600	13.51271700	10.46539100	H	8.57724000	11.44364000	-0.76962400
C	12.62186100	12.58935700	8.97656200	C	9.43619100	14.66432600	-0.08962700
H	13.52615800	12.67256100	9.57408400	H	10.46668600	15.31676300	1.69713400
C	12.68301500	12.00708700	7.71052800	H	8.42976200	13.70243600	-1.73979100
H	13.63676100	11.64539500	7.33847100	H	9.36191000	15.66068600	-0.51782500
C	12.66811500	12.35812200	4.34003800				
C	13.06095000	13.58249100	4.91042000				
H	12.78088300	13.82963500	5.92754100				
C	13.79818100	14.51607000	4.17588100				
H	14.07985100	15.45699100	4.64231800				
C	14.17153800	14.24704500	2.85766100				
H	14.74458300	14.97470400	2.28901000				
C	13.79044500	13.03563700	2.27702600				
H	14.05691600	12.80788800	1.24815700				
C	13.03894800	12.11417200	3.00653800				
H	12.71691100	11.20727900	2.51521500				
C	12.77470400	9.73859800	5.57844900				
C	12.67234200	9.02908000	6.79089700				
C	13.75503100	9.32878900	4.66145700				
C	13.51946400	7.95640400	7.07364600				
H	11.93121800	9.31088900	7.52856400				
C	14.59671400	8.24846800	4.93965300				
H	13.88064100	9.84720100	3.72003100				
C	14.48520700	7.55562100	6.14672900				
H	13.41195800	7.43014800	8.01849700				

Ni(PPh₃)₃



$$E = -3279.08460787$$

$$G_{\text{corr}} = 0.735357$$

Ni	8.54521400	10.27566900	3.62939900
P	9.38890200	10.48884300	1.65003000
C	8.18658000	9.78380600	0.43371600
C	7.92271300	10.34415900	-0.82408100
H	8.47227500	11.21982600	-1.15604700
C	6.94597000	9.78810300	-1.65629300
H	6.74934400	10.23612800	-2.62710400
C	6.22433600	8.66530600	-1.24403900
H	5.46333800	8.23767700	-1.89158500
C	6.48268300	8.09636500	0.00786100
H	5.92197500	7.22604400	0.33935800

C	7.45234400	8.65417300	0.84096400	C	6.85867900	5.19418900	5.88629900
H	7.63155300	8.23339300	1.82776900	H	7.04496800	4.19928600	6.28300400
C	10.95421900	9.57189200	1.28440000	C	7.92557200	6.07398400	5.69353900
C	11.96681300	9.63308600	2.25591000	H	8.93530200	5.75415900	5.93570900
H	11.78627900	10.18183800	3.17769100	C	9.49035900	9.19104500	6.60796000
C	13.18068300	8.97590500	2.06177000	C	9.15024000	8.53349200	7.79820400
H	13.95157700	9.02601700	2.82594400	C	10.12710900	10.44203400	6.68292100
C	13.39218700	8.22808700	0.89866800	C	9.42787100	9.12283600	9.03548700
H	14.33155600	7.70108800	0.75289100	H	8.64633400	7.57264300	7.76619700
C	12.38707800	8.14981500	-0.06788800	C	10.41070500	11.02824700	7.91623200
H	12.54499200	7.56717600	-0.97222400	H	10.36122600	10.97235700	5.76373300
C	11.17572000	8.82289900	0.12013500	C	10.05458100	10.37034500	9.09820700
H	10.40512200	8.76466200	-0.64345800	H	9.14678700	8.60802200	9.95086700
P	7.12552800	11.69629900	4.45904400	H	10.88627000	12.00493100	7.95258700
C	5.92922200	11.09785400	5.74359900	H	10.25847700	10.83070800	10.06150700
C	6.42341700	10.72140900	7.00607600	C	5.98866100	12.51927900	3.24632700
H	7.46196900	10.90828500	7.25740000	C	5.50258900	13.82811000	3.37923900
C	5.59485000	10.10256100	7.94085900	C	5.63781400	11.77678700	2.10680300
H	6.00016100	9.81771800	8.90843700	C	4.69013900	14.38344000	2.38666500
C	4.25667800	9.83790700	7.63086500	H	5.76615100	14.42234700	4.24956000
H	3.61359600	9.34584800	8.35586500	C	4.81384400	12.32473000	1.12300700
C	3.75417000	10.21040300	6.38278400	H	6.03854100	10.77504400	1.98186600
H	2.71435800	10.01452000	6.13238900	C	4.34270200	13.63399200	1.25892200
C	4.58234200	10.83829400	5.44688300	H	4.32960200	15.40349300	2.49427700
H	4.17427200	11.11504100	4.47938700	H	4.55973500	11.73600100	0.24535100
C	7.96901300	13.10545600	5.30704800	H	3.71394400	14.07084000	0.48734100
C	7.40462800	13.83818300	6.36275200	C	9.77915100	12.15450300	0.92525900
H	6.41021900	13.59240600	6.72331500	C	10.84143500	12.39242300	0.03835900
C	8.11980000	14.87532100	6.96668500	C	8.95482300	13.23097300	1.29046700
H	7.67233100	15.43154600	7.78651200	C	11.06987600	13.67502300	-0.46820600
C	9.40510800	15.19616600	6.52089800	H	11.49410500	11.57823800	-0.26143300
H	9.96046200	16.00159200	6.99448000	C	9.17501000	14.50939300	0.77677400
C	9.97518500	14.47485200	5.46778700	H	8.13720100	13.06340300	1.98114300
H	10.97593300	14.71580100	5.11840900	C	10.23740600	14.73627700	-0.10278600
C	9.26321100	13.43406300	4.86899100	H	11.89927100	13.84298000	-1.15083200
H	9.70959000	12.85636100	4.06374600	H	8.52114500	15.32624400	1.07191600
P	9.05279500	8.60018700	4.91027800	H	10.41792300	15.73287300	-0.49752100
C	10.45809000	7.46459600	4.49561900				
C	11.59952800	7.30476100	5.29227400				
H	11.68002600	7.83072000	6.23912600				
C	12.64119300	6.46592700	4.87947700				
H	13.52183900	6.35387400	5.50739300				
C	12.54896400	5.77083900	3.67293200				
H	13.35884200	5.12047500	3.35278900				
C	11.41154300	5.92359600	2.87129700				
H	11.33722000	5.39708400	1.92355700				
C	10.38242200	6.77021100	3.27498400				
H	9.51507000	6.90500300	2.63327800				
C	7.70169400	7.36439500	5.18441600				
C	6.39155900	7.74437900	4.85597900				
H	6.21598300	8.73364900	4.44808400				
C	5.32350400	6.86586200	5.05064400				
H	4.31457400	7.18151800	4.79853400				
C	5.55511700	5.58925000	5.56819600				
H	4.72645000	4.90202300	5.71872600				

Ni(PPh₃)₂							
Ph ₃ P—Ni—PPh ₃							
E	=	-2242.46752288					
G _{corr}	=	0.477374					
Ni	-1.29396100	1.93989600	-0.01465100				
P	-2.05630200	3.89533300	-0.39166100				
C	-2.90685900	4.68036000	1.04850900				
C	-2.92276700	6.06035900	1.30058700				
H	-2.40181000	6.74269100	0.63516600				
C	-3.60553500	6.56620100	2.41017600				
H	-3.60949100	7.63690600	2.59783800				
C	-4.27870200	5.70093400	3.27677500				
H	-4.80640700	6.09736800	4.14033600				
C	-4.26366600	4.32376000	3.03557600				
H	-4.77761800	3.64491300	3.71121400				

C	-3.57601800	3.81677800	1.93231600
H	-3.54156300	2.74450000	1.74904300
C	-0.78470300	5.13978400	-0.88779800
C	-1.04785300	6.24955800	-1.70535000
H	-2.04718800	6.41224100	-2.09864200
C	-0.02687200	7.14952800	-2.02181100
H	-0.24123400	8.00564900	-2.65643800
C	1.26493800	6.95041900	-1.52691400
H	2.05764200	7.65051300	-1.77757200
C	1.53733600	5.84367400	-0.71733100
H	2.54230200	5.67831000	-0.33770000
C	0.51954000	4.94131000	-0.40474100
H	0.72737100	4.06599400	0.20767900
P	-0.47832600	0.01037100	0.38061300
C	1.09461800	-0.35527400	-0.51672900
C	2.10583800	-1.19260200	-0.02196100
H	1.99775700	-1.66135400	0.95189900
C	3.25894700	-1.42675100	-0.77584300
H	4.03668800	-2.07642000	-0.38248100
C	3.41365400	-0.82803100	-2.02913600
H	4.31276800	-1.01033300	-2.61200500
C	2.41368000	0.01287200	-2.52683800
H	2.53273900	0.48932800	-3.49655900
C	1.26451500	0.25246300	-1.77215600
H	0.49088800	0.92178200	-2.14355500
C	-1.57299200	-1.41201000	-0.05621600
C	-2.95735100	-1.20192800	0.06102500
H	-3.31827600	-0.22294300	0.37062900
C	-3.85786300	-2.22858500	-0.22596000
H	-4.92633800	-2.05308900	-0.13074200
C	-3.38482500	-3.47489800	-0.64777600
H	-4.08451000	-4.27356600	-0.87978800
C	-2.01011300	-3.68896200	-0.77922500
H	-1.63877000	-4.65463100	-1.11278900
C	-1.10687800	-2.66398200	-0.48463500
H	-0.04054000	-2.84177500	-0.59080400
C	-0.05242300	-0.30101200	2.15104400
C	-0.08176900	-1.56651100	2.75636800
C	0.32370900	0.81441600	2.91803000
C	0.27180400	-1.71296900	4.10040400
H	-0.38169000	-2.43866600	2.18255000
C	0.68179500	0.66609100	4.25867400
H	0.32171400	1.79866900	2.45368900
C	0.65626500	-0.59946600	4.85234500
H	0.24485100	-2.69764900	4.56008100
H	0.97050500	1.53730500	4.84100100
H	0.92793100	-0.71650200	5.89823700
C	-3.31162200	3.99829400	-1.74319100
C	-3.18790800	3.07364400	-2.79387100
C	-4.35815000	4.93237500	-1.77651500
C	-4.08031700	3.09473600	-3.86658700
H	-2.39165800	2.33260200	-2.75441900
C	-5.25489300	4.94829200	-2.84821400
H	-4.47739400	5.64674900	-0.96685400
C	-5.11664300	4.03286300	-3.89504300

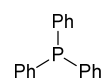
H	-3.97364100	2.37372500	-4.67299100
H	-6.06270100	5.67563100	-2.86345100
H	-5.81779200	4.04572700	-4.72549300

Ni(PPh₃)



E	=	-1205.85045751	
G _{corr}	=	0.227205	
Ni	9.72302200	9.91145400	3.80698600
P	9.17286800	8.33567900	4.96691400
C	10.27997700	6.85324400	4.86740700
C	10.52040500	5.98916200	5.94704100
H	10.05690100	6.17664400	6.91123100
C	11.35824500	4.88131700	5.79150200
H	11.53901600	4.22090100	6.63581900
C	11.96302800	4.62358500	4.55864900
H	12.61647000	3.76302300	4.44145500
C	11.73081900	5.48040000	3.47834600
H	12.20361500	5.28951000	2.51834800
C	10.89974700	6.59022700	3.63475500
H	10.73004800	7.27163600	2.80367600
C	7.49495200	7.63416900	4.61273500
C	6.49773300	8.52910500	4.19112600
H	6.75282300	9.57855900	4.05934100
C	5.20162400	8.08098700	3.93428700
H	4.43993700	8.78527700	3.60985700
C	4.88819000	6.72655400	4.08374700
H	3.88095300	6.37408500	3.87726900
C	5.87569200	5.82648700	4.49202900
H	5.63857700	4.77158100	4.60460100
C	7.17252900	6.27593400	4.75609500
H	7.92975400	5.56547400	5.07393300
C	9.10847500	8.68008700	6.78649000
C	8.16461000	8.11119900	7.65485400
C	10.07543400	9.55374800	7.31125700
C	8.19490600	8.40486400	9.02127000
H	7.40390300	7.43827000	7.27069200
C	10.11028500	9.83975800	8.67626800
H	10.79406500	10.01296300	6.63552100
C	9.16763900	9.26571500	9.53510200
H	7.45646400	7.95970600	9.68329900
H	10.86568000	10.51605800	9.06806900
H	9.18775600	9.49345700	10.59765400

PPh₃



E	=	-1036.54805321	
G _{corr}	=	0.228088	
P	-1.33822500	-0.20916800	-0.01106700

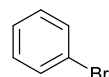
C	-0.49056200	0.65826200	-1.41058800
C	-1.08786100	0.55928300	-2.67884800
C	0.69563800	1.39704900	-1.27931000
C	-0.50573100	1.16860500	-3.79121200
H	-2.01393800	0.00067700	-2.79755200
C	1.27202100	2.01620100	-2.39123900
H	1.17486600	1.48781200	-0.30911600
C	0.67555600	1.90154900	-3.64912000
H	-0.97867100	1.07815100	-4.76575700
H	2.19061600	2.58559000	-2.27346300
H	1.12616600	2.38348700	-4.51284000
C	-0.49628800	0.52031500	1.46812700
C	-1.04301600	1.70211100	1.99702100
C	0.63639000	-0.03333400	2.08465800
C	-0.46285700	2.32381300	3.10358200
H	-1.92782100	2.13988000	1.53963200
C	1.21042300	0.58344600	3.19898000
H	1.07550200	-0.94690200	1.69537000
C	0.66520500	1.76377900	3.70925100
H	-0.89603700	3.23968000	3.49746900
H	2.08692800	0.14131200	3.66611400
H	1.11355500	2.24207700	4.57619200
C	-0.59117500	-1.90143100	-0.09580600
C	-1.25582700	-2.93147000	0.59084300
C	0.58661200	-2.20728600	-0.79589000
C	-0.74787500	-4.23162000	0.59154200
H	-2.17622700	-2.71534000	1.12918700
C	1.08920600	-3.51047700	-0.80332800
H	1.11558700	-1.42673100	-1.33446600
C	0.42562400	-4.52450000	-0.10823000
H	-1.27204200	-5.01638400	1.13092100
H	2.00170300	-3.73212600	-1.35122300
H	0.81808800	-5.53801100	-0.11533000

Phi



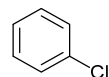
E	=	-243.107736972	
G _{corr}	=	0.058614	
C	2.37152000	-0.21742400	0.00004400
C	3.76861100	-0.23321200	0.00051100
C	4.46008500	0.98167600	-0.00005500
C	3.76413600	2.19271900	-0.00103700
C	2.36729000	2.19055000	-0.00148300
C	1.65935800	0.98487600	-0.00095000
H	4.31214000	-1.17186400	0.00128900
H	5.54689700	0.97369200	0.00029800
H	4.30771100	3.13330800	-0.00147300
H	1.81823800	3.12843600	-0.00226000
H	0.57433100	0.98727300	-0.00129000
I	1.31057300	-2.06376000	0.00090600

PhBr



E	=	-244.896841005	
G _{corr}	=	0.059764	
C	-0.85796100	0.70377900	0.00009600
C	0.53709300	0.72585000	0.00058500
C	1.25386900	1.92286100	-0.00001800
C	0.54635900	3.12815400	-0.00104900
C	-0.85051400	3.13003500	-0.00149500
C	-1.54762700	1.91946500	-0.00096300
H	-1.39816700	-0.23693400	0.00054500
H	2.33857700	1.91999100	0.00033700
H	1.09606600	4.06534300	-0.00150300
H	-1.39348900	4.07076600	-0.00228700
H	-2.63418700	1.91251600	-0.00132300
Br	1.50685400	-0.95204800	0.00213300

PhCl



E	=	-691.950425949	
G _{corr}	=	0.061491	
C	-0.85716900	0.70386000	0.00011200
C	0.53709400	0.72607000	0.00061000
C	1.25354400	1.92236600	-0.00000700
C	0.54680700	3.12722500	-0.00104300
C	-0.84999300	3.12910400	-0.00148800
C	-1.54697700	1.91855900	-0.00096300
H	-1.39124900	-0.24059900	0.00055500
H	2.33849700	1.91237000	0.00034100
H	1.09591200	4.06475600	-0.00151000
H	-1.39301300	4.06980900	-0.00229500
H	-2.63353100	1.91212000	-0.00133500
Cl	1.42199500	-0.80593300	0.00190100

PhH



E	=	-232.324141291	
G _{corr}	=	0.073358	
C	-0.58967400	0.46982000	0.00007300
C	0.80830200	0.46978900	0.00059400
C	1.50730200	1.68026600	-0.00009700
C	0.80833000	2.89101300	-0.00101000
C	-0.58944100	2.89104200	-0.00141100
C	-1.28854600	1.68039600	-0.00099600
H	-1.13306100	-0.47145200	0.00044300
H	1.35156700	-0.47156400	0.00138300

H	2.59421000	1.68036700	0.00014600
H	1.35195200	3.83214100	-0.00144800
H	-1.13292200	3.83226200	-0.00224200
H	-2.37546200	1.68056300	-0.00134700

Ph•



E	=	-231.634164717	
G _{corr}	=	0.059620	
C	1.08864700	-0.03769400	0.00006900
C	2.48722700	-0.02963100	0.00046900
C	3.19370500	1.17742900	-0.00006000
C	2.50180800	2.40134400	-0.00094100
C	1.12511300	2.33009200	-0.00131600
C	0.37481100	1.17352800	-0.00088100
H	0.54648100	-0.98062200	0.00048300
H	3.03049000	-0.97076800	0.00119500
H	4.28145500	1.17540900	0.00024800
H	3.03893100	3.34652400	-0.00135700
H	-0.71237300	1.18106900	-0.00119200

THF



E	=	-232.533046146	
G _{corr}	=	0.089224	
C	-1.56230200	-0.45607500	-0.24398700
O	-0.20588500	-0.90584700	-0.08615900
C	0.64395600	0.21838200	0.19170000
C	-0.17133000	1.46792000	-0.15074900
C	-1.59214100	1.00795700	0.20704100
H	-1.85390200	-0.55044800	-1.30149300
H	-2.22154100	-1.10312100	0.34786000
H	0.92674500	0.21260800	1.25650900
H	1.56037900	0.12037000	-0.40278100
H	0.15644900	2.35268300	0.40361300
H	-0.10111600	1.68671800	-1.22326500
H	-1.74999800	1.07166800	1.29050300
H	-2.37879700	1.58492900	-0.28879800

THF radical



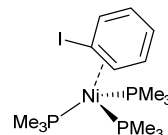
E	=	-231.874382497	
G _{corr}	=	0.075589	
C	-1.24722000	-0.70316900	0.08386900
O	0.10174200	-0.69340000	-0.43563800
C	0.60453000	0.57802300	-0.27297400

C	-0.47918200	1.56038500	0.07988100
C	-1.76070900	0.72121600	-0.13708100
H	-1.80208700	-1.47616200	-0.45435600
H	-1.22033300	-0.96284000	1.15191900
H	1.46881700	0.78697400	-0.89743500
H	-0.40745000	1.88985200	1.12873600
H	-0.45368500	2.46651100	-0.53792000
H	-2.57654100	0.98252500	0.54294400
H	-2.11662300	0.83286300	-1.16731300

H Abstraction TS: Ph• + THF

E	=	-464.165098393	
G _{corr}	=	0.161901	
v	=	-902.54 cm ⁻¹	
C	-1.83225600	0.60865000	0.00283100
C	-0.48010100	0.98016900	-0.00381900
C	-0.06053200	1.94830700	-0.90496600
C	-0.92424800	2.55791900	-1.80434300
C	-2.27557300	2.18081000	-1.79230100
C	-2.72469000	1.20981800	-0.89097300
H	-2.18644900	-0.14621200	0.70168700
H	0.22898300	0.52288900	0.68344600
H	-0.57330500	3.31260600	-2.50566400
H	-2.97413600	2.64468700	-2.48567200
H	-3.77274300	0.92112300	-0.88592900
C	2.66362800	2.10019400	-0.67812000
O	2.88774700	1.06445200	0.24846100
C	3.26725100	1.66796600	-2.00501800
H	2.99522800	3.05639800	-0.25961800
C	3.21888000	-0.15140200	-0.46370300
C	3.01532100	0.15209900	-1.95241100
H	4.34358300	1.88664200	-2.02737600
H	2.79627000	2.15951200	-2.86190900
H	4.26483000	-0.40086100	-0.23909900
H	2.58177700	-0.96078400	-0.09203600
H	3.68703000	-0.42773700	-2.59177300
H	1.98207700	-0.06356900	-2.24658200
H	1.44807700	2.19700900	-0.83631200

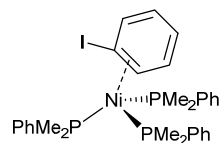
1-I-PMe₃



E	=	-1796.04683539	
G _{corr}	=	0.375599	
Ni	-1.26811300	-0.67801000	0.33288100
P	-0.49691400	0.41599500	-1.42677400
P	-0.41998400	-2.74211900	0.27898300
P	-3.49275500	-0.79442200	0.14759700

C	-0.64408300	0.70753700	1.96746700
C	-1.43510000	-0.15462000	2.77493900
C	0.77285400	0.58287800	2.01858100
C	-0.80473100	-1.08237600	3.63381500
H	-2.50027000	0.01709800	2.86637800
C	1.36575400	-0.35677900	2.85141500
H	1.38897500	1.24783800	1.42518800
C	0.57874000	-1.17944500	3.68269300
H	-1.42471600	-1.70667100	4.27268900
H	2.44965400	-0.44156600	2.86805400
H	1.05553600	-1.88671900	4.35609900
C	-4.44285100	-1.96379800	1.23501200
H	-4.31838800	-1.67142100	2.28393600
H	-5.51466100	-1.97781700	0.99779000
H	-4.04021300	-2.97649400	1.12037700
C	-4.55024100	0.72065100	0.33101800
H	-5.60908300	0.50714600	0.13461100
H	-4.45141200	1.12019800	1.34613800
H	-4.20507200	1.49143700	-0.36561900
C	-4.06364300	-1.38104300	-1.51866500
H	-3.70743500	-0.69010600	-2.28984300
H	-3.63621700	-2.36768700	-1.72659400
H	-5.15755600	-1.44600900	-1.58054600
C	-0.18396800	-0.62762500	-2.92948400
H	0.13470400	-0.01997800	-3.78578200
H	0.59583300	-1.36531700	-2.71329900
H	-1.10093600	-1.16298900	-3.19888300
C	-1.59011300	1.71185300	-2.18656800
H	-2.55887100	1.27203900	-2.44554400
H	-1.76238100	2.51509000	-1.46391700
H	-1.14299300	2.13825000	-3.09378500
C	1.09278500	1.36990000	-1.36062900
H	1.90379000	0.71876700	-1.01796100
H	1.35532600	1.78287000	-2.34264900
H	0.98995900	2.19729100	-0.65083400
C	1.41910900	-2.93097500	0.10034900
H	1.91456100	-2.44982700	0.95030800
H	1.72830400	-3.98326700	0.05299600
H	1.74728500	-2.42204500	-0.81304900
C	-0.99013200	-3.80969500	-1.13128200
H	-0.83253600	-3.29833400	-2.08530700
H	-0.45659100	-4.76855400	-1.15139400
H	-2.06214400	-4.00908500	-1.02617500
C	-0.72381800	-3.92968800	1.67408700
H	-0.23573200	-3.56738300	2.58242500
H	-1.80025700	-3.99008500	1.86934400
H	-0.34350600	-4.93215800	1.43972700
I	-1.40257900	2.78205300	1.67982500

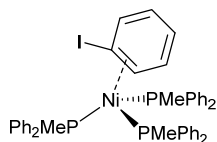
1-I-PMe₂Ph



E	=	-2371.43853795	
G _{corr}	=	0.523498	
Ni	-0.35032100	0.73709900	-0.43214600
P	0.16086700	0.76725700	-2.56401900
P	1.52361900	0.77784700	0.71676800
P	-1.92677800	2.20872300	-0.01240900
C	1.64705600	1.80645500	-2.91943100
C	1.55014700	3.20056600	-2.75606700
H	0.59812900	3.65163100	-2.49669800
C	2.67124900	4.01802000	-2.89440200
H	2.56899100	5.09189600	-2.75947000
C	3.91999600	3.45908300	-3.18594600
H	4.79647700	4.09438700	-3.28376700
C	4.03131600	2.07634100	-3.34794900
H	4.99629300	1.62985100	-3.57590100
C	2.90440000	1.25734800	-3.22021600
H	3.01860300	0.18520700	-3.35079600
C	-1.04503600	1.47237300	-3.79352400
H	-1.97498400	0.89634900	-3.73689100
H	-0.66101200	1.43668400	-4.82028600
H	-1.27236600	2.51052700	-3.53613700
C	0.56377900	-0.81857500	-3.44410500
H	-0.34874000	-1.42365800	-3.48017800
H	1.32109800	-1.38613100	-2.89429600
H	0.91381500	-0.65232700	-4.46955800
C	1.47031600	0.70449100	2.56692400
C	0.99771500	1.82851200	3.26934800
H	0.72377400	2.72690500	2.72300700
C	0.86984600	1.81104300	4.65697700
H	0.50797200	2.69504900	5.17660100
C	1.20289100	0.65908000	5.37914100
H	1.10159000	0.64230600	6.46120900
C	1.66855300	-0.46575100	4.69709200
H	1.93096300	-1.36636700	5.24705900
C	1.80340800	-0.44295100	3.30471100
H	2.17199300	-1.33165200	2.80099000
C	2.68606800	-0.61186000	0.30687500
H	2.17501900	-1.57631700	0.39735200
H	3.59218300	-0.62362900	0.92488500
H	2.97661400	-0.48381500	-0.74153000
C	2.68389800	2.20902400	0.48222200
H	2.17087300	3.15214600	0.68333500
H	3.01597700	2.22275700	-0.55862500
H	3.55831900	2.12430800	1.13764300
C	-1.34121200	3.89718700	-0.49873500
C	-1.79039800	4.56104500	-1.65241900
H	-2.57692700	4.12948400	-2.26316200
C	-1.23035900	5.78235400	-2.04362700

H	-1.58889700	6.27200000	-2.94581300
C	-0.21855500	6.37054100	-1.28251800
H	0.21793500	7.31789100	-1.58779600
C	0.22404700	5.73076800	-0.11926700
H	1.00577500	6.18142500	0.48729900
C	-0.32937800	4.50921300	0.26267200
H	0.03515400	4.01999300	1.16074000
C	-2.56023300	2.55145100	1.70302700
H	-3.16139800	1.69462900	2.02100300
H	-3.17768500	3.45677000	1.74241400
H	-1.72389400	2.64794700	2.40033600
C	-3.56797400	2.12295400	-0.88088300
H	-4.11114200	1.26490700	-0.47568600
H	-3.42880700	1.95085000	-1.95226200
H	-4.17015100	3.02699800	-0.73014700
C	-2.28197500	-1.10316800	1.60960400
C	-1.07563200	-1.29893500	0.90662100
H	-0.14760600	-1.41542200	1.45002800
C	-1.12880100	-1.54786500	-0.47938200
H	-0.23219700	-1.87209100	-0.99545300
C	-3.51297300	-1.13588200	0.96595500
H	-4.43465300	-0.98387400	1.51838500
C	-2.37684500	-1.57399200	-1.13676300
H	-2.41387100	-1.77764700	-2.20350700
C	-3.55122000	-1.37210500	-0.42165700
H	-4.51245900	-1.39831500	-0.92794400
I	-2.18505600	-0.77562200	3.70614600

1-I-PMePh₂



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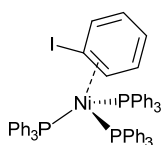
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C	7.91661900	7.63090000	1.43129600
H	8.30874800	8.44661000	0.82992200
C	6.75413400	6.97580600	1.02412600
H	6.26337400	7.27272200	0.10054500
C	6.21527600	5.94909200	1.80751700
H	5.30478500	5.44353400	1.49676600
C	6.85773700	5.57888000	2.99101900
H	6.44874800	4.78166300	3.60692100
C	8.02734700	6.23020200	3.39475200
H	8.50799600	5.93470000	4.32132700
C	10.80532800	7.33522500	4.51081100
C	11.01768200	7.96515900	5.74395500
H	10.68944200	8.99062500	5.86975200
C	11.63762300	7.29054600	6.79794200
H	11.78943500	7.80051300	7.74496900

C	12.04896600	5.96701900	6.62976700
H	12.52642300	5.43473500	7.44873000
C	11.84241500	5.32436500	5.40366500
H	12.15841900	4.29262100	5.26963700
C	11.22964700	6.00523800	4.35007700
H	11.06626800	5.49097000	3.40627400
C	11.18765000	8.03686400	1.77884300
H	11.42885000	6.97645600	1.64773800
H	12.10932700	8.58955700	1.98542400
H	10.75477700	8.41505700	0.84782200
P	8.38601300	11.73082900	2.29075000
C	7.86668600	13.29304100	3.13344900
C	8.85105000	14.17331800	3.62054200
H	9.89683600	14.00190300	3.37799600
C	8.50598000	15.26615200	4.41506300
H	9.28251200	15.93513200	4.77788100
C	7.16666300	15.49935800	4.74796400
H	6.89738100	16.34677600	5.37287100
C	6.18019500	14.63452700	4.26977800
H	5.13617500	14.80456000	4.52147000
C	6.52569800	13.54214600	3.46781300
H	5.74048100	12.87777700	3.12172800
C	9.46484600	12.38235000	0.92430700
C	9.19719600	13.58067500	0.24282200
H	8.34947900	14.19381700	0.53824000
C	10.01683400	13.99710800	-0.80808500
H	9.80092300	14.92844600	-1.32598000
C	11.11364400	13.21939000	-1.19538600
H	11.75166700	13.54671000	-2.01231600
C	11.38756100	12.02460400	-0.52573300
H	12.24111200	11.41711800	-0.81699900
C	10.56864200	11.61367200	0.52967900
H	10.78860400	10.69979700	1.07263500
C	6.88162700	11.30376900	1.28568700
H	6.50846500	12.16966600	0.72778200
H	6.09078700	10.90929400	1.92784800
H	7.16398100	10.51886900	0.57751600
P	7.89934200	10.37870700	5.52668400
C	8.00635100	9.06598800	6.83727500
C	8.61838700	9.28435900	8.08072400
H	8.96158100	10.27465700	8.35895600
C	8.81913700	8.22740600	8.97501500
H	9.30678100	8.41837000	9.92818700
C	8.40078500	6.93648400	8.64858500
H	8.56173300	6.11527500	9.34207600
C	7.77034900	6.71062500	7.42030600
H	7.43357100	5.71138000	7.15459700
C	7.58114600	7.76236300	6.52558000
H	7.10526300	7.56444800	5.57071000
C	6.10078500	10.28403300	5.09139800
C	5.72931900	9.40176000	4.06124400
H	6.49803300	8.82777500	3.55109000
C	4.39566600	9.28018300	3.66751800
H	4.13264700	8.58766800	2.87199600
C	3.41125900	10.06029900	4.28164800

H	2.37340000	9.97816100	3.96912900
C	3.77027100	10.95100800	5.29677300
H	3.01127700	11.56416400	5.77657600
C	5.10339800	11.05725200	5.70460500
H	5.35575400	11.75277400	6.49872700
C	8.01354000	11.92949200	6.53352100
H	7.39656800	11.90761000	7.43812300
H	7.71196700	12.77387000	5.90852800
H	9.05661500	12.07904200	6.82747500
C	11.65939000	11.83205200	5.04466600
H	10.82778400	12.43810800	5.38471300
C	12.46186900	11.12509300	5.94343400
C	13.52787000	10.33646900	5.50301700
H	14.13469500	9.77991400	6.20901900
C	11.95078100	11.75449600	3.67927300
H	11.34252300	12.30806200	2.97559900
C	13.01813800	10.97920800	3.22132500
H	13.23218200	10.93013900	2.15764700
C	13.80026300	10.26774600	4.13331800
H	14.62856800	9.65529300	3.78719700
I	12.04235400	11.22799100	8.02346000

1-I-PPh₃



$$E = -3522.20848963$$

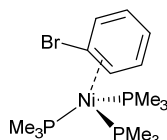
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C	9.02492700	9.39146600	1.01094400
C	7.77605900	9.18483900	1.61472400
H	7.52209600	9.73207800	2.51562300
C	6.85875200	8.28726600	1.06263200
H	5.88856100	8.15681900	1.53385600
C	7.18920600	7.56393900	-0.08561300
H	6.47831500	6.86113900	-0.51252600
C	8.44097400	7.74512800	-0.68201800
H	8.70678000	7.18217500	-1.57327100
C	9.35083800	8.65634200	-0.14164900
H	10.31395100	8.79956100	-0.62294000
C	11.78077900	10.14800500	1.08533000
C	12.34719700	8.99166700	1.64852400
H	11.78720000	8.42350400	2.38385600
C	13.63045400	8.57763100	1.29467100
H	14.05265300	7.68704400	1.75247700
C	14.37617600	9.31917400	0.37174900
H	15.38198600	9.00627900	0.10363300
C	13.82034500	10.46453100	-0.20215000
H	14.38963900	11.04330700	-0.92549700
C	12.52957900	10.87483700	0.14791500
H	12.11437400	11.77022100	-0.30390700

P	8.08400800	12.43759100	4.25442300
C	7.38743000	12.39178900	5.97250100
C	6.57900800	13.40649200	6.51036400
H	6.32535400	14.27660100	5.91178700
C	6.10507600	13.31369300	7.81987600
H	5.48673300	14.10947300	8.22801300
C	6.42576700	12.20105200	8.60529100
H	6.06142700	12.13212500	9.62721400
C	7.22367200	11.18554200	8.07569000
H	7.49369200	10.32690100	8.68229100
C	7.70474900	11.28323100	6.76796200
H	8.35228400	10.50947500	6.36440600
C	8.36729900	14.25016500	3.98895200
C	7.37441900	15.15901600	3.59041800
H	6.36101800	14.81361600	3.40974600
C	7.68075200	16.51030200	3.40756900
H	6.90135000	17.19953900	3.09244800
C	8.98039800	16.97557800	3.62684400
H	9.21583600	18.02653900	3.47991900
C	9.97550700	16.08083000	4.03049900
H	10.99356600	16.42473800	4.19531400
C	9.66919000	14.73094100	4.20505400
H	10.45178700	14.03438400	4.48645800
P	11.60352200	11.21891600	5.13972300
C	11.48232800	11.51471700	6.96856600
C	10.61033700	12.52396800	7.40744300
H	10.04901000	13.10032600	6.67920100
C	10.44282400	12.78664500	8.76774900
H	9.75784600	13.56926400	9.08306300
C	11.13165300	12.02643400	9.71657700
H	10.99205300	12.21818300	10.77737400
C	11.99904800	11.01565700	9.29314200
H	12.54147300	10.42098400	10.02427900
C	12.17850800	10.76511300	7.92996900
H	12.85790000	9.97714300	7.62106800
C	12.78906800	12.53442500	4.59222500
C	13.03329600	13.70822900	5.32144700
H	12.61040100	13.83524700	6.31288700
C	13.81755900	14.73219700	4.77946000
H	13.99285700	15.63521900	5.35910700
C	14.37745400	14.59607300	3.50741200
H	14.98535900	15.39357100	3.08819900
C	14.15429100	13.42233200	2.77985100
H	14.58864500	13.29692500	1.79117000
C	13.36425200	12.40554100	3.31438700
H	13.19621800	11.50395900	2.73695700
C	12.61030900	9.67218800	5.08226700
C	11.89329800	8.46902500	5.00284600
C	14.01129000	9.62707100	5.11580900
C	12.55634000	7.24205700	4.97081500
H	10.80938600	8.51046400	4.94754300
C	14.67889600	8.40021500	5.06364900
H	14.58414100	10.54769300	5.17794100
C	13.95455200	7.20633400	4.99561600
H	11.98625300	6.31835600	4.91163400

H	15.76567300	8.37734400	5.07954900
H	14.47657900	6.25371500	4.95767500
C	6.56710200	12.08443500	3.25162800
C	6.50102900	12.49821100	1.90874400
C	5.56317400	11.23359400	3.74250400
C	5.45852700	12.07637400	1.08395400
H	7.27065800	13.14609600	1.50228000
C	4.52333000	10.80609700	2.91195600
H	5.59801400	10.88766500	4.77132700
C	4.46661500	11.22458700	1.58035000
H	5.42896700	12.40662200	0.04868600
H	3.75729900	10.14495800	3.30984600
H	3.65922800	10.88936500	0.93451800
C	9.76264200	12.16537100	0.66706100
C	10.22113000	13.40974100	1.13234900
C	8.99627600	12.12414900	-0.50640600
C	9.90899900	14.58678500	0.45299200
H	10.80291800	13.45202900	2.04785500
C	8.67977400	13.30403800	-1.18665300
H	8.62514900	11.17648100	-0.88337100
C	9.12914600	14.53723000	-0.70720100
H	10.25512300	15.54008800	0.84320900
H	8.07413900	13.25772900	-2.08843900
H	8.87145400	15.45382700	-1.23160800
C	7.80575800	7.73887500	6.74728200
C	7.99227800	7.45094900	5.39253900
C	6.52564400	7.94048500	7.27119200
C	6.87693100	7.36890400	4.55481400
H	8.98485000	7.28841400	4.98818800
C	5.42067000	7.86371500	6.41805900
H	6.38643100	8.16415900	8.32294900
C	5.59266000	7.58129400	5.06088200
H	7.02266300	7.14542200	3.50342300
H	4.42543700	8.02702700	6.82273500
H	4.73114000	7.52333900	4.40165800
I	9.50022600	7.93387800	8.01184700

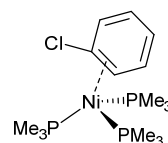
1-Br-PMe₃



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P		-0.53301100 0.31658100 -1.46597500
P		-0.52487800 -2.85111600 0.14705800
P		-3.52146500 -0.88934500 -0.01169600
C		-0.64872900 0.56034500 1.72586800
C		-1.45073200 -0.38760800 2.45563300
C		0.77447500 0.55081700 1.92940800
Br		-1.40745300 2.49600600 1.60739600
C		-0.80277500 -1.27845400 3.37164100

H	-2.50049100	-0.17436200	2.62947500
C	1.35950800	-0.37191600	2.76818400
H	1.38470700	1.28553200	1.41595500
C	0.56608200	-1.29132600	3.51144100
H	-1.42387900	-1.93454400	3.97825500
H	2.44208600	-0.38455900	2.87465800
H	1.04429600	-1.98115300	4.20243200
C	-4.42301500	-2.15916500	0.99657000
H	-4.22663700	-1.99063900	2.06118700
H	-5.50679500	-2.13368300	0.82561200
H	-4.05095100	-3.15679900	0.73842300
C	-4.56169000	0.60556300	0.32601400
H	-5.62913900	0.41252000	0.15888000
H	-4.41334900	0.92574100	1.36247900
H	-4.23859400	1.42587100	-0.32261800
C	-4.12455200	-1.35059700	-1.70441200
H	-3.79452800	-0.60541700	-2.43524400
H	-3.69795200	-2.31750800	-1.99240800
H	-5.21898100	-1.42060100	-1.74416300
C	-0.32714800	-0.70421900	-2.99747600
H	-0.04585900	-0.08420900	-3.85743900
H	0.45190100	-1.45732600	-2.83921600
H	-1.26579900	-1.21953700	-3.22528000
C	-1.60700800	1.67669400	-2.12107700
H	-2.60197300	1.28621400	-2.35604900
H	-1.71422100	2.44992800	-1.35524400
H	-1.18090100	2.12403000	-3.02786000
C	1.09928200	1.18794600	-1.42543600
H	1.88263300	0.49517900	-1.10080700
H	1.36186700	1.59213300	-2.41065500
H	1.04995100	2.01361500	-0.70907800
C	1.30806900	-3.08399000	-0.00967000
H	1.79864500	-2.64777800	0.86735200
H	1.58866400	-4.14187900	-0.09145900
H	1.66677800	-2.55078200	-0.89752400
C	-1.11515300	-3.85082500	-1.30098900
H	-0.87693900	-3.34735100	-2.24149000
H	-0.65877400	-4.84867900	-1.31055800
H	-2.20277800	-3.96775100	-1.24139900
C	-0.89750200	-4.06455000	1.49874600
H	-0.39704300	-3.75492500	2.41933300
H	-1.97662700	-4.08094400	1.68690200
H	-0.56490000	-5.07514300	1.23076300

1-Cl-PMe₃



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G _{corr}	=	0.378569
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P		-0.55764000 0.32899600 -1.47456200

P	-0.50777400	-2.82674800	0.17771900
P	-3.51805700	-0.89376200	-0.00703100
C	-0.59406700	0.59627900	1.71104100
C	-1.46808300	-0.29594400	2.42879500
C	0.82382600	0.49428600	1.92764600
C	-0.88558700	-1.22766600	3.34910700
H	-2.50052900	-0.00528300	2.59762200
C	1.33934600	-0.46079600	2.77370600
H	1.48020600	1.19298300	1.41974500
C	0.47753300	-1.32584600	3.50738700
H	-1.55329400	-1.84916800	3.94226400
H	2.41711000	-0.54250900	2.89470400
H	0.90129100	-2.04571900	4.20318100
C	-4.39426100	-2.18248400	0.99880900
H	-4.19054800	-2.01476600	2.06215300
H	-5.47960400	-2.17420700	0.83612900
H	-4.00689900	-3.17230900	0.73347900
C	-4.58973400	0.57941500	0.33857500
H	-5.65117600	0.37241700	0.15119700
H	-4.46855900	0.88300100	1.38431300
H	-4.27264400	1.41668200	-0.29216300
C	-4.11504300	-1.35409600	-1.70184300
H	-3.80613000	-0.59276300	-2.42532900
H	-3.66347600	-2.30625500	-2.00062900
H	-5.20730700	-1.45302000	-1.73958200
C	-0.38227600	-0.68312600	-3.01665300
H	-0.11037900	-0.05955400	-3.87717700
H	0.39509300	-1.44142500	-2.87567300
H	-1.32670100	-1.19230800	-3.23415900
C	-1.61742900	1.71007600	-2.11218400
H	-2.62273900	1.33498700	-2.32888800
H	-1.69838200	2.48422700	-1.34377700
H	-1.20137300	2.15318800	-3.02585200
C	1.09127700	1.17148800	-1.44863400
H	1.86611300	0.45870500	-1.14705700
H	1.34733300	1.58498900	-2.43186900
H	1.06908700	1.98630300	-0.71878000
C	1.32816300	-3.04576800	0.01607000
H	1.81876000	-2.61397800	0.89500400
H	1.61836300	-4.10030900	-0.07723300
H	1.67976500	-2.50045700	-0.86744700
C	-1.08328200	-3.83137500	-1.27504100
H	-0.84809400	-3.32278300	-2.21350800
H	-0.61695100	-4.82479800	-1.28730600
H	-2.16998900	-3.95903800	-1.21972400
C	-0.86466500	-4.06014700	1.51877600
H	-0.37954400	-3.74882800	2.44675600
H	-1.94477700	-4.10023600	1.69824500
H	-0.50969300	-5.06201500	1.24598100
Cl	-1.18004200	2.35007400	1.48821100

TS-1-2-I-PMe₃

E	=	-1796.04680227
G _{corr}	=	0.377806
Ni		-1.26352300 -0.67705500 0.33125100
P		-0.49319800 0.41808800 -1.42936700
P		-0.41738100 -2.74270800 0.27411300
P		-3.49025200 -0.79489900 0.14889000
C		-0.65193400 0.70142700 1.96673200
C		-1.44280400 -0.15226100 2.78351300
C		0.76455700 0.57089800 2.01407500
C		-0.81404600 -1.07608100 3.64661800
H		-2.50809500 0.02041900 2.87226800
C		1.35688900 -0.36446700 2.85298600
H		1.38125500 1.22873700 1.41348500
C		0.56977200 -1.17748700 3.69272200
H		-1.43435600 -1.69412000 4.29126800
H		2.44054500 -0.45291000 2.86681500
H		1.04588300 -1.88149200 4.37002200
C		-4.43865900 -1.96586900 1.23595600
H		-4.31304200 -1.67468600 2.28504300
H		-5.51070500 -1.97991700 0.99986300
H		-4.03589600 -2.97832000 1.11966400
C		-4.54746000 0.71984700 0.33490200
H		-5.60646200 0.50636100 0.13942400
H		-4.44758600 1.11844200 1.35027900
H		-4.20313300 1.49133800 -0.36135800
C		-4.06207600 -1.38003700 -1.51751400
H		-3.70690700 -0.68802900 -2.28820500
H		-3.63435300 -2.36624300 -1.72690300
H		-5.15599500 -1.44553600 -1.57852200
C		-0.18287300 -0.62635100 -2.93197200
H		0.13413800 -0.01920600 -3.78923600
H		0.59726400 -1.36402300 -2.71690300
H		-1.10040600 -1.16182500 -3.19925200
C		-1.58838100 1.71337300 -2.18706200
H		-2.55781100 1.27341800 -2.44323800
H		-1.75879000 2.51696500 -1.46436800
H		-1.14356200 2.13929900 -3.09562600
C		1.09624500 1.37259300 -1.36594500
H		1.90829200 0.72148800 -1.02563200
H		1.35648000 1.78629800 -2.34827400
H		0.99469600 2.19959900 -0.65545400
C		1.42129200 -2.93150200 0.09305000
H		1.91791200 -2.44999900 0.94211600
H		1.73015900 -3.98388700 0.04594600
H		1.74838300 -2.42319200 -0.82104000
C		-0.99030400 -3.81227700 -1.13325200
H		-0.83202400 -3.30318100 -2.08842200
H		-0.45848700 -4.77210500 -1.15143100
H		-2.06261600 -4.00945300 -1.02725500
C		-0.71949500 -3.92544100 1.67324900
H		-0.23214600 -3.55839400 2.58014700
H		-1.79584300 -3.98654700 1.86866400

H	-0.33746200	-4.92819900	1.44302300
I	-1.40252700	2.78389900	1.68028700

TS-1-2-I-PMe₂Ph

E = -2371.42764175

G_{corr} = 0.528074

Ni	-1.74979600	3.37904100	0.08652900
P	-1.25700300	3.37594500	-2.08759300
P	0.19711900	3.46751600	1.17526800
P	-3.18227900	5.04013700	0.40522900
C	0.22338400	4.42093300	-2.47338700
C	0.12527000	5.82191800	-2.40823400
H	-0.82953400	6.29058400	-2.20004500
C	1.24784300	6.63044500	-2.58942200
H	1.14155100	7.71072300	-2.53162200
C	2.49978000	6.05661500	-2.83037300
H	3.37608500	6.68546600	-2.96456000
C	2.61346800	4.66594500	-2.89686100
H	3.58044300	4.20562000	-3.08533700
C	1.48655800	3.85685500	-2.72331500
H	1.60475900	2.77882900	-2.77767200
C	-2.50073400	4.10732400	-3.26200000
H	-3.41017400	3.49793500	-3.21666000
H	-2.13243100	4.12789600	-4.29483200
H	-2.75563800	5.12511400	-2.95682300
C	-0.85705500	1.84842200	-3.07423800
H	-1.77636400	1.27079000	-3.19962100
H	-0.13015900	1.22072200	-2.55110100
H	-0.46549500	2.10619300	-4.06485600
C	0.24234300	3.44704000	3.02459400
C	-0.25474700	4.56762800	3.71409200
H	-0.58457500	5.43953200	3.15489500
C	-0.35315500	4.57278000	5.10413200
H	-0.73991700	5.45112500	5.61537700
C	0.03834500	3.44773700	5.83971900
H	-0.04235400	3.44663000	6.92364800
C	0.54217000	2.33120900	5.16939600
H	0.85635400	1.45479100	5.73133800
C	0.64694100	2.33235800	3.77487500
H	1.03395000	1.44757700	3.27831600
C	1.40661600	2.12423200	0.74234000
H	0.97113900	1.13194300	0.89424700
H	2.34332000	2.19499100	1.30800400
H	1.63028600	2.23060700	-0.32445000
C	1.31282600	4.92262400	0.86607800
H	0.80123700	5.85834500	1.09729000
H	1.58856400	4.94103400	-0.19000300
H	2.22334900	4.85146400	1.47217100
C	-2.56082600	6.69432400	-0.15126100
C	-3.03570300	7.34926300	-1.29970700
H	-3.84846000	6.92494800	-1.87980500
C	-2.46872700	8.55522400	-1.72606700
H	-2.84810000	9.03793300	-2.62337800

C	-1.42442100	9.13709100	-1.00537300
H	-0.98241500	10.07254500	-1.33809000
C	-0.95784600	8.50839300	0.15409900
H	-0.15194300	8.95575500	0.73055300
C	-1.52017900	7.30274600	0.57214200
H	-1.14300400	6.82738600	1.47262900
C	-3.79051200	5.50597200	2.10333900
H	-4.43818500	4.70724900	2.47627800
H	-4.35562600	6.44505800	2.08417500
H	-2.94894400	5.60133400	2.79471200
C	-4.83229400	4.97139400	-0.44672900
H	-5.40135700	4.14467800	-0.01413500
H	-4.71330800	4.76566300	-1.51383800
H	-5.40447300	5.89713800	-0.31434800
C	-3.21971500	1.72218200	1.21338600
C	-2.14833900	1.07133600	0.55982800
H	-1.22477100	0.87105200	1.08685500
C	-2.40958100	0.39599000	-0.65537000
H	-1.59866600	-0.15288700	-1.12404000
C	-4.51196600	1.71698500	0.63370700
H	-5.33892600	2.18327600	1.15866500
C	-3.67143900	0.41121200	-1.22996700
H	-3.85287700	-0.11360100	-2.16409100
C	-4.72380900	1.09001600	-0.58596400
H	-5.71782600	1.10152200	-1.02581500
I	-3.12594700	2.00355000	3.34339400

TS-1-2-I-PMePh₂

E = -2946.81030933

G_{corr} = 0.678608

Ni	-2.39362100	0.71517600	-0.00066400
P	-1.97553200	-1.34589900	-0.75826200
C	-3.46716100	-2.39100200	-1.13934200
C	-4.19916500	-2.13501700	-2.31230600
H	-3.84503600	-1.39603300	-3.02235300
C	-5.39338900	-2.80742800	-2.57788300
H	-5.94095600	-2.58930000	-3.49155000
C	-5.88432000	-3.75371700	-1.67353500
H	-6.81693100	-4.27385500	-1.87550400
C	-5.16004400	-4.02879000	-0.51138400
H	-5.52448300	-4.76930200	0.19637300
C	-3.96231900	-3.35842100	-0.24950500
H	-3.41730600	-3.59028800	0.65937100
C	-1.01087200	-2.48029200	0.34458700
C	-1.30303000	-2.44361900	1.71661400
H	-2.05411100	-1.75321800	2.07901600
C	-0.63199200	-3.26890800	2.61987900
H	-0.88676900	-3.22520400	3.67557900
C	0.37083600	-4.12941500	2.16666000
H	0.90613800	-4.76518000	2.86725400
C	0.68640600	-4.16278300	0.80512500
H	1.46993700	-4.82456000	0.44414500
C	-0.00365800	-3.35224300	-0.10054800

H	0.25729600	-3.40661400	-1.15208900
C	-1.06777900	-1.52894500	-2.36988200
H	-0.99566900	-2.56911400	-2.70341200
H	-0.06344800	-1.10781500	-2.26212400
H	-1.59578300	-0.95879300	-3.13773700
P	-3.25839000	2.05537400	-1.59018800
C	-4.07333600	3.56101100	-0.88658100
C	-3.28606600	4.60666800	-0.36820900
H	-2.20677400	4.57303900	-0.47262100
C	-3.87175000	5.69803100	0.27183700
H	-3.24296200	6.49645200	0.65807800
C	-5.26185400	5.76331400	0.42031300
H	-5.71955400	6.60920900	0.92644800
C	-6.05421600	4.73424500	-0.08969500
H	-7.13495100	4.76933800	0.02124400
C	-5.46665700	3.64548700	-0.74168100
H	-6.10799400	2.85529600	-1.11677400
C	-2.22450500	2.78935000	-2.95081300
C	-2.50595200	4.02674200	-3.55252600
H	-3.32329300	4.63919100	-3.18338400
C	-1.74299900	4.48489100	-4.62971400
H	-1.97263200	5.44717800	-5.08075700
C	-0.69488100	3.70813100	-5.13187200
H	-0.10292400	4.06545600	-5.97057400
C	-0.41192900	2.47167500	-4.54664400
H	0.40574800	1.86188300	-4.92312900
C	-1.16693000	2.02296100	-3.46076100
H	-0.91751800	1.08307000	-2.98402500
C	-4.59287400	1.39595700	-2.70795000
H	-5.06532100	2.20613000	-3.27369800
H	-5.35181500	0.84512600	-2.15150300
H	-4.11717400	0.71386800	-3.41761200
P	-3.91743700	0.90510500	1.67732800
C	-4.07925000	-0.32754700	3.06774200
C	-3.71234300	-0.04448600	4.39281300
H	-3.35767400	0.94346900	4.66626000
C	-3.78440000	-1.02906000	5.38327000
H	-3.49275800	-0.78508500	6.40207800
C	-4.22735300	-2.31578600	5.07032100
H	-4.27898500	-3.08104700	5.84046500
C	-4.61005300	-2.60718300	3.75735300
H	-4.96283900	-3.60217500	3.49679100
C	-4.53696700	-1.62344900	2.77147700
H	-4.83438700	-1.87259800	1.75843700
C	-5.68271400	0.85021300	1.10247000
C	-6.02087000	-0.07802200	0.10667100
H	-5.24592300	-0.70235700	-0.32210300
C	-7.33499600	-0.19830100	-0.35132000
H	-7.56760000	-0.92885300	-1.12174900
C	-8.33483700	0.62584400	0.17098200
H	-9.35699900	0.54460200	-0.18974700
C	-8.01101000	1.55575000	1.16333800
H	-8.78163200	2.20192200	1.57661300
C	-6.69890600	1.66212400	1.63079700
H	-6.47812000	2.39393800	2.40030200

C	-3.86736800	2.50621200	2.60884900
H	-4.57230400	2.54959900	3.44471900
H	-4.08538800	3.31658000	1.90957800
H	-2.85705100	2.65540600	2.99801300
C	-0.69183200	2.27190600	0.58059200
H	-1.33550500	2.92606400	1.15707600
C	-0.27938700	1.01983400	1.10003400
C	0.75866100	0.29311100	0.45467200
H	1.07724000	-0.65953100	0.86219600
C	-0.00205700	2.79576800	-0.54047000
H	-0.27624500	3.77806400	-0.91214900
C	1.01689300	2.08860400	-1.15405900
H	1.53187500	2.51159800	-2.01121700
C	1.37587700	0.81386700	-0.66962100
H	2.16482100	0.24586200	-1.15657500
I	-0.35864800	0.72468200	3.24761900

TS-1-2-I-PPh₃

E = -3522.177200

G_{corr} = 0.828053

Ni	-0.14490500	0.11140500	0.08611000
P	0.02944800	-0.36614700	-2.17758100
C	-1.39465200	-1.03523500	-3.17176500
C	-2.52690600	-0.22688700	-3.35940400
H	-2.53202200	0.78160300	-2.97240800
C	-3.64607700	-0.70173700	-4.04205400
H	-4.50529100	-0.04966200	-4.17537000
C	-3.66086300	-2.00620400	-4.54578800
H	-4.53455200	-2.38221400	-5.07192600
C	-2.53951100	-2.81899100	-4.37062000
H	-2.53469900	-3.83403500	-4.76021900
C	-1.41447900	-2.33723600	-3.69434400
H	-0.55931600	-2.99169000	-3.56869200
C	1.31662500	-1.61430600	-2.66574200
C	1.56642600	-2.67107400	-1.78039100
H	1.05511200	-2.68966800	-0.82479200
C	2.48072100	-3.67576700	-2.10772900
H	2.66322900	-4.48401600	-1.40516300
C	3.17699700	-3.62064900	-3.31647100
H	3.89981300	-4.39273600	-3.56721400
C	2.94502000	-2.56219700	-4.20148600
H	3.48670300	-2.51027400	-5.14265900
C	2.01367400	-1.57177400	-3.88465500
H	1.83730900	-0.76171400	-4.58530300
P	-1.20480000	2.22888300	0.23277800
C	-2.16678800	2.71576200	1.77750900
C	-1.68233500	3.72247700	2.63591400
H	-0.78013900	4.26687800	2.38532900
C	-2.33533200	4.04202000	3.82840000
H	-1.92912400	4.82558000	4.46317300
C	-3.50229500	3.37129200	4.19879400
H	-4.01687100	3.62539200	5.12161600
C	-3.99480700	2.36525400	3.36737900

H	-4.89409300	1.81887100	3.63959100	C	-4.18714600	3.02279200	-3.31397200
C	-3.32743100	2.03418400	2.18696600	H	-2.46351000	3.87146900	-4.30209700
H	-3.72657300	1.21328400	1.60786600	H	-5.68318300	2.09622400	-2.06431800
C	-0.14550600	3.75277600	0.08685700	H	-4.86262700	3.19338700	-4.14789900
C	-0.68894600	5.02422800	-0.17521800	C	0.51711600	1.09461300	-3.21514500
H	-1.75778000	5.13611900	-0.32850000	C	1.32662600	2.06259500	-2.60656000
C	0.13159800	6.14958400	-0.24035100	C	0.12335700	1.29298700	-4.54863500
H	-0.30591900	7.12229900	-0.45003100	C	1.73281000	3.20460900	-3.29756300
C	1.51077800	6.02973500	-0.03336300	H	1.61601400	1.92625200	-1.57483100
H	2.14898400	6.90788700	-0.08764700	C	0.51923300	2.43980200	-5.24162800
C	2.05849900	4.77755500	0.24592100	H	-0.50346300	0.56139200	-5.04780000
H	3.12668500	4.66324600	0.40810300	C	1.32292300	3.39993900	-4.61885600
C	1.22987100	3.65408600	0.30690100	H	2.34881000	3.94403300	-2.79313300
H	1.66152800	2.68773600	0.51770500	H	0.19710700	2.58314000	-6.27004400
P	1.91455700	0.00775700	1.11200600	H	1.62296100	4.29394800	-5.15947600
C	2.10253300	0.87485000	2.74900100	I	-1.39476300	-0.76157800	3.45212600
C	1.11595200	1.77135200	3.16628100	C	-1.23931100	-1.42545300	1.36322200
H	0.23684700	1.90409400	2.55245900	C	-2.26925500	-1.02580000	0.47308600
C	1.23361000	2.46765000	4.37178900	C	-0.68116500	-2.72605600	1.21632900
H	0.44377500	3.15028200	4.67307700	C	-2.74949000	-1.93421300	-0.49622800
C	2.35069500	2.26852100	5.18361500	H	-2.84801600	-0.13755200	0.66863300
H	2.44666700	2.80393000	6.12478600	C	-1.13780900	-3.57989000	0.22529200
C	3.34775400	1.37177800	4.78144400	H	0.08294100	-3.06357400	1.90395000
H	4.22171100	1.21020600	5.40738900	C	-2.19751900	-3.19742700	-0.62064800
C	3.22503200	0.68165800	3.57566000	H	-3.57157900	-1.62848800	-1.13512800
H	4.00886200	-0.00722800	3.27524200	H	-0.68692500	-4.56416500	0.12519200
C	3.35559100	0.75866200	0.18155900	H	-2.58038600	-3.88931600	-1.36414900
C	4.11824100	1.83226000	0.67477900				
H	3.91588800	2.24632600	1.65545200				
C	5.13803800	2.40250100	-0.09252200				
H	5.70580300	3.23620300	0.31306100				
C	5.42938100	1.90852200	-1.36563100				
H	6.22306900	2.35386600	-1.95958300				
C	4.68368600	0.84044300	-1.86771000				
H	4.88362800	0.44448500	-2.85995800				
C	3.65563000	0.28430800	-1.10630000				
H	3.07145100	-0.51784000	-1.53307600				
C	2.62631600	-1.64948900	1.60742700				
C	2.18822600	-2.23311400	2.81107900				
C	3.54570100	-2.36561600	0.82772100				
C	2.64057900	-3.49037100	3.21157500				
H	1.48853100	-1.70078900	3.44622900				
C	3.99934300	-3.62675800	1.22717000				
H	3.92810900	-1.95029300	-0.09570000				
C	3.54712000	-4.19804200	2.41705400				
H	2.28403800	-3.91369100	4.14735000				
H	4.71432700	-4.15656500	0.60271100				
H	3.90200800	-5.17742600	2.72713000				
C	-2.43095300	2.58603300	-1.13411400				
C	-1.98067600	3.18800800	-2.32545400				
C	-3.77716800	2.18803700	-1.07432900				
C	-2.84684000	3.40652800	-3.39781600				
H	-0.94582900	3.49002200	-2.42692100				
C	-4.64549300	2.40936600	-2.14656200				
H	-4.17342400	1.70313200	-0.19336700				

TS-1-2-Br-PMe₃							
E	=			-1797.83515434			
G _{corr}	=			0.376299			
Ni		-1.23515300	-0.74540800	0.35925700			
P		-0.41258600	0.27447900	-1.44617500			
P		-0.56820900	-2.88579000	0.02357100			
P		-3.53500700	-0.92565200	-0.03821600			
C		-0.78466100	0.45242300	1.72307400			
C		-1.47471000	-0.46800500	2.56445000			
C		0.60166700	0.68369200	1.94410100			
Br		-1.85127300	2.67100200	1.70112100			
C		-0.75085500	-1.17774000	3.56317300			
H		-2.55637000	-0.45026800	2.63177100			
C		1.28503400	-0.04644900	2.90206600			
H		1.12104700	1.42405300	1.34748300			
C		0.61016100	-0.98718800	3.71782800			
H		-1.29288100	-1.84363300	4.23182700			
H		2.35556300	0.10513900	3.02465900			
H		1.15922000	-1.53250900	4.48142200			
C		-4.39638400	-2.31153100	0.83984600			
H		-4.23455900	-2.21499800	1.91913400			
H		-5.47566900	-2.31718200	0.64251800			
H		-3.97408500	-3.26971700	0.51817800			
C		-4.60876700	0.50338300	0.42556400			
H		-5.66899500	0.29325700	0.23581700			

H	-4.46708700	0.73853400	1.48450400	C	-4.60245000	0.50020800	0.41607500
H	-4.30153500	1.38579700	-0.14299600	H	-5.66013600	0.30174700	0.20174900
C	-4.08395800	-1.23399800	-1.78089400	H	-4.48170900	0.71859000	1.48094100
H	-3.81880200	-0.37676400	-2.40858900	H	-4.27450400	1.38717300	-0.13347500
H	-3.57368000	-2.11892700	-2.17546500	C	-4.07187900	-1.23082000	-1.79378000
H	-5.16776000	-1.39176900	-1.84440100	H	-3.79102500	-0.37525400	-2.41735300
C	-0.42072400	-0.73219000	-2.99808900	H	-3.57117000	-2.12176200	-2.18684400
H	-0.13842600	-0.12391200	-3.86578700	H	-5.15711700	-1.37395200	-1.86547700
H	0.28324600	-1.56581700	-2.91077000	C	-0.45636600	-0.72279600	-3.00113400
H	-1.42325600	-1.14036500	-3.16057000	H	-0.18172500	-0.10704200	-3.86594400
C	-1.37056400	1.75597500	-1.98073000	H	0.23681900	-1.56759000	-2.93824900
H	-2.37675900	1.44853000	-2.28417200	H	-1.46779600	-1.11339400	-3.14716700
H	-1.46190000	2.44249600	-1.13415900	C	-1.32384400	1.77771300	-1.89879200
H	-0.88621900	2.26352600	-2.82404700	H	-2.35560200	1.50771900	-2.14761000
C	1.31388500	0.93451400	-1.45576800	H	-1.35048500	2.44937300	-1.03562800
H	2.00849700	0.17445700	-1.08407200	H	-0.87026200	2.28512000	-2.75914900
H	1.61313000	1.23419700	-2.46726800	C	1.35451100	0.86194300	-1.46994700
H	1.37736800	1.81015100	-0.80290400	H	2.03222800	0.06450200	-1.14802900
C	1.23979400	-3.11216200	-0.28563700	H	1.63497800	1.18886600	-2.47834700
H	1.79613700	-2.61872100	0.51870100	H	1.46772400	1.70860800	-0.78692800
H	1.51709000	-4.17296200	-0.31834800	C	1.22930100	-3.12577900	-0.32556500
H	1.52306200	-2.64260800	-1.23358900	H	1.78745700	-2.62066700	0.47013300
C	-1.31818000	-3.91937900	-1.31365900	H	1.51269400	-4.18510800	-0.35009000
H	-1.15531400	-3.45720700	-2.29154500	H	1.50186100	-2.66394300	-1.28037900
H	-0.88670800	-4.92763900	-1.32211200	C	-1.33708900	-3.94376900	-1.33217700
H	-2.39715500	-4.00121900	-1.14572100	H	-1.17889600	-3.48393000	-2.31216400
C	-0.81645000	-3.98245800	1.48861000	H	-0.90711400	-4.95260700	-1.34034200
H	-0.23750000	-3.59375900	2.33090400	H	-2.41506200	-4.02274200	-1.15721600
H	-1.87340400	-3.97990900	1.77336600	C	-0.81284400	-3.98595000	1.47473700
H	-0.50121400	-5.01054500	1.27372600	H	-0.23132700	-3.58125500	2.30809600
				H	-1.86824100	-3.98399200	1.76514200
				H	-0.49325500	-5.01532000	1.27318800
				Cl	-1.92004300	2.54502000	1.66250700

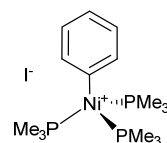
TS-1-2-Cl-PMe₃

$$E = -2244.88655801$$

$$G_{\text{corr}} = 0.375799$$

Ni	-1.23252900	-0.77061800	0.35454000
P	-0.39112000	0.25867200	-1.43565400
P	-0.57644300	-2.90774000	-0.00475400
P	-3.53626200	-0.93447600	-0.04528100
C	-0.81171000	0.42225500	1.71381400
C	-1.47089600	-0.49380800	2.58062200
C	0.55292000	0.73837300	1.94636900
C	-0.72318600	-1.14949700	3.59695800
H	-2.55301100	-0.53409500	2.63065500
C	1.26169900	0.06361700	2.92740900
H	1.03966300	1.49203100	1.33877400
C	0.62776900	-0.89436600	3.75400900
H	-1.23898100	-1.82481500	4.27664800
H	2.32172700	0.27205600	3.05724500
H	1.19668800	-1.39906200	4.53075000
C	-4.40836400	-2.31869500	0.82307900
H	-4.25148300	-2.22510400	1.90338200
H	-5.48661400	-2.31816000	0.62057300
H	-3.98935900	-3.27825100	0.50106900

2-I-PMe₃



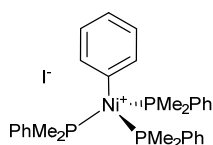
$$E = -1796.11261245$$

$$G_{\text{corr}} = 0.377983$$

Ni	-1.34730500	-1.28806300	-0.05416300
P	0.13800300	-0.01722600	-1.18121900
P	-0.74326100	-3.31385500	-0.98594800
P	-3.38744800	-1.83341900	0.77960900
C	-1.40212600	0.17175600	1.21355600
C	-0.58311700	-0.07766000	2.33232500
C	-2.13038100	1.37032500	1.19689000
C	-0.50799000	0.82572200	3.39705100
H	0.00752700	-0.99297300	2.37673000
C	-2.06431700	2.27712000	2.26125200
H	-2.74733200	1.61728900	0.33740200
C	-1.25519200	2.00708100	3.36738700

H	0.13665000	0.60906500	4.24593900	C	1.78079800	2.94429200	-2.11336300
H	-2.63841100	3.20024500	2.22009900	H	0.99525600	3.58972400	-1.72597600
H	-1.19802000	2.71332300	4.19147700	C	3.07396000	3.44542100	-2.25396700
C	-4.17399900	-3.48258900	0.51731200	H	3.28586700	4.47609100	-1.98256000
H	-3.71755800	-4.23001100	1.17070400	C	4.09701700	2.62168400	-2.73590100
H	-5.24152000	-3.41777800	0.75658500	H	5.10676600	3.00982600	-2.83720500
H	-4.06660900	-3.79909400	-0.52460100	C	3.81472900	1.30185700	-3.09310100
C	-3.72250400	-1.55861500	2.56705800	H	4.60250300	0.66018200	-3.47853500
H	-4.76834600	-1.79599500	2.79056600	C	2.51625700	0.79919600	-2.96166400
H	-3.07293400	-2.20615600	3.16517000	H	2.31275800	-0.22656100	-3.25384500
H	-3.51828600	-0.51916300	2.83195000	C	-1.10451400	2.08001100	-3.41792800
C	-4.60170000	-0.74448700	-0.07742700	H	-2.15989600	1.81491800	-3.49785400
H	-4.38939900	0.30462700	0.13486500	H	-0.63204500	1.93687000	-4.39520200
H	-4.53288800	-0.90699700	-1.15836500	H	-1.02745300	3.13158700	-3.13450600
H	-5.61960200	-0.97687200	0.25492300	C	-0.34322200	-0.63801200	-2.98027400
C	0.30723400	-0.41278500	-2.97778100	H	-1.40116300	-0.92107800	-2.96527500
H	1.02730700	0.27255900	-3.43854000	H	0.21637200	-1.38598600	-2.41389100
H	0.63944700	-1.43776400	-3.14998800	H	0.00159800	-0.62032500	-4.01913800
H	-0.66661300	-0.27684800	-3.46050400	C	1.14716200	-0.62951700	2.55119800
C	-0.19920200	1.78606700	-1.29012400	C	1.45641700	0.26353800	3.58868100
H	-1.20804000	1.95713700	-1.67873500	H	1.72115700	1.29385000	3.36992700
H	-0.10791900	2.25107200	-0.30809300	C	1.41400800	-0.15529900	4.92019600
H	0.52949200	2.24314900	-1.96761500	H	1.65607300	0.54785800	5.71276900
C	1.84127500	-0.06956900	-0.50175200	C	1.05762700	-1.46874400	5.23213400
H	2.21464300	-1.09595100	-0.47971500	H	1.01822900	-1.79257700	6.26864300
H	2.51211800	0.55459800	-1.10033800	C	0.74916600	-2.36439700	4.20474700
H	1.81716600	0.32185100	0.51907200	H	0.46676900	-3.38728700	4.43845000
C	1.07512900	-3.57170300	-1.19335200	C	0.79524300	-1.94965100	2.87368300
H	1.56618100	-3.46228800	-0.22087100	H	0.53333300	-2.65521100	2.09190400
H	1.25544700	-4.58580200	-1.56707500	C	1.86088200	-1.47795700	-0.10595000
H	1.51918100	-2.86034200	-1.89179100	H	1.14105000	-2.29705100	-0.18802700
C	-1.42120800	-3.78217700	-2.63240800	H	2.75963100	-1.83314900	0.40818900
H	-1.10520100	-3.05097000	-3.38243100	H	2.13178600	-1.14390100	-1.11082000
H	-1.07147600	-4.77688400	-2.93058100	C	2.47007900	1.19390400	0.77180600
H	-2.51570500	-3.78386200	-2.59297000	H	2.10410600	2.16724100	1.10966700
C	-1.12546400	-4.79071300	0.05803300	H	2.84129300	1.29838900	-0.24767800
H	-0.96087900	-4.55301400	1.11387900	H	3.29189900	0.87031300	1.41792400
H	-2.15987700	-5.10749500	-0.07955400	C	-2.92560300	3.11716200	-1.01631200
H	-0.47011100	-5.62201600	-0.22415700	C	-3.84648100	3.63320000	-1.93768500
I	2.81328000	3.68537600	0.96125000	H	-4.64668700	3.01278400	-2.32889900

2-I-PMe₂Ph



$$E = -2371.42764175$$

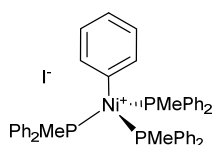
$$G_{\text{corr}} = 0.528074$$

Ni	-0.93316700	0.61845000	-0.00635200
P	-0.22208100	1.02092400	-2.19260500
P	1.11506900	-0.05969100	0.80551100
P	-2.99989100	1.40368700	-0.37598200
C	1.49144800	1.61233000	-2.45954500

C	1.78079800	2.94429200	-2.11336300
H	0.99525600	3.58972400	-1.72597600
C	3.07396000	3.44542100	-2.25396700
H	3.28586700	4.47609100	-1.98256000
C	4.09701700	2.62168400	-2.73590100
H	5.10676600	3.00982600	-2.83720500
C	3.81472900	1.30185700	-3.09310100
H	4.60250300	0.66018200	-3.47853500
C	2.51625700	0.79919600	-2.96166400
H	2.31275800	-0.22656100	-3.25384500
C	-1.10451400	2.08001100	-3.41792800
H	-2.15989600	1.81491800	-3.49785400
H	-0.63204500	1.93687000	-4.39520200
H	-1.02745300	3.13158700	-3.13450600
C	-0.34322200	-0.63801200	-2.98027400
H	-1.40116300	-0.92107800	-2.96527500
H	0.21637200	-1.38598600	-2.41389100
H	0.00159800	-0.62032500	-4.01913800
C	1.14716200	-0.62951700	2.55119800
C	1.45641700	0.26353800	3.58868100
H	1.72115700	1.29385000	3.36992700
C	1.41400800	-0.15529900	4.92019600
H	1.65607300	0.54785800	5.71276900
C	1.05762700	-1.46874400	5.23213400
H	1.01822900	-1.79257700	6.26864300
C	0.74916600	-2.36439700	4.20474700
H	0.46676900	-3.38728700	4.43845000
C	0.79524300	-1.94965100	2.87368300
H	0.53333300	-2.65521100	2.09190400
C	1.86088200	-1.47795700	-0.10595000
H	1.14105000	-2.29705100	-0.18802700
H	2.75963100	-1.83314900	0.40818900
H	2.13178600	-1.14390100	-1.11082000
C	2.47007900	1.19390400	0.77180600
H	2.10410600	2.16724100	1.10966700
H	2.84129300	1.29838900	-0.24767800
H	3.29189900	0.87031300	1.41792400
C	-2.92560300	3.11716200	-1.01631200
C	-3.84648100	3.63320000	-1.93768500
H	-4.64668700	3.01278400	-2.32889900
C	-3.71454600	4.94686000	-2.39407000
H	-4.42205500	5.33409000	-3.12193600
C	-2.67299200	5.75393500	-1.92877200
H	-2.57251200	6.77349900	-2.29092300
C	-1.75649100	5.24725500	-1.00150900
H	-0.94298900	5.87046400	-0.63946700
C	-1.87977500	3.93191500	-0.55199900
H	-1.14997600	3.52088600	0.14385500
C	-4.20131000	1.56148100	1.00890000
H	-4.44505300	0.57375100	1.40761400
H	-5.10956400	2.04289900	0.63083400
H	-3.77444200	2.17114000	1.80917200
C	-3.93471200	0.37476000	-1.57178800
H	-4.00956700	-0.63156400	-1.14541300
H	-3.41764900	0.31391800	-2.53077600

H	-4.94369100	0.76398300	-1.73494300
C	-1.73308900	-0.22470700	1.52769500
C	-2.26207200	-1.51159100	1.32920100
C	-1.81720100	0.32846600	2.81520800
C	-2.84055300	-2.22892000	2.38429000
H	-2.22579800	-1.96406100	0.33889500
C	-2.39034200	-0.38235700	3.87240400
H	-1.41541100	1.32170600	3.00190900
C	-2.90406000	-1.66633400	3.66151800
H	-3.23924500	-3.22563300	2.20631500
H	-2.43136800	0.06321800	4.86391100
H	-3.34887200	-2.22097100	4.48389400
I	-4.74170800	1.36343400	-5.45802900

2-I-PMePh₂



$$E = -2946.88279278$$

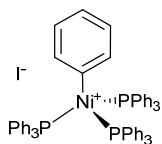
$$G_{\text{corr}} = 0.674795$$

Ni	9.47698500	10.32069500	4.06894500
P	10.06328100	11.20336200	2.04354300
C	8.80627800	11.80614100	0.83337800
C	8.42108500	13.15634000	0.82308500
H	8.86331700	13.86140400	1.51845800
C	7.44745700	13.60800500	-0.06972400
H	7.15909800	14.65531900	-0.05830100
C	6.84264300	12.72009400	-0.96165800
H	6.08412800	13.07365600	-1.65474000
C	7.22133100	11.37481000	-0.96096400
H	6.76247900	10.67705400	-1.65641000
C	8.19665500	10.92033400	-0.07163900
H	8.48402400	9.87361500	-0.09053500
C	10.86761100	9.83067600	1.12892900
C	10.39771800	8.52468500	1.34359600
H	9.59091200	8.35556500	2.05316100
C	10.98051200	7.44385500	0.68124500
H	10.61173500	6.43717000	0.85800600
C	12.04740400	7.65819800	-0.19585800
H	12.51093800	6.81750300	-0.70473200
C	12.52052800	8.95493400	-0.41360500
H	13.35159600	9.12448400	-1.09280000
C	11.93129800	10.03917800	0.24080200
H	12.31030400	11.04074000	0.06186000
C	11.28020400	12.58127900	2.08404100
H	11.45610200	12.98274200	1.08249500
H	12.21570800	12.21937700	2.51448200
H	10.88782000	13.37460700	2.72585400
P	7.23491000	10.94998900	4.04994400
C	6.31666000	10.72214100	5.62798400
C	6.74772400	11.43926700	6.75636800
H	7.58848900	12.12449000	6.68716800

C	6.10323300	11.27890200	7.98283200
H	6.45245900	11.84106500	8.84451500
C	5.02018200	10.40164300	8.09663400
H	4.51853400	10.27526000	9.05232000
C	4.58552200	9.68877100	6.97738100
H	3.74884100	9.00012500	7.05830200
C	5.22863600	9.84641700	5.74713800
H	4.88675700	9.26838700	4.89574600
C	7.21253800	12.77911900	3.85917100
C	6.11903200	13.46492600	3.31016600
H	5.24726600	12.92357100	2.95658300
C	6.14890300	14.85550900	3.19634900
H	5.30108700	15.37685100	2.76001800
C	7.26320700	15.57553100	3.63847800
H	7.28159600	16.65834500	3.54962100
C	8.34882600	14.90077800	4.20175100
H	9.21286700	15.45089500	4.56259300
C	8.32456300	13.50874100	4.30678000
H	9.17570900	12.99153300	4.73967400
C	6.08185600	10.32207900	2.76310700
H	5.06305000	10.68741600	2.91942100
H	6.07094900	9.22982900	2.78576700
H	6.43613300	10.64816400	1.78330600
P	9.42633400	8.77091800	5.70288600
C	10.76888300	7.51995600	5.55414600
C	11.86240200	7.51423500	6.43167900
H	11.91819700	8.22215000	7.25173100
C	12.91326400	6.61388900	6.24209300
H	13.75558200	6.62321100	6.92857500
C	12.88751900	5.71520700	5.17392500
H	13.70866800	5.01918000	5.02551700
C	11.79991100	5.71506600	4.29594600
H	11.77081200	5.01909800	3.46172100
C	10.74781000	6.61097700	4.48458900
H	9.91209500	6.59931600	3.79208300
C	7.91671300	7.72570900	5.66471700
C	7.38104100	7.39056200	4.41055800
H	7.84308200	7.78481500	3.50874300
C	6.25606900	6.57109500	4.31395300
H	5.85209200	6.31825600	3.33727200
C	5.64669000	6.08724300	5.47527100
H	4.76497600	5.45617600	5.40513300
C	6.17045500	6.42145900	6.72662700
H	5.69517400	6.05332700	7.63167500
C	7.30312600	7.23305200	6.82440900
H	7.69071200	7.48856900	7.80545300
C	9.56129200	9.41653700	7.41090900
H	9.72192700	8.61385300	8.13618900
H	8.64365300	9.95434000	7.65683300
H	10.39466500	10.12159500	7.45611300
C	11.39306200	10.42719000	4.45787000
C	11.70278400	11.45595700	5.36737400
C	12.45279500	9.66544700	3.94390100
C	13.02500500	11.72399000	5.73799300
H	10.91090300	12.05322100	5.81404200

C	13.77761500	9.93459500	4.30476000
H	12.25141600	8.84491600	3.26391700
C	14.07015100	10.96697000	5.20071200
H	13.22820400	12.52188700	6.44893500
H	14.58013300	9.32734800	3.89121300
H	15.09932400	11.17278100	5.48485100
I	9.81287400	13.92470900	8.17378800

2-I-PPh₃



$$E = -3522.24185588$$

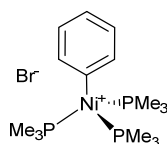
$$G_{\text{corr}} = 0.824754$$

Ni	9.35558800	10.48196500	4.19095400
P	9.33806700	10.20429700	1.79316600
C	7.96021900	9.26553800	1.03570300
C	6.75999300	9.90573200	0.68930600
H	6.67119500	10.98238100	0.76271200
C	5.66271600	9.16006700	0.25446200
H	4.74295500	9.67392600	-0.01081700
C	5.74405200	7.76823300	0.17010100
H	4.88745200	7.18989500	-0.16507500
C	6.92974900	7.12287300	0.52949300
H	7.00074900	6.03973600	0.48038800
C	8.02848900	7.86321200	0.96506700
H	8.93483300	7.34402000	1.25447900
C	10.89720200	9.46296200	1.13876800
C	12.09362300	9.81321300	1.78020900
H	12.06879800	10.40696400	2.68702200
C	13.32454900	9.41092100	1.26398900
H	14.23660900	9.67395500	1.79073000
C	13.37259200	8.63978400	0.10081400
H	14.32958700	8.31063000	-0.29470700
C	12.18677800	8.29392000	-0.55149900
H	12.21676800	7.70324600	-1.46330800
C	10.95417000	8.71282800	-0.04562100
H	10.04719400	8.45724500	-0.58271600
P	8.04590200	12.38190700	4.44131000
C	7.09975100	12.24380700	6.02106800
C	6.86620500	13.33692000	6.86596200
H	7.25012000	14.31984900	6.61613100
C	6.14643600	13.16785300	8.05203200
H	5.97861200	14.02306300	8.70103400
C	5.64975200	11.91157900	8.40592500
H	5.09282800	11.78504400	9.33023400
C	5.88304400	10.81568500	7.57066000
H	5.51540200	9.82962500	7.84167200
C	6.61042300	10.98117000	6.39299400
H	6.82715900	10.11817200	5.77501000
C	8.83714300	14.03860000	4.51089100
C	8.10737100	15.22525200	4.32243300

H	7.04216500	15.18746700	4.11804000
C	8.74761800	16.46347600	4.38881700
H	8.17374600	17.37319100	4.23476600
C	10.11855000	16.53340600	4.65202300
H	10.61529900	17.49863700	4.69962100
C	10.84696700	15.35922000	4.85643400
H	11.91197600	15.40314100	5.06682400
C	10.21050200	14.11893500	4.78675200
H	10.78320700	13.21277600	4.94473900
P	9.29762900	8.26094700	4.78439400
C	10.40071800	7.10217600	3.88040300
C	11.77144800	7.40577000	3.83196800
H	12.15872500	8.29896200	4.31275400
C	12.65761400	6.56899400	3.15319100
H	13.71202300	6.82592300	3.13266200
C	12.18320600	5.43529600	2.49110000
H	12.87236000	4.79292400	1.94967000
C	10.81904400	5.13517800	2.51930400
H	10.44058700	4.25818400	2.00070400
C	9.93082600	5.95882700	3.21342600
H	8.87545000	5.71215500	3.21699500
C	7.57902700	7.64624600	4.53624400
C	6.62033500	8.45692200	3.91284900
H	6.89426800	9.43961100	3.54904000
C	5.30540000	8.01510200	3.75644600
H	4.57989000	8.65993900	3.26970700
C	4.93614700	6.74987000	4.21461500
H	3.91466600	6.40091400	4.08961500
C	5.88291400	5.93249400	4.84119600
H	5.59909100	4.94913700	5.20580700
C	7.19346900	6.37884100	5.01010700
H	7.91473100	5.74456500	5.51682800
C	9.58452000	7.90507700	6.57131100
C	10.86257600	7.60673200	7.06489000
C	8.52453300	8.06961300	7.47848600
C	11.07343200	7.47630200	8.43875900
H	11.70226900	7.48055600	6.39174900
C	8.73863900	7.93428400	8.84990600
H	7.53023200	8.31331200	7.12094000
C	10.01539900	7.64173400	9.33514800
H	12.07079500	7.24810000	8.80418600
H	7.90759500	8.06725400	9.53760300
H	10.18502500	7.54333600	10.40396900
C	6.67956600	12.56409200	3.19951100
C	6.83045000	13.37612200	2.06206900
C	5.47541500	11.85705700	3.36363600
C	5.79883500	13.48971900	1.12777100
H	7.74619300	13.93096800	1.89960500
C	4.44953100	11.96674100	2.42354900
H	5.32103700	11.22525000	4.23070800
C	4.60456400	12.78695300	1.30366400
H	5.93816800	14.12725000	0.25933600
H	3.52548800	11.41529300	2.57471400
H	3.80354500	12.87681300	0.57503700
C	9.45268300	11.83337500	0.94571900

C	10.18258300	12.82161100	1.62179700
C	8.95366100	12.10261000	-0.33528100
C	10.37649400	14.07891900	1.04972600
H	10.58293500	12.60885300	2.60801100
C	9.14019200	13.36446300	-0.90392900
H	8.41293600	11.34053400	-0.88698000
C	9.84235300	14.35611700	-0.21165900
H	10.92543500	14.84008100	1.59695000
H	8.73708700	13.57204400	-1.89150100
H	9.97857800	15.33753600	-0.65758500
C	10.29692000	10.84724400	5.84082200
C	9.88322800	11.06101000	7.15975600
C	11.67531400	10.91487700	5.56393300
C	10.80842300	11.36991200	8.16368300
H	8.84090200	10.96629200	7.43094800
C	12.60294300	11.22961500	6.56329600
H	12.05447400	10.71609500	4.56488400
C	12.16990800	11.46515000	7.86977600
H	10.45676900	11.52515800	9.18136700
H	13.65995200	11.26353200	6.31408800
H	12.88804100	11.69946500	8.65141100
I	15.56255500	9.03535600	4.75823300

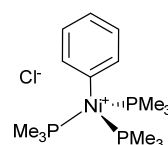
2-Br-PMe₃



E	=	-1797.88492862
G _{corr}	=	0.379868
Ni		-1.32885000 -1.27301000 -0.04172500
P		0.20292200 -0.14652300 -1.23590700
P		-0.87418800 -3.36374000 -0.90011100
P		-3.42015100 -1.63019400 0.77462500
C		-1.25284400 0.20514100 1.20714700
C		-0.47441800 -0.11853500 2.33617000
C		-1.88761100 1.45534300 1.19442200
Br		2.69629100 3.31741200 0.66042400
C		-0.36906200 0.75358300 3.42425100
H		0.05279800 -1.07220900 2.37381000
C		-1.78737100 2.33372800 2.28009300
H		-2.46682400 1.76182200 0.32812300
C		-1.03625400 1.98235200 3.40426700
H		0.23640300 0.47521800 4.28411300
H		-2.29350300 3.29595800 2.24360900
H		-0.95638800 2.66400500 4.24700000
C		-4.34160100 -3.21791200 0.58274300
H		-3.97045800 -3.96127900 1.29313500
H		-5.40466000 -3.04381500 0.78369600
H		-4.23552000 -3.60490400 -0.43505000
C		-3.78404900 -1.22210900 2.53140800
H		-4.84910200 -1.37713200 2.73658300
H		-3.19529100 -1.87180300 3.18710700

H	-3.51923500	-0.18352000	2.74081700
C	-4.50769000	-0.49347800	-0.18506100
H	-4.16326200	0.53766000	-0.08592700
H	-4.47383300	-0.77398000	-1.24336900
H	-5.54197100	-0.56287300	0.17031300
C	0.30829700	-0.65782500	-3.00936900
H	1.04754100	-0.03484300	-3.52519900
H	0.59150700	-1.70512100	-3.12700800
H	-0.66919600	-0.50673600	-3.47989600
C	-0.06454900	1.65830500	-1.44176900
H	-1.09584100	1.84923600	-1.75548500
H	0.14818800	2.18465000	-0.50979800
H	0.62015400	2.03415900	-2.20915600
C	1.91563800	-0.25285800	-0.58759700
H	2.16493100	-1.28617800	-0.33410000
H	2.62872200	0.13005000	-1.32481800
H	1.98860500	0.37485500	0.30564900
C	0.92668800	-3.74242100	-1.07265900
H	1.39957500	-3.66426900	-0.08803600
H	1.05246000	-4.76564300	-1.44367300
H	1.43185300	-3.05713100	-1.75559800
C	-1.57884400	-3.86745200	-2.52466800
H	-1.20206500	-3.21101400	-3.31416700
H	-1.31227900	-4.90387900	-2.76038700
H	-2.66974800	-3.77659400	-2.49376900
C	-1.36109200	-4.75926900	0.20736100
H	-1.15334800	-4.49717000	1.24987000
H	-2.42308700	-4.98396300	0.10305400
H	-0.79024100	-5.65686500	-0.05449800

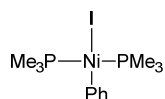
2-Cl-PMe₃



E	=	-2244.9507208
G _{corr}	=	0.382069
Ni		-1.31385700 -1.15926500 -0.02597300
P		0.87190400 -0.66263600 -0.52962100
P		-1.50140100 -2.82142200 -1.61872800
P		-3.40213100 -1.33931800 0.86406500
C		-1.04602300 0.14308100 1.37975500
C		-0.64618800 -0.24063400 2.67265600
C		-1.24315900 1.51413100 1.13611300
C		-0.44766500 0.70524400 3.68470100
H		-0.48415000 -1.29443200 2.89514900
C		-1.03507300 2.46586500 2.14035700
H		-1.57898700 1.82723100 0.14973500
C		-0.63699500 2.06569800 3.42057000
H		-0.14074000 0.38177600 4.67773100
H		-1.19220100 3.52142100 1.92576400
H		-0.47989100 2.80407900 4.20331800
C		-3.46710800 -2.77354900 2.02137300

H	-2.73170800	-2.62414100	2.81906200
H	-4.46187700	-2.88325400	2.46841600
H	-3.21061300	-3.69231500	1.48364200
C	-4.02328500	0.03787400	1.92121400
H	-5.01781500	-0.22354700	2.29968000
H	-3.35095300	0.22245000	2.76053200
H	-4.09465100	0.94976900	1.32131000
C	-4.87351300	-1.58555400	-0.22447900
H	-4.73343600	-0.99053900	-1.13103100
H	-5.00384100	-2.63660800	-0.48378900
H	-5.77379400	-1.24765700	0.29980100
C	2.06114500	-1.88818400	-1.24685900
H	2.98984900	-1.36955500	-1.51021800
H	2.29221800	-2.65228400	-0.49744600
H	1.67555200	-2.37963600	-2.14168400
C	0.87231700	0.69348700	-1.77115100
H	0.30067900	0.39382400	-2.65204000
H	0.37927200	1.56670500	-1.33641300
H	1.89819800	0.95519400	-2.05504200
C	1.95775600	0.01810400	0.79742400
H	2.05401000	-0.70455800	1.61293100
H	2.94988400	0.22045700	0.37853800
H	1.53955600	0.94248000	1.19943000
C	-1.00237500	-2.30761200	-3.31676700
H	0.00448600	-1.88636300	-3.34100700
H	-1.05097000	-3.15705300	-4.00781800
H	-1.70066300	-1.52537500	-3.62915300
C	-3.09176800	-3.66586200	-2.02131300
H	-3.80594600	-2.95359600	-2.43965900
H	-2.90017800	-4.44996100	-2.76296100
H	-3.51814100	-4.12966900	-1.12755200
C	-0.47920200	-4.31413200	-1.23834000
H	0.55240700	-4.05168500	-1.00078700
H	-0.90888700	-4.81262900	-0.36176000
H	-0.48608800	-5.01724100	-2.07927600
Cl	-2.83582000	0.67862500	-2.23140800

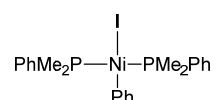
3-I-PMe₃



E	=	-1334.92584591	
G _{corr}	=	0.268058	
Ni	-1.11476700	0.34353300	-0.80171100
P	-2.83254200	1.74712700	-0.38873500
C	-4.00662500	0.92538200	0.76281300
C	-3.88587800	2.27764000	-1.80325600
C	-2.49905500	3.35681700	0.43969900
H	-4.84991500	1.58086500	1.00756600
H	-3.47554500	0.66042300	1.68321000
H	-4.66215500	2.97009300	-1.45845000
H	-4.35282900	1.40770400	-2.27045600
H	-1.83979900	3.96578500	-0.18646000

H	-2.00807800	3.19413800	1.40200500
P	0.67196600	-1.01929300	-1.00227300
C	1.20444200	-1.43400100	-2.71524700
C	2.26611400	-0.53010400	-0.22479400
C	0.33173900	-2.65216500	-0.22606000
H	1.50239900	-0.51567800	-3.23271500
H	0.37503800	-1.88799600	-3.26277500
H	2.62661500	0.40042500	-0.67276500
H	3.01206500	-1.31778000	-0.37822100
H	0.08847000	-2.50008300	0.83094700
H	1.20153800	-3.31416100	-0.30369400
H	-4.37744700	0.00685200	0.29839000
H	-3.26325900	2.78024000	-2.55092300
H	-3.44119600	3.89392800	0.59659400
H	2.05372800	-2.12634000	-2.69588600
H	2.12586500	-0.36330300	0.84626900
H	-0.52734600	-3.11633300	-0.71862200
C	-0.15254900	1.29019700	0.52112300
C	-0.26054300	0.91129300	1.87044600
C	0.43879600	1.59412800	2.87347000
C	1.26406700	2.67393200	2.54440800
C	1.38251300	3.06221400	1.20580200
C	0.68143200	2.37678600	0.20850500
H	-0.90022700	0.07401900	2.14459000
H	0.33846200	1.28235600	3.91130400
H	1.80787900	3.20608300	3.32099000
H	2.02175900	3.90131500	0.93810200
H	0.78509800	2.69294300	-0.82780600
I	-2.57756700	-1.17052900	-2.44665100

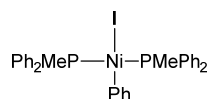
3-I-PMe₂Ph



E	=	-1718.51055427	
G _{corr}	=	0.367239	
Ni	-0.88779600	1.28886800	0.17164000
P	-1.92336000	0.82913900	-1.78754000
P	0.26010600	1.35214600	2.12148600
C	-0.67528100	0.97875500	-3.12273600
C	0.17869600	2.09458200	-3.08611000
H	0.07412500	2.82157300	-2.28383300
C	1.16445900	2.26221000	-4.05888300
H	1.81846800	3.12936100	-4.02106900
C	1.31626700	1.31002200	-5.07201300
H	2.08868300	1.43527000	-5.82615300
C	0.47624200	0.19482700	-5.10936500
H	0.59386700	-0.55021000	-5.89191200
C	-0.51654700	0.02775000	-4.13975100
H	-1.15528700	-0.84925400	-4.17888600
C	-3.30824500	1.89345700	-2.38107900
H	-4.11875700	1.87470800	-1.64533200
H	-3.67703700	1.52215900	-3.34353200

H	-2.96523600	2.92386300	-2.49482700	H	-0.85929600	-0.71651200	-5.95666500
C	-2.66097000	-0.84540100	-1.96651600	C	0.16694300	-0.11053300	-4.16546000
H	-3.37488400	-0.99081900	-1.14915000	H	0.49602000	-1.11775700	-3.93265000
H	-1.89174700	-1.61607000	-1.89342700	P	-1.64881200	1.91993700	1.32409500
H	-3.19204100	-0.93927300	-2.91917200	C	-2.53698900	3.20179400	0.35907200
C	-0.74057700	0.45272400	3.36839800	C	-2.70189200	2.99081300	-1.02110200
C	-2.11951100	0.72377300	3.40708900	C	-3.02546600	4.38427800	0.93415000
H	-2.54218400	1.44772000	2.71415900	C	-3.34331000	3.94576800	-1.81030600
C	-2.94526900	0.06053800	4.31509500	H	-2.31910900	2.08136000	-1.47616500
H	-4.00955900	0.27958400	4.33633200	C	-3.66543400	5.33960900	0.14042800
C	-2.40512000	-0.89018000	5.18704500	H	-2.90872200	4.57015300	1.99726000
H	-3.04869500	-1.41293900	5.88961000	C	-3.82457700	5.12336500	-1.23076800
C	-1.03722900	-1.16952100	5.14929900	H	-3.45904100	3.77006000	-2.87640100
H	-0.61333600	-1.91059800	5.82194200	H	-4.03749300	6.25394500	0.59497900
C	-0.20644700	-0.50179600	4.24501200	H	-4.31958300	5.87072000	-1.84522100
H	0.85305700	-0.73741600	4.22634800	C	0.99270800	2.54184100	0.50622100
C	1.92462100	0.57195000	2.14644100	C	1.99885500	2.30174600	1.45884700
H	1.86061600	-0.48950200	1.90095000	H	2.15173200	1.29291700	1.83856700
H	2.40016800	0.69913700	3.12415800	C	2.81231800	3.33790700	1.92999500
H	2.54105900	1.06613500	1.38830000	H	3.58366200	3.12686800	2.66803500
C	0.61216400	2.96358700	2.94520800	C	0.83268500	3.85612300	0.03627600
H	-0.32225000	3.48455000	3.16372400	H	0.05976600	4.07476300	-0.69649800
H	1.21182800	3.58905000	2.27601100	C	2.63609800	4.64213700	1.45598800
H	1.16223600	2.79221700	3.87704000	H	3.26658000	5.44889200	1.82150900
C	-0.19393500	-0.48166100	0.02175500	C	1.64277500	4.89679000	0.50605500
C	0.93378300	-0.74482900	-0.77601900	H	1.49655500	5.90690800	0.12853200
C	-0.78247000	-1.56246300	0.70173200	I	-1.53780000	-1.02051600	-0.82798900
C	1.45418100	-2.03833900	-0.89251800	C	2.24490000	-0.88259200	-1.75666400
H	1.40930000	0.06749900	-1.31981000	C	2.17290500	-1.68922300	-0.61165000
C	-0.26443000	-2.85765800	0.59114200	C	3.02320500	-1.30195300	-2.84790100
H	-1.65219600	-1.39181000	1.33091600	C	2.86529300	-2.90079000	-0.55788600
C	0.85690500	-3.10151300	-0.20804800	H	1.56421400	-1.36838000	0.22875500
H	2.32713000	-2.21452900	-1.51788300	C	3.70454300	-2.51880900	-2.79644100
H	-0.73844700	-3.67613600	1.12924400	H	3.08976900	-0.68643900	-3.74089600
H	1.26023700	-4.10739200	-0.29617100	C	3.62724000	-3.31853400	-1.65183000
I	-1.80826200	3.77488400	0.35355800	H	2.80247600	-3.51883100	0.33361100
				H	4.29705900	-2.84137100	-3.64839300
				H	4.16025400	-4.26482200	-1.61396900
				C	2.82720400	1.90142600	-1.92388000
				H	2.46800800	2.92885400	-2.01405300
				H	3.45830700	1.83463500	-1.03348000
				H	3.41217000	1.63694500	-2.80995400
				C	-2.95066600	0.81062100	1.99636100
				C	-4.31644900	1.01067400	1.75986800
				C	-2.54009000	-0.27427200	2.78799600
				C	-5.25943400	0.14033000	2.31480100
				H	-4.64904400	1.83976300	1.14302600
				C	-3.48318400	-1.13481900	3.34827600
				H	-1.48089300	-0.45454400	2.95614500
				C	-4.84662200	-0.92997400	3.11073600
				H	-6.31695700	0.30210000	2.12302500
				H	-3.15507100	-1.96990600	3.96148400
				H	-5.58165500	-1.60475500	3.54132800
				C	-1.07891600	2.75963700	2.86319800
				H	-0.47654100	2.04690600	3.43454700

3-I-PMePh₂



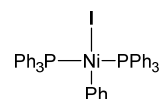
$$E = -2102.09126305$$

$$G_{\text{corr}} = 0.464839$$

Ni	-0.08211300	1.08796500	-0.07821600
P	1.40454700	0.74332100	-1.73438000
C	0.50619900	0.95557600	-3.32110600
C	0.04501500	2.24782700	-3.62684300
H	0.27767600	3.08052200	-2.96833400
C	-0.72810000	2.47045300	-4.76675600
H	-1.07753100	3.47454800	-4.99252800
C	-1.05479900	1.40449000	-5.61045700
H	-1.65854100	1.57655400	-6.49748300
C	-0.60502200	0.11715900	-5.30748700

H	-0.45721800	3.62292700	2.61751200
H	-1.93080700	3.06926300	3.47524500

3-I-PPh₃



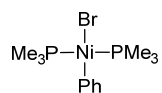
$$E = -2485.66788399$$

$$G_{\text{corr}} = 0.564945$$

Ni	-1.16813600	0.06610900	0.00127000
P	0.33072600	-0.35533400	-1.66331400
C	-0.18342600	-1.11965200	-3.26507600
C	-1.15088600	-0.43098300	-4.01739300
H	-1.58399100	0.48721600	-3.63162500
C	-1.56026900	-0.91475700	-5.25804200
H	-2.30787400	-0.36970500	-5.82798200
C	-1.01632400	-2.10096700	-5.76221500
H	-1.33917600	-2.48173800	-6.72752700
C	-0.05459500	-2.78936600	-5.02213000
H	0.37922600	-3.70747700	-5.40962900
C	0.36583600	-2.30055100	-3.78079900
H	1.12644300	-2.84267500	-3.23008000
C	1.68749500	-1.40972400	-1.02902300
C	2.96838700	-0.92242800	-0.74061500
H	3.23212200	0.10220000	-0.97736600
C	3.90584900	-1.74443300	-0.11055400
H	4.89354600	-1.35246200	0.11663100
C	3.57548400	-3.05638100	0.23437100
H	4.30765500	-3.69239000	0.72461500
C	2.29514000	-3.54527800	-0.04149100
H	2.02589400	-4.56150400	0.23363400
C	1.35175500	-2.72375100	-0.65761200
H	0.34893100	-3.10112400	-0.84149100
P	-2.42605900	0.95622900	1.66722300
C	-2.96952800	-0.28390200	2.90345200
C	-2.74442700	-1.64295200	2.63930300
H	-2.26819300	-1.93495400	1.70968200
C	-3.13215100	-2.61556300	3.56324600
H	-2.95211300	-3.66493600	3.34639100
C	-3.74524900	-2.23870600	4.76016100
H	-4.04849900	-2.99538600	5.47878000
C	-3.96093300	-0.88527500	5.03756000
H	-4.42855200	-0.58685600	5.97189700
C	-3.56938500	0.08906100	4.11899700
H	-3.71916800	1.13826300	4.35521900
C	-1.64899100	2.27388100	2.69854600
C	-1.73667600	3.62429300	2.32978200
H	-2.34210600	3.92371300	1.48006200
C	-1.04944700	4.60123900	3.05469500
H	-1.12951400	5.64382500	2.75819100
C	-0.27075400	4.24213800	4.15644500
H	0.26367700	5.00304200	4.71898300
C	-0.18233800	2.89866000	4.53187000
H	0.42558300	2.60746700	5.38411200
C	-0.86349000	1.92082300	3.80836400
H	-0.76625400	0.88042200	4.09876900

C	-3.92362000	1.78267300	0.99108700
C	-3.77366500	2.46539400	-0.22773900
C	-5.17343900	1.77347700	1.62295700
C	-4.84918800	3.15012100	-0.79234400
H	-2.81599700	2.44115300	-0.74207200
C	-6.25400600	2.44672600	1.04674400
H	-5.31733400	1.23176000	2.55163800
C	-6.09378200	3.13985900	-0.15534200
H	-4.72018700	3.67645100	-1.73425000
H	-7.22250500	2.42597400	1.53919600
H	-6.93684500	3.66233200	-0.59932800
C	1.04647700	1.21400000	-2.29543500
C	2.16829200	1.23232500	-3.13932300
C	0.36811000	2.41199400	-2.02887200
C	2.62306400	2.43764400	-3.67502300
H	2.68190000	0.30650300	-3.38243300
C	0.81705500	3.61581600	-2.57587000
H	-0.51053400	2.39731100	-1.38834000
C	1.94924800	3.63047800	-3.39345600
H	3.49750600	2.44444500	-4.32012300
H	0.28398500	4.53830900	-2.36180900
H	2.30330300	4.56684000	-3.81621700
C	0.36021900	0.43346100	1.09332000
C	0.73319500	-0.62022500	1.94787200
H	0.16774800	-1.54868900	1.94035700
C	1.83427000	-0.50620100	2.80156400
H	2.10458200	-1.33950900	3.44659100
C	1.11981200	1.61117000	1.13441000
H	0.84936100	2.45645700	0.51090900
C	2.58850700	0.67122600	2.82065800
H	3.44665500	0.76252600	3.48199000
C	2.22573100	1.72909100	1.98388000
H	2.79703400	2.65493300	1.99616900
I	-3.25565200	-1.14711300	-1.14193200

3-Br-PMe₃



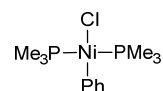
$$E = -1336.71315151$$

$$G_{\text{corr}} = 0.270212$$

Ni	2.07944600	0.17680000	-0.62344700
P	0.35120200	1.57309300	-0.28472500
C	-1.11884300	0.73094700	0.43233300
C	-0.28499500	2.34146800	-1.83066800
C	0.55356800	3.02613500	0.82478300
H	-1.95671700	1.42892800	0.54074500
H	-0.85674000	0.32924500	1.41723600
H	-1.16282200	2.96420200	-1.62415200
H	-0.54822900	1.55271000	-2.53996400
H	1.34103600	3.68097500	0.44121600
H	0.84768300	2.69261200	1.82399500
P	3.84578700	-1.17240100	-0.94103700

C	4.32071000	-1.37831800	-2.70653300
C	5.45458400	-0.76998500	-0.14695300
C	3.52929900	-2.88862900	-0.35829900
H	4.62482100	-0.40769000	-3.11310800
H	3.45613200	-1.73659400	-3.27085900
H	5.80498600	0.20738500	-0.49079400
H	6.20038500	-1.53251900	-0.39722700
H	3.34465300	-2.87380000	0.72141600
H	4.38509100	-3.54018300	-0.56874500
H	-1.40832200	-0.09996600	-0.21630900
H	0.49952900	2.96285500	-2.27605400
H	-0.38549700	3.58691000	0.88956400
H	5.15157600	-2.08575600	-2.80724400
H	5.33142400	-0.72330800	0.93854600
H	2.63742500	-3.27504200	-0.85893600
C	3.11041500	1.20800400	0.57785400
C	3.13036300	0.90450000	1.95084000
C	3.88880900	1.65948200	2.85351000
C	4.64930700	2.74197000	2.40037300
C	4.64267400	3.05876200	1.03839400
C	3.88237500	2.29912700	0.14173000
H	2.54431000	0.06544600	2.32320700
H	3.88543400	1.40210200	3.91107000
H	5.23915500	3.33032900	3.09899800
H	5.23104900	3.89843500	0.67302700
H	3.89164900	2.56112000	-0.91520000
Br	0.70472600	-1.19764500	-2.14301000

3-Cl-PMe₃



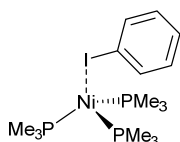
$$E = -1783.76597845$$

$$G_{\text{corr}} = 0.270514$$

Ni	0.11907600	0.69356100	0.02506100
C	2.00844400	0.65361100	-0.01394400
C	2.72715300	0.37054900	-1.18893900
C	2.75051500	0.90674000	1.15459800
C	4.12679400	0.33042200	-1.19756300
H	2.18664200	0.17396800	-2.11328100
C	4.14887700	0.87220900	1.15340900
H	2.22720700	1.13148400	2.08271800
C	4.84505900	0.58137200	-0.02470000
H	4.65628300	0.10573900	-2.12164200
H	4.69623600	1.07031500	2.07315800
H	5.93196800	0.55208800	-0.02812900
P	0.18217600	2.89527700	-0.39461500
P	0.18101400	-1.53705400	0.29706600
C	-0.46549900	3.86221500	1.02900500
H	-0.47734300	4.93623800	0.81132000
H	-1.47940000	3.51916900	1.25336300
H	0.16586900	3.67923000	1.90513600
C	1.78219600	3.71981300	-0.76708500

H	2.47367100	3.58424100	0.06913500
H	2.23331300	3.26887300	-1.65596700
H	1.62694100	4.79004400	-0.94338100
C	-0.87574100	3.41302800	-1.80640100
H	-1.89675200	3.06545900	-1.63091400
H	-0.86711500	4.50230200	-1.92561900
H	-0.50337700	2.94840900	-2.72589800
C	1.62394300	-2.30126100	1.14465600
H	2.54576900	-2.04227700	0.61825400
H	1.69338700	-1.92361800	2.16984900
H	1.51331300	-3.39110100	1.17131700
C	0.19754500	-2.34026000	-1.35903900
H	0.19609500	-3.43256700	-1.27018100
H	-0.68529700	-2.02049800	-1.92203800
H	1.09286400	-2.02432900	-1.90333100
C	-1.24283300	-2.33409100	1.14452200
H	-2.16881000	-2.05824600	0.63505600
H	-1.12880400	-3.42401100	1.14777700
H	-1.30037500	-1.97320400	2.17670600
Cl	-2.17902600	0.77818700	0.10558400

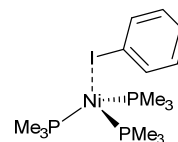
4-I-PMe₃



E	=	-1796.05427209	
G _{corr}	=	0.373122	
Ni	-2.68722900	0.81089200	-0.14483600
P	-3.66742600	2.35298400	-1.33936100
C	-4.12724100	3.96460900	-0.53499200
C	-5.27247300	1.96983200	-2.19612200
C	-2.68564800	2.99467000	-2.77863100
H	-4.59588600	4.66484600	-1.23905400
H	-3.22643400	4.43177500	-0.12107500
H	-5.63388500	2.80809800	-2.80629500
H	-6.03329400	1.72259800	-1.44666700
H	-2.49795800	2.17853500	-3.48385000
H	-1.71667800	3.36283000	-2.42427900
P	-1.16623200	1.73310900	1.13600600
P	-2.16836800	-0.96629500	-1.31013500
C	-0.15786000	3.08249200	0.34966300
C	0.21609300	0.75998900	1.91728000
C	-1.77927200	2.62888000	2.64378100
C	-2.08702200	-0.78017200	-3.15849700
C	-0.52550600	-1.79587300	-1.03129300
C	-3.28329900	-2.44705400	-1.19171800
H	0.56071800	3.52279600	1.05330600
H	-0.82054900	3.87287800	-0.01911800
H	0.90206800	1.40457900	2.48294300
H	0.78301900	0.23440000	1.14048900
H	-2.26883000	1.91306100	3.31371800
H	-2.52689100	3.37087000	2.34221100

H	-1.33754000	-0.02307900	-3.41440900
H	-3.05842500	-0.43812200	-3.53216600
H	0.27656600	-1.06442700	-1.18173000
H	-0.36514000	-2.64298000	-1.71165300
H	-3.31824700	-2.79186400	-0.15241400
H	-2.94596400	-3.27342000	-1.83071700
H	-4.81923500	3.77538200	0.29348600
H	-5.13810600	1.09232100	-2.83907800
H	-3.20690300	3.80573300	-3.30358300
H	-1.82479400	-1.72166200	-3.65894800
H	-0.46399900	-2.15854600	0.00041500
H	-4.29954000	-2.16130000	-1.48505500
H	-0.97077700	3.13259200	3.18940300
H	0.39084100	2.67317000	-0.50596000
H	-0.20104600	0.01164600	2.59919800
I	-4.60759000	0.05979400	1.50943800
C	-3.74504700	-1.46738800	2.74648800
C	-2.43050900	-1.84774600	2.48064100
C	-4.47725900	-2.05610400	3.77933100
C	-1.83481600	-2.83877200	3.26661500
H	-1.88769500	-1.36727400	1.67052800
C	-3.86942000	-3.04600100	4.55892400
H	-5.50138600	-1.75347900	3.97802900
C	-2.55145300	-3.43845900	4.30574800
H	-0.80943300	-3.13812100	3.06324900
H	-4.43136300	-3.50910000	5.36603500
H	-2.08648300	-4.20792900	4.91599800

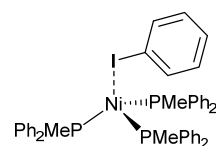
4-I-PMe₂Ph



E	=	-2371.44101625	
G _{corr}	=	0.520621	
Ni	-0.28787400	0.20661100	0.10664600
P	0.18039100	-0.32849400	-1.95012300
P	-1.74657500	-1.18795100	0.91742300
P	1.46724900	0.60923200	1.33973400
C	1.61298000	0.59628900	-2.66746200
C	1.47843700	1.98279500	-2.86850200
H	0.52004800	2.46489900	-2.68310900
C	2.55999000	2.75773000	-3.28437200
H	2.43089800	3.82639400	-3.43845200
C	3.81111000	2.16521800	-3.49236800
H	4.65804800	2.76987800	-3.80596100
C	3.96111900	0.79188200	-3.29249900
H	4.92758500	0.31986400	-3.45297300
C	2.87073800	0.01314200	-2.88869100
H	3.01475900	-1.05299800	-2.73942200
C	-1.10912300	-0.07017100	-3.26413700
H	-1.99249400	-0.66237800	-3.00145200
H	-0.75710400	-0.36467000	-4.26014900

H	-1.40721100	0.98290500	-3.28583900
C	0.61424100	-2.09892900	-2.29105100
H	-0.28291200	-2.69809000	-2.10241900
H	1.39836600	-2.43854600	-1.60728400
H	0.93577700	-2.26519300	-3.32624100
C	-3.00827200	-1.69701000	-0.33282300
C	-2.96309900	-2.92414800	-1.01450400
H	-2.23113400	-3.67770800	-0.73846900
C	-3.85221600	-3.19710200	-2.05973100
H	-3.79710700	-4.15286700	-2.57558700
C	-4.80864300	-2.25238100	-2.43683000
H	-5.49953800	-2.46517300	-3.24840900
C	-4.87090700	-1.02923800	-1.75853000
H	-5.61410300	-0.28721200	-2.04068700
C	-3.97706600	-0.75346100	-0.72453700
H	-4.02516700	0.20937200	-0.22172100
C	-2.84710400	-0.80550700	2.36607400
H	-3.49937000	0.03885200	2.13020300
H	-2.21855800	-0.51622200	3.21427500
H	-3.46533500	-1.66717100	2.64662300
C	-1.04631200	-2.80893700	1.48643900
H	-0.47370300	-2.61701800	2.40044200
H	-0.35382300	-3.20563600	0.73755800
H	-1.81890700	-3.55575300	1.70644800
C	1.12589300	1.41583100	2.96775900
C	0.48538900	0.67063700	3.97603200
H	0.28811500	-0.38751700	3.82115100
C	0.08073100	1.27022600	5.16821100
H	-0.40898700	0.67290000	5.93354000
C	0.29374900	2.63825800	5.37586700
H	-0.02987300	3.10943100	6.30019900
C	0.92366400	3.39189500	4.38345300
H	1.09363300	4.45545500	4.53249800
C	1.33880400	2.78651000	3.19214400
H	1.82243900	3.39574100	2.43437900
C	2.48281000	-0.85742600	1.85992600
H	1.86678700	-1.55922500	2.43073300
H	3.35425300	-0.57241100	2.46171700
H	2.82229200	-1.37101700	0.95331500
C	2.81483700	1.67729600	0.64188200
H	2.40139500	2.62710900	0.28881400
H	3.22727500	1.15696900	-0.22871100
H	3.62138500	1.87582800	1.35837600
I	-1.44110400	2.56136600	-0.15989300
C	-2.88546900	2.68983000	1.40893200
C	-2.44280900	2.66714800	2.73407600
C	-4.24858100	2.71056600	1.10017200
C	-3.38648500	2.66309400	3.76427800
H	-1.38431600	2.63012300	2.96203500
C	-5.18139700	2.69849300	2.14307900
H	-4.58209300	2.72224300	0.06702800
C	-4.75368400	2.67389600	3.47322300
H	-3.04317000	2.64091500	4.79518300
H	-6.24290800	2.70607800	1.90916900
H	-5.48305000	2.66175100	4.27856200

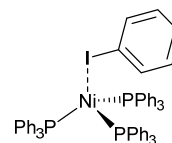
4-I-PMePh₂



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P	-0.98543800	0.74676200	-2.20350100
C	-2.46391900	0.01537400	-3.04233100
C	-3.61960600	0.79480500	-3.22201200
H	-3.60552300	1.85136600	-2.97239200
C	-4.79905600	0.22532700	-3.70660800
H	-5.68150400	0.84645100	-3.84011900
C	-4.84660400	-1.13715700	-4.01751500
H	-5.76548600	-1.58200400	-4.39025100
C	-3.70187900	-1.92070100	-3.84828100
H	-3.72587800	-2.98049800	-4.09003300
C	-2.52141000	-1.35023300	-3.36710700
H	-1.64344600	-1.97464500	-3.23504500
C	0.39138000	-0.25575400	-2.94565300
C	1.18449900	-1.03439800	-2.09175000
H	0.96426900	-1.04090500	-1.02982800
C	2.23077300	-1.81398100	-2.59398500
H	2.82480800	-2.41859800	-1.91409100
C	2.49685100	-1.82319900	-3.96430600
H	3.30987700	-2.42678100	-4.35989700
C	1.70702000	-1.05770200	-4.82960000
H	1.90518800	-1.06707300	-5.89864100
C	0.66061500	-0.28426800	-4.32503700
H	0.04632500	0.28864500	-5.01445200
C	-0.78944600	2.33820500	-3.15305800
H	-0.82484600	2.20361600	-4.23914700
H	0.17414600	2.78176200	-2.87966800
H	-1.57822800	3.03544700	-2.85646400
P	-2.59696000	2.30255300	0.77589800
C	-3.09004900	1.98731700	2.53046200
C	-2.24945500	2.37455000	3.58974200
H	-1.37184100	2.98029000	3.39117400
C	-2.52910400	1.99133200	4.90165500
H	-1.86381200	2.30540100	5.70186800
C	-3.65046100	1.20396800	5.18342600
H	-3.86481800	0.89995500	6.20478600
C	-4.49255700	0.81211900	4.14008000
H	-5.36581900	0.19719000	4.34320100
C	-4.21670500	1.20110800	2.82645600
H	-4.87655200	0.86660500	2.03243800
C	-2.05284300	4.07554500	0.82333500
C	-2.61771100	5.04128200	1.67162800
H	-3.39580200	4.75717300	2.37494000
C	-2.17460300	6.36504900	1.63519000
H	-2.61238700	7.09952400	2.30677000

C	-1.17321600	6.74740400	0.73623700
H	-0.83063500	7.77862600	0.70852200
C	-0.61460200	5.79768200	-0.12315900
H	0.16733100	6.08516500	-0.82180700
C	-1.04623500	4.46932000	-0.07001900
H	-0.58746200	3.71734300	-0.70439200
C	-4.26025600	2.53190400	-0.03134400
H	-4.91882100	3.16858300	0.57025600
H	-4.74084100	1.56432200	-0.19812600
H	-4.10098100	3.00756100	-1.00373700
P	-1.59155900	-1.08339300	1.02844700
C	-0.74825800	-2.61659900	0.42818400
C	0.52126900	-2.97649600	0.91420600
H	0.96757100	-2.42630100	1.73814600
C	1.23219800	-4.03503800	0.34129500
H	2.21227200	-4.29783500	0.73239300
C	0.68893100	-4.75432000	-0.72624800
H	1.24368200	-5.57492000	-1.17338100
C	-0.57602200	-4.40998200	-1.21250200
H	-1.01228900	-4.96539300	-2.03936400
C	-1.28515600	-3.35212500	-0.64263700
H	-2.26299300	-3.09261400	-1.03765600
C	-3.36699800	-1.60737000	1.03797600
C	-4.17455300	-1.19359900	-0.03314300
H	-3.73459800	-0.60023200	-0.82723100
C	-5.53278600	-1.51760000	-0.07462600
H	-6.13660600	-1.19138300	-0.91749800
C	-6.10821200	-2.24791300	0.96849900
H	-7.16748900	-2.49134000	0.94720000
C	-5.31408000	-2.66464000	2.04152500
H	-5.75564300	-3.23295600	2.85655900
C	-3.95232300	-2.35382600	2.07271000
H	-3.35499700	-2.68736000	2.91593200
C	-1.16001000	-1.11230300	2.83297500
H	-1.18345200	-2.11477000	3.27272900
H	-1.85851100	-0.46227000	3.36640300
H	-0.15758300	-0.69365200	2.95449400
I	1.25347100	1.44898500	0.79240700
C	1.25550300	2.52196600	2.64009800
C	1.32151900	1.81616300	3.84508600
C	1.10414600	3.91211600	2.62940300
C	1.21945500	2.51433100	5.05198400
H	1.43824000	0.73751400	3.84889000
C	0.99805600	4.59680100	3.84374000
H	1.04129600	4.45465800	1.69375700
C	1.04986400	3.90167100	5.05486900
H	1.26484100	1.96641100	5.98954200
H	0.86355400	5.67516400	3.83365400
H	0.95955600	4.43733200	5.99579600

4-I-PPh₃

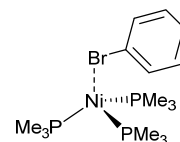


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G _{corr}	=	0.823783	
Ni	0.02935700	0.56132300	-0.37060700
P	0.50429900	0.70327600	-2.53514000
C	-0.53935200	-0.20767600	-3.77843700
C	-1.93168500	-0.21016300	-3.59155400
H	-2.35782600	0.29819200	-2.73554300
C	-2.77614300	-0.85984800	-4.49292800
H	-3.85000400	-0.84005600	-4.32754200
C	-2.24089600	-1.53054800	-5.59620900
H	-2.89526700	-2.04383500	-6.29610500
C	-0.85786500	-1.53513800	-5.79396200
H	-0.43120100	-2.04987000	-6.65135800
C	-0.01361900	-0.87353100	-4.89733500
H	1.05651100	-0.87856300	-5.07651700
C	2.19871000	0.20660400	-3.10240100
C	2.65172900	-1.06901700	-2.72932400
H	1.99749500	-1.72251900	-2.16197600
C	3.93652100	-1.49710600	-3.06047200
H	4.27089400	-2.48271400	-2.74884600
C	4.79657100	-0.64802500	-3.76471600
H	5.80447100	-0.97259100	-4.01024900
C	4.35432400	0.61974700	-4.14918200
H	5.01490900	1.28376200	-4.70130400
C	3.06068400	1.04288900	-3.82782800
H	2.73146200	2.03160800	-4.13216400
P	-1.58635600	1.99558400	0.19124100
C	-2.59999600	1.62418800	1.71017600
C	-3.69269300	2.40950900	2.11564600
H	-3.97404400	3.28858800	1.54402500
C	-4.43324500	2.06332500	3.24586600
H	-5.27595100	2.68017500	3.54845200
C	-4.09804900	0.92223900	3.98562800
H	-4.68060100	0.65250500	4.86304100
C	-3.01475400	0.13577700	3.59201700
H	-2.73922500	-0.75188300	4.15511600
C	-2.27240800	0.49230700	2.46240900
H	-1.42163200	-0.10353900	2.16075700
C	-1.13005700	3.77149600	0.49944100
C	-2.00247700	4.85813100	0.32263100
H	-3.00952400	4.69557300	-0.04786300
C	-1.57943400	6.16159400	0.59264800
H	-2.26649200	6.99064100	0.44225700
C	-0.28037500	6.40248900	1.05032500
H	0.04630100	7.41875200	1.25544500
C	0.59524700	5.32959900	1.23452200
H	1.61273400	5.49790900	1.57800600
C	0.17002900	4.02918700	0.95706700

H	0.86339800	3.20528900	1.06900300
P	1.77700200	0.31179100	0.95767400
C	1.51056500	0.15083100	2.79403800
C	0.66707200	1.08383800	3.41996000
H	0.21352600	1.87433100	2.83176200
C	0.38975800	1.00257100	4.78449200
H	-0.27007900	1.73480700	5.24231800
C	0.93698100	-0.03054900	5.55046300
H	0.70968900	-0.10565900	6.61066000
C	1.77751600	-0.96580200	4.94222400
H	2.21428100	-1.77040900	5.52875600
C	2.07033600	-0.87089200	3.57812800
H	2.73128900	-1.60449100	3.12865100
C	2.96404500	1.74367800	0.88744700
C	3.32148700	2.53237900	1.99175800
H	2.94763300	2.29327900	2.98144800
C	4.15602100	3.64428300	1.83305500
H	4.41446700	4.24591800	2.70104700
C	4.65989800	3.97714200	0.57406500
H	5.30661900	4.84230700	0.45371000
C	4.32910700	3.18367900	-0.52885400
H	4.71806500	3.42206500	-1.51566200
C	3.48736500	2.08380100	-0.37194400
H	3.23976100	1.48044300	-1.23634000
C	2.93420700	-1.11610100	0.66893100
C	2.37878400	-2.36632400	0.35380400
C	4.32959100	-1.01293700	0.77656000
C	3.19076000	-3.48361300	0.15265100
H	1.30404700	-2.46202600	0.24452000
C	5.14582200	-2.12630700	0.55982600
H	4.78801000	-0.06181700	1.02798700
C	4.58034800	-3.36561200	0.24971500
H	2.73781200	-4.44137800	-0.09116500
H	6.22528300	-2.02383900	0.63825500
H	5.21629300	-4.23119800	0.08307000
C	-2.94579300	2.14193800	-1.05880600
C	-2.82373300	2.99324800	-2.17149200
C	-4.03860100	1.25676600	-1.01330400
C	-3.76586200	2.96410000	-3.20067300
H	-1.98823700	3.68112500	-2.24038000
C	-4.97914500	1.22679100	-2.04587600
H	-4.15336700	0.58022700	-0.17200600
C	-4.84676400	2.08006700	-3.14488100
H	-3.64721900	3.63122300	-4.05057300
H	-5.81545500	0.53428600	-1.98929700
H	-5.57729300	2.05528600	-3.94920900
C	0.38895900	2.44260700	-3.16102900
C	0.82892200	3.46096200	-2.30126500
C	-0.15086000	2.79597500	-4.40635700
C	0.71984100	4.80297500	-2.66546900
H	1.23260100	3.19608000	-1.33119800
C	-0.26819200	4.14054300	-4.77021000
H	-0.49706300	2.02653900	-5.08940600
C	0.16115700	5.14699300	-3.90041100
H	1.04968300	5.57485500	-1.97511400

H	-0.70102400	4.40075300	-5.73305300
H	0.05879400	6.19190700	-4.18197000
I	-1.45173800	-1.75913200	-0.47396100
C	-1.80793800	-2.74648800	1.38587500
C	-3.02818200	-3.39465700	1.59685800
C	-0.84161700	-2.68650400	2.39243300
C	-3.27630500	-3.99091900	2.83716800
H	-3.77974900	-3.42873500	0.81380700
C	-1.10528900	-3.28054100	3.62979500
H	0.09408800	-2.16544500	2.23222700
C	-2.32021100	-3.93330800	3.85510900
H	-4.22449500	-4.49503900	3.00539900
H	-0.35713000	-3.21825600	4.41555000
H	-2.52264000	-4.39247800	4.81886600

4-Br-PMe₃



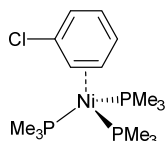
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$$G_{\text{corr}} = 0.373538$$

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C	1.04476600	10.88616800	11.53358300
C	-0.17310000	8.90367600	9.92072400
C	2.35001800	9.98124900	9.18057700
H	0.53744900	11.59665800	10.86742900
H	1.95751700	11.35489500	11.91808400
H	-0.59229100	9.75315700	9.36510200
H	-0.87690800	8.61839000	10.71145800
H	2.52272700	9.17751700	8.45700800
H	3.32577300	10.37950200	9.48024300
P	4.07279100	8.75247700	13.05470700
P	3.14001000	6.01293600	10.61320100
C	5.03007700	10.13205700	12.25640800
C	5.49159000	7.84249800	13.85119400
C	3.41930000	9.63857100	14.55162000
C	3.22336100	6.18681700	8.76240800
C	4.78883800	5.19064500	10.89178700
C	2.03526500	4.52359700	10.73607800
H	5.73103400	10.60910000	12.95390200
H	4.33601000	10.88988100	11.87719500
H	6.16212800	8.51879300	14.39820600
H	6.06852900	7.31664700	13.08201000
H	2.94351500	8.91342300	15.22134700
H	2.65300800	10.35484500	14.23632200
H	3.94726900	6.96783700	8.50407600
H	2.24290900	6.49184000	8.38055300
H	5.58779700	5.92142100	10.72188300
H	4.94673300	4.33248700	10.22454000
H	2.00854200	4.17335600	11.77368500
H	2.37444500	3.70160900	10.09218000

H	0.39063600	10.67328000	12.38705700
H	-0.07021500	8.05016400	9.24130100
H	1.76915800	10.77816700	8.69836200
H	3.52067800	5.25109200	8.27049300
H	4.86066600	4.84527900	11.92885700
H	1.01547500	4.80380500	10.45015900
H	4.20618100	10.16954000	15.10315200
H	5.59316500	9.73434600	11.40472600
H	5.10300000	7.09690700	14.55306600
Br	0.78679500	6.93691200	13.42165500
C	1.54549600	5.54112800	14.54133900
C	2.88301100	5.21043900	14.34091400
C	0.76483800	4.90026100	15.50304200
C	3.45709900	4.20897300	15.12831300
H	3.44872100	5.73774400	13.57797200
C	1.35345300	3.89972500	16.28322600
H	-0.27741900	5.16971800	15.64471900
C	2.69538000	3.55277200	16.09917700
H	4.50105000	3.94497200	14.97879400
H	0.75658000	3.39264500	17.03666600
H	3.14419900	2.77438900	16.70997000

4-Cl-PMe₃



$$E = -2244.8916434$$

$$G_{\text{corr}} = 0.374356$$

Ni	2.96763800	1.19341500	-0.21067500
P	1.42451200	2.48576500	-1.01080600
C	0.61658500	3.83252300	-0.01261100
C	-0.08931100	1.74478400	-1.79610600
C	2.06728700	3.50082600	-2.42905000
H	-0.06989300	4.44155200	-0.61589300
H	1.39024500	4.48423300	0.40926700
H	-0.75313000	2.50747900	-2.22445900
H	-0.64922800	1.17437300	-1.04681500
H	2.48475700	2.83889600	-3.19503800
H	2.87412600	4.14927200	-2.07020400
P	4.17358500	1.96282900	1.41499500
P	3.38857800	-0.52025200	-1.46374200
C	5.06139000	3.55136100	1.03556400
C	5.57838200	0.99280200	2.15839500
C	3.28210000	2.43981400	2.97221000
C	3.67382100	-0.12280300	-3.25687100
C	4.82943300	-1.66474500	-1.17488700
C	2.03958200	-1.78884300	-1.63713600
H	5.66345000	3.90083400	1.88423000
H	4.32835100	4.32330900	0.77664500
H	6.07691900	1.52891100	2.97689800
H	6.31561000	0.76872800	1.37865900

H	2.86132300	1.54411300	3.43911100
H	2.45402400	3.11187300	2.72367200
H	4.50796300	0.58145600	-3.35034000
H	2.77796200	0.35372100	-3.66926400
H	5.76047800	-1.08677100	-1.20425100
H	4.88281100	-2.46816500	-1.92134800
H	1.84976700	-2.26542900	-0.66925100
H	2.30257100	-2.56801300	-2.36409100
H	0.05845900	3.38731200	0.81762700
H	0.21670600	1.05495000	-2.59061700
H	1.28270200	4.12317700	-2.87819900
H	3.89982600	-1.02128200	-3.84548600
H	4.74629200	-2.11182400	-0.17735200
H	1.11713900	-1.29443500	-1.96033000
H	3.94746900	2.93379800	3.69217000
H	5.71772900	3.40626400	0.17018100
H	5.19280700	0.04063300	2.54049000
C	0.27772800	0.11414900	2.65444300
C	1.12778100	-0.45978700	1.71067700
C	0.49229800	-0.02861200	4.02533200
C	2.22525300	-1.20031700	2.16197600
H	0.94328500	-0.33277500	0.64952100
C	1.59497800	-0.77038200	4.45747900
H	-0.18581200	0.42879700	4.73825800
C	2.46123300	-1.35690500	3.52964800
H	2.89605900	-1.64127200	1.43265600
H	1.77273300	-0.88744000	5.52293500
H	3.31695800	-1.93198300	3.87178500
Cl	-1.12298600	1.03953700	2.09739300

TS-4-5-I-PMe₃

$$E(\text{OSS}) = -1796.04522643$$

$$E(\text{T}) = -1796.02982302$$

$$S^2(\text{OSS}) = 0.5095$$

$$G_{\text{corr}} = 0.371742$$

$$v = -270.05 \text{ cm}^{-1}$$

Ni	-2.77813800	0.80421700	-0.02224200
P	-3.57721000	2.39008800	-1.38115000
C	-3.99742900	4.01400400	-0.60033400
C	-5.15366100	2.00546100	-2.26987200
C	-2.50314000	2.94822300	-2.78148200
H	-4.43538900	4.71222600	-1.32468500
H	-3.09097100	4.46403300	-0.18160900
H	-5.45994800	2.82258900	-2.93510800
H	-5.94413500	1.82251000	-1.53430800
H	-2.33323500	2.11347300	-3.46787900
H	-1.53204900	3.27180900	-2.39245000
P	-1.23823500	1.85676400	1.23939000
P	-2.29799600	-1.00269400	-1.27498800
C	-0.08894000	3.00078500	0.34243500
C	-0.01836000	0.89022300	2.24729000

C	-1.91564400	2.98860800	2.53835100	C	4.07651300	1.80578500	-3.35211200
C	-2.27862900	-0.79961800	-3.11662200	H	5.01953100	2.28344800	-3.60462800
C	-0.66522600	-1.85110300	-1.03576200	C	4.00723200	0.41876600	-3.20805900
C	-3.45658000	-2.43370100	-1.09571500	H	4.89699700	-0.18917600	-3.35284500
H	0.62494300	3.47568900	1.02696100	C	2.79376100	-0.19783300	-2.88301000
H	-0.66179500	3.78404000	-0.16544300	H	2.76314800	-1.27867200	-2.78019400
H	0.69312600	1.54968000	2.76036000	C	-1.13608100	0.37873000	-3.42406300
H	0.53632100	0.20553300	1.59624300	H	-2.10967800	-0.08174100	-3.22527700
H	-2.52675700	2.40545000	3.23548600	H	-0.78970600	0.08226300	-4.42096500
H	-2.56546400	3.73232300	2.06560700	H	-1.26287600	1.46488700	-3.39174200
H	-1.48434700	-0.10029100	-3.39835900	C	0.19298300	-1.95197600	-2.46805600
H	-3.23581800	-0.38839200	-3.45414900	H	-0.78881200	-2.40778800	-2.30127800
H	0.14566800	-1.13011300	-1.18887300	H	0.90570600	-2.42060200	-1.78232000
H	-0.53339600	-2.68860600	-1.73293600	H	0.50180200	-2.14282000	-3.50221400
H	-3.46471100	-2.76340900	-0.05171200	C	-2.93155400	-1.72693300	-0.32548100
H	-3.17153000	-3.27582400	-1.73866400	C	-3.12564100	-3.06345900	-0.70374700
H	-4.70685500	3.84997200	0.21723700	H	-2.53585600	-3.85551200	-0.25205700
H	-5.02475500	1.09176400	-2.86038000	C	-4.07750100	-3.39532300	-1.67461500
H	-2.96088400	3.77677700	-3.33580200	H	-4.21161800	-4.43527800	-1.96198200
H	-2.10501400	-1.75569100	-3.62601200	C	-4.85374200	-2.39915500	-2.26950400
H	-0.59466600	-2.23262800	-0.01216500	H	-5.59344500	-2.65934900	-3.02206200
H	-4.47091900	-2.11143600	-1.35410500	C	-4.67139700	-1.06290300	-1.89469000
H	-1.12299400	3.50235500	3.09668800	H	-5.26834200	-0.28005400	-2.35578800
H	0.46634000	2.43755200	-0.41580700	C	-3.71058900	-0.72958800	-0.94064600
H	-0.55110400	0.29366600	2.99452000	H	-3.54314200	0.31287100	-0.67970400
I	-4.66198400	0.10816400	1.61614300	C	-2.70025400	-0.68253200	2.32275600
C	-3.62568100	-1.68183400	2.85939700	H	-3.39975500	0.10166800	2.02409600
C	-2.31065100	-1.92961300	2.50047200	H	-2.05839300	-0.28326300	3.11300700
C	-4.27305700	-2.41823600	3.84406600	H	-3.26388100	-1.54298700	2.70225700
C	-1.60563700	-2.95235600	3.14808300	C	-0.87203400	-2.71058300	1.48975300
H	-1.84267400	-1.32410300	1.72179800	H	-0.22346500	-2.44385400	2.33086900
C	-3.56458500	-3.44244100	4.49029300	H	-0.25010500	-3.16342000	0.71107900
H	-5.30708100	-2.21152000	4.11400400	H	-1.61026100	-3.44072400	1.84058600
C	-2.23529900	-3.70814600	4.14309300	C	1.11372000	1.44228000	2.94453100
H	-0.57091400	-3.15713700	2.87905200	C	0.53631600	0.61846200	3.92818900
H	-4.05209700	-4.03127400	5.26479300	H	0.40522500	-0.44337600	3.73634900
H	-1.69165900	-4.50262000	4.64814100	C	0.11582800	1.14466200	5.14967100

TS-4-5-I-PMe₂Ph

$$E(\text{OSS}) = -2371.43028050$$

$$E(\text{T}) = -2371.41605770$$

$$S^2(\text{OSS}) = 0.5479$$

$$G_{\text{corr}} = 0.519749$$

$$v = -276.90 \text{ cm}^{-1}$$

Ni	-0.34083600	0.44923300	0.01234500
P	0.04180000	-0.14834500	-2.09720300
P	-1.65254700	-1.15548400	0.87201600
P	1.49086700	0.73557400	1.28600800
C	1.63446600	0.56804900	-2.68673000
C	1.71899800	1.96512500	-2.82581100
H	0.83959500	2.57708400	-2.63917300
C	2.92418800	2.57764300	-3.16521600
H	2.96855600	3.65870500	-3.27125600

C	4.07651300	1.80578500	-3.35211200
H	5.01953100	2.28344800	-3.60462800
C	4.00723200	0.41876600	-3.20805900
H	4.89699700	-0.18917600	-3.35284500
C	2.79376100	-0.19783300	-2.88301000
H	2.76314800	-1.27867200	-2.78019400
C	-1.13608100	0.37873000	-3.42406300
H	-2.10967800	-0.08174100	-3.22527700
H	-0.78970600	0.08226300	-4.42096500
H	-1.26287600	1.46488700	-3.39174200
C	0.19298300	-1.95197600	-2.46805600
H	-0.78881200	-2.40778800	-2.30127800
H	0.90570600	-2.42060200	-1.78232000
H	0.50180200	-2.14282000	-3.50221400
C	-2.93155400	-1.72693300	-0.32548100
C	-3.12564100	-3.06345900	-0.70374700
H	-2.53585600	-3.85551200	-0.25205700
C	-4.07750100	-3.39532300	-1.67461500
H	-4.21161800	-4.43527800	-1.96198200
C	-4.85374200	-2.39915500	-2.26950400
H	-5.59344500	-2.65934900	-3.02206200
C	-4.67139700	-1.06290300	-1.89469000
H	-5.26834200	-0.28005400	-2.35578800
C	-3.71058900	-0.72958800	-0.94064600
H	-3.54314200	0.31287100	-0.67970400
C	-2.70025400	-0.68253200	2.32275600
H	-3.39975500	0.10166800	2.02409600
H	-2.05839300	-0.28326300	3.11300700
H	-3.26388100	-1.54298700	2.70225700
C	-0.87203400	-2.71058300	1.48975300
H	-0.22346500	-2.44385400	2.33086900
H	-0.25010500	-3.16342000	0.71107900
H	-1.61026100	-3.44072400	1.84058600
C	1.11372000	1.44228000	2.94453100
C	0.53631600	0.61846200	3.92818900
H	0.40522500	-0.44337600	3.73634900
C	0.11582800	1.14466200	5.14967100
H	-0.32522300	0.48829200	5.89577000
C	0.25727100	2.51138300	5.41235600
H	-0.07455400	2.92376700	6.36148800
C	0.82641000	3.34120800	4.44380000
H	0.94099900	4.40488700	4.63696800
C	1.25049800	2.81289800	3.22032500
H	1.68555700	3.47993300	2.48255200
C	2.50053500	-0.76197700	1.70263900
H	1.88374500	-1.51390100	2.20244000
H	3.35860300	-0.51858300	2.33993300
H	2.86142000	-1.19586000	0.76296700
C	2.81951200	1.84452200	0.63293900
H	2.39899400	2.81219400	0.34492300
H	3.22601500	1.37704100	-0.26962700
H	3.62897800	1.99818000	1.35641100
I	-1.41107600	2.77213000	-0.03817500
C	-3.14736900	2.83441200	1.65270000
C	-2.73549400	2.83192300	2.98302400

C	-4.47000300	2.58088400	1.29879100	H	-5.38415500	0.17874700	4.36796000
C	-3.67916900	2.57981000	3.98680900	C	-4.25479800	1.13757100	2.80788100
H	-1.69349800	3.00022500	3.24416500	H	-4.95185500	0.82572200	2.03685600
C	-5.40920000	2.32666900	2.30906200	C	-2.09985600	3.98965800	0.77852800
H	-4.77373500	2.56384700	0.25395200	C	-2.72667300	4.96273000	1.57352100
C	-5.01291900	2.32344900	3.65047000	H	-3.55357600	4.68485200	2.22156000
H	-3.36740300	2.57338800	5.02938900	C	-2.28185000	6.28538300	1.55264100
H	-6.44596700	2.12573300	2.04633000	H	-2.76711900	7.02814000	2.18068800
H	-5.74104200	2.11813200	4.43117300	C	-1.21577900	6.65540100	0.72538800

TS-4-5-I-PMPh₂

$$E(\text{OSS}) = -2946.81831720$$

$$E(\text{T}) = -2946.80534049$$

$$S^2(\text{OSS}) = 0.5464$$

$$G_{\text{corr}} = 0.670258$$

$$v = -273.91 \text{ cm}^{-1}$$

Ni	-1.08585700	0.77954500	-0.00087100	P	-1.55764100	-1.15549600	1.09171900
P	-0.89894500	0.78396000	-2.22754300	C	-0.70577800	-2.65071600	0.43225700
C	-2.43407500	0.14098400	-3.02770700	C	0.57095100	-3.00738400	0.89911800
C	-3.53982500	0.98642500	-3.21420900	H	1.02328200	-2.46501900	1.72464200
H	-3.45687800	2.04703700	-2.99927300	C	1.27912000	-4.05282300	0.30073200
C	-4.75937800	0.47823700	-3.66745400	H	2.26491500	-4.31687800	0.67556600
H	-5.60297700	1.14969800	-3.80619300	C	0.72699500	-4.75528700	-0.77374800
C	-4.89487400	-0.88585800	-3.94075100	H	1.28120000	-5.56490700	-1.24096400
H	-5.84457600	-1.28213400	-4.29003300	C	-0.54308900	-4.40877500	-1.24305800
C	-3.79847700	-1.73504700	-3.76570600	H	-0.98377400	-4.95023000	-2.07653300
H	-3.89127800	-2.79687300	-3.97921000	C	-1.25248000	-3.36565400	-0.64643700
C	-2.57902400	-1.22717600	-3.31416300	H	-2.23593300	-3.10396000	-1.02536000
H	-1.73932400	-1.90094300	-3.17644900	C	-3.33459400	-1.64616500	1.06729500
C	0.40267400	-0.29059800	-2.97945700	C	-4.11956000	-1.20700300	-0.01002400
C	1.20097500	-1.08318600	-2.14430900	H	-3.66062700	-0.61475600	-0.79432500
H	1.04585900	-1.04417700	-1.07155400	C	-5.48230300	-1.50852900	-0.07148100
C	2.17970300	-1.92406800	-2.68236000	H	-6.07039900	-1.16386500	-0.91781800
H	2.78199500	-2.53818800	-2.01901700	C	-6.08132900	-2.24070700	0.95675700
C	2.36918800	-1.98016700	-4.06411900	H	-7.14391000	-2.46665300	0.91975300
H	3.12973400	-2.63264000	-4.48548200	C	-5.30806400	-2.68306600	2.03501400
C	1.57186100	-1.19868600	-4.90807100	H	-5.76913700	-3.25350300	2.83740500
H	1.71150600	-1.24369100	-5.98525100	C	-3.94254600	-2.39482200	2.08716900
C	0.59264900	-0.36314700	-4.37036900	H	-3.35921000	-2.74596400	2.93303600
H	-0.03313400	0.22202600	-5.03910800	C	-1.12660600	-1.19721700	2.88892000
C	-0.62840100	2.38742000	-3.11998100	H	-1.12375800	-2.20798000	3.30885500
H	-0.67104700	2.27944600	-4.20838800	H	-1.84582000	-0.57654500	3.42959900
H	0.35653100	2.77114000	-2.83443300	H	-0.13714400	-0.74818100	3.01481300
H	-1.38128500	3.11459700	-2.80242500	I	1.24983500	1.32001300	0.98080100
P	-2.67353700	2.23587300	0.72406700	C	1.34745100	2.74765900	2.96125300
C	-3.11322700	1.88510200	2.47752300	C	1.34790700	2.13156500	4.21011500
C	-2.21973400	2.24641600	3.50106100	C	1.11494500	4.11433700	2.82747100
H	-1.32534500	2.81299500	3.26524500	C	1.12129100	2.90714900	5.35552100
C	-2.47052200	1.87956200	4.82320400	H	1.50390100	1.05837800	4.30013000
H	-1.76781200	2.17209100	5.59838500	C	0.87746600	4.88298400	3.97525900
C	-3.60967100	1.13367300	5.14391600	H	1.09039900	4.58077500	1.84725700
H	-3.80105500	0.84261000	6.17352300	C	0.87918400	4.28010800	5.23733800
C	-4.49879500	0.76362400	4.13225400	H	1.12352900	2.43644100	6.33667900

H	0.68245100	5.94900000	3.87800100
H	0.68797000	4.87649300	6.12584200

TS-4-5-I-PPh₃

E (OSS) = -3522.19654393

E (T) = -3522.18625046

S²(OSS) = 0.5756

G_{corr} = 0.820685

v = -295.63 cm⁻¹

Ni	-0.29723200	0.75225900	0.25707900
P	0.00769200	0.44789300	-2.00073400
C	-1.30551500	-0.54709000	-2.83998100
C	-2.61550100	-0.48756900	-2.34282700
H	-2.82791500	0.10892000	-1.46568600
C	-3.64135500	-1.21066400	-2.95462400
H	-4.65025000	-1.14914800	-2.55636500
C	-3.36631900	-2.01790400	-4.06175700
H	-4.16195900	-2.59031700	-4.53148400
C	-2.06142400	-2.09271200	-4.55830800
H	-1.83831600	-2.72258900	-5.41565400
C	-1.03750900	-1.36056000	-3.95321200
H	-0.02759500	-1.42999800	-4.34550700
C	1.51585600	-0.52096200	-2.43602800
C	1.66212200	-1.78269800	-1.83365400
H	0.90823800	-2.14300000	-1.14163300
C	2.76875800	-2.57858100	-2.12145400
H	2.86202600	-3.55153700	-1.64872200
C	3.76164800	-2.11387300	-2.99031300
H	4.63217900	-2.72908600	-3.20259000
C	3.63292100	-0.85440800	-3.57894900
H	4.40034900	-0.48610700	-4.25525200
C	2.51017800	-0.06361800	-3.31203000
H	2.41232200	0.90672300	-3.78999800
P	-1.73877800	2.51313600	0.53492500
C	-2.50765700	2.73414300	2.21553600
C	-2.46926600	3.95790900	2.90341300
H	-2.02370600	4.83258900	2.44314500
C	-2.99722000	4.06877600	4.19275700
H	-2.94865500	5.02404300	4.70921900
C	-3.58390200	2.96483300	4.81407200
H	-3.99301300	3.05311000	5.81706300
C	-3.63698100	1.74365600	4.13608400
H	-4.08923400	0.87427500	4.60615800
C	-3.09540000	1.62906800	2.85501500
H	-3.11706300	0.66596500	2.35660000
C	-1.02002700	4.19480300	0.25846700
C	-1.73256000	5.27971100	-0.27573500
H	-2.76687100	5.15939300	-0.58041300
C	-1.11718800	6.52506900	-0.42321900
H	-1.67809500	7.35335000	-0.84835200
C	0.20937200	6.70862500	-0.02297100
H	0.68587100	7.67827600	-0.14176300
C	0.91794500	5.64088500	0.53444800

H	1.94919500	5.76665800	0.85072400
C	0.30420600	4.39508900	0.67037400
H	0.86132100	3.56396900	1.08393000
P	1.75103800	0.68483600	1.35838500
C	1.61365500	0.78262400	3.19907800
C	0.37508900	1.12772000	3.75336200
H	-0.46646800	1.29858700	3.09289600
C	0.21499600	1.22826200	5.13807800
H	-0.75555800	1.49719900	5.54670900
C	1.29778000	0.97602100	5.98290300
H	1.17798200	1.04878400	7.06081800
C	2.53805700	0.62086700	5.43959800
H	3.38139600	0.41759400	6.09464900
C	2.69615900	0.52220400	4.05669600
H	3.66125600	0.24218300	3.64297700
C	2.91165100	2.06243400	0.93807700
C	3.36979400	3.00796800	1.86849100
H	3.08684900	2.93046200	2.91312400
C	4.18774200	4.06659000	1.46126700
H	4.53060300	4.79050500	2.19615000
C	4.56478000	4.19441000	0.12244700
H	5.19946000	5.01895400	-0.19122500
C	4.11805200	3.25483300	-0.81126900
H	4.40113800	3.34234400	-1.85704200
C	3.29601700	2.20318600	-0.40731600
H	2.95802000	1.47999800	-1.14211400
C	2.84899600	-0.80566000	1.20134000
C	2.31009400	-2.04423100	1.59061600
C	4.17196300	-0.76550700	0.73834700
C	3.07189000	-3.20914000	1.51392300
H	1.28916600	-2.09604200	1.95372400
C	4.93260400	-1.93561600	0.65651500
H	4.62176700	0.17425200	0.43810300
C	4.38756500	-3.16049700	1.04374400
H	2.63414000	-4.15651200	1.81473000
H	5.95478100	-1.88353900	0.29019900
H	4.97987900	-4.06951900	0.97892300
C	-3.19677500	2.50097900	-0.60872800
C	-3.00309100	2.86850100	-1.95342600
C	-4.44983100	1.99891100	-0.22634700
C	-4.03171500	2.73820100	-2.88522200
H	-2.04459400	3.25598900	-2.27829800
C	-5.47750300	1.86119500	-1.16464900
H	-4.63709000	1.71122800	0.80252600
C	-5.27346700	2.22807900	-2.49628600
H	-3.85501800	3.02654500	-3.91809300
H	-6.44043700	1.46923600	-0.84735600
H	-6.07308800	2.11749500	-3.22381000
C	0.13849600	1.95937800	-3.04818200
C	0.71209700	3.09304600	-2.45364000
C	-0.34777900	2.05352100	-4.36150100
C	0.80138000	4.29888200	-3.14982400
H	1.06324800	3.03572800	-1.43142400
C	-0.26756600	3.26290700	-5.05618300
H	-0.80550700	1.19290500	-4.83900400

C	0.30476600	4.38746800	-4.45295500
H	1.23643400	5.16741900	-2.66310100
H	-0.65690300	3.32729500	-6.06907200
H	0.35656700	5.32846100	-4.99445700
I	-1.49822600	-1.37237200	1.16386300
C	-1.01442700	-3.53541600	0.12960900
C	-1.39873600	-3.75953700	-1.18988800
C	-0.17601200	-4.41960000	0.80285900
C	-0.92536600	-4.89990000	-1.85241900
H	-2.04456900	-3.05897400	-1.70845700
C	0.29115200	-5.56035400	0.13497200
H	0.12338200	-4.22859800	1.83060500
C	-0.07818000	-5.79632800	-1.19324700
H	-1.21529600	-5.07891200	-2.88569200
H	0.94715900	-6.25861200	0.65098000
H	0.29374400	-6.67605700	-1.71236800

TS-4-5-Br-PMe₃

$$E(\text{OSS}) = -1797.8223389$$

$$E(\text{T}) = -1797.8047425$$

$$S^2(\text{OSS}) = 0.5443$$

$$G_{\text{corr}} = 0.372202$$

$$v = -285.62 \text{ cm}^{-1}$$

Ni	0.99546000	-0.07223400	0.07217300
P	0.12096300	1.50120700	-1.24164800
C	-0.36548300	3.08635000	-0.41914600
C	-1.44055900	1.07806300	-2.14034600
C	1.16432600	2.13654800	-2.63311300
H	-0.82714400	3.78808800	-1.12516400
H	0.51919300	3.55982400	0.02003500
H	-1.78383000	1.90318900	-2.77723400
H	-2.22111300	0.83728100	-1.41113400
H	1.35894200	1.32549200	-3.34215000
H	2.12659700	2.48331800	-2.24182400
P	2.51779900	0.98121600	1.35517700
P	1.61970200	-1.83514700	-1.16992200
C	3.50039800	2.33052700	0.54655600
C	3.89444600	0.03185600	2.16081800
C	1.82978200	1.87549900	2.82187100
C	1.66641800	-1.63559500	-3.01245000
C	3.31093400	-2.54471500	-0.88508300
C	0.57668500	-3.35639600	-1.01513000
H	4.19289000	2.80747800	1.25161500
H	2.82650400	3.09393300	0.14424400
H	4.56635100	0.69299200	2.72341800
H	4.47408600	-0.49736400	1.39627100
H	1.32960900	1.15272900	3.47513300
H	1.07779000	2.59592900	2.48250600
H	2.39584400	-0.86278100	-3.27782900
H	0.68163900	-1.31768400	-3.37143900
H	4.06172200	-1.76360900	-1.04969800
H	3.52163700	-3.38749900	-1.55618400
H	0.54864300	-3.67050100	0.03306100

H	0.95826500	-4.18057000	-1.63092700
H	-1.07310300	2.87134200	0.38822600
H	-1.27410600	0.19161100	-2.76265700
H	0.67575200	2.96250200	-3.16477800
H	1.94320400	-2.57037100	-3.51642000
H	3.39716200	-2.88907400	0.15066500
H	-0.44838800	-3.12182700	-1.32116300
H	2.60606200	2.40149100	3.39159900
H	4.07712000	1.91167200	-0.28564100
H	3.47691800	-0.71042100	2.84824700
Br	-0.81011600	-0.80367700	1.55217200
C	0.08242600	-2.41655400	2.90350700
C	1.40610800	-2.68568300	2.61234000
C	-0.61198000	-3.07278000	3.90868300
C	2.08141000	-3.65962200	3.35939800
H	1.90069700	-2.13413400	1.80923600
C	0.06764700	-4.04789800	4.65586600
H	-1.65516500	-2.84472100	4.12039700
C	1.40860300	-4.33975800	4.38138500
H	3.12451900	-3.88705500	3.14619100
H	-0.45156500	-4.57822200	5.45194900
H	1.92809400	-5.09660700	4.96373300

TS-4-5-Cl-PMe₃

$$E(\text{OSS}) = -2244.86583598$$

$$E(\text{T}) = -2244.84805196$$

$$S^2(\text{OSS}) = 0.5347$$

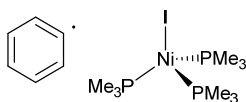
$$G_{\text{corr}} = 0.371917$$

$$v = -165.37 \text{ cm}^{-1}$$

Ni	2.29970700	1.34803400	0.02861300
P	1.34468700	2.88316800	-1.26710600
C	0.84037600	4.46645100	-0.45066700
C	-0.22682300	2.42246400	-2.13208900
C	2.34618200	3.52981500	-2.68364000
H	0.35124800	5.15219600	-1.15382700
H	1.72470900	4.96057200	-0.03375000
H	-0.59616800	3.23475700	-2.77082600
H	-0.99092900	2.17717200	-1.38673800
H	2.54725400	2.71816500	-3.38984700
H	3.30706900	3.90304200	-2.31363700
P	3.83065200	2.41819200	1.28125100
P	2.92298000	-0.40494300	-1.22331800
C	4.77074500	3.77788500	0.44173200
C	5.23677700	1.48829100	2.05976300
C	3.17122100	3.30849900	2.76573200
C	2.99173600	-0.18998600	-3.06369800
C	4.59360900	-1.16107000	-0.93329200
C	1.84342000	-1.90442800	-1.09353100
H	5.46985500	4.27552000	1.12546700
H	4.07101600	4.52276500	0.04847000
H	5.91880300	2.15836600	2.59902300
H	5.80057500	0.95405700	1.28696400
H	2.68065000	2.58427000	3.42521700

H	2.41640200	4.03447000	2.44444700
H	3.73626000	0.57294600	-3.31582200
H	2.01643300	0.14653900	-3.43125800
H	5.36644900	-0.39899200	-1.08428400
H	4.78798000	-2.00238800	-1.61114200
H	1.80844300	-2.23611100	-0.05066600
H	2.20508400	-2.72785600	-1.72208100
H	0.15352600	4.24596000	0.37325600
H	-0.05731300	1.53207300	-2.74789800
H	1.82761300	4.33918800	-3.21224600
H	3.25863100	-1.12502500	-3.57233800
H	4.66306500	-1.51868600	0.09934400
H	0.82396100	-1.64130100	-1.39611900
H	3.95837500	3.82913600	3.32538800
H	5.33548900	3.36299400	-0.40055700
H	4.84072600	0.75050000	2.76497300
C	1.34825100	-0.93052300	2.76971700
C	2.67623400	-1.21251400	2.53262400
C	0.58388500	-1.58523100	3.71963300
C	3.29384600	-2.21466200	3.29191600
H	3.21361000	-0.65300100	1.76225400
C	1.20799400	-2.58950500	4.47732100
H	-0.46353700	-1.33788900	3.88025800
C	2.55569100	-2.90133700	4.26349700
H	4.34166500	-2.45919400	3.12703300
H	0.63961800	-3.12686500	5.23401400
H	3.03027300	-3.68048400	4.85448100
Cl	0.60732300	0.62395700	1.48038700

5-I-PMe₃



$$E(\text{OSS}) = -1796.05732288$$

$$E(\text{T}) = -1796.05665155$$

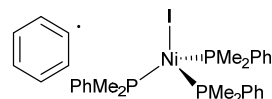
$$S^2(\text{OSS}) = 1.0067$$

$$G_{\text{corr}} = 0.366149$$

Ni	-0.62583000	0.66902000	0.02368500
P	-1.21459500	2.27719400	-1.52055600
C	-1.59541400	3.90919700	-0.75042900
C	-2.77287800	1.91895600	-2.43877600
C	-0.05852400	2.75157000	-2.88104000
H	-1.97593900	4.62646200	-1.48736700
H	-0.69109300	4.31914200	-0.28898500
H	-3.05842200	2.75133400	-3.09273100
H	-3.57373000	1.73183400	-1.71626900
H	0.12216000	1.88801300	-3.52897800
H	0.90012900	3.06789400	-2.45640200
P	0.92071400	1.77038500	1.30936900
P	-0.26235200	-1.26585900	-1.16032400
C	2.12032600	2.82469800	0.37654700
C	2.06860700	0.74664000	2.33593400

C	0.26492700	2.95787400	2.56069700
C	-0.16078800	-1.11491800	-2.99818900
C	1.30647700	-2.17209800	-0.78691700
C	-1.52133500	-2.59788800	-0.95439900
H	2.85500800	3.28431000	1.04878900
H	1.58525200	3.61957000	-0.15311000
H	2.81516600	1.37188400	2.84023000
H	2.58287300	0.02253400	1.69481000
H	-0.36872100	2.41590900	3.27036800
H	-0.35733100	3.70565100	2.05863600
H	0.65928700	-0.44046000	-3.26536700
H	-1.09532300	-0.69701800	-3.38561700
H	2.16302400	-1.51127900	-0.96005400
H	1.41230300	-3.06662600	-1.41297600
H	-1.60216400	-2.85326500	0.10709600
H	-1.26058900	-3.49684900	-1.52601400
H	-2.34527600	3.76313300	0.03365500
H	-2.64378500	1.01588800	-3.04443300
H	-0.46855800	3.56929700	-3.48536100
H	0.01268700	-2.09024600	-3.46882800
H	1.30932100	-2.47695500	0.26381400
H	-2.49641600	-2.22573200	-1.28606900
H	1.07238800	3.46179400	3.10567800
H	2.64622400	2.21133000	-0.36302000
H	1.49876700	0.19883500	3.09219700
I	-2.96508700	0.44484800	1.44693400
C	-1.47822700	-2.52553600	3.01822400
C	-0.23174800	-2.08815200	2.62358400
C	-1.72649500	-3.63587100	3.79857000
C	0.87411600	-2.83807600	3.05980500
H	-0.10690000	-1.20774200	1.99961100
C	-0.60705200	-4.37576700	4.22059300
H	-2.73196900	-3.93678500	4.08205200
C	0.68184100	-3.97531400	3.85215200
H	1.87862600	-2.52927800	2.77919000
H	-0.74930700	-5.26110300	4.83629900
H	1.54082800	-4.55158800	4.18574000

5-I-PMe₂Ph



$$E(\text{OSS}) = -2371.44147589$$

$$E(\text{T}) = -2371.44128873$$

$$S^2(\text{OSS}) = 1.0117$$

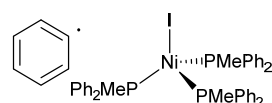
$$G_{\text{corr}} = 0.516916$$

Ni	-0.47346700	0.63783000	-0.19883400
P	0.06944800	-0.28957200	-2.22969100
P	-1.77334800	-1.00075600	0.75351400
P	1.27933300	1.02946800	1.22852300
C	1.72350300	0.37709700	-2.67487600
C	1.82564600	1.73960900	-3.01012100

H	0.93005200	2.35218100	-3.06378600
C	3.07097700	2.32152000	-3.24730600
H	3.13070500	3.37519000	-3.50746700
C	4.23769300	1.55763100	-3.13818400
H	5.20809300	2.01367500	-3.31551800
C	4.14785300	0.20593500	-2.79814800
H	5.04911400	-0.39598300	-2.71299700
C	2.89988100	-0.38244800	-2.57006600
H	2.85365000	-1.43611700	-2.31149000
C	-0.94539100	0.06111500	-3.73245500
H	-1.91550900	-0.43272800	-3.61589000
H	-0.45945200	-0.29782600	-4.64640100
H	-1.12152700	1.13809800	-3.80884900
C	0.25863000	-2.12250800	-2.32155000
H	-0.73520000	-2.56498100	-2.19506700
H	0.89639600	-2.47955500	-1.50738600
H	0.67544200	-2.45050900	-3.28037800
C	-3.01961200	-1.60297100	-0.45885600
C	-3.39308700	-2.94689600	-0.60966400
H	-2.95377100	-3.71600300	0.01893300
C	-4.33358400	-3.31424100	-1.57711600
H	-4.61004800	-4.35964500	-1.68904100
C	-4.91799600	-2.34396300	-2.39488000
H	-5.64967200	-2.63258200	-3.14491300
C	-4.55403400	-1.00137000	-2.24921500
H	-4.99837400	-0.24157800	-2.88686300
C	-3.60306800	-0.63526300	-1.29566500
H	-3.28803500	0.40257300	-1.20859800
C	-2.81318200	-0.52293600	2.20035500
H	-3.47238600	0.29658100	1.90639500
H	-2.16652000	-0.16877200	3.00791400
H	-3.41636800	-1.36732800	2.55272500
C	-0.93729100	-2.52434900	1.36880800
H	-0.23065100	-2.22880900	2.15081100
H	-0.37498900	-2.99982600	0.55941100
H	-1.64192300	-3.24519900	1.79721200
C	0.92661400	1.50088400	2.96959000
C	0.49585100	0.51734300	3.87805100
H	0.42743200	-0.52111000	3.56397900
C	0.15072600	0.85648600	5.18659900
H	-0.17497200	0.08168400	5.87606800
C	0.22096500	2.18804400	5.60956100
H	-0.04885400	2.45310900	6.62831600
C	0.63853800	3.17440700	4.71309500
H	0.69331900	4.21241900	5.03077600
C	0.98964300	2.83485900	3.40316900
H	1.30739100	3.61770500	2.72133600
C	2.44183800	-0.39760800	1.41990400
H	1.91324400	-1.26829200	1.81899800
H	3.28633600	-0.15686200	2.07515000
H	2.81887100	-0.65716800	0.42452800
C	2.41760000	2.34891400	0.62647300
H	1.85049200	3.25909100	0.41202400
H	2.86031500	2.00346000	-0.31288500
H	3.21656100	2.56698000	1.34384900

I	-1.41186000	3.09657400	-0.84530200
C	-3.57582800	3.09596400	1.93138800
C	-2.74140000	2.99272600	3.02567700
C	-4.88991200	2.67410500	1.88712300
C	-3.28619800	2.42351800	4.18922500
H	-1.70533300	3.31642400	2.99949200
C	-5.41472100	2.10270700	3.06017200
H	-5.50044700	2.77065100	0.99261800
C	-4.61329000	1.98008800	4.20069500
H	-2.66285400	2.31810200	5.07373300
H	-6.44509100	1.75404200	3.07561000
H	-5.02530300	1.53405600	5.10232000

5-I-PMePh₂



$$E(\text{OSS}) = -2946.82852389$$

$$E(\text{T}) = -2946.82830820$$

$$S^2(\text{OSS}) = 1.0113$$

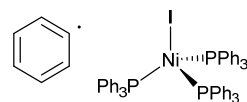
$$G_{\text{corr}} = 0.66871$$

Ni	-0.82914300	0.81738700	-0.09476500
P	-0.99630500	0.75977400	-2.40028600
C	-2.54665700	-0.02156100	-3.02420600
C	-3.67366400	0.73562300	-3.37850400
H	-3.62706100	1.81968900	-3.38636900
C	-4.87373800	0.10522400	-3.72136900
H	-5.73711400	0.70722500	-3.99324100
C	-4.96352400	-1.28862200	-3.71853900
H	-5.89726000	-1.77734800	-3.98348900
C	-3.84138200	-2.05153800	-3.37884000
H	-3.89810000	-3.13707200	-3.37903600
C	-2.64446000	-1.42436600	-3.03468300
H	-1.78352200	-2.02842700	-2.76401600
C	0.29435000	-0.23603600	-3.25418400
C	1.06201600	-1.12705100	-2.49144600
H	0.91198300	-1.17991300	-1.41940300
C	2.01792000	-1.94238600	-3.10279300
H	2.59833200	-2.63255500	-2.49726500
C	2.22124900	-1.86587700	-4.48188100
H	2.96814900	-2.49504600	-4.95919700
C	1.46020200	-0.97834800	-5.25070600
H	1.61404100	-0.91852700	-6.32513600
C	0.49784400	-0.17174000	-4.64250700
H	-0.09830400	0.49887500	-5.25516100
C	-0.94003000	2.38719900	-3.27172900
H	-1.16629000	2.31215900	-4.33994700
H	0.06631700	2.79801600	-3.14315200
H	-1.64902800	3.07600300	-2.80417400
P	-2.46799400	2.31900000	0.60307100
C	-3.22162100	1.97850000	2.24412000
C	-2.38971900	1.98245400	3.37648900

H	-1.33999600	2.23856300	3.27703900
C	-2.90162100	1.64812100	4.63075400
H	-2.24367700	1.66290300	5.49438800
C	-4.24566200	1.28956500	4.77031100
H	-4.63974300	1.01791800	5.74611500
C	-5.07752500	1.27869500	3.64917000
H	-6.12205800	0.99474000	3.74512500
C	-4.57170600	1.62702700	2.39414300
H	-5.23537700	1.60081700	1.53694300
C	-1.78701500	4.02238300	0.76219600
C	-2.35495300	4.98949200	1.60570300
H	-3.20059600	4.73254300	2.23747000
C	-1.82836800	6.28162100	1.64940800
H	-2.27040600	7.02185900	2.31135200
C	-0.73512000	6.62282400	0.84607100
H	-0.32545700	7.62876400	0.88354700
C	-0.16648300	5.66540600	0.00162700
H	0.69047000	5.92008000	-0.61623700
C	-0.68572200	4.36893300	-0.03467000
H	-0.22256500	3.61480300	-0.66345500
C	-3.93018600	2.62740100	-0.48317700
H	-4.62772900	3.33521400	-0.02371100
H	-4.44595500	1.69086400	-0.70964700
H	-3.56481600	3.05566600	-1.41987200
P	-1.24389700	-1.01566300	1.24096100
C	-0.51546300	-2.54330400	0.50794500
C	0.84949900	-2.81468600	0.70796000
H	1.44604200	-2.17411100	1.35049300
C	1.45909500	-3.89466800	0.06601500
H	2.51522700	-4.09053700	0.23246400
C	0.71899300	-4.71485200	-0.79014000
H	1.19630400	-5.55111000	-1.29382100
C	-0.63809400	-4.45256900	-0.99350300
H	-1.22403400	-5.08710200	-1.65374900
C	-1.25201600	-3.37612200	-0.34928300
H	-2.30675500	-3.18487100	-0.52058100
C	-3.03073200	-1.40900300	1.41072000
C	-3.86702800	-1.07740700	0.33195700
H	-3.43996300	-0.59752100	-0.54297800
C	-5.23542800	-1.34711200	0.38150100
H	-5.86392000	-1.09526200	-0.46859000
C	-5.78957000	-1.92716800	1.52588100
H	-6.85671600	-2.12757600	1.57434800
C	-4.96797800	-2.24366500	2.61154600
H	-5.39621200	-2.68796700	3.50631700
C	-3.59444000	-1.99498900	2.55323900
H	-2.97189300	-2.25181800	3.40479000
C	-0.57820800	-1.05408700	2.96262700
H	-0.60538400	-2.05779600	3.39807100
H	-1.15787000	-0.36633900	3.58248600
H	0.45531300	-0.69812000	2.93593200
I	1.79383400	1.32691500	0.41308500
C	1.30058500	2.90209500	3.41749700
C	1.26057200	2.02587700	4.48494000
C	0.69834600	4.14460000	3.39023300

C	0.56788000	2.44624600	5.63350900
H	1.73858200	1.05029100	4.44880300
C	0.00561900	4.54507700	4.54540200
H	0.73315100	4.78567100	2.51438100
C	-0.05468600	3.69965900	5.65831000
H	0.51327300	1.79163800	6.50079000
H	-0.49205900	5.51185300	4.56347700
H	-0.59671000	4.01433800	6.54630900

5-I-PPh₃

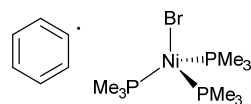


E (OSS) =	-3522.20750246		
E (T) =	-3522.20736581		
S ² (OSS) =	1.0130		
G _{corr} =	0.817883		
Ni	-0.40588100	0.68315600	0.44006400
P	-0.13489200	0.36030300	-1.86713900
C	-1.48976200	-0.56292200	-2.70445400
C	-2.76485500	-0.56204000	-2.12300600
H	-2.92697900	-0.04271400	-1.18684000
C	-3.82188700	-1.23799200	-2.73649600
H	-4.80454200	-1.22761900	-2.27369400
C	-3.61264800	-1.92540000	-3.93452300
H	-4.43374700	-2.45593700	-4.40952400
C	-2.34197800	-1.93510500	-4.51896700
H	-2.17230400	-2.47300100	-5.44811700
C	-1.28423400	-1.26230500	-3.90518400
H	-0.29726200	-1.29058900	-4.35720600
C	1.35227300	-0.63351900	-2.29498000
C	1.63618300	-1.74050100	-1.48068500
H	0.98102200	-1.97856100	-0.64952300
C	2.76525300	-2.52282800	-1.72522300
H	2.97720100	-3.36729800	-1.07832000
C	3.62349400	-2.20336000	-2.78058400
H	4.50963000	-2.80580400	-2.96316100
C	3.34415400	-1.10460600	-3.59844600
H	4.00830200	-0.85304800	-4.42148200
C	2.21153300	-0.32210300	-3.35996100
H	2.00588100	0.53446700	-3.99491000
P	-1.82372700	2.58387300	0.61679400
C	-2.59607900	2.84107100	2.28168700
C	-2.59040300	4.08745400	2.92931300
H	-2.15907900	4.95648100	2.44479600
C	-3.13634300	4.22500600	4.20764900
H	-3.11984300	5.19680200	4.69429100
C	-3.70074100	3.12470400	4.85746100
H	-4.12409700	3.23477800	5.85236700

C	-3.71351700	1.88107100	4.22070900
H	-4.14516200	1.01513300	4.71570400
C	-3.15992400	1.73884000	2.94692700
H	-3.14961600	0.76149100	2.47733500
C	-1.04349600	4.22527500	0.31405700
C	-1.71789100	5.32598900	-0.23655300
H	-2.75410000	5.23439300	-0.54573200
C	-1.06068800	6.54842900	-0.39345700
H	-1.59072600	7.39054600	-0.83060400
C	0.26881700	6.69113200	0.01339900
H	0.77784500	7.64321700	-0.11173900
C	0.94079800	5.60526000	0.58125500
H	1.97606000	5.70068600	0.89507100
C	0.28696800	4.38172800	0.72606900
H	0.81672400	3.53346000	1.14420000
P	1.76003800	0.63596600	1.45006800
C	1.61419700	1.02358300	3.24760000
C	0.35435700	1.34367800	3.76936000
H	-0.51350900	1.34541700	3.12114900
C	0.19870900	1.64004200	5.12618600
H	-0.78820000	1.88499300	5.50943500
C	1.30694900	1.61415300	5.97448200
H	1.19124300	1.84382800	7.03050000
C	2.56816500	1.28196000	5.46567000
H	3.43088700	1.25169800	6.12605700
C	2.72159100	0.98310000	4.11197300
H	3.70154100	0.71780700	3.72430100
C	2.96175900	1.88106700	0.80786600
C	3.37699600	3.00442200	1.53911300
H	3.03939100	3.14825800	2.56014100
C	4.22208700	3.95533900	0.95903900
H	4.53233300	4.81966700	1.54058500
C	4.66680600	3.79757800	-0.35527400
H	5.32176700	4.53972500	-0.80373600
C	4.26613000	2.67692500	-1.08858500
H	4.60398700	2.54000200	-2.11239200
C	3.41880200	1.73020000	-0.51395700
H	3.11466300	0.86734000	-1.09668000
C	2.77779900	-0.91180800	1.52095900
C	2.13290200	-2.09221900	1.92725200
C	4.14777000	-0.95829400	1.22367600
C	2.84134000	-3.28958300	2.02740700
H	1.07152700	-2.08073300	2.15251900
C	4.85285700	-2.16161200	1.31555100
H	4.67512500	-0.06306000	0.91320800
C	4.20394300	-3.33053200	1.71684200
H	2.32474000	-4.19150300	2.34358300
H	5.91285600	-2.17963000	1.07508700
H	4.75397400	-4.26522200	1.78874500

C	-3.25323200	2.54371700	-0.55156200
C	-3.04432200	2.89675500	-1.89669900
C	-4.50264500	2.02577000	-0.17706500
C	-4.05769700	2.73445300	-2.84079300
H	-2.08922800	3.29998400	-2.21157500
C	-5.51452500	1.86098900	-1.12672400
H	-4.69613800	1.74421200	0.85246800
C	-5.29598100	2.21064700	-2.46113300
H	-3.87135100	3.00983400	-3.87548800
H	-6.47549900	1.45805200	-0.81779800
H	-6.08310800	2.07604900	-3.19809800
C	0.06073000	1.89231200	-2.86807900
C	0.74273000	2.95674200	-2.26082200
C	-0.46449100	2.06683700	-4.15775400
C	0.90015700	4.17458100	-2.92287600
H	1.12886400	2.83789600	-1.25614000
C	-0.31310600	3.28829200	-4.81826900
H	-1.01010500	1.26275100	-4.64055100
C	0.36657100	4.34434100	-4.20286700
H	1.41867400	4.98990600	-2.42678400
H	-0.73247500	3.41621700	-5.81291700
H	0.47345400	5.29582100	-4.71720700
I	-1.71863700	-1.49268900	1.40740900
C	-0.68932000	-4.30022600	-0.44170500
C	-1.10708800	-4.02038000	-1.72671900
C	0.38617900	-5.09841400	-0.10791500
C	-0.37889700	-4.61075900	-2.77306200
H	-1.94645400	-3.36352900	-1.93217900
C	1.10013200	-5.68127800	-1.16965500
H	0.67953800	-5.27447800	0.92346500
C	0.71610100	-5.43485000	-2.49236000
H	-0.66684400	-4.41262100	-3.80257800
H	1.95642700	-6.31808400	-0.95758600
H	1.27831100	-5.88132500	-3.30843500

5-Br-PMe₃



$$E(\text{OSS}) = -1797.83450227$$

$$E(\text{T}) = -1797.83414397$$

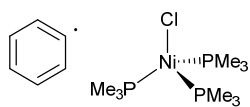
$$S^2(\text{OSS}) = 1.0115$$

$$G_{\text{corr}} = 0.368688$$

Ni	-0.52646100	0.51920300	0.11520900
P	-1.03997200	2.06473100	-1.51557600
C	-1.42631300	3.72917300	-0.81907400
C	-2.59719800	1.66490900	-2.41914000
C	0.11530300	2.49095400	-2.89387400

H	-1.79433000	4.41688200	-1.58995200
H	-0.52683600	4.15598100	-0.36337400
H	-2.90587200	2.47993200	-3.08457900
H	-3.38389700	1.47166000	-1.68295500
H	0.31938200	1.59814900	-3.49366700
H	1.06447500	2.84831300	-2.47981100
P	1.03040700	1.65022300	1.36496800
P	-0.09244600	-1.45615200	-0.97251200
C	2.25490800	2.67407800	0.42725800
C	2.15241700	0.66673300	2.45797200
C	0.36023400	2.88318800	2.56550700
C	0.10131400	-1.35316700	-2.80825500
C	1.44831400	-2.37213500	-0.51399800
C	-1.37002500	-2.77764800	-0.80861200
H	2.98539300	3.14266300	1.09823000
H	1.73326900	3.46241400	-0.12574400
H	2.89546400	1.30627100	2.94968800
H	2.66967600	-0.09317300	1.86277500
H	-0.28906500	2.36540100	3.27876600
H	-0.25073800	3.61649700	2.02946700
H	0.94081200	-0.69281900	-3.04955300
H	-0.80728900	-0.93341200	-3.25180000
H	2.31928000	-1.73121600	-0.69074700
H	1.55776000	-3.29401600	-1.09859300
H	-1.51614200	-3.00782400	0.25122300
H	-1.08436900	-3.69150900	-1.34388000
H	-2.18704700	3.61769000	-0.03997200
H	-2.45523800	0.75444900	-3.01115800
H	-0.30399200	3.26756600	-3.54465100
H	0.28665300	-2.34035100	-3.24915300
H	1.41719600	-2.62924600	0.54910800
H	-2.32156600	-2.40563500	-1.20299500
H	1.15903400	3.40245500	3.10936300
H	2.78560500	2.04210200	-0.29313400
H	1.55995300	0.16142200	3.22666500
Br	-2.69413700	0.39703300	1.41336500
C	-1.39611700	-2.90546100	3.02771100
C	-0.24156200	-2.17690000	2.83695700
C	-1.48129600	-4.14069000	3.63498000
C	0.95034100	-2.75368600	3.31042000
H	-0.25430800	-1.21121000	2.33860700
C	-0.27637600	-4.69855300	4.09947400
H	-2.42400500	-4.66812100	3.75781300
C	0.92768500	-4.00582000	3.93544500
H	1.89044700	-2.22209400	3.18669600
H	-0.28666700	-5.67107200	4.58643900
H	1.85407100	-4.44311900	4.29842700

5-Cl-PMe₃

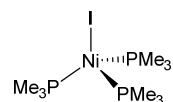


$$E(\text{OSS}) = -2244.88718919$$

E (T)	=	-2244.88685062	
S ² (OSS)	=	1.0118	
G _{corr}	=	0.370729	
Ni	1.55939600	1.02993200	0.06773100
P	1.04825600	2.57899500	-1.56715400
C	0.70765900	4.26514800	-0.89608100
C	-0.52776500	2.20181400	-2.44952300
C	2.19308300	2.96344700	-2.96638200
H	0.35866800	4.94908200	-1.67891300
H	1.61833100	4.67552900	-0.44749100
H	-0.82126400	3.01148300	-3.12816800
H	-1.31737300	2.04269800	-1.70812500
H	2.36051000	2.06418000	-3.56739000
H	3.15912300	3.29502900	-2.57040900
P	3.14451200	2.15052800	1.29508500
P	2.01828400	-0.93475900	-1.03686400
C	4.36990300	3.14620100	0.32855300
C	4.27115900	1.16728500	2.38392700
C	2.51152200	3.40874100	2.49158400
C	2.22532100	-0.82001700	-2.87031200
C	3.55355400	-1.85948900	-0.57730800
C	0.73865200	-2.25829400	-0.89125900
H	5.11802800	3.61091800	0.98258200
H	3.85238500	3.93654800	-0.22533100
H	5.02233300	1.80499100	2.86561100
H	4.77967600	0.40239300	1.78756600
H	1.87482100	2.90929700	3.22954500
H	1.89618400	4.14049600	1.95788100
H	3.07626400	-0.17022700	-3.09997100
H	1.32617200	-0.38313200	-3.31676500
H	4.42774900	-1.22032100	-0.74409600
H	3.66359800	-2.77651900	-1.16934400
H	0.58548900	-2.49827600	0.16578600
H	1.02730800	-3.16861300	-1.43074800
H	-0.05682800	4.19294300	-0.11575800
H	-0.41277400	1.27685600	-3.02492000
H	1.78570500	3.75014000	-3.61250100
H	2.39937500	-1.80582900	-3.31870400
H	3.51683300	-2.12683800	0.48315200
H	-0.21062200	-1.88502100	-1.29104400
H	3.32608200	3.92850700	3.01070900
H	4.88037700	2.49875300	-0.39274700
H	3.68349800	0.66830000	3.16033600
C	0.68597800	-2.34195600	2.94746600
C	1.85798100	-1.64349800	2.75283900
C	0.56468800	-3.55656800	3.58863100
C	3.03056700	-2.23191100	3.25952600
H	1.87552500	-0.69278400	2.22682300
C	1.75067100	-4.12626300	4.08616800
H	-0.39103800	-4.05952800	3.71303700
C	2.97177800	-3.46452800	3.91950700
H	3.98335100	-1.72384500	3.13391400
H	1.71235800	-5.08358100	4.60100600
H	3.88322600	-3.91105500	4.30813000

Cl -0.47285000 0.85701500 1.30676200

6-I-PMe₃

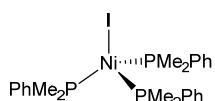


E = -1564.41378215

G_{corr} = 0.285068

Ni	3.19335000	7.61491500	11.71328600
P	1.42114100	8.89806000	11.02938100
C	0.92926700	10.20501400	12.23542700
C	-0.14454400	7.94826000	10.80984700
C	1.53713400	9.85467100	9.45469000
H	0.00722700	10.71403700	11.93061000
H	1.73419900	10.94368500	12.31335900
H	-0.99097200	8.60345000	10.57235500
H	-0.35757600	7.39969300	11.73337800
H	1.66951500	9.16654200	8.61384500
H	2.41126400	10.51382600	9.49478900
P	4.67452100	9.10374900	12.61927200
P	3.72089000	6.19142300	10.00155600
C	5.17192800	10.56633900	11.60707600
C	6.29539000	8.30412600	12.99476300
C	4.24443100	9.87664900	14.23909700
C	3.47263200	6.77897500	8.26781500
C	5.51298200	5.74015200	9.99938200
C	2.91216400	4.53276300	9.96311700
H	5.94598000	11.16362400	12.10392800
H	4.29733600	11.20149600	11.42812700
H	6.99713300	9.00042000	13.46914000
H	6.73882700	7.92256500	12.06883300
H	4.00335100	9.08339400	14.95427800
H	3.35683100	10.50649200	14.12017600
H	3.98225500	7.73855400	8.13028300
H	2.40375800	6.92744900	8.08120600
H	6.11448200	6.64307500	9.84946500
H	5.74919300	5.01732500	9.20899900
H	3.14119400	4.00121000	10.89240200
H	3.25166400	3.93374700	9.10942800
H	0.78299700	9.74791500	13.21948000
H	-0.01831900	7.21718900	10.00393800
H	0.63923400	10.46021600	9.28337800
H	3.86141000	6.05808400	7.53849000
H	5.77644700	5.30789500	10.97047500
H	1.82558000	4.65920500	9.90808200
H	5.06726700	10.48533600	14.63304300
H	5.55019000	10.22549200	10.63698000
H	6.12182700	7.45502400	13.66458500
I	2.49872700	6.02825200	13.83966400

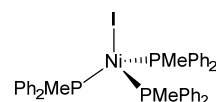
6-I-PMe₂Ph



E	=	-2139.7985927
G _{corr}	=	0.434689
Ni		-0.46362800 1.21841800 -0.09111500
P		0.03894400 0.13975600 -2.06019400
P		-1.93893900 -0.17262100 0.98647200
P		1.30022600 1.36634700 1.36474300
C		1.73705100 0.66483800 -2.54471300
C		2.03141300 2.03737700 -2.44873600
H		1.26480900 2.72544300 -2.09743600
C		3.30133900 2.51779400 -2.77160900
H		3.51084800 3.58162000 -2.69537400
C		4.30389700 1.63001400 -3.17500400
H		5.29639100 2.00072800 -3.41734100
C		4.02606400 0.26374900 -3.25997500
H		4.80234000 -0.43143000 -3.56966700
C		2.74963700 -0.21745700 -2.95155500
H		2.55443100 -1.28303400 -3.02847300
C		-0.91300800 0.40014300 -3.62396700
H		-1.92519300 0.00436800 -3.49237300
H		-0.43513600 -0.09777100 -4.47535000
H		-0.98541400 1.47388900 -3.82410200
C		0.11997800 -1.69945500 -1.96995800
H		-0.88360200 -2.06743700 -1.73433200
H		0.79409100 -1.99752900 -1.16076200
H		0.44883200 -2.15868800 -2.90864800
C		-3.06485900 -1.02538300 -0.18939800
C		-3.37660600 -2.39189900 -0.13477600
H		-2.96891600 -3.01912700 0.65274100
C		-4.21194000 -2.96474000 -1.09948100
H		-4.44108500 -4.02627000 -1.05077900
C		-4.75161400 -2.17831300 -2.11983200
H		-5.40136400 -2.62574100 -2.86736200
C		-4.44970400 -0.81369900 -2.17889200
H		-4.86207400 -0.19631800 -2.97274700
C		-3.60417000 -0.24352600 -1.22659000
H		-3.33774700 0.80923100 -1.29436200
C		-3.12167600 0.67428000 2.12405600
H		-3.63549900 1.46960800 1.57583500
H		-2.56304200 1.12996400 2.94744400
H		-3.85875700 -0.02914800 2.52687800
C		-1.25313000 -1.50644300 2.05520100
H		-0.61949000 -1.02932300 2.81014600
H		-0.63339000 -2.18297300 1.45792500
H		-2.03328700 -2.08257400 2.56450900
C		0.83291800 1.51040900 3.13717500
C		1.42179900 0.76664800 4.17103900
H		2.22347900 0.06583000 3.95828900
C		0.97962900 0.91500400 5.48958500
H		1.44043200 0.32852400 6.28045400

C		-0.04558100 1.81404600 5.79150300
H		-0.38593700 1.92848000 6.81729900
C		-0.63738600 2.56121500 4.76757500
H		-1.44175400 3.25663100 4.99298900
C		-0.20922500 2.40174900 3.44913600
H		-0.69712200 2.95188800 2.64746900
C		2.48677900 -0.04467300 1.29934200
H		1.97514100 -0.97590500 1.56313200
H		3.35185000 0.09365500 1.95762500
H		2.84201300 -0.12808800 0.26660300
C		2.42416700 2.81434900 1.12461400
H		1.83768800 3.73674200 1.18115000
H		2.87084900 2.75110500 0.12724700
H		3.21752200 2.83730700 1.87984100
I		-1.56805600 3.63130000 -0.51879800

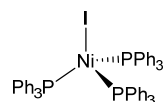
6-I-PMePh₂



E	=	-2715.18416817
G _{corr}	=	0.58561
Ni		0.77183100 0.79556700 0.03949200
P		0.80753700 0.85591400 -2.25606400
C		-0.73225800 0.13153800 -2.96427300
C		-1.86958400 0.92691100 -3.17833600
H		-1.81996300 2.00293400 -3.04201500
C		-3.07996900 0.34641000 -3.56649900
H		-3.95010200 0.97711200 -3.72994600
C		-3.17188300 -1.03620100 -3.74701900
H		-4.11407400 -1.48696800 -4.04679000
C		-2.04229000 -1.83481700 -3.54444600
H		-2.10170200 -2.91071900 -3.68719500
C		-0.83281000 -1.25731500 -3.15659200
H		0.03346700 -1.89137700 -2.99336500
C		2.12623800 -0.15772600 -3.03843200
C		2.82698600 -1.06694800 -2.23298700
H		2.60346100 -1.12769900 -1.17319300
C		3.80774000 -1.89444400 -2.78586900
H		4.33557800 -2.59776300 -2.14857500
C		4.10164700 -1.81383900 -4.14826700
H		4.86726000 -2.45330900 -4.58002800
C		3.40761800 -0.90906000 -4.95924000
H		3.63246800 -0.84615600 -6.02089300
C		2.42187100 -0.08853600 -4.40998500
H		1.88017800 0.59721400 -5.05552200
C		0.94198700 2.49319800 -3.10153700
H		0.78656700 2.42615600 -4.18275000
H		1.93987600 2.89549600 -2.90102600
H		0.20800000 3.18389100 -2.67726600
P		-0.80083700 2.33419500 0.77010800
C		-1.11560400 2.07575800 2.56197400
C		-0.12738300 2.45055500 3.48903300

H	0.76617000	2.96655600	3.14873800
C	-0.28338900	2.15943400	4.84405600
H	0.48635500	2.45921500	5.55024200
C	-1.41985700	1.47653700	5.29084700
H	-1.53697000	1.24391000	6.34598200
C	-2.40106700	1.09200800	4.37444000
H	-3.28401900	0.55462300	4.71065300
C	-2.25246000	1.39024800	3.01699800
H	-3.02015200	1.07053000	2.31977800
C	-0.21380800	4.07512300	0.67898400
C	-0.93476600	5.13050100	1.26172900
H	-1.84861800	4.92615000	1.81372000
C	-0.47645500	6.44279100	1.14607800
H	-1.03777600	7.25394800	1.60258900
C	0.70524000	6.71440700	0.44663100
H	1.06064500	7.73780600	0.35901800
C	1.42880400	5.66993400	-0.13206400
H	2.35084000	5.87389900	-0.67008700
C	0.97243900	4.35398900	-0.01306300
H	1.54197800	3.53571200	-0.44170200
C	-2.49890700	2.48286000	0.05334800
H	-3.12140300	3.16284400	0.64422000
H	-2.98224300	1.50498600	0.00030900
H	-2.40790100	2.87820700	-0.96193300
P	0.19163300	-1.07276100	1.26852400
C	1.02094300	-2.56613000	0.58144500
C	2.34977100	-2.84887800	0.94144000
H	2.85660400	-2.24075300	1.68467500
C	3.03911800	-3.89985400	0.33203200
H	4.06602400	-4.10688800	0.62192100
C	2.41603100	-4.67713500	-0.64809600
H	2.95533300	-5.49117200	-1.12471300
C	1.09574700	-4.40028900	-1.01287600
H	0.60206100	-5.00019500	-1.77325200
C	0.40268500	-3.35217800	-0.40422500
H	-0.62092400	-3.14537600	-0.70148900
C	-1.59326500	-1.50545800	1.26658500
C	-2.35936000	-1.10658800	0.16031500
H	-1.88049100	-0.57110900	-0.65303400
C	-3.72869200	-1.37774500	0.10706200
H	-4.30371000	-1.06682900	-0.76078100
C	-4.35057300	-2.03580900	1.17119000
H	-5.41800700	-2.23791000	1.13912300
C	-3.59556800	-2.43462900	2.27894700
H	-4.07553100	-2.94713100	3.10864600
C	-2.22364700	-2.17842800	2.32475400
H	-1.65253800	-2.49597800	3.19181500
C	0.67114600	-1.10269600	3.04895800
H	0.63805300	-2.10899900	3.47753600
H	0.00065900	-0.44258800	3.60485300
H	1.68550300	-0.70314100	3.13386400
I	3.28360800	1.28260500	0.98221000

6-I-PPh₃

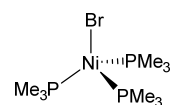


E	=	-3290.56151807	
G _{corr}	=	0.735468	
Ni	0.65210800	1.08207100	0.07069000
P	1.06762700	1.08895100	-2.24545900
C	-0.09917500	0.12626300	-3.29572800
C	-1.41722500	-0.04978300	-2.85304800
H	-1.71419600	0.33553700	-1.88643100
C	-2.34323600	-0.73336300	-3.64338600
H	-3.36210200	-0.85646600	-3.28732700
C	-1.95764100	-1.25910500	-4.87865100
H	-2.67699200	-1.79609000	-5.49158200
C	-0.64096900	-1.10029200	-5.32188100
H	-0.33289800	-1.51307700	-6.27902800
C	0.28480300	-0.41250700	-4.53520500
H	1.30587400	-0.29664700	-4.88680100
C	2.68730900	0.35110200	-2.71217400
C	2.97978200	-0.92370400	-2.19944300
H	2.26755500	-1.41771500	-1.54437600
C	4.18325700	-1.55101100	-2.51858600
H	4.40116100	-2.53221600	-2.10836200
C	5.11651800	-0.90629100	-3.33611800
H	6.05982900	-1.39156800	-3.57230100
C	4.83524600	0.36390700	-3.84371600
H	5.55606700	0.86969800	-4.48101100
C	3.62204000	0.98939000	-3.54015500
H	3.40824300	1.97326500	-3.94719100
P	-1.02854700	2.72145200	0.38293300
C	-1.99148500	2.58561200	1.95748800
C	-2.84358200	3.61406900	2.39506400
H	-2.94762000	4.52399800	1.81175800
C	-3.55882200	3.47903300	3.58467800
H	-4.21280400	4.28247900	3.91367100
C	-3.43420800	2.31626400	4.35333000
H	-3.99047900	2.21529900	5.28159000
C	-2.59275400	1.28885400	3.92425800
H	-2.48569000	0.38229800	4.51386400
C	-1.87539600	1.42355500	2.73195300
H	-1.22038500	0.62402400	2.40452500
C	-0.47535100	4.48437900	0.43464500
C	-1.24807100	5.56489400	-0.01858000
H	-2.22889500	5.39409700	-0.45000600
C	-0.75782100	6.87023400	0.06658700
H	-1.36509900	7.69549400	-0.29594500
C	0.50499700	7.11522100	0.61213200
H	0.88566400	8.13139800	0.67183500
C	1.27725000	6.04661800	1.07644200
H	2.26535000	6.21956600	1.49328400
C	0.78860100	4.74318400	0.98560700
H	1.40466800	3.91796500	1.32333900

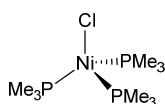
P	2.76321600	1.16772100	1.13998300
C	2.51953200	1.18296600	2.96962200
C	1.37166000	1.80951800	3.47578700
H	0.65546000	2.24586100	2.79050000
C	1.13661100	1.87047800	4.85002000
H	0.23310900	2.34763700	5.21967400
C	2.05259500	1.30113600	5.73766800
H	1.87040500	1.33859600	6.80843600
C	3.20253400	0.67727200	5.24403200
H	3.91849400	0.23327900	5.93072500
C	3.43796100	0.61846500	3.86898200
H	4.33456400	0.13080300	3.49910000
C	3.78498500	2.67723400	0.84518900
C	4.08707400	3.59904600	1.85947600
H	3.76279000	3.41577800	2.87864500
C	4.80103000	4.76462900	1.56692200
H	5.02401200	5.46961900	2.36364300
C	5.22952400	5.02125500	0.26244500
H	5.78278400	5.92914900	0.03752200
C	4.94593400	4.10117000	-0.75086300
H	5.27620400	4.28716900	-1.76938100
C	4.22616300	2.94166000	-0.46283700
H	4.01535700	2.23512000	-1.25868000
C	3.97233600	-0.21212100	0.92805300
C	3.49718500	-1.52124300	1.11757700
C	5.32639000	-0.02064500	0.61940600
C	4.35738400	-2.61218200	0.99936500
H	2.45072200	-1.68756000	1.35148100
C	6.18367800	-1.11695200	0.48928600
H	5.72271800	0.97872300	0.47677800
C	5.70438300	-2.41401900	0.67987100
H	3.97244300	-3.61734700	1.14996100
H	7.22929300	-0.95150500	0.24274100
H	6.37395000	-3.26430300	0.58029900
C	-2.35542400	2.69637300	-0.89541600
C	-2.15345800	3.30042000	-2.14826100
C	-3.52257200	1.94400900	-0.68532600
C	-3.09895300	3.15732100	-3.16419600
H	-1.26045400	3.88542500	-2.33450400
C	-4.46411200	1.79892400	-1.70689100
H	-3.69688400	1.46403100	0.27279900
C	-4.25551500	2.40351700	-2.94908600
H	-2.92376900	3.63123200	-4.12640100
H	-5.36135500	1.21218000	-1.52825900
H	-4.98794200	2.28701600	-3.74334600
C	1.09151600	2.75940000	-3.01563700
C	1.50748000	3.82219600	-2.20117600
C	0.66929500	3.02977600	-4.32644000
C	1.50174400	5.13364000	-2.67742600
H	1.81019000	3.62105400	-1.18158200
C	0.65644700	4.34280300	-4.80205200
H	0.33190600	2.22372100	-4.97022500
C	1.06867100	5.39660000	-3.97929300
H	1.81161400	5.94268700	-2.02210700
H	0.31835900	4.54385500	-5.81528600

H	1.04612200	6.41759200	-4.35111500
I	-0.38680000	-1.41962600	0.48720400

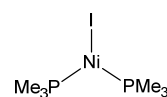
6-Br-PMe₃



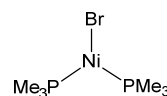
E	=	-1566.19226774	
G _{corr}	=	0.287107	
Ni	3.03250300	7.55801000	11.77588700
P	1.26707200	8.91609400	11.22903400
C	0.71294900	10.24606300	12.38905900
C	-0.30556700	7.98865100	10.95138800
C	1.43712400	9.86729000	9.65241700
H	-0.20052100	10.73924000	12.03408100
H	1.50308000	10.99816300	12.48689900
H	-1.12900900	8.65216400	10.66040500
H	-0.57256200	7.46031800	11.87237500
H	1.60521500	9.17079500	8.82402100
H	2.31162200	10.52378100	9.72105600
P	4.69473000	9.01283400	12.41539700
P	3.87791600	6.22789200	10.11080600
C	5.18975900	10.40823500	11.30993800
C	6.32322800	8.24707400	12.82857400
C	4.29040500	9.88914300	13.98952400
C	3.85611800	6.93305800	8.39969400
C	5.61548900	5.60194400	10.20979500
C	2.93378000	4.65832100	9.87645600
H	5.99141400	11.01175800	11.75214900
H	4.32400600	11.05260800	11.12227000
H	7.00328700	8.96836300	13.29741600
H	6.79269500	7.85599200	11.92056800
H	4.08020700	9.14482000	14.76482500
H	3.39004000	10.49700100	13.85278900
H	4.43130600	7.86548100	8.37817100
H	2.82389300	7.16564700	8.11611800
H	6.31260900	6.44377200	10.14364900
H	5.83757700	4.89632600	9.39968500
H	2.96854100	4.08178800	10.80615900
H	3.33826000	4.05644300	9.05377700
H	0.52646300	9.81292300	13.37745100
H	-0.15283200	7.23965100	10.16647900
H	0.54932600	10.47422600	9.43620700
H	4.27697300	6.23664600	7.66368600
H	5.77052200	5.10305800	11.17251700
H	1.88442800	4.89440100	9.66881100
H	5.11394400	10.53360200	14.31962900
H	5.53176100	10.00999600	10.34822900
H	6.15886600	7.40893700	13.51435400
Br	2.16865300	6.00315200	13.55847300

6-Cl-PMe₃

E	=	-2013.24570877	
G _{corr}	=	0.288220	
Ni	3.13193200	7.56706800	11.78039300
P	1.39241000	8.89649000	11.06173500
C	0.91569400	10.26053500	12.21291300
C	-0.20563000	7.99951200	10.83466200
C	1.56338700	9.80056800	9.46056100
H	0.01767500	10.78848200	11.87044400
H	1.74179900	10.97619500	12.28550900
H	-1.02067300	8.67595700	10.55071700
H	-0.46854600	7.49247600	11.76949400
H	1.63355700	9.08155800	8.63873500
H	2.48697200	10.38948600	9.47418800
P	4.64697400	9.06403100	12.63199100
P	3.69287900	6.21567100	10.00838200
C	5.13628800	10.51214700	11.59046400
C	6.27965600	8.28483100	13.00422700
C	4.25553800	9.88272600	14.24367100
C	3.47508900	6.80296500	8.26818500
C	5.49320600	5.79245600	10.03306000
C	2.92526000	4.53645200	9.92720000
H	5.92939100	11.10670100	12.06012000
H	4.26603900	11.15702500	11.42490400
H	6.97713600	8.99130500	13.47024000
H	6.72423600	7.90224600	12.07950100
H	4.04560800	9.11184800	14.99270000
H	3.35726500	10.49937500	14.13232600
H	3.94183800	7.78698300	8.14992400
H	2.40666000	6.90161000	8.04714800
H	6.08352800	6.70420400	9.89196600
H	5.75566500	5.07245500	9.24812500
H	3.09691300	4.02097700	10.87752200
H	3.33908600	3.93654300	9.10751300
H	0.73204800	9.84483800	13.20932400
H	-0.08544600	7.23548700	10.05867600
H	0.71301400	10.46817600	9.27756300
H	3.91887800	6.10725300	7.54562600
H	5.74667400	5.36740100	11.00989900
H	1.84292100	4.63718300	9.78877000
H	5.08143400	10.51256400	14.59650200
H	5.48712100	10.15781700	10.61465400
H	6.11816500	7.43771600	13.67900700
Cl	3.04333600	5.96742800	13.55335800

7-I-PMe₃

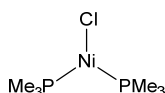
E	=	-1103.2070108	
G _{corr}	=	0.179439	
Ni	2.97694000	7.32161000	11.59716800
P	1.73021300	9.18358400	11.27788600
P	2.70143200	6.70177000	13.75815800
C	1.70482100	10.41968700	12.64600500
C	-0.06337500	8.85994600	10.99769100
C	2.19514000	10.20294200	9.81453500
C	3.65263600	7.70893400	14.97502300
C	0.98472800	6.78048000	14.42808800
C	3.21436900	4.97799400	14.16182700
H	1.07966700	11.28397700	12.39281700
H	2.72509900	10.76340100	12.84689300
H	-0.62405900	9.79195600	10.86137400
H	-0.47347300	8.31492500	11.85440400
H	2.13865400	9.58357700	8.91309500
H	3.22875700	10.54772200	9.92509800
H	3.32940300	8.75349700	14.91538100
H	4.71855300	7.66652200	14.72699200
H	0.61255400	7.80871700	14.36719700
H	0.95020100	6.44977000	15.47257900
H	2.62461700	4.27620500	13.56246900
H	3.07226000	4.75373200	15.22547000
H	1.31206900	9.95248300	13.55527300
H	-0.18205900	8.23511300	10.10619900
H	1.53561000	11.07105500	9.69924500
H	4.26945600	4.84342600	13.90105200
H	0.32944100	6.14002000	13.82804800
H	3.50701300	7.34509900	15.99878000
I	4.39144600	6.13458900	9.80203900

7-Br-PMe₃

E	=	-1104.992075	
G _{corr}	=	0.179718	
Ni	3.06750900	7.33061100	11.59571600
P	1.74691600	9.13568400	11.25518400
P	2.71524600	6.74593800	13.75887300
C	1.74732400	10.42266800	12.57785300
C	-0.04991700	8.75641800	11.07634700
C	2.09770600	10.12367900	9.73841800
C	3.61912600	7.78251000	14.98855800
C	0.97869700	6.82627000	14.37854000
C	3.22139600	5.03455200	14.22185100
H	1.09164700	11.26209700	12.31807200
H	2.76615200	10.79705000	12.72400900

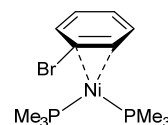
H	-0.63894700	9.66859100	10.92555600
H	-0.40746900	8.24202200	11.97458600
H	2.00818700	9.47756100	8.85860400
H	3.12519500	10.50112900	9.78008200
H	3.30674200	8.82693100	14.88426500
H	4.69483900	7.72734000	14.78979100
H	0.60383200	7.85200200	14.29823900
H	0.91473000	6.50504100	15.42473400
H	2.65338700	4.31490100	13.62245200
H	3.04688500	4.83554700	15.28569700
H	1.40338200	9.98270000	13.51978600
H	-0.19563400	8.08955500	10.21980800
H	1.40658800	10.96868500	9.63695700
H	4.28453600	4.89796700	13.99716200
H	0.34253200	6.17763100	13.76685600
H	3.42509900	7.45088900	16.01528300
Br	4.53599100	6.21555900	10.09098800

7-Cl-PMe₃

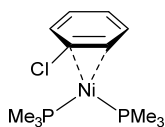


E	=	-1552.04429788	
G _{corr}	=	0.182396	
Ni	3.06690600	7.31937300	11.59599400
P	1.74836800	9.13061000	11.26473000
P	2.71674300	6.73966600	13.75863800
C	1.75110000	10.42370600	12.58137900
C	-0.04942500	8.75621200	11.08430600
C	2.10425400	10.11132300	9.74422700
C	3.61372800	7.78534000	14.98584800
C	0.97752200	6.82259700	14.37053800
C	3.22257200	5.03196700	14.23742400
H	1.09763500	11.26343500	12.31708900
H	2.77060800	10.79661300	12.72617400
H	-0.63554900	9.66943900	10.92877800
H	-0.41092700	8.24613200	11.98340600
H	2.01797900	9.46003300	8.86785500
H	3.13183700	10.48837100	9.78745900
H	3.30995100	8.83052900	14.86563400
H	4.69117300	7.72105900	14.79995800
H	0.60416200	7.84876200	14.28846800
H	0.90943800	6.50226200	15.41673000
H	2.65683600	4.30686900	13.64236600
H	3.04474700	4.84114800	15.30220000
H	1.40565700	9.98978900	13.52562700
H	-0.19540500	8.08665500	10.22995400
H	1.41414600	10.95618100	9.63525300
H	4.28681600	4.89428500	14.01789200
H	0.34264000	6.17451400	13.75709700
H	3.40581100	7.46753900	16.01420800
Cl	4.40937900	6.34932800	10.08462500

8-Br-PMe₃



E	=	-1336.64535174	
G _{corr}	=	0.267601	
Ni	-2.51527500	1.80090200	-0.03276900
P	-4.38851900	1.48763400	-1.18364500
C	-5.42814700	0.19073800	-0.37829600
C	-4.42043900	0.95404800	-2.95305400
C	-5.53034900	2.93934200	-1.21686000
H	-6.41317600	0.10190500	-0.85156400
H	-5.55218000	0.44260700	0.68028500
H	-5.44824200	0.86884900	-3.32584000
H	-3.92640700	-0.01728000	-3.05528200
H	-5.04366800	3.77575200	-1.73080100
H	-5.74682800	3.24839400	-0.18913800
P	-0.74211000	1.01423100	-1.07728500
C	0.28074000	2.30221200	-1.91782500
C	0.50677000	0.16478500	-0.01508200
C	-0.97523200	-0.22175500	-2.43164100
H	0.59936000	3.04152600	-1.17650700
H	-0.32606200	2.81174100	-2.67435900
H	0.84549400	0.85788600	0.76098000
H	1.37125500	-0.16925600	-0.60104700
H	-1.55022300	0.23092300	-3.24509000
H	-1.53560100	-1.08148600	-2.04845000
H	-4.91174100	-0.77349200	-0.43968200
H	-3.88047200	1.68260200	-3.56781700
H	-6.47074300	2.70394900	-1.72917700
H	1.16291800	1.86504700	-2.40074200
H	0.04842400	-0.70315200	0.47080400
H	-0.01359900	-0.57019400	-2.82716000
C	-1.89536400	2.30945900	1.70060600
C	-3.20549600	2.91896000	1.56358300
C	-4.27868400	2.46159500	2.39853800
C	-4.11752400	1.38229200	3.23408300
C	-2.84792000	0.73501200	3.31437900
C	-1.76043100	1.20286900	2.61272000
H	-3.29064200	3.91571200	1.13276200
H	-5.22225000	3.00345500	2.37495700
H	-4.93930000	1.03241300	3.85335300
H	-2.72962000	-0.13192800	3.96092500
H	-0.78725900	0.73589600	2.72885000
Br	-0.24806100	3.61851900	1.78727200

8-Cl-PMe₃

E	=	-1783.69729748
G _{corr}	=	0.268563
Ni		-0.77264000 0.67024800 -0.11353400
P		-2.62002100 0.41448600 -1.30633200
C		-3.85748200 -0.68813000 -0.48957900
C		-2.60606000 -0.27437400 -3.02303900
C		-3.59831700 1.96390000 -1.55118500
H		-4.81212500 -0.69266500 -1.02898500
H		-4.01944000 -0.34904800 0.53838900
H		-3.61853000 -0.32332700 -3.44209400
H		-2.18007700 -1.28272300 -3.01082600
H		-2.99298100 2.69954900 -2.09219100
H		-3.85641200 2.38761000 -0.57498400
P		1.03005200 -0.04754100 -1.15728700
C		1.98296500 1.30675800 -1.97944100
C		2.33378800 -0.84511100 -0.11922200
C		0.86900000 -1.26924700 -2.53617800
H		2.25451000 2.05616400 -1.22951300
H		1.35156300 1.78860200 -2.73419800
H		2.65430300 -0.14217600 0.65568100
H		3.20288000 -1.13792300 -0.72039500
H		0.25954100 -0.84058000 -3.33749500
H		0.36964100 -2.17283900 -2.16964600
H		-3.46427800 -1.71004700 -0.45014100
H		-1.98564300 0.35603700 -3.66933000
H		-4.51969000 1.77559000 -2.11529400
H		2.89234300 0.92832900 -2.46195400
H		1.92253600 -1.73473500 0.36951400
H		1.84848600 -1.54580500 -2.94432900
C		-0.11382200 1.21953900 1.61916100
C		-1.46586700 1.74168200 1.49147700
C		-2.49964500 1.19115500 2.32480200
C		-2.26171000 0.10997300 3.13673200
C		-0.94586700 -0.44362300 3.21152500
C		0.10363200 0.11840500 2.52555900
H		-1.61106800 2.74967900 1.10419300
H		-3.47989100 1.66371800 2.31171400
H		-3.05641900 -0.31055300 3.74741200
H		-0.76369300 -1.30599900 3.84910900
H		1.11229600 -0.26592100 2.64325800
Cl		1.29374000 2.45807500 1.59130600

TS-8-9-Br-PMe₃

E	=	-1336.64193985
G _{corr}	=	0.268325
v	=	-85.30 cm ⁻¹
Ni		-2.60106300 1.65679100 0.00721300

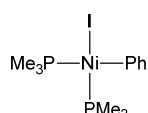
P		-4.43035800 1.38936200 -1.25685000
C		-5.67221000 0.32762000 -0.40282800
C		-4.41498800 0.68646800 -2.96083100
C		-5.34476000 2.97279200 -1.49828700
H		-6.62787000 0.31574300 -0.93969400
H		-5.82724300 0.70560800 0.61310700
H		-5.42976200 0.64071500 -3.37322800
H		-3.99472300 -0.32379600 -2.94164500
H		-4.72600500 3.66909800 -2.07467900
H		-5.55127000 3.42468200 -0.52272900
P		-0.79349100 1.05740800 -1.08144400
C		0.09006700 2.48410400 -1.83706700
C		0.49552800 0.26730800 -0.03497900
C		-0.94246200 -0.12575500 -2.48744000
H		0.32035600 3.20423200 -1.04622900
H		-0.55868300 2.96591800 -2.57671800
H		0.75004800 0.95431600 0.77722100
H		1.39427800 0.04030800 -0.61995700
H		-1.55800300 0.31103100 -3.27890800
H		-1.42172200 -1.04826700 -2.14277300
H		-5.28819200 -0.69581500 -0.33083700
H		-3.79535600 1.31120700 -3.61263500
H		-6.29011900 2.81036300 -2.02875400
H		1.01741600 2.16198800 -2.32530800
H		0.10302600 -0.66114000 0.39283400
H		0.04413900 -0.37003500 -2.89799200
C		-2.05804200 2.02438900 1.71394600
C		-3.29554500 2.74234100 1.69264100
C		-4.30822000 2.40404500 2.63487700
C		-4.12055200 1.35653700 3.51744900
C		-2.89924300 0.63829800 3.51313500
C		-1.86780200 0.98055500 2.65368600
H		-3.37806200 3.69102400 1.16416100
H		-5.21167500 3.00854600 2.68189900
H		-4.89704300 1.09177600 4.23012300
H		-2.76978600 -0.20198800 4.19198100
H		-0.92739600 0.43926400 2.67196600
Br		-0.07981500 3.56567100 1.89055600

TS-8-9-Cl-PMe₃

E	=	-1783.69289962
G _{corr}	=	0.269087
v	=	-104.13 cm ⁻¹
Ni		-0.80924900 0.56031400 -0.12550700
P		-2.62462800 0.31269600 -1.41950500
C		-3.87651500 -0.74462300 -0.57466800
C		-2.59668600 -0.38744400 -3.12368600
C		-3.52644800 1.90271600 -1.66166200
H		-4.82870800 -0.75306200 -1.11777200
H		-4.03689400 -0.36607800 0.44028600
H		-3.60905400 -0.43552300 -3.54164000
H		-2.17372500 -1.39652500 -3.10276600
H		-2.89955300 2.59644500 -2.23223200

H	-3.73523500	2.35284500	-0.68570900
P	1.01236900	-0.01240000	-1.19417700
C	1.88322300	1.43784500	-1.91600300
C	2.29460600	-0.80464900	-0.14344800
C	0.88123500	-1.17463300	-2.61848000
H	2.09870700	2.14004200	-1.10542100
H	1.23283200	1.92717600	-2.64912600
H	2.54061600	-0.11599400	0.66969900
H	3.19637700	-1.02920100	-0.72468500
H	0.26698400	-0.73054600	-3.40681800
H	0.40886000	-2.10731100	-2.29229400
H	-3.49610100	-1.76919200	-0.50014600
H	-1.97534700	0.23979600	-3.77135500
H	-4.46998900	1.74813900	-2.19765000
H	2.81651300	1.13513000	-2.40511100
H	1.90088700	-1.73443700	0.28017100
H	1.87296300	-1.40251600	-3.02621100
C	-0.26389700	0.89777900	1.57388900
C	-1.48043000	1.64497900	1.58429900
C	-2.46202600	1.35060100	2.57063200
C	-2.25290000	0.32877100	3.47975100
C	-1.04186200	-0.40352200	3.45485700
C	-0.04191400	-0.10999700	2.54017200
H	-1.57265600	2.57271800	1.02021100
H	-3.35556200	1.96828700	2.63128500
H	-3.00507000	0.09778900	4.22923400
H	-0.89647800	-1.22104300	4.15783900
H	0.88930700	-0.66726300	2.53491200
Cl	1.67504400	2.36902100	1.66149600

9-I-PMe₃



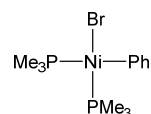
$$E = -1334.70742817$$

$$G_{\text{corr}} = 0.268779$$

Ni	2.37440000	3.95863200	5.57007600
P	1.01244700	5.02022200	4.03544600
C	0.13548000	6.39191800	4.90358800
C	-0.34992600	4.06672700	3.24739600
C	1.71661700	5.93965900	2.59506000
H	-0.47430500	6.96501300	4.19612800
H	0.87311500	7.05837400	5.36408400
H	-0.98519700	4.72020300	2.63856400
H	-0.95502500	3.58966100	4.02361100
H	2.00331700	5.25135900	1.79738800
H	2.59675300	6.51204500	2.90619900
P	4.10747000	3.35992700	4.35495700
C	3.95981600	3.41180600	2.51789900
C	5.72806700	4.18411300	4.62391500
C	4.46099000	1.57603100	4.63198100
H	4.02651100	4.44136800	2.16033500
H	3.00530800	2.97906600	2.20368500

H	5.63172100	5.25719500	4.42790800
H	6.47646000	3.76275800	3.94347900
H	4.82627900	1.42293400	5.64899000
H	5.21243100	1.22333900	3.91729300
H	-0.50247200	5.98773800	5.69272000
H	0.07494800	3.28474900	2.60871700
H	0.96615400	6.63378100	2.20016500
H	4.77631600	2.83345100	2.07112500
H	6.05335200	4.04509100	5.65695400
H	3.53901100	1.00006200	4.50172000
C	3.54282700	3.67092200	7.05768900
C	3.74568300	2.49242100	7.79311500
C	4.53579300	2.48287000	8.94715900
C	5.13508200	3.66278200	9.40098800
C	4.94125100	4.84782500	8.68616900
C	4.16416300	4.84416500	7.52089500
H	3.26352900	1.57227600	7.47281100
H	4.67414000	1.55561800	9.49972900
H	5.74449000	3.65805600	10.30149400
H	5.40176900	5.77283800	9.02759100
H	4.04627800	5.77341900	6.96355900
I	0.27331600	3.31344500	7.08271300

9-Br-PMe₃



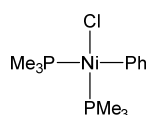
$$E = -1336.69800763$$

$$G_{\text{corr}} = 0.271175$$

Ni	-3.52707500	1.70041900	0.12845700
P	-4.53274900	1.68518200	-1.96134900
C	-6.32780600	1.27132300	-1.93998200
C	-3.96597700	0.51692500	-3.27871500
C	-4.49898100	3.32033400	-2.80758700
H	-6.72635800	1.26545000	-2.96082100
H	-6.86607800	2.00207000	-1.33354800
H	-4.55048300	0.67072000	-4.19293900
H	-4.12263800	-0.51060100	-2.93353700
H	-3.46455100	3.60310800	-3.02845100
H	-4.92536800	4.07113300	-2.13466300
P	-1.48573000	1.23291500	-0.55457100
C	-0.92567800	2.24031900	-1.99401000
C	-0.07656800	1.49765000	0.59744200
C	-1.24035400	-0.51828400	-1.05826300
H	-0.92212700	3.29479100	-1.69811700
H	-1.58704500	2.12698500	-2.85424500
H	-0.08743300	2.52704600	0.96616000
H	0.86494700	1.31035100	0.06883000
H	-1.94179400	-0.79260700	-1.84966400
H	-1.42887200	-1.15790900	-0.18974300
H	-6.46977700	0.28261300	-1.49088100
H	-2.90695000	0.64543500	-3.51482900
H	-5.07397000	3.30019100	-3.74038400

H	0.09047200	1.95098500	-2.28487300
H	-0.15631500	0.82236800	1.45203100
H	-0.21468400	-0.68257500	-1.40693500
C	-2.86027200	1.38547500	1.88710500
C	-2.42448100	2.38335800	2.77399600
C	-1.99047800	2.06959500	4.06501500
C	-1.98751600	0.74050000	4.50530300
C	-2.42208600	-0.26661800	3.63999300
C	-2.84608400	0.05664800	2.34376700
H	-2.43524700	3.42245900	2.45338300
H	-1.65832100	2.86267500	4.73269400
H	-1.65129800	0.49487100	5.50991700
H	-2.42715300	-1.30415300	3.96929700
H	-3.16539300	-0.74504200	1.67834600
Br	-5.46833100	2.83660700	1.08135400

9-Cl-PMe₃



E	=	-1783.75121852	
G _{corr}	=	0.270617	
Ni	-1.66158000	0.51749800	-0.01575800
P	-2.30701100	1.54735800	-2.00573100
C	-4.08047500	1.31200400	-2.44171000
C	-1.52814700	1.35978300	-3.67301600
C	-2.15312400	3.36519500	-1.74458700
H	-4.36201600	1.95000900	-3.28712100
H	-4.69830600	1.55097700	-1.57331700
H	-1.93007300	2.12187500	-4.35053200
H	-1.76065200	0.37627600	-4.09193800
H	-1.09764900	3.62182300	-1.60012600
H	-2.70278700	3.64094400	-0.84116300
P	0.06814000	-0.59646800	-0.78501100
C	-0.25808500	-1.67144600	-2.24476100
C	1.41503500	0.53898200	-1.31709500
C	0.97016900	-1.77457600	0.30184400
H	-0.64348800	-1.09464500	-3.08592800
H	-1.00441400	-2.42349000	-1.96741100
H	1.04172500	1.25541700	-2.05261600
H	2.25247900	-0.02224600	-1.74669400
H	0.28983000	-2.55781000	0.64690900
H	1.36588700	-1.25486600	1.17708300
H	-4.25032800	0.26394300	-2.71238400
H	-0.44204300	1.47641000	-3.62466000
H	-2.54500700	3.92261200	-2.60290600
H	0.66335200	-2.17943800	-2.55081500
H	1.76743800	1.09601800	-0.44257900
H	1.79359300	-2.22822100	-0.26072600
C	-1.11421900	-0.05512300	1.71575000
C	-1.64229100	-1.20161900	2.33062500
C	-1.25877000	-1.57575700	3.62297900
C	-0.33041100	-0.80674200	4.33251900

C	0.20438500	0.33980800	3.73776700
C	-0.18425200	0.70618000	2.44326900
H	-2.36473700	-1.81380500	1.79358500
H	-1.68410200	-2.46893400	4.07731500
H	-0.02854500	-1.09726400	5.33606100
H	0.92565100	0.94858100	4.28021200
H	0.25068000	1.59778400	1.99309300
Cl	-3.47625700	1.53010200	0.95223600

TS-9-3-I-PMe₃

E	=	-1334.89533628	
G _{corr}	=	0.265005	
V	=	-88.03 cm ⁻¹	
Ni	-1.30498100	0.12127600	0.00974500
P	-2.55981600	1.85759200	-0.96668600
C	-3.50474300	2.75682700	0.33863900
C	-3.86857500	1.45652700	-2.20150000
C	-1.63704600	3.22647900	-1.79412800
H	-4.08081900	3.58892600	-0.08302700
H	-2.80818100	3.14409900	1.09010700
H	-4.41774000	2.35269400	-2.51393200
H	-4.56679700	0.73834600	-1.75962400
H	-1.12426000	2.84186300	-2.68257900
H	-0.88343200	3.62882400	-1.10828700
P	0.49890900	-0.48730700	-0.96608300
C	-0.01624600	-0.95849900	-2.66636700
C	1.81787600	0.76136100	-1.21863300
C	1.37052500	-1.96769200	-0.33022300
H	-0.44193000	-0.08849800	-3.17569900
H	-0.78242100	-1.73703700	-2.60445200
H	1.38624400	1.65414800	-1.68237200
H	2.60357900	0.35953800	-1.86796200
H	1.81275500	-1.74305300	0.64412900
H	2.15689200	-2.27781800	-1.02707000
H	-4.18707400	2.05746200	0.83295700
H	-3.41409300	0.98891500	-3.08171300
H	-2.30803800	4.03867100	-2.09876700
H	0.84195100	-1.33018600	-3.23813900
H	2.25033000	1.04067700	-0.25413800
H	0.64828300	-2.78085300	-0.20896900
C	-0.21023300	0.38033000	1.48376800
C	-0.12258300	-0.59811600	2.48617700
C	0.37255900	-0.26586100	3.75185500
C	0.81192100	1.03529500	4.01787100
C	0.75835100	2.00583300	3.01269400
C	0.26516000	1.67560600	1.74506500
H	-0.46111800	-1.60940900	2.28111500
H	0.41706700	-1.02564300	4.52901300
H	1.20103100	1.28940300	5.00058300
H	1.10710000	3.01703300	3.21063800
H	0.23973600	2.42962100	0.96181300
I	-3.06747900	-1.97892200	0.15291800

TS-9-3-Br-PMe₃

E	=	-1336.67631292
G _{corr}	=	0.267521
v	=	-84.67 cm ⁻¹
Ni	0.71481000	1.22553000 -0.03001400
P	-0.48274500	3.04627000 -0.97831300
C	-1.43605900	3.86803000 0.37238000
C	-1.79203400	2.73018900 -2.23942500
C	0.43314200	4.47372200 -1.71463700
H	-1.99258300	4.73828700 0.00432300
H	-0.74611400	4.18705700 1.16113300
H	-2.36664500	3.63650700 -2.46558400
H	-2.46880000	1.95688300 -1.86152800
H	0.95310000	4.15027800 -2.62328100
H	1.18002400	4.83812400 -1.00043600
P	2.55352300	0.68320500 -0.99142800
C	2.07818300	0.17636500 -2.69552300
C	3.85228400	1.95522600 -1.24535800
C	3.46790400	-0.76434000 -0.33444100
H	1.63524700	1.02841400 -3.22081700
H	1.33202600	-0.62227400 -2.63956000
H	3.41084000	2.83675000 -1.72116700
H	4.65372200	1.56320600 -1.88157800
H	3.86903200	-0.52168200 0.65353600
H	4.28885400	-1.04096500 -1.00519500
H	-2.13681500	3.14760800 0.80730900
H	-1.33223900	2.35883500 -3.16211700
H	-0.24207700	5.29949800 -1.97049200
H	2.95228900	-0.17970200 -3.25290600
H	4.26977000	2.25072600 -0.27888100
H	2.77825400	-1.60817000 -0.23344800
C	1.78582400	1.56724300 1.44928400
C	1.89417200	0.62190200 2.48113600
C	2.41474600	0.99301400 3.72550100
C	2.85479000	2.30303000 3.94479800
C	2.77585200	3.24220600 2.91225300
C	2.25860000	2.87139400 1.66522300
H	1.54544100	-0.39262500 2.31388300
H	2.47598300	0.25731700 4.52466200
H	3.26216600	2.58759100 4.91169100
H	3.12375300	4.26058900 3.07196300
H	2.21411400	3.60036800 0.85929000
Br	-1.02463200	-0.51900700 0.31646300

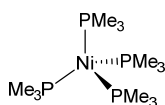
C	-3.06930000	2.73735600 -2.13063400
C	-0.73396700	4.36403600 -1.77616600
H	-2.99353200	4.69559700 0.16325900
H	-1.66705800	4.07639600 1.18972200
H	-3.61427400	3.67491400 -2.29368500
H	-3.75377800	1.99244000 -1.71155100
H	-0.30145700	4.02943400 -2.72578300
H	0.08218000	4.69493800 -1.12454700
P	1.42783300	0.58471500 -1.01476000
C	1.01142800	0.02274900 -2.71781500
C	2.67583000	1.90731600 -1.26916000
C	2.39569400	-0.80108000 -0.30271100
H	0.52911500	0.84145300 -3.26176600
H	0.30915100	-0.81494400 -2.65949700
H	2.20776100	2.76421100 -1.76405500
H	3.50144200	1.53853400 -1.88815600
H	2.76119500	-0.51452100 0.68758400
H	3.24529300	-1.05633600 -0.94580400
H	-3.12120500	3.09414500 0.94730000
H	-2.70771400	2.36253400 -3.09479200
H	-1.39559900	5.21675400 -1.97225700
H	1.91154300	-0.29267700 -3.25791200
H	3.06925900	2.23205800 -0.30192300
H	1.74445100	-1.67410300 -0.19336700
C	0.53808000	1.47616000 1.39532500
C	0.61168700	0.54703000 2.44488500
C	1.09468400	0.93620000 3.69919300
C	1.53292000	2.24747900 3.91203700
C	1.49146500	3.16910300 2.86180400
C	1.00994900	2.78106400 1.60599400
H	0.27003800	-0.47133900 2.28502000
H	1.12998800	0.21166100 4.50999600
H	1.91073800	2.54603500 4.88664400
H	1.83802400	4.18884900 3.01542500
H	0.99451800	3.49789200 0.78876300
Cl	-2.15901000	-0.48711900 0.26577700

TS-9-3-Cl-PMe₃

E	=	-1783.72865959
G _{corr}	=	0.268487
v	=	-88.55 cm ⁻¹
Ni	-0.46345900	1.07262600 -0.11445600
P	-1.64277900	2.96437400 -0.98048100
C	-2.43743500	3.79902700 0.46244500

In Toluene

Ni(PMe₃)₄



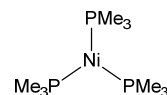
E = -2014.13708291

G_{corr} = 0.403970

Ni	2.97381100	7.50344000	11.85409900
P	1.37483900	8.84210700	11.13366300
P	2.20722400	6.27725200	13.51149600
C	0.88536800	10.24856200	12.25337300
C	-0.31697100	8.16396700	10.75098000
C	1.64143500	9.81555100	9.56776600
C	2.55556300	6.82503300	15.25803600
C	0.36860200	6.01592500	13.67682000
C	2.74379500	4.49927900	13.67361100
H	0.05074000	10.83875800	11.85235300
H	1.74639700	10.91117200	12.39388100
H	-0.99515300	8.92925400	10.35015700
H	-0.76077600	7.74282600	11.65808900
H	1.69439100	9.13211500	8.71510100
H	2.59567600	10.35007200	9.62535100
H	2.18758700	7.84642100	15.40103200
H	3.63692500	6.82627000	15.43416100
H	-0.12338400	6.97858500	13.85513400
H	0.11669700	5.33787300	14.50319500
H	2.36144500	3.92489400	12.82404700
H	2.37823100	4.03591700	14.59981200
P	4.57278300	8.84210700	12.57453600
P	3.74039800	6.27725100	10.19670300
C	5.06225400	10.24856200	11.45482600
C	6.26459200	8.16396600	12.95721900
C	4.30618600	9.81555100	14.14043300
C	3.39205800	6.82503300	8.45016300
C	5.57901900	6.01592500	10.03137800
C	3.20382600	4.49927900	10.03458800
H	5.89688200	10.83875700	11.85584600
H	4.20122600	10.91117200	11.31431800
H	6.94277500	8.92925400	13.35804300
H	6.70839800	7.74282500	12.05011000
H	4.25323000	9.13211500	14.99309800
H	3.35194600	10.35007200	14.08284800
H	3.76003400	7.84642100	8.30716700
H	2.31069700	6.82627000	8.27403800
H	6.07100500	6.97858500	9.85306500
H	5.83092400	5.33787300	9.20500400
H	3.58617600	3.92489400	10.88415200
H	3.56939100	4.03591700	9.10838700
H	0.60305900	9.85393000	13.23550800
H	-0.22469800	7.35334000	10.01912300
H	0.83650600	10.53989700	9.38505300

H	3.86490100	6.17035700	7.70594000
H	5.97358000	5.60061000	10.96487800
H	2.10969600	4.44342100	10.05054800
H	3.83792600	4.44342100	13.65765100
H	-0.02595900	5.60061000	12.74332100
H	2.08272000	6.17035800	16.00225900
H	5.11111600	10.53989700	14.32314600
H	5.34456300	9.85392900	10.47269100
H	6.17231900	7.35333900	13.68907600

Ni(PMe₃)₃



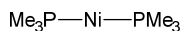
E = -1552.92426336

G_{corr} = 0.294185

Ni	-0.37837600	1.29416200	-0.03109900
P	-1.59146500	2.98753900	-0.59201400
P	-0.61818900	0.48827300	1.95583800
C	-1.65730000	4.43136800	0.58038000
C	-3.40670900	2.62804300	-0.77096400
C	-1.29768300	3.90778500	-2.18441500
C	0.44962100	1.34553100	3.21291700
C	-2.25996400	0.56294700	2.83011800
C	-0.18076400	-1.28545500	2.32129700
H	-2.32478500	5.22823500	0.22713300
H	-0.65035900	4.84505700	0.70753100
H	-3.98395600	3.52092500	-1.04389700
H	-3.78933400	2.22797500	0.17437000
H	-1.37319200	3.20596000	-3.02228600
H	-0.28166700	4.31859600	-2.18123800
H	0.18761500	2.40858700	3.24441100
H	1.49972900	1.27013200	2.91047300
H	-2.59566300	1.60479000	2.88108800
H	-2.21362400	0.15511200	3.84879900
H	-0.81105800	-1.94614300	1.71516300
H	-0.31398100	-1.54403800	3.38037000
P	1.12325800	0.41662900	-1.30785200
C	1.30644200	0.96266900	-3.07865600
C	2.87662000	0.64088600	-0.73043800
C	1.09510100	-1.42544500	-1.56013100
H	1.50425300	2.04006300	-3.09967900
H	0.36415100	0.78646600	-3.61020900
H	3.09499200	1.71042600	-0.63615900
H	3.60360400	0.18967800	-1.41805000
H	1.15910700	-1.92528600	-0.58757800
H	1.91848100	-1.77372800	-2.19737400
H	-2.00274300	4.08627900	1.56132700
H	-3.55380400	1.86238100	-1.54075200
H	-2.00997800	4.72896700	-2.34330400
H	2.11528200	0.44143500	-3.60851400
H	2.99325500	0.18688600	0.25968000
H	0.14457600	-1.71537200	-2.02228400

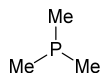
H	0.86298900	-1.46747800	2.04174300
H	-3.00486100	-0.00272300	2.25874800
H	0.33526600	0.91787100	4.21737200

Ni(PMe₃)₂



E	=	-1091.70878163
G _{corr}	=	0.186059
Ni		2.97653100 7.45427600 11.84232000
P		1.82795000 9.14246000 11.22109500
P		4.14393200 5.80034500 12.51666300
C		1.88573500 10.63545200 12.32156800
C		-0.00517300 8.91423100 11.04646100
C		2.23965600 9.90648800 9.58127300
C		5.41142300 6.14879300 13.82612300
C		3.24381700 4.37090300 13.28343600
C		5.18372900 4.91534300 11.26115800
H		1.26234000 11.45165600 11.93504300
H		2.92012100 10.98512800 12.40776900
H		-0.50279800 9.84149100 10.73504100
H		-0.42457300 8.58604800 12.00350800
H		2.14014300 9.15418500 8.79142000
H		3.28041500 10.24787900 9.59046600
H		4.91633300 6.55807700 14.71323900
H		6.12009100 6.89925000 13.45983000
H		2.66092700 4.72481400 14.14044200
H		3.93479200 3.58754600 13.61952600
H		4.54196200 4.52317100 10.46499000
H		5.74499000 4.08580600 11.70958700
H		1.53836800 10.36244300 13.32377500
H		-0.20799900 8.13331600 10.30567500
H		1.58494200 10.75684500 9.35259500
H		5.88904600 5.62001800 10.80771500
H		2.54610100 3.94431300 12.55477600
H		5.96277700 5.24313800 14.10964700

PMe₃



E	=	-461.172525307
G _{corr}	=	0.084469
P		1.67484700 -0.11566400 -0.01330200
C		2.55783100 0.74151800 -1.41288500
H		2.39837900 0.18879300 -2.34593100
H		2.14845100 1.74901800 -1.54919800
H		3.63817000 0.82334900 -1.23581400
C		2.37136300 0.85366700 1.41672300
H		1.97765200 1.87654400 1.39773100
H		2.05965700 0.39537400 2.36235600
H		3.46792000 0.90020800 1.39517500
C		2.73439300 -1.64250600 0.11665500

H	2.46666600	-2.20518100	1.01842200
H	2.55297500	-2.29344900	-0.74633300
H	3.80560600	-1.40598700	0.15666900

PhI



E	=	-243.107411301
G _{corr}	=	0.058655
C		2.37157500 -0.21732900 0.00004300
C		3.76822800 -0.23265400 0.00051000
C		4.45944700 0.98171500 -0.00005600
C		3.76393600 2.19238200 -0.00103400
C		2.36761900 2.19011800 -0.00148000
C		1.66000600 0.98489800 -0.00094800
H		4.31110600 -1.17155600 0.00129100
H		5.54623300 0.97381700 0.00029700
H		4.30742100 3.13298200 -0.00147600
H		1.81887400 3.12816300 -0.00226200
H		0.57508200 0.98662000 -0.00129100
I		1.31136300 -2.06288500 0.00090300

Ph•



E	=	-231.634469524
G _{corr}	=	0.059636
C		1.08903600 -0.03726000 0.00006800
C		2.48710300 -0.02944900 0.00046800
C		3.19309100 1.17730400 -0.00006300
C		2.50138000 2.40050800 -0.00093800
C		1.12511000 2.33023600 -0.00131100
C		0.37584200 1.17352000 -0.00088100
H		0.54732900 -0.98048800 0.00048500
H		3.03023100 -0.97063200 0.00119900
H		4.28086300 1.17485100 0.00024600
H		3.03752200 3.34612200 -0.00135700
H		-0.71121200 1.18196800 -0.00119500

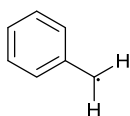
Toluene



E	=	-271.655265649
G _{corr}	=	0.098610
C		5.36852300 -0.42567700 0.02178100
H		4.47301500 -0.85535400 0.49141000
H		5.87686300 0.17269100 0.78652500
H		6.02627100 -1.25953500 -0.24677800

C	5.00528800	0.40794500	-1.18421600
C	4.60796100	1.74478800	-1.03725900
C	5.03057800	-0.13799500	-2.47461600
C	4.24480600	2.51280100	-2.14452200
H	4.58602300	2.18782400	-0.04364900
C	4.66816900	0.62597900	-3.58604900
H	5.33961500	-1.17241400	-2.60986700
C	4.27322300	1.95542100	-3.42513600
H	3.94332800	3.54841800	-2.00750700
H	4.69804800	0.18236500	-4.57820700
H	3.99451800	2.55299600	-4.28916600

Toluene radical



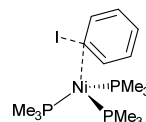
E	=	-271.002248804	
G _{corr}	=	0.085412	
C	6.50908800	1.27618600	-0.21000700
H	6.67673200	1.81105700	0.71994700
H	6.69715200	0.20676400	-0.21611400
C	6.06368900	1.94410500	-1.36490400
C	5.81901300	3.35063500	-1.36239100
C	5.83781300	1.24266900	-2.58778000
C	5.37988800	4.00260500	-2.50438500
H	5.98439800	3.90922400	-0.44413800
C	5.39869600	1.90613500	-3.72307600
H	6.01733000	0.17054000	-2.61621900
C	5.16527600	3.28938000	-3.69350100
H	5.20012900	5.07449300	-2.47747600
H	5.23410300	1.34969400	-4.64248800
H	4.82056800	3.80490100	-4.58553300

H Abstraction TS: Ph• + Toluene

E	=	-503.285594423	
G _{corr}	=	0.170965	
v	=	-1107.17 cm ⁻¹	
C	0.48657400	-0.67541400	0.05715700
C	1.87801500	-0.62389000	0.22491400
C	2.62063300	0.06446100	-0.72007300
C	2.06170500	0.70079100	-1.81565800
C	0.66967500	0.64194600	-1.97270200
C	-0.11121200	-0.04442600	-1.03795100
H	-0.12625600	-1.20779900	0.78132700
H	2.35048400	-1.11237100	1.07427100
H	2.68330000	1.23079800	-2.53388300
H	0.19919300	1.13087700	-2.82283500
H	-1.19007900	-0.08773700	-1.16298900
C	5.34497900	0.34502300	-0.68351400

H	4.12462700	0.17578200	-0.63411700
H	5.57819400	0.84416900	0.26109900
H	5.75058500	-0.67043500	-0.70122800
C	5.65257400	1.14709700	-1.89141800
C	5.63552400	2.55332100	-1.84745900
C	5.89697600	0.52463700	-3.12910900
C	5.86516100	3.30919600	-2.99612700
H	5.44017300	3.05209700	-0.90071900
C	6.12706200	1.27939000	-4.27842200
H	5.90665200	-0.56165800	-3.18358100
C	6.11232800	2.67569400	-4.21740000
H	5.85249700	4.39477700	-2.93889600
H	6.31910800	0.77746900	-5.22345500
H	6.29291200	3.26445000	-5.11287900

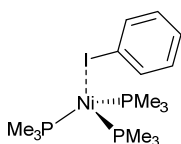
TS-1-2-I-PMe₃



E	=	-1796.04472876	
G _{corr}	=	0.377611	
v	=	-45.52 cm ⁻¹	
Ni	-1.22766800	-0.66595800	0.31022100
P	-0.47472200	0.44258700	-1.45468100
P	-0.40115100	-2.73170400	0.26434200
P	-3.45091400	-0.79752000	0.16192500
C	-0.71802400	0.67184700	1.97539500
C	-1.50084000	-0.12509200	2.85331200
C	0.68906900	0.47397000	1.95915700
C	-0.88127800	-1.04110400	3.71839800
H	-2.56354100	0.06567900	2.94323100
C	1.28291200	-0.44784400	2.82156700
H	1.30783200	1.09218600	1.32082900
C	0.50441700	-1.18979600	3.72128100
H	-1.49831700	-1.61883400	4.40218300
H	2.36310100	-0.57000800	2.80122800
H	0.97917800	-1.88261200	4.41100100
C	-4.37843200	-1.98627000	1.25045300
H	-4.18701500	-1.74348200	2.30142400
H	-5.46151500	-1.96581900	1.07230200
H	-4.01237000	-3.00380100	1.07441100
C	-4.51571300	0.70895000	0.37071900
H	-5.57470200	0.49466800	0.17592900
H	-4.41527000	1.09855600	1.38922100
H	-4.17561500	1.49190000	-0.31434900
C	-4.04610300	-1.37437100	-1.50097300
H	-3.72014300	-0.66715000	-2.27068000
H	-3.60295100	-2.34834000	-1.73363900
H	-5.13929400	-1.46184700	-1.54502900
C	-0.16525900	-0.60209000	-2.95954300
H	0.13981500	0.00089100	-3.82426500
H	0.62301100	-1.33242500	-2.74812300

H	-1.07907800	-1.14842200	-3.21718200
C	-1.58327900	1.72918500	-2.21069300
H	-2.55308800	1.28478000	-2.45789700
H	-1.75385600	2.53182100	-1.48716200
H	-1.15156000	2.15870700	-3.12399100
C	1.10859500	1.41180000	-1.41396100
H	1.93124100	0.76377600	-1.09313300
H	1.35249700	1.83686700	-2.39577000
H	1.01419100	2.23274900	-0.69533800
C	1.43623300	-2.94819300	0.09344800
H	1.93439800	-2.46371100	0.93915200
H	1.73335600	-4.00446900	0.05888000
H	1.77569000	-2.45389800	-0.82404200
C	-0.97329800	-3.81515600	-1.13499200
H	-0.80027600	-3.31943000	-2.09495000
H	-0.45420400	-4.78211900	-1.13931100
H	-2.04858900	-4.00076800	-1.04013200
C	-0.72683400	-3.88963700	1.67755700
H	-0.24516300	-3.50857800	2.58141700
H	-1.80498400	-3.93183600	1.86601300
H	-0.35507000	-4.90178600	1.47294700
I	-1.41225000	2.76794000	1.66203000

4-I-PMe₃



$$E = -1796.05331975$$

$$G_{\text{corr}} = 0.374202$$

Ni	2.49049200	7.76494000	11.86972100
P	1.46795900	9.29256500	10.69778800
C	1.23004600	10.98173200	11.44135700
C	-0.26941500	8.98593600	10.10796100
C	2.26339900	9.77627500	9.08974300
H	0.71601800	11.67288700	10.76046300
H	2.20467600	11.40681300	11.70368600
H	-0.65036100	9.79746700	9.47359200
H	-0.93252400	8.87671300	10.97421500
H	2.24374600	8.92718800	8.39963000
H	3.31173000	10.03838600	9.26806600
P	4.03338300	8.70826300	13.10119900
P	3.06058600	6.00247100	10.71197300
C	5.09107700	9.95087300	12.20812800
C	5.38654800	7.74459800	13.94588800
C	3.47063200	9.73357100	14.54534400
C	3.17482300	6.18102000	8.86327100
C	4.72276900	5.21689300	11.01566600
C	1.98720300	4.48897900	10.81096500
H	5.85312900	10.39602800	12.86130700
H	4.46386700	10.75333700	11.80533800
H	6.10153700	8.40062200	14.46018000
H	5.92868200	7.14340300	13.20744600

H	2.95672900	9.08490900	15.26386500
H	2.74859000	10.48094100	14.19931400
H	3.88197400	6.98150100	8.61922200
H	2.19394100	6.45953900	8.46356800
H	5.50704200	5.96923500	10.87452100
H	4.91693700	4.37303300	10.34013400
H	1.94903500	4.13711200	11.84752800
H	2.35241600	3.67435300	10.17203500
H	0.64554800	10.89092200	12.36357700
H	-0.30258100	8.04654900	9.54503100
H	1.75577600	10.62692100	8.61665300
H	3.50436100	5.25456000	8.37465100
H	4.78181200	4.85623200	12.04789700
H	0.96640800	4.74911200	10.51028600
H	4.29982300	10.24140200	15.05539300
H	5.58894700	9.45884100	11.36488800
H	4.94959700	7.06209400	14.68234200
I	0.59453300	6.98089800	13.52685400
C	1.45960400	5.42557000	14.72272300
C	2.79055200	5.09202400	14.47767900
C	0.71528100	4.76832200	15.70376700
C	3.39016200	4.07971400	15.23186900
H	3.33811700	5.62536400	13.70451000
C	1.32683100	3.75690800	16.45108800
H	-0.32175800	5.03495800	15.88610100
C	2.66091900	3.41105300	16.21827100
H	4.42855300	3.81632700	15.04511600
H	0.75494300	3.23962200	17.21731800
H	3.12889900	2.62401500	16.80328400

TS-4-5-I-PMe₃

$$E (\text{OSS}) = -1796.04305854$$

$$E (\text{T}) = -1796.02642847$$

$$S^2(\text{OSS}) = 0.6013$$

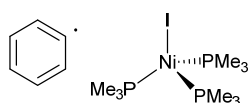
$$G_{\text{corr}} = 0.371398$$

$$v = -188.75 \text{ cm}^{-1}$$

Ni	-1.68677000	1.86665100	0.02369100
P	-2.46821200	3.47045700	-1.33098600
C	-2.90535100	5.07052300	-0.51227800
C	-4.04720400	3.07810500	-2.21132200
C	-1.41106300	4.05967500	-2.73263100
H	-3.35449100	5.78567100	-1.21276600
H	-2.00617800	5.52123800	-0.07845000
H	-4.37313500	3.89673900	-2.86532600
H	-4.82580700	2.87387400	-1.46938800
H	-1.22267500	3.22874000	-3.41973500
H	-0.44546900	4.40303100	-2.34672300
P	-0.07963000	2.83781900	1.27305500
P	-1.22264000	0.05003200	-1.22720200
C	0.94934800	4.13485700	0.43559100
C	1.26296400	1.80468200	2.02669300
C	-0.67492000	3.75738700	2.76343800
C	-1.20260400	0.23833100	-3.07170800

C	0.41963400	-0.77736700	-0.97731300	H	-4.14553400	1.98576200	-1.57438100
C	-2.37039300	-1.38483300	-1.02731600	H	-0.55882500	2.36754600	-3.57638600
H	1.69157200	4.57156700	1.11560300	H	0.14376400	3.67306700	-2.60742700
H	0.30690900	4.93831700	0.06014500	P	0.78266800	2.07515300	1.31078900
H	2.00658300	2.42106800	2.54787000	P	-0.48629200	-0.58500000	-1.04271400
H	1.76656200	1.22770700	1.24335500	C	2.03733200	2.99424600	0.30419700
H	-1.19030600	3.05496000	3.42672400	C	1.88259800	0.96208000	2.29957800
H	-1.40437900	4.51318400	2.45334900	C	0.30580400	3.33260500	2.57283600
H	-0.42017000	0.94911800	-3.35864600	C	-0.30324700	-0.49879900	-2.88041900
H	-2.16555100	0.63131600	-3.41492100	C	1.02325600	-1.54509900	-0.58284900
H	1.22355300	-0.05301800	-1.14907300	C	-1.83063400	-1.83041000	-0.84432000
H	0.56035000	-1.62996900	-1.65421900	H	2.84907800	3.39997700	0.92088600
H	-2.37013500	-1.69977000	0.02112900	H	1.54675200	3.82077900	-0.22116400
H	-2.08954000	-2.23479400	-1.66189200	H	2.69803900	1.52275100	2.77288200
H	-3.60897100	4.87046700	0.30204900	H	2.31496100	0.19395300	1.64982700
H	-3.91471100	2.17167900	-2.81193300	H	-0.33503000	2.85446300	3.32035200
H	-1.88385200	4.87845600	-3.28893000	H	-0.28343900	4.12084900	2.09248200
H	-1.01364300	-0.71619100	-3.57880100	H	0.54863600	0.14054700	-3.13607400
H	0.49753300	-1.13509700	0.05408200	H	-1.20589700	-0.06309000	-3.32103200
H	-3.38861100	-1.06841100	-1.27609600	H	1.91387300	-0.92876300	-0.74762500
H	0.14072400	4.24407600	3.31301300	H	1.11549600	-2.46502200	-1.17291300
H	1.47246600	3.68961900	-0.41810200	H	-1.95150100	-2.06263700	0.21774800
H	0.82721000	1.10117000	2.74235500	H	-1.62111000	-2.75232200	-1.40000000
I	-3.62365500	1.24820000	1.63132900	H	-3.01981700	4.22531400	0.00490000
C	-2.57836600	-0.54034600	2.98269400	H	-3.22226400	1.28341100	-2.91140800
C	-1.27683000	-0.82185300	2.60465500	H	-1.30259000	3.98501800	-3.60293900
C	-3.20369700	-1.20546300	4.02838600	H	-0.14507600	-1.49159900	-3.31879500
C	-0.56117000	-1.80824500	3.29568400	H	0.97346300	-1.81391500	0.47586500
H	-0.82701800	-0.26730500	1.77817100	H	-2.77265900	-1.39647600	-1.19490900
C	-2.48529900	-2.19255400	4.71931400	H	1.17756100	3.77834900	3.06699200
H	-4.22802500	-0.97094200	4.31212500	H	2.46570400	2.32401600	-0.44988400
C	-1.16858400	-2.49223600	4.35396300	H	1.29744900	0.46964000	3.08133700
H	0.46423300	-2.04138400	3.01287800	I	-3.13896800	1.25303300	1.74196900
H	-2.95471500	-2.72598700	5.54380000	C	-1.99922700	-2.02430900	3.07063500
H	-0.61716200	-3.25769100	4.89431700	C	-0.72747500	-1.58913100	2.76067300

5-I-PMe₃



$$E(\text{OSS}) = -1796.04908611$$

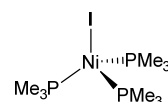
$$E(\text{T}) = -1796.04880792$$

$$S^2(\text{OSS}) = 1.0098$$

$$G_{\text{corr}} = 0.369947$$

Ni	-1.01348900	1.33721100	0.10126100
P	-1.84396800	2.74744200	-1.52362800
C	-2.33544900	4.38923200	-0.83349200
C	-3.40414500	2.20609300	-2.34909300
C	-0.79847400	3.24576700	-2.96855300
H	-2.82310400	5.02208300	-1.58497700
H	-1.44924900	4.90885900	-0.45251300
H	-3.80187500	2.96734300	-3.03134500

6-I-PMe₃



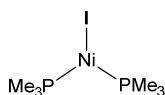
$$E = -1564.40705784$$

$$G_{\text{corr}} = 0.287279$$

Ni	-1.84324800	-0.47041800	0.07921600
P	-3.67235000	0.83299800	-0.33312000

C	-4.17073000	2.07806700	0.93713600	C	0.98561800	6.78770700	14.52758800
C	-5.20502000	-0.18462800	-0.49073500	C	3.21612900	5.00879800	14.14315600
C	-3.71537500	1.84136500	-1.88501700	H	1.06731200	11.36551300	12.18679200
H	-5.13735100	2.54125700	0.70425000	H	2.70003000	10.85700500	12.69592800
H	-3.40975300	2.86365600	0.99811800	H	-0.66755400	9.73261700	10.80900900
H	-6.09094100	0.42899800	-0.69384000	H	-0.48658800	8.32496400	11.89205900
H	-5.35087600	-0.74269800	0.43972200	H	2.09272000	9.40044900	8.84533200
H	-3.55483700	1.18376100	-2.74671500	H	3.16784900	10.45810900	9.76951400
H	-2.90261900	2.57640500	-1.86908300	H	3.34566500	8.75787800	15.02748100
P	-0.14197700	0.93142700	0.69769200	H	4.72298100	7.67434800	14.76902600
P	-0.96025700	-1.86388100	-1.49890000	H	0.59966400	7.81254300	14.50468800
C	0.36832000	2.34285100	-0.38093900	H	0.97072900	6.42970200	15.56371600
C	1.45901800	0.06443300	1.00569400	H	2.61246500	4.32647600	13.53548700
C	-0.45114800	1.75441900	2.31875600	H	3.11262400	4.74087500	15.20133100
C	0.06553300	-1.13883000	-2.85632700	H	1.27001500	10.12157700	13.44506400
C	0.10925200	-3.24578600	-0.90411300	H	-0.21515500	8.13603900	10.15179000
C	-2.26680500	-2.77092200	-2.43936500	H	1.46406800	10.93554000	9.51324400
H	1.20553300	2.91013500	0.04293100	H	4.26021300	4.88926600	13.83718800
H	-0.48304700	3.01876100	-0.51857700	H	0.32163600	6.15787600	13.92568000
H	2.21298200	0.72914500	1.44426200	H	3.54516700	7.31616200	16.06226700
H	1.85020500	-0.34044000	0.06586400	I	4.75342400	6.19204700	10.24449700
H	-0.70886200	0.98519200	3.05354400				
H	-1.30629200	2.43263400	2.23085400				
H	0.97406800	-0.69586400	-2.43361700				
H	-0.49920900	-0.34275900	-3.35401200				
H	0.99547200	-2.83431100	-0.40903800				
H	0.42646300	-3.91106000	-1.71673700				
H	-2.91041000	-3.29548200	-1.72511300				
H	-1.84768200	-3.49675300	-3.14646500				
H	-4.23258200	1.58340400	1.91170300				
H	-5.07727700	-0.91280700	-1.29921900				
H	-4.66769300	2.37070500	-2.01253700				
H	0.35840700	-1.88907400	-3.60093100				
H	-0.44854300	-3.82098000	-0.15809500				
H	-2.88296300	-2.05157500	-2.99025600				
H	0.42104200	2.31937900	2.66880900				
H	0.65791700	1.96145200	-1.36634900				
H	1.27410900	-0.77149300	1.68817600				
I	-2.49900300	-2.01070500	2.17983600				

7-I-PMe₃



E	=	-1103.20076166	
G _{corr}	=	0.179104	
Ni	3.02107300	7.39600400	11.66721000
P	1.70436400	9.17505000	11.23412200
P	2.68797800	6.74339800	13.81325500
C	1.67778300	10.51280700	12.50681500
C	-0.09120800	8.81947700	10.99845700
C	2.13905100	10.09063600	9.69413400
C	3.66405900	7.70987000	15.04595400

In *n*-Hexane

PhH



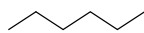
E	=	-232.323983605
G _{corr}	=	0.073465
C		3.70589900 1.91299500 0.09731400
C		5.02855700 2.16828700 -0.27308500
C		5.30158700 2.86508100 -1.45295300
C		4.25182000 3.30556600 -2.26273300
C		2.92907100 3.05022800 -1.89226100
C		2.65602400 2.35345000 -0.71257900
H		3.49371700 1.37081000 1.01535700
H		5.84529900 1.82523200 0.35707100
H		4.46380500 3.84788300 -3.18074700
H		2.11242000 3.39344200 -2.52243700
H		1.62680800 2.15474600 -0.42445400
H		6.33077500 3.06381900 -1.74109800

Ph•



E	=	-231.634151943
G _{corr}	=	0.059624
C		1.08911600 -0.03717900 0.00006800
C		2.48709500 -0.02944000 0.00046700
C		3.19297100 1.17727300 -0.00006400
C		2.50128200 2.40032400 -0.00093700
C		1.12504800 2.33036600 -0.00131100
C		0.37606800 1.17352000 -0.00088000
H		0.54753700 -0.98047900 0.00048500
H		3.03019000 -0.97061800 0.00119900
H		4.28073200 1.17470000 0.00024600
H		3.03719100 3.34602400 -0.00135700
H		-0.71093500 1.18219000 -0.00119600

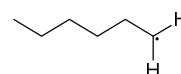
Hexane



E	=	-237.171989133
G _{corr}	=	0.158283
C		4.30635300 1.65426000 -0.70126800
H		4.96429200 2.26450200 -1.33697500
H		3.30432200 1.72035900 -1.14707800
C		4.77290600 0.19029800 -0.75004600
H		4.10385100 -0.42259700 -0.12725000
H		4.66001800 -0.18425700 -1.77768600
C		6.22335100 -0.03257900 -0.30206500

H		6.34756100 0.28332200 0.74293000
H		6.88905900 0.61119400 -0.89710500
C		6.67864400 -1.49139000 -0.43553600
H		6.56112500 -1.81377000 -1.48005700
H		6.01260300 -2.13369600 0.15855000
C		8.12800200 -1.71011000 0.00700500
H		8.26850600 -1.42712900 1.05812900
H		8.82056400 -1.10520200 -0.59220700
H		8.42765400 -2.75989700 -0.09717400
C		4.26433400 2.25193400 0.70936300
H		3.62672900 1.65261400 1.37246800
H		5.26111700 2.29885900 1.16216400
H		3.86304900 3.27239900 0.69494500

Hexane radical



E	=	-236.505625587
G _{corr}	=	0.141932
C		4.14198600 2.86583800 -0.96927300
H		4.23676800 3.61890500 -1.75033400
C		4.75210000 1.52116800 -1.20420800
H		4.19636700 0.75627200 -0.63878900
H		4.67249900 1.24756100 -2.26589200
C		6.24224800 1.43280300 -0.78679900
H		6.33332700 1.68981200 0.27804700
H		6.81666200 2.19115900 -1.33755900
C		6.85294300 0.04756400 -1.03109700
H		6.75786500 -0.20720300 -2.09633400
H		6.26968800 -0.70652800 -0.48329700
C		8.32334400 -0.03860800 -0.61293100
H		8.44486700 0.18218900 0.45520600
H		8.93659900 0.68085000 -1.17024700
H		8.73559700 -1.03841200 -0.79466400
C		3.77452800 3.32159200 0.40386400
H		3.36364600 2.49827000 1.00472000
H		4.64357400 3.71218500 0.96547700
H		3.03197300 4.12949100 0.38295500

H Abstraction TS: Ph• + Hexane

E	=	-468.799635792
G _{corr}	=	0.228793
v	=	-1304.15 cm ⁻¹
C		0.55681800 -0.96172200 0.05857600
C		1.92526500 -0.67751400 0.15994000
C		2.49884800 0.16891700 -0.77780100
C		1.76974000 0.74242900 -1.80926800
C		0.40163500 0.45395200 -1.90396200
C		-0.20007000 -0.39613100 -0.97151900
H		0.08461400 -1.62301700 0.78183600
H		2.51910700 -1.11513500 0.95975500

H	2.24418000	1.40278500	-2.53235200	H	9.92103100	-1.49168100	0.26597300
H	-0.19135800	0.89186500	-2.70395800	H	9.90679100	-1.42357600	-1.50253200
H	-1.26129000	-0.61873800	-1.04778100	H	9.97536600	-2.98950200	-0.67811700
C	5.15691000	0.66655100	-0.54524300	C	5.31896300	1.48871800	0.72097900
H	5.39731900	1.24462000	-1.44718000	H	5.00364400	0.91841000	1.60424500
H	3.92261800	0.45474300	-0.67194100	H	6.36411000	1.78915300	0.87951600
C	5.82140000	-0.70265900	-0.55585400	H	4.71734900	2.40425700	0.68133600
H	5.48939900	-1.27445800	0.32354600				
H	5.47745400	-1.26359200	-1.43635800				
C	7.35937700	-0.65076200	-0.56795900				
H	7.71936500	-0.12366500	0.32654300				
H	7.69465200	-0.05641300	-1.43097500				
C	8.00628800	-2.04019400	-0.62570700				
H	7.65072900	-2.56801500	-1.52205000				
H	7.66481200	-2.63414000	0.23423000				
C	9.53651900	-1.98552100	-0.63559200				

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