Advances in Nickel-Catalyzed C-N Cross-Coupling Enabled by Tailored Ancillary Ligand Design

by

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ABSTRACT

The nickel-catalyzed C_{sp2}-N cross-coupling of NH substrates and (hetero)aryl (pseudo)halides for the synthesis of (hetero)anilines is in the midst of a resurgence. Reactivity breakthroughs that have been achieved in this field within the past five years have served to establish Ni catalysis as being competitive with, and in some cases superior to, more well-established Pd- or Cu-based protocols. Whereas the repurposing of useful ancillary ligands from the Pd domain has been the most frequently employed approach in the quest to develop effective Ni-based catalysts for such transformations, considerable progress has been made as of late in the design of ancillary ligands tailored specifically for use with Ni. Bisphosphine ancillary ligands have proven to be well-suited for such an approach, given their modular and facile syntheses. As part of this thesis research, several new bidentate phosphine ancillary ligands were developed that are particularly effective in enabling a range of otherwise challenging Ni-catalyzed C_{sp2}-N cross-couplings. Presented herein is a comprehensive summary of my contributions to the field of Ni-catalyzed C_{sp2}-N cross-coupling, achieved by the application of a newly developed PAd-DalPhos ancillary ligand class. It is anticipated that the discussion of key ancillary ligand design concepts and mechanistic considerations presented herein will provide a useful platform for researchers to initiate ancillary ligand design efforts for the continued development of high-performing Ni cross-coupling catalysts.

LIST OF ABBREVIATIONS AND SYMBOLS USED

acac	acetylacetone
Ar	aryl
bpy	bipyridine
BHA	Buchwald-Hartwig amination
BINAP	2,2′-bis(diphenylphosphino)-1,1′-binaphthalene
Boc	*tert*-butyloxycarbonyl
CgP	1,3,5,7-tetramethyl-2,4,8-trioxa-6-phosphaadamantane
CgPPh	phenyl-1,3,5,7-tetramethyl-2,4,6-trioxaphosphaadamanatane
cod	1,5-cycylooctadiene
δ	chemical shift
Cp	cyclopentadienyl
CyPF-Cy	(R)-(-)-1-[(S)-2-(Dicyclohexylphosphino)ferrocenyl]ethyldicyclohexylphosphine
CyPF-*t*Bu	(R)-(-)-1-[(S)-2-(Dicyclohexylphosphino)ferrocenyl]ethyldi-t-butylphosphine
CPME	cyclopentyl methyl ether
DFT	Density-Functional Theory
DMA	dimethylacetamide
dme	1,2-dimethoxyethane
dppe	1,2-bis(diphenylphosphino)ethane
dtbpy	4,4’-di-*tert*-butyl-2,2’-dipyridyl
d	doublet
dppf	1,1′-ferrocenediyl-bis(diphenylphosphine)
DIPAMP	Ethane-1,2-dylbis[(2-methoxyphenyl)phenylphosphane]
ESI	electrospray ionization
GC	gas chromatography

GP	general procedure
Hz	hertz
h	hour(s)
HRMS	high-resolution mass spectrometery
i.d.	Internal diameter
int. std.	internal standard
IPr	1,3-bis-(2,6-diisopropylphenyl)imidazol-2-ylidene
IMes	1,3-bis-(1,3,5-trimethylphenyl)imidazol-2-ylidene
J	scalar coupling constant
K	kelvin
κ	denticity
L	neutral 2-electron donor ligand
L-DOPA	3,4-dihydroxyphenylalanine
M	mol / L
m	multiplet
η	hapticity
NHC	*N*-heterocyclic carbene
NMR	nuclear magnetic resonance
phen	phenanthroline
PhBPin	phenylboronic acid pinacol ester
PGMs	platinum-group metals
PS	polystyrene
PTFE	poly(tetrafluoroethylene)
***rac*-BINAP**	racemic 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl
RVC	reticulated vitreous carbon
rt	room-temperature

SGE	scientific glass engineering
SET	single electron transfer
TEMPO	2,2,6,6-tetramethylpiperine-1-oxyl
THF	tetrahydrofuran
TLC	thin layer chromatography
X	halide substituent or anionic ligand
XantPhos	4,5-Bis(diphenylphosphino)-9,9-dimethylxanthene
XDM	exchange-hole dipole moment

COMPOUND NUMBERING NOTE: For the purposes of this Thesis document, ligands are labeled as (**L#),** nickel(II) pre-catalysts labeled as (**C#**), and all other compounds are denoted by **#.#**; separated by chapters, or by their common name.

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Chapter 1

Introduction

1.1. GENERAL CONCEPTS OF CATALYSIS

The large-scale manufacturing of commodity chemicals (e.g., petrochemicals, pharmaceuticals, fertilizers, dyes, etc.) comprises a significant sector of the global economy.[1,2] Satisfying the growing demand of commercial chemicals has become a daunting task for the chemical community, who face increased pressure to reduce the energy consumption, depletion of natural resources, and associated costs of chemical manufacturing technologies. In this vein, no discovery has had a greater impact on the chemical industry than catalysis – chemical reactions that are accelerated by action of an un-consumed molecular entity, which provides an alternative, energetically favorable mechanism to the non-catalytic reaction (Fig. 1-1). The use of catalytic procedures allows for many industrial processes to be carried out under feasible conditions of reaction time, temperature and pressure, which collectively improve the cost-efficiency (e.g., cost

of materials, waste removal) and safety of a given protocol. Whereas the chemical industry of the 20th century relied heavily on wasteful stoichiometric procedures for the production of commodity chemicals, catalysis now figures prominently in virtually all sectors of organic synthesis, with up to 90% of all chemical products featuring at least one catalytic step in its manufacturing.[1-3]

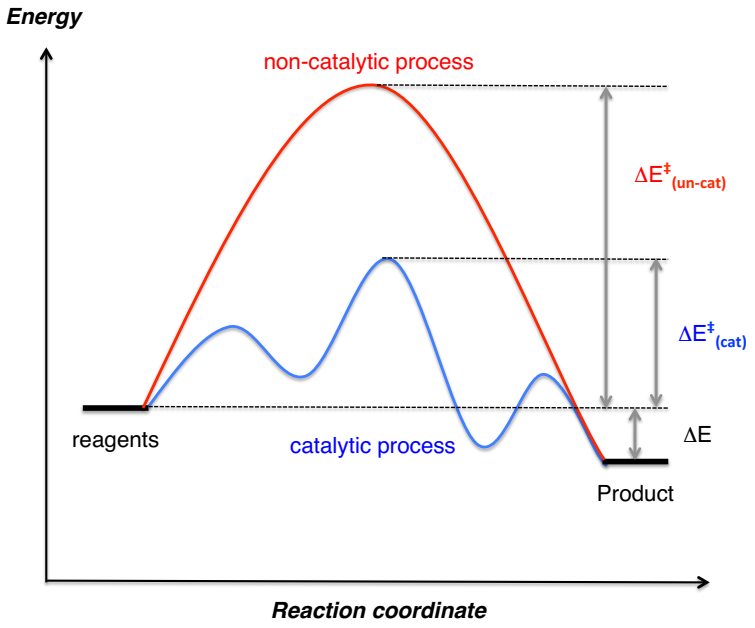


Figure 1-1. Energetics associated with catalyzed and non-catalyzed chemical transformations.

One of the foremost goals of catalytic methodology development is the conversion of abundant feedstock chemicals (e.g., H_2, H_2O, NH_3, CO, olefins, alkanes, etc.) into value-added compounds (e.g., plastics, organic electronic devices, pharmaceuticals, etc.). The utilization of transition metal coordination complexes as catalysts has figured prominently in achieving this goal.[2-4] In particular, organometallic complexes comprised of late second and third row transition metals (i.e., platinum-group metals, PGMs) have proven unique in their

capacity to bind and activate a broad range of synthetically useful small molecules, which is attributable to the capacity of PGMs to access a diversity of stable oxidation states and structural geometries.[5, 6] Furthermore, the typically excellent functional group tolerance exhibited by PGMs, in conjunction with the ability to mediate many substrate transformations under mild conditions, has contributed to their extensive application as catalysts in organic synthesis.[3] Given the relevance of transition metal catalysis to this thesis research, a more detailed discussion is provided below.

1.2. TRANSITION METAL CATALYSIS

It is difficult to overstate the impact of transition metal catalysis in the continued development of organic synthesis. Discoveries in this area are driven largely by the design of ancillary ligands,[7, 8] which strongly influence the steric and electronic properties of the coordination complex, thereby providing a useful handle for fine-tuning the activity and selectivity (e.g., chemo-, regio-, and stereoselectivity) exhibited by the metal catalyst. The identification of optimally configured catalysts for enabling a particular chemical transformation is by no means a trivial process, and is complicated by numerous important considerations, including: the nature of ligand-metal bonding modes; the influence of ancillary ligand coordination on discrete catalytic steps; the identification of catalyst decomposition pathways, among others. Nonetheless, advances in modern chemical technology (e.g., spectroscopic, crystallographic, and computational methods) have streamlined the development of remarkably effective catalysts, which is exemplified by the awarding of three separate Nobel Prizes in Chemistry to the field of transition metal

catalysis (Fig. 1-2): catalytic asymmetric synthesis (2001),[9] olefin metathesis (2005),[10] and palladium-catalyzed C-C cross-coupling (2010).[11, 12] A brief description of the research that led to each of these awards is provided below to provide further context on catalyst design strategies.

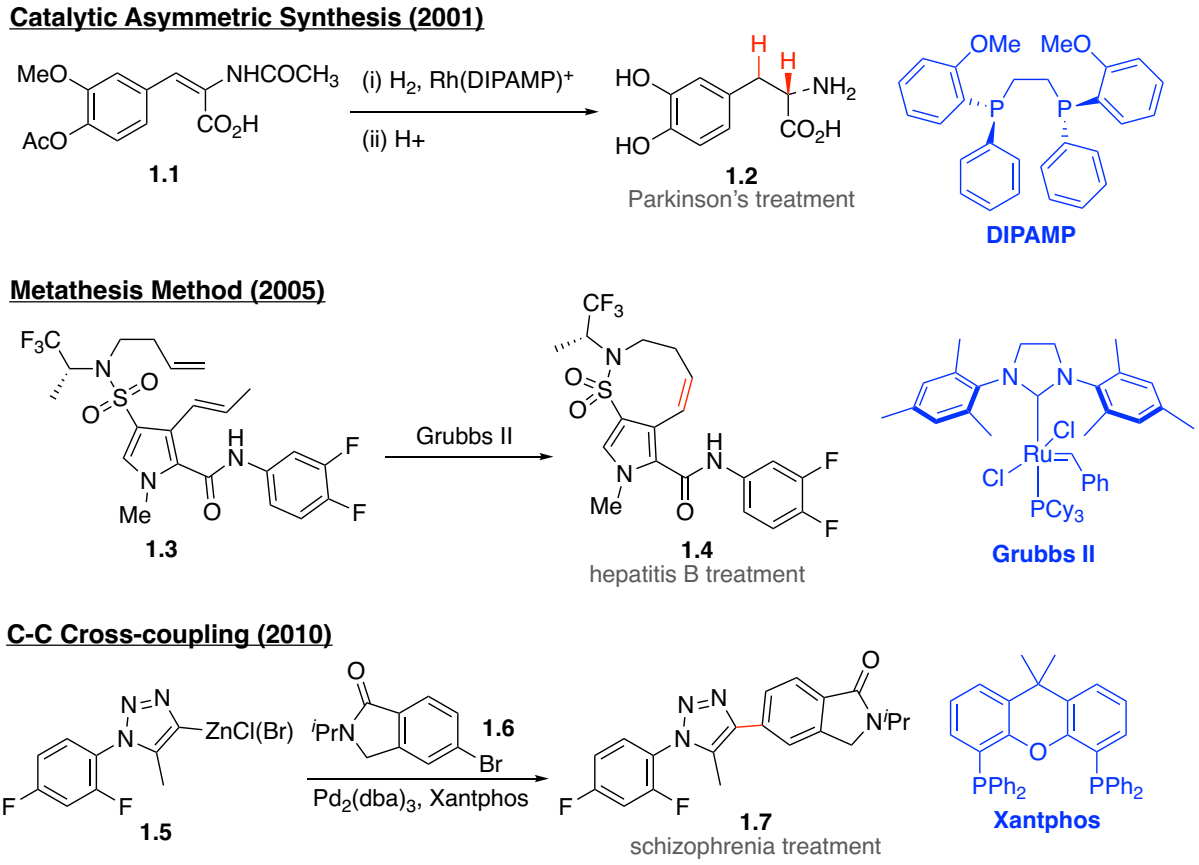


Figure 1-2. Selected applications of Nobel Prize winning chemistry research in the synthesis of pharmaceuticals. Bonds formed in the reaction are highlighted in red.

In 2001, the Nobel Prize in Chemistry was awarded to Ryoji Noyori, William Knowles, and Barry Sharpless for their independent contributions to the development of asymmetric catalysis.[9] While the research focus of these laureates is distinct, a unifying theme is their success in utilizing ligand design to achieve exquisite control over the reactivity and selectivity in asymmetric transformations.

One notable example reported by Knowles, involved the application of a C_2-symmetric diphosphine DIPAMP in conjunction with rhodium to achieve the enantioselective synthesis of the Parkinson's treatment drug L-DOPA (**1.2**),[13] which was the first industrial-scale synthesis involving asymmetric catalysis (Fig. 1-2).

The 2005 Nobel Prize in Chemistry[10] – awarded to Robert Grubbs, Richard Schrock, and Yves Chauvin for their contributions to the development of the metathesis method, well illustrates the importance of mechanistic organometallic chemistry. While the olefin metathesis reaction had been known since the 1950s,[10, 14] the mechanism of this transformation was not considerably understood until the 1970s, when Chauvin[15] invoked the intermediacy of metal-carbene complexes, coordination compounds with M=C double bonds. This proposal stimulated an intense period of research into the development of new classes of metal-carbene complexes as potential catalysts.[16-18] One prominent example is an *N*-heterocyclic carbene supported ruthenium(III) complex (Fig. 1-2) developed by Grubbs and coworkers (i.e., second generation Grubbs catalyst, G2),[19, 20] which is one of the most widely-used homogenous metathesis catalysts. Janssen and coworkers[21] recently utilized the G2 catalyst to prepare a series of cyclic sulfonamides *via* ring-closing metathesis, for their evaluation as hepatitis B medication.

In 2010, the Nobel Prize in Chemistry[11, 12] was awarded to Akira Suzuki, Richard Heck, and Ei-ichi Negishi for their contributions to the development of palladium-catalyzed carbon-carbon cross-coupling, an incredibly general transformation which figures prominently in many chemical manufacturing processes.[22, 23] As the cross-coupling method is the major focus of the thesis work presented herein, a more detailed discussion is given below.

1.3. CROSS-COUPLING CATALYSIS

The cross-coupling methodology offers a convenient synthetic strategy for forming new carbon-carbon and carbon-heteroatom bonds (e.g., C-N, C-O, C-S, C-F) between two or more often inexpensive and easily procured chemical reagents.[24] Increased research efforts in this area over the last several decades has led to the development of an enriched library of cross-coupling transformations (Fig. 1-3), which collectively serve as an indispensable tools for synthetic chemists.[25] As previously noted, the broad utility of Pd-catalyzed cross-coupling chemistry and its impact on organic synthesis was acknowledged through awarding of the 2010 Nobel Prize in Chemistry to Heck, Suzuki and Negishi.

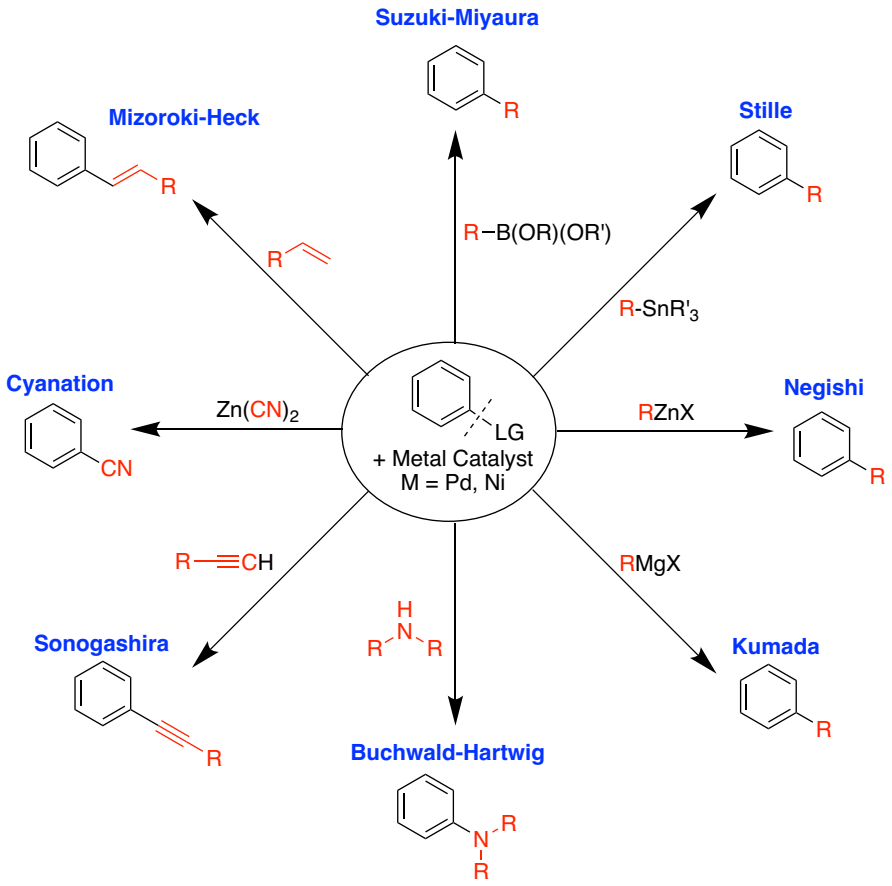


Figure 1-3. Various palladium-catalyzed cross-coupling catalytic transformations. LG = leaving group (i.e., Cl, Br, I, OTs, OTf, etc.).

While each of these transformations appear distinct from one another with regard to the structural composition of reaction products afforded through catalysis (i.e., biaryls, anilines, nitriles, olefins *etc.*), there are mechanistic similarities between many transformations considered to be cross-coupling reactions (Fig. 1-4).[24, 26] The catalytic cycle for Pd-catalyzed cross-coupling transformations is initiated by oxidative addition of the aryl (pseudo)halide to the catalytically active $L_nPd(0)$ species. The so-formed aryl (pseudo)halide $L_nPd(II)$ species then undergoes transmetallation with an organometallic reagent to generate a $L_nPd(II)$ species bearing both 'to-be-eliminated' organic fragments. Of the three major elementary steps that govern many cross-coupling catalytic cycles, the

transmetalation event; and more specifically the type of the organometallic reagent employed, is often what distinguishes the different classes of cross-coupling from one another. Notably, several forms of cross-coupling reaction types (e.g., Mizorozi-Heck and Buchwald-Hartwig amination, BHA) do not involve formal transmetalations, and the installation of the second organic coupling fragment is achieved *via* other elementary processes (e.g., alkene binding/migratory insertion for Mizoroki-Heck coupling). Subsequent C-C or C-heteroatom bond reductive elimination furnishes the organic product, and regenerates the catalytically active $L_nPd(0)$ species.

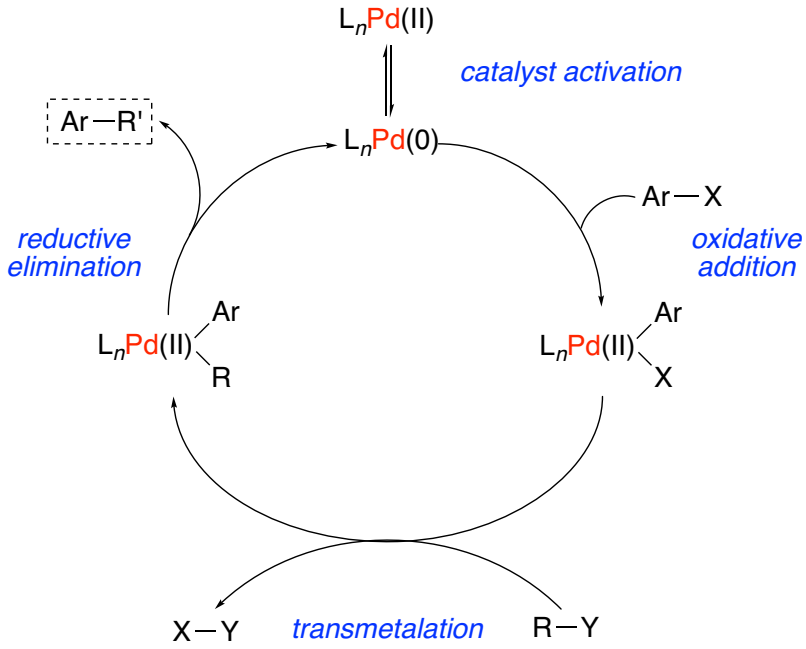


Figure 1-4. A general catalytic cycle applicable to many Pd-catalyzed cross-coupling transformations. Ar = aryl.

The C-N bond forming variant of cross-coupling (i.e., Buchwald-Hartwig amination, BHA) constitutes the major area of research focus for the thesis work presented herein. The following section describes the development of BHA

protocols, with a particular focus on the utilization of ligand design as a powerful approach for the pursuit of superlative C-N cross-coupling catalysts.

1.4. BUCHWALD-HARTWIG AMINATION

The palladium-catalyzed C(sp^2)-N cross-coupling (herein C-N) of NH substrates and (hetero)aryl (pseudo)halides (i.e., Buchwald-Hartwig Amination, BHA) represents a widely employed method, along with Chan-Lam coupling, for the synthesis of (hetero)anilines, with applications in the preparation of natural products, pharmaceuticals, functional materials, and beyond.[27-32] The rapid evolution of BHA chemistry over the past two decades is due in large part to advances in ancillary ligand and pre-catalyst design,[33-36] which afforded generalized protocols devoid of salient limitations associated with early precursors to BHA chemistry (e.g., the use of toxic tin amido reagents, limited functional group compatibility, and elevated reaction temperatures). The development of broadly useful ligand classes for application in BHA was guided by extensive mechanistic analysis, wherein the preponderance of empirical data led to the identification of sterically demanding, relatively electron-rich ancillary ligands as being optimal (Fig. 1-5).[37-39]

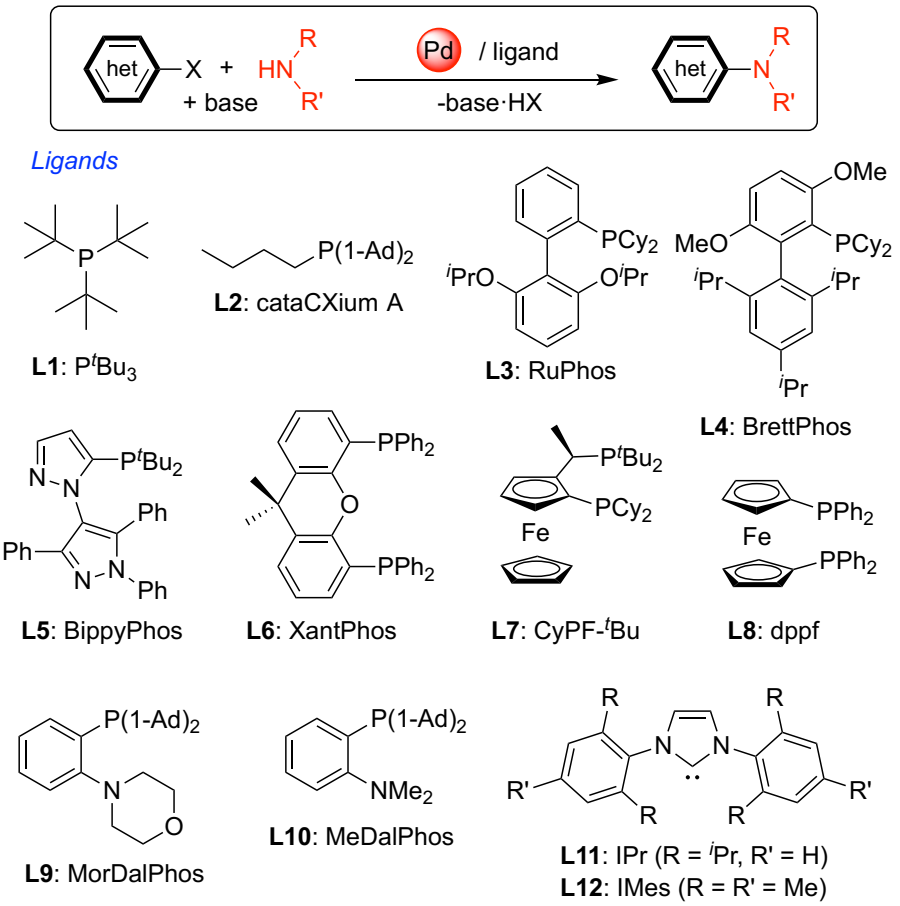


Figure 1-5. Prominent bulky, electron-rich ligands used in BHA chemistry.

These ancillary ligand characteristics promote the formation of electron-rich, low-coordinate L_nPd^0 species that are pre-disposed towards challenging oxidative additions (e.g., C_{sp2}-Cl). Prominent ancillary ligand classes adhering to these basic design principles include trialkylphosphines (e.g., P^{t}Bu$_3$ (**L1**),[40] cataCXium A (**L2**),[41]), (hetero)biaryl monophosphines (e.g., RuPhos (**L3**),[38, 42] BrettPhos (**L4**),[42] BippyPhos (**L5**),[43, 44]), large bite angle bisphosphines (e.g., XantPhos (**L6**),[45] CyPF-^{t}Bu JosiPhos (**L7**),[46-48] dppf (**L8**),[49, 50]), mixed P,N donors (e.g., Mor-DalPhos (**L9**),[51-54] Me-DalPhos (**L10**),[55] and sterically demanding *N*-heterocyclic carbenes (NHCs) (e.g., IPr (**L11**), IMes (**L12**),[56, 57])[58] which collectively give rise to Pd

catalysts capable of promoting the cross-coupling of a broad spectrum of synthetically useful (hetero)aryl electrophiles and NH reagents.

1.5. SHIFTING TOWARDS NICKEL CATALYSIS

Notwithstanding the broad impact of BHA in synthetic chemistry, both cost and supply limitations of Pd have steered research efforts in the direction of more sustainable amination methodologies that utilize inexpensive, non-precious metals. Among such metals, catalysts based on Ni, Cu, and Fe have each proven effective in enabling C-N cross-coupling (Fig. 1-6). However the scope of compatible reaction partners and mild reaction conditions enabled by use of Ni catalysts currently far exceeds that of Cu[59-62] or Fe catalysts,[63-66] making Ni the most promising substitute for Pd in such reactions.

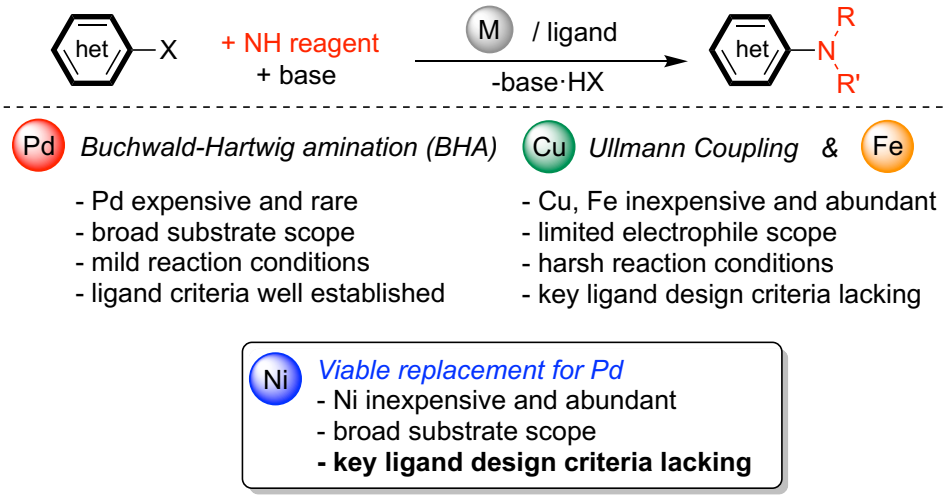


Figure 1-6. Approaches to metal-catalyzed C-N cross-coupling.

Beyond the significant cost benefits associated with using Ni in place of Pd, the reactivity profile of Ni can provide useful advantages in cross-coupling chemistry.[67, 68] For example, the relatively low electronegativity of Ni serves to

enhance reactivity with sought-after (hetero)aryl chlorides and phenol derivatives (e.g., ethers, tosylates, mesylates, triflates, sulfamates, etc.),[68] which are comparatively less reactive electrophiles under BHA conditions. Furthermore, the expanded range of readily accessible oxidation states (commonly 0 to III),[67, 68] and greater propensity for single-electron transfer (SET) for Ni leads to an inherently more complex, but potentially useful, mechanistic landscape versus Pd. Whereas Pd^0/Pd^{II} cycles involving $2e^-$ elementary steps are commonly observed in BHA,[39] the situation is much less clear in the case of Ni. Whereas both Ni^0/Ni^{II} [69-72] and Ni^I/Ni^{III} [72-74] catalytic cycles have been invoked in Ni variants of BHA (Fig. 1-7), the existence of elementary processes that link these manifolds (e.g., comproportionation, disproportionation, and SET) creates ambiguity regarding the dominant operative mechanism of catalysis. In fact, the tendency of Ni species to engage in SET processes has been exploited by pairing Ni catalysts with photosensitizers (e.g., $[Ir(dtbpy)_3]^{3+}$, dtbpy = 4,4'-di-*tert*-butyl-2,2'-dipyridyl),[75] which are presumed to facilitate otherwise challenging cross-couplings (e.g., C_{sp2}-N,[76] C_{sp2}-O,[77] C_{sp3}-C_{sp2}[78]) by modulating the oxidation state of Ni.

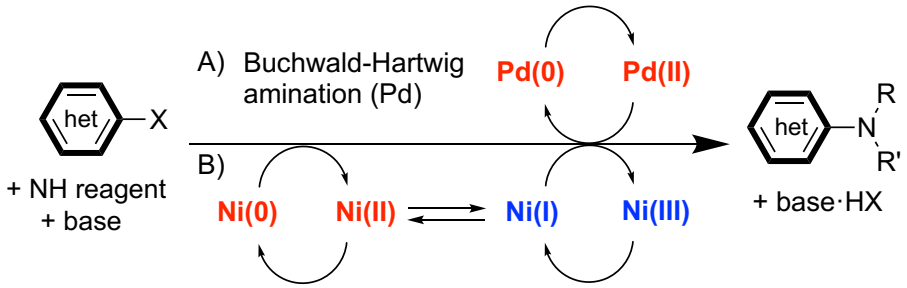


Figure 1-7. A comparison of palladium- and nickel-catalyzed C-N cross-coupling.

Given the inherent advantages associated with using Ni in place of Pd, it is surprising that Ni has received comparatively little attention in C-N cross-coupling over the past two decades. The potential for more diverse reactivity and a broader range of accessible oxidation states undoubtedly discouraged Ni catalyst development, thereby contributing in part to the preferential study of Pd catalysts for C-N cross-coupling. Indeed, the complex reactivity characteristics of Ni complicate mechanistic analysis of such catalyst systems, rendering the identification of key ancillary ligand design criteria, and thus the development of high-performing Ni catalysts, rather problematic.[79] Faced with these challenges, chemists have routinely defaulted to repurposing ligands that function well in BHA chemistry as a means of developing new Ni-based amination protocols – an approach that is predicated on the assumption that Ni catalysis is governed by Pd-like mechanisms (e.g., a Pd^{0}/Pd^{II} cycle), with analogous rate-limiting steps (e.g., oxidative addition). This strategy has proven somewhat effective for the cross-coupling of a limited selection NH substrate/electrophile pairings, with Ni catalysts based on PPh_3,[80] IPr,[81-83] JosiPhos,[71, 84-86] dppf,[87-90] BINAP[69, 70] and DPEPhos,[91] each exhibiting useful performance. Given the smaller atomic radius and distinct electronic properties of nickel, it is unlikely that the 're-purposing' of ancillary ligands that function well with palladium will be a university effective strategy in the

pursuit of superlative Ni-catalysts for challenging C(sp^2)-N cross-couplings; the design and application of new ancillary ligands tailored specifically for use in Ni-catalysis represents a promising and complimentary approach.

To provide context for the main discussion of this Thesis regarding the design and application of new bisphosphine ancillary ligands in Ni-catalyzed C-N cross-coupling, a brief overview of prominent ligand classes employed in such transformations is given below.

1.6. AN OVERVIEW OF EFFECTIVE ANCILLARY LIGANDS IN NI-CATALYZED C-N CROSS-COUPLING

1.6.1. Chelating N,N-Donor Ligands

The field of Ni-catalyzed C-N cross-coupling employing aryl chlorides was initiated in 1997, when Wolfe and Buchwald[87] reported the cross-coupling of electronically varied electrophiles with selected primary and secondary amines, enabled by use of *in situ* generated Ni catalysts based on dppf (**L8**) or 1,10-phenanthroline (phen), and employing sodium *tert*-butoxide as the base. While **L8** has since been exploited in a plethora of Ni cross-couplings (e.g., selected examples: C_{sp2}-N,[88, 89, 92] C_{sp2}-C_{sp2},[93, 94] C_{sp2}-SCF_3,[95, 96] C_{sp2}-CF_2H,[97] C_{sp2}-CN[98]; chelating N,N-donor ligands (e.g., phen,[87] 3,5,6,8-tetrabromo-1,10-phenanthroline,[99] and bipyridine[100, 101] (bpy)) have seen limited use in Ni-catalyzed C-N cross-coupling since the mid 2000s. This is despite the fact that Wolfe and Buchwald[87] observed that the use of phen in place of **L8** in some cross-couplings led to improved reactivity and selectivity. Recently there has been considerable

interest in the use of Ni catalysts supported by such N,N-donor ligands in the context of metallophotoredox-enabled cross-coupling applications.[75]

1.6.2. Monodentate Phosphine Ligands

Despite figuring prominently in BHA chemistry, monophosphine ancillary ligands including some of those featured in Figure 1-5 have generally proven inferior to bisphosphines in challenging Ni-catalyzed C-N cross-couplings (e.g., ammonia monoarylation[102]). Among the useful Ni amination catalysts based on monophosphines that have been reported, most feature simple ligands such as PPh_3[103] or PMe_3,[104] and in no cases do such catalysts represent the state-of-the-art. It is unclear as to why monophosphines that perform well in BHA are generally ineffective in Ni-catalyzed C-N cross-couplings. However, the enhanced stability of Ni complexes supported by chelating bisphosphines presumably plays an important role in suppressing catalyst deactivation pathways, which are likely more prevalent in Ni chemistry versus Pd (*vide supra*).[79] For example, recent computational analyses conducted by Maseras and co-workers[105] predicts that halide abstraction is competitive with aryl halide oxidative addition for complexes of the type $Ni(PMe_nPh_{(3-n)})_4$, thus providing a direct route to paramagnetic intermediates (e.g., Ni^{I}, Ni^{III}), which may diminish catalytic activity under circumstances where a product-forming Ni^0/Ni^{II} cycle is operative. It is noteworthy, however, that well-defined Ni coordination complexes supported by monophosphines, including $[Ni(PPh_3)_2Cl_2]$[81, 103] and $[Ni(PPh_3)_2(1\text{-naphthyl})Cl]$,[106, 107] can serve as useful pre-catalyst precursors, wherein the target pre-catalyst may be obtained *via* PPh_3 substitution with a desired ancillary ligand.

1.6.3. *N*-Heterocyclic Carbenes (NHCs)

In contrast to monophosphine ligands, NHCs have proven highly effective in enabling both Pd- and Ni-catalyzed C-N cross-coupling chemistry. The seminal report of such Ni-catalyzed aminations utilizing NHC ancillary ligation was disclosed by Fort and co-workers in 2001,[108] wherein the coupling of (hetero)aryl chlorides with anilines and secondary cyclic and acyclic amines was enabled by employing mixtures (1:4) of $Ni(acac)_2$ and SIPr•HCl (SIPr = 1,3-bis(2,6-diisopropylphenyl)dihydroimidazol-2-ylidene), in the presence of NaH and *t*-BuOH. Tremendous progress has been made since, and Ni catalysts based on NHCs have been shown to promote cross-couplings of a broad spectrum of both (hetero)aryl electrophiles (chlorides,[109-111] bromides,[81] tosylates,[82, 107] phosphates,[106] pivalates,[83] methyl ethers,[112] carbamates,[113] and sulfamates[114]) and NH reagents (primary[106, 113, 115] and secondary amines,[82, 83, 106, 110, 113] anilines,[82, 110, 111] hydrazones,[81, 110] indole,[109] and carbazole[109]). A common feature of highly effective amination protocols of this type is the application of well-defined Ni pre-catalysts (e.g., [Ni(NHC)CpCl],[110] [Ni(NHC)(allyl)Cl],[111] [Ni(NHC)$(styrene)_2$],[82, 109] etc.). This has proven to be a superior approach to catalysis, relative to *in situ* catalyst generation *via* ligand exchange between a Ni source (e.g., $Ni(acac)_2$, $Ni(cod)_2$, etc.) and the NHC. While only limited mechanistic data pertaining to Ni-catalyzed C-N cross-couplings employing NHC ancillary ligation are available, current literature findings implicate a Ni^0/Ni^{II} cycle analogous to that proposed for BHA, involving oxidative addition, amine binding and deprotonation, and product forming C-N reductive elimination;[116-118] the last of these steps has been predicted to be rate-limiting for the cross-coupling of aryl carbamates with secondary amines

on the basis of DFT analysis.[113] Complementary mechanisms involving a Ni^{I}/Ni^{III} cycle have also been postulated[73] when employing mononuclear, Y-shaped Ni^{I}(NHC)X pre-catalysts. In these systems it is proposed that initial amine binding and HX loss, followed by aryl halide oxidative addition to the resultant [Ni^{I}(NHC)(amido)] intermediate, and subsequent product-forming C-N reductive elimination from a [Ni^{III}(NHC)(aryl)(amido)X] species occurs.

1.6.4. Bidentate Phosphine Ligands

Whereas electron-rich, sterically demanding monodentate phosphines (e.g., **L1-L5**; Fig. 1-5) currently represent some of the most effective ancillary ligands known for application in BHA, these ligands often perform poorly when applied in Ni-catalyzed C-N cross-coupling. Conversely, building on the pioneering 1997 report by Wolfe and Buchwald[87] regarding the use of dppf (**L8**),[119-121] several other bisphosphines repurposed from BHA chemistry have proven effective for such Ni-catalyzed transformations, including BINAP (**L13**),[69] DPEPhos (**L14**),[91] variants of JosiPhos (**L15**-**L17**),[71, 84-86] and *ortho*-phenylene bridged bisphosphines (**L18-L22**),[102, 122-125] with most reports of this type appearing within the past five years (Fig. 1-8). Nonetheless, given the frequent failure of prominent ancillary ligands from the BHA domain in enabling more challenging Ni-catalyzed C-N cross-couplings involving sought after NH substrates, and in consideration of the divergent properties of Ni versus Pd (*vide supra*), it is unlikely that repurposing BHA ligands will be a universal solution for developing superlative Ni catalysts for C-N cross-coupling. Consequently, the tremendous potential of Ni in C-N cross-coupling catalysis will remain untapped until our understanding of the mechanistic

landscape of Ni-catalyzed C-N cross-coupling, and the influence of ancillary ligation on the elementary steps therein, rivals that of BHA chemistry.

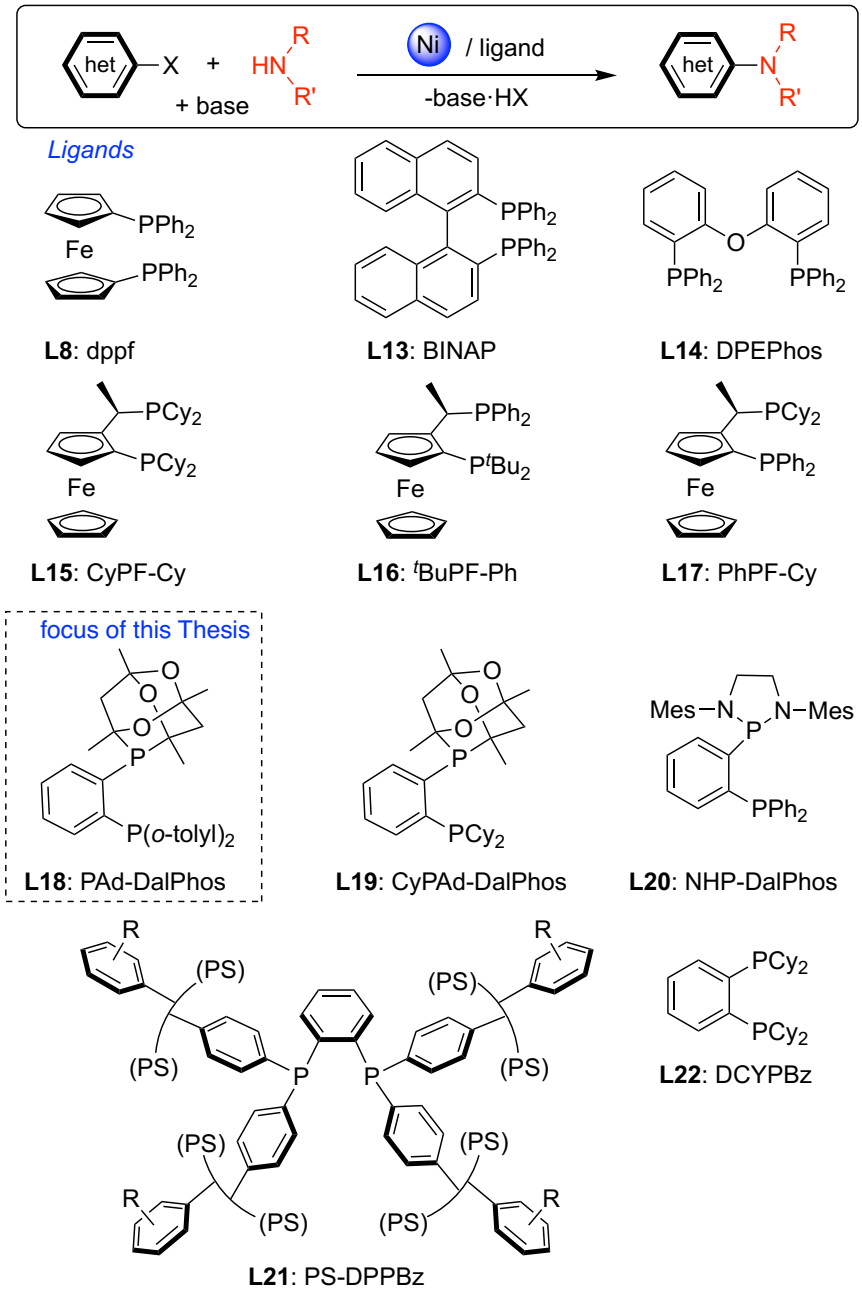


Figure 1-8. Effective bisphosphine ancillary ligands utilized in Ni-catalyzed C-N cross-coupling. The development and application of **L18** is the major focus of this thesis. For **L21**, PS = polystyrene.

1.7. OVERVIEW OF THESIS

The research encompassed within this thesis builds upon the Stradiotto research group's ongoing interest in the design and application of new ligand architectures in synthetically useful Ni-catalyzed C-N cross-coupling transformations. Previous group work in this area has documented the utilization of sterically demanding, relatively electron-rich ferrocene-based JosiPhos ligands in achieving the first Ni-catalyzed ammonia monoarylation with (hetero)aryl chlorides for primary arylamine synthesis (Fig. 1-8).[84] While an important breakthrough, the use of air- and moisture-sensitive $Ni(cod)_2$ (cod = 1,5-cyclooctadiene) represents an impediment with regard to uptake by end users, and creates problems arising from potential cod inhibition. Moreover, there are a number of drawbacks associated with the use of JosiPhos type ligands, including: i) the cost of JosiPhos ligands, which are sold commercially as single enantiomers, ii) the need for elevated reaction temperatures (>100 ^{o}C), and iii) the lack of clarity pertaining the structural features of the JosiPhos ligand responsible for enabling desired reactivity.

In light of these challenges, my thesis work is dedicated to the tailored design of new ancillary ligand and pre-catalyst classes, which may offer improved advantages (e.g., materials cost, catalyst loading, mild reaction conditions, scope of suitable coupling partners) over previously mentioned processes, and provide useful information regarding ideal ligand design concepts. Presented herein is a comprehensive summary of advancements within the field of Ni-catalyzed C-N cross-coupling that have arisen from the collective efforts of this author and other contributors.

Chapter 2 details the design and application of a new *ortho*-phenylene bisphosphine PAd-DalPhos (**L18**), which is uniquely effective in enabling otherwise challenging Ni-catalyzed amine arylations involving ammonia and primary alkylamines. Chapter 3 describes the extension of the scope of reactivity enabled by the new **L18**/Ni system to include primary amides and lactam reagents, substrates that had not been utilized under Ni-catalyzed C-N cross-coupling conditions prior. Chapter 4 details a combined experimental and theoretical investigation into the mechanistic underpinnings of the **L18**/Ni amination system, which includes a comparison of potential parallel reaction mechanisms involving either Ni^{0}/Ni^{II} or Ni^{I}/Ni^{III} cycles. Chapter 5 features a combined experimental and theoretical examination of the influence of the **L18** structural features in Ni-catalyzed ammonia arylations, which revealed a particularly critical role exerted by the ligands steric parameters. It is anticipated that the key ancillary ligand design concepts and mechanistic considerations presented herein will provide a useful platform for researchers initiate ancillary ligand design efforts for the development of high-performing Ni cross-coupling catalysts. Such an outcome is pivotal in my view, in the pursuit of more sustainable C-N cross-coupling protocols that may be adopted by end users in favor of Pd technology.

Chapter 2

The Design and Application of Bidentate Phosphine Ligands for Nickel-Catalyzed Amine Arylations

2.1. RESEARCH OVERVIEW AND CONTRIBUTION REPORT

This author wishes to clarify his contributions to the research described in Chapter 2 of this Thesis document. This chapter describes the development of a new, air-stable *ortho*-phenylene bisphosphine ligand PAd-DalPhos (**L18**), which embodies design criteria viewed by our group as essential for forming active amination Ni-catalysts. The derived air-stable pre-catalyst (**L18**)NiCl(*o*-tolyl) (**C1**) is effective in catalyzing otherwise challenging C(sp^2)-N cross-coupling transformations at relatively low catalyst loadings, accommodating the broadest combination of (hetero)aryl (pseudo)halide and NH coupling partners reported to date for any single nickel catalyst, without the need for precious metal co-catalysts or other additives. The use of **C1** enabled the first examples of room-temperature Ni-catalyzed cross-couplings involving primary alkylamines and ammonia, as well as examples of sought-after ammonia monoarylations employing (hetero)aryl mesylate electrophiles, for which no capable catalyst system of any type is known.

My contributions to this study include: designed parts of the research, performed all of the ligand and coordination complexes syntheses, participated in developing the scope of reactivity with ammonia alongside Dr. Andrey Borzenko, Nick L. Rotta-Loria, and Ryan S. Sawatzky, contributed to the interpretation of the results, and provided feedback on the manuscript, which was written by Prof. Mark Stradiotto. Authors R. McDonald and M. Ferguson carried out the X-ray diffraction analyses of (**L18**)$NiCl_2$ and **C1**. Where appropriate, the specific contributions of each author are stated explicitly in the text. This work has been published in Nature Communications.

Reference: Lavoie, C.M.; MacQueen, P.M.; Rotta-Loria, N.L.; Sawatzky, R.S.; Chisholm, A.J.; Hargreaves, B.K.V.; McDonald, R.; Ferguson, M.J.; Stradiotto, M., Challenging Nickel-catalysed Amine Arylations Enabled by Tailored Ancillary Ligand Design *Nat*. *Commun*. **2016**, *7*, 11073.

2.2. INTRODUCTION

By far the most common strategy employed thus far for identifying competent nickel catalysts for cross-coupling transformations has involved screening of ancillary ligands that have proven effective in analogous Pd-driven processes. For less challenging N-H substrates such as secondary amines, this has proven to be an effective approach, with nickel catalyst systems based on on triphenylphosphine,[80] dppf,[87, 89] NHCs,[82, 83, 126] and also phenanthrolines[99] exhibiting desirable performance. Conversely, nickel catalysts capable of promoting the cross-coupling of other useful NH substrates (e.g., primary alkylamines,

ammonia, azoles and others) are rare, limited in scope, and commonly require forcing conditions.

Therefore it appears unlikely that simply “re-purposing” ancillary ligands that function well with palladium will be an effective strategy for identifying superlative Ni-catalysts for challenging C-N cross-couplings. Furthermore, given the distinct chemical properties of Ni, it stands to reason that the rational design and application of new ancillary ligands targeted specifically for use in enabling Ni catalysis represents a complementary and potentially more powerful approach.

Despite such opportunities, the design of ancillary ligands specifically tailored for use in enabling Ni-catalyzed C-N cross-coupling was not reported prior to the work presented in Chapter 2 of this Thesis. While other promising approaches to achieving Ni-catalyzed C-N cross-coupling have emerged as of late (e.g., photo-,[76] and electrochemically-driven[127] processes, Fig. 2-1), the demonstrated scope of reactivity and generality of such protocols in no cases represent the state-of-the-art. Therefore there is tremendous room for growth within Ni-catalyzed amination chemistry, and it is the belief of this author that the rational development of ancillary ligands specifically tailored for use with Ni represents the most promising approach to addressing outstanding reactivity challenges within this area.

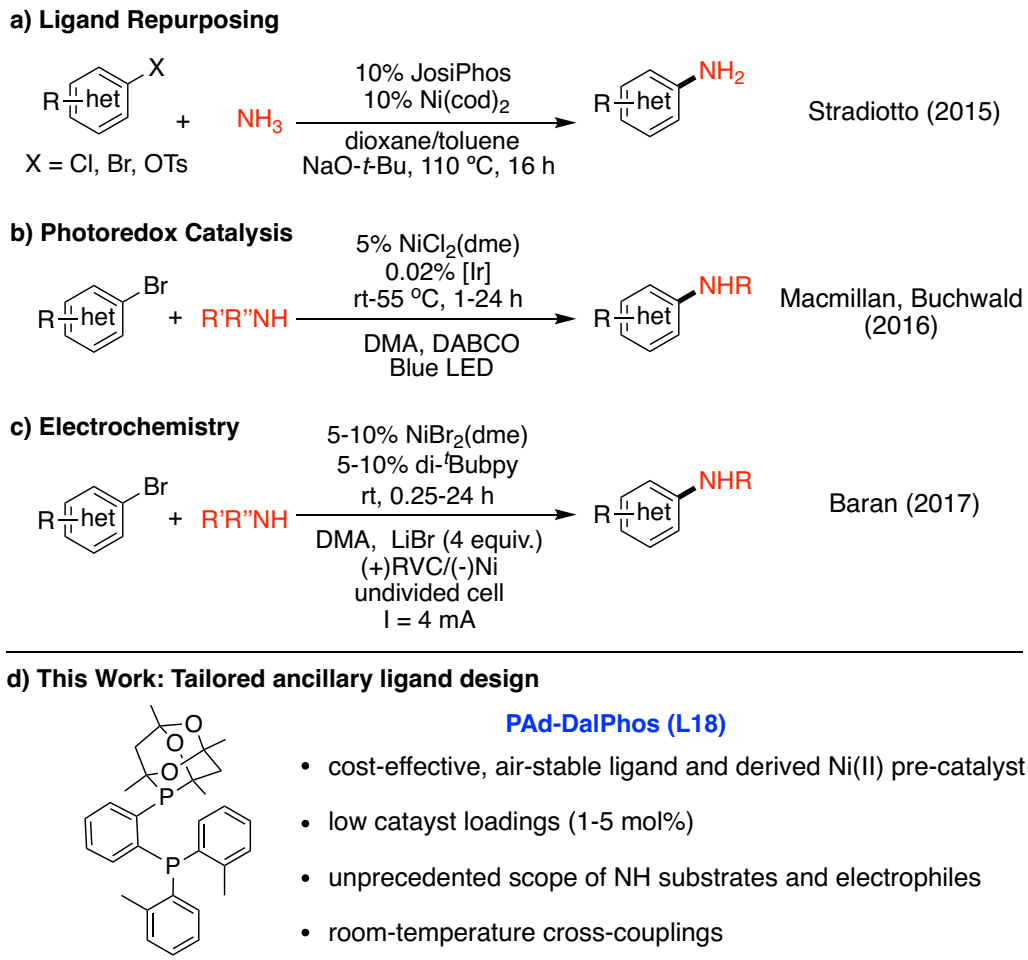


Figure 2-1. Approaches to nickel-catalyzed C-N cross-coupling (a-c) and the focus of this Thesis (d).

2.3. RESULTS AND DISCUSSION

2.3.1. Ancillary Ligand Design

Unlike the bulky *electron-rich* ancillary ligands that have proven optimal for use with palladium (Fig. 1-5), we envisioned that sterically demanding yet relatively *electron-poor* bisphosphines might be well-suited for use with nickel, given the greater propensity for C(sp^2)-Cl oxidative additions to Ni(0) versus Pd(0),[128, 129] and the associated potential for rate-limiting C(sp^2)-N reductive elimination within a presumptive Ni^0/Ni^{II} catalytic cycle.[113, 118] In the pursuit of bulky electron-poor bisphosphine ancillary ligands that would function well in nickel-catalyzed

amination chemistry, possibly by promoting C(sp^2)-N reductive elimination, I sought tuneable *ortho*-phenylene bisphosphines, featuring the 1,3,5,7-tetramethyl-2,4,8-trioxa-6-phosphaadamantane (CgP) group with an adjacent phosphorus donor fragment that could be modified easily. Prior structural analyses have established that CgP is as sterically demanding as a P(^{t}Bu)$_2$ fragment, while also being a relatively electron-poor phosphorus donor comparable to a P(OR)$_2$ group,[130] thus making such a fragment well-matched to these ancillary ligand design criteria. The use of CgPPh and related monophosphine ancillary ligand derivatives in palladium-catalyzed cross-couplings dates to 2003,[131] with subsequent reports involving (carbonylative) BHA chemistry featuring only a limited scope of secondary amines and anilines.[132] Conversely, journal publications documenting the application of CgP-based ligands in nickel catalysis are limited to a single report focused on CgPOR-type phosphinites for the hydrocyanation of 3-pentenenitrile.[133]

2.3.2. Ancillary Ligand Synthesis

With the aforementioned ligand design criteria in mind, I generated a small library of *ortho*-phenylene bisphosphines containing structurally varied *ortho* PR$_2$ donor fragments (PR$_2$ = P(*o*-tolyl)$_2$ (**L18**), PCy$_2$ (**L19**), PPh$_2$ (**L23**), and P^{i}Pr$_2$ (**L24**); Fig. 2-2). The new air-stable phosphaadamantane ligands were prepared straightforwardly in a two-step synthesis from relatively inexpensive, commercially available components via the common synthetic intermediate **2.1**. The new air-stable bisphosphine **L25**, a complementary variant of **L18** featuring a P(*t*Bu)$_2$ donor in place of the CgP group, was prepared analogously from synthon **2.2**. Several structurally varied monophosphines featuring the CgP moiety (**L26-L28**) were prepared straightforwardly in a one-step synthesis from *ortho*-substituted

bromobenzenes to compare the effects of mono- and bis-ligation on catalytic efficiency.

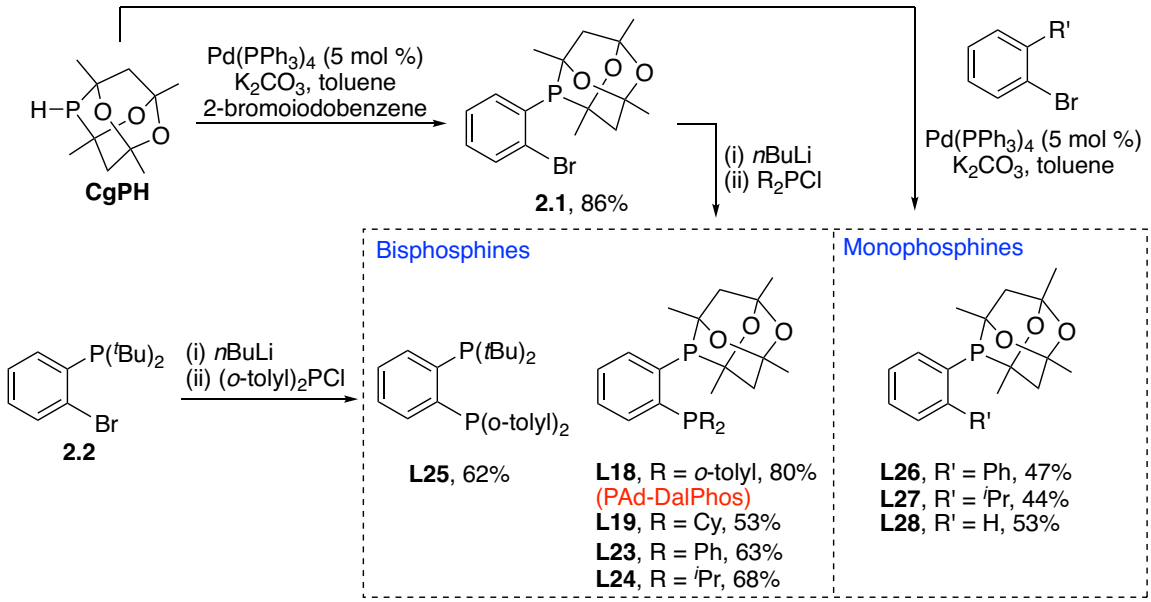


Figure 2-2. Synthesis of the mono- and bisphosphine ligands used in this study.

2.3.3. Ligand Screening in Ni-catalyzed Ammonia Arylations

The utilization of ammonia (NH_3) in transition metal-catalyzed carbon-nitrogen (herein C-N) cross-coupling transformations involving aryl chlorides constitutes an incredibly attractive methodology for the production of primary arylamines, which are ubiquitous structural units found in a range of commodity chemicals (e.g., pharmaceuticals, agrochemicals, natural products, and beyond).[31, 134, 135] While appealing, the successful use of NH_3 in cross-coupling methods is difficult to achieve on account of several salient challenges, which include: catalyst deactivation via ammonia induced ancillary ligand dissociation;[136] slow C-N bond reductive elimination from sterically unencumbered parent amido intermediates;[137] uncontrolled polyarylation of the initial primary arylamine product, [39] among others.

Nonetheless, in 2015 our group[84] along with the Hartwig group[71] independently reported the first Ni-catalyzed ammonia monoarylation with (hetero)aryl chlorides for the synthesis of primary arylamines, a breakthrough that was enabled in both instances by the application of electron-rich, sterically bulky ferrocene-based JosiPhos ligands (**L15, L17**). Notwithstanding such progress, the limitations of these protocols (*vide supra*), along with the failure of other top-performing bulky and electron-rich ancillary ligands from the domain of palladium-catalyzed ammonia monoarylation (e.g., CyPF-*t*Bu JosiPhos, Mor-DalPhos, BippyPhos)[84] underscores the inconsistent nature of simply re-purposing ancillary ligands from palladium chemistry in the pursuit of nickel catalysts for such challenging C(sp^2)-N cross-couplings.

Against this background, I selected the C-N cross-coupling of ammonia with 4-chlorobiphenyl (**2.3**) as a testing ground on which to evaluate the catalytic abilities of the newly prepared ligands (Fig. 2.3). While poor conversion and/or poor selectivity was achieved when employing $Ni(cod)_2$/(**L19, L23**-**L24**) catalyst mixtures, the use of **L18** (PAd-DalPhos) resulted in high conversion (>90%) of **2.3** to the target 4-aminobiphenyl (**2.4**). These findings are in keeping with the view that sterically demanding yet relatively *electron-poor* bisphosphine ancillary ligands should support particularly effective nickel catalysts for such challenging cross-couplings (*vide supra*). Nonetheless, the competent performance of the $P(^tBu)_2$/$P(o\text{-tolyl})_2$ ancillary ligand **L25**, though inferior to the CgP/$P(o\text{-tolyl})_2$ variant **L18** in the test reaction employed (Fig. 2-3), suggests that ancillary ligand sterics are particularly important in engendering useful catalytic behaviour within the nickel-catalyzed C(sp^2)-N cross-couplings under scrutiny herein. The poor

performance of the new structurally related CgPPh derivatives (**L26/L27**), along with the monophosphines CgPPh (**L28**),[131] P(*o*-tolyl)$_2$Ph (**L29**),[138] which did not vary when using Ni:L = 1:1 or 1:2 in the case of **L26**, confirms the benefit of bisphosphine ligation by **L18**. Finally, the observation that [Pd(cinnamyl)Cl]$_2$/**L18** mixtures afforded no conversion of **2.3** under analogous conditions underscores that the design of **L18** (PAd-DalPhos) is particularly well-matched to the properties of nickel, rather than those of palladium, in this reaction setting.

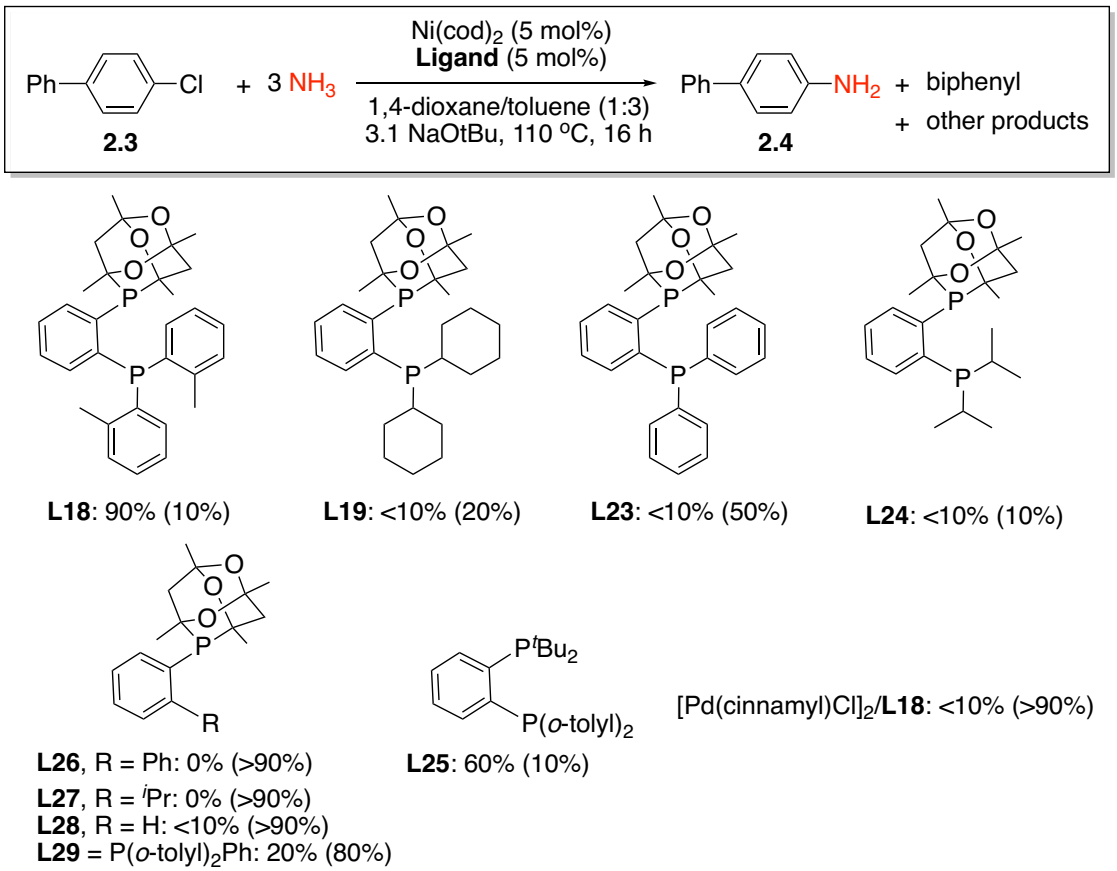


Figure 2-3. Preliminary ligand screen in the Ni-catalyzed monoarylation of ammonia with 4-chlorobiphenyl, **2.3** (0.12 mmol), using 0.5 M stock solutions of ammonia in 1,4-dioxane (0.72 mL) and toluene (1.00 mL). Conversions estimated on the basis of gas chromatographic data, reported as % 4-aminobiphenyl, **2.4**, (% **2.3** unreacted); mass balance attributable to biphenyl and/or other unidentified products; cod = 1,5-cyclooctadiene.

2.3.4. Synthesis of L18-derived Ni(II) Pre-catalysts

After establishing the new CgPPh ligand class as a competent alternative to the JosiPhos family for use in Ni-catalyzed ammonia monoarylations, we subsequently sought to circumvent the use of expensive and air-sensitive $Ni(cod)_2$. Notwithstanding the reactivity benefits associated with the use of nitriles as co-ligands/additives,[69, 71, 95] and the utility of precious metal/nickel photoredox dual catalysis,[75, 76] to facilitate end-user uptake, operationally simple, air-stable nickel pre-catalysts were targeted without recourse to the aforementioned experimental modifications. Buchwald and coworkers recently reported on the development of an air-stable dppf-ligated LNiCl(*o*-tolyl) pre-catalyst for the amination of aryl (pseudo)halides, including challenging sulfamates, mesylates, and triflates.[89] As pre-catalysts of this type (i.e., $L_nNiX(aryl)$) resemble oxidative addition products, they are readily activated through amido/halide ligand exchange and reductive elimination of catalytic quantities of the (*ortho*-tolyl)NR_2 by-product, which generates the active Ni(0) species.

I thus turned my attention to the synthesis of (**L18**)NiCl(*o*-tolyl), **C1**, which could be reduced to a requisite (**L18**)Ni(0) species under the amination conditions employed without the formation of inhibiting by-products.[68, 89] Combination of **L18** with $NiCl_2$(dme) afforded (**L18**)$NiCl_2$, in 77% isolated yield, and subsequent treatment with (*o*-tolyl)MgCl afforded (**L18**)NiCl(*o*-tolyl), **C1**, in 93% isolated yield (Fig. 2-4). Each complex was obtained as an analytically pure solid, and was characterized by use of spectroscopic and crystallographic techniques. The κ^2-*P*,*P*-bidentate nature of **L18** is evident in the solid state structures of both complexes (Fig. 2-5), which are best described as exhibiting a distorted square planar

geometry at nickel ($\Sigma_{\text{angles at Ni}}$ ~ 360º). The catalytic performance of **C1** was found to be identical to that of Ni(cod)$_2$/**L18** mixtures in the test reaction featured in Fig. 2-3, with no loss of performance observed following storage of **L18** or **C1** in air for an extended period (months). Moreover, the performance of **C1** was found to be vastly superior to that of Ni(cod)$_2$/**L18** under more challenging reaction conditions (i.e., room temperature, lower catalyst loadings), in keeping with catalyst inhibition by cod.[139]

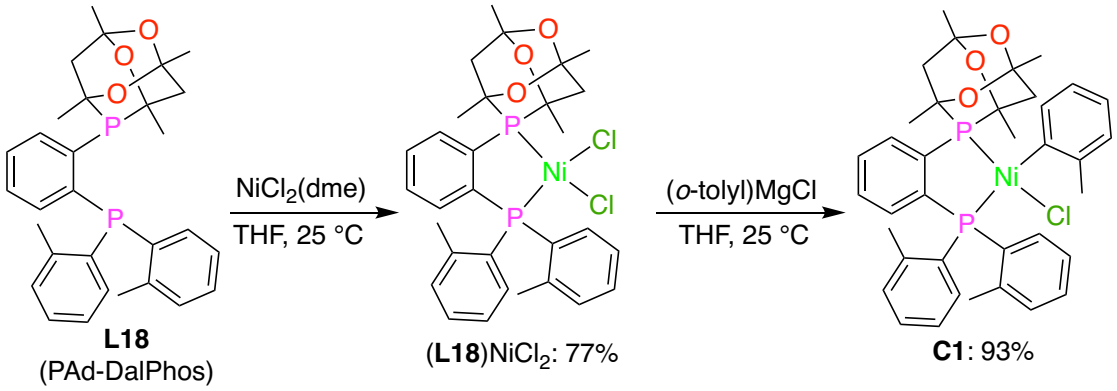


Figure 2-4. Synthesis of the **L18**-derived nickel complexes (**L18**)NiCl$_2$, and **C1**.

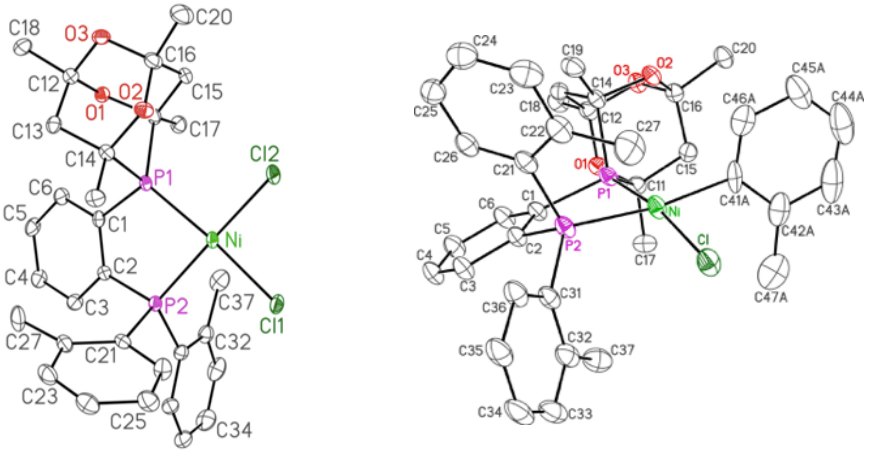


Figure 2-5. Single-crystal X-ray structures of (**L18**)NiCl$_2$ (left) and **C1** (right) depicted with hydrogen atoms omitted for clarity. Selected interatomic distances (Å) and angles (º): for (**L18**)NiCl$_2$ Ni-P1 2.1903(12), Ni-P2 2.1691(13), Ni-Cl1

2.2195(13), Ni-Cl2 2.1865(13), P1-Ni-P2 86.74(5), P1-Ni-Cl2 94.03(5), P2-Ni-Cl1 88.88(5), Cl1-Ni-Cl2 90.37(5); for **C1**: Ni-P1 2.1766(8), Ni-P2 2.2263(8), Ni-Cl 2.1916(8), Ni-C(aryl) 1.971(3), P1-Ni-P2 86.52(3), P1-Ni-C(aryl) 95.79(10), P2-Ni-C1 92.72(3), Cl-Ni-C(aryl) 87.53(10).

2.4. SELECTED NMR CHARACTERIZATION FOR L18 AND C1

The complete characterization data for previously described ligands (**L18**, **L19**, **L23**-**L29**) and the **L18** derived Ni(II) pre-catalyst (**C1**) are detailed in Section 2.8. Several noteworthy aspects regarding the NMR behavior of these aforementioned compounds however warrant further commentary. For instance, the NMR spectral assignments for several ligands and **C1** in some cases, were rendered complex by: the C_1-symmetric nature of these species due to the chiral (racemic) phosphaadamantane group; second-order coupling; dynamic behaviour (as evidenced in the temperature-dependent $^{31}P\{^1H\}$ NMR spectra of **L18**); and possibly in the case of C_1 dynamic equilibria involving rotamers and/or between tetrahedral and square planar species of **C1**.

2.4.1. NMR Analyses of PAd-DalPhos (L18)

In the case of **L18** (PAd-DalPhos), not only are its corresponding NMR spectra complicated by second-order coupling, they are also accompanied by dynamic equilibrium phenomena, evidenced by the appearance of a broad resonance in the $^{31}P\{^1H\}$ NMR spectrum where a doublet would otherwise be expected. The dynamic effects associated with **L18** in solution – which are presumably the result of restricted P-C(tolyl) bond rotation in the P(*o*-tolyl)$_2$ fragment as well as the chiral (racemic) phosphaadamantanyl group, were confirmed by conducting variable temperature NMR experiments (Figures 2-6 and 2-7). Cooling of a sample of **L18** from 300 K down to 223 K allowed the broad peak

at -24.1 ppm to decoalesce, revealing the expected doublet, and also revealed two new sets of doublets (-30.2 ppm and -38.8 ppm), that can be attributed to a minor diastereomer.

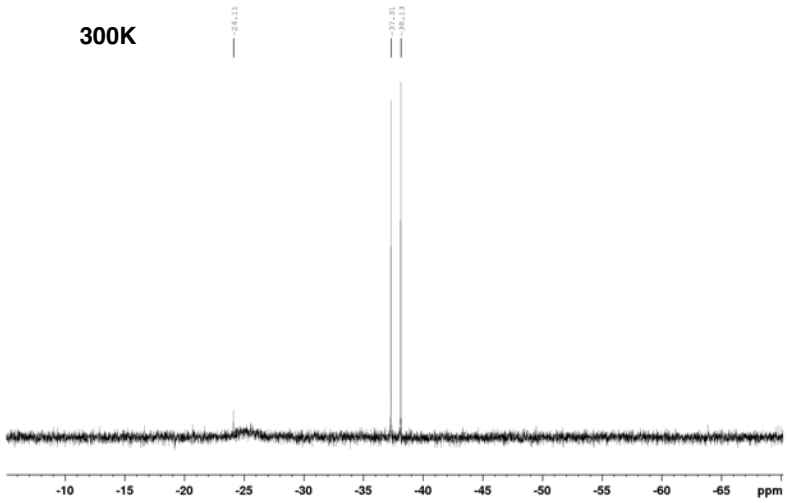


Figure 2-6. $^{31}P\{^{1}H\}$ NMR spectrum of PAd-DalPhos (**L18**) collected at 300 K.

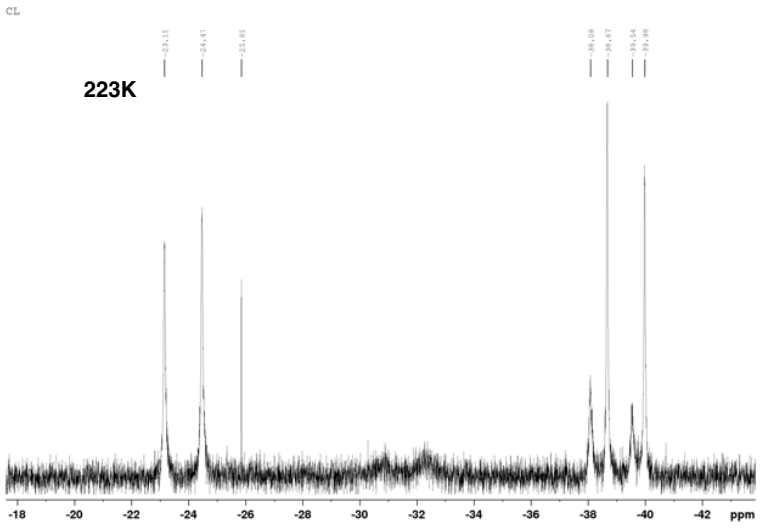


Figure 2-7. $^{31}P\{^{1}H\}$ NMR spectrum of PAd-DalPhos (**L18**) collected at 223 K.

2.4.2. NMR and X-ray Crystallographic Analysis of C1

The $^{31}P\{^{1}H\}$ NMR spectrum of the **L18** derived (**L18**)NiCl(*o*-tolyl) pre-catalyst (**C1**) (Fig. 2-8) appears to feature an AB quartet, however there are in fact four sets of doublet resonances, existing as major and minor disastereomers (ca. 2:1) in solution (J = 4.3 Hz for minor species, J = 4.6 Hz for major). On the basis of the observed positional disorder associated with the Ni-bound *ortho*-tolyl fragment within the X-ray structure of **C1**, arising from Ni-C(tolyl) bond rotation (80:20 occupancy ratio), the major and minor species can be assigned as being rotamers of this type.

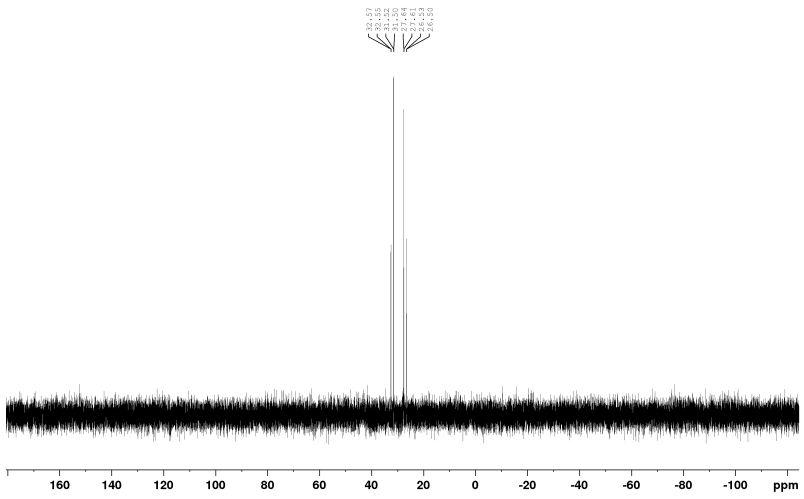


Figure 2-8. $^{31}P\{^{1}H\}$ NMR spectrum of **C1** collected at 300 K.

2.5. SCOPE OF REACTIVITY IN AMMONIA ARYLATIONS ENABLED BY C1

Following the synthesis and characterization of the desired air-stable (**L18**)NiCl(*o*-tolyl) (**C1**) pre-catalyst, the scope and limitations exhibited by **C1** in the context of C-N cross-couplings were examined. This investigation revealed that the scope of reactivity enabled by **C1** in the monoarylation of ammonia exceeds that

demonstrated previously for any catalyst (i.e., palladium, copper, nickel, or other), both in terms of the breadth of electrophilic partner (e.g., chlorides, bromides, iodides, mesylates, tosylates, triflates, and imidazolylsulfonates) and the varied reaction conditions (e.g., room temperature; microwave conditions; use of gaseous ammonia). This authors contribution to the scope was the isolation of reaction products derived from cross-couplings involving non-heteroatom containing aryl chlorides, as well as select pairings involving aryl bromides and tosylates (Fig. 2-9); a more thorough account of other aspects of the reaction scope has been described in several previous Stradiotto group members' theses,[140-142] which readers are directed to for further inquiry.

In keeping with the preliminary ligand screening experiments (Fig. 2-3), 4-aminobiphenyl monoarylation products (**2.4-2.6**) were isolated in synthetically useful yields, as were 1- or 2-naphthylamines (**2.7**-**2.8**) derived from an unprecedentedly wide array of 1-(pseudo)halonaphthalenes (e.g., X = Cl, Br, I OTs, OTf, OMs; only entries derived from aryl chlorides, bromides, and tosylates were isolated by this author). Electrophiles featuring or lacking *ortho*-substitution were also accommodated, including variants incorporating pyrrole (**2.9**), methoxy (**2.5**, **2.10**, **2.11**), cyano (**2.12**), methyl (**2.6**, **2.12**, **2.13**), and phenyl (**2.14**) functionalities. Given the importance of biologically active (hetero)anilines in pharmaceutical chemistry, other members of Stradiotto group turned their attention to **C1**-catalyzed ammonia monoarylations employing (hetero)aryl (pseudo)halide electrophiles (work conducted exclusively by P.M.M., N.R.L., and R.S.S.) We were pleased to find that quinoline, isoquinoline, quinaldine, pyrimidine, quinoxaline,

quinazoline, benzothiophene, and benzothiazole core structures each proved compatible with this chemistry.

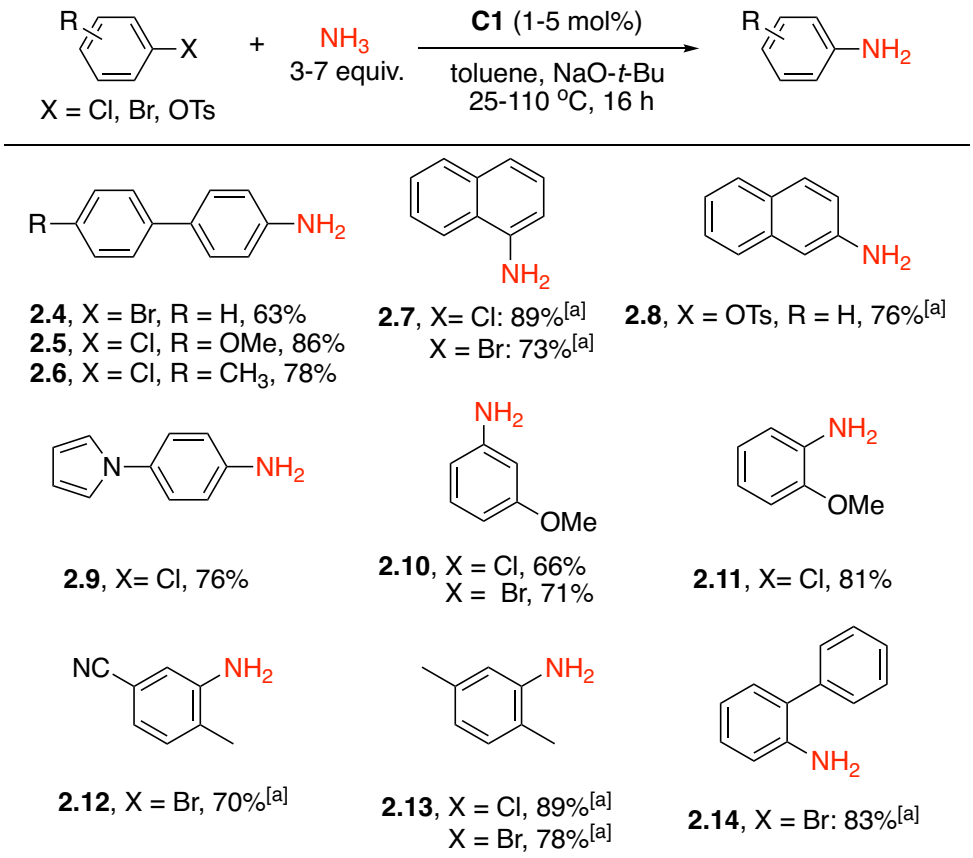


Figure 2-9. Scope of ammonia monoarylation using **C1**. Unless stated otherwise, reactions were conducted employing **C1** (1-5 mol %), NaO-*t*-Bu 2.0-3.0 equiv.), NH_3 (from 0.5 M solutions in 1,4-dioxane; 3-7 equiv.), in toluene at 110 ˚C for 16 h (un-optimized), with yields of isolated products reported. See section 2.7 for complete experimental details. [a] 25 ˚C.

Other distinguishing facets of the above-mentioned reactivity warrant further commentary. Whereas room temperature C(sp^2)-N cross-couplings are attractive in terms of operational simplicity and reduced energy footprint, ammonia monoarylation has proven difficult; only a small number of such transformations have been achieved using palladium catalysis,[143] and none involving nickel catalysis. The ability of **C1** to catalyze room temperature ammonia monoarylations

is demonstrated in entries **2.7**, **2.8**, **2.12-2.14** covering chloride, bromide, tosylate electrophiles. Furthermore, the ability to conduct such room temperature ammonia monoarylation reactions on preparative (multi-gram) scale was confirmed by coworker R.S.S. in the reaction of 1-chloronaphthalene with ammonia leading to **2.7** (2 mol % **C4**, 2.28 g, 76 % isolated yield). While efforts to optimize the reaction times was not made, the monoarylation of ammonia using 1-chloronaphthalene was found to be complete (>90% conversion to **2.7** on the basis of GC data) after only 15 minutes when using 5 mol % **C1**, thereby underscoring the highly active nature of **C1** under room temperature conditions. While no loss in catalytic activity was observed in the monoarylation of ammonia using 1-chloronaphthalene when the solid reaction components including **C1** were handled in air, followed by delivery of the ammonia stock solution on the benchtop within a nitrogen-purged glove-bag, identical reactions conducted under an ambient atmosphere were unsuccessful.

The first examples of ammonia monoarylation employing (hetero)aryl mesylates involving any catalyst system was also achieved (work performed by P.M.M.) There is significant interest in the development of cross-couplings involving such electrophiles, given their low cost and greater atom economy relative to (hetero)aryl tosylates and triflates, and in the context that the generated methanesulfonic acid is naturally occurring and can undergo biodegradation under conventional waste-water processing.[144] Finally, scalability issues in ammonia monoarylation would suggest the use of gaseous ammonia, while the application of ammonium salts[145] offers operational simplicity in bench-scale syntheses. The ability of **C1** to function effectively both when using high pressures of gaseous

ammonia (work done by P.M.M.) and alternatively ammonium acetate under microwave reaction conditions (work done by R.S.S.) at elevated reaction temperatures is unique among all previously reported catalyst systems for ammonia monoarylation.

2.6. INEFFECTIVE APPLICATIONS OF THE DEVELOPED METHODOLOGY

Several limitations of the previously described **L18**/Ni catalyst system warrant further discussion. Whereas activated (pseudo)halide electrophiles (e.g., 4-chlorobenzonitrile) could be efficiently aminated under conditions of low temperature (e.g., room-temp.) and catalyst loading (1-5% **C1**), employing electron-neutral (e.g., chlorobenzene) or deactivated (pseudo)halide partners (e.g., 4-chloroanisole) in conjunction with ammonia required comparatively more forcing conditions (e.g., 110 ^{o}C, 10 mol % **C1**). Recent computational analysis (featured in Chapter 4 of this Thesis)[72] of **C1** based ammonia monoarylation indicates that the origin of the poor reactivity of the latter substrates may be attributed to a comparatively higher energy barrier to rate-limiting C-N reductive elimination involving (**L18**)Ni(aryl)NH_2 intermediates that feature electron-neutral or electron–rich aryl groups.

A number of electrophiles were not-tolerated by **C1** during the survey of electrophile coupling partners in reactions with ammonia (Fig. 2-10). Although the ability for **C1** to tolerate sterically hindered *ortho*-substituted aryl halides was demonstrated (e.g., **2.11**-**2.14**, Fig. 2-9), incorporation of a second group at the *ortho*-position (i.e., 2,6-dimethylchlorobenzene) proved detrimental, yielding <10% of the corresponding product **2.15** even at elevated temperatures (110 ^{o}C). Several

primary aniline products derived from mono-*ortho*-substituted aryl halides proved elusive even at elevated temperatures (110 ^{o}C), including 2-(trifluoromethyl)aniline (**2.16**), and 2',6'-dimethoxybiphenyl-2-ylamine (**2.17**). Notably, a structural derivative of **2.17** derived from a cross-coupling involving *n*-octylamine was isolated in high yield by coworker P.M.Q. It is possible that the weak nucleophilicity of ammonia relative to primary alkylamines (e.g., *n*-octylamine) may prevent efficient binding to a more congested Ni-coordination envirionment when sterically hindered aryl halides are used as substrates.

Aryl chlorides bearing certain functional groups were not tolerated by **C1**, including those containing *tert*-butyl (**2.18**), methyl ketone (**2.19**), nitro (**2.20**), primary alcohol (**2.21**), and primary amine (**2.22**) functionality. Despite giving rise to moderate conversion of starting aryl halide (ca. 30-50%), the cross-coupling to form **2.18**-**2.20** yielded substantial quantities of un-identified high-molecular weight products. Full consumption of starting material was observed in the cross-coupling to form **2.21** under room-temperature conditions, however the major product was not the expected primary aniline. While the identity of the byproduct formed was not confirmed, it is plausible that **C1** catalyzed the C-O cross-coupling between two molecules of 4-chlorobenzyl alcohol; **C1** and a structurally related nickel pre-catalyst based on **L19** have recently been demonstrated by our group[146] to be efficient catalysts for enabling such C-O transformations.

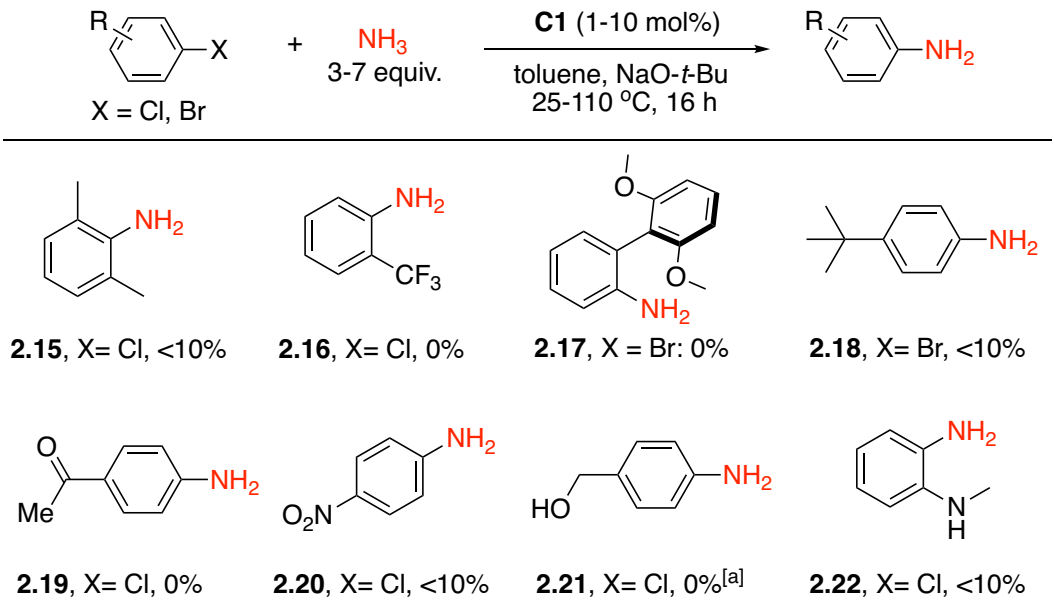


Figure 2-10. Examples of unsuccessful ammonia arylations using **C1**. Unless stated otherwise, reactions were conducted employing **C1** (1-5 mol %), NaO-*t*-Bu 2.0-3.0 equiv.), NH_3 (from 0.5 M solutions in 1,4-dioxane; 3-7 equiv.), in toluene at 110 ˚C for 16 h (un-optimized), with yields reported on the basis of GC data. [a] 25 ˚C.

2.7. SUMMARY

The pre-catalyst **C1**, featuring the new sterically demanding and electron-poor bisphosphine ancillary ligand (**L18**, PAd-DalPhos), enables unprecedented nickel-catalyzed C(sp^2)-N cross-coupling chemistry under mild conditions and without the need for a precious metal co-catalyst. The utility of **C1** is showcased in the first reports of room-temperature nickel-catalyzed reactions involving and ammonia, including reactions involving (hetero)aryl mesylates, for which no capable catalyst system of any type had been described previously.

The “re-purposing” of ancillary ligands that function well with palladium has in some cases proven useful in the development of nickel catalysts for use in cross-coupling chemistry. Nonetheless, the outstanding performance of **L18** in the challenging nickel-catalyzed C(sp^2)-N cross-coupling chemistry presented herein confirms that hindered and electron-poor bisphosphines, the properties of which

can be viewed as complementing the inherent reactivity profile of nickel, represent an effective class of ancillary ligands for such applications. Unlike palladium chemistry, the applicability of diverse ancillary ligand strategies for use in enabling varied nickel-catalyzed cross-couplings is crucial not only in terms of promoting elementary catalytic steps, but also as a means of favoring desired oxidation states of nickel, given the established viability of both Ni(0)/Ni(II) and Ni(I)/Ni(III) catalytic cycles. In this regard, the ancillary ligand design strategies employed herein are likely to contribute toward the development of high-performing nickel catalysts for use in a range of synthetically important cross-coupling applications, so as to enable more sustainable chemical practices that circumvent the use of precious metals such as palladium.

2.8. EXPERIMENTAL

2.8.1. General Considerations

General Considerations. Unless otherwise stated, all reactions were setup inside a nitrogen-filled inert atmosphere glovebox, and were worked up in air using benchtop procedures. Toluene was deoxygenated by sparging with nitrogen followed by passage through a double column solvent purification system packed with alumina and copper-Q5 reactant, and storage over activated 4 Å molecular sieves. 1,4-Dioxane was dried over Na/benzophenone followed by distillation under a nitrogen atmosphere. Otherwise, all reagents, solvents and materials were used as received from commercial sources. Column chromatography was carried out using Silicycle SiliaFlash 60 silica (particle size 40-63 μm; 230-400 mesh) or using neutral alumina (150 mesh; Brockmann-III; activated), as indicated. Unless stated

NMR spectra were recorded at 300 K in $CDCl_3$ with chemical shifts expressed in parts per million (ppm) using the residual $CHCl_3$ solvent signal (^1H, 7.26 ppm; ^{13}C, 71.4 ppm) as an internal reference, or H_3PO_4 as an external reference (^{31}P, 0 ppm). Splitting patterns are indicated as follows: br, broad; s, singlet; d, doublet; m, multiplet, with all coupling constants (*J*) reported in Hertz (Hz). In some cases fewer than expected independent ^{13}C NMR resonances were observed despite prolonged acquisition times. Mass spectra were obtained using ion trap (ESI) instruments operating in positive mode, and GC data were obtained on an instrument equipped with a SGE BP-5 column (30 m, 0.25 mm i.d.). The accompanying NMR spectra for the reported compounds in this chapter can be found in Appendix A of this document.

2.8.2. Catalytic Procedures

General Catalytic Procedure 2-1 (GP2-1). C1 (8.3-20.7 mg, 0.0012-0.030 mmol, 2-5 mol %), aryl (pseudo)halide (0.60 mmol, 1 equiv.), and NaO-*t*-Bu or (1.20-1.80 mmol, 2.0-3.0 equiv.) were added to a screw-capped vial containing a magnetic stir bar, to which was added toluene (9 mL) and NH_3 as a 0.5 M solution in 1,4-dioxane (1.8-4.2 mmol, 3-7 equiv., 3.0-8.4 mL). The vial was sealed with a cap containing a PTFE septum, was removed from the glovebox and placed in a temperature-controlled aluminum heating block set at 25°C or 110°C, and was allowed to react under the influence of magnetic stirring for 16 h (unoptimized). The vial was then removed from the heating block and was left to cool to ambient temperature, after which the reaction mixture was worked up as described.

Workup Method 1 (Purification by Chromatography): The crude reaction mixture was filtered through a short Celite plug, and the volatile materials were

evaporated *in vacuo*. The crude product was purified by flash-column chromatography to afford the purified product.

Workup Method 2 (Purification by Extraction): The volatile materials were evaporated *in vacuo*. The residue was dissolved in EtOAc. The product was extracted with aqueous 1 M HCl (3 x 25 mL). The combined aqueous layers were then washed with EtOAc (3 x 10 mL). Solid sodium bicarbonate was added to the acidic aqueous layer until it was fully neutralized (monitored with pH paper). The product was extracted with EtOAc (3 x 25 mL). The organic layers were combined, dried over anhydrous sodium sulfate, and filtered through a silica plug with ethyl acetate (~ 30 mL). The residual solvent was removed *in vacuo* and the product was allowed to dry overnight.

2.8.3. Synthesis and Characterization Data

Synthesis of 1,3,5,7-tetramethyl-2,4,6-trioxaphosphaadamanatane-phenylbromide (2.1) To a glass screw-capped vial containing a magnetic stir bar was added 2-bromoiodobenzene (0.73 mL, 5.7 mmol, 1.05 equiv.), toluene (9.0 mL), $Pd(PPh_3)_4$ (0.330 g, 0.285 mmol), K_2CO_3 (1.571 g, 11.4 mmol, 2.0 equiv.), and 1,3,5,7-tetramethyl-2,4,8-trioxaphosphaadamantane, CgPPh, (1.14 g, 5.3 mmol). The vial was sealed with a PTFE-lined cap and was removed from the glovebox. The vial was placed in an oil bath set to 110 °C and magnetic stirring was initiated. After 48 h (unoptimized) the reaction mixture was cooled, diluted with CH_2Cl_2 (50 mL), and washed with distilled water (3 x 50 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered, and the collected eluent solution was

concentrated under reduced pressure by use of a rotary evaporator. The resulting yellow oil was filtered through an alumina plug (ca. 50 g) eluting with 90% hexanes/CH_2Cl_2; the solvent was then removed from the collected eluent under reduced pressure by use of a rotary evaporator. The resulting yellow solid was purified by flash chromatography over silica, eluting with 10% ethyl acetate/hexanes to afford **2.1** as a white solid (1.69 g, 86 % yield). ^{1}H NMR: ($CDCl_3$, 500 MHz) 8.29 (d, *J* = 7.7, 1H), 7.66-7.64 (m, 1H), 7.37 (apparent t, *J* = 7.5 Hz, 1H), 7.25 (apparent t, *J* = 7.6 Hz, 1H), 2.14 (m, 1H), 2.02-1.89 (m, 2H), 1.55-1.44 (m, 13H). ^{13}C{^{1}H} NMR: ($CDCl_3$, 125.8 MHz) 135.3 (d, *J* = 22.6 Hz), 135.2, 133.8 (d, *J* = 2.5 Hz), 133.2 (d, *J* = 37.7 Hz), 131.0, 127.5, 97.0, 96.2, 74.5 (d, J = 10.1 Hz), 73.9 (d, *J* = 25.2 Hz), 45.8 (d, *J* = 20.1 Hz), 36.5, 28.7 (d, *J* = 18.9 Hz), 28.2, 27.9, 26.7 (d, *J* = 11.3 Hz). ^{31}P{^{1}H} NMR: ($CDCl_3$, 202.5 MHz) -29.6. HRMS-ESI (m/z) Calcd for $C_{16}H_{20\ 79}BrNaO_3P$ [M+ Na]: 393.0226; Found: 393.0214.

General Procedure for the synthesis of L18-L19, **L23-L24** (**GP2-2**)

Compound **2.1** and diethyl ether (~0.3M in **2.1**) were added to a glass screw-capped vial containing a magnetic stir bar. The vial was sealed with a cap featuring a PTFE septum. The solution was then cooled to -33^{o}C and magnetic stirring was initiated, followed by drop-wise addition of *n*-butyllithium (1.5 eq, 2.5 M in hexanes) via syringe. The resulting mixture was left to stir for 30 minutes while warming to ambient temperature. At this point the appropriate chlorophosphine (R_2ClP, R = *o*-tol, Ph, ^{i}Pr, Cy; 1.2 equiv) was added dropwise via syringe with continued stirring. The resulting mixture was left to stir for 48 h (unoptimized) at ambient temperature, after which the crude reaction mixture was opened to air on the benchtop and was

filtered through a short Celite plug; the collected eluent was concentrated by use of a rotary evaporator. The residue was adsorbed onto silica (ca. 1 g) and was then concentrated to dryness by use of a rotary evaporator. The so-formed silica dry pack was added to a silica plug (ca. 50 g), and 10% EtOAc/hexanes (ca. 300 mL) was passed through the plug. The collected eluent was then concentrated to dryness by use of a rotary evaporator, was washed with cold pentane (3 x 1.5 mL), and was then dried *in vacuo* to afford the desired bisphosphine as a white to off-white solid (R = *o*-tolyl, **L18**: 80%; R = Cy, **L19**: 53% R = Ph, **L23**: 63%; R = ^{i}Pr, **L24**: 68%). Please note that the cyclohexyl variant **L19** was purified by flash chromatography over silica (ca. 50 g) eluting with 10% EtOAc/hexanes.

Characterization Data for Ligand Variants L18-L19, **L23-L24**

L18 (PAd-DalPhos): ^{1}H NMR: ($CDCl_3$, 300 MHz) 8.32 (m, 1H), 7.39 (m, 1H), 7.29-7.21 (m, 5H), 7.11-7.04 (m, 2H), 6.89-6.87 (m, 1H), 6.79 (dd, *J* = 7.2, 3.1 Hz, 1H), 6.64 (m, 1H), 2.42 (s, 3H), 2.36 (s, 3H), 2.14-1.79 (m, 3H), 1.57-1.21 (m, 13H). $^{13}C\{^{1}H\}$ NMR: (CDCl3, 125.8 MHz) 142.7-142.2 (m), 134.2, 133.5, 130.3-130.0 (m), 128.8-128.6 (m), 126.4, 125.8, 97.2, 96.3, 74.5-74.2 (m), 46.1 (d, J = 18.9 Hz), 36.6, 28.4-28.0 (m), 26.3 (d, J = 11.3 Hz), 21.7, 21.5. $^{31}P\{^{1}H\}$ NMR: (CDCl3, 202.5 MHz, 298K) -24.1 (broad m), -37.7 (d, *J* = 166 Hz). $^{31}P\{^{1}H\}$R: (CDCl3, 121.5 MHz, 223K) -23.8 (d, *J* = 160 Hz, major species), -30.2 to -33.0 (broad m, minor species), -38.8 (d, *J* = 177 Hz, minor species), -39.4 (d, J = 160 Hz, major species). HRMS-ESI (m/z) Calcd for $C_{30}H_{34}NaO_3P_2$ [M+Na]: 527.1881; Found: 527.1875. Anal. Calcd for $C_{30}H_{34}NaO_3P_2$: C, 71.42; H, 6.79. Found: C, 71.12; H, 6.84.

L19: ^{1}H NMR: ($CDCl_3$, 500 MHz) 8.35-8.33 (m, 1H), 7.68 (broad s, 1H), 7.42-7.40 (m, 2H), 2.19-1.09 (m, 38H). $^{13}C\{^{1}H\}$ NMR: (CDCl3, 125.8 MHz) 134.0, 133.1, 128.8, 128.5,97.1, 96.2, 74.7 (two signals), 74.2 (m), 46.4 (d, *J* = 18.9 Hz), 37.0-36.4 (m), 33.0-32.8 (m), 31.1-30.0 (m), 28.4-26.6(m). $^{31}P\{^{1}H\}$ NMR: (CDCl3, 202.5 MHz) -14.0 (broad m), -39.6 (broad m). HRMS-ESI (m/z) Calcd for $C_{28}H_{43}O_3P_2$ [M+H]: 489.2687; Found: 489.2682.

L23: ^{1}H NMR: ($CDCl_3$, 500 MHz) 8.36-8.33 (m, 1H), 7.40-7.30 (m, 10H), 7.23-7.19 (m, 2H), 7.02-6.99 (m, 1H), 2.12-2.07 (m, 2H), 1.94 (m, 1H), 1.56-1.53 (m, 1H), 1.49 (s, 3H), 1.43-1.40 (m, 6H), 1.33 (d, *J* = 12.4 Hz, 3H). $^{13}C\{^{1}H\}$ NMR: ($CDCl_3$, 125.8 MHz) 147.5-147.1 (m), 140.5-140.0 (m), 137.9-137.5 (m), 134.6 (m), 134.2 (m), 133.5 (m), 129.9, 128.9-128.6 (m), 128.4 (two signals), 97.1, 96.2, 74.6, 74.5 (m), 46.1 (d, J = 18.9 Hz), 36.6, 28.4-28.0 (m), 26.5 (d, J = 11.3 Hz). $^{31}P\{^{1}H\}$ NMR: ($CDCl_3$, 202.5 MHz) -12.5 (d, J = 168 Hz, 1P), -37.6 (d, J = 168 Hz, 1P). HRMS-ESI (m/z) Calcd for $C_{30}H_{34}NaO_3P_2$ [M+Na]: 499.1562; Found: 499.1562.

L24: ^{1}H NMR: ($CDCl_3$, 300 MHz) 8.36-8.31 (m, 1H), 7.59 (m, 1H), 7.40 7.36 (m, 2H), 2.42- 2.36 (m, 1H), 2.20-1.87 (m, 4H), 1.46-1.36 (m, 13H), 1.24 (dd, *J* = 15.4, 6.8 Hz, 3H), 1.14 (m, 3H), 1.01-0.90 (m, 6H). $^{13}C\{^{1}H\}$ NMR: ($CDCl_3$, 125.8 MHz) 134.1, 133.5 (m), 132.4 (m), 129.1 (two signals), 128.7 (m), 97.1, 96.2, 74.8. 74.7, 74.3-74.0 (m), 46.3 (d, *J* = 20.1 Hz), 36.4, 28.4-28.0 (m), 26.7 (d, J = 11.3 Hz), 22.9 (m), 20.7-19.8 (m), 18.0. $^{31}P\{^{1}H\}$ NMR: ($CDCl_3$, 202.5 MHz) -38.5 to -39.2 (m). HRMS-ESI (m/z) Calcd for $C_{30}H_{34}NaO_3P_2$ [M+Na]: 431.1875; Found: 431.1867.

Synthesis and characterization of L25. To a glass screw-capped vial containing a magnetic stir bar was added (2-bromophenyl)-di-*tert*-butylphosphine (**2.2**, 145.1 mg, 0.482 mmol, 1.0 equiv.) and diethyl ether (1.5 mL). The vial was sealed with a cap featuring a PTFE septum. The solution was then cooled to -33 ºC and magnetic stirring was initiated, followed by drop-wise addition of *n*-butyllithium (0.29 mL, 2.5 M in hexanes, 1.5 equiv.) via syringe. The resulting mixture was left to stir for 30 minutes while warming to ambient temperature. At this point chlorodi(*o*-tolyl)phosphine (126 mg, 0.506 mmol, 1.05 equiv.) was dissolved in diethyl ether (1.0 mL) and was added dropwise via syringe to the reaction vial with continued stirring. The resulting mixture was left to stir for 48 h (unoptimized) at ambient temperature, after which the crude reaction was opened to air on the benchtop and was filtered through a short Celite plug; the collected eluent was concentrated by use of a rotary evaporator. The residue was adsorbed onto silica (ca. 1 g) and was then concentrated to dryness by use of a rotary evaporator. The so-formed silica dry pack was added to a silica plug (ca. 50 g), and 1% EtOAc/hexanes (ca. 200 mL) was passed through the plug. The collected eluent was then concentrated to dryness by use of a rotary evaporator, was washed with cold pentane (3 x 1.5 mL), and was then dried *in vacuo* to afford **L25** as an off-yellow solid (0.130 g, 62% yield). ^{1}H NMR (300.1 MHz, $CDCl_3$): δ 7.78 (br s, 1H), 7.34-7.19 (m, 6H), 7.07-6.98 (m, 3H), 6.86-6.82 (m, 2H), 2.47 (br s, 6H), 1.11-1.07 (br d, J = 10.5 Hz, 18H); ^{13}C{^{1}H} NMR (125.8 MHz, $CDCl_3$): δ 143.1 (m), 135.4, 135.1, 133.2, 130.1, 129.2, 128.4, 127.4, 126.0, 33.3 (m), 30.7 (d, J = 11.3 Hz), 21.8, 21.7; ^{31}P{^{1}H} NMR (121.5 MHz, $CDCl_3$): δ 20.7 (d, J = 167 Hz, 1P), -27.5 (d, J = 166 Hz, 1P). HRMS-ESI (m/z) Calcd for $C_{28}H_{37}P_2$ [M+H]: 435.2292; Found: 435.2365.

Synthesis and characterization of L26. To a glass screw-capped vial containing a magnetic stir bar was added 2-iodobiphenyl (0.176 mL, 1.0 mmol, 1.05 equiv.), toluene (3.0 mL), $Pd(PPh_3)_4$ (36.3 mg, 0.0314 mmol), K_2CO_3 (1.571 g, 2.0 mmol, 2.0 equiv.), and 1,3,5,7-tetramethyl-2,4,8-trioxaphosphaadamantane, CgPPh, (0.2 g, 0.95 mmol, 1.0 equiv.). The vial was sealed with a PTFE-lined cap and was removed from the glovebox. The vial was placed in an oil bath set to 110 °C and magnetic stirring was initiated. The resulting mixture was left to stir for 48 h (unoptimized) at ambient temperature, after which the crude reaction mixture was opened to air on the benchtop and was filtered through a short Celite plug; the collected eluent was concentrated by use of a rotary evaporator. The residue was adsorbed onto silica (ca. 1 g) and was then concentrated to dryness by use of a rotary evaporator. The so-formed silica dry pack was added to a silica plug (ca. 50 g), and 10% EtOAc/hexanes (ca. 300 mL) was passed through the plug. The collected eluent was then concentrated to dryness by use of a rotary evaporator, was washed with cold pentane (3 x 1.5 mL), and was then dried *in vacuo* to afford **L26** as a white solid (0.159 g, 47% yield). ^{1}H NMR (300.1 MHz, $CDCl_3$): δ 8.38-8.36 (m, 1H), 7.43-7.34 (m, 7H), 7.32-7.28 (m, 1H), 2.08-2.01 (m, 1H), 1.97-1.84 (m, 2H), 1.56-1.52 (m, 3H), 1.45-1.39 (m, 4H), 1.34 (s, 3H), 0.95-0.91 (m, 3H); ^{13}C{ ^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 151.2, 150.8, 141.8, 141.7, 133.8, 132.5, 132.1, 131.0, 130.9, 129.1, 127.6, 127.1, 127.0, 96.7, 95.9, 73.9, 73.8, 73.6, 46.1, 45.8, 36.0, 28.1, 27.8, 27.7, 26.9, 26.7; ^{31}P{ ^{1}H} NMR (121.5 MHz, $CDCl_3$): δ -39.0 (s, 1P).

Synthesis and characterization of L27. To a glass screw-capped vial containing a magnetic stir bar was added 1-bromo-2-isopropylbenzene (0.153 mL, 1.0 mmol, 1.05 equiv.), toluene (3.0 mL), $Pd(PPh_3)_4$ (36.3 mg, 0.0314 mmol), K_2CO_3 (1.571 g, 2.0 mmol, 2.0 equiv.), and 1,3,5,7-tetramethyl-2,4,8-trioxaphosphaadamantane, CgPPh, (0.20 g, 0.95 mmol, 1.0 equiv.). The vial was sealed with a PTFE-lined cap and was removed from the glovebox. The vial was placed in an oil bath set to 110 °C and magnetic stirring was initiated. The resulting mixture was left to stir for 48 h (unoptimized) at ambient temperature, after which the crude reaction mixture was opened to air on the benchtop and was filtered through a short Celite plug; the collected eluent was concentrated by use of a rotary evaporator. The residue was adsorbed onto silica (ca. 1 g) and was then concentrated to dryness by use of a rotary evaporator. The so-formed silica dry pack was added to a silica plug (ca. 50 g), and 10% EtOAc/hexanes (ca. 300 mL) was passed through the plug. The collected eluent was then concentrated to dryness by use of a rotary evaporator, was washed with cold pentane (3 x 1.5 mL), and was then dried *in vacuo* to afford **L27** as a white solid (0.140 g, 44% yield). ^{1}H NMR (300.1 MHz, $CDCl_3$): δ 8.19-8.16 (m, 1H), 7.39-7.35 (m. 2H), 7.22-7.17 (m, 1H), 4.13-3.99 (m, 1H), 2.19-2.11 (m, 1H), 2.05-1.92 (m, 2H), 1.52-1.44 (m, 10H), 1.32-1.28 (m, 6H), 1.24-1.22 (m, 3H); ^{13}C{ ^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 156.4, 156.1, 133.2, 130.8, 130.5, 129.8, 125.7, 96.9, 96.0, 73.8, 73.7, 73.3, 46.4, 46.2, 35.9, 30.9, 30.6, 28.1, 27.9, 27.8, 27.7, 26.7, 26.5, 25.4, 22.3; ^{31}P{ ^{1}H} NMR (121.5 MHz, $CDCl_3$): δ -40.9 (s, 1P).

Synthesis of (L18)$NiCl_2$. In a dinitrogen filled glovebox, a 100 mL oven-dried round bottom flask containing a magnetic stir bar was charged with $NiCl_2$(dme) (1.78 g, 8.10 mmol) and **L18** (PAd-DalPhos; 4.54 g, 9.00 mmol, 1.1 equiv.). The

solid mixture was dissolved in ca 90 ml of tetrahydrofuran (THF) and the resulting solution was stirred magnetically at room temperature for 1 h. The crude reaction mixture was poured directly onto a glass frit and was washed with pentane (5 x 30 ml). The remaining solid on the frit was dissolved by passing CH_2Cl_2 through the frit (ca 50 ml), followed by collection of the eluent. The solvent was removed *in vacuo* affording the desired product as a dark purple paramagnetic solid (3.93 g, 77%). Anal. calculated for $C_{30}H_{34}Cl_2NiO_3P_2$ C, 56.82; H, 5.40. Found: C, 56.72; H, 5.65. A single crystal suitable for X-ray diffraction analysis was prepared by slow evaporation of pentane into a solution of CH_2Cl_2 at room temperature.

Synthesis of C1. In a dinitrogen filled glovebox, (**L18**)$NiCl_2$ (3.90 g, 6.15 mmol) and THF (62 mL) were added to an oven-dried 100 mL round-bottom flask containing a magnetic stir bar. Magnetic stirring was initiated and *ortho*-tolylmagnesium chloride was then added drop-wise (7.40 mL, 7.40 mmol, 1.2 equiv., 1.0 M in THF) to the heterogeneous mixture, resulting in an immediate color change from red to orange. The reaction mixture was allowed to stir at room temperature for 2 h. The reaction mixture was subsequently treated with MeOH (5 mL) in air, and then was reduced to dryness *in vacuo*. The residue was treated with cold MeOH (0 ^{o}C, 15 mL), and the crude reaction mixture was then filtered through a glass frit, affording a retained orange solid that was washed with additional cold MeOH (0^{o}C, 3 x 10 mL), followed by pentane (3 x 50 mL). The orange solid on the frit was then dissolved via addition of CH_2Cl_2 (50 mL). Collection of the eluent followed by removal solvent afforded (**L18**)NiCl(*o*-tolyl), **C1**, as an orange solid (3.95 g, 93 % yield). The existence of a major and minor diastereomers (ca. 2:1) in

solution is suggested on the basis of $^{31}P\{^{1}H\}$ NMR data (*vide supra*). ^{1}H NMR: ($CDCl_3$, 500 MHz) 8.74 (m, 1H), 7.59-7.09 (m, 10H), 6.86-6.67 (m, 5H), 3.33-2.59 (m, 9H), 1.98-1.93 (m, 1H), 1.59-1.53 (m, 6H), 1.42 (s, 3H), 1.10- S8 0.92 (s, 6H). $^{13}C\{^{1}H\}$ NMR: ($CDCl_3$, 125.8 MHz) 145.9 (m), 145.8 (m), 143.4-143.2 (m), 136.7-133.1 (m), 132.0-130.9 (m), 129.6-128.6 (m), 126.3-125.8 (m), 124.7 (m), 123.8 (m), 122.7, 97.8-96.2 (m), 40.2-39.6 (m), 28.8-24.2 (m). $^{31}P\{^{1}H\}$ NMR: ($CDCl_3$, 202.5 MHz) 32.6 (d, *J* = 4.3 Hz, minor species), 31.5 (d, *J* = 4.6 Hz, major species), 27.6 (d, *J* = 4.6 Hz, major species), 26.5 (d, *J* = 4.3 Hz, minor species). On the basis of the observed positional disorder associated with the Ni-bound ortho-tolyl fragment within the X-ray structure of **C4**, arising from Ni-C(tolyl) bond rotation (80:20 occupancy ratio), we interpret the major and minor species as being rotamers of this type. Anal. Calcd for $C_{37}H_{41}ClNiO_3P_2$ C, 64.42; H, 5.99. Found: C, 64.11; H, 5.84. A single crystal suitable for X-ray diffraction analysis was prepared by slow evaporation of pentane into a solution of CH_2Cl_2 at room temperature.

2.8.4. Crystallographic Solution and Refinement Details

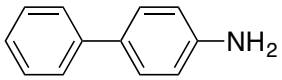
Crystallographic data for **C1**•$0.5C_5H_{12}$•$0.5C_4H_8O$ and [(**L18**)$NiCl_2$]•$0.5CH_2Cl_2$ were obtained at -100(±2) °C on a Bruker PLATFORM or D8/APEX II CCD diffractometer using graphite-monochromated Mo $K\alpha$ (λ = 0.71073 Å) radiation, employing samples that were mounted in inert oil and transferred to a cold gas stream on the diffractometer. Programs for diffractometer operation, data collection, and data reduction (including SAINT) were supplied by Bruker. Gaussian integration (face-indexed) was employed as the absorption correction method for **C1**, while multi-scan (TWINABS) was employed for (**L18**)$NiCl_2$. The structure of **C1** was solved by

use of intrinsic phasing methods, while (**L18**)$NiCl_2$ was solved by use of a Patterson/structure expansion; both were refined by use of full-matrix least-squares procedures (on F^2) with R_1 based on $F_o^2 \geq -2\sigma(F_o^2)$ and wR_2 based on $F_o^2 \geq -3\sigma(F_o^2)$. In the case of **C1**, attempts to refine peaks of residual electron density as disordered or partial-occupancy solvent pentane and/or tetrahydrofuran oxygen or carbon atoms were unsuccessful. The data were corrected for disordered electron density through use of the SQUEEZE procedure as implemented in PLATON. A total solvent-accessible void volume of 1666 $Å^3$ with a total electron count of 323 (consistent with 4 molecules of solvent pentane and 4 molecules of tetrahydrofuran, or 0.5 molecules each of pentane and tetrahydrofuran per formula unit of the Ni complex) was found in the unit cell. Positional disorder that was observed in the Ni-bound *ortho*-tolyl fragment during the solution and refinement of **C1** was modeled in a satisfactory manner (80:20 occupancy ratio); only the larger of these is discussed in the text. In the case of (**L18**)$NiCl_2$, the crystal used for data collection was found to display non-merohedral twinning. Both components of the twin were indexed with the program CELL_NOW (Bruker AXS Inc., Madison, WI, 2004). The second twin component can be related to the first component by 180º rotation about the [-0.2 -0.25 1] axis in real space and about the [0 0 1] axis in reciprocal space. Integrated intensities for the reflections from the two components were written into a SHELXL-2014 HKLF 5 reflection file with the data integration program SAINT (version 8.34A), using all reflection data (exactly overlapped, partially overlapped and non-overlapped). The refined value of the twin fraction (SHELXL- 2014 BASF parameter) was 0.4855(13). Furthermore, in the case of (**L18**)$NiCl_2$ attempts to refine peaks of residual electron density as disordered or

partial-occupancy solvent dichloromethane chlorine or carbon atoms were unsuccessful. The data were corrected for disordered electron density through use of the SQUEEZE procedure as implemented in PLATON. A total solvent-accessible void volume of 156.7 Å 3 with a total electron count of 39 (consistent with one molecule of solvent dichloromethane, or one-half molecule of CH_2Cl_2 per formula unit of the Ni complex molecule) was found in the unit cell. Anisotropic displacement parameters were employed for all the non-hydrogen atoms. In all cases non-hydrogen atoms are represented by Gaussian ellipsoids at the 30% probability level. Additional crystallographic information is provided in the accompanying CIFs (CCDC 1403891 and 1403892).

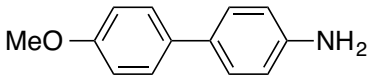
2.8.5. Characterization Data for Isolated Reaction Products

4-phenylaniline (2.4)



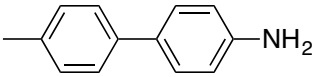
Following **GP2-1 (110 °C)**: Purified by column chromatography on SiO_2 (10:1, hexanes/EtOAc) to yield **2.4** as a beige yellow solid in 63% yield from the corresponding bromide. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.58-7.56 (m, 2H), 7.46-7.40 (m, 4H), 7.32-7.28 (m, 1H), 6.80-6.77 (m, 2H), 3.72 (br s, 2H), 2.41; ^{13}C{ ^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 145.8, 141.2, 131.6, 128.7, 128.0, 126.4, 126.3, 115.4. Agrees with data previously reported in the literature.[84]

4'-methoxybiphenyl-4-amine (2.5)



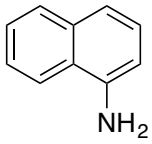
Following **GP2-1 (110°C)**: Purified by column chromatography on SiO_2 (5:1, hexanes/EtOAc) to yield **2.5** as a yellow solid in 86% yield from the corresponding chloride. ^1H NMR (500 MHz, $CDCl_3$): δ 7.50-7.48 (m, 2H), 7.40-7.39 (m, 2H), 6.99-6.97 (m, 2H), 6.79-6.78 (m, 2H), 3.87 (s, 3H), 3.73 (br s, 2H); $^{13}C\{^1H\}$ NMR (125.8 MHz, $CDCl_3$): δ 158.7, 145.5, 134.1, 131.6, 127.8, 127.6, 115.7, 114.3, 55.6. Agrees with data previously reported in the literature.[84]

4'-methylbiphenyl-4-amine (2.6)



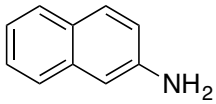
Following **GP2-1 (110°C)**: Purified by column chromatography on SiO_2 (5:1, hexanes/EtOAc) to yield **2.6** as a yellow solid in 78% yield from the corresponding chloride. ^1H NMR (500 MHz, $CDCl_3$): δ 7.48-7.43 (m, 4H), 7.29-7.24 (m, 2H), 6.79-6.78 (m, 2H), 3.76 (br s, 2H), 2.41 (s, 3H); $^{13}C\{^1H\}$ NMR (125.8 MHz, $CDCl_3$): δ 145.8, 138.5, 136.1, 131.9, 129.7, 128.0, 126.49, 115.63, 21.2, Agrees with data previously reported in the literature.[84]

Naphthalen-1-amine (2.7)



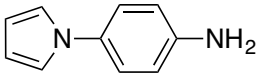
Following **GP2-1 (25°C)**: Purified by column chromatography on SiO_2 (10:1, hexanes/EtOAc) to yield **2.7** as a purple solid from the corresponding halide. ^1H NMR (500 MHz, $CDCl_3$): δ 7.88-7.84 (m, 2H), 7.51-7.49 (m, 2H), 7.36-7.29(m, 2H), 6.82 (dd, *J* = 1.4 Hz, 1H), 4,17 (br s, 2H); $^{13}C\{^1H\}$ NMR (125.8 MHz, $CDCl_3$): δ 142.25, 134.62, 128.76, 126.52, 126.04, 125.06, 123.89, 120.98, 109.102. Agrees with data previously reported in the literature.[84]

Naphthalen-2-amine (2.8)



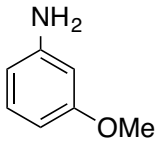
Following **GP2-1 (25°C)**: Purified by column chromatography on SiO_2 (5:1, hexanes/EtOAc) to yield **2.8** as a purple solid in 76% yield from the corresponding tosylate. ^1H NMR (300 MHz, $CDCl_3$): δ 7.77-7.67 (m, 2H), 7.62-7.59 (d, 1H), 7.40-7.36 (m, 1H), 7.26-7.24 (m, 1H), 7.0-6.95 (m, 2H), 3.84 (br s, 2H); $^{13}C\{^1H\}$ NMR (125.8 MHz, $CDCl_3$): δ 144.27, 135.14, 129.42, 127.92, 126.55, 126.01, 122.70, 118.45, 108.85. Agrees with data previously reported in the literature.[53]

4-(1H-pyrrol-1yl)aniline, (2.9)



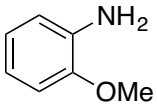
Following **GP2-1 (110°C)**: Purified by column chromatography on SiO_2 (10:1, hexanes/EtOAc) to yield **2.9** as a light brown solid in 76% yield from the corresponding chloride. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.23-7.22 (m, 2H), 7.02 (t, *J* = 2.1 Hz, 2H), 6.77-6.75 (m, 2H), 6.35 (t, *J* = 2.1 Hz, 2H), 3.76 (br s, 2H); ^{13}C{ ^{1}H} NMR (125.8 MHz, $CDCl_3$): δ 144.7, 133.1, 122.6, 119.9, 115.9, 109.7. Agrees with data previously reported in the literature.[84]

3-anisidine (2.10)



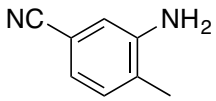
Following **GP2-1 (110°C)**: Purified by extraction with 1.0 M $HCl_{(aq)}$. The title compound **2.10** was isolated as a brown oil in 66% yield from the corresponding chloride and in 71% yield from the corresponding bromide. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.12-7.09 (m, 1H), 6.39-6.33 (m, 2H), 6.29 (s, 1H), 3.80 (s, 3H), 3.74 (br s, 2H); ^{13}C{ ^{1}H} NMR (125.8 MHz, $CDCl_3$): δ 160.9, 147.7, 130.3, 108.3, 104.4, 101.4, 55.3. Agrees with data previously reported in the literature.[147]

2-anisidine (2.11)



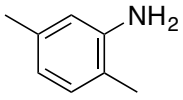
Following **GP2-1 (110°C)**: Purified by extraction with 1.0 M $HCl_{(aq)}$. The title compound **2.11** was isolated as a brown oil in 81% yield from the corresponding chloride. ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.85-6.76 (m, 4H), 3.96 (br s, 2H), 3.89 (s, 3H); $^{13}C\{^{1}H\}$ NMR (125.8 MHz, $CDCl_3$): δ 147.6, 136.2, 121.3, 118.8, 115.3, 110.7, 55.8. Agrees with data previously reported in the literature.[53]

3-amino-4-methylbenzonitrile (2.12)



Following **GP2-1 (25°C)**: Purified by extraction with 1.0 M $HCl_{(aq)}$. The title compound **2.12** was isolated as a solid in 70% yield from the corresponding bromide. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.14-7.12 (d, *J* = 7.5 Hz, 1H), 7.01-7.00 (d, *J* = 1.2 Hz, 1H), 6.93 (s, 1H), 3.82 (br s, 2H), 2.22 (s, 3H); $^{13}C\{^{1}H\}$ NMR (125.8 MHz, $CDCl_3$): δ 145.2, 131.3, 127.9, 122.5, 119.6, 117.5, 110.6, 17.9. Agrees with commercial source (CAS: 60710-80-7).

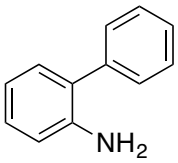
2,5-dimethylaniline (2.13)



Following **GP2-1 (25°C)**: Purified by column chromatography on SiO_2 (10:1, hexanes/EtOAc) to yield **2.13** as a colorless oil in 89% yield from the corresponding chloride and in 78% yield from the corresponding bromide. ^{1}H NMR (500 MHz,

$CDCl_3$): δ 7.02-7.00 (d, *J* = 7.5 Hz, 1H), 6.62-6.60 (d, *J* = 8 Hz, 1H), 6.57 (s, 1H), 3.61 (br s, 2H), 2.33 (s, 3H), 2.20 (s, 3H); $^{13}C\{^{1}H\}$ NMR (125.8 MHz, $CDCl_3$): δ 144.6, 136.8, 130.5, 119.5, 115.9, 21.2, 17.0. Agrees with data previously reported in the literature.[53]

[1,1'-Biphenyl]-2-amine (2.14)



Following **GP2-1 (25°C)**: Purified by column chromatography on SiO_2 (10:1, hexanes/EtOAc) to yield **2.14** as a solid in 83% yield from the corresponding bromide. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.48-7.47 (m, 4H), 7.39-7.33 (m, 1H), 7.19-7.14 (m, 2H), 6.85 (td, *J* = 7.4, 1.1 Hz, 1H), 6.79 (d, *J* = 7.9 Hz, 1H), 3.78 (br s, 2H); $^{13}C\{^{1}H\}$ NMR (125.8 MHz, $CDCl_3$): δ 143.71, 139.76, 130.66, 129.30, 129.01, 128.69, 127.86, 127.36, 118.85, 115.80. Agrees with data previously reported in the literature.[71]

Chapter 3

Nickel-Catalyzed N-Arylation of Primary Amides and Lactams

3.1. RESEARCH OVERVIEW AND CONTRIBUTION REPORT

This author wishes to clarify his contributions to the research described in Chapter 3 of this Thesis document. This chapter describes the development of the first nickel-catalyzed *N*-arylation of amides with (hetero)aryl (pseudo)halides, which was enabled by use of the air-stable pre-catalyst (PAd-DalPhos)NiCl(o-tolyl) (**C1**). A range of structurally diverse primary amides and lactams were cross-coupled successfully with activated (hetero)aryl chloride, bromide, triflate, tosylate, mesylate, and sulfamate electrophiles.

My contribution to this study includes: initial discovery, ancillary ligand screening, control reactions, initial optimization, isolation of reaction products derived from cross-couplings involving primary amides and aryl chlorides and bromides, characterization of compounds reported herein, and writing the majority of the manuscript. This project was conducted in collaboration with Preston M.

MacQueen, who contributed the following: optimization of reaction conditions involving pseudohalide coupling partners; isolation of reaction products derived from cross-couplings involving primary amides and lactams with aryl pseudohalides; characterization of isolated reaction products; and writing of the manuscript section involving the use lactams as coupling partners. Where appropriate, the specific contributions of each author are stated explicitly in the text. This work has been published in Chemistry – A European Journal.

Reference: Lavoie, C.M.; MacQueen, P.M.; M.J.; Stradiotto, M., Nickel-Catalyzed *N*-Arylation of Primary Amides and Lactams with Activated (Hetero)aryl Electrophiles. *Chem*. *Eur*. *J*. **2016**, *22*, 18572-18575.

3.2. INTRODUCTION

3.2.1. Palladium Catalyzed C-N Cross-coupling Involving Amides

The prevalence of amides in biologically active molecules (e.g., those depicted in Fig. 3-1[148]) and functional materials[149] has inspired the development of efficient synthetic routes to such compounds, including metal-catalyzed protocols.[150-154] In this context, the Pd-catalyzed intermolecular C*(sp*^{2})-N cross-coupling of amides and (hetero)aryl electrophiles, initially reported by Shakespeare[155] and shortly thereafter expanded by Yin and Buchwald,[156] has emerged as a useful protocol for the assembly of *N*-aryl amides.[154, 157-161] Advances in ancillary ligand design[36] have facilitated the evolution of Pd-catalyzed amide *N*-arylation, whereby state-of-the-art Pd-catalysts can enable C*(sp*^{2})-N cross-couplings between a range of (hetero)aryl electrophiles including chlorides and phenol-derived sulfonates,[44, 162-166] with both primary[44, 156, 163, 165-167] and

secondary amides[156, 164, 168] as well as related nucleophiles including sulfonamides, lactams, carbamates, ureas, and others.[44, 155, 156, 163, 164, 166, 168-171] Notably, the Pd-catalyzed C(sp^2)-N cross-coupling of amides, relative to other amines, has proven challenging, owing in part to the weakly nucleophilic nature of amides, along with their tendency to bind in a κ^2-N,O fashion to Pd,[172, 173] thus inhibiting C-N reductive elimination.

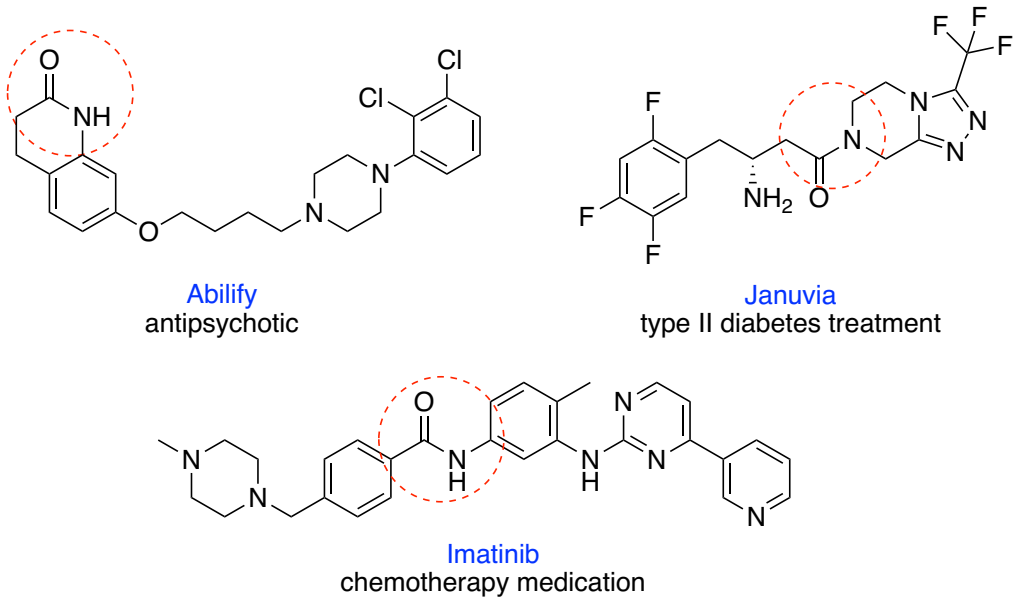


Figure 3-1. Examples of pharmaceutical compounds containing amide functionality

3.2.2. Overview of Nickel Catalyzed Cross-coupling Involving Amides

Notwithstanding the utility of Pd-based cross-coupling methods, both cost and supply limitations provide motivation for the development of cross-coupling protocols that utilize non-precious metals.[174] Cu catalysis is the most established in this regard,[62] with a number of synthetically useful protocols[175-182] having been developed since the pioneering report by Goldberg.[183] Nonetheless, the frequent inability of Cu-catalysts to accommodate (hetero)aryl chlorides and phenol-derived

electrophiles remains a significant limitation. The use of Fe-based catalysts in amide *N*-arylation chemistry has been limited to reactions of aryl iodides at elevated temperatures (≥ 130 ˚C).[184, 185]

Conversely, Ni-based catalysts have proven to be exceptionally competent in C*(sp*^{2})-N cross-coupling chemistry,[186, 187] in some cases out-performing state-of-the-art Pd catalysts in transformations of (hetero)aryl chlorides.[102] Moreover, the use of Ni-based catalysts in C*(sp*^{2})-N cross-coupling chemistry has enabled the application of an array of phenol-derived electrophiles that are typically challenging for Pd-based catalysts, including sulfamates, carbamates, ethers, and mesylates.[83, 102, 112, 114, 126, 188, 189] Despite such progress, *the Ni-catalyzed N-arylation of amides with (hetero)aryl electrophiles is unknown*. This is despite work by Garg,[190-194] Szostak,[195, 196] and Shi,[197] who have disclosed a remarkable class of Ni-catalyzed transformations, whereby 'twisted' amide reagents undergo C-N oxidative addition followed by substitution at the acyl carbon to furnish a range of products including esters,[190] biaryls,[195] organoboronates,[197] ketones,[191, 192] and amides[193, 194] (Fig. 3-2A-C).

Recently our group reported[102] on the synthesis and application of an air-stable nickel pre-catalyst (PAd-DalPhos)NiCl(*o*-tolyl) (**C1**), which enabled the first examples of room-temperature Ni-catalyzed arylations of primary alkylamines and ammonia in combination with an unprecedented scope of (hetero)aryl electrophiles. Notably, more acidic NH reagents such as indole and carbazole were also viable coupling partners, giving rise to a scope of nucleophilic partners that span over 20 orders of magnitude in terms of NH acidity. Intrigued by i) the capacity of pre-catalyst **C1** to selectively arylate NH nucleophiles covering a wide pKa range and ii)

the orthogonal ideal ancillary ligand characteristics for enabling Pd-catalyzed amidations (sterically demanding, bidentate), and un-desirable Ni-catalyzed amide N-C oxidative additions (electron-rich, monodendate), I began probing for the competency of pre-catalyst **C1** to catalyze *N*-arylations of amides, whose typical pKa's fall into the range of viable NH reagents for *N*-arylation by **C1**. Disclosed herein is the first Ni-catalyzed *N*-arylation of amides with (hetero)aryl (pseudo)halides (Fig. 3-2D), which is enabled by use of the pre-catalyst (PAd-DalPhos)NiCl(*o*-tolyl) (**C1**).

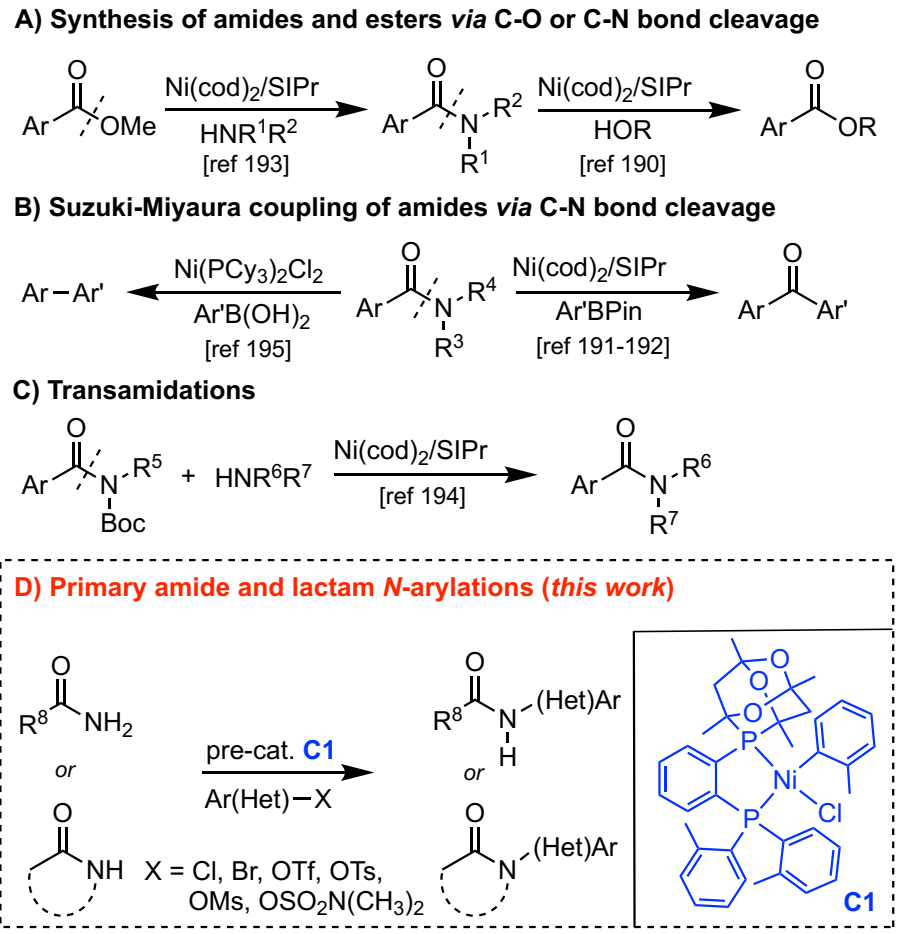


Figure 3-2. Selected Ni-catalyzed transformations of amides (A–C), and the new Ni-catalyzed C(*sp*^{2})-N cross-coupling of amides or lactams with (hetero) aryl electrophiles (D) reported here.

3.3. RESULTS AND DISCUSSION

3.3.1. Ancillary Ligand Screening

I commenced by examining the cross-coupling of benzamide (**3.1**) and 4-chlorobenzonitrile (**3.2**) using a selection of commercially available phosphine and NHC ancillary ligands with $Ni(cod)_2$ (Fig. 3-3). I initially targeted ligands that proved successful in the Pd-catalyzed C*(sp*^{2})-N cross-coupling of amides, including BippyPhos (**L5**),[44] XantPhos (**L6**),[168] dppf (**L8**),[155] and JackiePhos (**L30**);[164] notably, **L8** is also effective in the Ni-catalyzed *N*-arylation of secondary amines and anilines.[186] Moderate conversion to the target product (**2a**) was observed when using the bisphosphines XantPhos and dppf and negligible conversion was achieved with the monophosphines JackiePhos and BippyPhos. The poor performance of these ligands reaffirms the notion that re-purposing ancillary ligands that function well with Pd is not a universal strategy for establishing effective Ni-based cross-coupling protocols.[102]

I then turned my attention to the application of other ancillary ligands that have proven effective in Ni-catalyzed C*(sp*^{2})-N cross-couplings involving alternative nucleophile classes. Whereas each of *rac*-BINAP (**L13**)[69] and SIPr (**L31**)[113, 114] performed poorly, both JosiPhos (CyPF-Cy) (**L15**)[84, 85] and PAd-DalPhos (**L18**)[102] afforded high conversion to **3.3**. In an effort to differentiate the catalytic abilities of **L15** and **L18**, I examined the cross-coupling of nicotinamide and 1-chloronapthalene (see the Experimental Section **3.6.1**), employing air-stable pre-catalysts (**L**)NiCl(*o*-tolyl) (**L** = **L18**, **C1;**[102] **L** = **L15**, **C2**[92]),[139] which out-perform related $Ni(cod)_2$/**L** mixtures in ammonia monoarylation. Whereas negligible conversion was achieved with **C2**, high conversion to the target cross-coupling

product **3.7** was realized by use of **C1** (10 mol % Ni). In using **C1**, products **3.3** and **3.7** were isolated in 82% and 80% yield, respectively (Fig. 3-4).

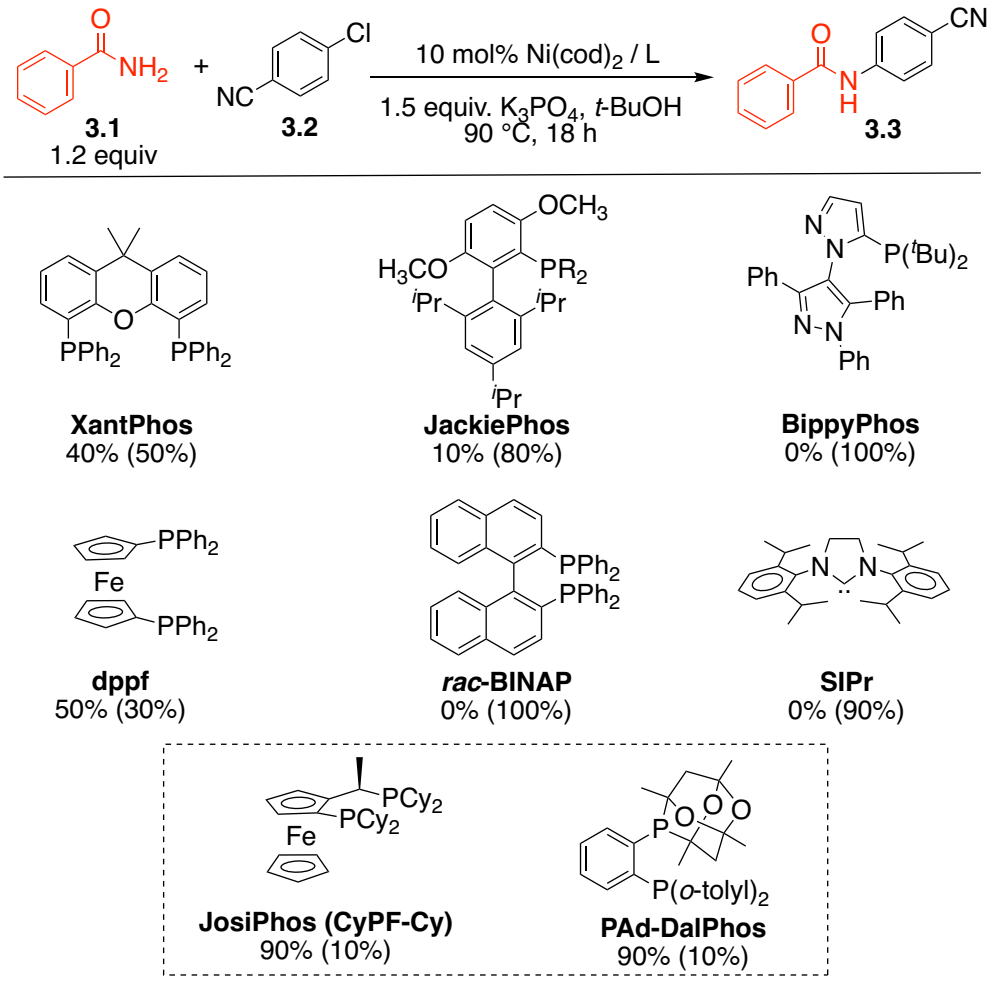


Figure 3-3. Ligand screen for the Ni-catalyzed N-arylation of benzamide (**3.1**) with 4-chlorobenzonitrile (**3.2**). Conversions estimated on the basis of GC data, reported as % **3.3** (% **3.2** remaining); mass balance attributable to unidentified products. For JackiePhos, R = 3,5-bis(trifluoromethyl)phenyl.

3.3.2. Optimization of Reaction Conditions

Preliminary investigations indicated that a 5-10 mol % loading of **C1** relative to the limiting reagent was sufficient to enable suitable conversion of starting material into product when reactions were conducted at 90 °C for 16-20 hours

(unoptimized); reactions conducted at lower loadings and/or temperatures resulted in significant decrease in catalyst performance. Gratifyingly, high levels of starting material conversion can be obtained when employing 1.0–1.1 equivalents of the amide reagent, and the majority of reaction products featured in Figure 3-4 could be accessed through the use of a single equivalent of amide. Several solvent/base combinations were found to be useful (i.e., toluene/NaO-*t*-Bu, 1,4-dioxane/Cs_2CO_3, and *t*-BuOH/K_3PO_4) which allowed for conditions to be optimized. Substrate concentration proved to be a key reaction parameter,[168] and it was found that substrate concentrations of 0.06 to 0.24 M are most effective for amidations catalyzed by **C1**.

For operational convenience the cross-couplings reported herein using **C1** were conducted using a glovebox. However, control experiments confirmed that the use of such inert-atmosphere apparatus *is not required*. High conversion (>80%) to **3.3** was achieved when the reaction components (including **C1**) were added in air to a glass vial that was subsequently sparged with argon gas, and sealed with a PTFE cap prior to heating. The potential scalability of our C*(sp*^{2})-N cross-coupling of amides and (hetero)aryl electrophiles using **C1** (5 mol %) was demonstrated via the gram-scale coupling of **3.1** and **3.2** (6.75 mmol) to afford **3.3** (1.14 g, 76% isolated yield).

3.3.3. Scope of Reaction Products Generated using C1

Having identified standard conditions for **C1**-mediated C*(sp*^{2})-N cross-coupling of amides and aryl chlorides, we then sought to explore the scope of reactivity. A range of functionalized (hetero)aryl (pseudo)halides (X = Cl, Br, OTf,

OTs, OMs, $OSO_2N(CH_3)_2$) were successfully cross-coupled with structurally diverse primary amides and lactams in synthetically useful yields using **C1** (Fig. 3-4); note, this author worked exclusively with (hetero)aryl chlorides and bromides with primary amides. Parent benzamide, electron-rich 4-methoxybenzamide, and electron-poor 3,5-bis(trifluoromethyl)benzamide, were successful reaction partners, as were nicotinamide and isonicotinamide, affording **3.3-3.7**. The smaller nucleophiles acetamide and acrylamide were also suitable reagents, undergoing *N*-arylations with 6-chloroquinoxaline to afford **3.8-3.9**. The heterocyclic amides 2-thiophene carboxamide and 2-furamide proved to be effective coupling partners in combination with heterocyclic electrophiles (isoquinoline, quinaldine, and 4,6-dimethoxypyrimidine derivatives) leading to **3.10**, **3.11**, and **3.14**. The ability of **C1** to tolerate ketone functionality and *ortho*-methyl substitution on the electrophile was demonstrated in formation of **3.12-3.13**. The primary alkyl amides cyclopropanecarboxamide and cyclohexanecarboxamide also proved compatible, whereby cross-couplings employing 2-chloro-4,6-dimethoxypyrimidine[159] afforded **3.15** and **3.16**. Throughout, the use of **C1** proved tolerant to fragments that are susceptible to Ni-mediated bond activation (e.g., nitrile, ketones, ether groups).[83, 112, 198-201]

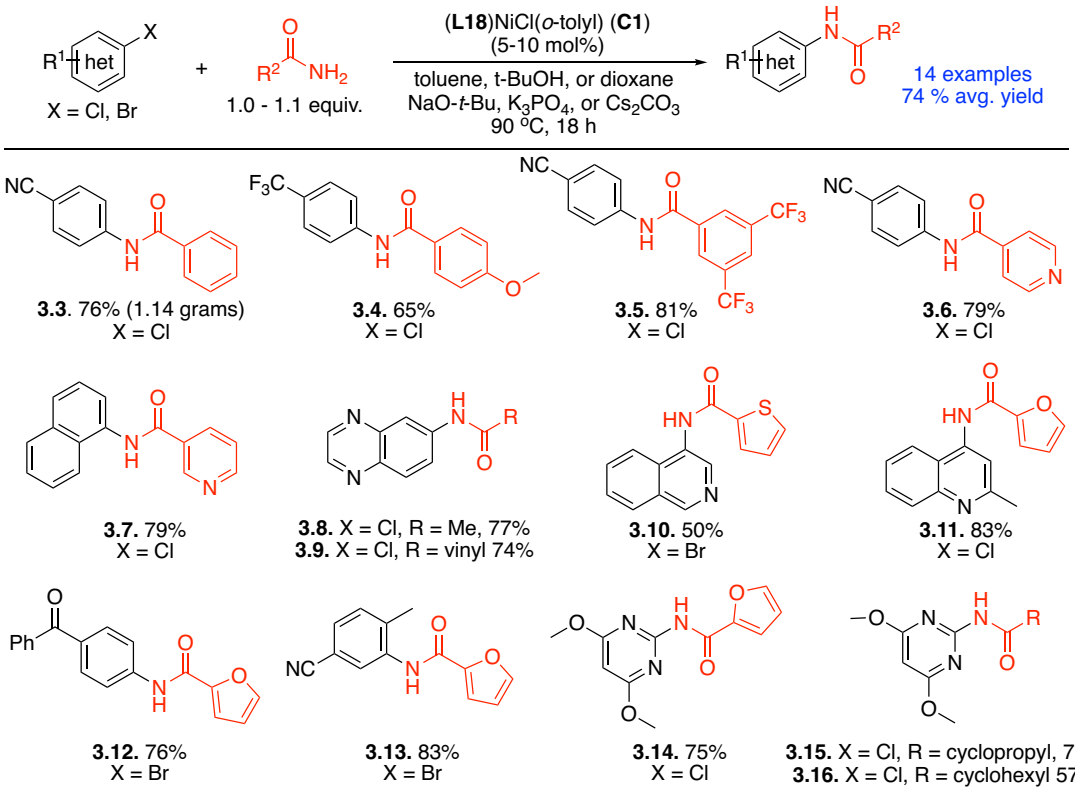
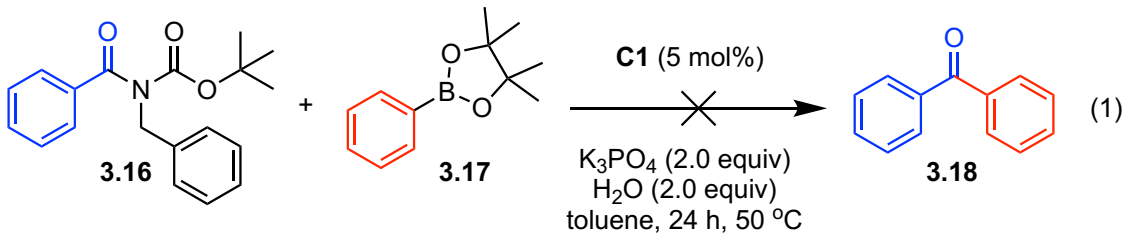


Figure 3-4. Scope of Ni-catalyzed *N*-arylation of primary amides and sulfonamides with (hetero)aryl halides (yields of isolated products reported). [1] = 5 mol % **C1**. [2] = 10 mol % **C1**. [a] X = Cl. [b] X = Br. See Experimental Section **3.3.2** for details regarding solvent, base and substrate concentration used for specific cross-couplings.

Other distinguishing facets of the above-mentioned methodology warrant further commentary. Notably, while acyclic secondary amides were not effective substrates, coworker Preston MacQueen was able to demonstrate that cyclic lactams of various ring sizes (*n* = 4-7) can be efficiently *N*-arylated by **C1** with structurally diverse (pseudo)halides. This includes a chiral enantiopure oxazolidinone – a commonly used Evans auxiliary, which did not undergo racemization during cross-coupling.

3.3.4. Control Experiments Probing for Potential C-N Bond Cleavage

The potential for **C1** to undergo unwanted insertion into amide C-N bonds (Fig. 3-2A-C) was probed. In examining the cross-coupling reaction between the (*N*-Boc)-activated amide **3.16** and PhBPin (**3.17**) under conditions whereby Ni(cod)$_2$/**L31** mixtures afford benzophenone (**3.18**),[191] negligible conversion of the starting materials was achieved when using **C1** as a catalyst (Eq. 3-1). This result, when considered alongside the poor catalytic performance of Ni(cod)$_2$/**L31** in the cross-coupling of **3.1** and **3.2** (Fig. 3-3), suggests that ancillary ligand characteristics that facilitate the oxidative addition of amide C-N bonds are divergent from those needed to enable the *N*-arylation of amides with (hetero)aryl (pseudo)halides.



3.4. INEFFECTIVE APPLICATIONS OF THE DEVELOPED METHODOLOGY

Several limitations of the previously described **L18**/Ni catalyst system warrant further discussion. Whereas activated (pseudo)halide electrophiles (e.g., 4-chlorobenzonitrile) could be efficiently amidated under standard conditions, deactivated (pseudo)halide partners (e.g., 4-chloroanisole) could not be tolerated even under more forcing conditions (e.g., 15 mol % **C1**, 110 °C). It is possible that oxidative addition complexes of the type (**L**)Ni(aryl)X derived from deactivated electrophiles, are not sufficiently electrophilic to promote coordination of weakly

nucleophilic amides under reaction conditions scrutinized herein. In support of this claim, Buchwald and coworkers[164] have demonstrated for mechanistically related Pd-catalyzed amidations involving secondary amides, that the use of an electron-deficient ligand is critical for facilitating rate-limiting amide binding to (**L**)Pd(aryl)X intermediates.

A number of ineffective amide coupling partners were encountered in reactions involving **C1** (Fig. 3-5). Whereas benzamide could be efficiently *N*-arylated under standard conditions (e.g., **3.3** in Fig. 3-4), its sulfur containing analogue thiobenzamide was not tolerated under any examined conditions (e.g., **3.20** in Fig. 3-5). It is possible that thiobenzamide deactivates **C1** through formation of unreactive N,S-chelates; Ni(II) coordination complexes based on thiobenzamide are known.[202] Other ineffective coupling partners include formamide (**3.21**), and trifluoroacetamide (**3.22**), despite their structurally similarity to the highly effective substrate acetamide. The electron-withdrawing trifluromethyl (CF_3) groups on acetamide presumably decrease its nucleophilicity by such an extent that binding to Ni is not favored under the examined reaction conditions.

Other limitations encountered in this chemistry when using **C1** include the use of acyclic secondary amide reaction partners (e.g., **3.23**-**3.26**). Notably however, secondary amides such as *N*-methylbenzamide do not poison **C1**, as evidenced by the uninhibited cross-coupling of **3.1** and **3.2** to give **3.3** when conducted in the presence of *N*-methylbenzamide (1 equiv. vs. **3.1**). Whereas a number of catalysts based on Pd are known to effect primary amide *N*-arylations (*vide supra*), analogous cross-couplings involving secondary amides are rare,[156, 164, 168] and require relatively forcing conditions. This is likely attributed to the

increased size of secondary amides along with their relatively low nuclephilicity, both of which inhibit amide binding. Addressing the aforementioned challenges necessitated significant tailoring of both the ligand structure and reaction conditions for the development of Pd-driven secondary amide *N*-arylations. For example, Buchwald and coworkers[164] achieved the first Pd-catalyzed C-N cross-coupling of aryl (pseudo)halides with secondary acylic amides through a combination of modifications to primary amide arylation protocols, including: i) the use of aryl triflates to generate cationic Pd(II) intermediates sufficiently electrophilic enough to encourage amide binding; ii) employing electronic-deficient ligands to facilitate amide binding; iii) the use of a gross excess of amide reagent; and iv) the use of high reaction temperatures (130 ^{o}C). It is anticipated that achieving a general protocol for Ni-catalyzed *N*-arylations of secondary amides will require a similarly intensive investigation into the reaction components. A proposal for future work in this regard is featured in Chapter 6 of this Thesis.

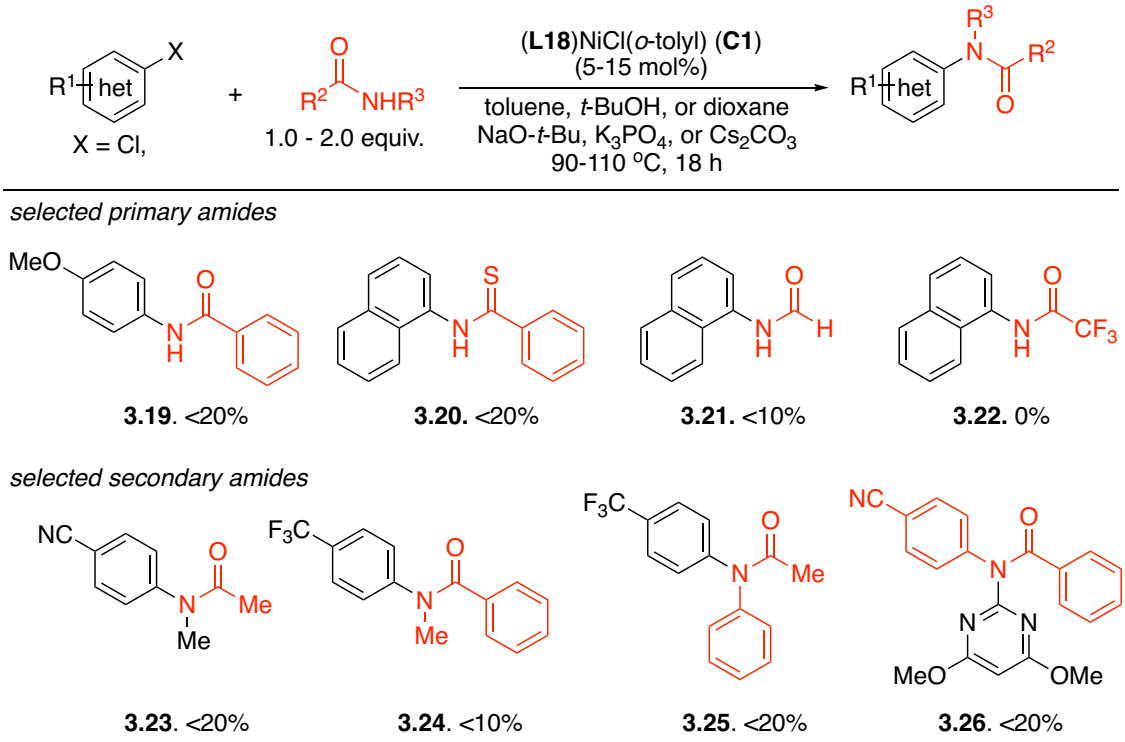


Figure 3-5. Examples of low yielding amidation products using **C1**. Reactions were conducted employing **C1** (10-15 mol %), 1.5 equiv. of base, 1-2 equiv. of amide) at 90-110 ˚C for 18 h (un-optimized), with yields on the basis of GC data reported.

3.5. SUMMARY

In summary, we have established the first Ni-catalyzed C(sp^2)-N cross-coupling of amides and (hetero)aryl (pseudo)halides by use of the pre-catalyst **C1**. Structurally diverse primary amides and lactams were cross-coupled with an unprecedented scope of (hetero)aryl halide, sulfonate, and sulfamate electrophiles, relative to any previously reported catalyst system (i.e., Pd, Cu, or other). In addition to complementing the diverse chemistry emerging from the activation and functionalization of amides by use of Ni catalysis, the results herein contribute toward the development of base-metal catalysts to supplant precious metal catalysts in synthetically useful C-N bond-forming chemistry.

3.6. EXPERIMENTAL

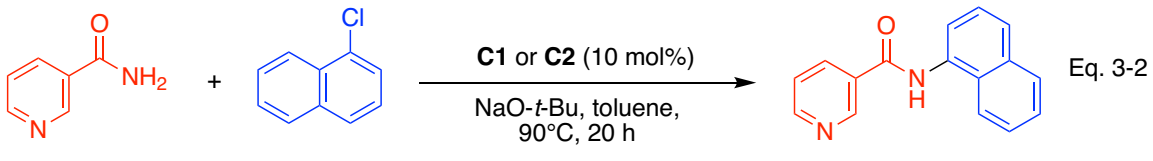
3.6.1. General Considerations and Procedures

General Information. All reactions were set up inside a nitrogen-filled, inert atmosphere glovebox (unless otherwise indicated) and isolated under standard benchtop conditions. Toluene used in the glovebox was deoxygenated by purging with dinitrogen followed by passage through a double column solvent purification system equipped with one alumina-packed column and one column packed with copper-Q5 reactant. 1,4-Dioxane used in the glovebox was deoxygenated by purging with nitrogen followed by storage over activated 4 Å molecular sieves for 48 h. *tert*-butanol was dried over CaH_2 followed by distillation under an atmosphere of dinitrogen. All solvents used within the glovebox were stored over activated 4 Å molecular sieves. Pre-catalysts **C1** and **C2** were synthesized following literature procedures.[92, 102] *tert*-Butyl benzoyl(benzyl)carbamate was synthesized following a literature procedure.[203] Otherwise chemicals were obtained from commercial sources and were used as-received. Flash column chromatography was performed on silica gel (SiliaFlash P60, Silicycle) or using neutral alumina (150 mesh; Brockmann-III; activated), as indicated. All ^{1}H NMR (500.1 MHz or 300.1 MHz) and ^{13}C NMR (125.8 MHz or 75.4 MHz) spectra were recorded at 300 K. Chemical shifts are expressed in parts per million (ppm) using the solvent signal CD_3CN (^{1}H 1.94 ppm, ^{13}C 1.32 and 118.3 ppm) or DMSO-d_6 (^{1}H 2.50 ppm, ^{13}C 39.5 ppm) as an internal reference. Splitting patterns are indicated as follows: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublets. All coupling constants (*J*) are reported in Hertz (Hz). In some cases, fewer than expected independent carbon resonances were observed despite prolonged

acquisition times. Mass spectra were obtained using ion trap (ESI) instruments operating in positive mode and GC data were obtained on an instrument equipped with a SGE BP-5, 30 m, 0.25 mm i.d. column. The accompanying NMR spectra for the reported compounds in this chapter can be found in Appendix A of this document.

General Procedure for Commercial Ligand Reaction Screening (GP3-1). In a nitrogen-filled glovebox, $Ni(cod)_2$ (3.3 mg, 0.012 mmol, 0.1 equiv), ligand (0.012 mmol, 0.1 equiv), 4-chlorobenzonitrile (**3.2**) (16.5 mg, 0.12 mmol, 1.0 equiv), K_3PO_4 (38.2 mg, 0.18 mmol, 1.50 equiv), and benzamide (**3.1**) (17.4 mg, 0.14 mmol, 1.2 equiv) were added to a screw capped vial containing a magnetic stir bar, followed by the addition of *tert*-butanol (1.0 mL). The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 90°C for 18 h with magnetic stirring. GC analysis of reaction aliquots was used to estimate starting material conversions and percentage of product.

Nicotinamide/1-Chloronaphthalene Competition Involving C1 and C2



3.27 **3.28** **3.7**

(**L18**)NiCl(*o*-tolyl), **C1**: 90% (0% **3.27**))
(**L15**)NiCl(*o*-tolyl), **C2**: 0% (100% **3.27**)

Eq. 3-2

In a nitrogen-filled glovebox, pre-catalyst **C1** (8.2 mg, 0.012 mmol, 0.10 equiv.) or **C2** (9.5 mg, 0.012 mmol, 0.10 equiv.), NaO-*t*-Bu (0.0173 g, 0.18 mmol, 1.5 equiv.),

nicotinamide, (**3.27)** (0.0146 g, 0.12 mmol, 1.0 equiv.), and 1-chloronaphthalene (**3.28**) (16.3 µL, 0.12 mmol, 1.0 equiv.) were added to a screw capped vial containing a magnetic stir bar, followed by the addition of toluene (2 mL). The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 90 °C for 20 h with magnetic stirring. The vial was then removed from the heating block and left to cool to ambient temperature. GC analysis of reaction aliquots was used to estimate starting material conversions and percentage of product.

Representative Procedure for Suzuki-Miyaura Coupling Using C1. In a nitrogen-filled glovebox, pre-catalyst **C1** (8.2 mg, 0.012 mmol, 0.05 equiv.), *tert*-butyl benzoyl(benzyl)carbamate (74.8 mg, 0.24 mmol, 1.0 equiv.), PhBPin (122.0 mg, 0.60 mmol, 2.5 equiv), K_3PO_4 (101.8 mg, 0.48 mmol, 2.0 equiv.), and 1,3,5-trimethoxybenzene (as an internal standard; 12.1 mg, 0.072 mmol, 0.3 equiv.) were added to a screw capped vial containing a magnetic stir bar, followed by the addition of toluene (0.24 mL). The vial was sealed with a cap containing a PTFE septum, removed from the glovebox, followed by the addition of degassed water (8.6 µL, 0.400 mmol, 2.0 equiv.). The vial was placed in a temperature-controlled aluminum heating block set to 50 °C for 24 h with magnetic stirring. After cooling to room-temperature, the reaction mixture was diluted with hexanes (1.0 mL) and filtered over a plug of silica gel eluting with ethyl acetate (10 mL). The eluent was collected and the volatiles were removed *in vacuo*; the yield of benzophenone was determined by ^{1}H NMR analysis using 1,3,5-trimethoxybenzene as an internal standard. ^{1}H NMR analysis revealed only starting materials present and no

formation of the benzophenone Suzuki-Miyaura coupling product.

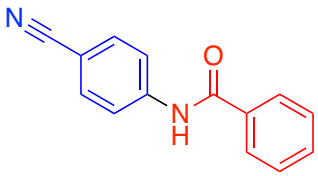
General Procedure for the *N*-Arylation of Primary Amides with Aryl Halides (GP3-2). In a nitrogen-filled glovebox, pre-catalyst **C1** (5-10 mol %), aryl halide (1.0 equiv.), base (1.5 equiv.), and amide or lactam (1.0-1.1 equiv.) were added to a screw capped vial containing a magnetic stir bar, followed by the addition of either toluene, 1,4-dioxane or *tert*-butanol. The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 90°C for 18 h with magnetic stirring. The vial was then removed from the heating block and left to cool to ambient temperature. The crude reaction mixture was then filtered through a short Celite/SiO_2 plug (5:1 v/v) eluting with ethyl acetate, and the volatile materials were evaporated *in vacuo*. Unless stated otherwise, the crude product was purified by flash-column chromatography to afford the purified product.

Gram-scale coupling protocol. In a nitrogen-filled glovebox, a 300 mL Schlenk flask was charged with a magnetic stir bar, **C1** (0.233 g, 0.338 mmol, 0.05 equiv.), K_3PO_4 (2.15 g, 10.1 mmol, 1.5 equiv.), benzamide (0.900 g, 7.43 mmol, 1.1 equiv.), and 4-chlorobenzonitrile (0.930 g, 6.75 mmol, 1.0 equiv.) followed by the addition of *tert*-butanol (56 mL). The reaction flask was sealed with a SubaSeal rubber septa, removed from the glovebox and placed in an oil bath set to 90 °C. The flask was equipped with a reflux condenser, and magnetic stirring was initiated. After 18 h, the reaction was allowed to cool to room-temperature, followed by passage of the crude reaction through a Celite/silica plug (1/5: v/v) eluting with ethyl acetate (300 mL); the collected eluent was concentrated by use of a rotary evaporator. The

residue was adsorbed onto silica (ca. 25 g) and was then concentrated to dryness by use of a rotary evaporator. The so-formed silica dry pack was purified by flash column chromatography on silica gel using 20% ethyl acetate/hexanes to afford *N*-(4-cyanophenyl)-benzamide (**3.3**) in a 76% isolated yield (1.14 g, 5.13 mmol) as a white solid.

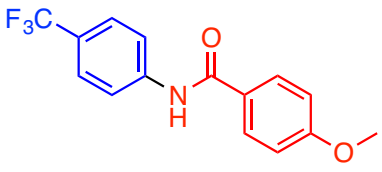
3.6.2. Synthesis and Characterization Data

***N*-(4-cyanophenyl)-benzamide (2a)**



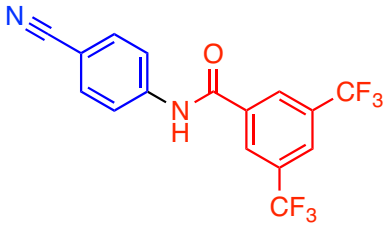
The title compound was synthesized from the corresponding aryl chloride using 5 mol % **C1**, K_3PO_4 and *tert*-butanol ([ArCl] = 0.12 M), and purified by flash column chromatography on silica gel using 20% ethyl acetate/hexanes to afford **3.3** in an 82% isolated yield (81.9 mg, 0.37 mmol) as an off-white solid. ^{1}H NMR (500.1 MHz, CD_3CN): δ 9.04 (br. s, 1H), 7.97-7.93 (m, 4H), 7.75-7.73 (m, 2H), 7.66-7.63 (m, 1H), 7.58-7.55 (m, 2H); $^{13}C\{^1H\}$ NMR (125.8 MHz, CD_3CN): δ 167.1, 144.3, 135.6, 134.2, 133.2, 129.7, 128.7, 121.3, 120.0, 107.6. Spectral data are in good agreement with previously reported ^{1}H and ^{13}C NMR characterization data (recorded in $CDCl_3$) for the title compound.[204]

4-methoxy-*N*-[4-(trifluoromethyl)phenyl]-benzamide (3.4)



The title compound was synthesized from the corresponding aryl chloride using 10 mol % **C1**, K_3PO_4 and toluene ([ArCl] = 0.12 M), and purified by flash column chromatography on silica gel using 20% ethyl acetate/hexanes to afford **3.4** in a 65% isolated yield (65.0 mg, 0.22 mmol) as an off-white solid. ^{1}H NMR (500.1 MHz, DMSO-d_6): δ 10.41 (br. s, 1H), 8.02-7.98 (m, 4H), 7.72-7.71 (m, 2H), 7.10-7.08 (m, 2H), 3.86 (s, 3H); ^{13}C{^{1}H} NMR (125.8 MHz, DMSO-d_6): δ 165.3, 162.2, 143.0, 129.8, 129.4, 126.6, 126.4, 125.8, 123.4, 123.2, 119.9, 113.7, 113.6, 55.4. *m/z* ESI$^+$ found 318.0712 [M+Na]$^+$ calculated for $C_{15}H_{12}F_3NNaO_2$ 318.0718.

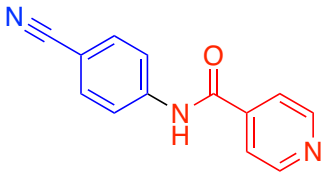
***N*-(4-cyanophenyl)-3,5-bis(trifluoromethyl)-benzamide (3.5)**



The title compound was synthesized from the corresponding aryl chloride using 10 mol % **C1**, NaO^{t}Bu and toluene ([ArCl] = 0.12 M), and purified by flash column chromatography on silica gel using 20% ethyl acetate/hexanes to afford **3.5** in a 81% isolated yield (81 mg, 0.23 mmol) as a white solid. ^{1}H NMR (500.1 MHz, DMSO-d_6): δ 10.99 (br. s, 1H), 8.61 (s, 1H), 8.41 (s, 1H), 7.99-7.97 (m, 2H), 7.89-7.87 (m, 2H); ^{13}C{^{1}H} NMR (125.8 MHz, DMSO-d_6): δ 163.2, 142.8, 136.7, 133.2, 130.6, 130.4, 130.1, 128.8, 128.7, 125.5, 125.4, 124.1, 121.9 120.6, 120.5, 118.9,

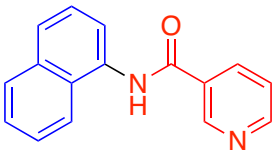
106.0; *m/z* ESI$^+$ found 381.0433 $[M+Na]^+$ calculated for $C_{16}H_8F_6N_2NaO$ 381.0433.

_N_-(4-cyanophenyl)-4-pyridinecarboxamide (3.6)



The title compound was synthesized from the corresponding aryl chloride using 10 mol % **C1**, K_3PO_4 and *tert*-butanol ([ArCl] = 0.12 M), and purified by flash column chromatography on silica gel using ethyl acetate to afford **3.6** in a 79% isolated yield (79 mg, 0.35 mmol) as an off-white solid. ^{1}H NMR (500.1 MHz, CD_3CN): δ 9.19 (br s, 1H), 8.81 (dd, 2H, *J* = 4.4, 1.6 Hz, 2H), 7.95 (d, 2H, *J* = 8.8 Hz, 2H), 7.81 (dd, 2H, *J* = 4.4, 1.6 Hz, 2H), 7.77 (d, 2H, *J* = 8.8 Hz); $^{13}C\{^1H\}$ NMR (125.8 MHz, CD_3CN): δ 165.9, 151.8, 143.8, 142.8, 134.5, 122.6, 121.7, 120.0, 108.3; *m/z* ESI$^+$ found 224.0818 $[M+H]^+$ calculated for $C_{13}H_{10}N_3O$ 224.0824.

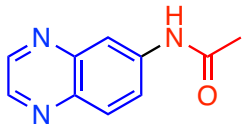
_N_-1-naphthalenyl-3-pyridinecarboxamide (3.7)



The title compound was synthesized from the corresponding aryl chloride, using 5 mol % **C1**, NaO^{t}Bu and toluene ([ArCl] = 0.06M), and purified by flash column chromatography on silica gel using ethyl acetate to afford **3.7** in 80% isolated yield (146 mg, 0.58 mmol) from the aryl chloride as a white solid. ^{1}H NMR (500.1 MHz, DMSO-d_6): δ 10.62 (br. s, 1H), 9.26 (s, 1H), 8.82 (dd, *J* = 4.8, 1.4 Hz, 1H), 8.44 (d, *J* = 7.9 Hz, 1H), 8.06-8.04 (m, 1H), 8.01-7.99 (m, 1H), 7.91 (d, *J* = 8.2 Hz, 1H),

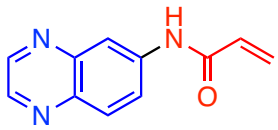
7.66-7.56 (m, 5H); $^{13}C\{^{1}H\}$ NMR (125.8 MHz, DMSO-d_6): δ 164.7, 152.2, 148.8, 135.5, 133.7, 133.4, 130.3, 130.1, 128.9, 128.0, 126.4, 126.1, 126.0, 125.5, 123.8, 123.5, 123.3; *m/z* ESI^+ found 271.0842 $[M+Na]^+$ calculated for $C_{16}H_{12}N_2NaO$ 271.0847. CAS registry #: 75358-96-2.

***N*-6-quinoxalinyl-acetamide (3.8)**



The title compound was synthesized from the corresponding aryl chloride using 5 mol % **C1**, Cs_2CO_3 and 1,4-dioxane ([ArCl] = 0.06 M). The crude reaction mixture was poured over a Celite/silica gel plug (5:1 v/v) and the solvent was removed *in vacuo*. The resulting residue was washed with room-temperature hexanes (5 x 5 mL) and dried *in vacuo* to afford **3.8** in a 77 % isolated yield (77 mg, 0.41 mmol) as a yellow solid. ^{1}H NMR (500.1 MHz, DMSO-d_6): δ 10.53 (br. s, 1H), 8.87-8.80 (m, 2H), 8.51 (s, 1H), 8.04 (d, *J* = 9.0 Hz, 1H), 7.93 (d, *J* = 8.6 Hz, 1H), 2.16 (s, 3H); $^{13}C\{^{1}H\}$ NMR (125.8 MHz, DMSO-d_6): δ 169.1, 145.8, 143.8, 143.0, 138.9, 129.4, 123.6, 115.2, 24.1; *m/z* ESI^+ found 210.0638 $[M+Na]^+$ calculated for $C_{10}H_9N_3NaO$ 210.0643.

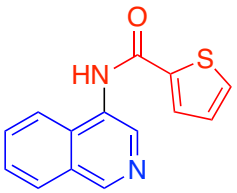
***N*-6-quinoxalinyl-2-propenamide (3.9)**



The title compound was synthesized from the corresponding aryl chloride using 10 mol % **C1**, Cs_2CO_3 and 1,4-dioxane ([ArCl] = 0.12 M), and purified by flash column chromatography on silica gel using ethyl acetate to afford **3.9** in a 74% isolated

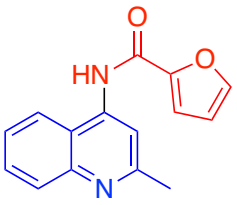
yield (74 mg, 0.371 mmol) as a yellow solid. ^{1}H NMR (300.1 MHz, CD_3CN): δ 8.90 (br. s, 1H), 8.82 (d, *J* = 1.9 Hz, 1H), 8.76 (d, *J* = 1.9 Hz, 1H), 8.54 (d, *J* = 2.3 Hz, 1H), 8.05 (d, *J* = 9.1 Hz, 1H), 7.96 (dd, *J* = 9.1, 2.3 Hz, 1H), 6.46 (d, *J* = 3.1 Hz, 1H), 6.43 (s, 1H), 5,85 (dd, *J* = 7.4, 4.9 Hz, 1H); ^{13}C{^{1}H} NMR (125.8 MHz, CD_3CN): δ 163.8, 145.9, 144.0, 142.9, 140.1, 139.2, 131.5, 129.6, 127.9, 123.8, 115.9; *m/z* ESI^{+} found 222.0638 $[M+Na]^{+}$ calculated for $C_{11}H_9N_3NaO$ 222.0643. CAS #: 1183129-19-2.

***N*-4-isoquinolinyl-2-thiophenecarboxamide (3.10)**



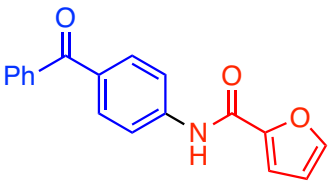
The title compound was synthesized from the corresponding aryl bromide using 10 mo l% **C1**, K_3PO_4 and toluene ([ArBr] = 0.06 M), and purified by flash column chromatography on silica gel using 80% ethyl acetate/hexanes to afford **3.10** in a 50% isolated yield (46 mg, 0.18 mmol) as a beige solid. ^{1}H NMR (500.1 MHz, DMSO-d_6): δ 10.60 (br. s, 1H), 9.28 (s, 1H), 8.62 (s, 1H), 8.21-8.18 (m, 2H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.92-7.91 (m, 1H), 7.86-7.83 (m, 1H), 7.76-7.73 (m, 1H), 7.31-7.29 (m, 1H); ^{13}C{^{1}H} NMR (125.8 MHz, DMSO-d_6): δ 160.9, 150.4, 140.5, 139.1, 132.0, 131.7, 130.5, 129.7, 128.5, 128.4, 128.2, 127.7, 127.6, 122.5; *m/z* ESI^{+} found 255.0587 $[M+H]^{+}$ calculated for $C_{14}H_{11}N_2OS$ 255.0592.

***N*-(2-methyl-4-quinolinyl)-2-furancarboxamide (3.11)**



The title compound was synthesized from the corresponding aryl chloride using 10 mo l% **C1**, NaO^{t}Bu and toluene ([ArCl] = 0.12 M), and purified by flash column chromatography on silica gel using 70% ethyl acetate/hexanes to afford **3.11** in an 83 % isolated yield (84 mg, 0.33 mmol) as a beige solid. ^{1}H NMR (500.1 MHz, CD_3CN): δ 9.07 (br. s, 1H), 8.08 (s, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.79-7.78 (m, 1H), 7.77-7.74 (m, 1H), 7.61-7.58 (m, 1H), 7.36 (m, 1H), 6.72-7.71 (m, 1H), 2.70 (s, 3H); ^{13}C{^{1}H} NMR (125.8 MHz, DMSO-d_6): δ 160.7, 157.7, 149.8, 148.6, 146.9, 141.5, 130.5, 130.3, 126.5, 122.0, 120.6, 116.7, 113.9, 113.7, 25.9; *m/z* ESI$^+$ found 253.0972 $[M+H]^+$ calculated for $C_{15}H_{13}N_2O_2$ 253.0977. CAS #: 901365-28-4.

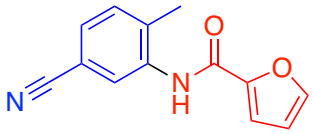
***N*-(4-benzoylphenyl)- 2-furancarboxamide (3.12)**



The title compound was synthesized from the corresponding aryl bromide using 10 mol % **C1**, NaO^{t}Bu and toluene ([ArBr] = 0.06 M), and purified by flash column chromatography on silica gel using 60% ethyl acetate/hexanes to afford **3.12** in a 76 % isolated yield (72.3 mg, 0.25 mmol) as a yellow solid. ^{1}H NMR (300.1 MHz, DMSO-d_6): δ 10.54 (br. s, 1H), 8.00-7.96 (m, 3H), 7.79-7.71 (m, 4H), 7.68-7.63 (m,

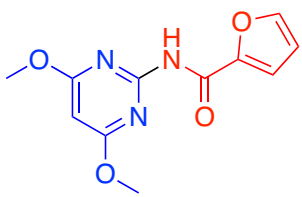
1H), 7.58-7.52 (m, 2H), 7.43-7.42 (m, 1H), 6.73-6.72 (m, 1H); $^{13}C\{^{1}H\}$ NMR (125.8 MHz, DMSO-d_6): δ 194.6, 156.4, 147.1, 146.1, 142.8, 137.5, 132.2, 131.8, 130.1, 129.4, 129.1, 128.4, 128.3, 119.4, 115.5, 112.3; *m/z* ESI^+ found 314.0788 $[M+Na]^+$ calculated for $C_{18}H_{13}NNaO_3$ 314.0793. CAS#: 723257-50-9.

***N*-(5-cyano-2-methylphenyl)-2-furancarboxamide (3.13)**



The title compound was synthesized from the corresponding aryl bromide using 10 mo l% **C1**, NaO^{t}Bu and toluene ([ArBr] = 0.06 M), and purified by flash column chromatography on silica gel using 50% ethyl acetate/hexanes to afford **3.13** in an 83 % isolated yield (82.6 mg, 0.37 mmol) as a yellow solid. ^{1}H NMR (500.1 MHz, DMSO-d_6): δ 9.95 (br. s, 1H), 7.97 (d, *J* = 1.0 Hz, 1H), 7.84 (d, *J* = 1.5 Hz, 1H), 7.64 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.34 (d, *J* = 3.4 Hz, 1H), 6.73 (dd, *J* = 3.5, 1.7 Hz, 1H), 2.33 (s, 3H); $^{13}C\{^{1}H\}$ NMR (125.8 MHz, DMSO-d_6): δ 156.3, 147.1, 145.8, 139.8, 136.5, 131.7, 129.5, 129.4, 118.5, 115.1, 112.2, 108.8, 18.1; *m/z* ESI^+ found 249.0634 $[M+Na]^+$ calculated for $C_{13}H_{10}N_2NaO_2$ 249.0640. CAS#: 1282732-11-9.

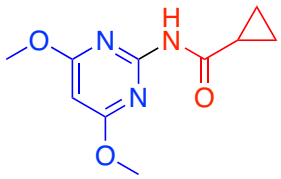
***N*-(4,6-dimethoxy-2-pyrimidinyl)-2-furancarboxamide (3.14)**



The title compound was synthesized from the corresponding aryl chloride using 10 mol % **C1**, NaO^{t}Bu and toluene ([ArCl] = 0.06 M), and purified by flash column

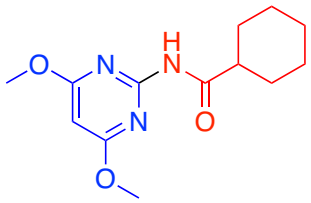
chromatography on silica gel using 50% ethyl acetate/hexanes to afford **3.14** in a 75% isolated yield (67 mg, 0.27 mmol) as a beige solid. ^{1}H NMR (500.1 MHz, DMSO-d_6): δ 10.48 (br. s, 1H), 7.94-7.93 (m, 1H), 7.51 (d, J = 3.6 Hz, 1H), 6.69 (dd, J = 3.6 Hz, 1.7 Hz, 1H), 5.97 (s, 1H), 3.89 (s, 6H); ^{13}C{^{1}H} NMR (125.8 MHz, DMSO-d_6): δ 171.6, 156.5, 155.6, 147.0, 146.4, 115.8, 112.0, 84.5, 54.0; *m/z* ESI^{+} found 272.0642 [M+Na]$^{+}$ calculated for $C_{11}H_{11}N_3NaO_4$ 272.0647. CAS#: 943417-94-5.

***N*-(4,6-dimethoxy-2-pyrimidinyl)-cyclopropanecarboxamide (3.15)**



The title compound was synthesized from the corresponding aryl chloride using 10 mol % **C1**, NaO^{t}Bu and toluene ([ArCl] = 0.06 M), and purified by flash column chromatography on silica gel using 30% ethyl acetate/hexanes to afford **3.15** in a 78 % isolated yield (78 mg, 0.35 mmol) as light yellow solid. ^{1}H NMR (500.1 MHz, CD_3CN): δ 8.61 (br. s, 1H), 5.82 (s, 1H), 3.90 (s, 6H), 2.54-2.49 (m, 1H), 0.99-9.96 (m, 2H), 0.93-0.89 (m, 2H); ^{13}C{^{1}H} NMR (125.8 MHz, CD_3CN): δ 174.2, 173.2, 157.8, 85.0, 54.9, 15.4, 9.3; *m/z* ESI^{+} found 246.0849 [M+Na]$^{+}$ calculated for $C_{10}H_{13}N_3NaO_3$ 246.0855. CAS#: 517869-79-3

***N*-(4,6-dimethoxy-2-pyrimidinyl)-cyclohexanecarboxamide (3.16)**



The title compound was synthesized from the corresponding aryl chloride using 10 mol % **C1**, Cs_2CO_3 and 1,4-dioxane ([ArCl] = 0.12 M) and purified by flash column chromatography on silica gel using 20% ethyl acetate/hexanes to afford **3.16** in a 57 % isolated yield (57 mg, 0.21 mmol) as a beige solid. ^{1}H NMR (500.1 MHz, DMSO-d_6): δ 8.35 (br. s, 1H), 5.81 (s, 1H), 3.91 (s, 6H), 2.98-2.96 (m, 1H), 1.94-1.91 (m, 2H), 1.83-1.79 (m, 2H), 1.72-1.69 (m, 1H), 1.51-1.43 (m, 2H), 1.39-1.24 (m, 3H); ^{13}C{^{1}H} NMR (125.8 MHz, DMSO-d_6): δ 173.2, 157.8, 85.0, 54.9, 45.5, 30.1, 26.7, 26.5; *m/z* ESI$^+$ found 288.1319 $[M+Na]^+$ calculated for $C_{13}H_{19}N_3NaO_3$ 288.1324. CAS#: 943417-92-3.

Chapter 4

Bisphosphine-Ligated Nickel Pre-Catalysts in C(sp^2)-N Cross-Couplings of Aryl Chlorides: a Comparison of Ni(I) and Ni(II)

4.1. RESEARCH OVERVIEW AND CONTRIBUTION REPORT

This author wishes to clarify his contributions to the research described in Chapter 4 of this Thesis document. This chapter details the findings of a combined experimental and computational examination of the influence of ancillary ligand and Ni oxidation state in the Ni-catalyzed C(sp^2)-N cross-coupling of aryl chlorides, focusing on (**L**)NiCl and (**L**)NiCl(*o*-tolyl) pre-catalysts (PAd-DalPhos, **L18**; dppf, **L8**). Whereas Ni(II) pre-catalysts generally out-performed Ni(I) species in our study, the viability and in some cases superiority of Ni(I) pre-catalysts in challenging aminations is established. Computational analyses support the viability of Ni(0)/Ni(II) cycles featuring rate-limiting C-N reductive elimination, as well as parallel Ni(I)/Ni(III) mechanisms involving rate-limiting C-Cl oxidative addition.

This authors contributions to this work include: conceived of the project idea; synthesis of all compounds; conducted all of the catalytic reactions; performed the

majority of the DFT calculations; characterization of compounds reported herein; interpreted all of the data; and wrote the manuscript. This project was conducted in collaboration with Prof. Erin Johnson of Dalhousie, who mentored this author in DFT analysis, and located all of the oxidative addition transition state species reported herein. Author M. Ferguson carried out the X-ray diffraction analyses of (**L18**)NiCl (**^{PAd}Ni^{I}**) and (**L18**)Ni(Ph)(Cl). This work has been published in Advanced Synthesis and Catalysis.

Reference: Lavoie, C.M.; McDonald, R.; Johnson, E.R.; M.J.; Stradiotto, M., Bisphosphine-Ligated Nickel Pre-catalysts in C(sp^2)-N Cross-couplings of Aryl Chlorides: A Comparison of Nickel(I) and Nickel(II). *Adv. Synth. Catal.* **2017**, *359*, 2972-2980.

4.2. INTRODUCTION

4.2.1. Overview of Mechanistic Studies in Nickel Catalyzed C-N Cross-coupling

The Pd-catalyzed cross-coupling of NH substrates and (hetero)aryl (pseudo)halides (i.e., Buchwald-Hartwig amination, BHA) is widely employed for the synthesis of (hetero)anilines.[31] The preponderance of evidence supports a Pd(0)/Pd(II) mechanism for BHA (Fig. 4-1A),[205, 206] which has guided the development of Pd(0) or Pd(II) pre-catalysts featuring bulky, electron-rich alkylphosphine and *N*-heterocyclic carbene ancillary ligands[31, 186] that give rise to $L_nPd(0)$ (n = 1 or 2)[37] species capable of challenging C(sp^2)-X oxidative additions (e.g. X = Cl[128]).[207]

The high cost and scarcity of Pd, as well as the desire to effect transformations for which Pd has proven ineffective, provides motivation for the development of base-metal variations of BHA. This has contributed to a renaissance in Ni-catalyzed C(sp^2)-N (herein C-N) cross-coupling chemistry,[186, 187] leading to outstanding Ni catalysts for transformations involving relatively inexpensive (hetero)aryl chlorides and phenol-derived electrophiles.[187, 198] Nonetheless, our understanding of the factors that give rise to effective Ni catalysts in such transformations is primitive. The smaller size of Ni versus Pd, as well as the greater propensity of Ni(0) to engage in C(sp^2)-X oxidative additions,[128, 208] suggest that ancillary ligands optimized for BHA are unlikely to be broadly effective with Ni. Furthermore, the widely accessible oxidation state range (commonly 0 to III) and propensity for single-electron chemistry creates a complex mechanistic landscape for Ni-catalyzed C-N cross-coupling, whereby Ni(0)/Ni(II) and Ni(I)/Ni(III) cycles, as well as single-electron transfer linking these reaction manifolds, must be considered (Fig. 4-1B).[68, 209]

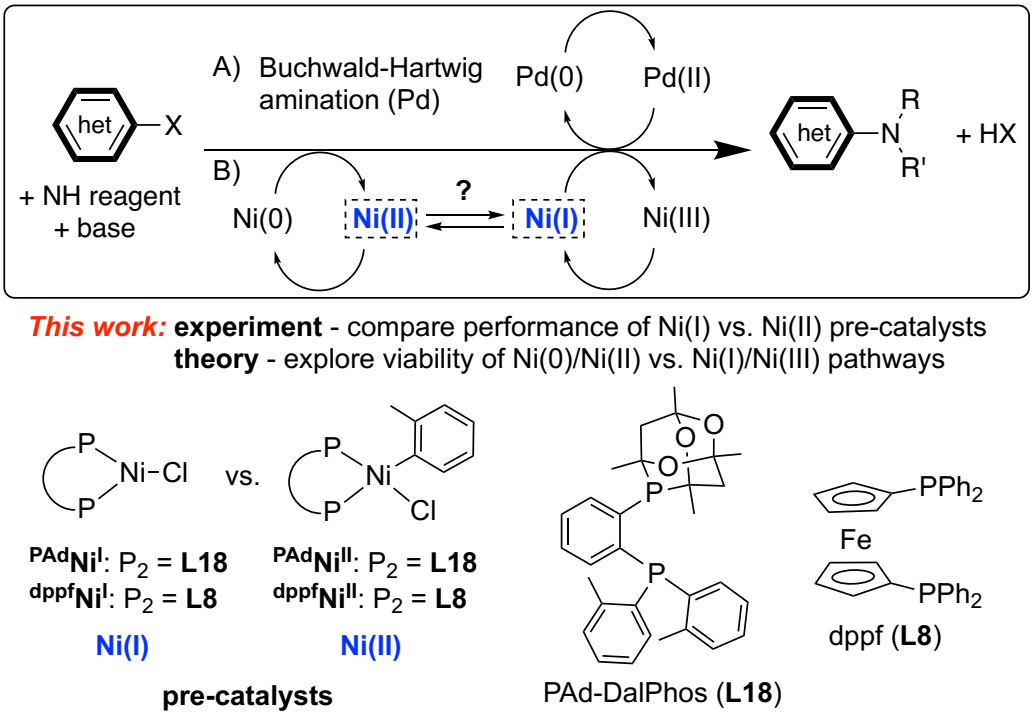


Figure 4-1. Palladium- and nickel-catalyzed C(*sp*^{2})–N cross-coupling, and the Ni(I) and Ni(II) pre-catalysts under investigation herein.

While Ni(0) and Ni(II) pre-catalysts are commonly employed in C-N cross-coupling,[35] data pertaining to the mechanism of such reactions are limited.[93-96] In the context of reactions of aryl chlorides,[113] the Ni(I) pre-catalyst [(BINAP)Ni(μ-Cl)]$_2$ proved inactive[69] for alkylamine arylation under conditions whereby high conversion was achieved by use of a Ni(II)[69] or Ni(0)[70] pre-catalyst. Control experiments conducted by Green and Hartwig[71] demonstrate that JosiPhos-ligated Ni(0) and Ni(II) pre-catalysts promote C-N cross-couplings of ammonia or primary alkylamines in the absence of free aryl radicals. Conversely, the intermediacy of Ni(I) species in C-N cross-couplings of haloarenes and diarylamines has been invoked given the efficacy of [(IPr)Ni(μ-Cl)]$_2$ and (**L**)Ni(IPr)Cl Ni(I) pre-catalysts,[73, 74]

and based on the lack of reactivity observed between main group diphenylamides and Ni(II) catalytic intermediates of the type $(PPh_3)_2Ni(aryl)X$.[210]

Collectively, these isolated reports support the viability of either Ni(0)/Ni(II) or Ni(I)/Ni(III) catalytic cycles. However, more systematic comparative analyses are required to inform the rational development of superlative Ni pre-catalysts for C-N cross-coupling. Herein we disclose the results of a combined experimental and DFT study focusing on PAd-DalPhos (**L18**) and dppf (**L8**) ligated Ni(I) and Ni(II) pre-catalysts (Fig. 4-1) in the C-N cross-coupling of aryl chlorides. Computational analyses support the feasibility of both Ni(0)/Ni(II) and Ni(I)/Ni(III) mechanisms. Moreover, we establish that while the performance of the Ni(II) pre-catalysts (**^{PAd}Ni^{II}** and **^{dppf}Ni^{II}**) is in general superior to that of Ni(I) species (**^{PAd}Ni^{I}** and **^{dppf}Ni^{I}**), dramatic exceptions to this trend are possible for given ancillary ligand and substrate combinations.

4.3. RESULTS AND DISCUSSION

4.3.1. Synthesis of Ni(I) and Ni(II) Pre-catalysts

PAd-DalPhos (**L18**)[102] and dppf (**L8**)[89] were selected for our study, given the utility of derived (**L**)NiCl(*o*-tolyl) pre-catalysts in catalyzing a broad scope of C-N cross-couplings. Whereas (**L8**)NiCl (**^{dppf}Ni^{I}**) is known,[94, 95] its use as a pre-catalyst in C-N cross-coupling chemistry has not been described. The new Ni(I) complex (**L18**)NiCl (**^{PAd}Ni^{I}**) was prepared as a red paramagnetic solid via comproportionation of (**L18**)$NiCl_2$ and putative (**L18**)Ni(cod) (see section 4.5.2 for details). Single-crystal X-ray analysis established **^{PAd}Ni^{I}** as a mononuclear species

featuring a distorted Y-shape geometry at Ni, in keeping with other L_2NiCl complexes (Fig. **4-2**).[73, 95, 211]

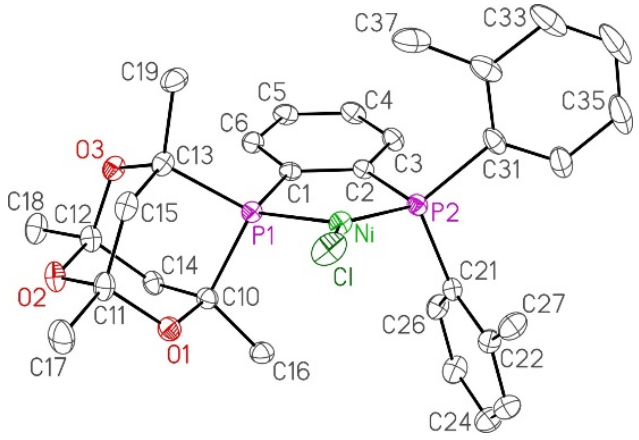


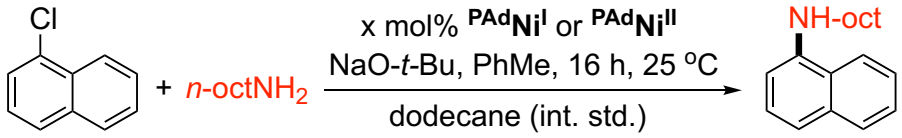
Figure 4-2. Single-crystal X-ray structure of ^{PAd}**Ni**^{I}, with one of the two independent molecules shown at the 30% probability level with H atoms omitted for clarity. Selected interatomic distances (Å) and angles (º): Ni-P1 2.1646(6), Ni-P2 2.1830(6), Ni-Cl 2.1503(6), P1-Ni-P2 88.47(2), P1-Ni-Cl 126.90(3), P2-Ni-Cl 144.61(3).

4.3.2. Reactivity Comparisons of Ni(I) and Ni(II) Pre-catalysts

The room temperature cross-coupling of 1-chloronaphthalene (**3.28**) and *n*-octylamine (**4.1**) to afford **4.2** was selected to compare the catalytic abilities of ^{PAd}**Ni**^{I} and ^{PAd}**Ni**^{II}, given the established utility of ^{PAd}**Ni**^{II} in this transformation (Table 4-1). The performance of ^{PAd}**Ni**^{I} and ^{PAd}**Ni**^{II} proved indistinguishable at 5 mol % loading (entries 1 and 2). The efficacy of ^{PAd}**Ni**^{I} under these mild conditions is significant, in that it represents the first example of a Ni(I) pre-catalyst being employed competitively in Ni-catalyzed C-N cross-couplings beyond diphenylamine variants, and contrasts the inactivity of $[(BINAP)Ni(\mu\text{-}Cl)]_2$ in an analogous transformation of **4.1**.[69] On lowering the loading to 0.5 mol % Ni, ^{PAd}**Ni**^{I} proved inferior to ^{PAd}**Ni**^{II} (entries 3 and 4), and poor performance for both pre-catalysts was

noted at 0.1 mol % Ni (entries 5 and 6). Addition of catalytic quantities of TEMPO (2,2,6,6-tetramethylpiperine-1-oxyl) caused a significant decrease in product formation in the case of ^{PAd}**Ni**^{I} (entry 7); a lesser effect was found with ^{PAd}**Ni**^{II} (entry 8). Observations by Wolf and co-workers[212] establishing that Ni(I) species can be trapped by TEMPO support a similar inhibitory processes involving ^{PAd}**Ni**^{I}.

Table 4-1. Comparative cross-coupling of 1-chloronaphthalene and *n*-octylamine employing ^{PAd}**Ni**^{I} or ^{PAd}**Ni**^{II}.[a]



3.28 **4.1** **4.2**

Entry	Ni cat.	mol% Ni	Additive	% Yield **4.2**
1	^{PAd}**Ni**^{I}	5	--	91
2	^{PAd}**Ni**^{II}	5	--	94
3	^{PAd}**Ni**^{I}	0.5	--	8
4	^{PAd}**Ni**^{II}	0.5	--	87
5	^{PAd}**Ni**^{I}	0.1	--	<5
6	^{PAd}**Ni**^{II}	0.1	--	27
7	^{PAd}**Ni**^{I}	5	0.10 equiv TEMPO	22
8	^{PAd}**Ni**^{II}	5	0.10 equiv TEMPO	79
9	^{PAd}**Ni**^{I}	0.5	0.15 equiv PhBPin	93
10	^{PAd}**Ni**^{II}	0.1	0.15 equiv PhBPin	80

[a]Reaction conditions: **3.28** (1.0 equiv), **4.1** (1.1 equiv), toluene (2 mL), NaO-*t*-Bu (1.5 equiv). Conversion to product (**4.2**) determined on the basis of calibrated GC analysis using dodecane as an internal standard.

The superior performance of ^{PAd}**Ni**^{II} over ^{PAd}**Ni**^{I} (Table 4-1) may suggest that maintaining a higher concentration of (**L18**)Ni(0/II) intermediates should lead to more productive catalysis. In this vein, substantially higher yields were achieved in the presence of phenylboronic acid pinacol ester (PhBPin) as a reducing agent, using either ^{PAd}**Ni**^{I} (entry 9) or ^{PAd}**Ni**^{II} (entry 10). The latter result (entry 10) is

significant in that 0.1 mol % represents the lowest reported loading of a Ni-based pre-catalyst in C-N cross-coupling chemistry. Subsequent experimentation (Fig. 4-3) confirmed that using ^{PAd}**Ni**^{I} with added PhBPin accelerates the reaction through the formation of (**L18**)Ni(0) species which, upon addition of cod, can be trapped as presumptive (**L18**)Ni(cod) on the basis of ^{31}P NMR data (see **GP4-14** of the experimental section)

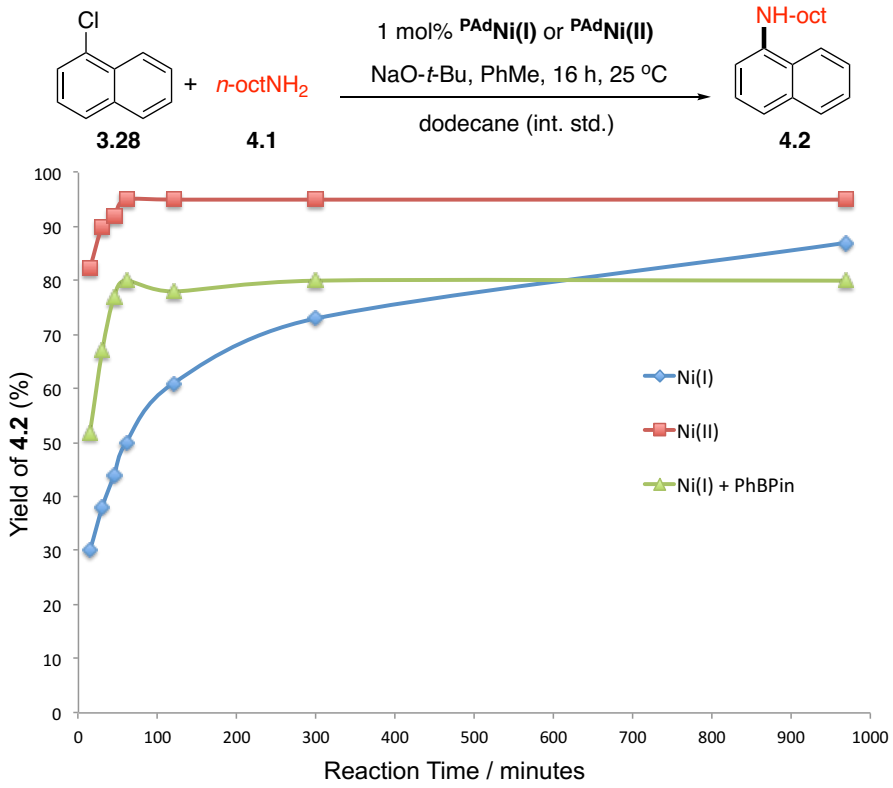
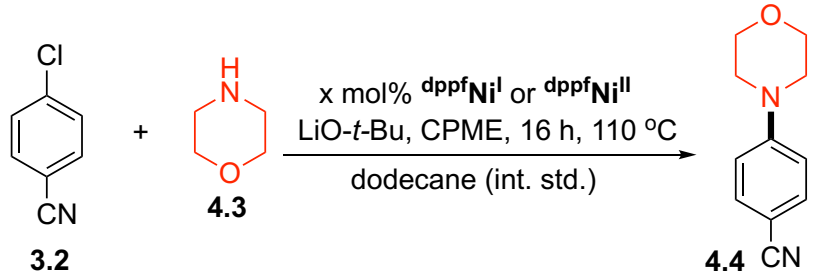


Figure 4-3. PAd-DalPhos-based pre-catalyst conversion versus time comparison for the C-N cross-coupling between 1-chloronapthalene (**3.28**) and *n*-octylamine (**4.1**) (product = *N*-(1-naphthyl)-octylamine, **4.2**).

I then sought to evaluate the performance of ^{dppf}**Ni**^{I} and ^{dppf}**Ni**^{II} in the cross-coupling of 4-chlorobenzonitrile (**3.2**) and morpholine (**4.3**) to afford **4.4** (Table 4-2). Although ^{dppf}**Ni**^{II} is known to be competent for this transformation,[92] ^{dppf}**Ni**^{I} had yet to be applied in any Ni-catalyzed C-N cross-coupling chemistry. Unlike ^{PAd}**Ni**^{I} and

^{PAd}**Ni**^{II} (Table 4-1), similar catalytic performance was observed by use of either ^{dppf}**Ni**^{I} or ^{dppf}**Ni**^{II}, with excellent conversion realized at the 5 mol % Ni level (entries 1 and 2), but less so at 0.5 mol % Ni (entries 3 and 4). The observation that catalytic quantities of TEMPO significantly inhibited product formation for both ^{dppf}**Ni**^{I} and ^{dppf}**Ni**^{II} (entries 5 and 6) suggests that **L8**-derived Ni(II) pre-catalysts may be more prone to Ni(I) formation than **L18** pre-catalysts.[93] Addition of PhBPin resulted in an increase in product formation for reactions employing 0.5 mol % of either ^{dppf}**Ni**^{I} (entry 7) or ^{dppf}**Ni**^{II} (entry 8).

Table 4-2. Comparative cross-coupling of 4-chlorobenzonitrile (**3.2**) and morpholine (**4.3**) employing ^{dppf}**Ni**^{I} or ^{dppf}**Ni**^{II}.



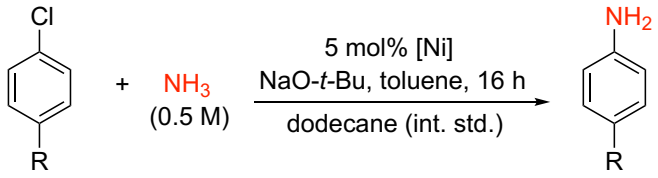
Entry	Ni cat.	mol% Ni	Additive	% Yield **4.4**
1	^{dppf}**Ni**^{I}	5	--	88
2	^{dppf}**Ni**^{II}	5	--	79
3	^{dppf}**Ni**^{I}	0.5	--	27
4	^{dppf}**Ni**^{II}	0.5	--	42
5	^{dppf}**Ni**^{I}	5	0.10 equiv TEMPO	5
6	^{dppf}**Ni**^{II}	5	0.10 equiv TEMPO	12
7	^{dppf}**Ni**^{I}	0.5	0.30 equiv PhBPin	68
8	^{dppf}**Ni**^{II}	0.5	0.30 equiv PhBPin	78

[a]Reaction conditions: **3.2** (1.0 equiv), **4.3** (1.1 equiv), CPME (0.25 mL), LiO-*t*-Bu (1.5 equiv). Conversion to product (**4.4**) on the basis of calibrated GC analysis using dodecane as an internal standard.

In examining the performance of the pre-catalysts in reactions involving morpholine, aniline (Tables 4-4 and 4-5 of the experimental section), and ammonia

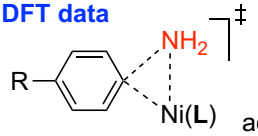
(Table 4-3), we observed that: **L18** and **L8** displayed their established nucleophile preferences, with **L8**-ligated pre-catalysts proving superior in transformations of morpholine and aniline, and **L18**-ligated pre-catalysts being better-suited for the monoarylation of ammonia; the Ni(II) pre-catalysts (^{PAd}**Ni**^{II} and ^{dppf}**Ni**^{II}) were found to be competitive with or superior to their Ni(I) counterparts (^{PAd}**Ni**^{I} and ^{dppf}**Ni**^{I}); and where competent catalysis was observed, higher substrate conversions (including in some cases polyarylation) were achieved by use of electron-poor electrophiles.

Table 4-3. Comparative experimental and computational survey of the cross-coupling of ammonia and substituted aryl chlorides.[a]



Entry	Ni pre-cat.	R	Reaction temp.[°C]	% Aniline yield
1	^{PAd}**Ni**^{I}	H	110	62
2	^{PAd}**Ni**^{II}	H	110	69
3	^{dppf}**Ni**^{I}	H	110	6
4	^{dppf}**Ni**^{II}	H	110	7
5	^{PAd}**Ni**^{I}	CN	25	11[b]
6	^{PAd}**Ni**^{II}	CN	25	8[b]
7	^{dppf}**Ni**^{I}	CN	25	0
8	^{dppf}**Ni**^{II}	CN	25	0
9	^{PAd}**Ni**^{I}	OMe	110	29
10	^{PAd}**Ni**^{II}	OMe	110	28
11	^{dppf}**Ni**^{I}	OMe	110	0
12	^{dppf}**Ni**^{II}	OMe	110	0

DFT data

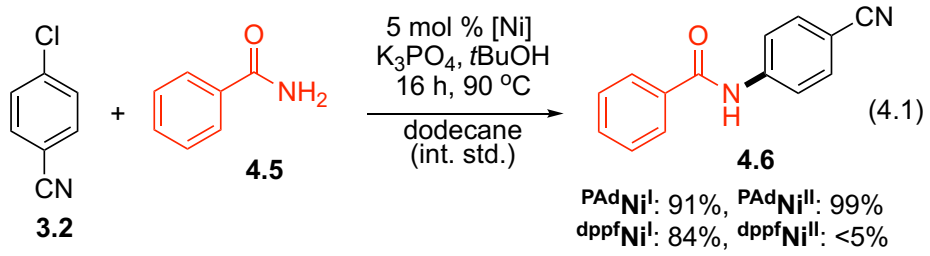


R = H	R = CN	R = OMe
L1: 18.6	**L1**: 15.3	**L1**: 20.9
L2: 18.5	**L2**: 14.0	**L2**: 20.3

activation free energies ($\Delta G^{\ddagger}$, kcal mol^{-1})

[a]Reaction conditions: aryl chloride (1.0 equiv.), NH_3 (0.5M in 1,4-dioxane, 7.0 equiv.), toluene (0.50 mL), NaO-*t*-Bu (3.0 equiv.). Conversion to the aniline product on the basis of calibrated GC analysis using dodecane as an internal standard. [b]Complete conversion of the aryl chloride observed, accompanied by substantial quantities of the presumptive polyarylation products.

A notable exception was observed in the cross-coupling of 4-chlorobenzonitrile (**3.2**) with benzamide (**4.5**) (eq. 4-1). Whereas ^{PAd}**Ni**^{I} and ^{PAd}**Ni**^{II}[213] performed similarly well, a striking difference was noted with the dppf-derived pre-catalysts: ^{dppf}**Ni**^{II} proved *inactive*, while ^{dppf}**Ni**^{I} afforded **4.6** in high yield. Notwithstanding recent reports documenting the undesirable nature of Ni(I) species in C(sp^2)-E (E = C, S, N) cross-coupling catalysis[69, 94, 95] the observed superiority of ^{dppf}**Ni**^{I} over ^{dppf}**Ni**^{II} in this transformation highlights the potential value of surveying Ni pre-catalysts in varied oxidation states in reaction development.



4.3.3. Computational Analysis of Potential Reaction Pathways

In considering viable mechanistic pathways, the Ni(I) pre-catalysts ^{PAd}**Ni**^{I} and ^{dppf}**Ni**^{I} could give rise to substrate turnover in C-N cross-coupling by way of a Ni(I)/Ni(III) cycle, or via redox chemistry that provides entry into a Ni(0)/Ni(II) cycle. We assessed the feasibility of these scenarios via DFT calculations using the B3LYP-XDM method[214-216] and the 6-311+G(2d,2p) basis set, which is well-suited for calculating 3d transition metal-ligand binding energies.[217] The geometry optimizations and frequency calculations were performed with a smaller, mixed basis set, and frequencies were used to assign stationary points as either minima (no imaginary frequencies) or transition states (one imaginary frequency).

Computed data for Ni(0)/Ni(II) pathways involving dppf (**L8**) or PAd-DalPhos

(**L18**) for the cross-coupling of chlorobenzene and either ammonia, aniline, morpholine, or formamide are provided in Figure 4-3 and Tables 4-7/4-8. Calculated bond lengths and angles for ^{PAd}**Ni**^{I}, ^{PAd}**Ni**^{II}, and (**L18**)Ni(Ph)Cl are in excellent agreement with X-ray data (Table 4-6 of the experimental section).

In examining the Ni(0)/Ni(II) pathway for the monoarylation of ammonia with chlorobenzene (**4.7**) to furnish aniline (**4.8**), each of the **L18** and **L8** (Fig. 4-4) derived Ni catalyst systems were modeled, including: a) arene exchange with (**L**)Ni(η^2-toluene) to afford (**L**)Ni(η^2-PhCl); b) C-Cl oxidative addition to give (**L**)Ni(Ph)Cl via **TS-1**; c) reaction with NH_3 and base to give (**L**)Ni(Ph)NH_2; and d) C-N reductive elimination to afford (**L**)Ni(η^2-PhNH_2) via **TS-2**. In examining the Ni(0)/Ni(II) pathway for the monoarylation of ammonia with chlorobenzene (**4.7**) to furnish aniline (**4.8**), each of the **L18** and **L8** (Fig. 4-4) derived Ni catalyst systems were modeled, including: a) arene exchange with (**L**)Ni(h^2-toluene) to afford (**L**)Ni(η^2-PhCl); b) C-Cl oxidative addition to give (**L**)Ni(Ph)Cl via **TS-1**; c) reaction with NH_3 and base to give (**L**)Ni(Ph)NH_2; and d) C-N reductive elimination to afford (**L**)Ni(η^2-PhNH_2) via **TS-2**. The free energy activation barriers to C-Cl oxidative addition (**TS-1**) are small (**L18**: 7.2 kcal mol^{-1}, **L8**: 8.7 kcal mol^{-1}), and ground state calculations show that formation of (**L**)Ni(Ph)NH_2 is exergonic by 8.3 kcal mol^{-1} (**L18**) and 8.6 kcal mol^{-1} (**L8**). Notably, both pathways suffer from comparatively high free energy barriers to C-N reductive elimination of the product aniline (**TS-2**) (**L18**: 18.6 kcal mol^{-1}, **L8**: 18.5 kcal mol^{-1}). These data suggest that sterically encumbered yet electron-poor ancillary ligands, which promote C-N reductive elimination, are likely to prove useful in such transformations.[102] By comparison

(Table 4-3) the free energy activation barriers to C-N reductive elimination for electron-rich *para*-anisidine were computed to be high (**L18**: 20.9 kcal mol^{-1}, **L8**: 20.3 kcal mol^{-1}) versus electron-poor *para*-aminobenzonitrile (**L18**: 15.3 kcal mol^{-1}, **L8**: 14.0 kcal mol^{-1}). The empirically observed poor performance of **L8** in this ammonia chemistry (Table 4-3) may arise from catalyst inhibition processes not captured by the computational survey.

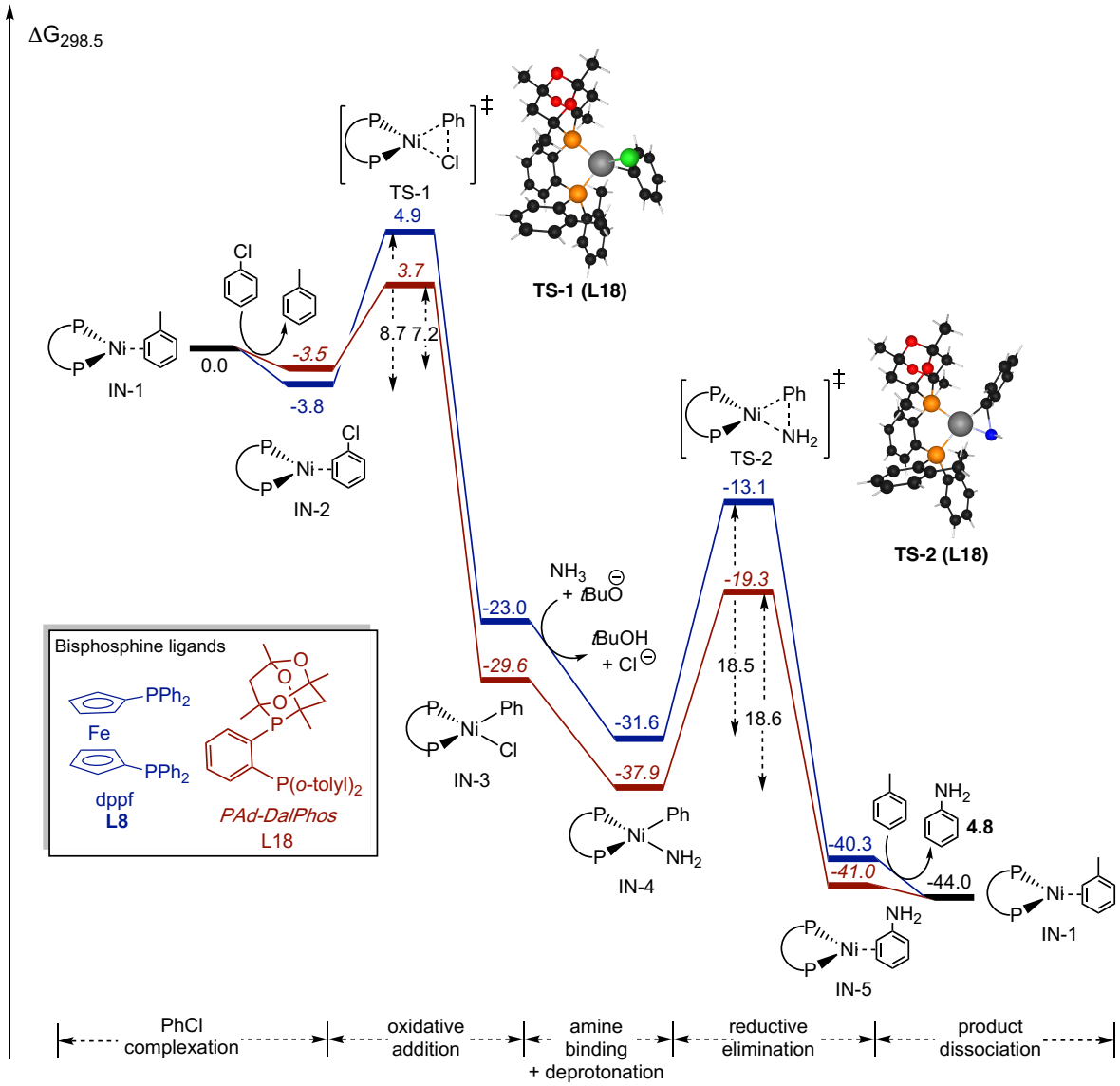


Figure 4-4. Relative free energies (kcal mol^{-1}) calculated for C-N cross-coupling reaction steps involving (**L8/L18**)Ni species within a Ni(0)/Ni(II) cycle. The **L18**-based transition state structures for **TS-1** and **TS-2** are depicted with hydrogen atoms represented as sticks.

It is generally accepted that for C-N cross-couplings involving weakly nucleophilic NH reagents (e.g., ammonia, amides, among others), aryl amido intermediates of the type (L)Ni(aryl)NRR' are formed via initial amine coordination, followed by deprotonation by base.[218-220] Indeed this is how we modeled the formation of **IN-4** from **IN-3.** However given that an excess of sodium *tert*-butoxide is employed in catalytic reactions, a pathway in which **IN-3** is formed via reaction between ammonia and an aryl *tert*-butoxy intermediate of the type (**L18**)Ni(Ph)(O^tBu)[221] **IN-6** was also considered. The calculated energies of all modeled reactions are presented in Figure 4-5. Initial complexation of *tert*-butoxide to form **IN-6** is highly exothermic and exergonic, even more so than the formation of **IN-4** via reaction of **IN-3** with ammonia and *tert*-butoxide. At this point (i.e., after the formation of **IN-6**), several routes to form catalytically active species were considered, including: i) reaction of **IN-6** with ammonia to form **IN-4**, which then undergoes C-N reductive elimination to form product aniline; and ii) initial C-O reductive elimination from **IN-6** via **TS-3** to form **IN-7**, which may navigate towards catalytically active species via ligand exchange processes (i.e., with aryl chloride substrate).

The formation of **IN-4** through the reaction of ammonia and **IN-6** is energetically disfavored, which coupled with the relatively high barrier to C-O reductive elimination occurring from **IN-6** via **TS-3**, indicates that the formation of **IN-6** may be deleterious to productive amination catalysis. It is possible that **IN-6** is

the catalytic resting state of ammonia-based C-N cross-couplings involving **L18**, which may have repercussions on the necessary catalyst loading, reaction temperature and equivalency of amine. While the synthesis and isolation of (**L18**)Ni(Ph)(O^{t}Bu) type species was beyond the scope of this investigation, our group demonstrated recently[146] that the **L18**-derived Ni(II) pre-catalyst **C1** catalyzes conceptually related C-O cross-couplings between aryl chlorides and primary and secondary alcohols. These reactions presumably proceed through catalytic cycles involving (**L18**)Ni(aryl)(OR) intermediates, lending credence to the feasibility of **IN-6** forming under amination conditions when **C1** is employed. It is noteworthy that comparatively more forcing conditions are necessary for the **C1**-catalyzed C-O cross-coupling methodology than for C-N cross-coupling protocols (e.g., higher catalyst loading, higher reaction temperatures), which may be due in part to the substantially higher barrier to potentially rate-limiting C-O reductive elimination versus C-N reductive elimination (Fig. 4-5).

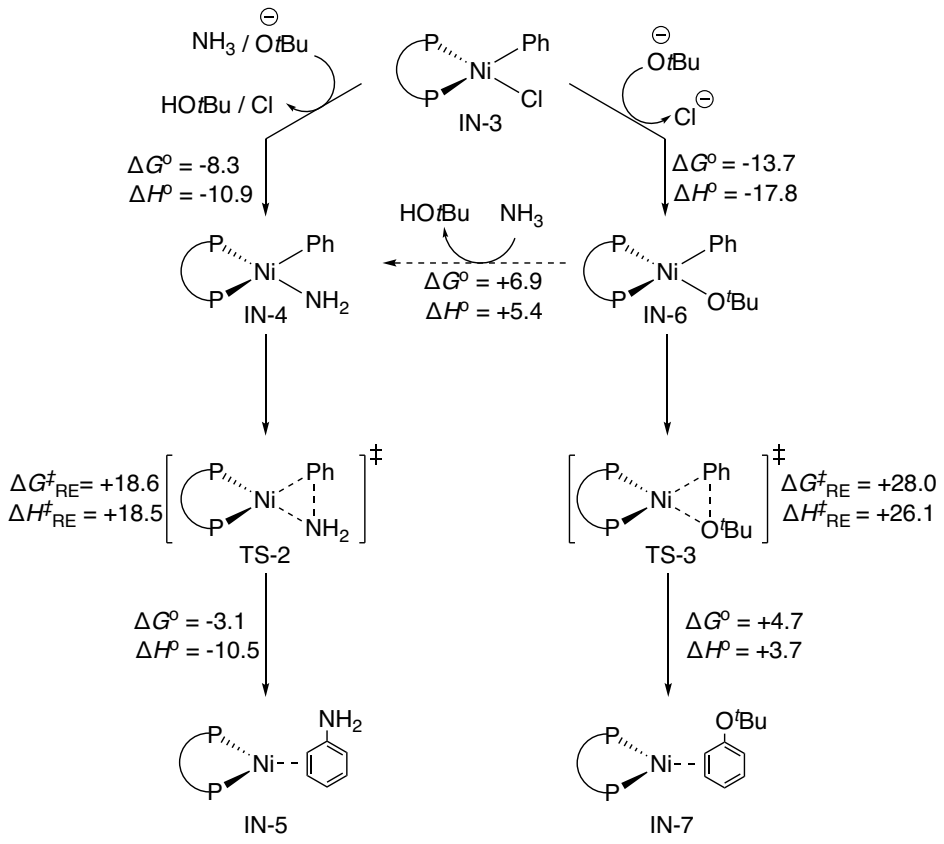


Figure 4-5. Potential reaction pathways involving *tert*-butoxide. Energies are reported in kcal mol^{-1}. P-P = PAd-DalPhos (**L18**).

In modelling the comproportionation[93, 96] of (**L18**)NiCl(*o*-tolyl) and (**L18**)Ni(η^2-toluene) to form (**L18**)NiCl(η^2-toluene) and (**L18**)Ni(*o*-tolyl), the reaction was calculated to have an associated free energy change of -5.3 kcal mol^{-1}. Calibrated GC analysis of catalytically relevant stoichiometric reactions involving the combination of $^{\mathbf{PAd}}\mathbf{Ni}^{\mathbf{II}}$ (1 equiv.), **3.28** (1 equiv.), **4.1** (1.2 equiv.), and NaO-*t*-Bu (1.5 equiv.) confirmed the presence of 2,2'-dimethylbiphenyl (**4.9**) in the product mixture, along with unreacted **3.28**. The formation of **4.9** may be viewed as being in keeping with comproportionation involving (**L18**)NiCl(*o*-tolyl) ($^{\mathbf{PAd}}\mathbf{Ni}^{\mathbf{II}}$) outlined above, whereby **4.9** arises from the subsequent disproportionation of (**L18**)Ni(*o*-tolyl) to (**L18**)Ni(0) and (**L18**)Ni(*o*-tolyl)$_2$, followed by biaryl reductive elimination.[222]

In using excess amine (**4.2**) (2.2 equiv), neither residual aryl chloride (**3.28**) nor biaryl **4.9** was observed, suggesting that comproportionation to form (**L18**)Ni(I)X species is inefficient from (**L18**)Ni(aryl)(*n*-octNH). Analogous stoichiometric reactions conducted in the absence of aryl chloride **3.28**, utilizing 1.1 equiv. of *n*-octylamine yielded only the expected 2-methyl-*N*-octylamine activation product, and no 2,2'-dimethylbiphenyl was observed, indicating that comproportionation to form Ni(I) likely involves σ-arylhalide complexes of the type (L)NiCl(aryl), as has been proposed by others.[93]

Two plausible **L18**-ligated Ni(I)/Ni(III) pathways for the monoarylation of ammonia with chlorobenzene were then modelled (Fig. 4-6 and 4-7), each leading to the common intermediate (**L18**)Ni(Ph)(Cl)NH_2 (**IN-10**). The first (Pathway A) involves: a) C-Cl oxidative addition involving (**L18**)NiCl(η^2-PhCl) (**IN-8**) to yield (**L18**)Ni(Ph)Cl_2 (**IN-9**); b) reaction with *tert*-butoxide and NH_3 to give (**L18**)Ni(Ph)(Cl)NH_2 (**IN-10**); and c) C-N reductive elimination to generate (**L18**)NiCl(η^2-PhNH_2) (**IN-11**). Although steps b) and c) are thermodynamically favourable on the basis of the computed free energies (-12.5 and -40.1 kcal mol^{-1} respectively), the C-Cl oxidative addition step was calculated to be endergonic by 6.4 kcal mol^{-1} and to have a free energy barrier (**TS-4**) of 17.5 kcal mol^{-1}. On the basis of these data, this Ni(I)/Ni(III) pathway, when compared to the Ni(0)/Ni(II) cycle (Fig. 4-4), is less feasible. An alternative Ni(I)/Ni(III) pathway was considered, whereby the aforementioned intermediate (**L18**)Ni(Ph)(Cl)NH_2 (**IN-10**) was instead accessed via thermodynamically favourable amination of (**L1**)NiCl(η^2-PhCl) (**IN-8**)

to yield (**L1**)Ni(NH_2)(η^2-PhCl) (**IN-12**) (-1.9 kcal mol^{-1}), followed by binding of chlorobenzene and subsequent C-Cl oxidative addition (Fig. 4-7).

In contrast to the previous scenario, C-Cl oxidative addition from **IN-12** to give **IN-10** is thermodynamically favoured (-6.0 kcal mol^{-1}). Given that the free energy barrier to C-N reductive elimination from the common intermediate **IN-8** (**TS-5**: 6.3 kcal mol^{-1}) is small relative to that of C-Cl oxidative addition involving **IN-11** (**TS-4'**: 18.0 kcal mol^{-1}), the latter is apparently rate-limiting. Thus, we view a Ni(I)/Ni(III) cycle involving the binding of chlorobenzene to (**L1**)Ni(NH_2), followed by rate-limiting C-Cl oxidative addition, as being a viable competitor to the Ni(0)/Ni(II) pathway (Fig. 4-4) for C-N cross-couplings of ammonia, and possibly other substrates.

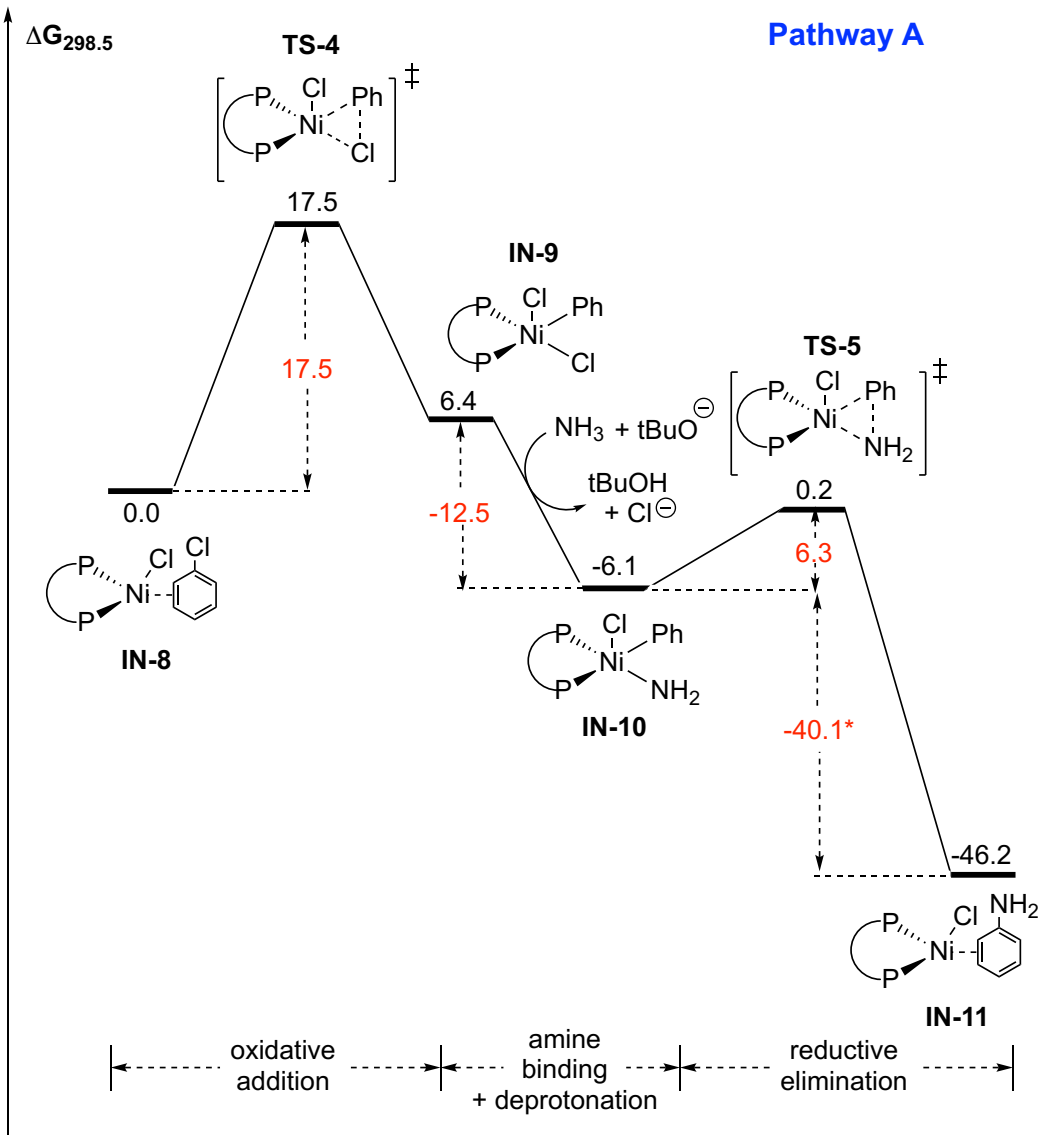


Figure 4-6. Pathway A for the DFT-computed Ni^{I}/Ni^{III} catalytic cycle for the C−N cross-coupling of chlorobenzene and ammonia. P-P = PAd-DalPhos (**L18**). Gibbs Free energies are reported. The B3LYP-XDM method and the 6-311+G(2d,2p) basis set were used for DFT calculations. *Not drawn to scale.

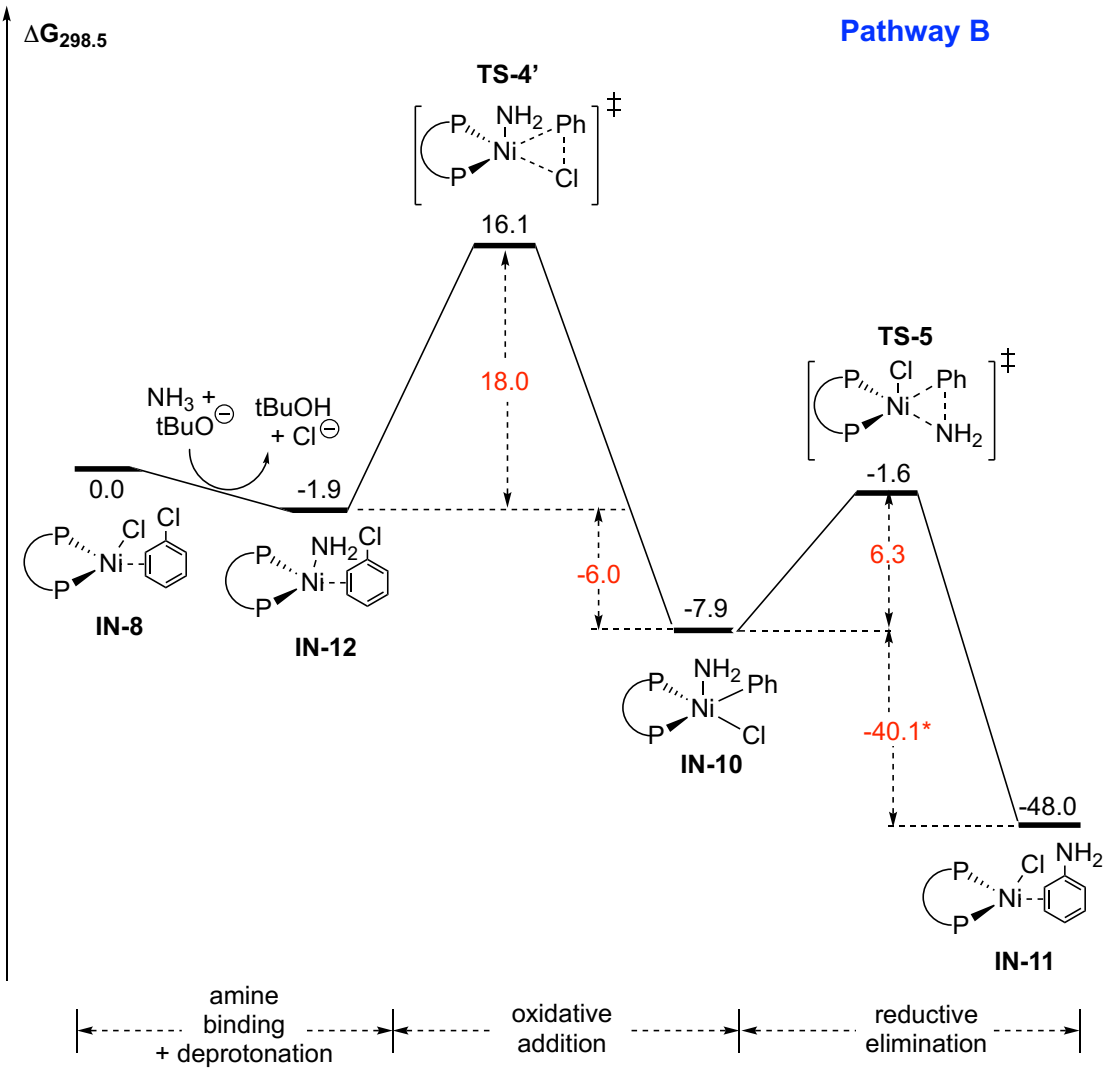


Figure 4-7. Pathway B for the DFT-computed Ni^{I}/Ni^{III} catalytic cycle for the C−N cross-coupling of chlorobenzene and ammonia. P-P = PAd-DalPhos (**L18**). Gibbs Free energies are reported. The B3LYP-XDM method and the 6-311+G(2d,2p) basis set were used for DFT calculations. *Not drawn to scale.

4.4. SUMMARY

In summary, we have explored the influence of bisphosphine ancillary ligation and nickel oxidation state on Ni-catalyzed C-N cross-coupling. This was accomplished via a combined experimental and theoretical investigation focusing on [Ni^{I}(**L**)Cl] and [Ni^{II}(**L**)Cl(*o*-tolyl)] pre-catalysts (**L** = **L8** or **L18**) in the amination of

aryl chlorides with various nitrogen nucleophiles. In particular we were curious as to whether Ni^0/Ni^{II} or parallel Ni^I/Ni^{III} manifolds are dominant under particular conditions, given that both catalytic cycles may be plausible,[69-71, 73, 74] and that elementary chemical processes linking these mechanistic manifolds likely exist.

While both [Ni^I(bisphosphine)Cl] and [Ni^{II}(bisphosphine)Cl(*o*-tolyl)] pre-catalysts proved active in a selection of test C-N cross-couplings, the latter were generally more effective. A dramatic exception to this trend was observed in challenging amide cross-couplings when employing dppf (**L8**) ligation, whereby the Ni^I pre-catalyst out-performed the Ni^{II} pre-catalyst, thereby underscoring the complex interplay between the nature of substrates, Ni oxidation state, and ancillary ligand in influencing catalytic behavior. The efficacy of mononuclear [Ni^I(**L**)Cl] (**L** = **L8** or **L18**) pre-catalysts in enabling C-N cross-coupling is notable, given the observation by Hartwig and co-workers[69] that BINAP-derived [Ni(**L13**)(μ-Cl)]$_2$ species are inactive for the amination of aryl chlorides with primary alkylamines. Although structurally similar [Ni(**L8**)(μ-Br)]$_2$[208] and [Ni(**L8**)(Cl)]$_2$(μ-dppf)][94] species have been shown to form under cross-coupling conditions, related species featuring **L18** ligation are as-yet unknown. It is plausible that the greater steric demand of **L18** is potentially beneficial in favoring the formation of what might be more kinetically competent mononuclear Ni^I species. Computational analyses of bisphosphine-ligated Ni species support the *via*bility of Ni^0/Ni^{II} cycles featuring rate-limiting C-N reductive elimination from [Ni^{II}(**L**)(Ph)amido] species, as well as competitive Ni^I/Ni^{III} mechanisms involving rate-limiting C-Cl oxidative addition to a [Ni^I(**L**)(amido)] intermediate (Fig. 4-5). Given that ideal ancillary design characteristics are likely divergent for these two competing mechanistic manifolds

(Ni^0/Ni^{II} versus Ni^I/Ni^{III}), opportunities and challenges exist with regard to the design of ancillary ligands that serve both to favor one manifold over the other, while optimizing catalytic performance therein. Future efforts related to this research should be devoted to the isolation and characterization of potential intermediates for both Ni^0/Ni^{II} and Ni^I/Ni^{III} pathways, so as to explore their relevance to catalysis.

4.5. EXPERIMENTAL

4.5.1. General Considerations

Unless otherwise stated, all reactions were setup inside a nitrogen-filled inert atmosphere glovebox using oven-dried glassware, and were worked up in air using benchtop procedures. Toluene and hexanes were deoxygenated by sparging with nitrogen followed by passage through a double column solvent purification system packed with alumina and copper-Q5 reactant, and storage over activated 4 Å molecular sieves. Cyclopentyl methyl ether (CPME) was degassed by use of three repeated freeze-pump-thaw cycles and was stored over activated 4 Å molecular sieves. 1,4-Dioxane was dried over Na/benzophenone followed by distillation under a nitrogen atmosphere. Pre-catalysts (**L18**)$NiCl_2$,[102] ^{PAd}**Ni^{II}**,[102] ^{dppf}**Ni^{I}**,[94] and ^{dppf}**Ni^{II}**,[89] were synthesized following literature procedures. Gas chromatography data were obtained on an instrument equipped with a SGE BP-5 column (30 m, 0.25 mm i.d.), and were calibrated by using authentic materials using dodecane as an internal standard. Authentic reaction products 4-(4-methoxyphenyl)morpholine,[88] 4-morpholinobenzonitrile,[92] napthelen-1-amine,[102] *N*-(1-naphthyl)-octylamine,[102] and 4-(cyanophenyl)benzamide,[213] used for calibrated GC analysis were synthesized following literature procedures. All catalytic

experiments were conducted in duplicate (minimum). The magnetism of ^{PAd}**Ni**^{I} was examined by use of Evans' method.[223] Otherwise, all other GC standards, reagents, solvents, and materials were used as received from commercial sources.

4.5.2. Synthesis and Characterization Data

Synthesis of ^{PAd}Ni^{I}. Within a glovebox, a vial containing a magnetic stir bar was charged with **L18** (0.243 g, 0.481 mmol, 1.05 equiv.) and $Ni(cod)_2$ (0.126 g, 0.458 mmol, 1.0 equiv.). To the solid mixture was added benzene (6.0 mL), and the resulting heterogeneous mixture was stirred magnetically at 25 ˚C for 0.5 h. Analysis of the reaction mixture at this stage by use of $^{31}P\{^{1}H\}$ NMR methods revealed partial consumption of **L1** and the appearance of two resonances at 46.1 and 38.4 ppm (J_{PP} = 40.5 Hz), which we tentatively assign to (**L18**)Ni(cod). The reaction vial was then charged with pre-formed (**L18**)$NiCl_2$ (0.290 g, 0.16 mmol, 1.0 equiv.), and the reaction mixture was stirred magnetically at 25 ˚C for 0.5 h. Within a glovebox, hexanes (ca. 4 mL) was added to the crude reaction mixture to induce precipitation of the complex, and the resulting mixture was filtered through a glass sintered frit. The retained solid on the frit was washed with hexanes (ca. 5 x 3 mL) and dried *in vacuo* to afford ^{PAd}**Ni**^{I} as a red paramagnetic solid (0.443 g, 81%). Anal. Found (Calcd) for $C_{30}H_{34}ClNiO_3P_2$: C 59.94 (60.17), H 5.53 (5.73), N <0.5 (0.0) %. μeff = 1.2 μB (25 ^{o}C, C_6H_6; Evan's method). A single crystal suitable for X-ray diffraction analysis was obtained via slow evaporation of a toluene solution of the target complex.

4.5.3. General Procedures

Protocol for the cross-coupling of 1-chloronapthalene and octylamine (GP4-1). In a nitrogen-filled glovebox, pre-catalyst $^{PAd}Ni^{I}$ (3.6 mg, 0.006 mmol, 5 mol %) or $^{PAd}Ni^{II}$ (4.1 mg, 0.006 mmol, 5 mol %), 1-chloronaphthalene (16.3 mL, 0.12 mmol, 1.0 equiv.), sodium *tert*-butoxide (17.3 mg, 0.18 mmol, 1.5 equiv.), and *n*-octylamine (21.8 mL, 0.13 mmol, 1.1 equiv.) were added to a screw capped vial containing a magnetic stir bar, followed by the addition of toluene (2.0 mL). The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to the 25 ^{o}C for 16 h. The reaction vial was then removed from the heating block, followed by addition of dodecane internal standard (1.0 equiv.). The product yield was determined by calibrated GC analysis using authentic products according to the **Workup Method 4-1**.

Protocol for the cross-coupling of 1-chloronapthalene and octylamine using stock solutions of pre-catalyst (GP4-2). For reactions requiring <3 mg of pre-catalyst, the pre-catalyst was delivered by use of stock solutions. $^{PAd}Ni^{I}$: 42.9 mL (0.10 mol %) or 214.5 mL (0.50 mol %) taken from a 0.0084 M toluene stock solution, $^{PAd}Ni^{II}$: 98.8 mL (0.10 mol %) or 494.0 mL (0.50 mol %) taken from a 0.0036 M toluene stock solution.

Protocol for the cross-coupling of 1-chloronapthalene and octylamine with TEMPO (GP4-2). Reactions were conducted on a 0.36 mmol scale otherwise as per **GPA**, with the only deviation being the addition of TEMPO (5.6 mg, 0.036

mmol, 0.1 equiv.) following addition of base, prior to the addition of octylamine. The product yield was determined by calibrated GC analysis using authentic products according to the **Workup Method 4-1**.

Protocol for the cross-coupling of 1-chloronapthalene and octylamine with PhBPin (GP4-4). Reactions were conducted on a 0.36 mmol scale otherwise as per **GPB**, with the only deviation being the addition of PhBPin (12.3 mL, 0.054 mmol, 0.15 equiv.) following addition of base, prior to the addition of octylamine. The product yield was determined by calibrated GC analysis using authentic products according to the **Workup Method 4-1**.

Protocol for the cross-coupling of 4-chlorobenzonitrile and morpholine (GP4-5). In a nitrogen-filled glovebox, pre-catalyst ^{dppf}**Ni**^{I} (3.9 mg, 0.006 mmol, 5 mol %) or ^{dppf}**Ni**^{II} (4.4 mg, 0.006 mmol, 5 mol %), 4-chlorobenzonitrile (16.5 mg, 0.12 mmol, 1.0 equiv.), lithium *tert*-butoxide (14.4 mg, 0.18 mmol, 1.5 equiv.), and morpholine (11.4 mL, 0.13 mmol, 1.1 equiv.) were added to a screw capped vial containing a magnetic stir bar, followed by the addition of CPME (0.25 mL). The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 110 ^{o}C for 16 h. The reaction vial was then removed from the heating block and left to cool to ambient temperature, followed by addition of dodecane internal standard (1.0 equiv.). The product yield was determined by calibrated GC analysis using authentic products according to the **Workup Method 4-1**.

Protocol for the cross-coupling of 4-chlorobenzonitrile and morpholine using stock solutions of pre-catalyst (GP4-6). For reactions requiring <3 mg of pre-catalyst, the pre-catalyst was delivered by use of stock solutions. $^{dppf}Ni^{I}$: 233.0 mL (0.50 mol taken from a 0.008 M toluene stock solution, $^{dppf}Ni^{II}$: 494.0 mL (0.50 mol %) taken from a 0.003 M toluene stock solution. After all reaction components were added, CPME was added to bring the total volume of solvent to 0.75 mL.

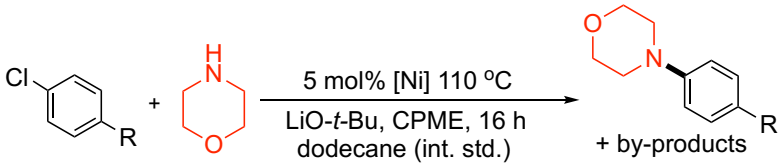
Protocol for the cross-coupling of 4-chlorobenzonitrile and morpholine with TEMPO (GP4-7). Reactions were conducted on a 0.36 mmol scale otherwise as per **GPE**, the only deviation being the addition of TEMPO (5.6 mg, 0.036 mmol, 0.1 equiv.) following addition of base, prior to the addition of octylamine. The product yield was determined by calibrated GC analysis using authentic products according to the **Workup Method 4-1**.

Protocol for the cross-coupling of 4-chlorobenzonitrile and morpholine with PhBPin (GP4-8). Reactions were conducted on a 0.36 mmol scale otherwise as per **GPF**, with the only deviation being the addition of PhBPin (24.6 mL, 0.108 mmol, 0.30 equiv.) following addition of base, prior to the addition of octylamine. The product yield was determined by calibrated GC analysis using authentic products according to the **Workup Method 4-1**.

Protocol for the pre-catalyst reactivity comparison in the cross-coupling of chloroarenes with morpholine (GP4-9). In a nitrogen-filled glovebox, pre-catalyst (0.006 mmol, 5 mol %), aryl chloride (0.12 mmol, 1.0 equiv), lithium *tert*-butoxide (14.4 mg, 0.18 mmol, 1.5 equiv.), and morpholine (11.4 mL, 0.13 mmol, 1.1 equiv.)

were added to a screw capped vial containing a magnetic stir bar, followed by the addition of CPME (0.25 mL). The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to the stated temperature for 16 h. The reaction vial was then removed from the heating block and left to cool to ambient temperature, followed by addition of dodecane internal standard (1.0 equiv.). The product yield was determined by calibrated GC analysis using authentic products according to the **Workup Method 4-1**.

Table 4-4. Pre-catalyst reactivity comparison for the cross-coupling of chlorobenzene and aniline.



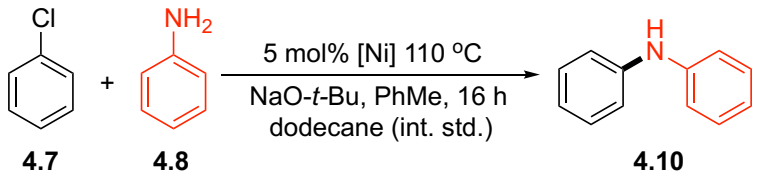
Entry	Ni cat.	R	% Yield
1	(PAd-DalPhos)NiCl (^{PAd}**Ni**^{I})	OMe	3
2	(PAd-DalPhos)NiCl(o-tolyl) (^{PAd}**Ni**^{II})	OMe	8
3	(dppf)NiCl (^{dppf}**Ni**^{I})	OMe	48
4	(dppf)NiCl(o-tolyl) (^{dppf}**Ni**^{II})	OMe	62
5	(PAd-DalPhos)NiCl (^{PAd}**Ni**^{I})	CN	2
6	(PAd-DalPhos)NiCl(o-tolyl) (^{PAd}**Ni**^{II})	CN	2
7	(dppf)NiCl (^{dppf}**Ni**^{I})	CN	88
8	(dppf)NiCl(o-tolyl) (^{dppf}**Ni**^{II})	CN	79

Protocol for the pre-catalyst reactivity comparison in the cross-coupling of ammonia and chloroarenes (GP4-10). In a nitrogen-filled glovebox, pre-catalyst (0.006 mmol, 5 mol %), aryl chloride (0.12 mmol, 1.0 equiv.), sodium *tert*-butoxide (34.6 mg, 0.36 mmol, 3.0 equiv.), and ammonia as a 0.5 M solution in 1,4-dioxane

(1.68 mL, 0.84 mmol, 7.0 equiv.), were added to a screw capped vial containing a magnetic stir bar, followed by the addition of toluene (0.5 mL). The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to the stated temperature for 16 h. The reaction vial was then removed from the heating block and left to cool to ambient temperature, followed by addition of dodecane internal standard (1.0 equiv.). The product yield was determined by calibrated GC analysis using authentic products according to the **Workup Method 4-1**.

Protocol for the pre-catalyst reactivity comparison in the cross-coupling of aniline and chlorobenzene (GP4-11). In a nitrogen-filled glovebox, pre-catalyst (0.006 mmol, 5 mol %), chlorobenzene (12.3 mL, 0.12 mmol, 1.0 equiv.), sodium *tert*-butoxide (17.3 mg, 0.18 mmol, 1.5 equiv.), and aniline (12.1 mL, 0.132 mmol, 1.1 equiv.), were added to a screw capped vial containing a magnetic stir bar, followed by the addition of toluene (2.0 mL). The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 110 ^{o}C for 16 h. The reaction vial was then removed from the heating block and left to cool to ambient temperature, followed by addition of dodecane internal standard (1.0 equiv.). The product yield was determined by calibrated GC analysis using authentic products according to the **Workup Method**.

Table 4-5. Pre-catalyst reactivity comparison for the cross-coupling of chlorobenzene and aniline.



4.7 **4.8** **4.10**

Entry	Ni cat.	% Yield **4.10**
1	(PAd-DalPhos)NiCl (^{PAd}**Ni**^{I})	2
2	(PAd-DalPhos)NiCl(o-tolyl) (^{PAd}**Ni**^{II})	22
3	(dppf)NiCl (^{dppf}**Ni**^{I})	49
4	(dppf)NiCl(o-tolyl) (^{dppf}**Ni**^{II})	86

Protocol for the pre-catalyst reactivity comparison in the cross-coupling of benzamide and 4-chlorobenzonitrile (GP4-12). In a nitrogen-filled glovebox, pre-catalyst (0.006 mmol, 5 mol %), 4-chlorobenzonitrile (16.5 mg, 0.12 mmol, 1.0 equiv.), tripotassium monophosphate (38.2 mg, 0.18 mmol, 1.5 equiv.), and benzamide (16.0 mg, 0.13 mmol, 1.1 equiv.), were added to a screw capped vial containing a magnetic stir bar, followed by the addition of *tert*-butanol (1.0 mL). The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 90 °C for 16 h. The reaction vial was then removed from the heating block and left to cool to ambient temperature, followed by addition of dodecane internal standard (1.0 equiv.). The product yield was determined by calibrated GC analysis using authentic products according to the **Workup Method 4-1**.

Protocol for the reaction rate comparison for pre-catalysts in the cross-coupling of octylamine and 1-chloronaphthalene (GP4-13). In a nitrogen-filled glovebox, pre-catalyst (0.0024 mmol, 1.0 mol %), 1-chloronaphthalene (32.6 mL, 0.24 mmol, 1.0 equiv.), sodium *tert*-butoxide (34.6 mg, 0.36 mmol, 1.5 equiv.), PhBPin (11.0 mL, 0.048 mmol, 0.20 equiv., *where applicable*), dodecane internal standard (1.0 equiv.), and octylamine (45.6 mL, 0.26 mmol, 1.1 equiv.), were added to a screw capped vial containing a magnetic stir bar, followed by the addition of toluene (4.0 mL). The vial was sealed with a cap containing a PTFE septum, and placed on a stir plate *inside* the glovebox; 200 mL aliquots were taken at the designated time intervals and the product yield (*N*-(1-naphthyl)-octylamine, **3**) was determined by calibrated GC analysis using authentic products according to the **Workup Method 4-1**.

Protocol for the reaction of $^{PAd}Ni^{I}$ with PhBPin, cod and base (GP4-14). $^{PAd}Ni^{I}$ (10 mg, 0.17 mmol, 1.0 equiv.), sodium *tert*-butoxide (32.7 mg, 0.34 mmol, 2.0 equiv.), PhBPin (7.6 mL, 0.033 mmol, 2.0 equiv.), and 1,5-cyclooctadiene (750 mL from a 0.05 M C_6D_6 stock solution, 0.037 mmol, 2.2 equiv.), were added to a screw capped vial containing a magnetic stir bar. The vial was sealed with a cap containing a PTFE septum, and placed on a temperature-controlled aluminum heating block set to 65 ^{o}C for 4 h. The vial was then brought into the glovebox, and an NMR sample was prepared. The $^{31}P\{^{1}H\}$ NMR spectra of the crude reaction mixture revealed mutual doublets with chemical shifts of 46.1 and 38.4 ppm, which we attribute to the putative (**L1**)Ni(cod) species (see **Synthesis of $^{PAd}Ni^{I}$** above).

Workup Method 4-1 (Procedure for GC Sample Preparation). Following **GP1-GP14**, after the reaction vial was allowed to cool to room temperature, dodecane was added (1.0 equiv. relative to limiting reagent) to the reaction mixture. The mixture was diluted using ethyl acetate and methanol, was passed through a Kimwipe filter containing a Celite/silica gel pad, and was eluted into a GC vial. Calibrated GC yields are reported by comparison to authentic samples.

4.5.4. Crystallographic Solution and Refinement Data

Crystallographic Solution and Refinement DataCrystallographic data for **PAdNi^{I}** and (**L1$_8$**)Ni(Ph)Cl (Fig. 4-6, below) were obtained at -100 °C on a Bruker D8/APEX II CCD diffractometer equipped with a CCD area detector using graphite monochromated Mo Kα (α = 0.71073 Å) radiation employing a sample that was mounted in inert oil and transferred to a cold gas stream on the diffractometer. Data reduction, correction for Lorentz polarization, and absorption correction (Gaussian integration; face-indexed) were each performed. Structure solution by using the Patterson method was carried out, followed by least-squares refinement on F^2. All non-hydrogen atoms were refined with anisotropic displacement parameters, while all hydrogen atoms were added at calculated positions and refined by use of a riding model employing isotropic displacement parameters based on the isotropic displacement parameter of the attached atom. In the case of **PAdNi^{I}**, two crystallographically independent molecules of the parent compound (along with a half-occupied toluene solvate) were located in the asymmetric unit; for simplicity only one of the crystallographically independent molecules is described in the text. A minute quantity of crystalline (**L1$_8$**)Ni(Ph)Cl (featuring a fully occupied chloroform

solvate) were obtained via slow evaporation of a reaction mixture in which L1, $Ni(cod)_2$ and PhCl were combined in chloroform; see Figure 4-6 below for a thermal ellipsoid plot of (**L18**)Ni(Ph)Cl. Complete crystallographic data in CIF format are available. CCDC 1538174 [(**L18**)Ni(Ph)Cl] and CCDC 1538175 (**PAdNi^{I}**) contain the supplementary crystallographic data for this study. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

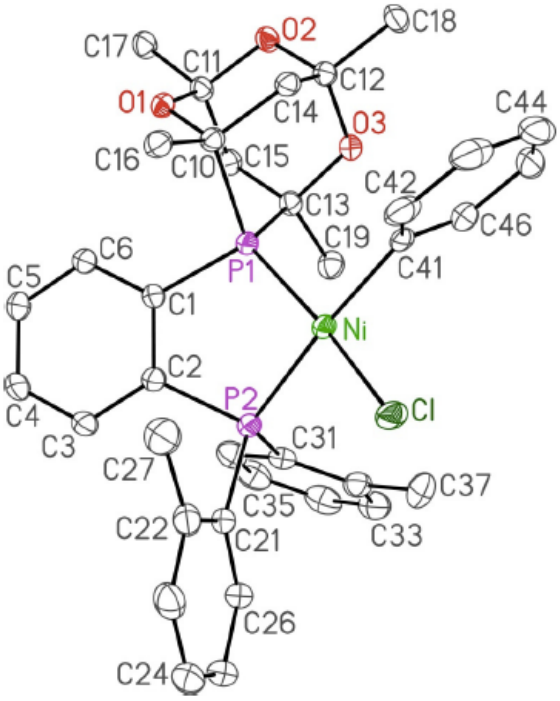


Figure 4-8. Single-crystal X-ray structure of (**L18**)Ni(Ph)Cl, shown at the 30% probability level with H atoms omitted for clarity.

4.5.5. General Computational Details

Geometry optimizations and frequency calculations were performed on all species with the B3LYP functional[214, 215] and the XDM[216, 217] dispersion correction. A mixed

basis set was used, consisting of 6-31G* for C and H, and 6-31+G* for all other elements. Single-point energy calculations on the optimized geometries were carried out using the same B3LYP-XDM method with the 6-311+G(2d,2p) basis set. The XDM damping parameters were a_1=0, a_2=3.7737 Å for the geometry optimizations and a_1=0.4376, a_2=2.1607 Å for the single-point energies. All calculations were performed using the Gaussian 09 software package, along with the postg program for the dispersion energies. The postg program is available at: http://schooner.chem.dal.ca. The thermochemical energies and Cartesian coordinates for all computed species can be found in accompanying Thesis Appendix document.

Table 4-6. Metrical Paramaters: DFT *vs.* Single-crystal X-ray diffraction analysis (XRD)

Compound	Ni-Cl (Å) (XRD)	Ni-Cl (Å) (DFT)	P-Ni-P (°) (XRD)	P-Ni-P (°) (DFT)
^{PAd}**Ni**^{I}	2.150	2.170	88.5	88.3
^{PAd}**Ni**^{Ii}	2.192	2.222	86.6	86.5
(**L18**)Ni(Ph)Cl	2.219	2.197	86.7	86.7

4.5.6. Summary of Computationally Modelled Amination Pathways

Reaction steps are as follows: (1) ligand exchange between chloroarene and LNi(η^2 toluene) to afford LNi(η^2-ArCl), (2) oxidative addition of chloroarene to give LNi(aryl)Cl, (3) transition state barrier for oxidative addition, (4) generation of the amido complex LNi(Ar)NRR', (5) reductive elimination of aniline product, (6) reductive elimination transition state barrier, (7) ligand exchange between toluene

and LNi(η^2-ArNRR') to liberate product and regenerate the active LNi(η^2-toluene) species.

Table 4-7. Summary of DFT calculated free energies for each modelled reaction step for the C-N cross-couping between chlorobenzene and various N-based nucleophiles for the PAd-DalPhos (**L18**) based pathway. Transition state barriers are highlighted in red.

	Nucleophiles / Free Energies (kcal mol^{-1})			
Reaction Step	Ammonia	Aniline	Morpholine	Formamide
1	-3.5	-3.5	-3.5	-3.5
2	-26.1	-26.1	-26.1	-26.1
3	7.2	7.2	7.2	7.2
4	-8.3	-12.2	-8.2	-16.2
5	-3.1	-3.8	-14.0	0.7
6	18.6	16.7	14.4	24.0
7	-2.3	3.5	7.2	3.8

Table 4-8. Summary of DFT calculated free energies for each modelled reaction step for the C-N cross-couping between chlorobenzene and various N-based nucleophiles for the dppf (**L8**) based pathway. Transition state barriers are highlighted in red.

	Nucleophiles / Free Energies (kcal mol^{-1})		
Reaction Step	Ammonia	Aniline	Morpholine
1	-3.8	-3.8	-3.8
2	-19.2	-19.2	-19.2
3	8.7	8.7	8.7
4	-8.6	-14.3	-7.8
5	-8.7	-6.8	-15.1
6	18.5	18.3	13.1
7	-2.9	1.9	1.3

Chapter 5

Probing the Influence of PAd-DalPhos Ancillary Ligand Structure on Nickel-Catalyzed Ammonia Arylations

5.1. RESEARCH OVERVIEW AND CONTRIBUTION REPORT

This author wishes to clarify his contributions to the research described in Chapter 5 of this Thesis document. This chapter details the results of a combined experimental/computational study directed toward gaining insight regarding the catalytic performance of the PAd-DalPhos (**L18**) ligand family in nickel-catalyzed ammonia arylations for aniline synthesis. Primary arylamine C-N reductive eliminations occurring from arylnickel(II) parent amido complexes of the type (**L**)Ni(Ph)(NH_2) were modeled by use of density-functional theory (DFT) methods, for a series of **L18** derivatives. The dual aims were to assess the impact of structural modifications to **L18** on potentially rate-limiting C-N reductive elimination, and to identify promising candidates for experimental inquiry. Increasing the steric demand of the P_{aryl} groups from *o*-tolyl (in **L18**) to mesityl (in **L43**) resulted in a

significant lowering of the barrier to C-N reductive elimination ($\Delta G^{\ddagger}_{RE}$), which can be attributed in part to interactions between the ligand P_{aryl} groups and the nickel-bound amido ligand, as observed in non-covalent interaction (NCI) plots of the reductive elimination transition-state structures. Despite the favorability of **L43** predicted on the basis of computational analysis focusing on C-N reductive elimination, this ancillary ligand performed poorly in experimental testing versus **L18**, suggesting that in practice the significant steric demands of **L43** may discourage formation of key catalytic intermediates. Modifications to the steric profile of the P_{aryl} groups in **L18** led to dramatic changes in catalytic performance, with the presence of an *ortho*-methyl proving to be important, amongst the **L18** variants tested, in achieving useful catalytic performance in the Ni-catalyzed monoarylation of ammonia.

My contributions to this work include: conceived of the project idea; synthesis of all compounds; conducted all of the catalytic reactions; performed the majority of the DFT calculations; characterization of compounds reported herein with the exception of (**L23**)$NiCl_2$ (completed by J.P.T.); interpreted all of the data; and wrote the manuscript. This project was conducted in collaboration with Prof. Erin Johnson of Dalhousie, who located all of the oxidative addition transition state species reported herein, and conducted the non-covalent interaction (NCI) calculations. Authors M.J. Ferguson and Y. Zhou conducted the X-ray diffraction analyses of **L43** and (**L43**)$NiCl_2$. This work has been published in Organometallics. **Reference:** Lavoie, C.M.; Tassone, J.P.; Ferguson, M.J.; Zhou, Y.; Johnson, E.R.; Stradiotto, M. Probing the Influence of PAd-DalPhos Ancillary Ligand Structure on

Nickel-Catalyzed Ammonia C-N Cross-Coupling. *Organometallics*. **2018**, *37*, 4015-4023.

5.2. INTRODUCTION

The significance of utilizing ammonia (NH_3) in transition metal-catalyzed carbon-nitrogen (herein C-N) cross-coupling transformations for the production of primary arylamines, has been described previously in this document (Chapter 2, section 2.3). Therefore only a brief introduction is provided for the current chapter. As described prior, the successful use of NH_3 in cross-coupling methods is difficult to achieve on account of several salient challenges, which include but are not restricted to: catalyst deactivation via ammonia induced ancillary ligand dissociation;[136] slow C-N bond reductive elimination from sterically unencumbered parent amido intermediates;[137] uncontrolled polyarylation of the initial primary arylamine product,[31, 39] among others. These challenges have largely been addressed in the domain of palladium-catalyzed C-N cross-coupling (i.e., Buchwald-Hartwig Amination, BHA) through the application of optimally configured ancillary ligands (e.g., JosiPhos,[47] AdBrettPhos,[224] Mor-DalPhos,[53, 225] BippyPhos,[44] DiMeIHept^{Cl},[226] among others), which collectively give rise to Pd-catalysts capable of effecting selective ammonia monoaryltions with a useful spectrum of electrophiles, including (hetero)aryl chlorides.

Recently there has been considerable progress made towards the development of complementary amination catalysts based on nickel.[186, 187] If utilized in sufficiently low quantities (e.g., <5 mol%), such protocols can offer economic and other advantages over conventional BHA protocols based on

palladium. To date, three ancillary ligands have emerged as being particularly effective in Ni-catalyzed ammonia monoarylation chemistry (**L15**, **L16**, and **L18**, Fig. 5-1). In 2015 our group[84] along with the Hartwig group[71] independently reported on the first Ni-catalyzed ammonia monoarylation with (hetero)aryl chlorides for the synthesis of primary arylamines (Fig. 5-1) - a breakthrough that was enabled in both instances by the application of relatively electron-rich, sterically bulky ferrocene-based JosiPhos ligands (**L15** and **L16**). In an effort to circumvent the use of expensive JosiPhos ligands which are sold commercially as single enantiomers, we reported[102] in 2016 on the development of the *ortho*-phenylene bridged bidentate phosphine PAd-DalPhos (**L18**), which when employed in its (**L18**)NiCl(*o*-tolyl) pre-catalyst form, enables the C-N cross-coupling of a broad scope of (hetero)aryl (pseudo)halides with ammonia[102] and related NH reagents (e.g., primary alkylamines,[102] primary amides[213]) under mild reaction conditions. The key design features of **L18** (i.e., high steric demand, modestly electron-donating) were intended to facilitate ammonia monoarylations, given that such ancillary ligands might promote rate-limiting primary aniline C-N reductive elimination and discourage subsequent diarylation, within a presumptive Ni^{0}/Ni^{II} cycle.[72, 122]

Given that only **L15**-**L16** and **L18** are known to enable Ni-catalyzed ammonia monoarylations with demonstrated substrate scope, there exists a need for fundamental studies directed towards probing the influence of ancillary ligation on catalytic performance in such transformations. With this in mind, we sought to probe the impact on catalytic performance in Ni-catalyzed C-N cross-coupling reactions involving ammonia arising from structural modifications to **L1**, with the

intention of leveraging new design concepts to inform the development of increasingly effective **L1** variants. In response, we have undertaken a combined computational and experimental investigation of Ni-catalyzed ammonia arylations, involving **L1** and related structural variants, which we disclose herein.

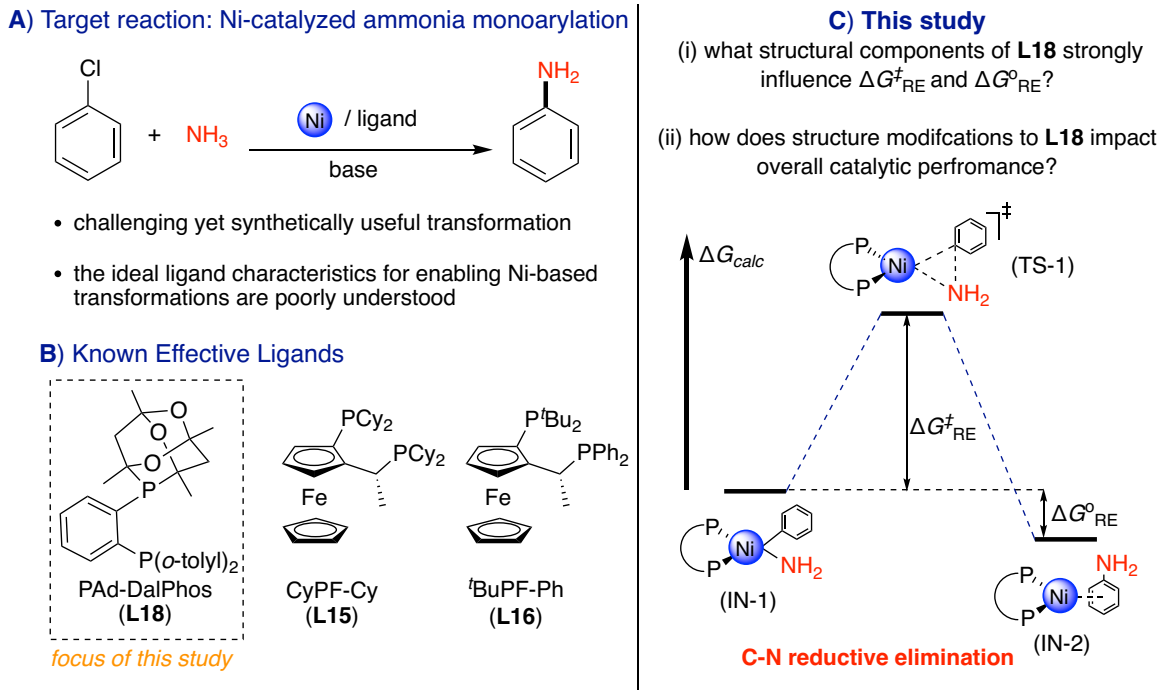


Figure 5-1. An overview of this research study. RE = reductive elimination.

5.3. RESULTS AND DISCUSSION

5.3.1. Computational Modeling of Aniline C-N Reductive Elimination

We have previously evaluated complete catalytic cycles for Ni-catalyzed C-N cross-coupling reactions involving **L18** by use of density-functional theory (DFT) methods.[72, 122] In all examined cases, these calculations predicted that within a a Ni^0/Ni^{II} cycle, C-N reductive elimination occurring from (**L**)Ni(aryl)(NHR) intermediates is rate-limiting. As such, for the purposes of this study we explored the cross-coupling of chlorobenzene and ammonia to furnish aniline by use of DFT

calculations, focusing exclusively on comparing $\Delta G°_{RE}$ and $\Delta G^{‡}_{RE}$ values associated with aniline C-N reductive elimination from (**L**)Ni(Ph)(NH_2) (**IN-1**) intermediates via **TS-1** to afford (**L**)Ni(η^2-aniline) (**IN-2**) for each of PAd-DalPhos (**L18**) and structural analogues (**L23,** and **L32-L43**; Fig. 5-2). The variants of **L18** that I selected to examine featured the following structural modifications: extension of the phosphaadamantane (CgP) group alkyl chain length (**L32**); incorporation of phenylene backbone substituents (**L33**-**L35**); incorporation of heteroatoms into the backbone (**L36**-**L37**); and varying the P_{aryl} substituents (**L23**, **L38**-**L43**). The B3LYP-XDM method[214-217] and the 6-311+G(2d,2p) basis set[217] were employed, and the geometry optimizations and frequency calculations were performed with a smaller, mixed basis set, and frequencies were used to assign stationary points as either minima (no imaginary frequencies) or transition-states (one imaginary frequency).

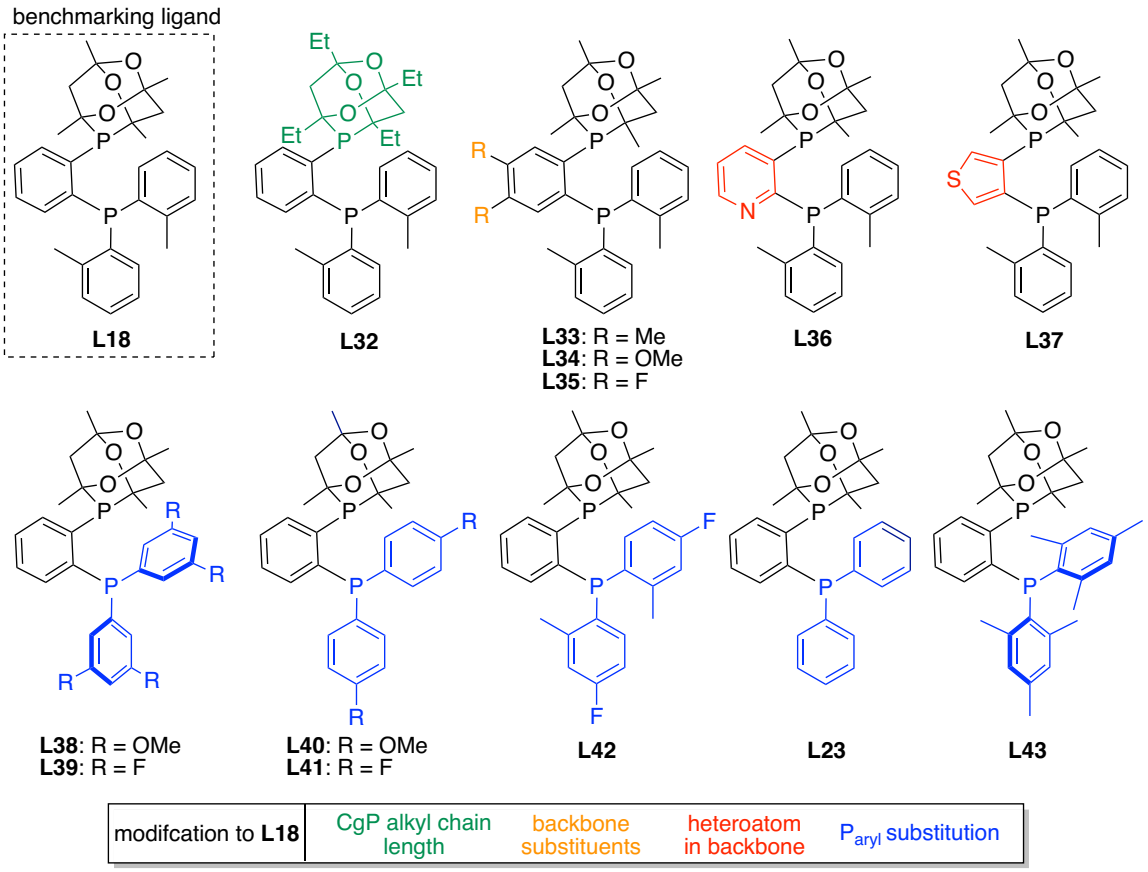


Figure 5-2. Structural analogues of **L18** selected for the current study.

The computed ΔG°_{RE} and $\Delta G^{\ddagger}_{RE}$ values for the C-N reductive elimination of aniline from complexes of the type (**L**)Ni(Ph)(NH_2) (**IN-1**) are presented in Figure 5-3. The overall reaction (ΔG°_{RE}) is predicted to be thermodynamically favored for each of the examined **IN-1** variants, with the ΔG°_{RE} spanning $-12.3 \leq \Delta G^{\circ}_{RE} \leq -1.7$ kcal mol^{-1}. Perhaps the most notable trend across the series is the observation that the computed free energy barrier ($\Delta G^{\ddagger}_{RE}$) for **IN-1** species featuring the modeled ligands is influenced by the presence of *ortho*-methyl substitution on the P_{aryl} groups, as found in the parent ligand **L18**: relatively low barriers ≤ 18.8 kcal mol^{-1} are calculated for **L18** variants featuring *ortho*-methyl substitution, whereas higher barriers (≥ 21.1 kcal mol^{-1}) are encountered in the absence of such substitution.

Our finding that the incorporation of *para*-fluoro substituents on the P(*o*-tolyl)$_2$ group in **L18** to give **L42** resulted in negligible variation of the $\Delta G°_{RE}$ and $\Delta G^{‡}_{RE}$ values, suggests that **L18** is relatively immune to such electronic perturbations. In exploring these ideas further, extension of the CgP alkyl length from Me to Et (**L32**), the addition of electronically and/or structurally varied substituents to the phenylene backbone (**L33**-**L35**), or incorporating heteroaryl backbones in place of phenylene in (**L36**-**L37**) each had minimal effect on the $\Delta G^{‡}_{RE}$ values (all within 0.4 kcal mol^{-1} of **IN-1** featuring **L18**). The $\Delta G°_{RE}$ values arising from **IN-1** complexes featuring the (aryl)P(*o*-tolyl)$_2$ type ligands **L32**-**L37** were found to be somewhat more varied, with the 3,4-substituted thiophene version (**L37**) in particular predicted to afford a significantly more exergonic C-N reductive elimination ($\Delta G°_{RE}$ = -12.3 kcal mol^{-1}) than the other **IN-1** variants. While we are currently unsure as to the specific origins of the differing $\Delta G°_{RE}$ values arising from **IN-1** complexes featuring **L18** (PAd-DalPhos) or **L37** (ThioPAd-DalPhos), we have observed that in selected Ni-catalyzed C-N cross-coupling applications involving primary alkylamines under low-loading conditions, the performance of **L37** is indeed superior to that of **L18**.[227]

In examining C-N reductive elimination from **IN-1** species featuring exclusively *meta* or *para*-substituted P$_{aryl}$ groups (e.g., **L38**-**L41**), or a simple (aryl)PPh$_2$ donor unit (PhPAd-DalPhos, **L23**), minimal impact on $\Delta G^{‡}_{RE}$ was noted; however, such modifications resulted in some modest changes to $\Delta G°_{RE}$, as seen in the comparison of **L38** ($\Delta G°_{RE}$ = -1.7 kcal mol^{-1}) and **L39** ($\Delta G°_{RE}$ = -5.6 kcal mol^{-1}). Given the apparent benefits of the P(*o*-tolyl)$_2$ moiety in **L18**, I speculated that

related ancillary ligand variants featuring di-*ortho*-methyl substitution on the P_{aryl} groups might give rise to even lower $\Delta G^{\ddagger}_{RE}$ values. Consistent with this hypothesis, replacement of the P(*o*-tolyl)$_2$ moiety in **L18** with a sterically demanding dimesitylphosphino (i.e., $PMes_2$) donor group (**L43**) led to a significant reduction in the calculated $\Delta G^{\ddagger}_{RE}$ value from the related **IN-1** species (16.4 versus 18.6 kcal mol^{-1} for **L43** and **L18**, respectively), as depicted in Figure 5-3.

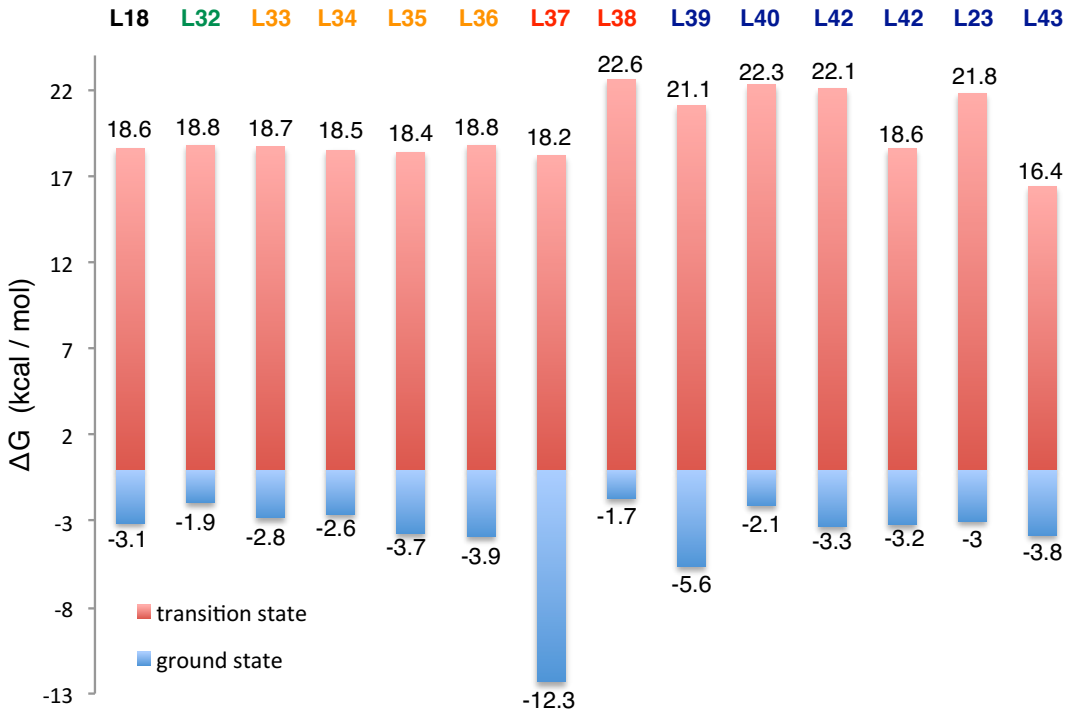


Figure 5-3. Computed ΔG°_{RE} (blue) and $\Delta G^{\ddagger}_{RE}$ (red) values associated with aniline C-N reductive elimination from (**L**)Ni(Ph)(NH_2) (**IN-1**) involving **L18** and structural analogues (**L23**, **L32**-**L43**).

In an effort to gain further insight into the potential role of P_{aryl} steric contributions to the observed difference in $\Delta G^{\ddagger}_{RE}$ values calculated for **IN-1** complexes featuring **L18** and its structural analogues, we generated non-covalent interaction (NCI) plots for the C-N reductive elimination transition-state species

(**TS-1**) based on **L18**, **L23**, and **L43** (Fig. 5-4). NCI plots provide a convenient visualization of inter- and intramolecular interactions in real space.[228, 229] These are generated by plotting the isosurface of the reduced density gradient for a defined region of space; the resulting colored isosurfaces indicate regions in space wherein the electron density of different domains of the ligand are interacting in a non-covalent manner (e.g., steric repulsion, π-π stacking, van der Waals interactions). The major NCI features of the defined region of the **L18** derived transition-state are: CH-π interactions between the CH_3 groups of the CgP unit and the Ni-bound phenyl ligand; and interactions between the *ortho*-methyl group of the P_{aryl} fragment and the Ni-bound amido ligand. While the CH-π interactions observed in the **L18**-based transition-state are present in both the **L23** and **L43** derived **TS-1** structures, there are no significant interactions between the Ni-bound amido group and the phenyl groups on **L23**, whereas interactions of this type are present in the **L43**-based transition-state structure. The observation that the NCI data correlate with the calculated $\Delta G^{\ddagger}_{RE}$ values (**L23** > **L18** > **L43**) highlights the benefits of steric loading on the P_{aryl} groups of **L18** ancillary ligand variants as a means of promoting C-N reductive elimination. Schoenebeck and coworkers[230] recently exploited this effect in achieving Pd-centered Ph-CF_3 reductive elimination by utilizing a CF_3-substituted bis(diphenylphosphino)ethane (dppe) ancillary ligand, which induces ground-state destabilization and thus a lowering of the transition-state barrier via electrostatic repulsion of the bisphosphine ancillary ligand and the reacting phenyl and CF_3 groups.

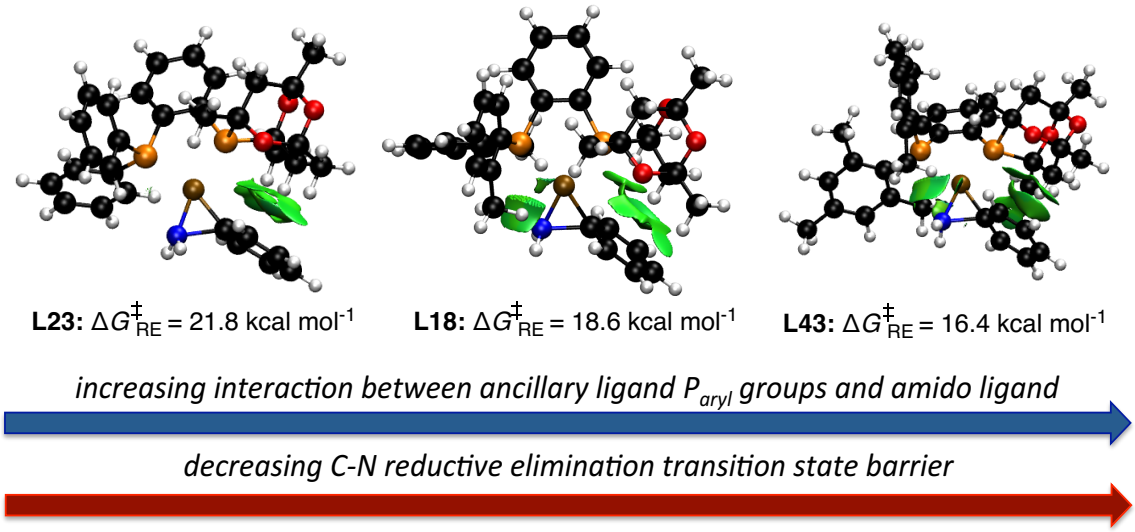


Figure 5-4. Non-covalent interaction (NCI) isosurfaces for **TS-1** structures featuring **L18**, **L23**, and **L43**. Atom colors: Ni (brown), C (black), H (white), O (red), P (orange), N (blue).

5.3.2. Synthesis of Hitherto Unknown L43

Our computational analyses indicated that the more sterically demanding **L43**, which exhibits a relatively low barrier for C-N reductive elimination, might give rise to more efficient ammonia monoarylation chemistry relative to **L18** and **L23**, assuming that arylnickel(II) parent amido intermediates of the type (**L**)Ni(Ph)NH_2 are accessed in a comparable manner for these ligands. I sought to test this assertion experimentally by comparing the catalytic behavior of nickel complexes supported by each of **L18**, **L23**, and **L43** in C-N cross-coupling test reactions involving ammonia and aryl chlorides. The new bisphosphine **L43** was prepared in a manner analogous to that used for the synthesis of **L18**[102] (Fig. 5-5A), and was fully characterized on the basis of NMR spectroscopy, high-resolution mass spectrometric data, and by use of X-ray crystallographic techniques (Fig. 5-5B).

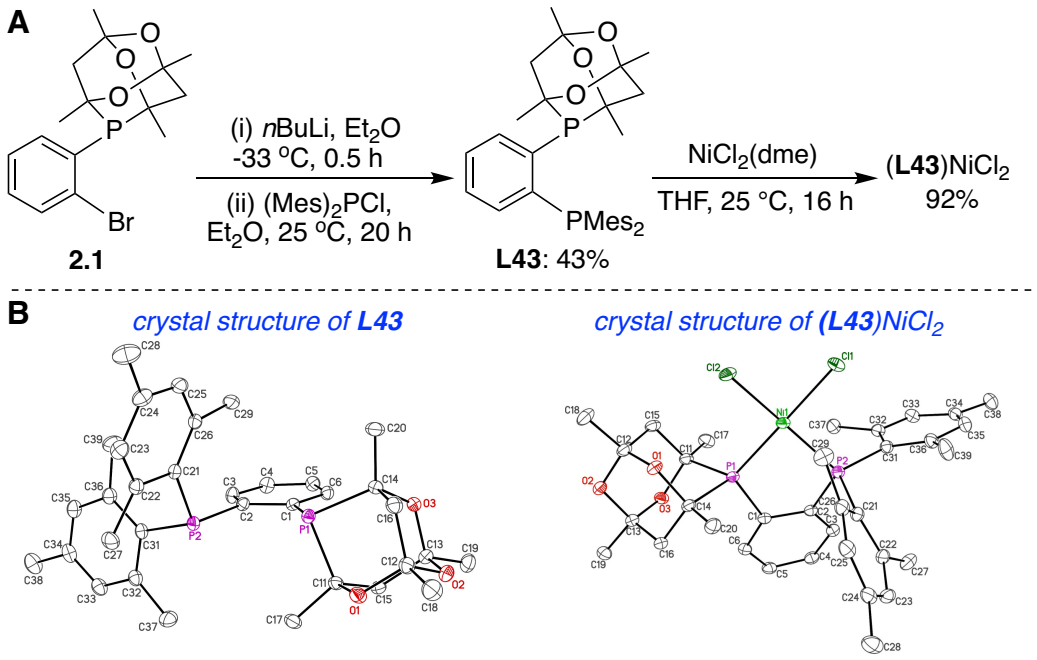
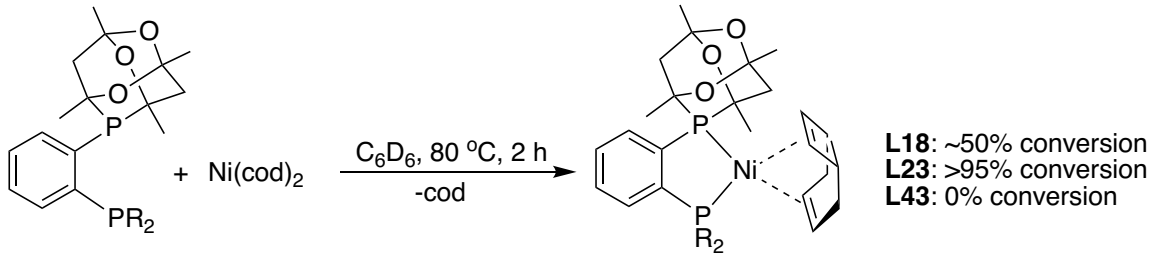


Figure 5-5. Synthesis (**A**) and single-crystal X-ray structures (**B**) of **L43** and (**L43**)$NiCl_2$, represented with thermal ellipsoids at the 30% probability level, and with hydrogen atoms omitted for clarity. Selected interatomic distances (Å) and angles (°) for (**L43**)$NiCl_2$: Ni-P1 2.1902(6); Ni-P2 2.1738(6); Ni-Cl1 2.2135(6); Ni-Cl2 2.1840(6), P1-Ni-P2 88.06(2). dme = 1,2-dimethoxyethane.

5.3.3. Experimental Testing of Select Ligand Variants

In a preliminary effort to assess the relative catalytic performance of catalysts based on **L18**, **L23**, and **L43**, I conducted nickel-catalyzed C(sp^2)-N test cross-couplings involving 4-chlorobiphenyl (**2.3**) and ammonia to furnish 4-aminobiphenyl (**2.4**), employing 5 mol % of ligand and $Ni(cod)_2$, under conditions we had established in a prior report.[102] Monitoring the consumption of **2.3** over time (Fig. 5-9 of the experimental section) revealed that catalyst mixtures of **L18**/$Ni(cod)_2$ were the most active, with complete conversion of **2.3** being observed after only 30 minutes. While our observation that the less hindered **L23** variant gave rise to slower turnover relative to **L18** was expected on the basis of their calculated $\Delta G^{\ddagger}_{RE}$ values (**L18**: 18.6 kcal mol^{-1}, **L23**: 21.8 kcal mol^{-1}), the

comparatively modest consumption of **2.3** (ca. 20 % conversion after 30 minutes) when employing **L43**/Ni(cod)$_2$ catalyst mixtures was not anticipated. Furthermore, the computed barriers to C-Cl oxidative addition occurring from intermediates of the type (**L**)Ni(η^2-PhCl) are comparatively low for both **L18** (7.2 kcal mol^{-1})[72] and **L43** (7.9 kcal mol^{-1}), indicating that the difference in observed activity is not likely the result of slow oxidative addition in the case of **L43**. I speculated that inefficient substitution of a diene ligand in Ni(cod)$_2$ by the sterically encumbered **L16** might explain in part its inferior activity. To examine this hypothesis, I prepared 1:1 mixtures of each of **L18**, **L23**, or **L43** and Ni(cod)$_2$ in C_6D_6 (2 h, 80 ^oC) and monitored the formation of putative (**L**)Ni(cod) species by use of $^{31}P\{^1H\}$ NMR analysis (Scheme 1); a structurally related 1,1'-bis(diphenylphosphino)ferrocene (dppf)-based (**L**)Ni(cod) complex was recently characterized by use of X-ray crystallographic techniques.[95] Whereas **L18** and **L23** each gave rise to partial (**L18**) or complete (**L23**) conversion to the putative (**L**)Ni(cod) species, only free ligand was detected in the case of **L43**. Collectively these observations confirm that while **L43** may indeed be efficient in promoting reductive elimination from **IN-1** type intermediates when formed, the significant steric demands of this ancillary ligand may lead to inefficient formation of requisite ligated pre-catalyst species (e.g., formation of pre-catalyst (**L16**)Ni(cod) from Ni(cod)$_2$ *in situ*).



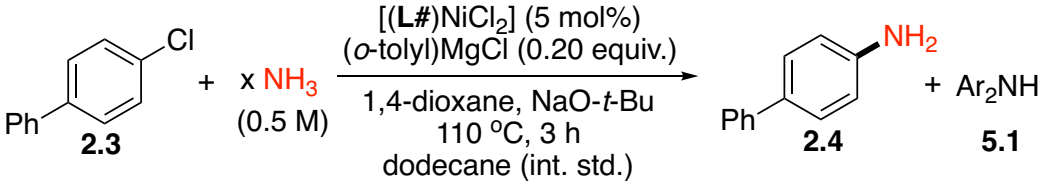
Scheme 5-1. Extent of ligand substitution reactions between **L18**, **L23**, or **L43** and $Ni(cod)_2$ on the basis of $^{31}P\{^1H\}$ NMR spectroscopic data. cod = 1,5-cyclooctadiene

In light of the poor reactivity observed between $Ni(cod)_2$ and **L43**, we turned our attention to the synthesis of an (**L43**)NiCl(*o*-tolyl) pre-catalyst. Such pre-catalysts routinely out-perform **L**/$Ni(cod)_2$ mixtures by virtue of avoiding potentially inhibiting cod,[35, 139] and by offering ancillary ligand pre-coordination to nickel. Treatment of $NiCl_2$(dme) with each of **L18**, **L23**, and **L43** resulted in the clean formation of the target (**L**)$NiCl_2$ complexes; the X-ray structure of (**L43**)$NiCl_2$ is presented in Figure 5-5. Treatment of (**L43**)$NiCl_2$ with (*o*-tolyl)MgCl under established conditions[102] resulted in the formation of a new product exhibiting two resonances appearing at 53.4 and 29.0 ppm (J_{PP} = 11.2 Hz) in the $^{31}P\{^1H\}$ NMR spectrum of the crude reaction mixture, which we tentatively assign to the target (**L43**)NiCl(*o*-tolyl) complex. Unfortunately, attempts to isolate pure material from such reactions led to decomposition of the putative target complex into unidentified paramagnetic impurities, an occurrence which has been observed for some other bidentate phosphine-based (**L**)NiCl(*o*-tolyl) complexes.[91, 139] Given the apparent complexity associated with the synthesis of (**L43**)NiCl(*o*-tolyl), in moving forward I opted to employ (**L**)$NiCl_2$/(*o*-tolyl)MgCl mixtures to achieve formation of the desired (**L**)NiCl(*o*-tolyl) catalyst precursor *in situ*; proof-of-principle experimentation comparing the catalytic performance of pre-formed (**L18**)NiCl(*o*-tolyl) and

(**L18**)$NiCl_2$/(*o*-tolyl)MgCl mixtures demonstrated the viability of this approach (see GP5-3 of the experimental section for details).

I began the reactivity survey by examining the impact of ammonia concentration on the selectivity of the (**L18**)$NiCl_2$/(*o*-tolyl)MgCl-based amination of 4-chlorobiphenyl (**2.3**, herein denoted as ArCl) with NH_3 (0.5 M in 1,4-dioxane) to produce 4-aminobiphenyl (**2.4**, herein denoted as $ArNH_2$), and potentially bis(4-biphenylyl)amine (**5.1**, herein denoted as Ar_2NH). Using (**L18**)$NiCl_2$ (5 mol %), (*o*-tolyl)MgCl (0.2 equiv), sodium *tert*-butoxide (2.0 equiv) as base, and ammonia (10 equiv) relative to ArCl, resulted in complete conversion of ArCl at 110 ˚C and relatively good selectivity for $ArNH_2$ (Table 1, entry 4). Decreasing the amount of ammonia (3 or 7 equiv), while keeping the concentration of ArCl the same, resulted in only a moderate decrease in the yield of $ArNH_2$ (Table 1, entries 2 and 3); however, modestly better selectivity was observed when using 7 equivalents of ammonia versus 3 equivalents. Utilizing 1 equivalent of ammonia led to incomplete conversion of ArCl, negligible quantities of $ArNH_2$, and significant formation of Ar_2NH (Table 1, entry 1). The trend of increased ammonia concentration leading to improved monoarylation selectivity is likely attributed to an increase in the ratio of (**L18**)Ni(aryl)(NH_2) to (**L18**)Ni(aryl)(NHaryl) intermediates, given that both ammonia and the monoarylation product $ArNH_2$ are competing substrates.

Table 5-1. Ancillary ligand screen in the nickel-catalyzed C-N cross-coupling of 4-chlorobiphenyl (**2**) with ammonia. Quantities of **2.3**, **2.4**, and **5.1** calculated on the basis of calibrated GC data, using dodecane and authentic products as internal standards.



Entry	Ligand	NH_3 equiv.	% **2.3**	% Yield **2.4**	% Yield **5.1**	$ArNH_2$ / Ar_2NH
1	L18	1	48	0	27	0
2	L18	3	0	72	15	4.8
3	L18	7	0	72	9	9
4	L18	10	0	81	8	10.1
5	L23	10	0	0	36	0
6	L43	10	0	12	37	0.3
7	L15	10	0	88	3	29.3

Having identified optimized conditions for achieving selectivity for $ArNH_2$ with pre-catalyst (**L18**)$NiCl_2$ (i.e., Table 1, entry 4), I then examined the reactivity profile of related (**L**)$NiCl_2$ pre-catalysts featuring **L23** and **L43**. While full consumption of ArCl was observed in both cases (Table 1, entries 5 and 6), the diarylated product Ar_2NH was obtained as the major product. Having shown **L18** to be superior to both **L23** and **L43** in this application, I subsequently probed the catalytic abilities of the analogous JosiPhos pre-catalyst (**L15**)$NiCl_2$,[84] to provide a comparison of what can be viewed as the two most highly effective ligands known for Ni-catalyzed ammonia arylations: CyPF-Cy (**L15**)[71, 85, 86, 231] and PAd-DalPhos (**L18**).[102, 186] Use of (**L15**)$NiCl_2$/(*o*-tolyl)MgCl catalyst mixtures under our optimized conditions resulted in the consumption of ArCl and somewhat improved selectivity for $ArNH_2$ over Ar_2NH (Table 1, entry 7) relative to that achieved by use of (**L18**)$NiCl_2$/(*o*-tolyl)MgCl (Table 1, entry 4).

In an effort to better understand the diverse reactivity profiles exhibited by each of the (**L**)$NiCl_2$ pre-catalysts examined above (**L** = **L15**, **L18**, **L23**, and **L43**), I monitored the reaction mixture product distribution at various time intervals throughout the course of catalytic experiments. Pre-catalysts (**L18**)$NiCl_2$ and (**L15**)$NiCl_2$ gave rise to the fastest consumption of ArCl, with each achieving full conversion within 60 minutes (Fig. 5-6). This was accompanied in both cases by a rapid increase in the yield of primary arylamine $ArNH_2$ (Fig. 5-7), and minimal formation (<10%) of diarylated Ar_2NH (Fig. 5-8). Pre-catalysts (**L23**)$NiCl_2$ and (**L43**)$NiCl_2$ gave rise to comparatively slow consumption of ArCl, with each requiring 120 minutes to achieve full conversion (Fig. 5-6). Despite substantial quantities of secondary arylamine Ar_2NH being formed throughout the reaction (Fig. 5-8), the amount of primary arylamine $ArNH_2$ detected was consistently low (<15%, Fig. 5-7), indicating that uptake of initially formed $ArNH_2$ is likely rapid for catalyst systems featuring **L23** or **L43**. For ligand-specific time course data, see Figures 5-10 - 5-13.

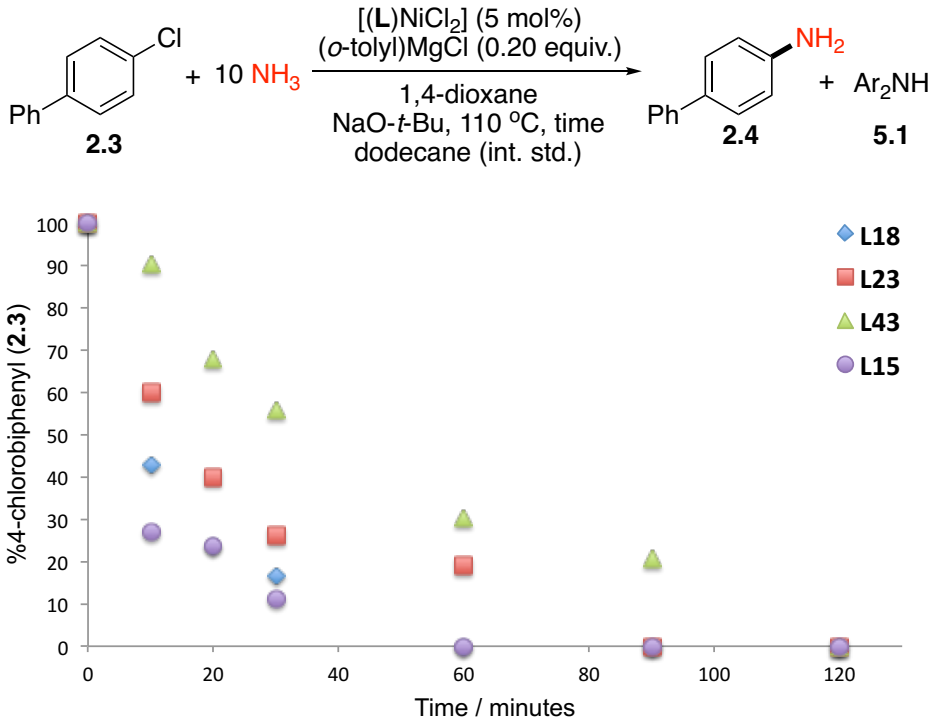


Figure 5-6. Time course for the conversion of 4-chlorobiphenyl (**2.3**) using the (**L**)$NiCl_2$/(*o*-tolyl)MgCl system. See **GP5-4** of the experimental section for details.

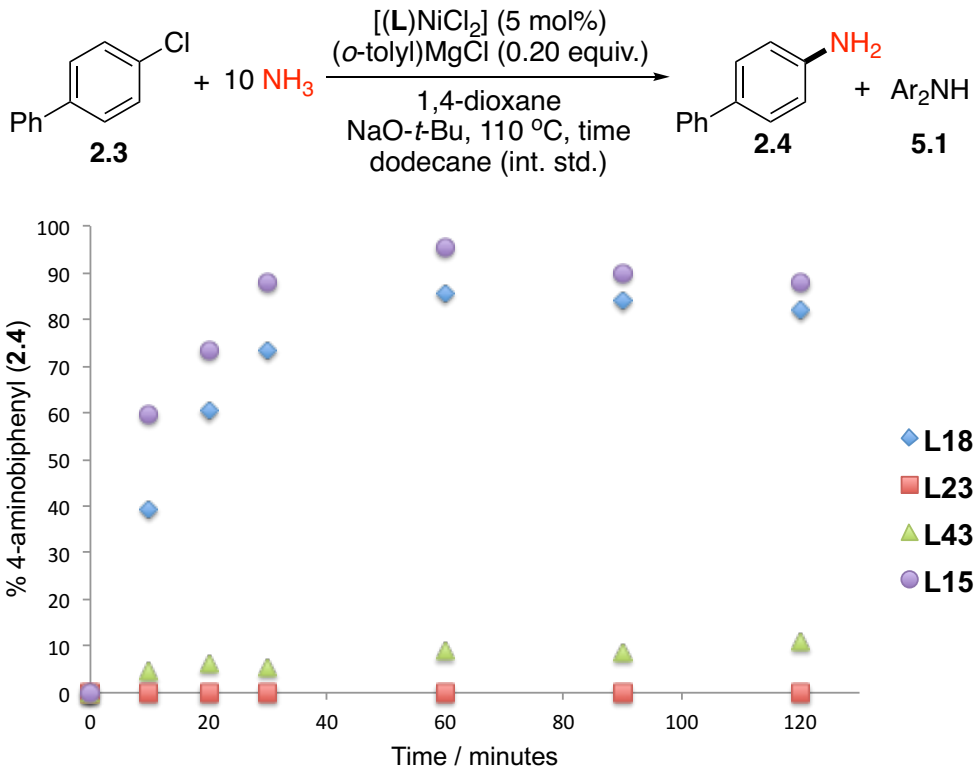


Figure 5-7. Time course for the conversion of **2.3** into 4-aminobiphenyl (**2.4**) using the (**L**)$NiCl_2$/(*o*-tolyl)MgCl system. See **GP5-4** of the experimental section for details.

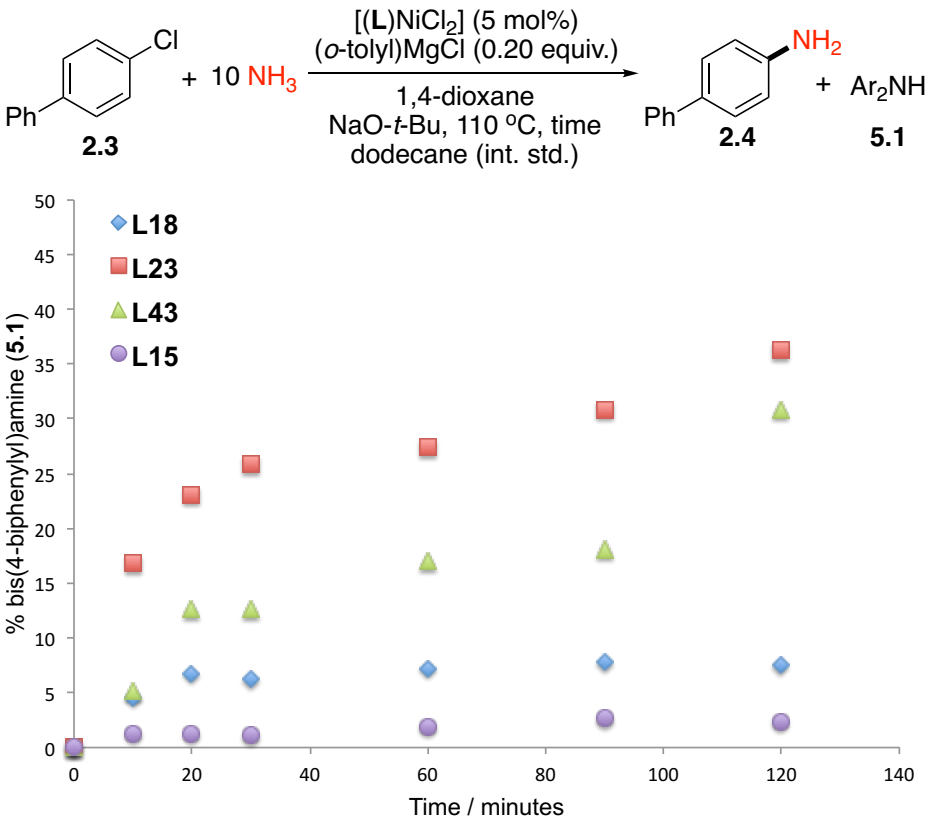


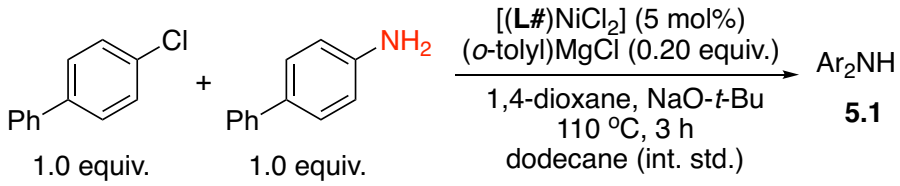
Figure 5-8. Time course for the conversion of 4-chlorobiphenyl into bis(4-biphenyl)amine (**5.1**) using the (**L**)$NiCl_2$/(*o*-tolyl)MgCl system. See **GP5-4** of the experimental section for details.

Whereas the poor monoarylation selectivity observed in Ni-catalyzed ammonia C-N cross-couplings involving the comparatively unhindered **L23** can be attributed to facile coordination/arylation of the initially formed primary aniline **A**, a similar rationale for the low conversion and monoarylation selectivity observed when using the hindered **L43** variant would not seem to be applicable.

We posited that the selectivity exhibited by the **L43**-derived pre-catalyst might be due to **L43** being an effective ligand for enabling primary aniline arylations. In testing the ability of the (**L**)$NiCl_2$ pre-catalysts herein to enable primary arylamine arylations, I examined the cross-coupling of **2.3** (1.0 equiv) with

4-aminobiphenyl (**2.4**) (1.0 equiv) to furnish bis(4-biphenylyl)amine (**5.1**) under conditions similar to those outlined in Table 5-1, but in the absence of ammonia (Table 5-2). The use of (**L23**)$NiCl_2$/(*o*-tolyl)MgCl catalyst mixtures resulted in the formation of substantial quantities of **5.1** (76%, Table 5-2, entry 2), which is consistent with the proposal that a less hindered coordination environment allows for facile primary arylamine coordination and thus decreased monoarylation selectivity in ammonia cross-couplings. In contrast, comparatively low consumption of **2.3** and **2.4** (29-41%) and poor formation of **5.1** (20-23%) was achieved by use of pre-catalysts based on **L15**, **L18**, or **L43** (Table 5-2, entries 1, 3, and 4). The poor reactivity (<5 % consumption of **2.3**) exhibited by $NiCl_2$(dme)/(*o*-tolyl)MgCl catalyst mixtures suggests that nickel species lacking phosphine ligation are unlikely to contribute significantly to the observed reactivity of (**L43**)$NiCl_2$/(*o*-tolyl) catalyst mixtures. Collectively, these observations reveal **L43** to be a relatively ineffective ligand for use in nickel-catalyzed C-N cross-couplings of ammonia or the primary arylamine **2.4** with electrophile **2.3**, despite the low barrier ($\Delta G^{\ddagger}_{RE}$) for C-N reductive elimination predicted for the **IN-1** species featuring κ^2-**L43** (Fig. 5-5). In this regard, it is possible that under catalytic conditions **L43** does not bind as a κ^2-bisphosphine ligand, despite crystallographic support for such connectivity in the pre-catalyst (**L43**)$NiCl_2$ (Fig. 5-5).

Table 5-2. Cross-coupling of 4-Aminobiphenyl and 4-Chlorobiphenyl using (**L**)$NiCl_2$ pre-catalysts (see **GP5-5** of the experimental section for details).



Entry	**L**(#)	% ArCl	% $ArNH_2$	% Yield **5.1**
1	15	71	59	23
2	23	7	8	76
3	43	66	64	21
4	18	70	59	20

5.4. SUMMARY

In an effort to better understand the desirable catalytic performance of PAd-DalPhos (**L18**) in the Ni-catalyzed monoarylation of ammonia, and to guide the development of increasingly effective variants of **L18**, we conducted a combined experimental/computational study. In computationally modeling C-N reductive eliminations occurring from arylnickel(II) parent amido complexes of the type (**L**)Ni(Ph)(NH_2), one key observation was that increasing the steric demand of the P_{aryl} groups from *o*-tolyl (in **L18**) to mesityl (in **L43**) resulted in a significant lowering of the barrier to C-N reductive elimination ($\Delta G^{\ddagger}_{RE}$). However, empirically the newly prepared **L43** performed poorly versus **L18**, suggesting that the significant steric demands of **L43** may discourage formation of key catalytic intermediates. Conversely, the poor monoarylation selectivity afforded by the **L18** variant featuring a PPh_2 donor fragment (**L23**) can be attributed to facile coordination/arylation of the initially formed primary aniline. Collectively these observations suggest that the intermediate steric profile of **L18**, relative to **L23** and **L43**, may be optimal in

achieving useful catalytic performance in the Ni-catalyzed monoarylation of ammonia.

We anticipate that the findings of this study will provide a useful platform for researchers to conduct their own ligand design efforts in the pursuit of superlative Ni-catalysts for use in ammonia monoarylations. Future efforts in the Stradiotto group will be focused on expanding our appreciation of the mechanistic subtleties of these transformations as part of our ongoing efforts to optimize the DalPhos ligand architecture.

5.5. EXPERIMENTAL

5.5.1. General Considerations

General Considerations. Unless otherwise stated, all reactions were setup inside a nitrogen-filled inert atmosphere glovebox using oven-dried glassware and purified solvents, and were worked up in air using bench-top procedures. Toluene and hexanes were deoxygenated by sparging with nitrogen followed by passage through a double column solvent purification system packed with alumina and copper-Q5 reactant, and storage over activated 4 Å molecular sieves. 1,4-Dioxane was dried over Na/benzophenone followed by distillation under a nitrogen atmosphere. All other commercial solvents, reagents, and materials were used as received. Deuterated NMR solvents were freeze−pump−thaw degassed three times. NMR spectra were recorded on a Bruker AV 300 MHz or Bruker AV 500 MHz spectrometer at 300 K, with chemical shifts (in ppm) referenced to residual protio solvent peaks (^{1}H), deuterated solvent peaks ($^{13}C\{^{1}H\}$), or external 85% H_3PO_4 ($^{31}P\{^{1}H\}$). Splitting patterns are indicated as follows: s, singlet; d, doublet;,

dd, doublet of doublets; t, triplet; m, multiplet. All coupling constants (*J*) are reported in hertz (Hz). In some cases, fewer than expected carbon resonances were observed despite prolonged acquisition times. Mass spectra were obtained using ion trap electrospray ionization (ESI) instruments operating in positive mode. Gas chromatography data were obtained on an instrument equipped with a SGE BP-5 column (30 m, 0.25 mm i.d.), and were calibrated by using authentic materials using dodecane as an internal standard. CyPF-Cy (JosiPhos) ligand **L15** was purchased from Strem Chemicals and was used as received. PAd-DalPhos (**L18**) was synthesized according to an existing literature procedure. Pre-catalysts (**L15**/**L18**)$NiCl_2$, were synthesized following literature procedures. The accompanying NMR spectra for the reported compounds in this chapter can be found in Appendix A of this document.

5.5.2. General Procedures

General Procedure for Monitoring the Reaction Progress for the cross-coupling of ammonia and 4-chlorobiphenyl time-trials using *in situ* Formed Catalyst (GP5-1). *Individual reactions were set up for each time interval.* In a nitrogen-filled glovebox, bis(cyclooctadiene)nickel(0) (1.7 mg, 0.006 mmol, 0.05 equiv.), ligand (0.006 mmol, 0.05 equiv.), 4-chlorobiphenyl (22.6 mg, 0.12 mmol, 1.0 equiv.), sodium *tert*-butoxide (34.6 mg, 0.36 mmol, 3.0 equiv.), ammonia as a 0.5 M solution in 1,4-dioxane (1.2 mL, 0.6 mmol, 5.0 equiv.), and toluene (0.466 mL; [ArCl] = 0.072 M) were added to a screw capped vial containing a magnetic stir bar. The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 110 ^{o}C. At the designated time, the reaction vial was removed from the heating block

and left to cool to ambient temperature, followed by addition of dodecane internal standard (0.12 mmol, 1.0 equiv.) to the reaction mixture, which was subsequently analyzed by use of GC methods following **Workup Method 5-1**.

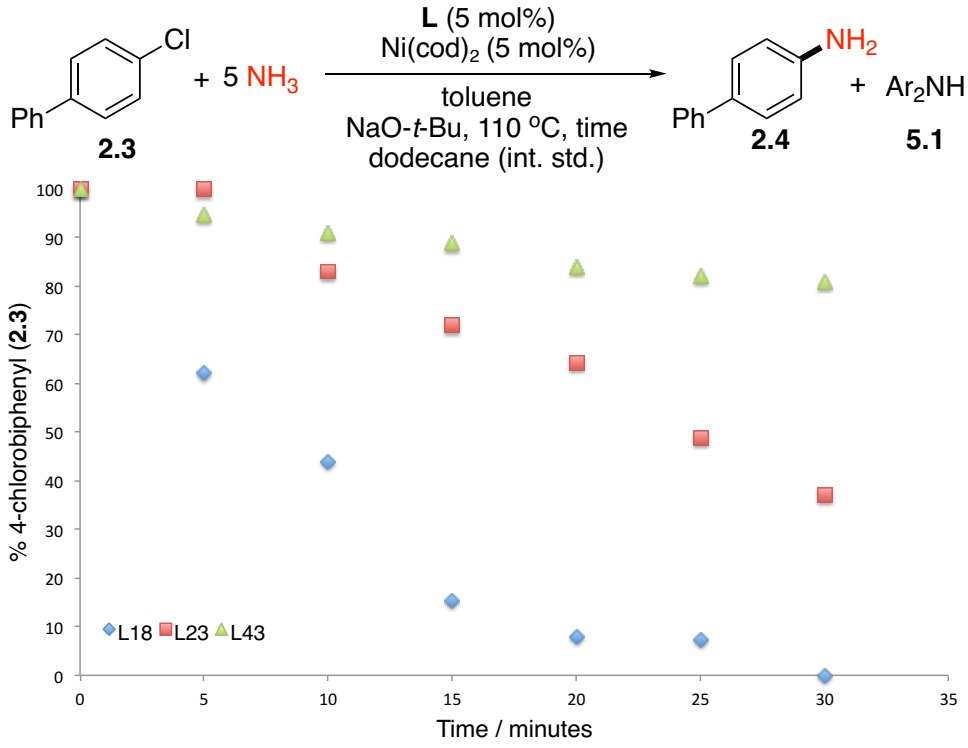


Figure 5-9. Time course for the conversion of 4-chlorobiphenyl (**2.3**) using the **L**/Ni(cod)$_2$ system.

General Procedure for the Cross-coupling of Ammonia and 4-Chlorobiphenyl Using (L#)NiCl$_2$ Pre-catalysts (GP5-2). In a nitrogen-filled glovebox, pre-catalyst (0.006 mmol, 5 mol %), 4-chlorobiphenyl (22.6 mg, 0.12 mmol, 1.0 equiv.), sodium *tert*-butoxide (23.1 mg, 0.24 mmol, 2.0 equiv.), *ortho*-tolylmagnesium chloride as a 1.0 M solution in THF (24.0 mL, 0.024 mmol, 0.2 equiv.), and ammonia as a 0.5 M solution in 1,4-dioxane (0.24-2.40 mL, 0.12-1.2 mmol, 1-10 equiv.), were added to a screw capped vial containing a magnetic stir bar, followed by the addition of 1,4-dixoane to make the [ArCl] = 0.05M. The vial was sealed with a cap containing a

PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 110 ^{o}C for 3 h. At the designated time, the reaction vial was removed from the heating block and left to cool to ambient temperature, followed by addition of dodecane internal standard (0.12 mmol, 1.0 equiv.) to the reaction mixture, which was subsequently analyzed by use of GC methods following **Workup Method 5-1**.

General Procedure for the Cross-coupling of Ammonia and 4-Chlorobiphenyl Using the [(L18)NiCl(*o*-tolyl)] Pre-catalyst (GP5-3). In a nitrogen-filled glovebox, pre-catalyst (0.006 mmol, 5 mol %), 4-chlorobiphenyl (22.6 mg, 0.12 mmol, 1.0 equiv.), sodium *tert*-butoxide (23.1 mg, 0.24 mmol, 2.0 equiv.), and ammonia as a 0.5 M solution in 1,4-dioxane (2.4 mL, 1.2 mmol, 10.0 equiv.), were added to a screw capped vial containing a magnetic stir bar. The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 110 ^{o}C. At the designated time, the reaction vial was removed from the heating block and left to cool to ambient temperature, followed by addition of dodecane internal standard (0.12 mmol, 1.0 equiv.) to the reaction mixture, which was subsequently analyzed by use of GC methods following **Workup Method 5-1**. *The product distribution observed when utilizing this method (0% unreacted ArCl, 71% $ArNH_2$, 11% Ar_2NH) is similar to that observed for analogous reactions employing [(**L18**)$NiCl_2$]/(o-tolyl)MgCl catalyst mixtures (**GP5-2**) (0% unreacted ArCl, 81% $ArNH_2$, 8% Ar_2NH).*

General Procedure for Monitoring the Reaction Progress for the Cross-coupling of Ammonia and 4-chlorobiphenyl Using (L#)$NiCl_2$ Pre-catalysts (GP5-4). *Individual reactions were set up for each time interval.* In a nitrogen-filled glovebox, pre-catalyst (0.006 mmol, 5 mol %), 4-chlorobiphenyl (22.6 mg, 0.12 mmol, 1.0 equiv.), sodium *tert*-butoxide (23.1 mg, 0.24 mmol, 2.0 equiv.), *ortho*-tolylmagnesium chloride as a 1.0 M solution in THF (24.0 mL, 0.024 mmol, 0.2 equiv.), and ammonia as a 0.5 M solution in 1,4-dioxane (2.4 mL, 1.2 mmol, 10.0 equiv.), were added to a screw capped vial containing a magnetic stir bar. The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 110 ^{o}C. At the designated time, the reaction vial was removed from the heating block and left to cool to ambient temperature, followed by addition of dodecane internal standard (0.12 mmol, 1.0 equiv.) to the reaction mixture, which was subsequently analyzed by use of GC methods following **Workup Method 5-1**.

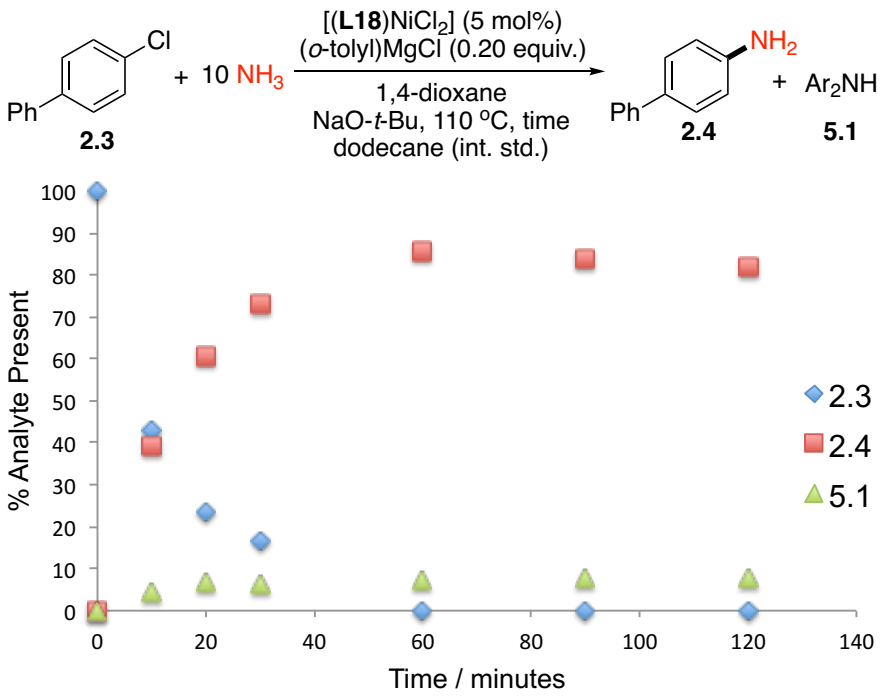


Figure 5-10. Time course for the cross-coupling 4-chlorobiphenyl and ammonia using the (**L18**)$NiCl_2$ system. Note: **2.3** is 4-chlorobiphenyl; **2.4** is 4-aminobiphenyl; **5.1** is bis(4-biphenyl)amine.

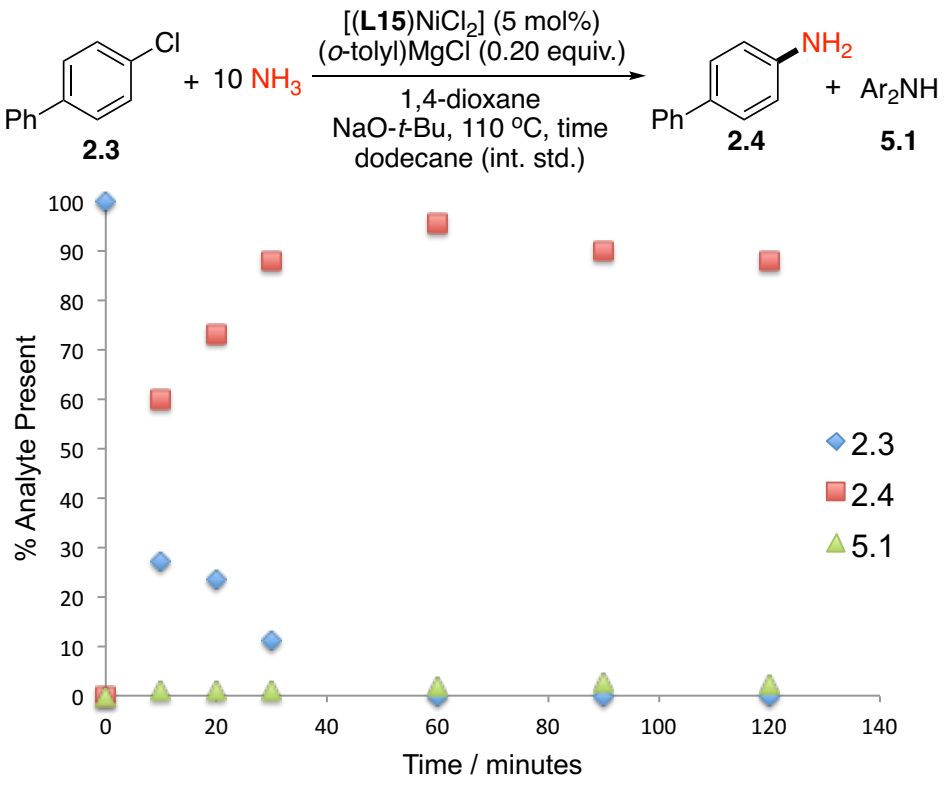


Figure 5-11. Time course for the cross-coupling 4-chlorobiphenyl and ammonia using the (**L15**)$NiCl_2$ system. Note: **2.3** is 4-chlorobiphenyl; **2.4** is 4-aminobiphenyl; **5.1** is bis(4-biphenyl)amine.

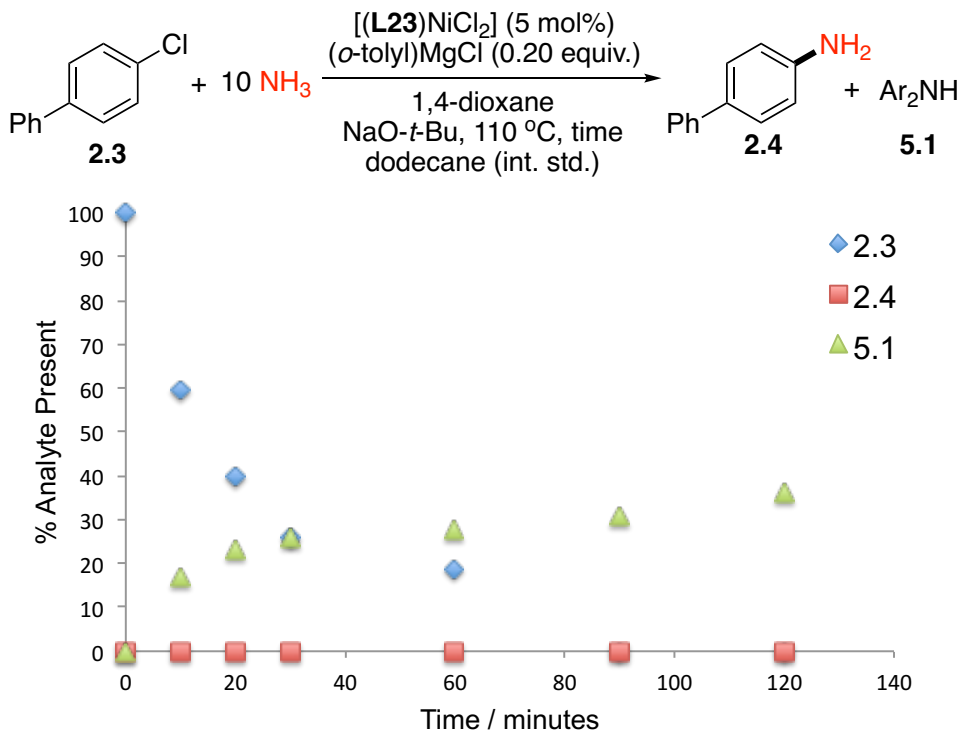


Figure 5-12. Time course for the cross-coupling 4-chlorobiphenyl and ammonia using the (**L23**)$NiCl_2$ system. Note: **2.3** is 4-chlorobiphenyl; **2.4** is 4-aminobiphenyl; **5.1** is bis(4-biphenyl)amine.

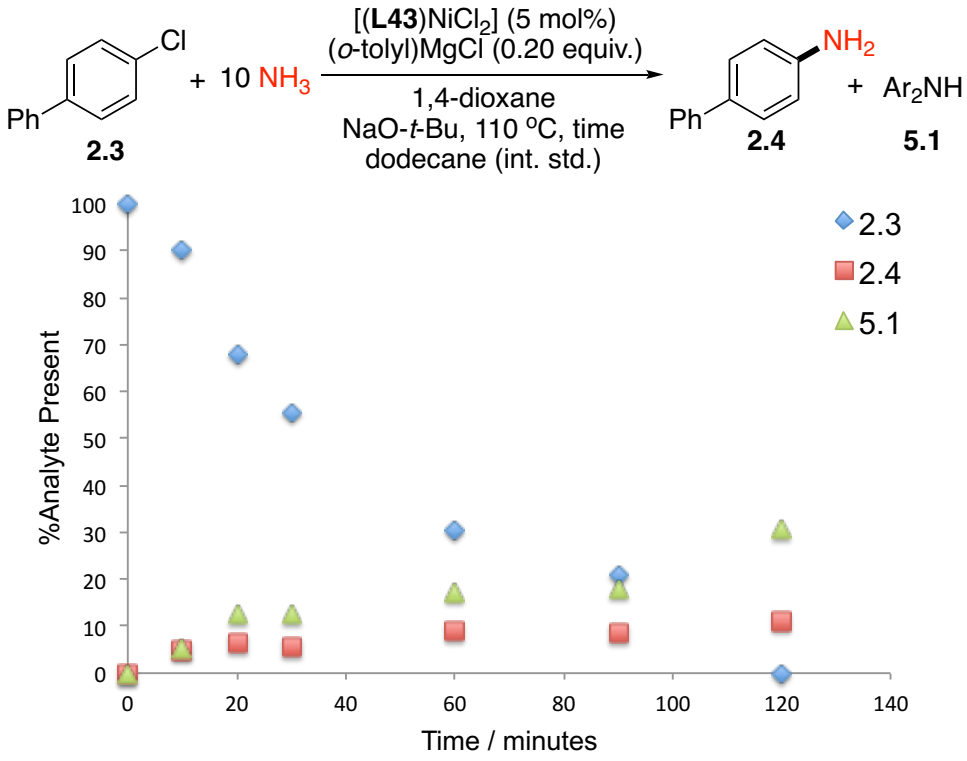


Figure 5-13. Time course for the cross-coupling 4-chlorobiphenyl and ammonia using the (**L43**)$NiCl_2$ system. Note: **2.3** is 4-chlorobiphenyl; **2.4** is 4-aminobiphenyl; **5.1** is bis(4-biphenyl)amine.

General Procedure for the Cross-coupling of 4-Aminobiphenyl and 4-Chlorobiphenyl Using (L)$NiCl_2$ Pre-catalysts (GP5-5). In a nitrogen-filled glovebox, pre-catalyst (0.006 mmol, 5 mol %), 4-chlorobiphenyl (22.6 mg, 0.12 mmol, 1.0 equiv.), sodium *tert*-butoxide (23.1 mg, 0.24 mmol, 2.0 equiv.), *ortho*-tolylmagnesium chloride as a 1.0 M solution in THF (24.0 mL, 0.024 mmol, 0.2 equiv.), and 4-aminobiphenyl (20.3 mg, 0.12 mmol, 1.0 equiv.), were added to a screw capped vial containing a magnetic stir bar, followed by the addition of 2.4 mL of 1,4-dixoane; [ArCl] = 0.05M. The vial was sealed with a cap containing a PTFE septum, removed from the glovebox and placed in a temperature-controlled aluminum heating block set to 110 °C for 2 h. At the designated time, the reaction

vial was removed from the heating block and left to cool to ambient temperature, followed by addition of dodecane internal standard (0.12 mmol, 1.0 equiv.) to the reaction mixture, which was subsequently analyzed by use of GC methods following **Workup Method 5-1**.

Workup Method 5-1 (Procedure for the Preparation of GC Samples). Following (**GP5-1)**-(**GP5-5)**, the reaction mixture was diluted using ethyl acetate and was passed through a Kimwipe filter containing Celite and silica gel, with the eluent collected in a GC vial. Calibrated GC estimates are given on the basis of data obtained from authentic materials using dodecane as an internal standard.

General Procedure for Ligand Substitution Reactions Involving L# and $Ni(cod)_2$ (GP5-6). In a nitrogen-filled glovebox, ligand (0.019 mmol, 1.0 equiv.), and bis(cyclooctadiene)nickel(0) (5.2 mg, 0.019 mmol, 1.0 equiv.) were added to a screw capped vial containing a magnetic stir bar, followed by the addition of 0.75 mL of C_6D_6. The vial was sealed with a cap containing a PTFE septum, and placed on a temperature-controlled aluminum heating block set to 80 ^oC for 2 h. After cooling to ambient temperature, the vial was brought into the glovebox, and an NMR sample was prepared. Analysis of the reaction mixture by use of $^{31}P\{^1H\}$ NMR methods revealed partial conversion of **L18**, and the appearance of two resonances at 46.1 and 38.4 ppm (J_{PP} = 40.5 Hz), which we tentatively assign to (**L18**)Ni(cod). For **L23**, analysis of the reaction mixture by use of $^{31}P\{^1H\}$ NMR methods revealed complete consumption of **L23**, and the appearance of two resonances at 51.2 and 38.5 ppm (J_{PP} = 40.5 Hz), which we tentatively assign to (**L23**)Ni(cod). For **L43**, only free ligand was detected upon analysis of the reaction

mixture by use of $^{31}P\{^{1}H\}$ NMR methods.

Procedure for the Synthesis of L43. In a nitrogen-filled glovebox, **1** (0.400 g, 1.08 mmol, 1.0 equiv.) and diethyl ether (ca. 6 mL) were combined in a 4-dram vial along with a magnetic stir bar. The vial was sealed and then cooled to -33 ˚C in the glovebox freezer. This vial was then removed from the freezer and a 2.5 M hexanes solution of cold (-33 ˚C) *n*-butyllithium (0.517 mL, 1.3 mmol, 1.2 equiv.) was added drop-wise under the influence of magnetic stirring, resulting in a yellowish-orange colored solution. This mixture was left to stir for 30 min at ambient temperature. At this time, a solution of dimesitylphosphorus chloride (395.0 mg, 1.3 mmol, 1.2 equiv.) in diethyl ether (ca. 6 mL) was added, resulting in an orange colored solution. This mixture was left to stir at ambient temperature for 20 h. On the bench-top, the reaction mixture was diluted with CH_2Cl_2 (ca. 10 mL) and filtered over Celite, eluting with CH_2Cl_2 (ca. 20 mL). The eluent was collected and the solvent was removed via rotary evaporation. The resulting yellow oil was purified by flash chromatography (SiO_2), eluting with 3% ethyl acetate/hexanes. The resulting beige waxy solid was recrystallized in cold pentane (0 ˚C) overnight, which following filtration afforded **L43** as a white crystalline solid (260.0 mg, 43 % yield). ^{1}H NMR ($CDCl_3$, 500.1 MHz): d 8.27 (m, 1H, ArH), 7.30-7.27 (m, 1H, ArH), 7.17-7.13 (m, 2H, ArH), 6.90 (d, *J* = 2.0 Hz, 2H, ArH), 6.76 (d, *J* = 2.5 Hz, 2H, ArH), 2.31 (s, 3H, Me), 2.27 (s, 3H, Me), 2.16-2.13 (m, 7H, Me/CgP), 2.04-2.02 (m, 7H, Me/CgP), 1.89 (m, 1H, CgP), 1.59-1.55 (m, 4H, CgP), 1.48 (s, 3H, Me), 1.39 (s, 3H, Me), 1.38 (d, *J* = 12.0 Hz, 3H, Me). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125.8 MHz): d 148.1 (dd, *J* = 33.9, 15.1 Hz, ArC), 144.5 (d, *J* = 16.3 Hz, ArC), 142.3 (d, *J* = 16.3 Hz, ArC),

140.7-140.2 (m, ArC), 138.8 (ArC), 137.3 (ArC), 134.1 (ArC), 133.4 (d, *J* = 7.5 Hz, ArC), 131.8 (d, *J* = 18.9 Hz, ArC), 130.8 (dd, *J* = 20.7, 11.3 Hz, ArC), 130.2 (dd, *J* = 35.2, 3.8 Hz, ArC), 129.4 (ArC), 128.1 (ArC), 97.0 (CgP), 96.2 (CgP), 74.7-74.3 (m, CgP), 46.2 (d, *J* = 20.1 Hz, CgP), 36.5 (CgP), 29.1 (dd, *J* = 18.9, 7.5 Hz, CgP), 28.4 (Me), 27.9 (Me), 26.8 (d, *J* = 11.3 Hz, Me), 23.6 (dd, *J* = 41.5, 16.3 Hz, Me), 21.2 (d, *J* = 10.0 Hz, Me). $^{31}P\{^{1}H\}$ (202.5 MHz, $CDCl_3$): d -24.9 (d, J_{PP} = 158 Hz, 1P), -36.8 (d, J_{PP} = 159 Hz, 1P). HRMS-ESI (m/z) calcd for $C_{34}H_{43}O_3P_2$ [M+H]: 561.2687; found: 561.2682. A single crystal suitable for X-ray diffraction was obtained by slow evaporation of **L43** in cold (0 ^{o}C) hexanes.

Synthesis of [(L23)NiCl$_2$]. In a nitrogen-filled glovebox, a 4-dram vial was charged with $NiCl_2$(dme) (219.6 mg, 0.999 mmol, 1.0 equiv.) and **L23** (500.0 mg, 1.05 mmol 1.05 equiv.). To these solids was added THF (ca 10 mL), affording a cloudy brown mixture. A magnetic stir bar was added, the vial was sealed, and stirring was initiated. After several minutes, a red precipitate formed. The resulting mixture was allowed to stir at ambient temperature for 2 h, after which time the vial was removed from the glovebox and pentane (5 mL) was added. The precipitated red solid was collected on a glass filter frit, and the retained solid was washed with cold (~0 ºC) pentane (3 x 3 mL). The collected solid product was then washed off of the frit by passing CH_2Cl_2 (ca 50 mL) through the frit, followed by evaporation of solvent from the intensely colored red eluent. The product was then dried *in vacuo* to afford the desired complex as a crimson solid (520 mg, 86%). ^{1}H NMR (500.1 MHz, $CDCl_3$): δ 8.45 (d, *J* = 8.0 Hz, 1H, ArH), 8.04 (d, *J* = 7.6 Hz, 2H, ArH), 7.64-7.61 (m, 3H, ArH), 7.56-7.54 (m, 2H, ArH), 7.51-7.48 (m, 2H, ArH), 7.45 (d, *J* = 7.1

Hz, 1H, ArH), 7.41-7.36 (m, 3H, ArH), 4.19 (d, *J* = 13.6 Hz, 1H, CgP), 2.20 (d, *J* = 13.9 Hz, 1H, CgP), 1.85 (d, *J* = 13.7 Hz, 2H, CgP), 1.61 (s, 3H, Me), 1.57 (s, 3H, Me), 1.52-1.51 (m, 6H, Me). $^{13}C\{^1H\}$ NMR (125.8 MHz, $CDCl_3$): δ 144.1 (ArC), 137.7 (ArC), 135.0 (ArC), 134.8 (ArC), 134.5 (ArC), 133.9 (ArC), 133.0 (ArC), 132.7 (ArC), 132.4 (ArC), 132.1 (ArC), 131.6 (ArC), 129.1 (ArC), 128.7 (ArC), 128.4 (ArC), 97.6 (CgP), 97.0 (CgP), 79.3 (CgP), 74.8 (CgP), 41.7 (CgP), 40.4 (CgP), 28.6 (Me), 27.8 (Me), 26.9 (Me), 25.7 (Me). $^{31}P\{^1H\}$ NMR (202.5 MHz, $CDCl_3$): There were no observable signals in the $^{31}P\{^1H\}$ NMR spectrum. Anal. Calc'd for $C_{28}H_{30}Cl_2NiO_3P_2$: C, 55.49; H, 4.99; N, 0. Found: C, 55.16; H, 5.21; N, <0.3.

Synthesis of [(L43)NiCl$_2$]. In a nitrogen-filled glovebox, a 4-dram vial containing a magnetic stir bar was charged with $NiCl_2$(dme) (48.9 mg, 0.223 mmol, 1.0 equiv.) and **L43** (150.0 mg, 0.268 mmol, 1.2 equiv.). The solid mixture was dissolved in THF (ca 2 mL), magnetic stirring was initiated, and the resulting solution was allowed to stir at room temperature for 16 h. The crude reaction mixture was directly poured into a glass frit and was washed thoroughly with pentane (5 x 5 mL). The product was collected by passing CH_2Cl_2 (ca 25 mL) through the frit, followed by evaporation of solvent from the eluent. The product was then dried *in vacuo* to afford the desired complex as a dark purple solid (145 mg, 92%). A single crystal suitable for X-ray diffraction was prepared by slow evaporation of a cold (0 ˚C) CH_2Cl_2 solution of (**L43**)$NiCl_2$. The ^1H NMR features of this compound were sufficiently broad to preclude meaningful interpretation, and no signals were observed in the $^{31}P\{^1H\}$ NMR spectrum. Anal. Calc'd for $C_{34}H_{42}Cl_2NiO_3P_2$: C, 59.14; H, 6.14; N, 0. Found: C, 59.32; H, 6.11; N, <0.3.

Crystallographic Solution and Refinement Details. Crystallographic data were obtained at or below 193(2) K on a Bruker D8/APEX II CCD diffractometer equipped with a CCD area detector, employing samples that were mounted in inert oil and transferred to a cold gas stream on the diffractometer. Data reduction, correction for Lorentz polarization, and absorption correction were each performed. Structure solution and least-squares refinement on F^2 were used throughout. All non-hydrogen atoms were refined with anisotropic displacement parameters. Full crystallographic solution and refinement details are provided in the deposited CIFs (1858791 and 1858792).

General Computational Information: Geometry optimizations and frequency calculations were performed on all species with the B3LYP functional[214, 215] and the XDM[216, 217] dispersion correction. A mixed basis set was used, consisting of 6-31G* for C and H, and 6-31+G* for all other elements. Single-point energy calculations on the optimized geometries were carried out using the same B3LYP-XDM method with the 6-311+G(2d,2p) basis set. The XDM damping parameters were a_1=0, a_2=3.7737 Å for the geometry optimizations and a_1=0.4376, a_2=2.1607 Å for the single-point energies. All calculations were performed using the Gaussian 09 software package, along with the postg program for the dispersion energies. NCI plots[228] were generated using the B3LYP/6-311+G(2d,2p) wavefunctions via the nciplot program.[229] Interactions between only the $PhNH_2$ moiety and the ancillary ligand are shown and are represented using a 0.5 a.u. reduced gradient isosurface. The nciplot program can be downloaded from http://schooner.chem.dal.ca.

Chapter 6

Conclusion

6.1. SUMMARY OF NI-CATALYZED C-N CROSS-COUPLING PROTOCOLS

A summary of the protocols described throughout this Thesis, both in the context of my research as well as those reported by others in literature, is presented in Figures 6-1 and 6-2, categorized by the type of NH nucleophile utilized. While intended as a useful condensation of the results described herein, these Figures also illustrate the areas of Ni-catalyzed C-N cross-coupling that require further development. For example, while several bisphosphine-based catalyst systems are now known that are capable of effecting primary alkylamine and aniline based cross-couplings, catalysts that are compatible with other important NH substrate classes such as ammonia, amides, and NH heterocycles are much less common and in some cases require forcing reaction conditions (i.e., higher reaction temperatures and catalyst loadings) to achieve suitable turnover. Addressing these and other shortcomings represent important unmet challenges in the field of Ni-catalyzed C-N cross-coupling.

Ammonia

Effective Ancillary Ligands	Catalyst Type	Conditions	Suitable Electrophiles (hetero)aryl-X	References
dppf (**L8**)	[Ni(**L8**)Cl_2]	5 mol% Ni 100 °C, 12 h K_3PO_4, 1,4-dioxane	X = OH (via Ar-O-TCT)	119
JosiPhos (**L15-L17**)	**L**/Ni(cod)2 [Ni(**L**)(η^2-NCPh)] [Ni(**L**)Cl(*o*-tolyl)] [Ni(**L**)(*p*-PhCN)Cl]	1-10 mol% Ni rt-110 °C, 3-16 h NaO-*t*-Bu/LiO-*t*-Bu 1,4-dioxane/toluene	X = Cl, Br, OTs, OSO_2NMe_2, OC(O)NEt_2	71, 84, 85, 86
PAd-DalPhos (**L18**)	[Ni(**L18**)Cl(*o*-tolyl)]	1-10 mol% Ni rt-110 °C, 16 h NaO-*t*-Bu/LiO-*t*-Bu 1,4-dioxane/toluene	X = Cl, Br, I, OTs, OMs, OTf, imidazolylSO_3	72, 102, 213

Primary Alkylamines and Anilines

Effective Ancillary Ligands	Catalyst Type	Conditions	Suitable Electrophiles (hetero)aryl-X	References
dppf (**L8**)	**L8**/Ni(cod)2 [Ni(**L8**)Cl_2] **L8**/Ni/C [Ni(**L8**)Cl(*o*-tolyl)] [Ni(**L8**)[P(OPh)$_3$]$_2$]	2-10 mol% Ni 70-130 °C, 2-52 h Na/LiO-*t*-Bu, K_3PO_4 1,4-dioxane, toluene, CPME	X = OH, Cl, Br OTf, OMs, OSO_2NMe_2	87, 88, 89, 90, 119
BINAP (**L13**)	[Ni(**L13**)(η^2-NCPh)] [Ni(**L13**)[P(OPh)$_3$]$_2$]	1-5 mol% Ni 50-80 °C, 18-24 h NaO-*t*-Bu, toluene	X = Cl, Br, OTs	69, 70
JosiPhos (**L15**)	[Ni(**L15**)Cl(*o*-tolyl)]	5-10 mol% Ni rt-110 °C, 16 h NaO-*t*-Bu, K_3PO_4 1,4-dioxane, toluene	X = OC(O)^{t}Bu OSO_2NMe_2, OC(O)NMe_2	85
PAd-DalPhos (**L18**)	[Ni(**L18**)Cl(*o*-tolyl)]	1-5 mol% Ni rt, 16 h NaO-*t*-Bu, K_3PO_4 1,4-dioxane/toluene	X = Cl, Br, OTs, OMs	102
CyPAd-DalPhos (**L19**)	[Ni(**L19**)Cl(*o*-tolyl)]	3-5 mol% Ni rt-110 °C, 16 h NaO-*t*-Bu, toluene	X = Cl, Br, OTs, OMs, OSO_2NMe_2, OC(O)NEt_2	123
NHP-DalPhos (**L20**)	[Ni(**L20**)Cl(*o*-tolyl)]	3-5 mol% Ni rt, 16 h NaO-*t*-Bu, toluene	X = Cl, Br	122
PS-DPPBz (**L21**)	**L21**/Ni(cod)2	1 mol% Ni 80-120 °C 20 h NaO-*t*-Bu, toluene	X = Cl	124
DCYPBz (**L22**)	**L22**/Ni(cod)2	7.5 mol% Ni 80-120 °C 20 h NaO-*t*-Bu, toluene	X = F	125

Figure 6-1. A summary of established (bisphosphine)Ni-catalyzed C-N cross-coupling methodologies involving ammonia, primary alkylamines, anilines, and related ammonium salts.

Secondary Amines

Effective Ancillary Ligands	Catalyst Type	Conditions	Suitable Electrophiles (hetero)aryl-X	References
dppf (**L8**)	**L8**/Ni(cod)$_2$ [Ni(**L8**)Cl$_2$] **L8**/Ni/C [Ni(**L8**)Cl(*o*-tolyl)] [Ni(**L8**)[P(OPh)$_3$]$_2$]	2-5 mol% Ni 70-130 °C, 2-52 h Na/LiO-*t*-Bu, K_3PO_4 1,4-dioxane, toluene, CPME	X = OH, Cl, Br ,I OTf, OTs, OSO_2NMe_2	87, 88, 89, 90, 119
DPEPhos (**L14**)	[Ni(**L14**)(2-mesityl)Br]	5 mol% Ni 5 mol% PhB(OH)$_2$ 110 °C, 16 h LiO-*t*-Bu, toluene	X = Cl	91

Primary Amides and Lactams

Effective Ancillary Ligands	Catalyst Type	Conditions	Suitable Electrophiles (hetero)aryl-X	References
PAd-DalPhos (**L18**)	[Ni(**L18**)Cl(*o*-tolyl)]	5-10 mol% Ni 90 °C, 18 h NaO-*t*-Bu, K_3PO_4, Cs_2CO_3 1,4-dioxane, toluene, ^{t}BuOH	X = Cl, Br, OTf OTs, OMs, OSO_2NMe_2	213

NH Heterocycles (carbazole, indole, indazole, imidazole, pyrazole, pyrole)

Effective Ancillary Ligands	Catalyst Type	Conditions	Suitable Electrophiles (hetero)aryl-X	References
dppf (**L8**)	[Ni(**L8**)Cl$_2$]	5 mol% Ni 100 °C, 12 h K_3PO_4, 1,4-dioxane	X = OH (via Ar-O-TCT)	119
DPEPhos (**L14**)	[Ni(**L14**)(2-mesityl)Br]	5 mol% Ni 5 mol% PhB(OH)$_2$ 110 °C, 16 h LiO-*t*-Bu, toluene	X = Cl	91

Figure 6-2. A summary of established (bisphosphine)Ni-catalyzed C-N cross-coupling methodologies involving secondary amines, primary amides, lactams, and NH heterocycles.

Much work is needed both in the quest to establish a more thorough understanding of Ni-catalyzed C-N cross-couplings, and to advance such experimental protocols to the point where they will be adopted with confidence by end-users. Important areas of combined experimental and mechanistic inquiry include:

i. increased emphasis regarding the design and application of new ancillary ligands to generate highly active, selective, and robust Ni catalysts;

ii. exploring the nature of the elementary steps involved in Ni-catalyzed C-N cross-coupling, including the identification of the active catalytic species, catalyst resting states, and rate-limiting steps as a function of the ancillary ligand, Ni oxidation state, and substrates involved;

iii. the identification of off-cycle reaction pathways, along with the mechanism of formation of deactivated catalytic species.

iv. increased commercialization of new ligand and pre-catalyst architectures so as to streamline the adoption of technology by end users in industrial settings.

6.2. NEW DIRECTIONS FOR PROJECTS DISCUSSED IN THIS THESIS

In the sections below, new potential areas to explore in the context of my Thesis work are presented with respect to the themes of chapters 2-5.

6.2.1. Chapter 2

The PAd-DalPhos/Ni pre-catalyst system (i.e., **C1**) described in Chapter 2 is unique among all previously reported transition metal catalysts in its capacity to accommodate a wide range of both electrophilic and nucleophilic partners, often under exceedingly mild conditions (e.g., room-temperature, low catalyst loadings). Nonetheless, several notable limitations were identified throughout the course of developing the **C1** based amination chemistry, which if addressed, would substantially improve the likelihood for end user uptake by the chemical community.

One such shortcoming encountered is the inability for **C1** to catalyze aminations involving sterically hindered di-*ortho*-substituted arylhalides (e.g, 2,6-

dimethylchlorobenzene), as well as hindered mono-*ortho*-substituted electrophiles (e.g., 2-chlorobenzotrifluoride). This limitation is not surprising given that the design of **L18** was intended to promote otherwise slow Ar-NH_2 reductive elimination, and to dissuade reuptake of the initially formed primary arylamine product. The design and application of a less-hindered **L18** variant would likely lead to improved reactivity within Ni-catalyzed aminations involving bulky electrophiles.

The investigation that is discussed in Chapter 5 of this Thesis revealed that the selectivity of **L18**-based Ni-catalyzed ammonia arylations is subpar in comparison to state-of-the-art Pd systems. This is discussed further in section 6.2.4 below.

6.2.2. Chapter 3

Described in Chapter 3 is the first documented example of Ni-mediated *N*-arylations of primary amides and lactams, achieved via the application of the **C1** pre-catalyst. While an important advance in the context of the burgeoning field of Ni-based C-N cross-coupling chemistry, the performance of **C1** is not on par with state-of-the-art Pd amidation catalysts, which collectively can accommodate a substantially broader scope of both electrophilic and nucleophilic reagents under low loadings of catalyst. Given however that **L18** was designed to facilitate selective monoarylations involving small NH nucleophiles (i.e., ammonia), it is not surprising that notable limitations exist with respect to the **C1** catalyzed amidation chemistry. Therefore it stands to reason that a ligand tailored specifically for mediating C-N cross-couplings involving amide and lactam reagents should offer significant improvements with regard to the performance of the **C1** system.

Salient limitations encountered in the **C1** amidation chemistry that ought to be addressed via ligand design include: the inability to accommodate non-activated arylhalides and secondary amides beyond lactams; and the need for relatively high catalyst loadings and reaction temperatures. While it is unlikely that each of the aforementioned limitations may be addressed by a single new ligand, a more feasible approach might be to diversify the **L18** architecture so as to develop a small library of **L18** based variants that enable unique reactivity when paired with Ni. For example, synthesizing a comparatively electron-deficient variant of **L18** containing electron-withdrawing groups (e.g., trifluoromethyl), might give rise to more electrophilic nickel species that encourage binding of weakly nucleophilic amide reagents, perhaps allowing for lower catalyst loadings and reaction temperatures to be utilized in comparison to **C1** (Fig. 6-3). It is also possible that such an alternation could expand the scope of effective substrates to include secondary amides; Buchwald and coworkers[164] have demonstrated that the use electron-deficient biaryl monophosphines in conjunction with with aryl triflates, is critical for achieving cationic Pd(II) complexes which are sufficiently electrophilic so as to facilitate secondary amide binding. It is anticipated that such a ligand design strategy would prove fruitful in the context of the Ni-catalyzed amidations involving the PAd-DalPhos ligand family.

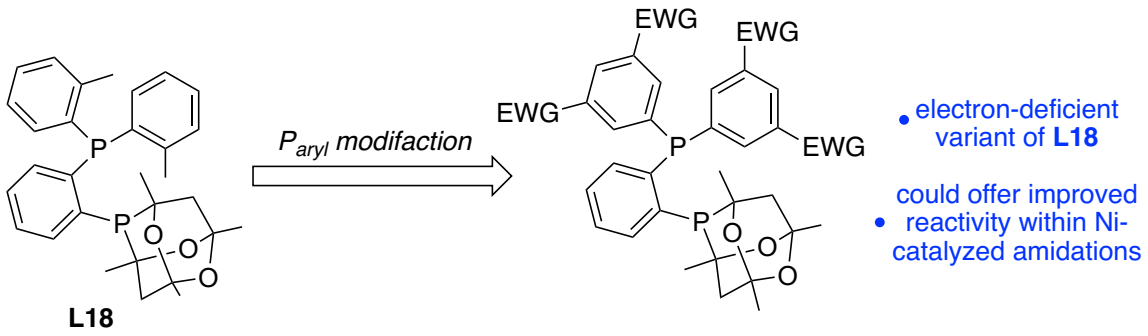


Figure 6-3. A hypothetical electron-deficient ligand variant of **L18**, which may offer improved reactivity in Ni-catalyzed C-N cross-couplings of amides. EWG = electron-withdrawing group.

6.2.3. Chapter 4

The research encompassed within Chapter 4 provides compelling evidence for the existence of productive parallel catalytic cycles involving either Ni^{0}/Ni^{II} or Ni^{I}/Ni^{III} couples for aminations catalyzed by **C1**. There is however ambiguity regarding the circumstances under which such manifolds may be operative, thus future efforts should be devoted towards understanding the dominant operative mechanism for Ni-catalyzed aminations catalyzed by **C1**. Furthermore, it is likely that the ideal ligand design principles are divergent for competing mechanistic pathways (i.e., Ni^{0}/Ni^{II} *versus* Ni^{I}/Ni^{III} cycles), therefore providing opportunities for the design of ligands tailored to favor one manifold over the other, while optimizing catalytic performance therein. For example, it was discovered throughout the course of the investigation described in Chapter 4, that the Ni(I) pre-catalyst based on dppf (**L8**) is catalytically active for primary amide *N*-arylations, whereas its corresponding Ni(II) pre-cursor is not. This finding lends credence to the proposal that ideal ligand characteristics are likely distinct for potentially competing Ni^{0}/Ni^{II} and Ni^{I}/Ni^{III} pathways. Given that C-Cl oxidative addition was predicted by DFT

analyses to be rate-limiting for the Ni^{I}/Ni^{III} pathway, it is possible that improved reactivity could be achieved by employing a relatively electron-rich variant of dppf, i.e., d*i*ppf. An investigation similar to the one featured in Chapter 4 is envisioned, whereby the reactivity of Ni(I) and Ni(II) pre-catalysts based electron-rich and electron-poor variants of the same ligand family are compared to interrogate the influence of ligand structure on potentially distinct reaction manifolds (Fig. 6-4). It is anticipated that such a study could unlock new modes of reactivity not possible for cycles involving Ni^{0}/N^{II} intermediates.

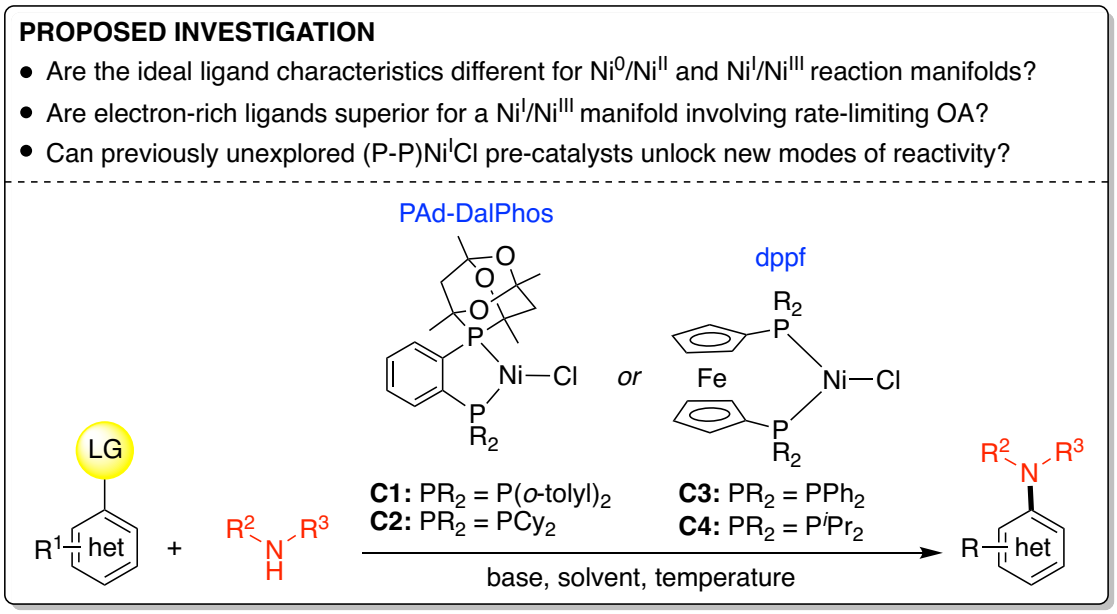


Figure 6-4. A proposal for future work involving the comparison of Ni(I) and Ni(II) pre-catalysts supported by electron-rich and electron-poor variants within the same ligand family.

6.2.4. Chapter 5

The findings of the research presented in Chapter 5 showcase that there is a tedious balance with respect to the ligands steric and electronic parameters with regard to its exhibited activity and selectivity within Ni-catalyzed ammonia

arylations. For example, the sterically distinct diphenyl (**L23**)- and dimesitylphosphino (**L43**) variants of **L18** exhibited comparably poor selectivity for monoarylation, whereas the sterically 'in-between' di-*ortho*-tolylphosphino analogue (**L18**) displayed satisfactory selectivity. Uncovering the origin of the observed selectivity exhibited by these ligands would provide a useful platform for the development of superlative **L18** variants for ammonia monoarylation. Although the selectivity exhibited by **L18**/Ni catalyst system (**C1**) was sufficient for our synthetic purposes, current state-of-the-art Pd systems exhibit superior selectivity in ammonia arylation chemistry in comparison to **C1**.

It was discovered throughout the investigation featured in chapter 5, that the Ni(II) pre-catalyst based on the JosiPhos ligand CyPF-Cy (**L15**) exhibited excellent monoarylation selectivity (>25:1). It is presently unclear why **L15** offers superior selectivity compared to PAd-DalPhos (**L18**) in Ni-catalyzed ammonia arylations. It is possible that the difference in the bite-angles for their respective (P-P)NiCl(*o*-tolyl) coordination complexes – 86.52(3)^{o} for **L18**[102] and 97.84(3)^{o} for **L15**,[92] contributes in part to their distinct reactivity profiles; the effect of bidentate phosphine bite angles on catalyst selectivity and activity in transition metal catalyzed cross-coupling is well documented.[232, 233] In light of these considerations, a new variant of **L18** containing a methylene bridged phosphine donor fragment is envisioned, which upon coordination would form a 6-membered chelate, as seen with **L15**. It is possible that the change in bite angle for this new ligand (Fig. 6-5) would give rise to improved activity and selectivity within Ni-catalyzed ammonia arylations.

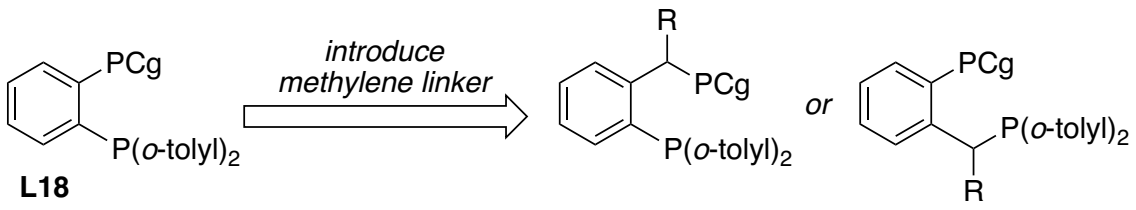


Figure 6-5. A hypothetical ligand variant of **L18** containing a methylene bridged phosphine donor fragment, which would enforce a 6-membered Ni chelate. PCg = 1,3,5,7-tetramethyl-2,4,8-trioxa-6-phosphaadamantane.

6.3. CONCLUDING REMARKS

The field of Ni-catalyzed C-N cross-coupling has evolved considerably over the past five years alone, and the advances gained within this timeframe – including those discovered in the context of my Thesis work, illustrate that the benefits of employing Ni catalysis in this context extend far beyond mere economic considerations. Whereas the initial exploration of Ni-catalyzed C-N cross-coupling chemistry involved efforts to repurpose prominent bisphosphine and other ancillary ligands from Pd-based transformations (i.e., BHA), the development of ancillary ligands tailored to engender desired Ni-based reactivity has recently gained traction, providing in-roads to otherwise challenging substrate classes (e.g., ammonia, amides). In this regard, the design and application of bisphosphine ancillary ligands has figured importantly, as demonstrated herein. Implementation of air-stable Ni^{II} pre-catalysts that activate under C-N cross-coupling conditions has permitted many of the developed methodologies to be conducted at room-temperature, utilizing relatively low concentrations of Ni (<5 mol%), and without recourse to additives and metal co-catalysts. From a practical perspective, a number of the bisphosphine ancillary ligands and derived Ni^{II} pre-catalysts are now

commercially available, including PAd-DalPhos (**L18**) and (**L18**)NiCl(*o*-tolyl) (**C1**) developed in my Thesis work.

It is my sincerest hope that the strong foundation in ligand design and mechanistic organometallic chemistry presented in this Thesis will serve as a useful guide for researchers seeking to address these aforementioned challenges, and for practitioners who wish to exploit recent advances in Ni-catalyzed C-N cross-coupling.

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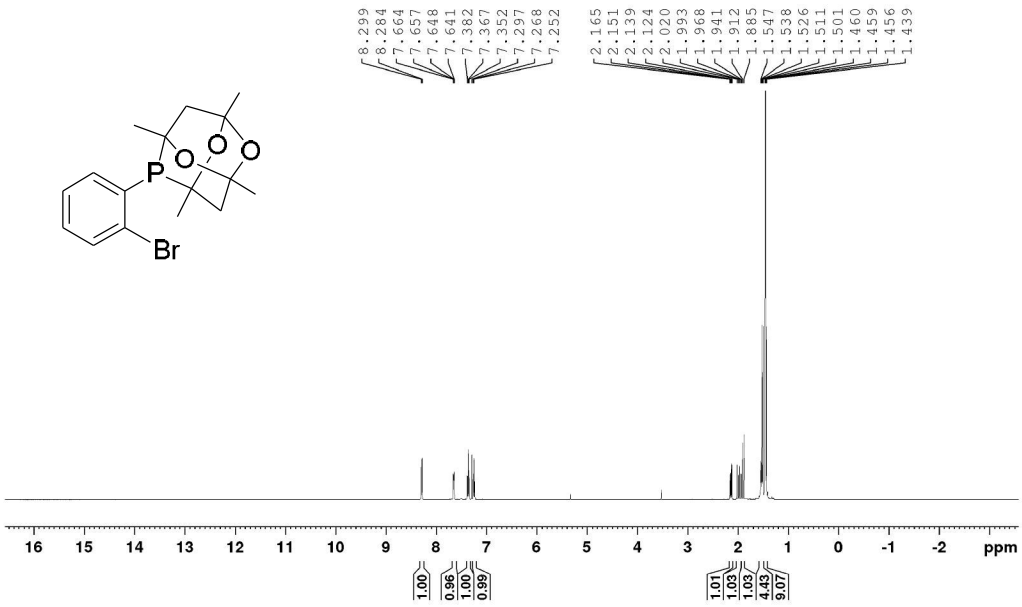
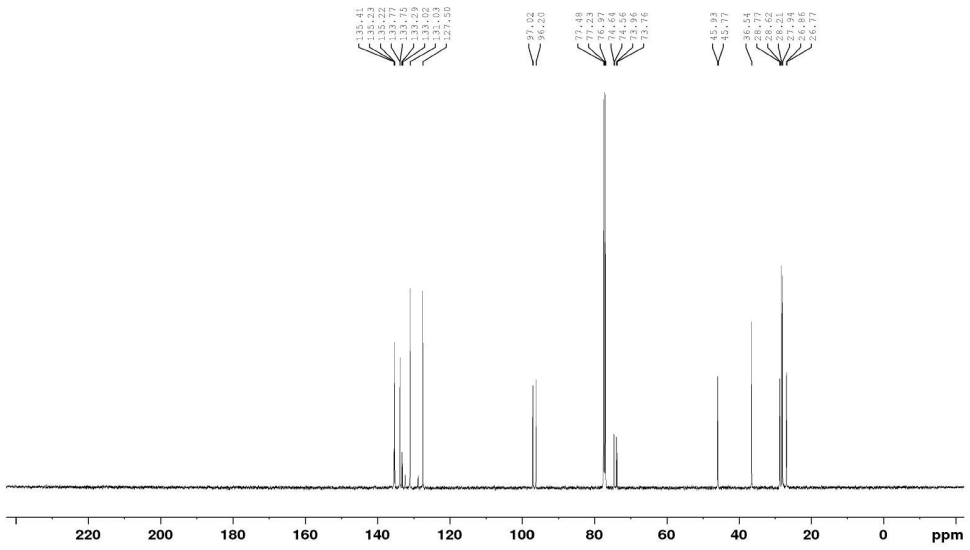
APPENDIX A. Representative NMR Spectra

Below are ^{1}H, $^{13}C\{^{1}H\}$, and $^{31}P\{^{1}H\}$ NMR spectra of all compounds reported in the experimental sections of Chapters 2-5.

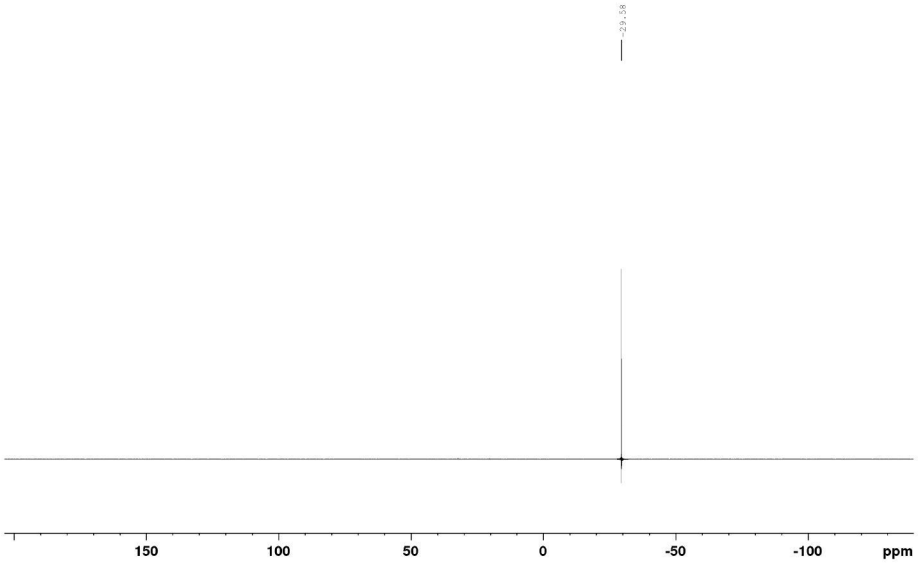
^{1}H NMR Spectrum of **2.1**, ($CDCl_3$, 500.1 MHz)



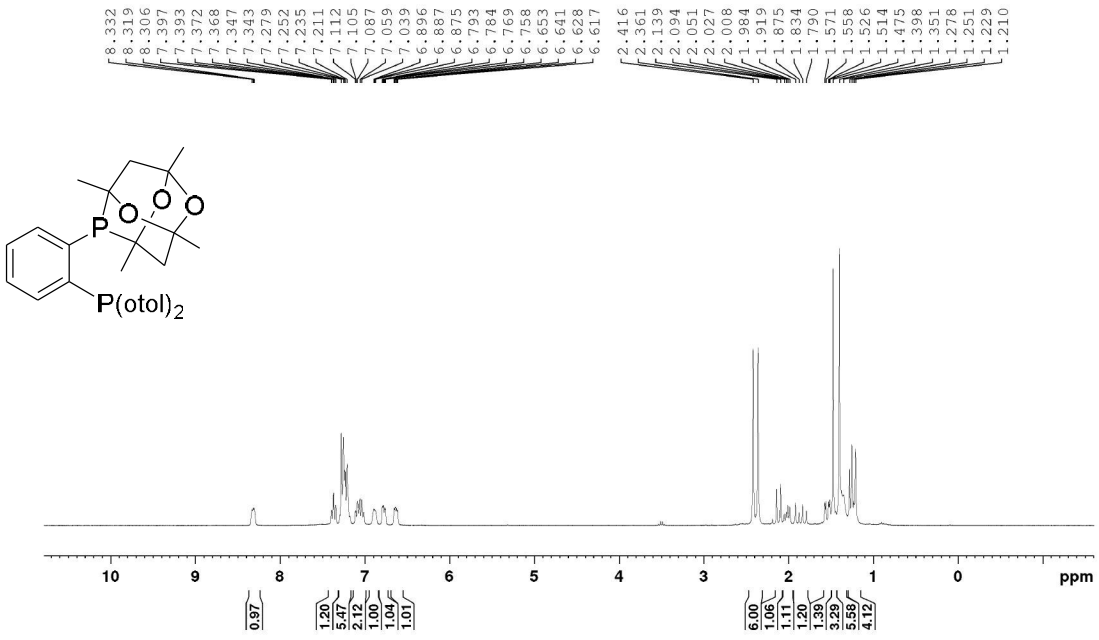
$^{13}C\{^{1}H\}$ NMR Spectrum of **2.1**, ($CDCl_3$, 125.8 MHz)



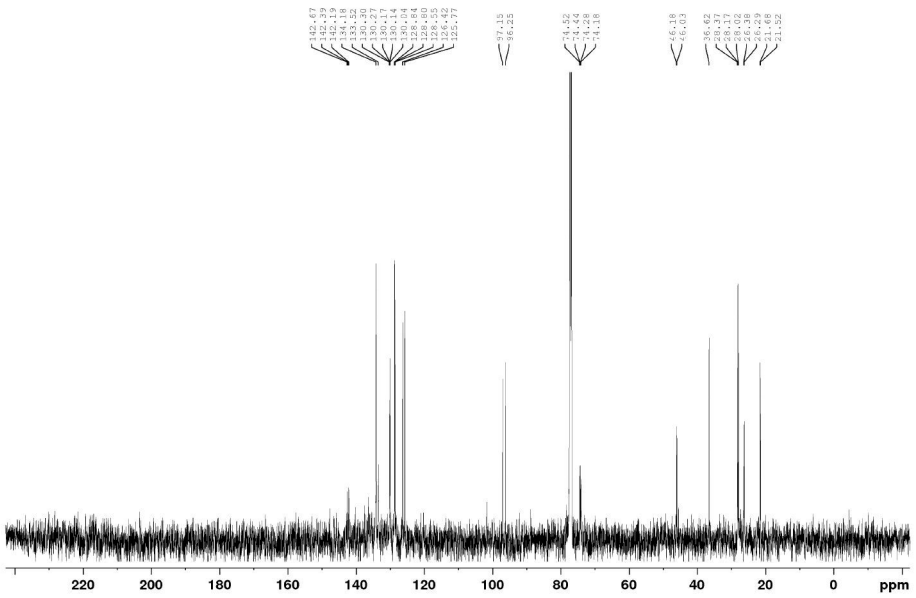
$^{31}P\{^{1}H\}$ NMR Spectrum of **2.1**, ($CDCl_3$, 202.5 MHz



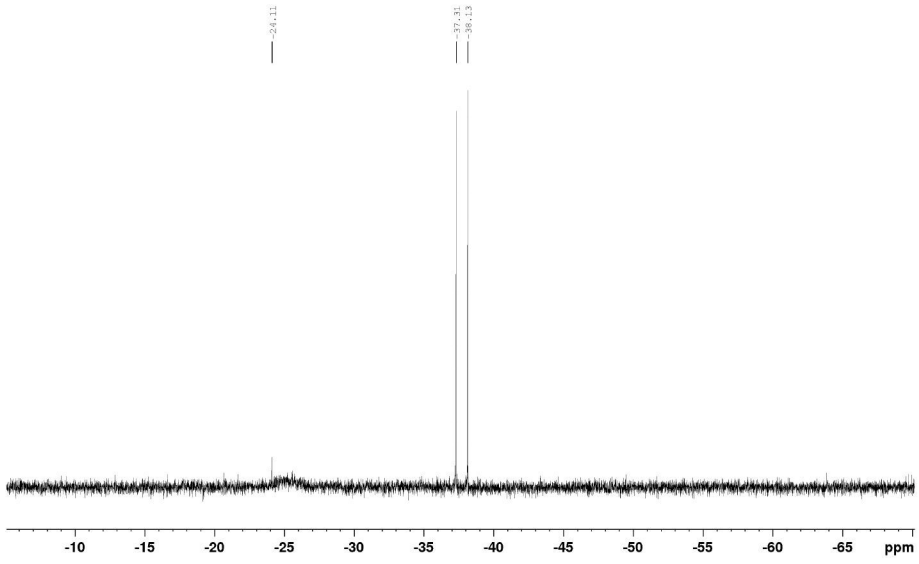
^{1}H NMR Spectrum of **L18**, ($CDCl_3$, 300.1 MHz)



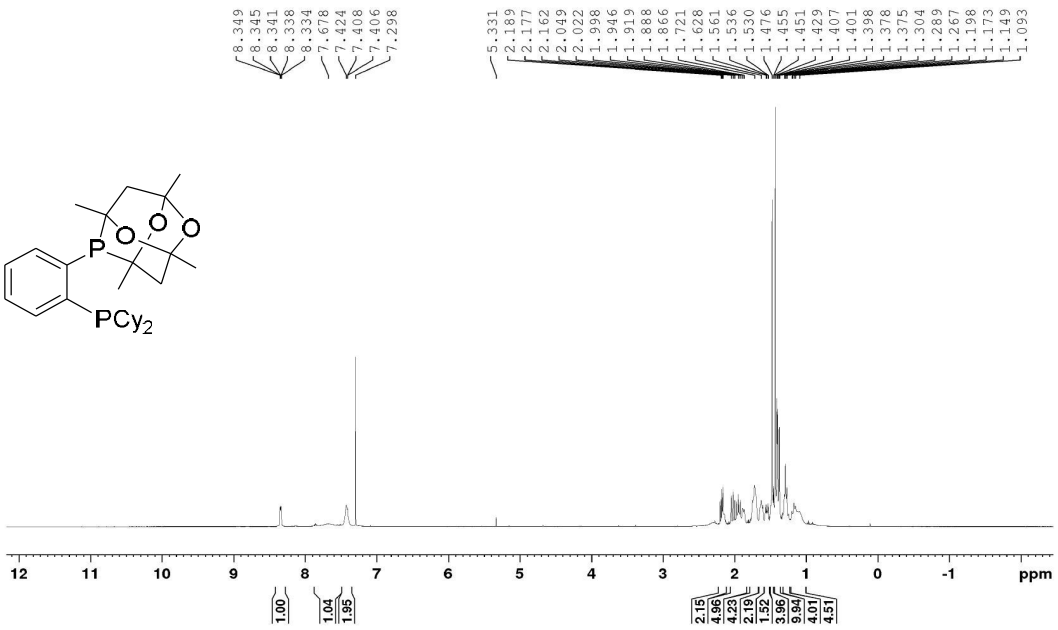
$^{13}C\{^{1}H\}$ NMR Spectrum of **L18**, ($CDCl_3$, 125.8 MHz)



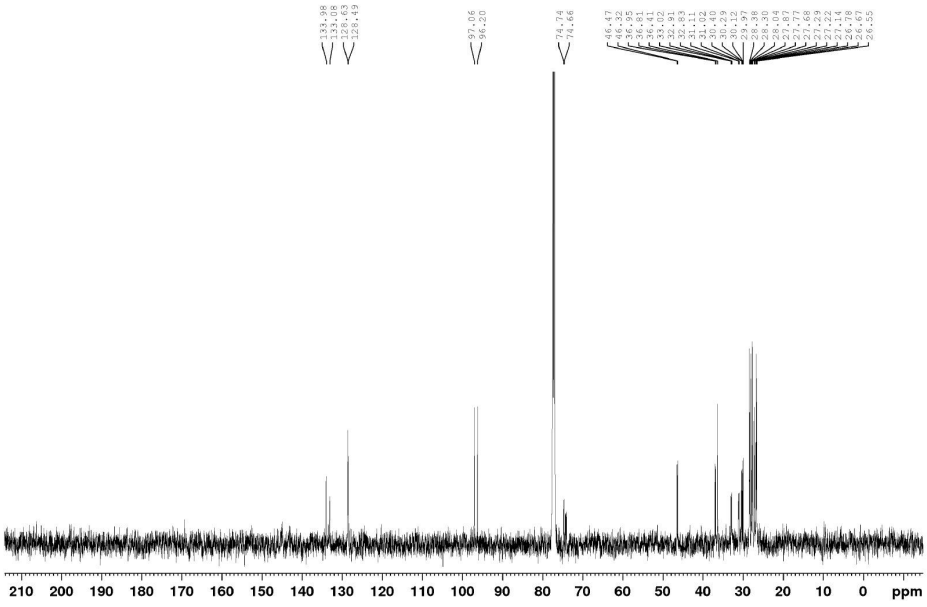
$^{31}P\{^{1}H\}$ NMR Spectrum of **L18**, ($CDCl_3$,202.5 MHz)



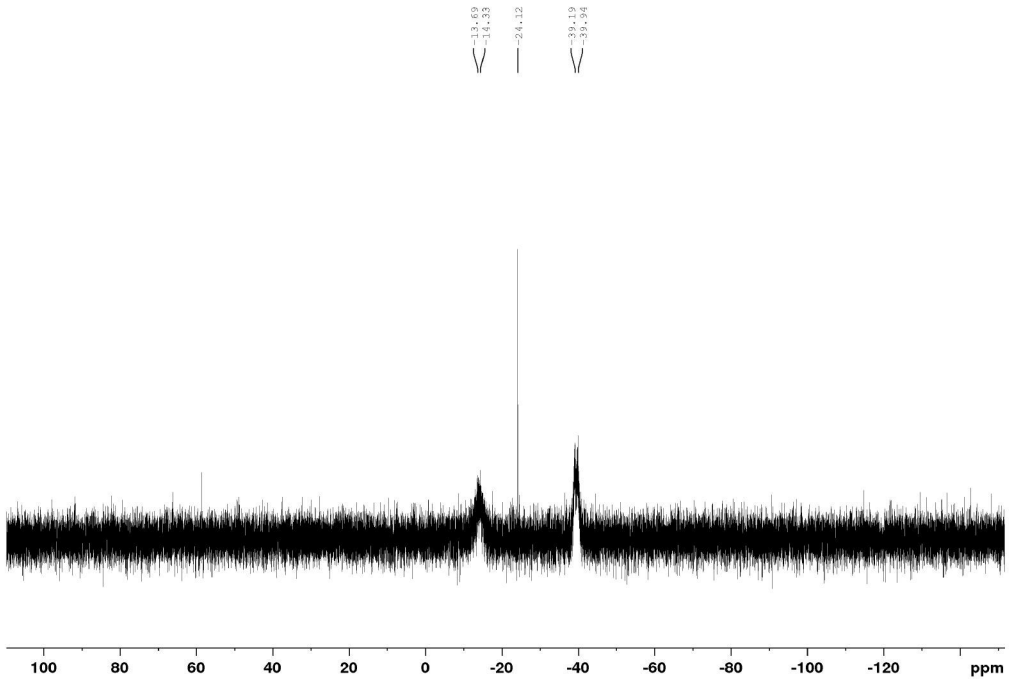
^{1}H NMR Spectrum of **L19**, ($CDCl_3$, 500.1 MHz)



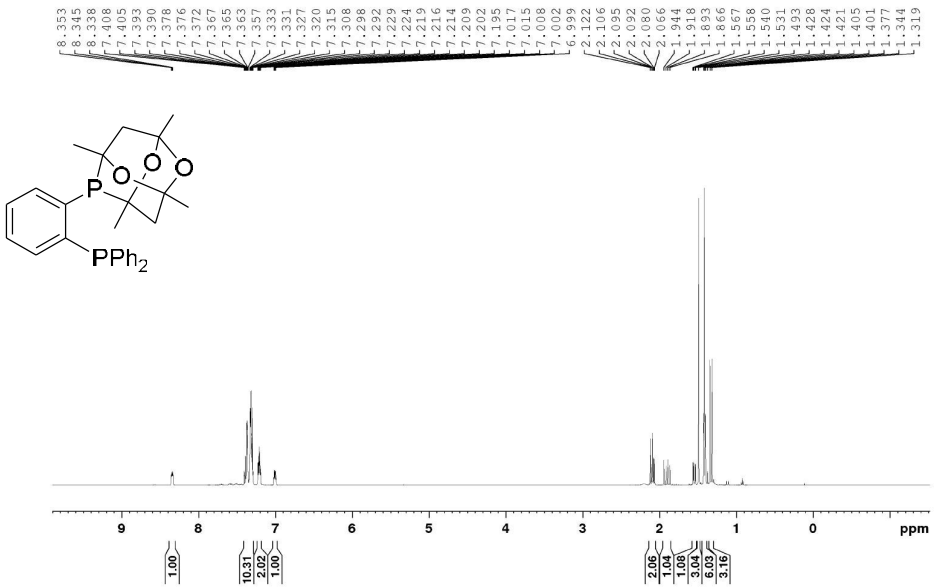
$^{13}C\{^{1}H\}$ NMR Spectrum of **L19**, ($CDCl_3$, 125.8 MHz)



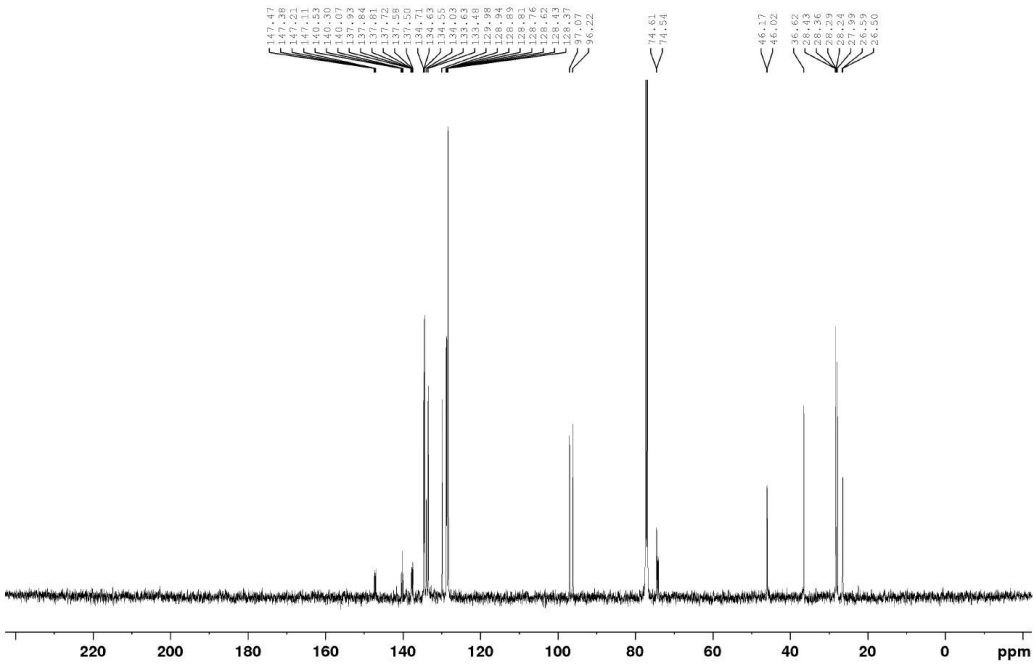
$^{31}P\{^{1}H\}$ NMR Spectrum of **L19**, ($CDCl_3$, 202.5 MHz)



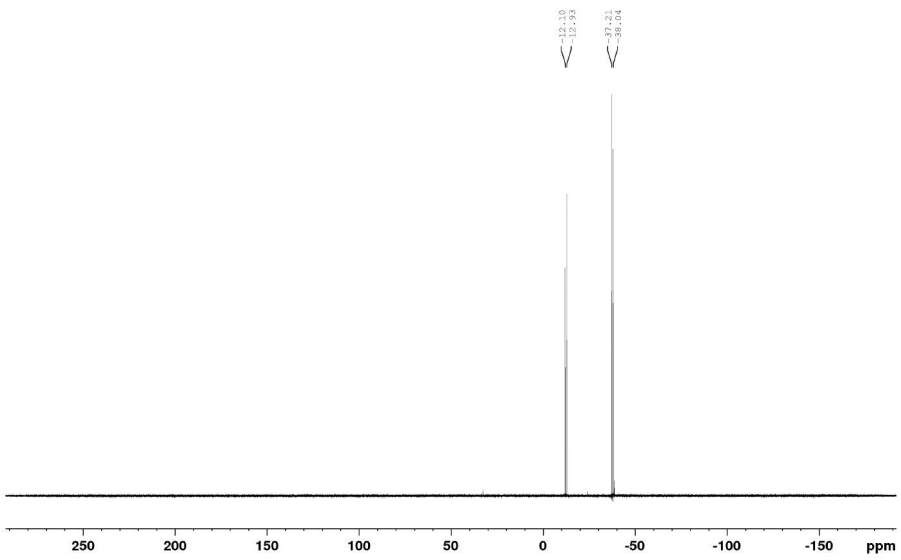
^{1}H NMR Spectrum of **L23**, ($CDCl_3$, 500.1 MHz)



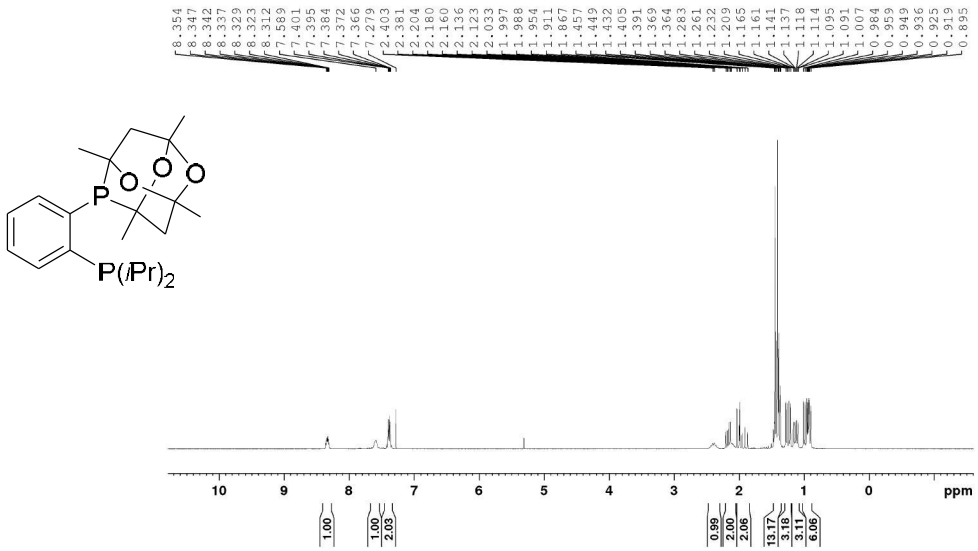
$^{13}C\{^{1}H\}$ NMR Spectrum of **L23**, ($CDCl_3$, 125.8 MHz)



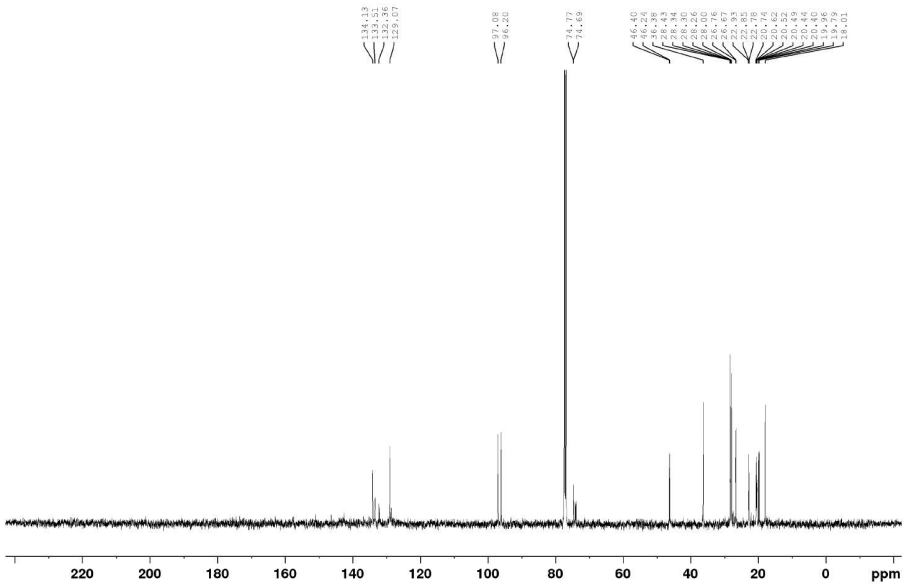
$^{31}P\{^{1}H\}$ NMR Spectrum of **L23**, ($CDCl_3$, 202.5 MHz)



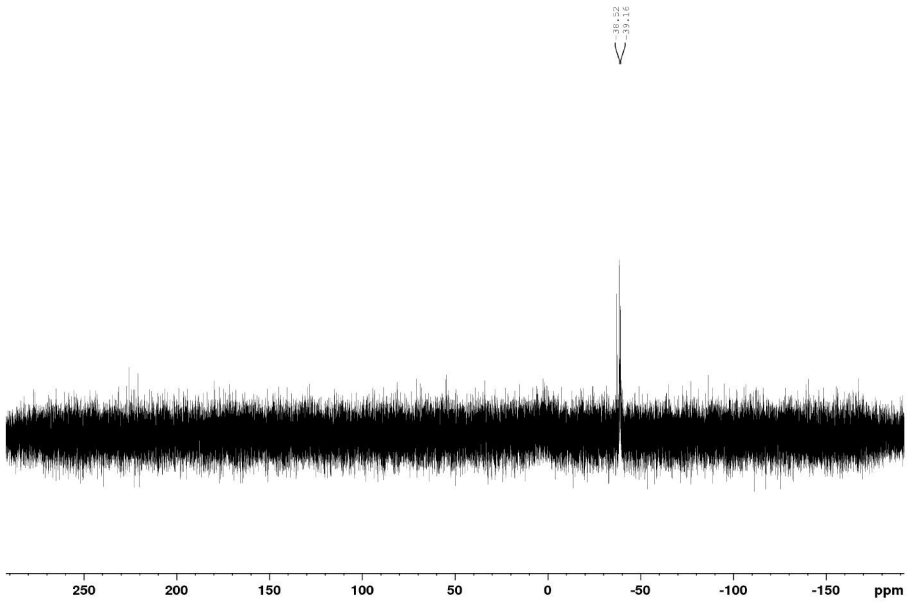
^{1}H NMR Spectrum of **L24**, ($CDCl_3$, 300.1 MHz)



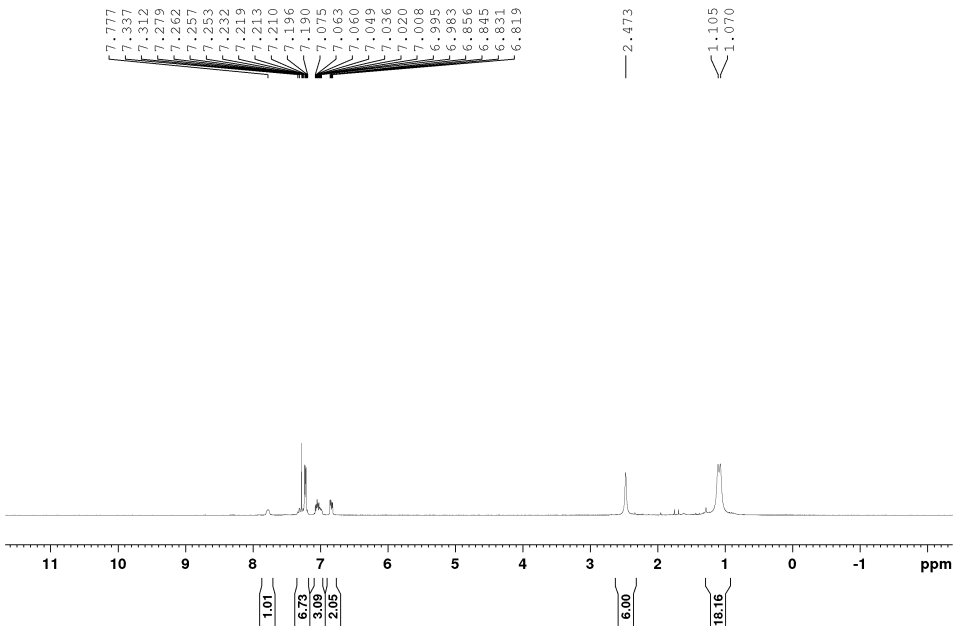
$^{13}C\{^{1}H\}$ NMR Spectrum of **L24**, ($CDCl_3$, 125.8 MHz)



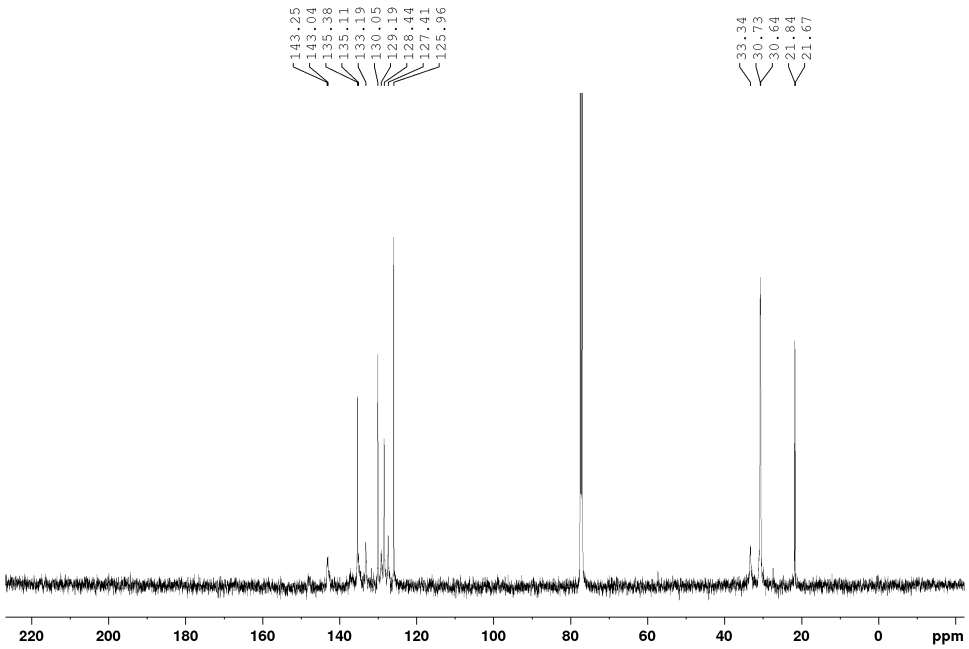
$^{31}P\{^{1}H\}$ NMR Spectrum of **L24**, ($CDCl_3$, 202.5 MHz)



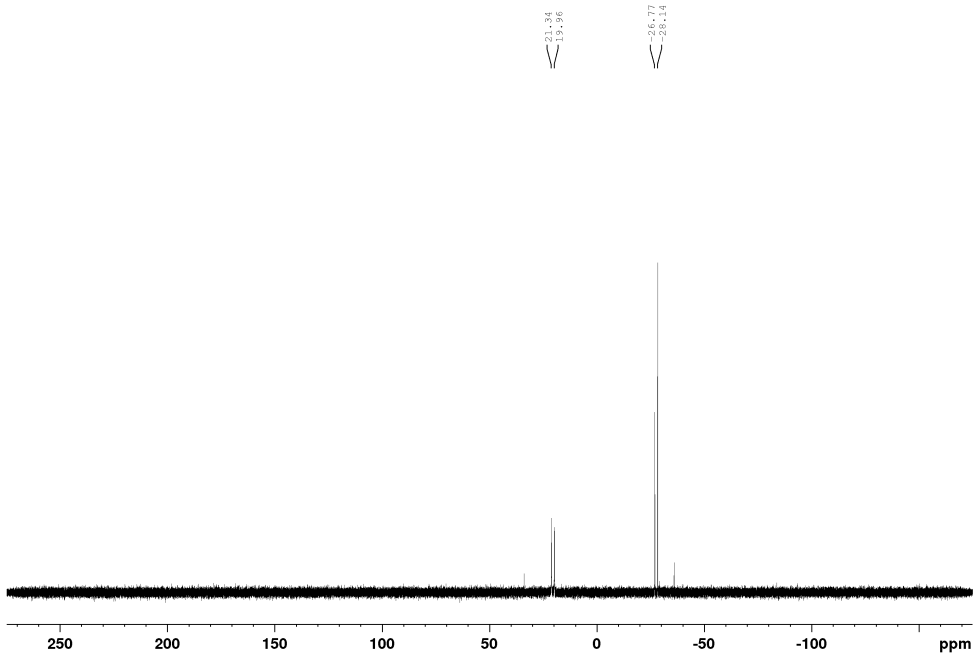
^{1}H NMR Spectrum of **L25**, ($CDCl_3$, 300.1 MHz)



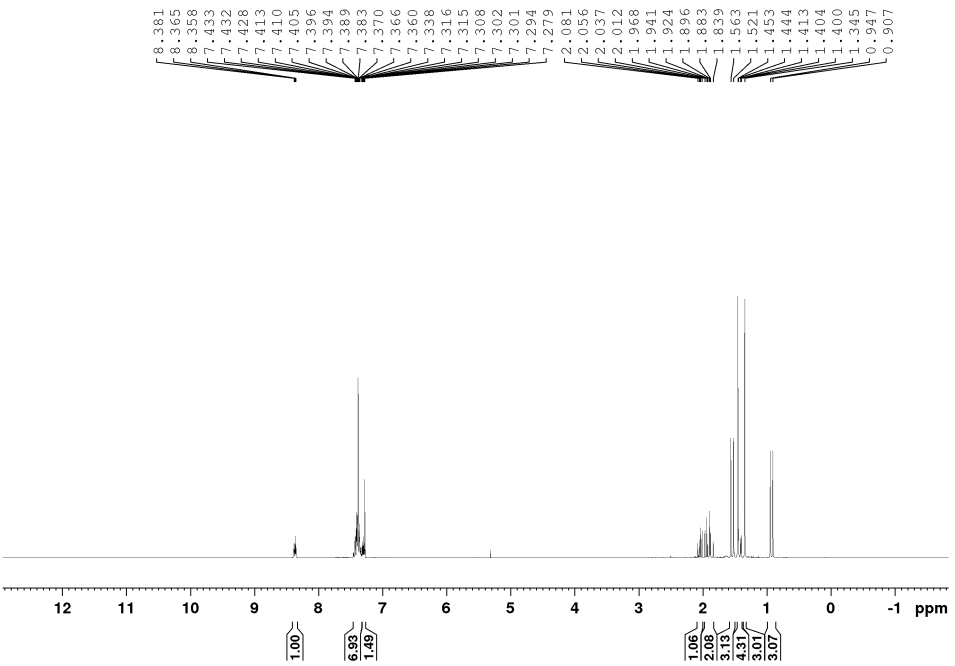
^{13}C NMR Spectrum of **L25**, ($CDCl_3$, 121.8 MHz)



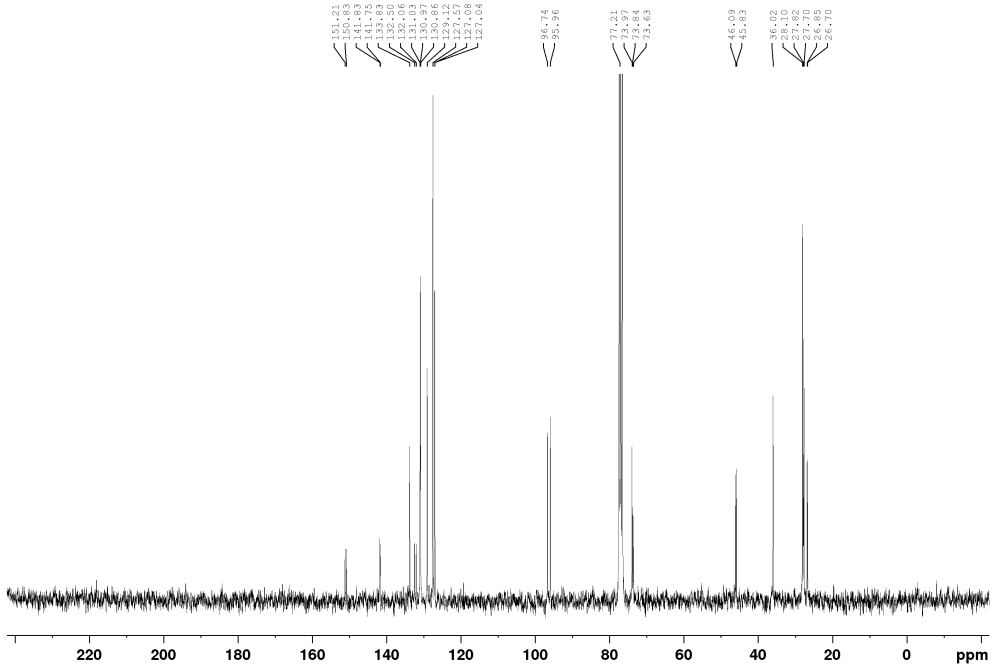
^{31}P NMR Spectrum of **L25**, ($CDCl_3$, 121.5 MHz)



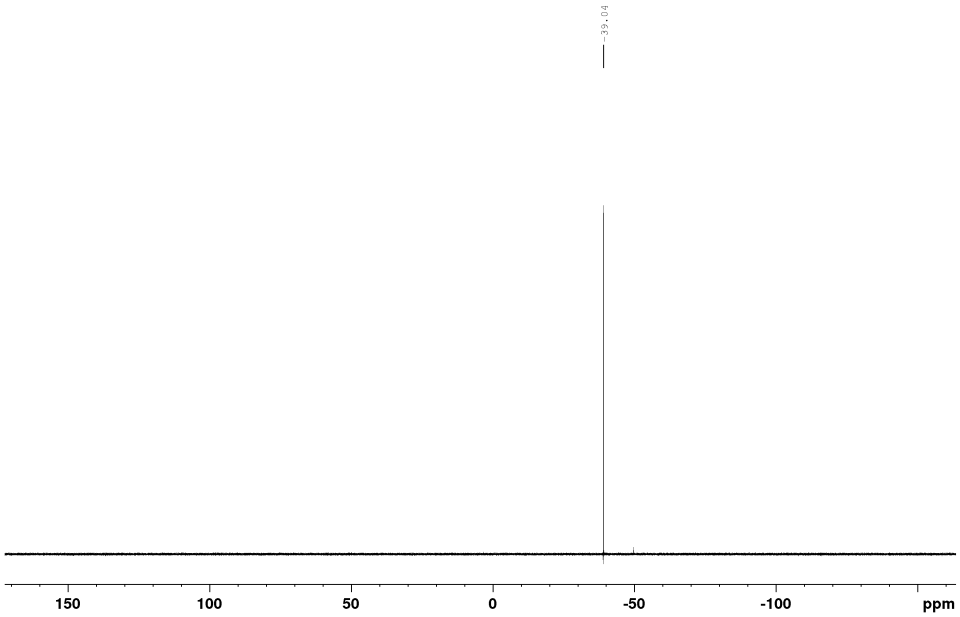
^{1}H NMR Spectrum of **L26**, ($CDCl_3$, 300.1 MHz)



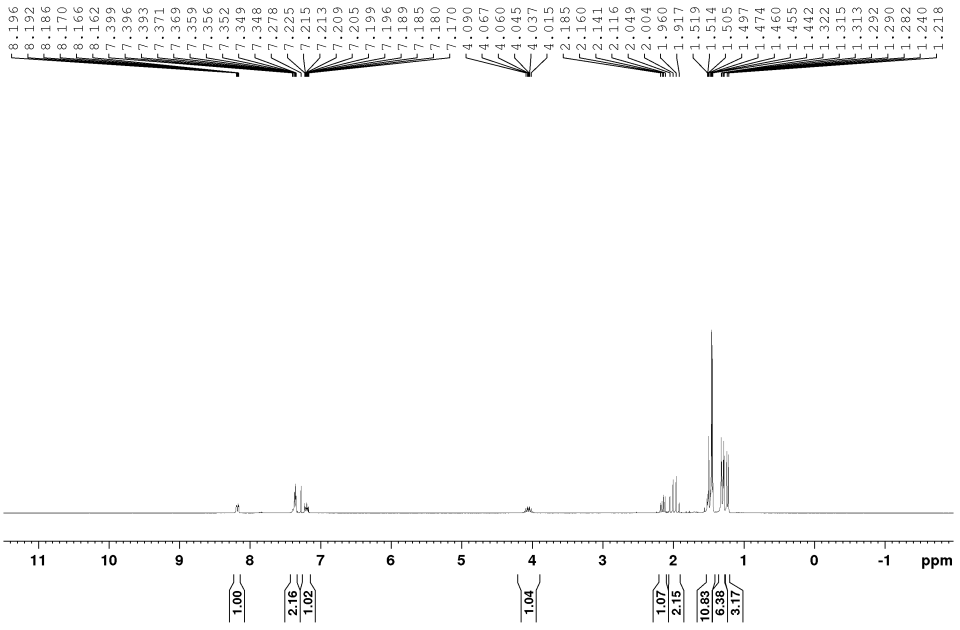
^{13}C NMR Spectrum of **L26**, ($CDCl_3$, 75.5 MHz)



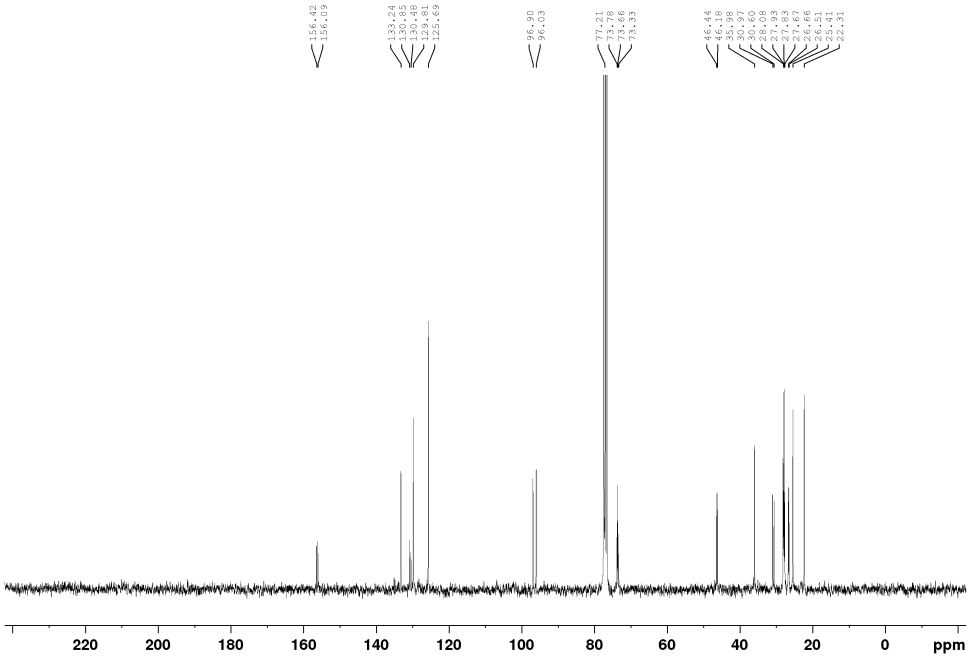
^{31}P NMR Spectrum of **L26**, ($CDCl_3$, 121.5 MHz)



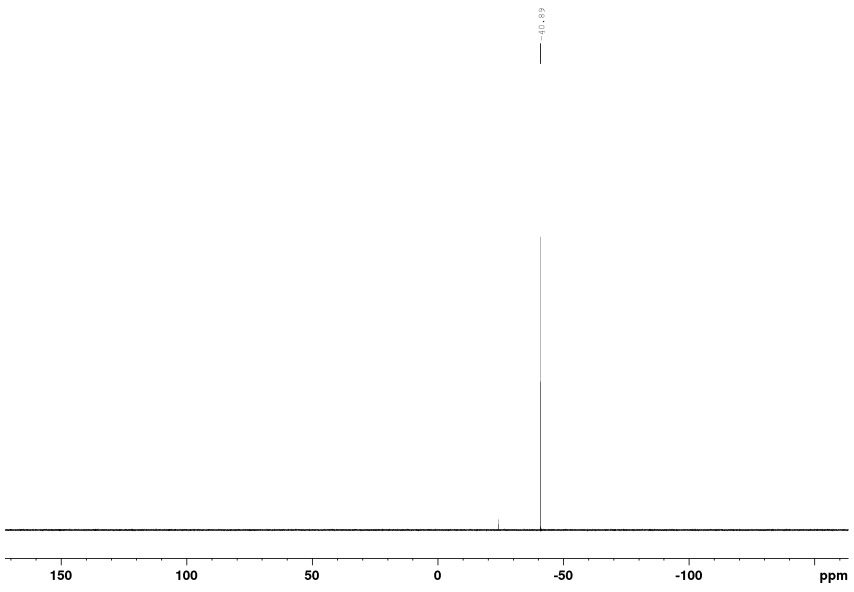
^{1}H NMR Spectrum of **L27**, ($CDCl_3$, 300.1 MHz)



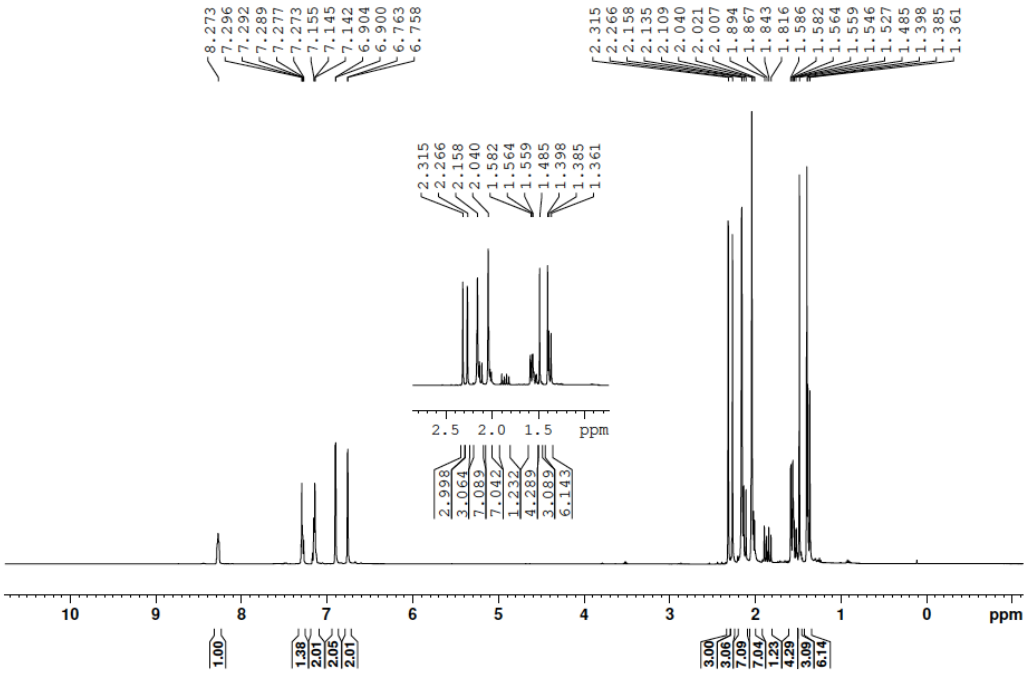
^{13}C NMR Spectrum of **L27**, ($CDCl_3$, 75.5 MHz)



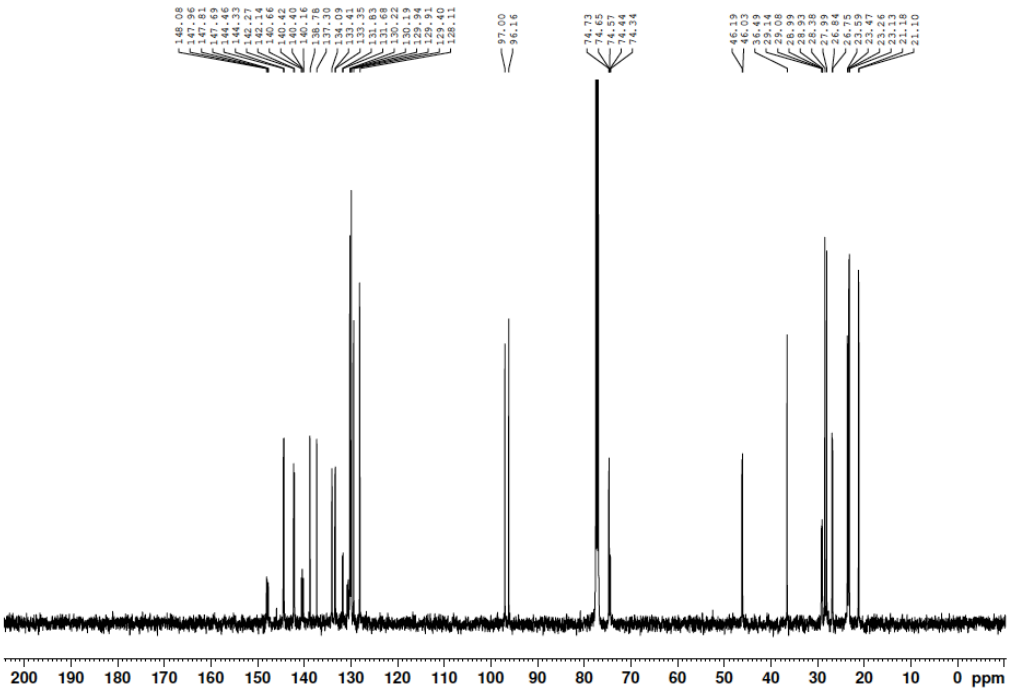
^{31}P NMR Spectrum of **L27**, ($CDCl_3$, 121.5 MHz)



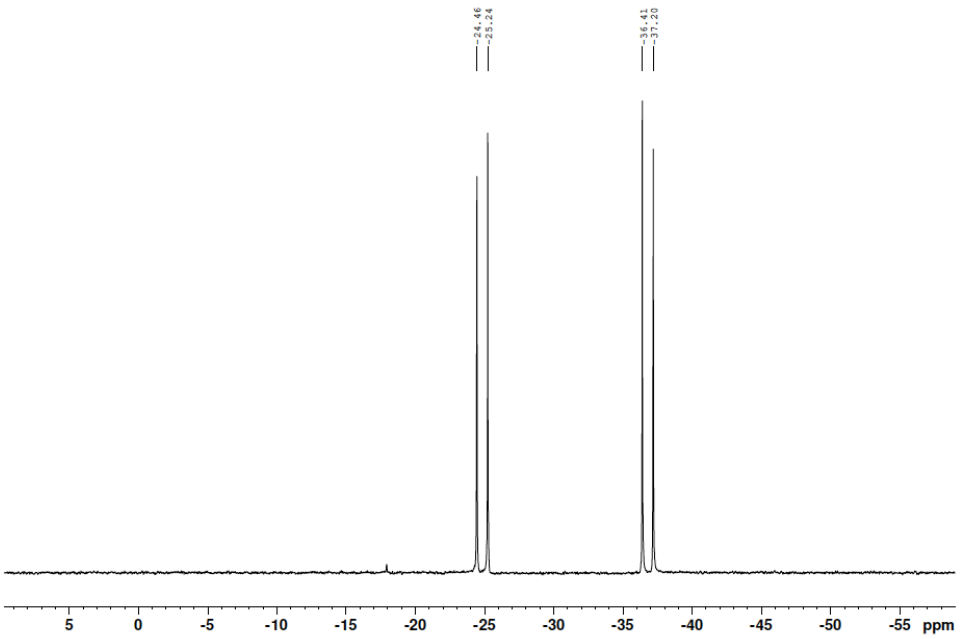
^{1}H NMR of **L43**, ($CDCl_3$, 500.1 MHz)



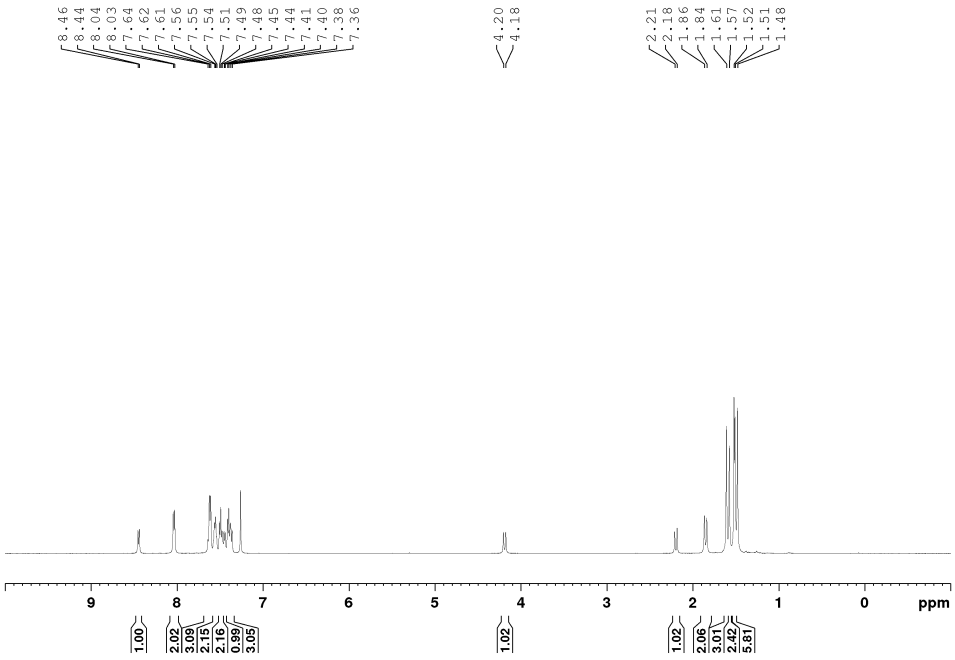
$^{13}C\{^{1}H\}$ NMR of **L43** ($CDCl_3$, 125.8 MHz)



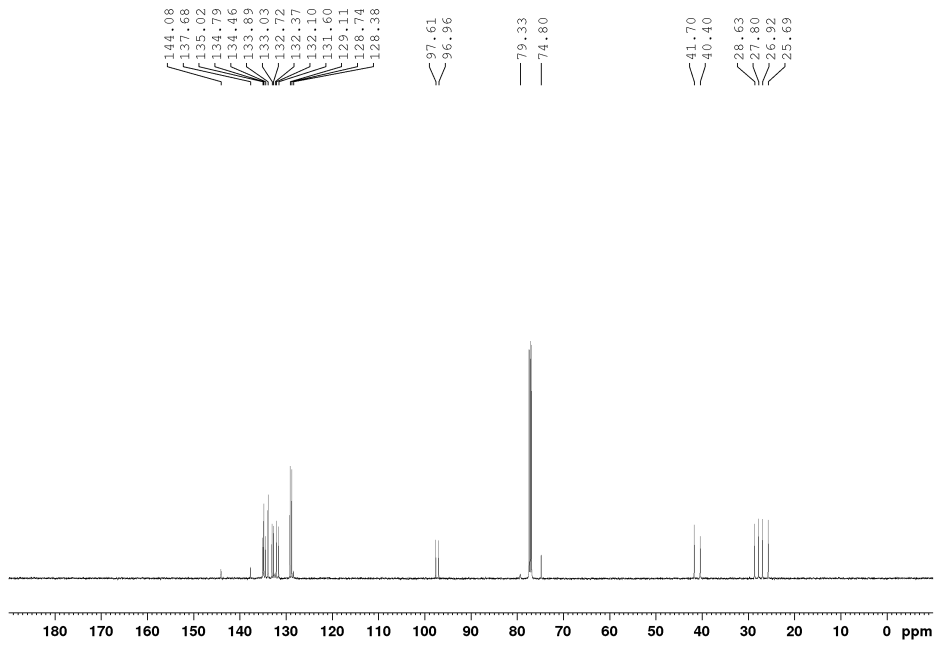
$^{31}P\{^{1}H\}$ NMR of **L43**, ($CDCl_3$, 202.5 MHz)



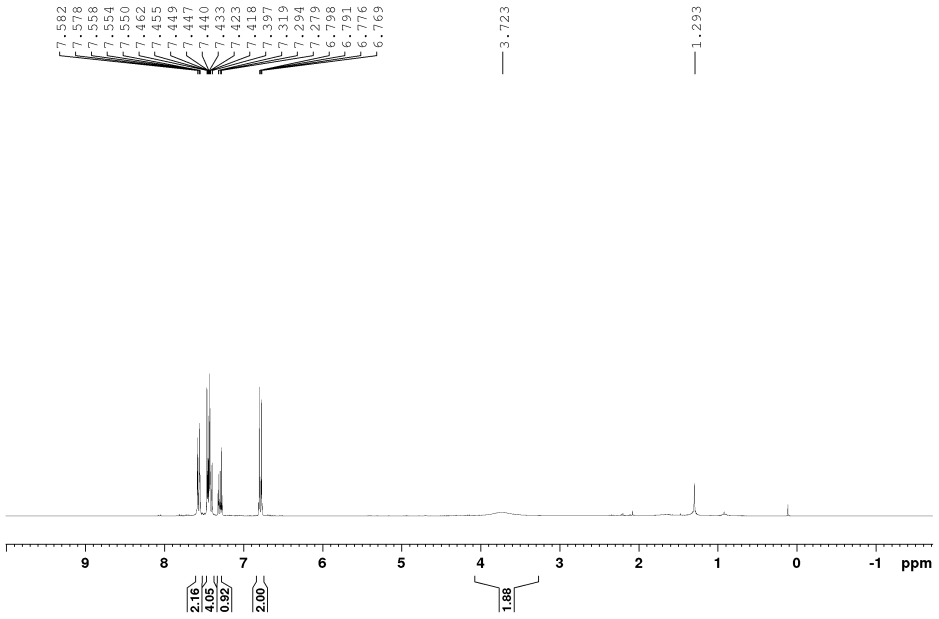
^{1}H NMR of (**L23**)$NiCl_2$, ($CDCl_3$, 500.1 MHz)



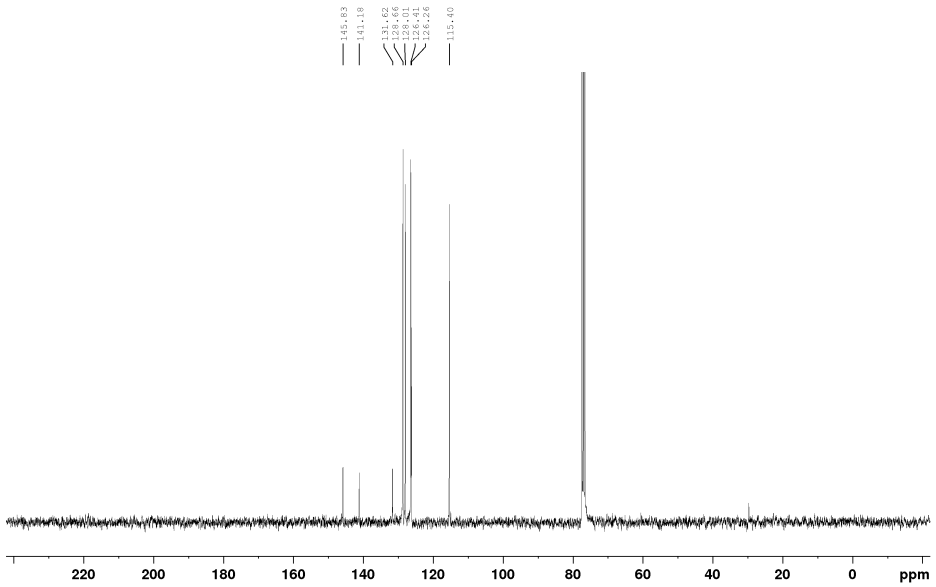
$^{13}C\{^{1}H\}$ NMR of (**L23**)$NiCl_2$ ($CDCl_3$, 125.8 MHz)



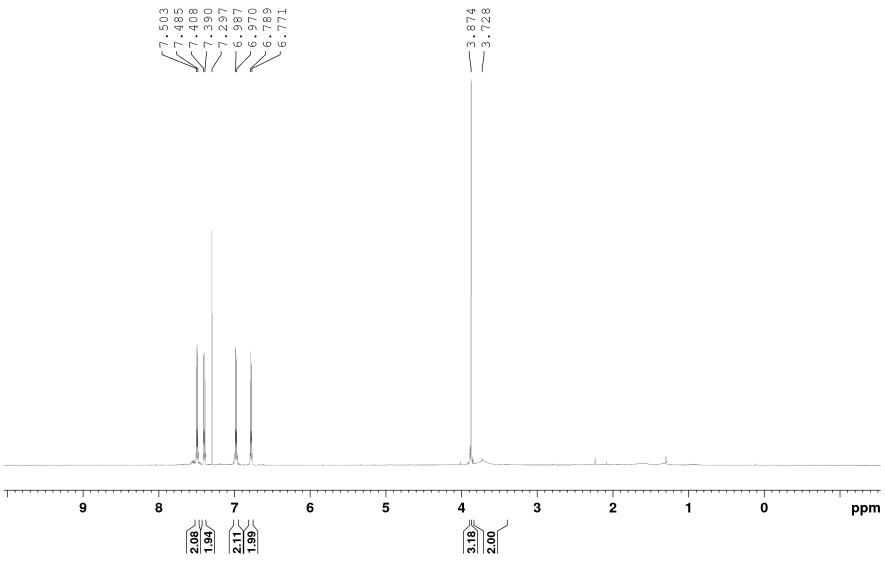
^{1}H NMR Spectrum of 4-phenylaniline (**2.4**), ($CDCl_3$, 300 MHz)



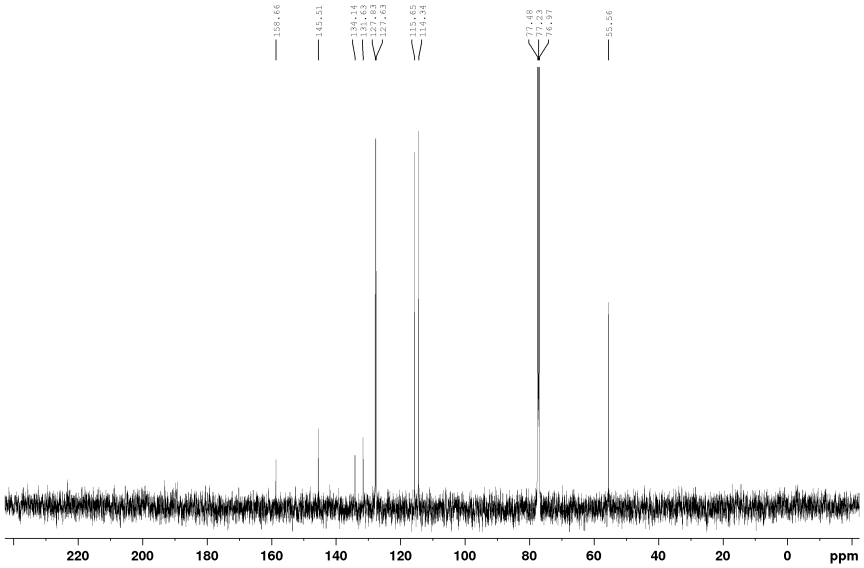
^{13}C NMR Spectrum of 4-phenylaniline (**2.4**), ($CDCl_3$, 300 MHz)



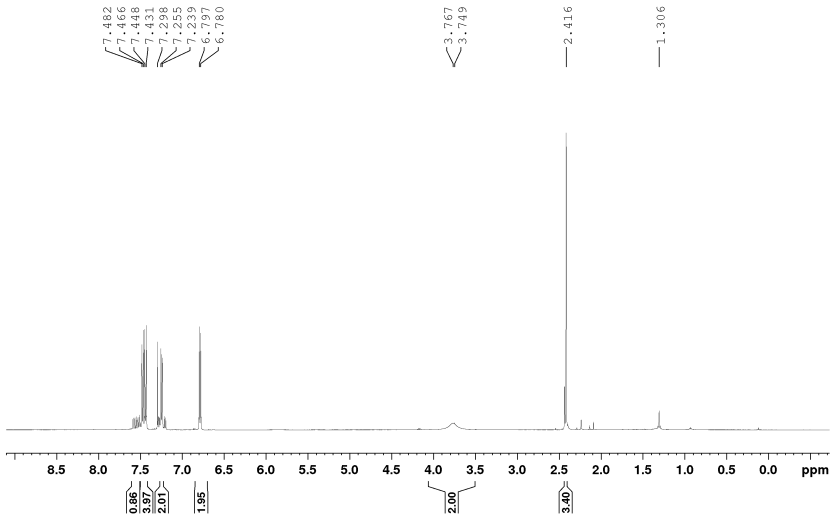
^{1}H NMR Spectrum of 4'-methoxylbiphenyl-4-amine (**2.5**), ($CDCl_3$)



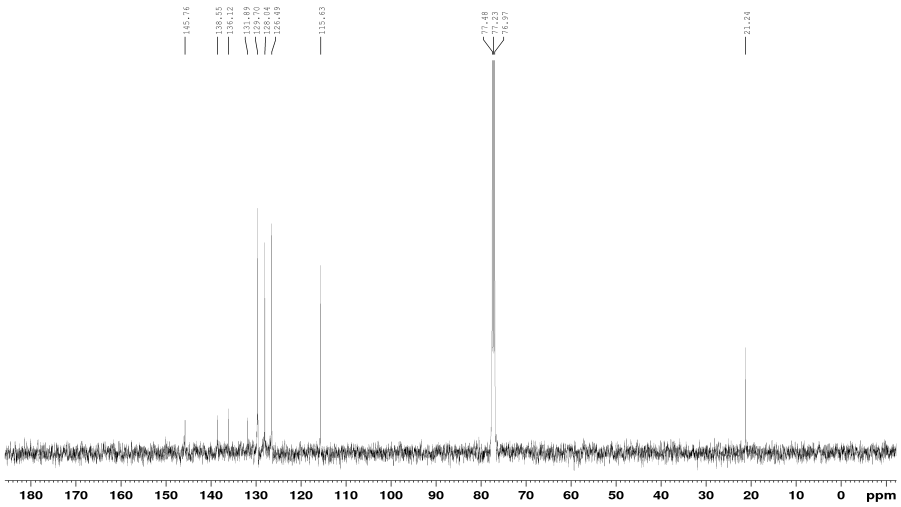
$^{13}C\{^{1}H\}$ NMR Spectrum of 4'-methoxybiphenyl-4-amine (**2.5**), ($CDCl_3$)



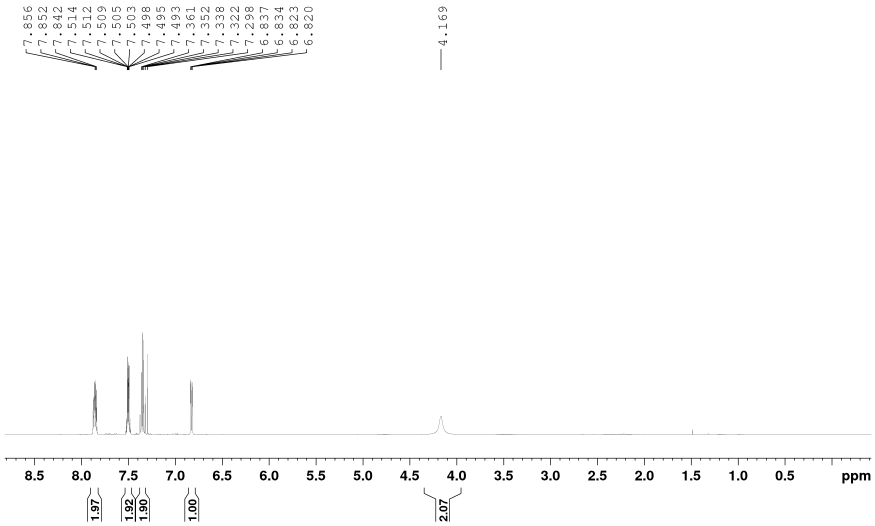
^{1}H NMR Spectrum of 4'-methylbiphenyl-4-amine (**2.6**), ($CDCl_3$)



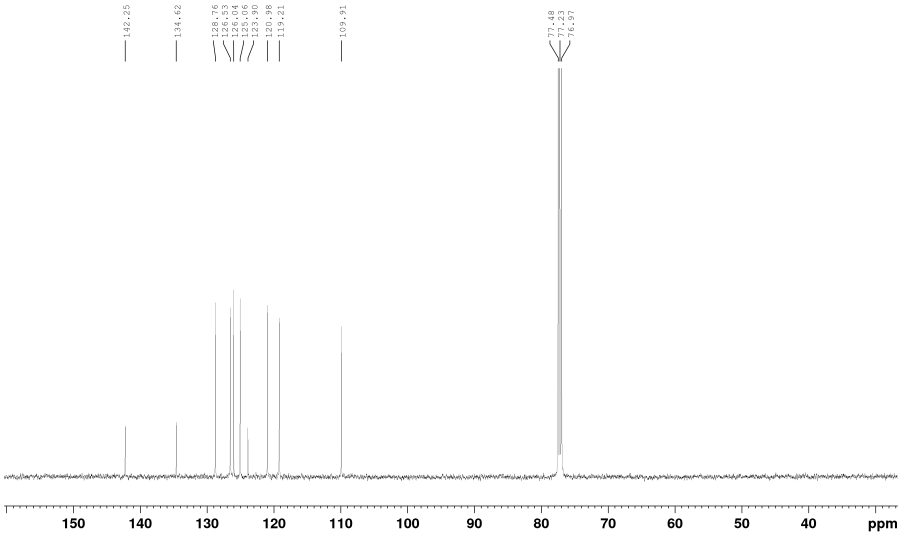
$^{13}C\{^{1}H\}$ NMR Spectrum of 4'-methylbiphenyl-4-amine (**2.6**), ($CDCl_3$)



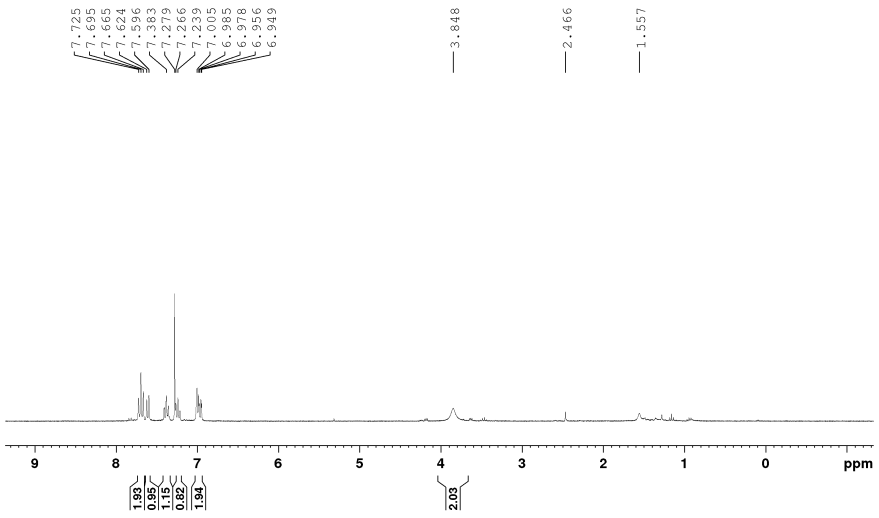
^{1}H NMR Spectrum of Naphthalen-1-amine (**2.7**), ($CDCl_3$)



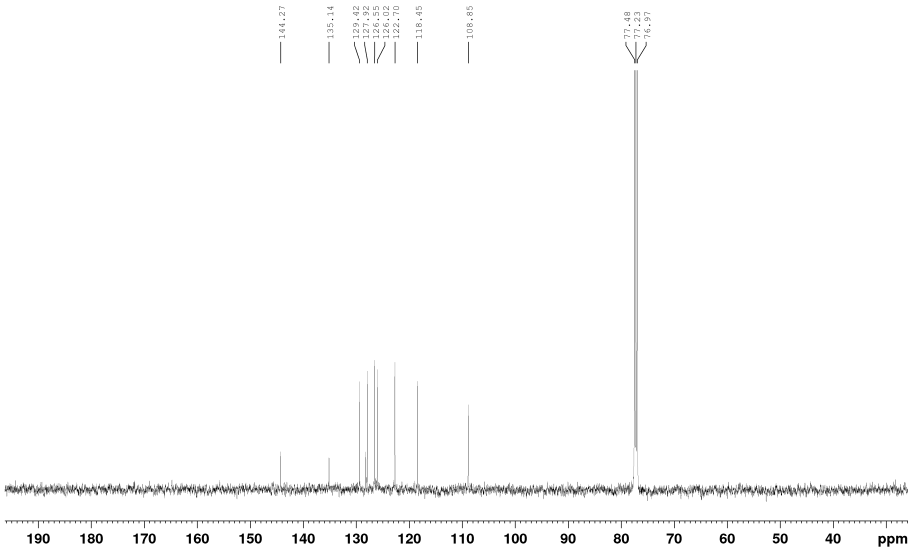
$^{13}C\{^{1}H\}$ NMR Spectrum of Naphthalen-1-amine (**2.7**), ($CDCl_3$)



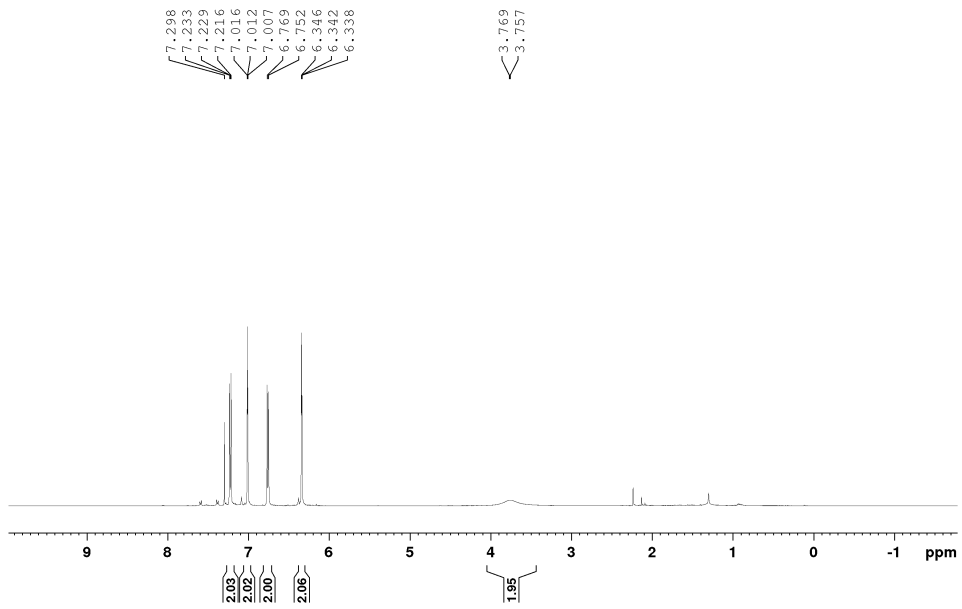
^{1}H NMR Spectrum of Naphthalen-2-amine (**2.8**), ($CDCl_3$)



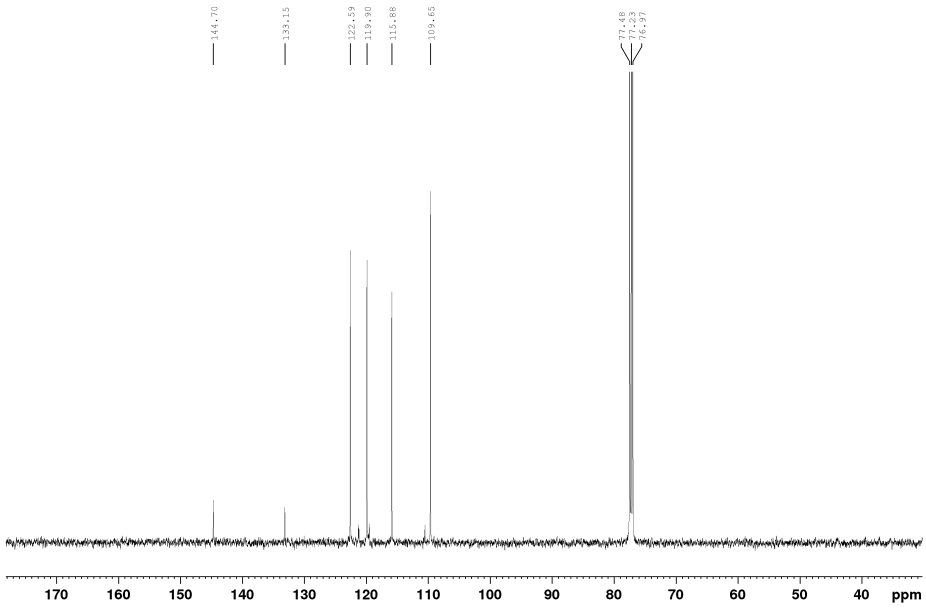
$^{13}C\{^{1}H\}$ NMR Spectrum of Naphthalen-2-amine (**2.8**), ($CDCl_3$)



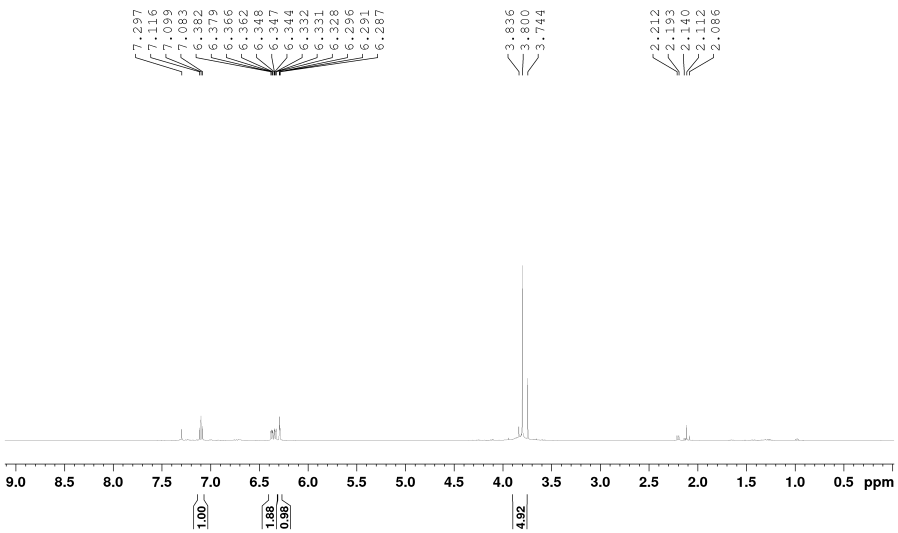
^{1}H NMR Spectrum of 4-(1H-pyrrol-1yl)aniline (**2.9**), ($CDCl_3$, 500 MHz)



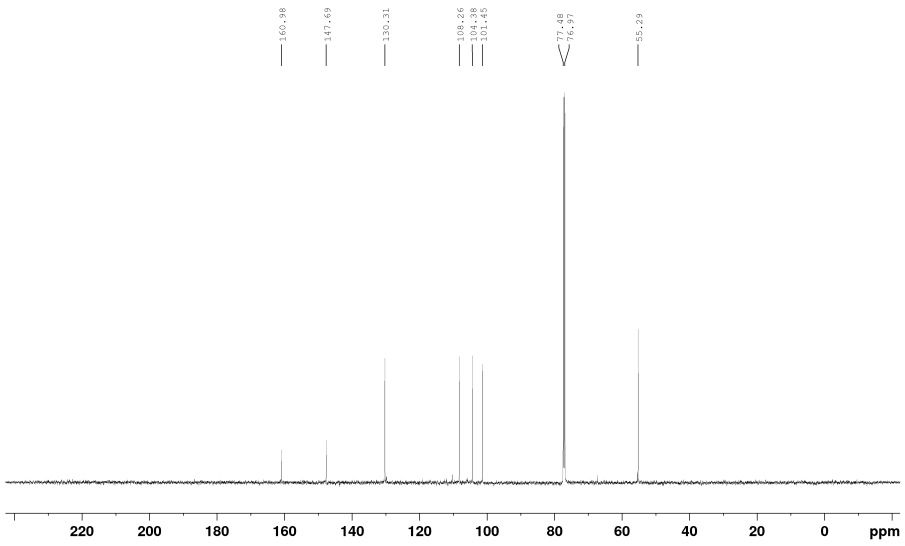
^{13}C NMR Spectrum of 4-(1H-pyrrol-1yl)aniline (**2.9**), ($CDCl_3$, 500 MHz)



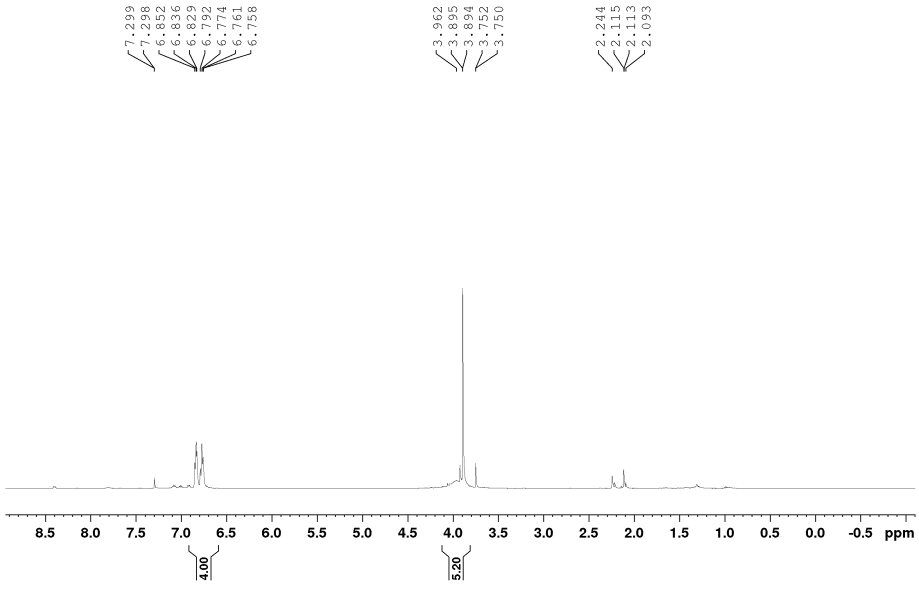
^{1}H NMR Spectrum of 3-methoxyaniline (**2.10**), ($CDCl_3$)



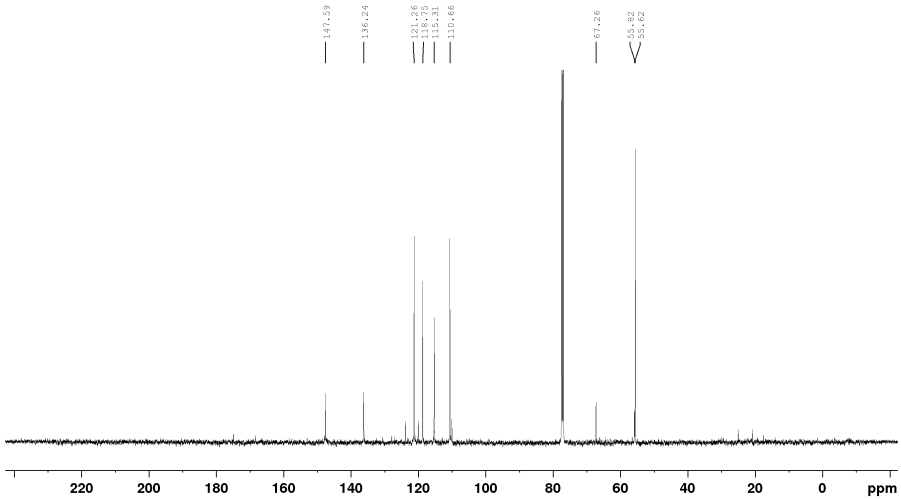
$^{13}C\{^{1}H\}$ NMR Spectrum of 3-methoxyaniline (**2.10**), ($CDCl_3$)



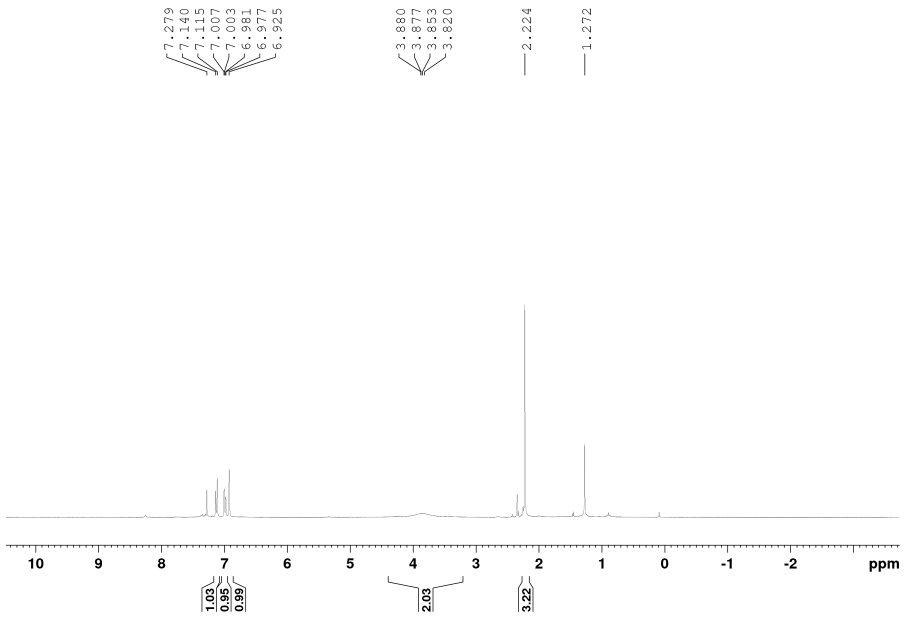
^{1}H NMR Spectrum of 2-methoxyaniline (**2.11**), ($CDCl_3$)



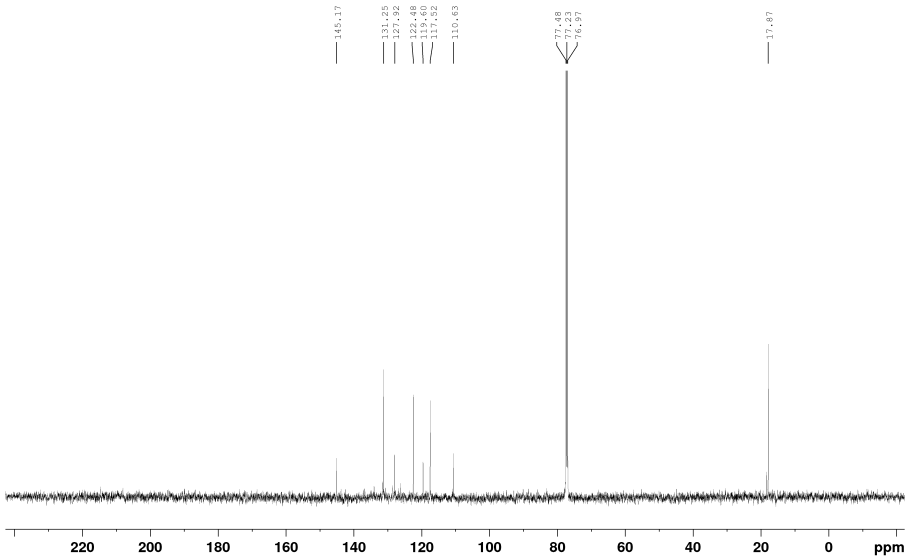
$^{13}C\{^{1}H\}$ NMR Spectrum of 2-methoxyaniline (**2.11**), ($CDCl_3$)



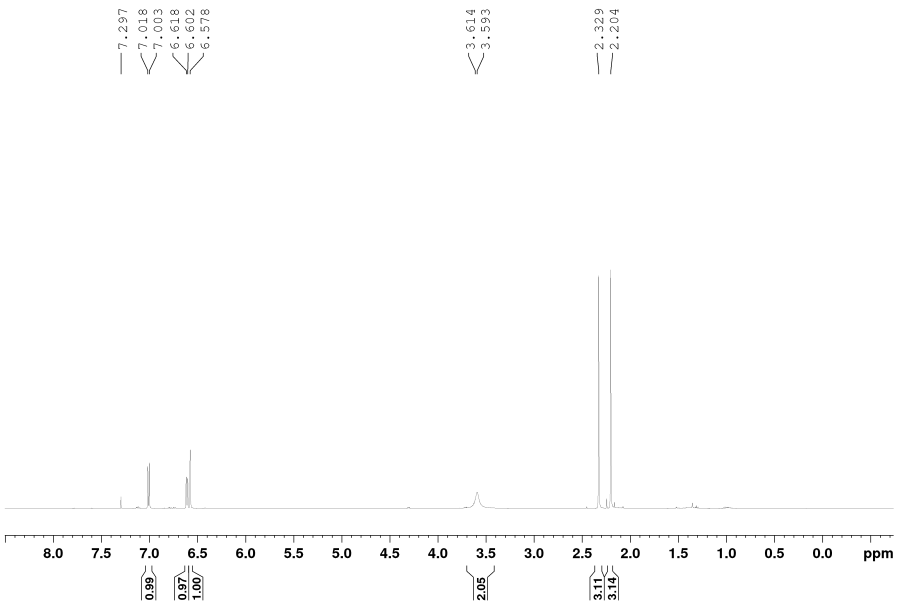
^{1}H NMR Spectrum of 3-amino-4-methylbenzonitrile (**2.12**), ($CDCl_3$)



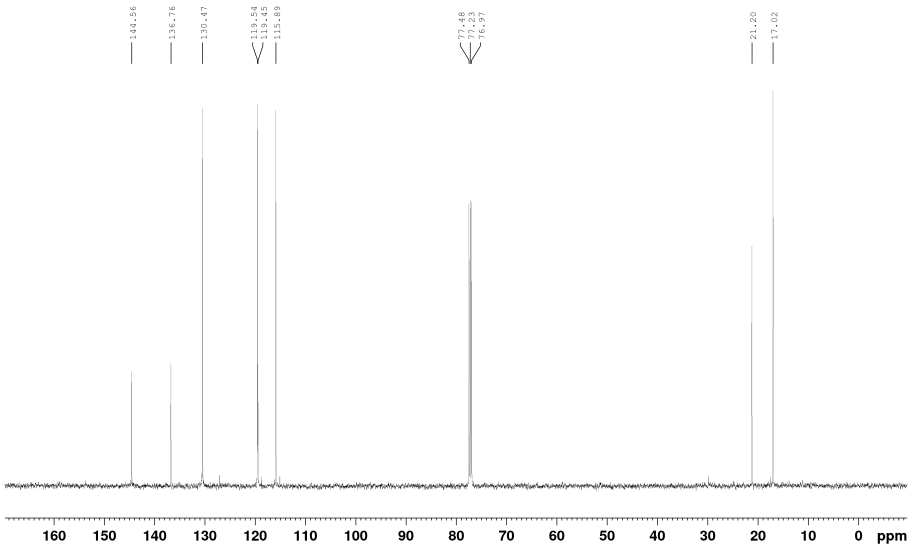
$^{13}C\{^{1}H\}$ NMR Spectrum of 3-amino-4-methylbenzonitrile (**2.12**), ($CDCl_3$)



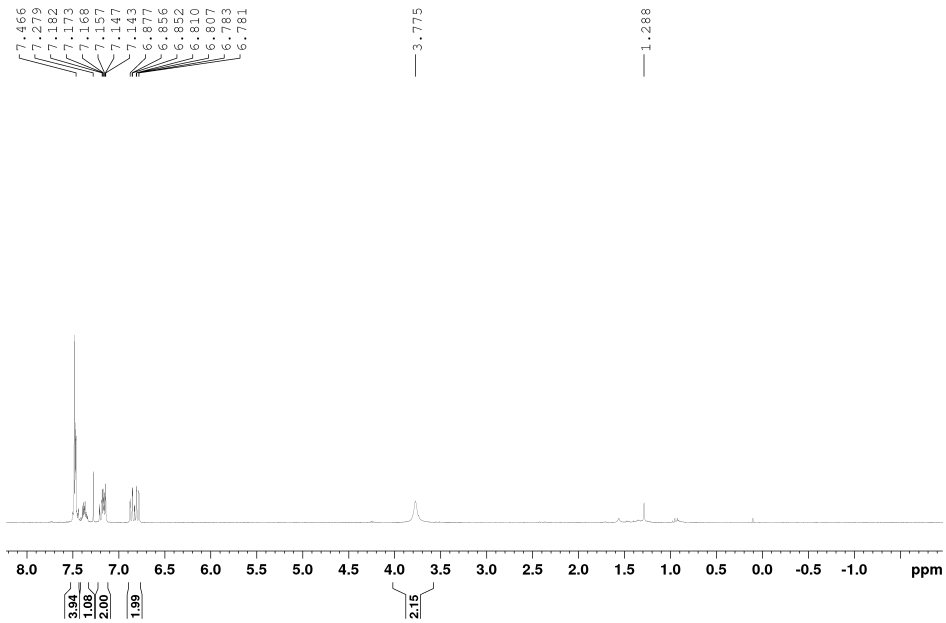
^{1}H NMR Spectrum of 2,5-dimethylaniline (**2.13**), ($CDCl_3$)



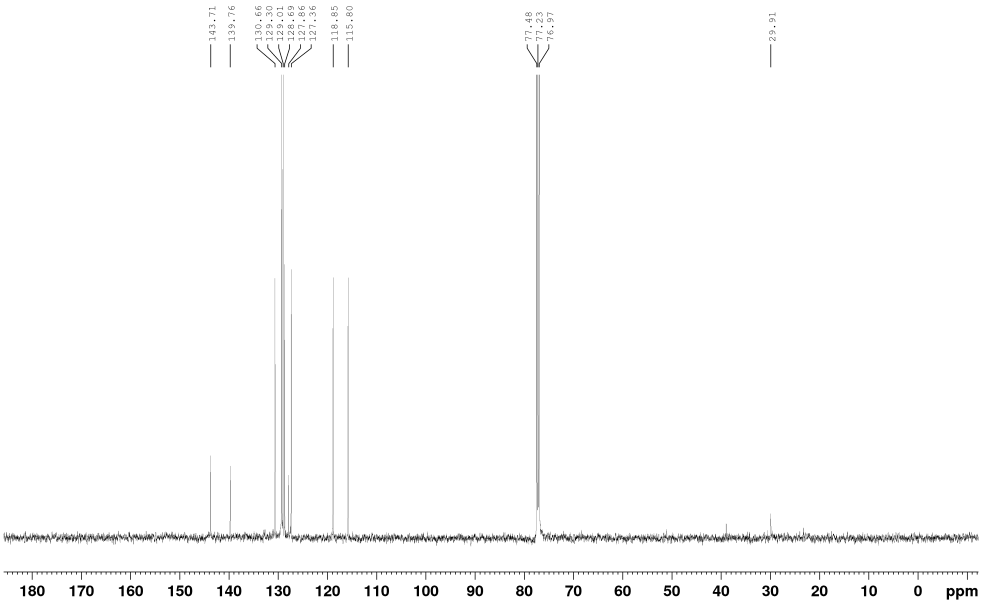
$^{13}C\{^{1}H\}$ NMR Spectrum of 2,5-dimethylaniline (**2.13**), ($CDCl_3$)



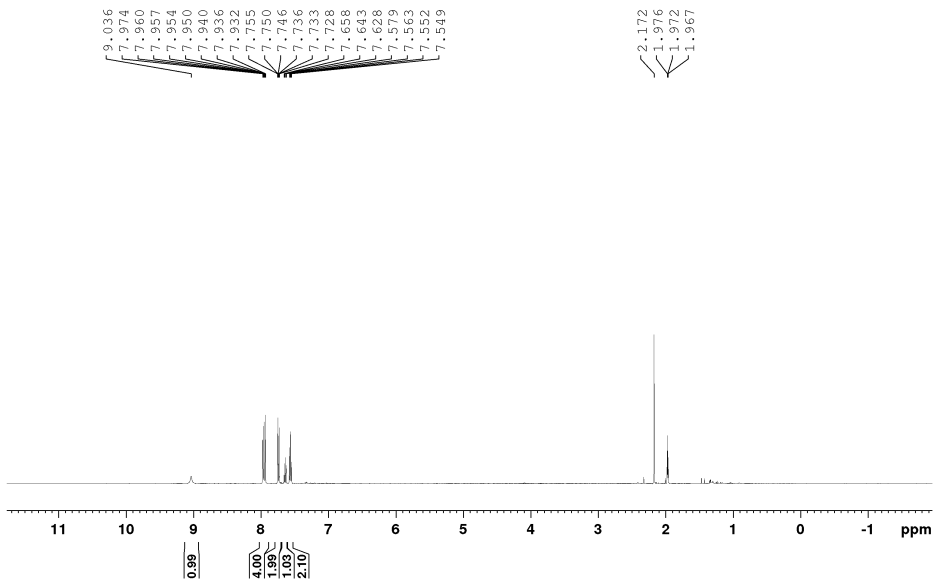
^{1}H NMR Spectrum of [1,1'-Biphenyl]-2-amine (**2.14**), ($CDCl_3$)



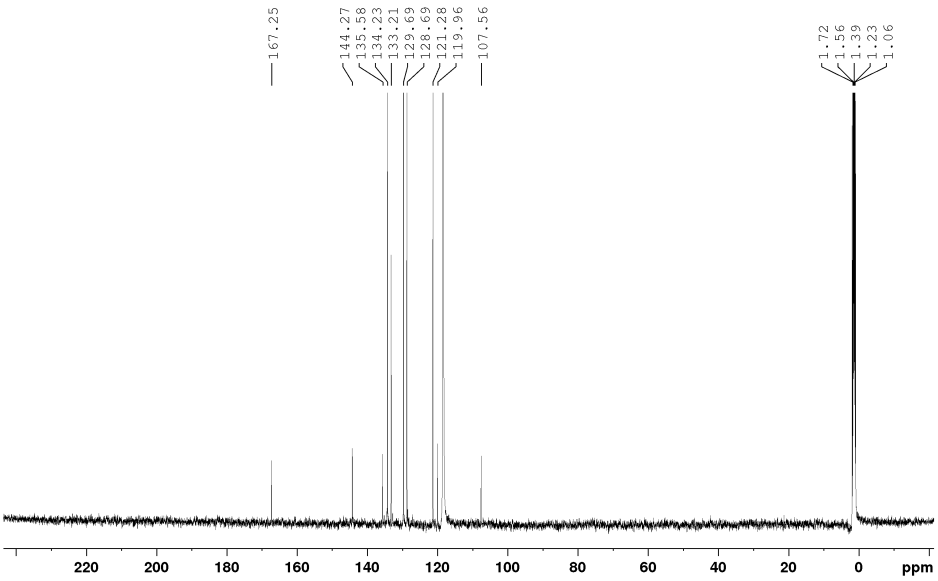
$^{13}C\{^{1}H\}$ Spectrum of [1,1'-Biphenyl]-2-amine (**2.14**), ($CDCl_3$)



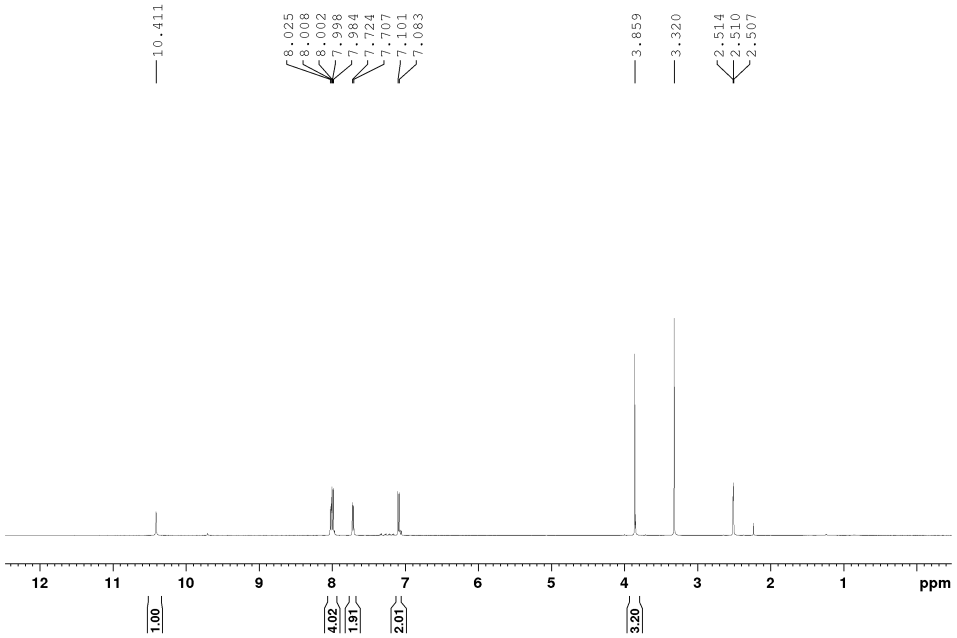
^{1}H NMR Spectrum of *N*-(4-cyanophenyl)-benzamide (**3.3**) (CD_3CN, 500.1 MHz)



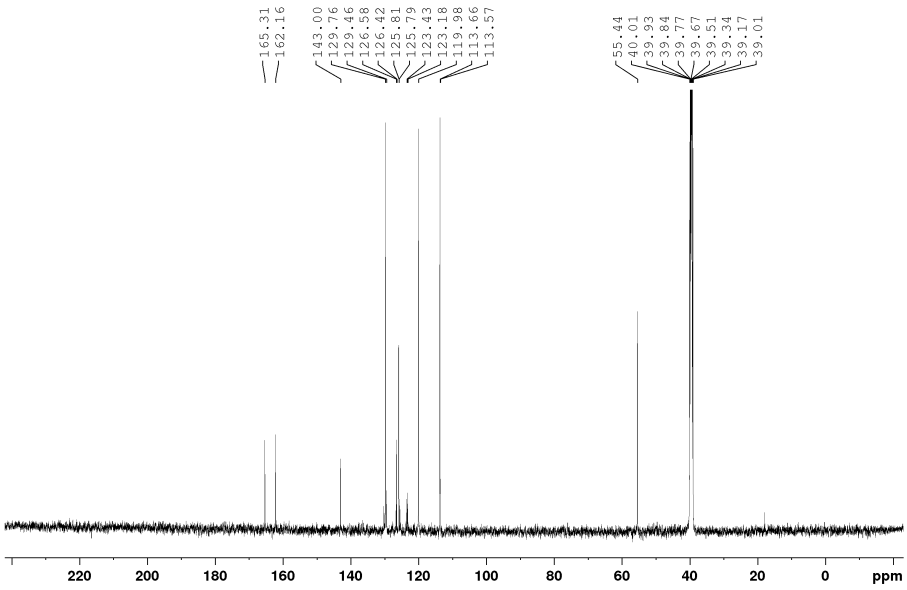
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-(4-cyanophenyl)-benzamide (**3.3**), (CD_3CN, 125.8 MHz)



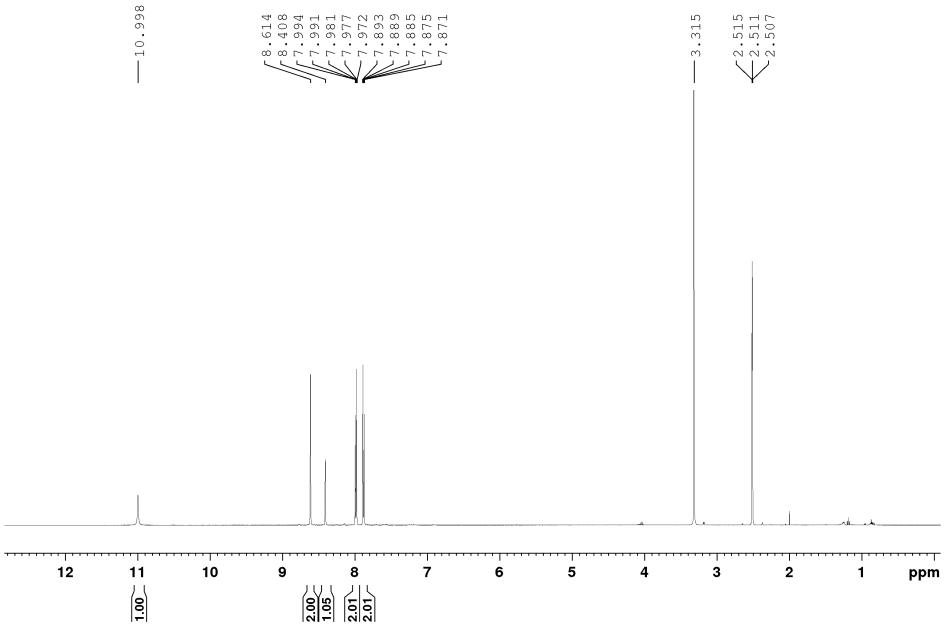
^{1}H NMR Spectrum of 4-methoxy-*N*-[4-(trifluoromethyl)phenyl]-benzamide (**3.4**), (DMSO-d_6, 500.1 MHz)



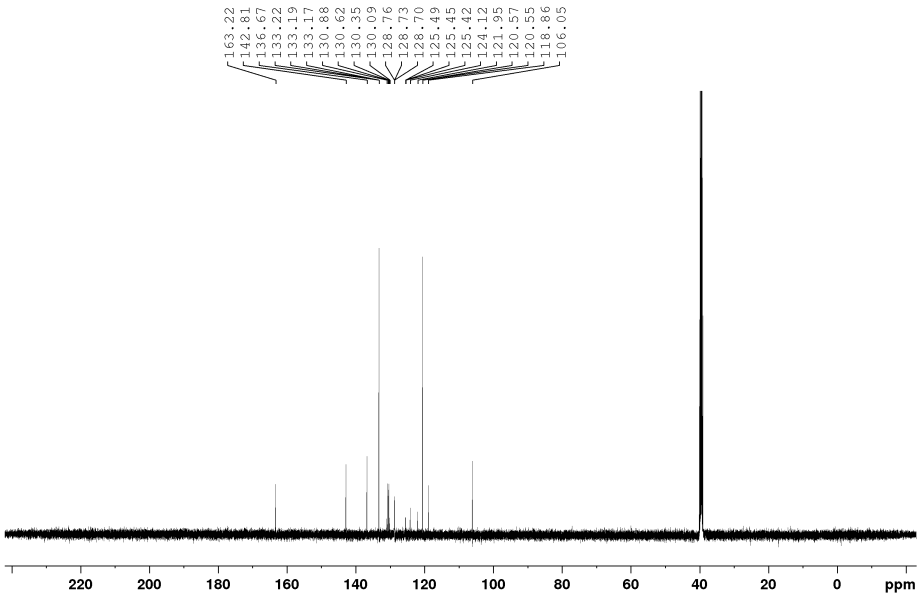
$^{13}C\{^{1}H\}$ NMR Spectrum of 4-methoxy-*N*-[4-(trifluoromethyl)phenyl]-benzamide, (**3.4**), (DMSO-d_6, 125.8 MHz)



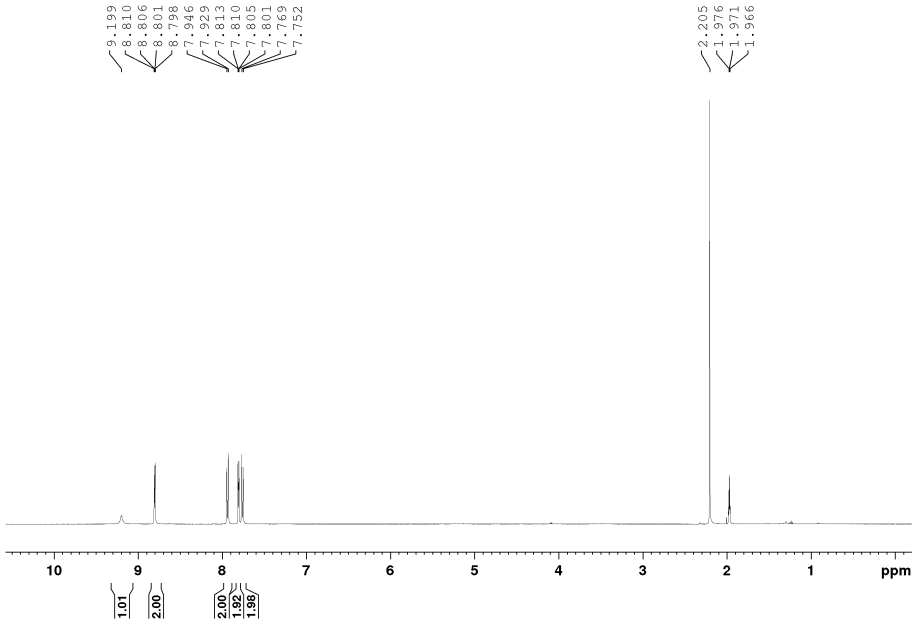
^{1}H NMR Spectrum of *N*-(4-cyanophenyl)-3,5-bis(trifluoromethyl)-benzamide (**3.5**), (DMSO-d_6, 500.1 MHz)



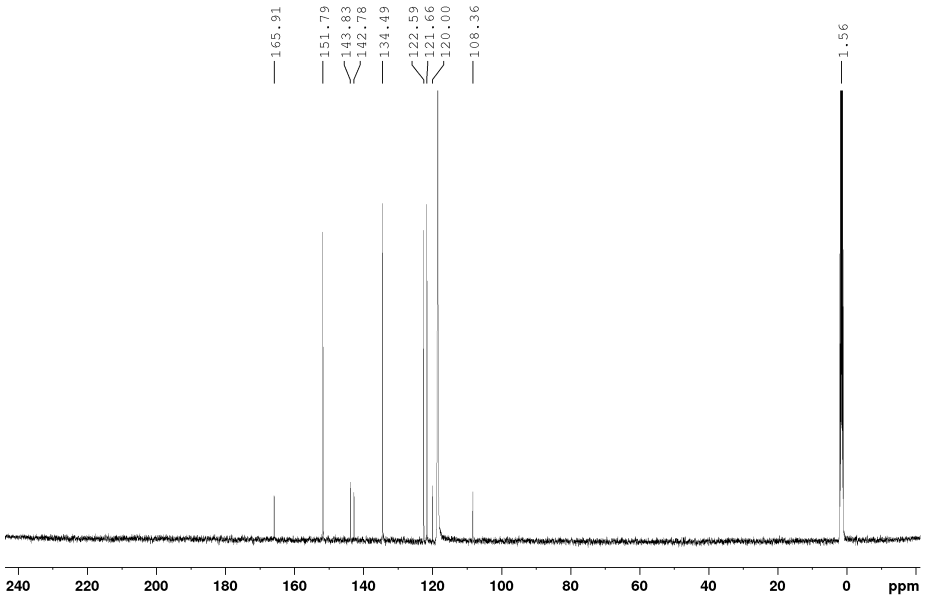
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-(4-cyanophenyl)-3,5-bis(trifluoromethyl)-benzamide (**3.5**), (DMSO-d_6, 125.8 MHz)



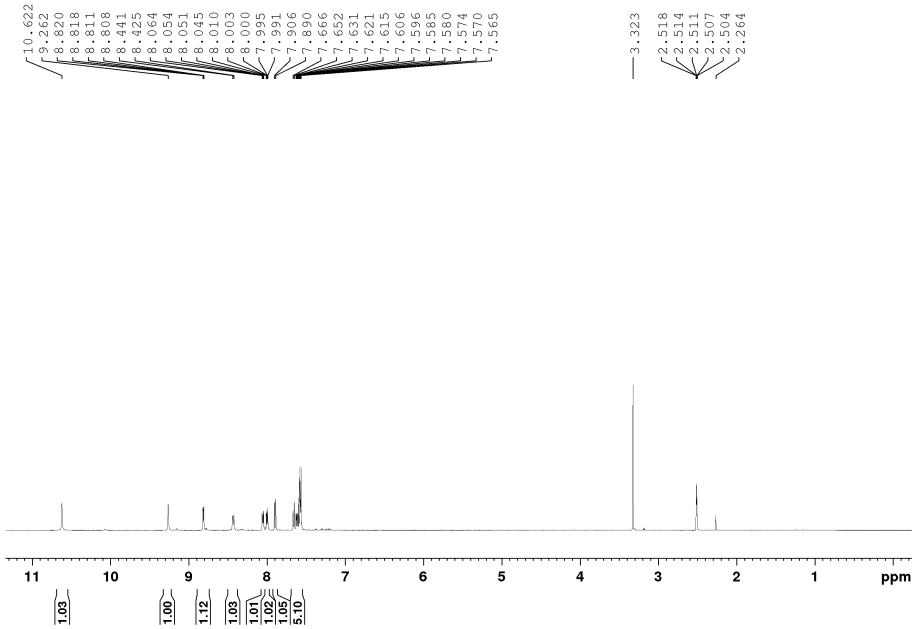
^{1}H NMR Spectrum of *N*-(4-cyanophenyl)-pyridinecarboxamide (**3.6**), (CD_3CN, 500.1 MHz)



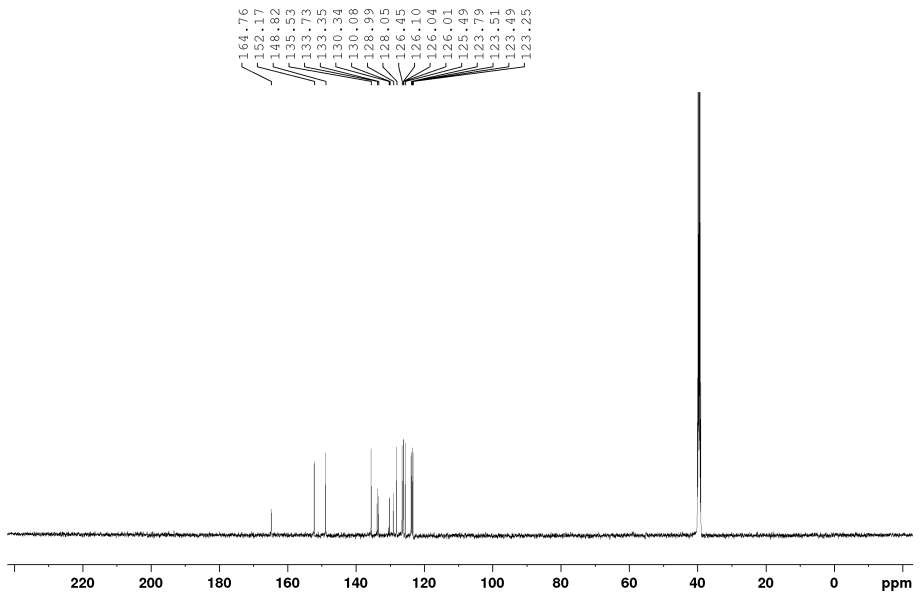
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-(4-cyanophenyl)-pyridinecarboxamide (**3.6**), (CD_3CN, 125.8 MHz)



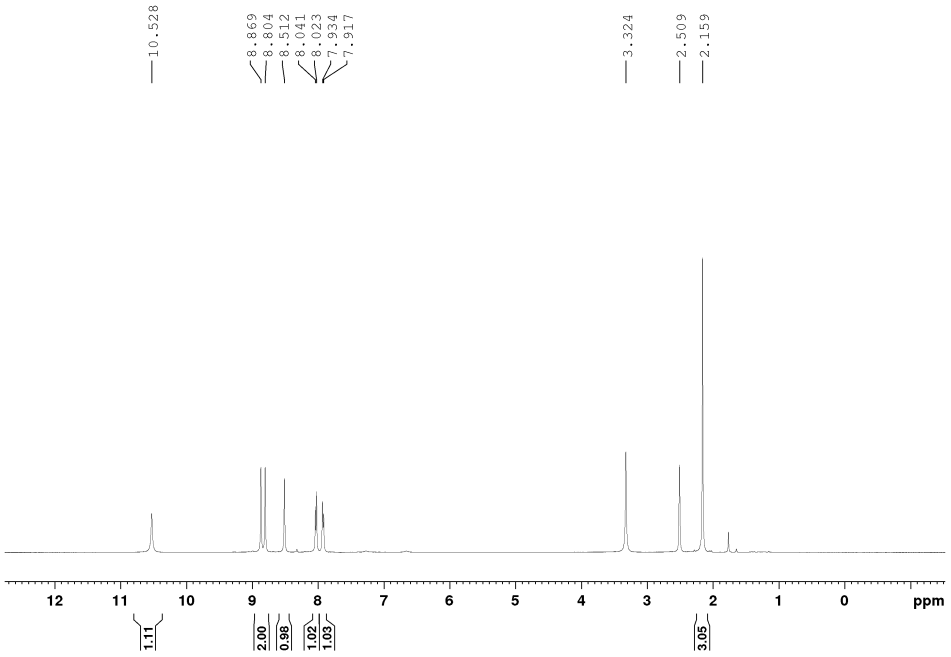
^{1}H NMR Spectrum of *N*-1-napthalenyl-3-pyridinecarboxamide (**3.7**), (DMSO-d_6, 500.1 MHz)



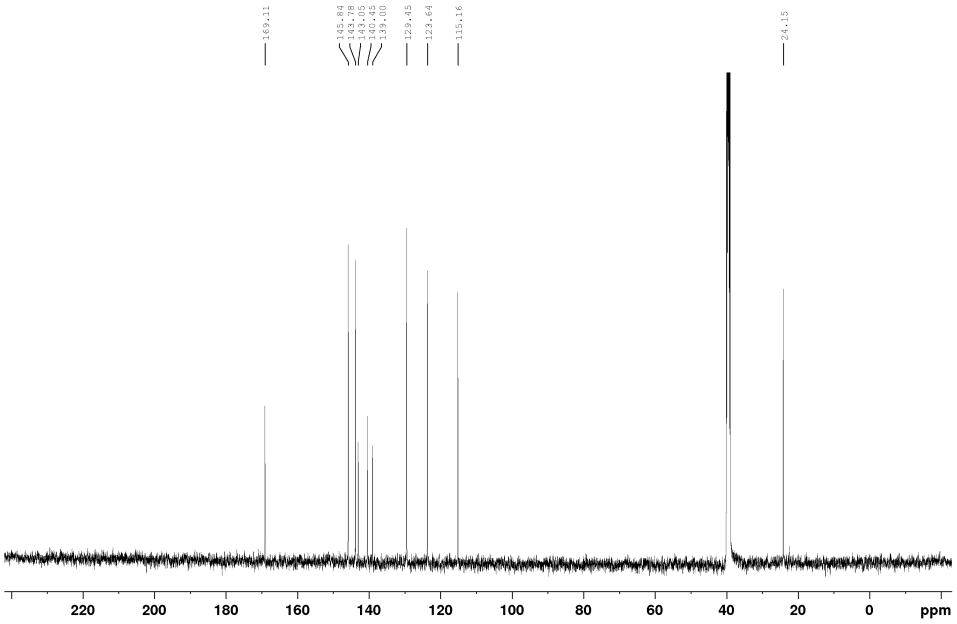
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-1-napthalenyl-3-pyridinecarboxamide (**3.7**), (DMSO-d_6, 125.8 MHz)



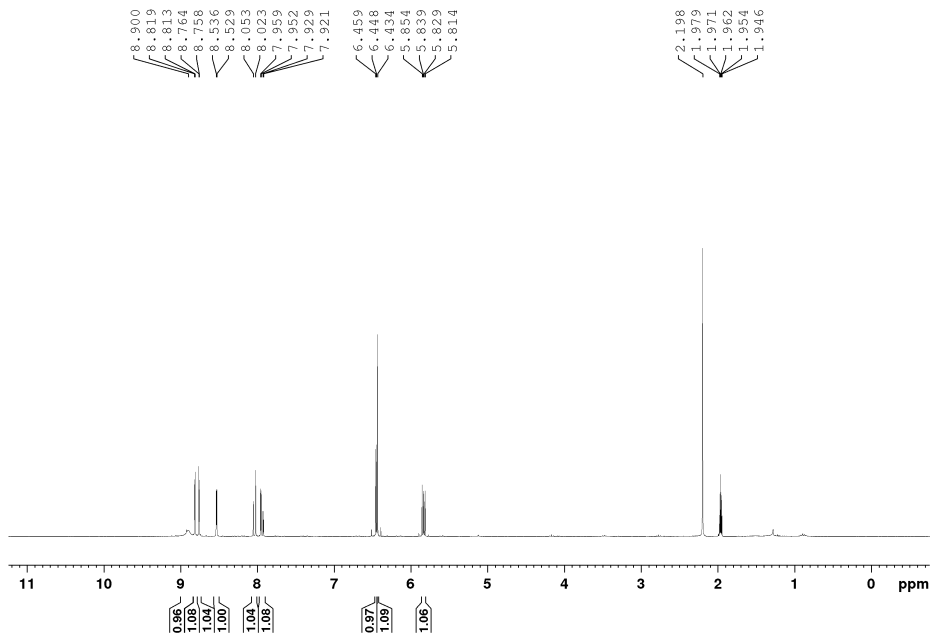
^{1}H NMR Spectrum of *N*-6-quinoxalinyl-acetamide (**3.8**), (DMSO-d_6, 500.1 MHz)



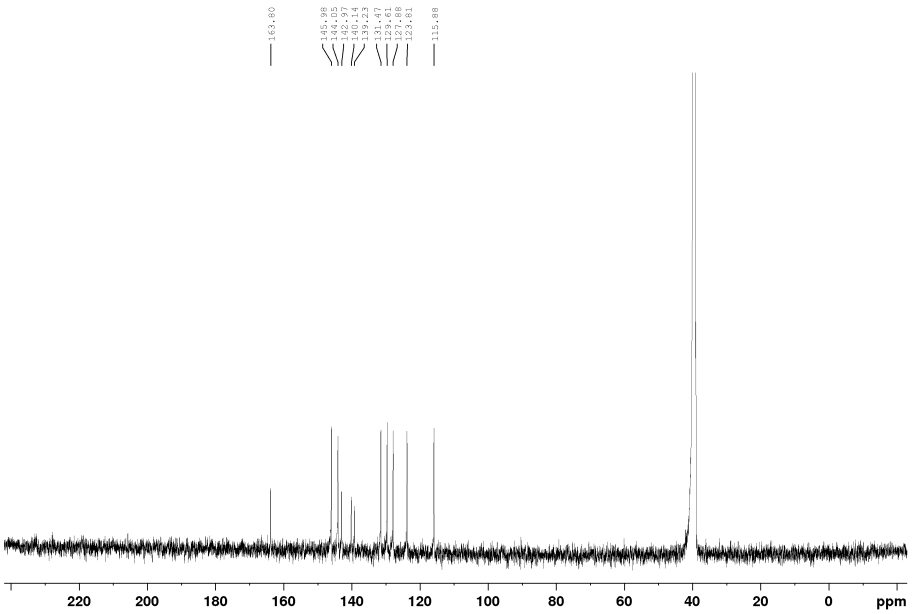
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-6-quinoxalinyl-acetamide (**3.8**), (DMSO-d_6, 125.8 MHz)



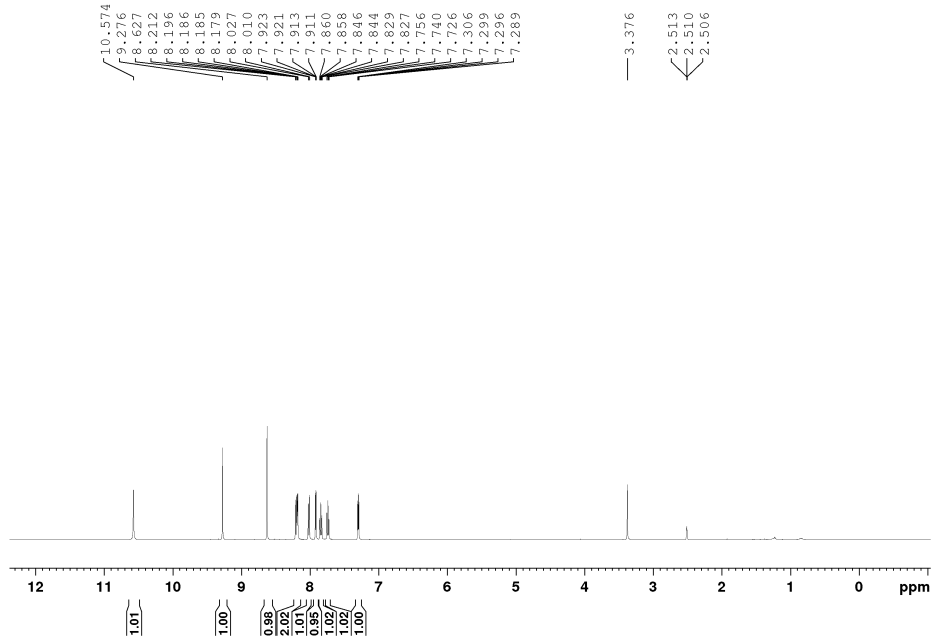
^{1}H NMR Spectrum of *N*-6-quinoxalinyl-2-propenamide (**3.9**), (DMSO-d_6, 300.1 MHz)



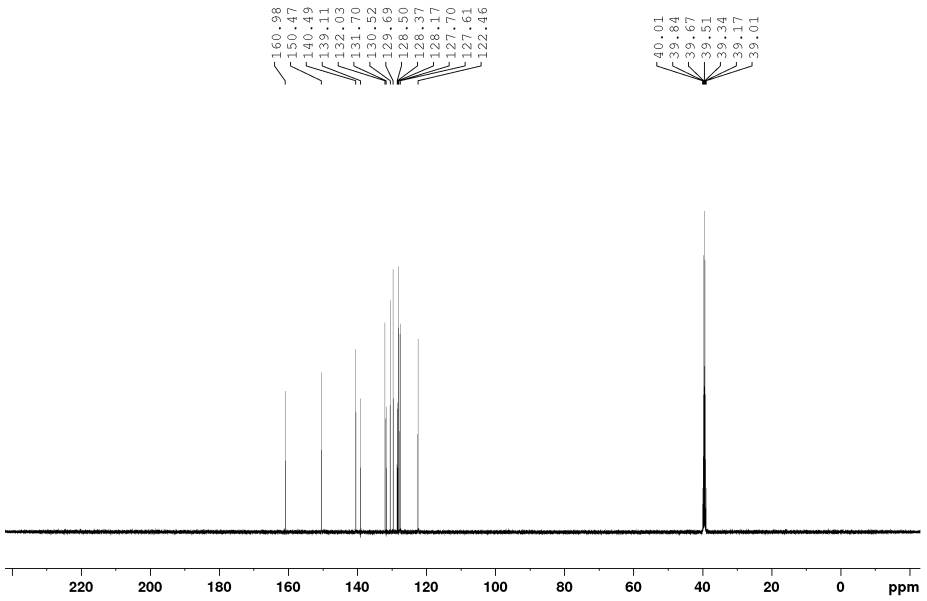
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-6-quinoxalinyl-2-propenamide (**3.9**), (DMSO-d_6, 125.8 MHz)



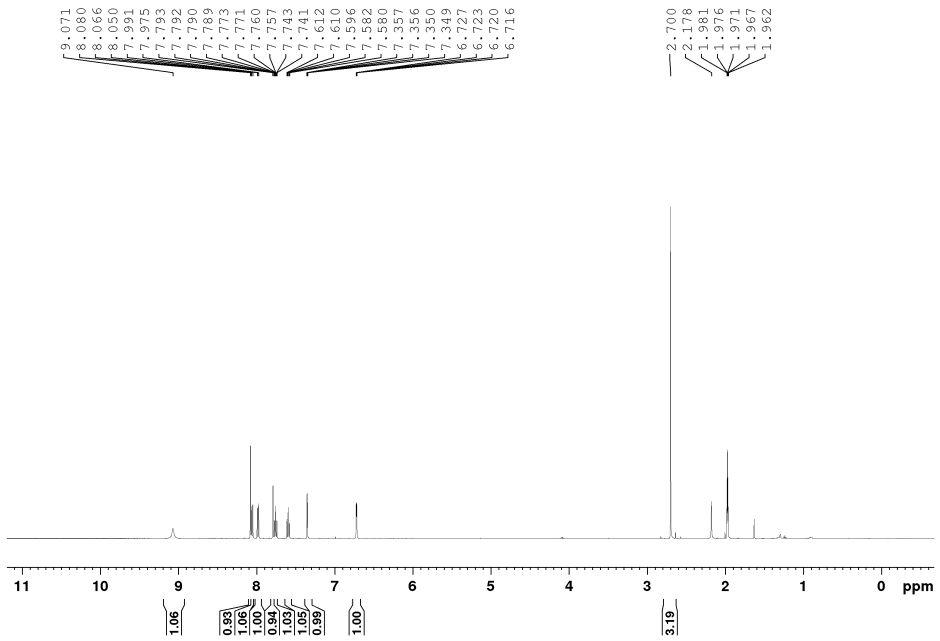
^{1}H NMR Spectrum of *N*-4-isoquinolinyl-2-thiophenecarboxamide (**3.10**), (DMSO-d_6, 500.1 MHz)



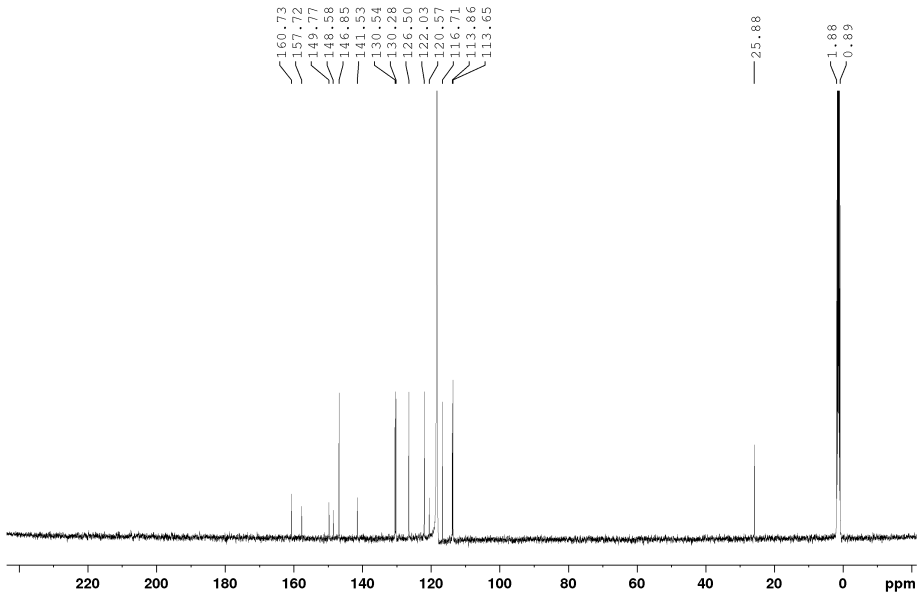
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-4-isoquinolinyl-2-thiophenecarboxamide (**3.10**), (DMSO-d_6, 125.8 MHz)



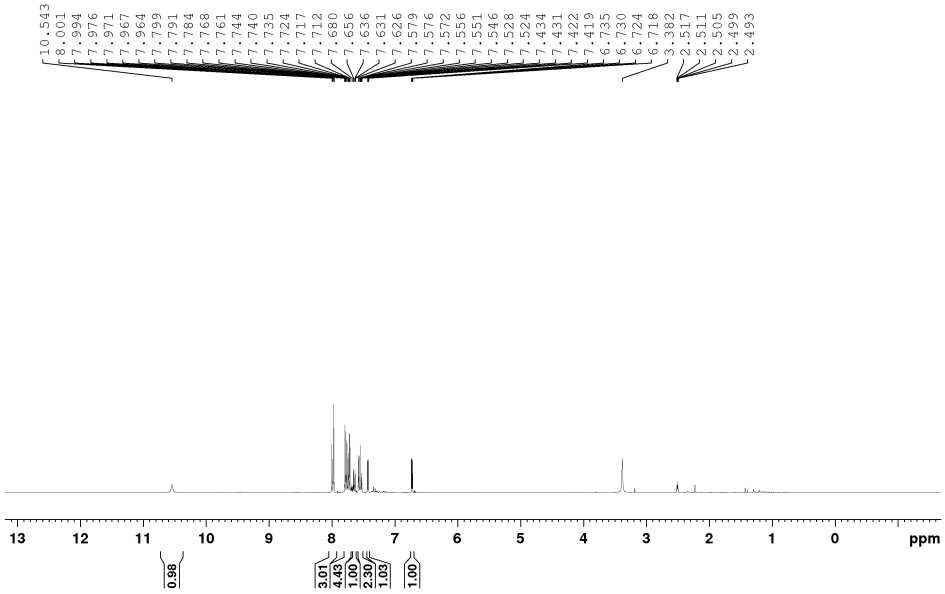
^{1}H NMR Spectrum of *N*-(2-methyl-4-quinolinyl)-2-furancarboxamide (**3.11**), (CD_3CN, 500.1 MHz)



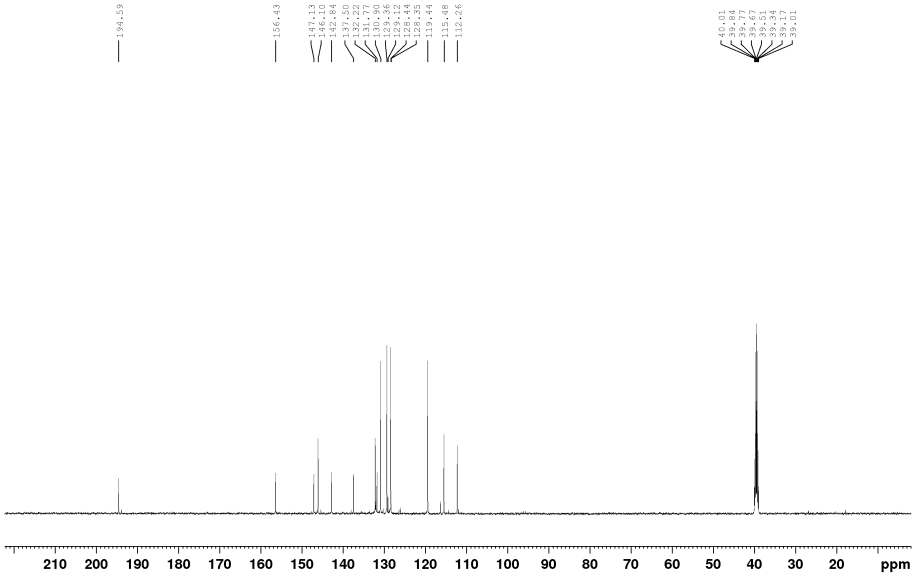
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-(2-methyl-4-quinolinyl)-2-furancarboxamide (**3.11**), (CD_3CN, 125.8 MHz)



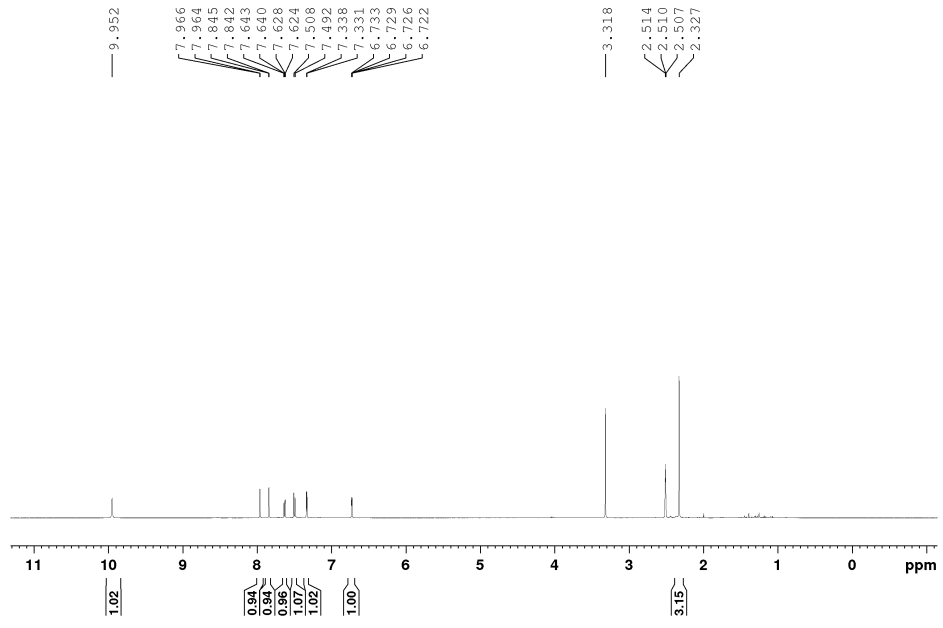
^{1}H NMR Spectrum of *N*-(4-benzoylphenyl)-2-furancarboxamide (**3.12**), (DMSO-d_6, 300.1 MHz)



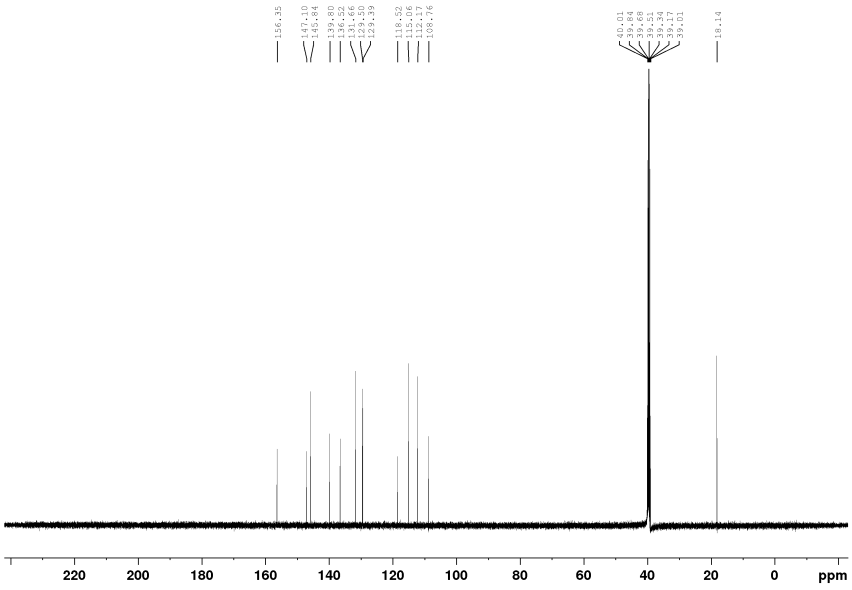
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-(4-benzoylphenyl)-2-furancarboxamide (**3.12**), (DMSO-d_6, 125.8 MHz)



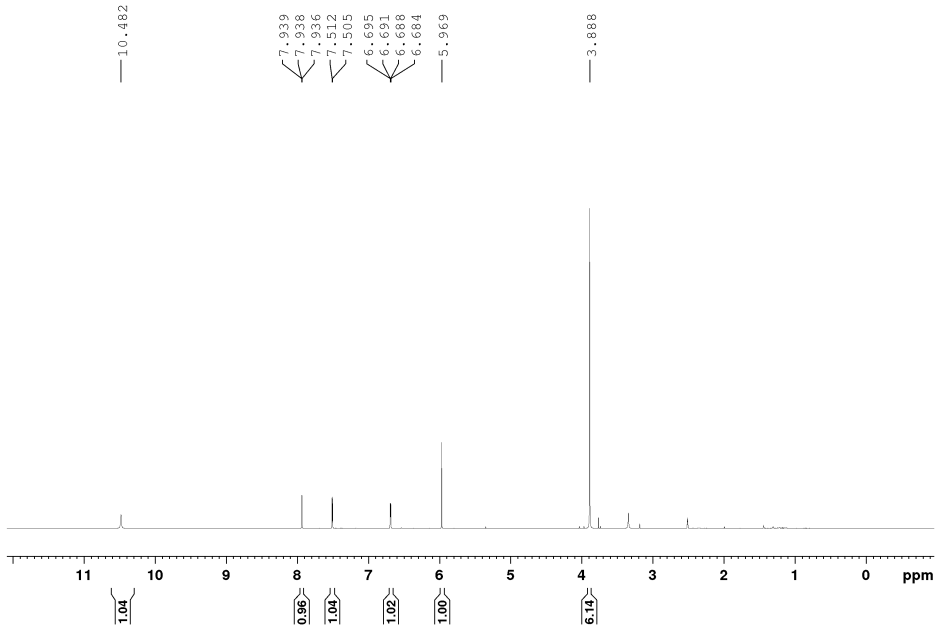
^{1}NMR Spectrum of *N*-(5-cyano-2-methylphenyl)-2-furancarboxamide (**3.13**), (DMSO-d_6, 500.1 MHz)



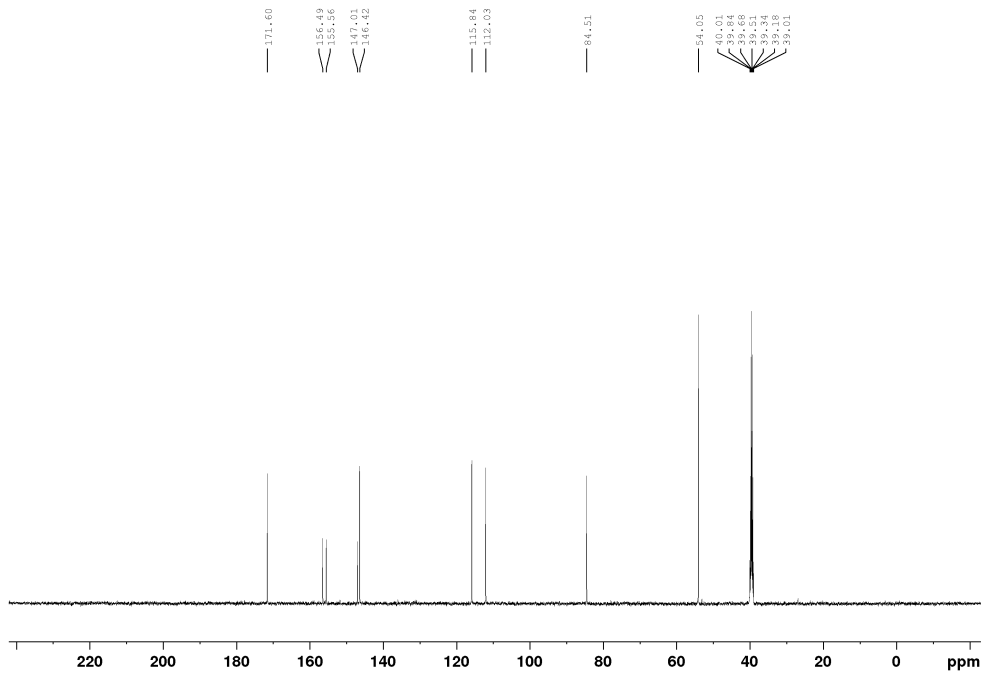
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-(5-cyano-2-methylphenyl)-2-furancarboxamide (**3.13**), (DMSO-d_6, 125.8 MHz)



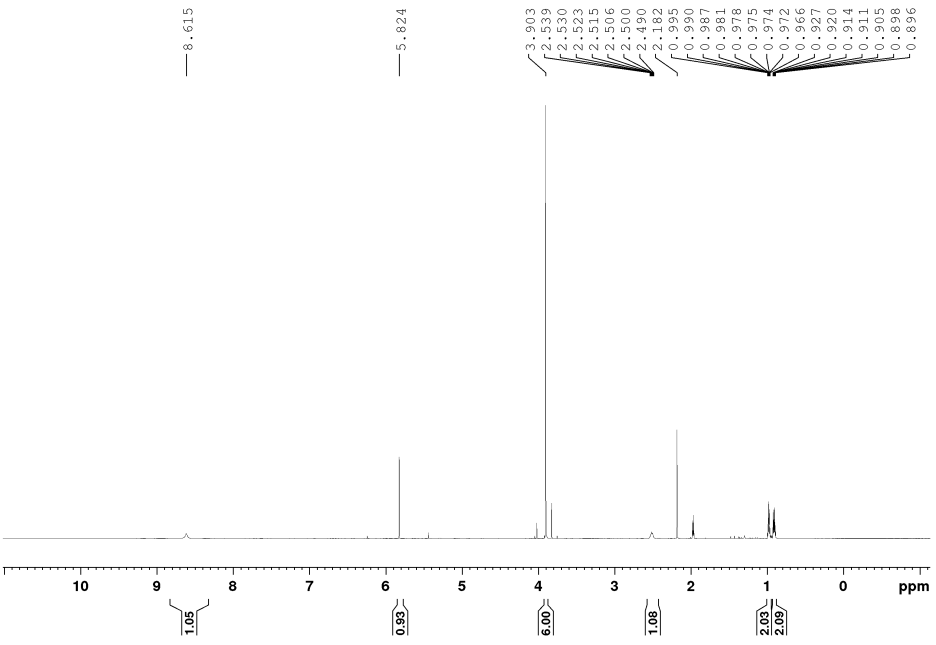
^{1}H NMR Spectrum of *N*-(4,6-dimethoxy-2-pyrimidinyl)-2-furancarboxamide (**3.14**), (DMSO-d_6, 500.1 MHz)



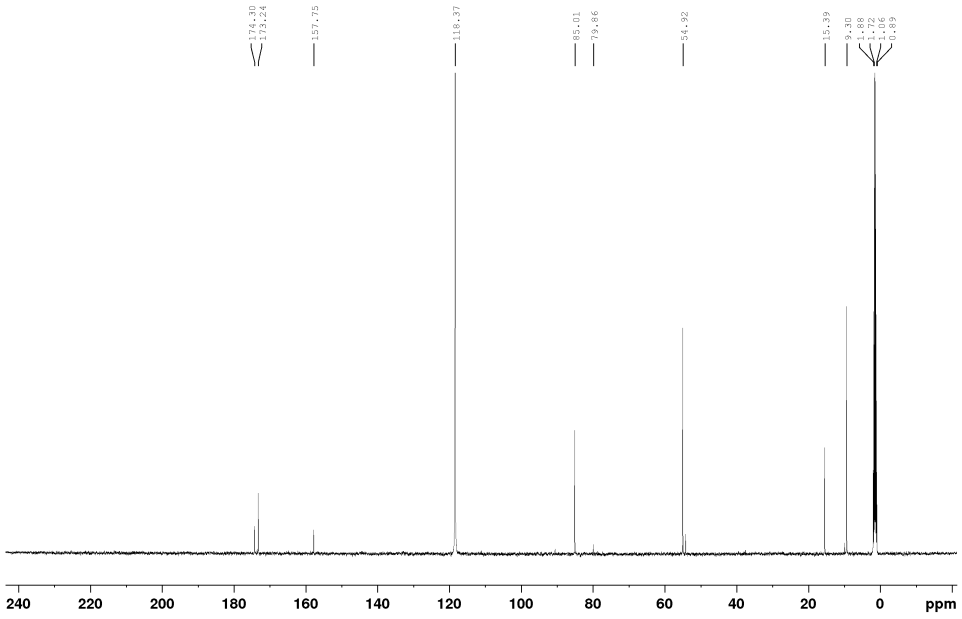
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-(4,6-dimethoxy-2-pyrimidinyl)-2-furancarboxamide (**3.14**), (DMSO-d_6, 125.8 MHz)



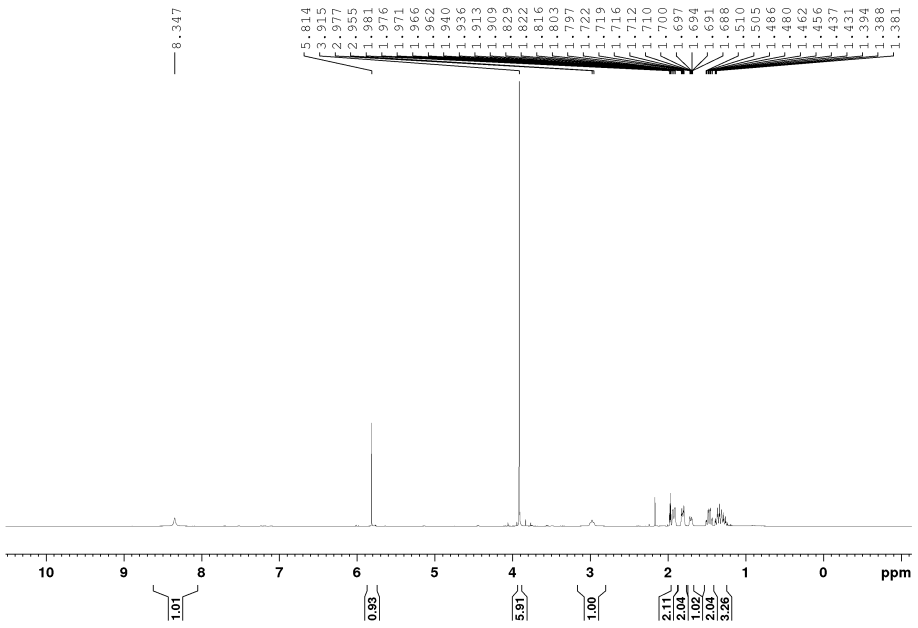
^{1}H NMR Spectrum of *N*-(4,6-dimethoxy-2-pyrimidinyl)-cyclopropanecarboxamide (**3.15**), (CD_3CN, 500.1 MHz)



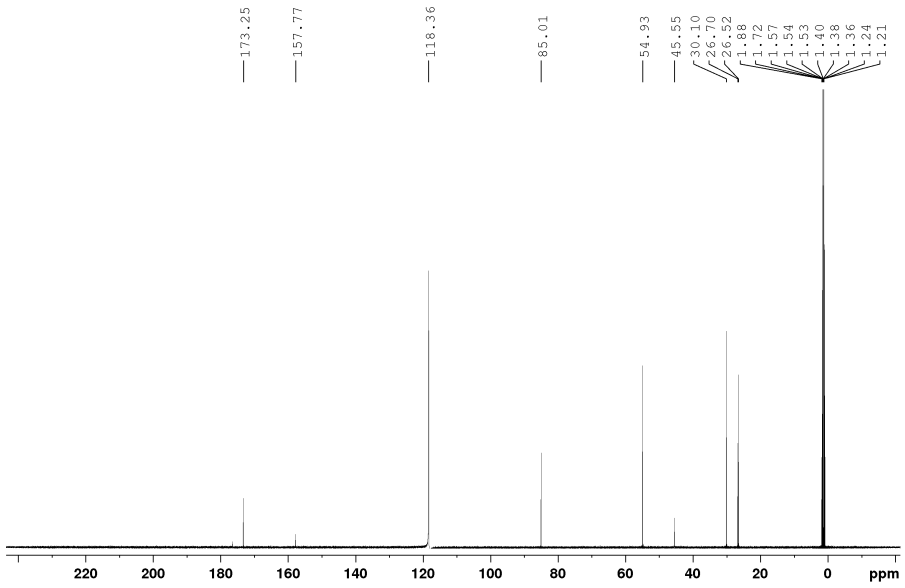
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-(4,6-dimethoxy-2-pyrimidinyl) cyclopropanecarboxamide (**3.15**), (CD_3CN, 125.8 MHz)



^{1}H NMR Spectrum of *N*-(4,6-dimethoxy-2-pyrimidinyl)-cyclohexaneecarboxamide (**3.16**), (CD_3CN, 500.1 MHz)



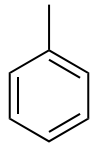
$^{13}C\{^{1}H\}$ NMR Spectrum of *N*-(4,6-dimethoxy-2-pyrimidinyl)-cyclohexanecarboxamide (**3.16**), (CD_3CN, 125.8 MHz)



APPENDIX B. Thermochemical Energies and Cartesian Coordinates for Computationally Modeled Compounds

Below are the DFT calculated thermochemical energies and Cartesian coordinates for all modeled compounds reported in Chapters 4-5.

Toluene



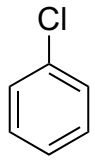
Zero-point correction= 0.128318 (Hartree/Particle)

Thermal correction to Energy= 0.134524
Thermal correction to Enthalpy= 0.135468
Thermal correction to Gibbs Free Energy= 0.097615
Sum of electronic and zero-point Energies= -271.443562
Sum of electronic and thermal Energies= -271.437355
Sum of electronic and thermal Enthalpies= -271.436411
Sum of electronic and thermal Free Energies= -271.474264

Single-point energy (6-311+G(2d,2p)) = -271.668522

C	-1.7827	-4.38255	-0.00067
C	-0.38648	-4.37962	0.01322
C	0.33403	-3.17691	0.01571
C	-0.38622	-1.97395	0.01061
C	-1.78231	-1.97079	-0.00329
C	-2.48671	-3.17663	-0.00967
H	-2.32022	-5.32764	0.00008
H	0.1533	-5.32444	0.02424
H	0.15371	-1.02915	0.0195
H	-2.31963	-1.02559	-0.00471
H	-3.57358	-3.17649	-0.0171
C	1.84666	-3.17674	-0.00051
H	2.23489	-3.16055	-1.02802
H	2.2541	-2.2985	0.51229
H	2.25376	-4.0705	0.48479

Chlorobenzene

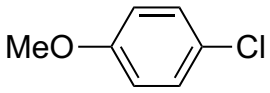


Zero-point correction= 0.091230 (Hartree/Particle)
Thermal correction to Energy= 0.096733
Thermal correction to Enthalpy= 0.097677
Thermal correction to Gibbs Free Energy= 0.061441
Sum of electronic and zero-point Energies= -691.758724
Sum of electronic and thermal Energies= -691.753221
Sum of electronic and thermal Enthalpies= -691.752277
Sum of electronic and thermal Free Energies= -691.788512

Single-point energy (6-311+G(2d,2p)) = -691.962808

C	-1.25523	1.38798	0.00026
C	0.14021	1.42833	0.00123
C	0.8129	2.65153	0.0006
C	0.06675	3.82944	-0.00106
C	-1.32728	3.81069	-0.00208
C	-1.9839	2.57879	-0.00139
H	-1.77234	0.43305	0.00077
H	0.71403	0.50575	0.00246
H	1.8968	2.69378	0.0013
H	-1.88451	4.74135	-0.0033
H	-3.0701	2.55506	-0.0021
Cl	0.90653	5.37899	-0.0019

***p*-chloroanisole**

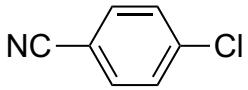


Zero-point correction= 0.124071 (Hartree/Particle)
Thermal correction to Energy= 0.132149
Thermal correction to Enthalpy= 0.133093
Thermal correction to Gibbs Free Energy= 0.090728
Sum of electronic and zero-point Energies= -806.253987
Sum of electronic and thermal Energies= -806.245910
Sum of electronic and thermal Enthalpies= -806.244965
Sum of electronic and thermal Free Energies= -806.287331

Single-point energy (6-311+G(2d,2p)) = -806.528269

C	3.48598	-1.55577	-2.11507
C	4.2085	-0.40498	-2.44722
C	3.60953	0.85583	-2.31538
C	2.30335	0.9684	-1.85694
C	1.58945	-0.18643	-1.52757
C	2.17133	-1.44234	-1.65371
H	3.92633	-2.54128	-2.20818
H	4.18537	1.73732	-2.57788
H	1.83952	1.94367	-1.75478
H	1.60827	-2.33287	-1.39528
C	6.15423	-1.65614	-3.06177
H	5.63291	-2.29247	-3.78815
H	6.23558	-2.18505	-2.10366
H	7.1525	-1.42292	-3.43377
O	5.49699	-0.40563	-2.90641
Cl	-0.06758	-0.04684	-0.94577

***p*-chlorobenzonitrile**

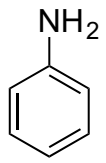


Zero-point correction= 0.089696 (Hartree/Particle)
Thermal correction to Energy= 0.096989
Thermal correction to Enthalpy= 0.097933
Thermal correction to Gibbs Free Energy= 0.057191
Sum of electronic and zero-point Energies= -784.007250
Sum of electronic and thermal Energies= -783.999957
Sum of electronic and thermal Enthalpies= -783.999013
Sum of electronic and thermal Free Energies= -784.039755

Single-point energy (6-311+G(2d,2p)) = -784.232536

C	-3.50425	-1.81632	1.72216
C	-4.26839	-0.75164	2.22882
C	-3.69773	0.52758	2.33887
C	-2.37937	0.74109	1.94752
C	-1.63437	-0.32828	1.44618
C	-2.18562	-1.60598	1.32999
H	-3.9458	-2.80375	1.63758
H	-4.28861	1.34908	2.73022
H	-1.93222	1.72562	2.02956
H	-1.58976	-2.42288	0.93806
C	-5.62758	-0.97009	2.63266
N	-6.7304	-1.14735	2.96034
Cl	0.02689	-0.06128	0.95257

Aniline

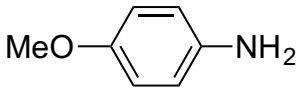


Zero-point correction= 0.117324 (Hartree/Particle)
Thermal correction to Energy= 0.123146
Thermal correction to Enthalpy= 0.124091
Thermal correction to Gibbs Free Energy= 0.088125
Sum of electronic and zero-point Energies= -287.493567
Sum of electronic and thermal Energies= -287.487744
Sum of electronic and thermal Enthalpies= -287.486800
Sum of electronic and thermal Free Energies= -287.522766

Single-point energy (6-311+G(2d,2p)) = -287.716336

C	-1.79937	-4.3975	0.07626
C	-0.4067	-4.44857	0.08069
C	0.34735	-3.26695	0.00674
C	-0.32741	-2.038	-0.07166
C	-1.71995	-1.99741	-0.07538
C	-2.46871	-3.17442	-0.00201
H	-2.36374	-5.32472	0.13253
H	0.10365	-5.4072	0.14535
H	0.24598	-1.115	-0.12616
H	-2.22249	-1.0357	-0.13828
H	-3.55385	-3.13857	-0.00617
H	2.22021	-2.5135	-0.34741
H	2.16626	-4.1805	-0.236
N	1.75157	-3.30849	0.07068

***para*-anisidine**

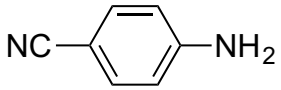


Zero-point correction= 0.150015 (Hartree/Particle)
Thermal correction to Energy= 0.158454
Thermal correction to Enthalpy= 0.159398
Thermal correction to Gibbs Free Energy= 0.117074
Sum of electronic and zero-point Energies= -401.986941
Sum of electronic and thermal Energies= -401.978502
Sum of electronic and thermal Enthalpies= -401.977558
Sum of electronic and thermal Free Energies= -402.019882

Single-point energy (6-311+G(2d,2p)) = -402.279158

C	3.45064	-1.51254	-2.14906
C	4.23125	-0.38468	-2.4132
C	3.68563	0.88688	-2.19517
C	2.38721	1.02764	-1.72272
C	1.58981	-0.09801	-1.4543
C	2.14299	-1.36325	-1.6748
H	3.84011	-2.5118	-2.30803
H	4.29758	1.75901	-2.40356
H	1.98362	2.02378	-1.55433
H	1.54964	-2.25205	-1.47104
C	6.1263	-1.67894	-3.10776
H	5.58197	-2.25467	-3.86853
H	6.18273	-2.26609	-2.18124
H	7.1361	-1.47215	-3.46628
O	5.5251	-0.41402	-2.88472
N	0.29226	0.05052	-0.91379

***para*-aminobenzonitrile**



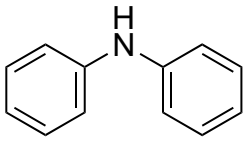
Zero-point correction= 0.115940 (Hartree/Particle)
Thermal correction to Energy= 0.123513
Thermal correction to Enthalpy= 0.124458
Thermal correction to Gibbs Free Energy= 0.084051
Sum of electronic and zero-point Energies= -379.747720
Sum of electronic and thermal Energies= -379.740146
Sum of electronic and thermal Enthalpies= -379.739202
Sum of electronic and thermal Free Energies= -379.779608

Single-point energy (6-311+G(2d,2p)) = -379.991086

C	-3.44353	-1.79537	1.81174
C	-4.2767	-0.74424	2.23659
C	-3.76984	0.56828	2.23276
C	-2.47071	0.82117	1.81884
C	-1.63465	-0.22943	1.39431
C	-2.14449	-1.54208	1.39779
H	-3.82347	-2.81201	1.81142
H	-4.40312	1.38688	2.55948
H	-2.09316	1.84061	1.81823
H	-1.51285	-2.36355	1.06916
C	-5.61575	-1.00581	2.66778

N	-6.70605	-1.21912	3.02015
N	-0.34977	0.03057	0.93045
H	0.0736	0.90253	1.22013
H	0.30128	-0.74378	0.92776

Diphenylamine

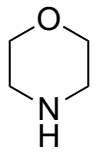


Zero-point correction= 0.198267 (Hartree/Particle)
Thermal correction to Energy= 0.208681
Thermal correction to Enthalpy= 0.209625
Thermal correction to Gibbs Free Energy= 0.160714
Sum of electronic and zero-point Energies= -518.468216
Sum of electronic and thermal Energies= -518.457802
Sum of electronic and thermal Enthalpies= -518.456857
Sum of electronic and thermal Free Energies= -518.505769

Single-point energy (6-311+G(2d,2p)) = -518.844857

C	-1.4889461105	-3.1049785245	-0.8845728182
C	-1.0576648088	-1.7948832873	-0.6951418746
C	-1.7625325055	-0.9246748416	0.1550114341
C	-2.9113632055	-1.4026131621	0.8087856794
C	-3.3221013728	-2.7217382078	0.6254063082
H	-2.9488176683	-4.6088581779	-0.3583370693
H	-0.9284141068	-3.7581819362	-1.5481511817
H	-0.1636198087	-1.4362691501	-1.2008540422
H	-3.4888791874	-0.7368820411	1.4402034969
H	-4.213563719	-3.0718293413	1.1394015937
N	-1.3202283113	0.3990132112	0.2772264453
H	-0.7819724587	0.7526188093	-0.5007745717
C	-1.5209805311	1.2984891276	1.3324588559
C	-1.452385618	2.6771121682	1.0648784118
C	-1.7379552733	0.877056577	2.6556441869
C	-1.597824671	3.6066453821	2.0910355203
H	-1.2910308314	3.0132312577	0.0428047915
C	-1.900732233	1.8178674352	3.6709741297
H	-1.7582154113	-0.1817214185	2.8879765624
C	-1.8329582624	3.1861066903	3.4019458126
H	-1.5390748712	4.66698649	1.8598964648
H	-2.0669078887	1.4716691232	4.6878274077
H	-1.9575054093	3.9119845654	4.1998410223

Morpholine

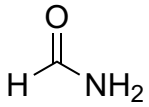


Zero-point correction= 0.135942 (Hartree/Particle)
Thermal correction to Energy= 0.141254
Thermal correction to Enthalpy= 0.142199
Thermal correction to Gibbs Free Energy= 0.107473
Sum of electronic and zero-point Energies= -287.671012
Sum of electronic and thermal Energies= -287.665700
Sum of electronic and thermal Enthalpies= -287.664755
Sum of electronic and thermal Free Energies= -287.699481

Single-point energy (6-311+G(2d,2p)) = -287.908242

C	-2.8034266198	-1.9778555175	0.0176958892
C	-0.8058688302	-0.6148087123	0.018761561
C	-1.3957106195	0.1983794745	1.1738918232
C	-3.3464006643	-1.1326955824	1.1728593249
H	0.2866621144	-0.6581023618	0.0994048569
H	-0.9627266258	-2.5307333476	0.7336334618
H	-3.1746158455	-1.5694508632	-0.9311099541
H	-3.1615343084	-3.0109976503	0.0975515249
H	-1.0590525658	-0.2161301735	2.1409671112
H	-1.093534401	1.2489380915	1.1240362113
H	-3.0838626377	-1.5977972654	2.1398891538
H	-4.4347791736	-1.0309974859	1.1222809044
H	-1.0501076341	-0.1197928865	-0.9299821348
O	-2.8221954507	0.194021986	1.128576484
N	-1.3354612381	-1.9838812057	-0.0427527179

Formamide

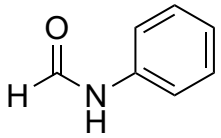


Zero-point correction= 0.045483 (Hartree/Particle)
Thermal correction to Energy= 0.049246
Thermal correction to Enthalpy= 0.050190
Thermal correction to Gibbs Free Energy= 0.020914
Sum of electronic and zero-point Energies= -169.855160
Sum of electronic and thermal Energies= -169.851397
Sum of electronic and thermal Enthalpies= -169.850453

Sum of electronic and thermal Free Energies= -169.879729
Single-point energy (6-311+G(2d,2p)) = -1.699625701843E+02

C	-1.7571365604	-0.4940208137	-0.000027055
O	-2.3974275863	-1.5321471553	0.000041912
N	-0.3966280052	-0.4209044618	-0.0000094624
H	-2.2375736481	0.5020948486	-0.0000028373
H	0.1472218785	-1.2749870684	-0.0000263038
H	0.0877987215	0.4652666506	-0.0000822535

Formanilide

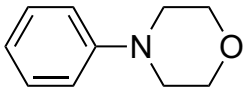


Zero-point correction= 0.127554 (Hartree/Particle)
Thermal correction to Energy= 0.135103
Thermal correction to Enthalpy= 0.136047
Thermal correction to Gibbs Free Energy= 0.094949
Sum of electronic and zero-point Energies= -400.828679
Sum of electronic and thermal Energies= -400.821130
Sum of electronic and thermal Enthalpies= -400.820186
Sum of electronic and thermal Free Energies= -400.861284

Single-point energy (6-311+G(2d,2p)) = -4.010911964652E+02

C	-2.1511348442	-0.4724062813	-0.5107149955
O	-2.776221624	-1.513605059	-0.3784883052
N	-1.03926574	-0.1516992684	0.2205773709
H	-2.4401628833	0.310005392	-1.2317615793
H	-0.8112952981	-0.8061102809	0.9619024381
C	-0.2876217496	1.0448069678	0.128113438
C	0.2806864326	1.5834343656	1.2900281612
C	-0.094022424	1.6886377146	-1.1014713088
C	1.0289590723	2.7568221688	1.2221033884
H	0.1229071515	1.0873198755	2.2444097044
C	0.6335885028	2.8772677325	-1.1532845855
H	-0.4877533916	1.2523627213	-2.0137881574
C	1.2005125207	3.4155235659	0.00283695
H	1.4677357661	3.1628973311	2.1290703486
H	0.774847165	3.3712575878	-2.1104184852
H	1.7772530438	4.3341679667	-0.0468402827

4-phenylmorpholine



Zero-point correction= 0.216860 (Hartree/Particle)
Thermal correction to Energy= 0.226606
Thermal correction to Enthalpy= 0.227550
Thermal correction to Gibbs Free Energy= 0.181337
Sum of electronic and zero-point Energies= -518.649228
Sum of electronic and thermal Energies= -518.639482
Sum of electronic and thermal Enthalpies= -518.638538
Sum of electronic and thermal Free Energies= -518.684751

Single-point energy (6-311+G(2d,2p)) = -519.041935

C	0.4155260908	-0.5252918472	0.7061707705
C	-0.170361881	0.5023893157	-0.0587639945
C	-1.3307078921	0.2022481202	-0.7920730073
C	-1.8792913969	-1.0825150581	-0.7618959802
H	-1.7304661795	-3.084630994	0.0300583063
H	0.3312869669	-2.5712888783	1.3368750349
H	1.3334782809	-0.328617357	1.2517287017
H	-1.8201698557	0.9685766932	-1.3820196623
H	-2.7769934062	-1.286879689	-1.3397548003
C	-0.0538768103	2.7420959323	-1.0706336157
C	0.6636674334	2.4270140908	1.2084714861
C	0.910955616	3.9218132675	-1.1677740953
H	-1.0594165611	3.1182457391	-0.8058662151
H	-0.119187908	2.2563301287	-2.0494940406
C	1.6041611671	3.6165362973	1.0481901217
H	-0.2947779766	2.7727403602	1.6365513534
H	1.1039389866	1.7127777283	1.9074656926
H	0.5102207133	4.6898790816	-1.8345017978
H	1.8795971948	3.575736042	-1.561737535
H	1.6994154306	4.1610787647	1.9913490615
H	2.6001215265	3.2648411519	0.7348496835
N	0.4439864731	1.7794579237	-0.0922142288
O	1.1034989473	4.549229421	0.0956015416

NH_3

Zero-point correction= 0.034529 (Hartree/Particle)
Thermal correction to Energy= 0.037393
Thermal correction to Enthalpy= 0.038338
Thermal correction to Gibbs Free Energy= 0.016489

Sum of electronic and zero-point Energies= -56.521852
Sum of electronic and thermal Energies= -56.518988
Sum of electronic and thermal Enthalpies= -56.518043
Sum of electronic and thermal Free Energies= -56.539892

Single-point energy (6-311+G(2d,2p)) = -56.586881

N	0.34314	3.02846	-2.77119
H	0.71278	2.07975	-2.77119
H	0.7128	3.50281	-1.94958
H	0.7128	3.50281	-3.59279

***tert*-Butoxide**

Zero-point correction= 0.121461 (Hartree/Particle)
Thermal correction to Energy= 0.127784
Thermal correction to Enthalpy= 0.128728
Thermal correction to Gibbs Free Energy= 0.092817
Sum of electronic and zero-point Energies= -232.952827
Sum of electronic and thermal Energies= -232.946504
Sum of electronic and thermal Enthalpies= -232.945560
Sum of electronic and thermal Free Energies= -232.981471

Single-point energy (6-311+G(2d,2p)) = -233.168725

C	1.06553	0.6917	-0.00238
C	1.64319	1.41899	1.2573
H	1.27333	2.45262	1.27595
H	1.27311	0.91851	2.16178
H	2.74715	1.44407	1.301
C	1.64335	1.41885	-1.26207
H	2.74731	1.44392	-1.30563
H	1.27338	0.91827	-2.16654
H	1.27349	2.45248	-1.28088
C	1.64303	-0.76292	-0.00226
H	1.27295	-1.29584	0.88349
H	1.27306	-1.29594	-0.888
H	2.74699	-0.81342	-0.00219
O	-0.2891	0.69185	-0.00247

***tert*- Butanol**

Zero-point correction= 0.136151 (Hartree/Particle)
Thermal correction to Energy= 0.142874
Thermal correction to Enthalpy= 0.143818
Thermal correction to Gibbs Free Energy= 0.107159
Sum of electronic and zero-point Energies= -233.547294

Sum of electronic and thermal Energies= -233.540571
Sum of electronic and thermal Enthalpies= -233.539627
Sum of electronic and thermal Free Energies= -233.576286

Single-point energy (6-311+G(2d,2p)) = -233.776853

C	1.16699	0.70144	-0.00237
C	1.64481	1.42733	1.26398
H	1.28536	2.46477	1.28012
H	1.26706	0.92096	2.15824
H	2.7394	1.45571	1.31678
C	1.64497	1.42719	-1.26875
H	2.73957	1.45557	-1.32141
H	1.26733	0.92072	-2.163
H	1.28552	2.46462	-1.28505
C	1.6232	-0.75936	-0.00226
H	1.24356	-1.27676	0.88477
H	1.24367	-1.27686	-0.88928
H	2.71672	-0.82454	-0.00219
O	-0.27716	0.63688	-0.00246
H	-0.62655	1.54246	-0.00253

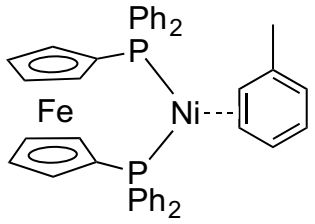
chloride

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015023
Sum of electronic and zero-point Energies= -460.271463
Sum of electronic and thermal Energies= -460.270047
Sum of electronic and thermal Enthalpies= -460.269103
Sum of electronic and thermal Free Energies= -460.286486

Single-point energy (6-311+G(2d,2p)) = -460.303727

Cl	4.77575	3.37673	-0.48322

(dppf)Ni(η^2-PhCH$_3$)



Zero-point correction= 0.649486 (Hartree/Particle)
Thermal correction to Energy= 0.689737
Thermal correction to Enthalpy= 0.690681
Thermal correction to Gibbs Free Energy= 0.575415
Sum of electronic and zero-point Energies= -5038.112428
Sum of electronic and thermal Energies= -5038.072177
Sum of electronic and thermal Enthalpies= -5038.071233
Sum of electronic and thermal Free Energies= -5038.186499

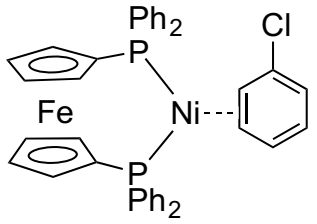
Single-point energy (6-311+G(2d,2p)) = -5039.549907

Fe	0.2415040	-2.5858810	-1.2285750
C	1.7483190	-1.2020460	-1.2045030
C	2.2996830	-2.5272700	-1.2353160
C	1.8371450	-3.1795730	-2.4155640
C	1.0058360	-2.2674660	-3.1306010
C	0.9461510	-1.0530380	-2.3889050
C	-1.2185060	-4.0568470	-1.1256360
C	-1.8097670	-2.7693440	-1.2830330
C	-1.3996000	-1.9417860	-0.1837440
C	-0.5506470	-2.7484190	0.6508460
C	-0.4453680	-4.0460550	0.0721840
P	1.8348400	0.0852820	0.0879010
P	-1.7182600	-0.1624110	0.1178360
C	3.2701030	1.1020940	-0.4673240
C	2.5550380	-0.8126860	1.5294990
C	-3.1600480	-0.2377820	1.2727170
C	-2.5108320	0.3647440	-1.4603010
C	3.6122010	1.2259710	-1.8211680
C	4.6056340	2.1215550	-2.2244540
C	5.2712810	2.9061320	-1.2820750
C	4.9394280	2.7886740	0.0705360
C	3.9460560	1.8980150	0.4732710
C	1.7816900	-0.9174250	2.6938450
C	2.2680470	-1.5915630	3.8159210
C	3.5405750	-2.1640820	3.7860590
C	4.3274230	-2.0512480	2.6361980
C	3.8399100	-1.3756930	1.5169860

C	-3.2618060	-1.2390180	2.2498440
C	-4.2797660	-1.2017410	3.2051240
C	-5.2127750	-0.1639570	3.1998800
C	-5.1236910	0.8355530	2.2281340
C	-4.1063970	0.8000860	1.2752910
C	-3.7355390	-0.1509510	-1.9111930
C	-4.2740760	0.2671190	-3.1281800
C	-3.5979370	1.2118340	-3.9059530
C	-2.3888160	1.7439650	-3.4567200
C	-1.8511560	1.3255110	-2.2379390
H	2.9119100	-2.9730610	-0.4640820
H	2.0448140	-4.2048540	-2.6950070
H	0.4721120	-2.4754520	-4.0491110
H	0.3570840	-0.1824040	-2.6414900
H	-1.3055420	-4.8826970	-1.8204270
H	-2.4158250	-2.4495250	-2.1186130
H	-0.0354460	-2.4110740	1.5388770
H	0.1576740	-4.8612800	0.4511860
H	3.1055670	0.6184040	-2.5645490
H	4.8606110	2.2013180	-3.2780800
H	6.0436610	3.6025050	-1.5968600
H	5.4537640	3.3935460	0.8128120
H	3.6944480	1.8185480	1.5273700
H	0.7956060	-0.4580890	2.7104720
H	1.6569280	-1.6632300	4.7117280
H	3.9237900	-2.6874580	4.6579230
H	5.3238910	-2.4846670	2.6138930
H	4.4648200	-1.2740570	0.6341250
H	-2.5507640	-2.0591190	2.2615510
H	-4.3449520	-1.9900020	3.9507640
H	-6.0051490	-0.1360960	3.9428350
H	-5.8490440	1.6449700	2.2102230
H	-4.0472900	1.5820360	0.5253160
H	-4.2735600	-0.8739490	-1.3044300
H	-5.2225160	-0.1407290	-3.4680610
H	-4.0200370	1.5386680	-4.8526530
H	-1.8675570	2.4931420	-4.0465790
H	-0.9250040	1.7595500	-1.8707350
Ni	-0.0185880	1.1059740	0.5840700
C	-1.0768370	2.3764840	2.9741970
C	-0.7572630	2.7978780	1.5499730
C	-1.7661870	3.4849730	0.7941470
C	-1.4657140	4.2003910	-0.3398480
C	-0.1157260	4.3072100	-0.7784040
C	0.8945420	3.7271140	-0.0468460
C	0.6103940	2.9582320	1.1299950

H	-2.7913960	3.4440430	1.1545040
H	-2.2559000	4.6972960	-0.8965390
H	0.1187790	4.8857630	-1.6685680
H	1.9316520	3.8615700	-0.3414460
H	1.4167530	2.7990340	1.8448570
H	-2.0550540	1.8891950	3.0371290
H	-1.0945380	3.2476450	3.6465000
H	-0.3276420	1.6798210	3.3664460

(dppf)Ni(η^2-PhCl)



Zero-point correction= 0.611919 (Hartree/Particle)
Thermal correction to Energy= 0.651835
Thermal correction to Enthalpy= 0.652779
Thermal correction to Gibbs Free Energy= 0.536907
Sum of electronic and zero-point Energies= -5458.434171
Sum of electronic and thermal Energies= -5458.394255
Sum of electronic and thermal Enthalpies= -5458.393311
Sum of electronic and thermal Free Energies= -5458.509183

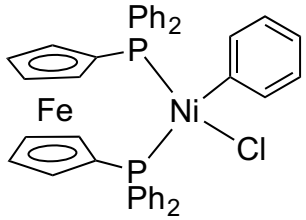
Single-point energy (6-311+G(2d,2p)) = -5459.847899

Fe	-0.3608910	2.8868970	-0.5516730
C	-1.8311210	1.5045740	-0.8879220
C	-2.4169380	2.7702670	-0.5466720
C	-1.9965180	3.7340400	-1.5091250
C	-1.1574120	3.0784060	-2.4576600
C	-1.0496740	1.7099560	-2.0781760
C	1.0496520	4.3258600	-0.0548030
C	1.6789000	3.1637700	-0.5892750
C	1.3301580	2.0396540	0.2328890
C	0.4806650	2.5361520	1.2817490
C	0.3139470	3.9392730	1.1037630
P	-1.8527240	-0.0816200	0.0128030
P	1.7031770	0.2617250	0.0275180
C	-3.2213400	-1.0001620	-0.8122640
C	-2.5998020	0.3519000	1.6381720
C	3.2255410	0.0631340	1.0479050
C	2.3488410	0.1518750	-1.6921390
C	-3.5160360	-0.8195460	-2.1706340

C	-4.4580710	-1.6314020	-2.8071080
C	-5.1179390	-2.6343140	-2.0963020
C	-4.8324530	-2.8209960	-0.7409980
C	-3.8902410	-2.0136390	-0.1056570
C	-1.8371550	0.1345440	2.7943200
C	-2.3511770	0.4519230	4.0535910
C	-3.6359790	0.9842290	4.1683370
C	-4.4112100	1.1872000	3.0226530
C	-3.8983980	0.8680990	1.7653620
C	3.3395630	0.7054240	2.2891350
C	4.4263860	0.4478740	3.1251260
C	5.4141930	-0.4582620	2.7353930
C	5.3105380	-1.1013070	1.5006390
C	4.2249960	-0.8438040	0.6636400
C	3.4897690	0.8428910	-2.1278070
C	3.9184270	0.7365180	-3.4510060
C	3.2178720	-0.0708400	-4.3519650
C	2.0956890	-0.7802240	-3.9220740
C	1.6664300	-0.6722480	-2.5977340
H	-3.0234840	2.9691360	0.3254590
H	-2.2371470	4.7895600	-1.4942910
H	-0.6490880	3.5458230	-3.2912260
H	-0.4421780	0.9619120	-2.5684130
H	1.0878010	5.3195960	-0.4829380
H	2.2673610	3.1246990	-1.4946690
H	0.0058860	1.9339630	2.0437360
H	-0.3043160	4.5858210	1.7132230
H	-3.0140720	-0.0395380	-2.7346490
H	-4.6777140	-1.4744270	-3.8599300
H	-5.8509570	-3.2646810	-2.5920940
H	-5.3434630	-3.5971830	-0.1774440
H	-3.6762960	-2.1691020	0.9480410
H	-0.8440090	-0.2998580	2.7029390
H	-1.7504560	0.2742920	4.9413670
H	-4.0390110	1.2296820	5.1472290
H	-5.4176970	1.5879060	3.1099180
H	-4.5135350	1.0075730	0.8807120
H	2.5792860	1.4126000	2.6061660
H	4.5003110	0.9572170	4.0823560
H	6.2594280	-0.6598200	3.3876960
H	6.0770180	-1.8048020	1.1859140
H	4.1565980	-1.3485830	-0.2945420
H	4.0529800	1.4529260	-1.4272880
H	4.8024180	1.2777890	-3.7778210
H	3.5551070	-0.1549740	-5.3816550
H	1.5583640	-1.4253630	-4.6118740

H	0.8079110	-1.2431420	-2.2521930
Ni	0.0422390	-1.1338420	0.2899790
Cl	1.2000730	-2.6276850	2.6608150
C	0.8486940	-2.8401940	0.8969310
C	1.9025760	-3.4094340	0.1086290
C	1.6138790	-3.9863180	-1.1023910
C	0.2637890	-4.1036630	-1.5477350
C	-0.7709310	-3.6799010	-0.7489460
C	-0.5293830	-3.0383010	0.5144250
H	2.9193390	-3.3545570	0.4814380
H	2.4198750	-4.3747140	-1.7191570
H	0.0539470	-4.5848150	-2.4993120
H	-1.8013090	-3.8503410	-1.0488200
H	-1.3088240	-3.0653210	1.2718980

(dppf)Ni(Ph)Cl



Zero-point correction= 0.612938 (Hartree/Particle)
Thermal correction to Energy= 0.652951
Thermal correction to Enthalpy= 0.653896
Thermal correction to Gibbs Free Energy= 0.538101
Sum of electronic and zero-point Energies= -5458.463439
Sum of electronic and thermal Energies= -5458.423425
Sum of electronic and thermal Enthalpies= -5458.422481
Sum of electronic and thermal Free Energies= -5458.538275

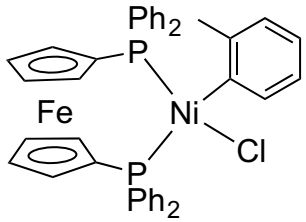
Single-point energy (6-311+G(2d,2p)) = -5459.879687405

Fe	0.9412970	2.8049880	-0.3536310
C	-0.8826580	2.0100620	-0.7160710
C	-1.0267920	3.3748380	-0.2892450
C	-0.3314250	4.2070100	-1.2130290
C	0.2361090	3.3756750	-2.2233190
C	-0.1041180	2.0255770	-1.9262220
C	2.7952320	3.5914650	0.1655230
C	2.9324050	2.2987100	-0.4159190
C	2.1781710	1.3609050	0.3707580
C	1.5841500	2.1076180	1.4491810
C	1.9686160	3.4727790	1.3197710
P	-1.5258260	0.4751090	0.0215170

P	1.8650270	-0.4065740	-0.0044400
C	-3.2634830	0.5144160	-0.5801800
C	-1.6955250	0.8016960	1.8200980
C	2.8855230	-1.2571340	1.2735860
C	2.8126830	-0.6225080	-1.5605050
C	-3.5611350	1.0658010	-1.8335530
C	-4.8656320	1.0285040	-2.3285900
C	-5.8838310	0.4424750	-1.5765690
C	-5.5934810	-0.1045620	-0.3251210
C	-4.2928730	-0.0688430	0.1719590
C	-0.9620650	0.0048670	2.7107270
C	-1.0331560	0.2288510	4.0868530
C	-1.8437620	1.2499350	4.5853500
C	-2.5961140	2.0342240	3.7064670
C	-2.5295360	1.8065200	2.3319200
C	3.5475540	-2.4573750	0.9707170
C	4.2577550	-3.1389730	1.9583490
C	4.3108540	-2.6417670	3.2617710
C	3.6526690	-1.4517710	3.5723680
C	2.9455810	-0.7632570	2.5848320
C	4.2027570	-0.4412130	-1.6099740
C	4.8873600	-0.5667540	-2.8187440
C	4.1895670	-0.8757830	-3.9893730
C	2.8082770	-1.0697050	-3.9453840
C	2.1238080	-0.9490400	-2.7350420
H	-1.5262000	3.7091160	0.6087030
H	-0.2155320	5.2803790	-1.1328970
H	0.8577350	3.7047880	-3.0458930
H	0.2082830	1.1516880	-2.4816030
H	3.2140310	4.5089570	-0.2276860
H	3.4665540	2.0680590	-1.3259440
H	0.9126530	1.7173160	2.1995900
H	1.6452450	4.2825930	1.9611390
H	-2.7781620	1.5254140	-2.4279880
H	-5.0829120	1.4591440	-3.3023130
H	-6.8984630	0.4098300	-1.9640750
H	-6.3783100	-0.5715490	0.2629280
H	-4.0749210	-0.5234170	1.1310960
H	-0.3377250	-0.7955270	2.3216570
H	-0.4603280	-0.3981750	4.7642000
H	-1.9016870	1.4262350	5.6558890
H	-3.2429860	2.8172390	4.0925890
H	-3.1426570	2.3981210	1.6589690
H	3.4961340	-2.8647150	-0.0310580
H	4.7636470	-4.0668890	1.7066220
H	4.8629130	-3.1773860	4.0292980

H	3.6927150	-1.0507690	4.5817230
H	2.4526000	0.1662800	2.8447830
H	4.7509970	-0.2088760	-0.7014950
H	5.9647240	-0.4277300	-2.8456210
H	4.7242590	-0.9773400	-4.9298850
H	2.2637950	-1.3329120	-4.8478550
H	1.0577700	-1.1490650	-2.6905820
Ni	-0.2758780	-1.2994060	-0.2460280
Cl	0.7306810	-3.2503430	-0.5458330
C	-1.9197400	-2.2595280	-0.3678680
C	-2.5806770	-2.4349460	-1.5900210
C	-2.4613680	-2.8558650	0.7778530
C	-3.7594040	-3.1799970	-1.6657340
H	-2.1803200	-1.9846010	-2.4960450
C	-3.6455060	-3.5977790	0.7062050
H	-1.9544270	-2.7607740	1.7354540
C	-4.3018850	-3.7581400	-0.5150220
H	-4.2570290	-3.3052220	-2.6249210
H	-4.0485290	-4.0565280	1.6069220
H	-5.2220090	-4.3341480	-0.5723010

(dppf)Ni(*ortho*-tolyl)Cl



Zero-point correction= 0.640828 (Hartree/Particle)
Thermal correction to Energy= 0.682387
Thermal correction to Enthalpy= 0.683331
Thermal correction to Gibbs Free Energy= 0.565568
Sum of electronic and zero-point Energies= -5497.759181
Sum of electronic and thermal Energies= -5497.717622
Sum of electronic and thermal Enthalpies= -5497.716677
Sum of electronic and thermal Free Energies= -5497.834441

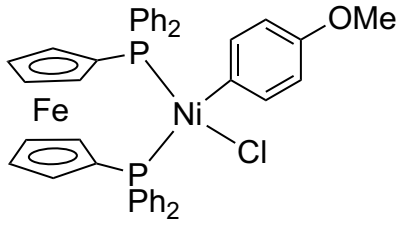
Single-point energy (6-311+G(2d,2p)) = -5499.217789

Fe	0.9624498078	2.7601235899	-0.3523743677
C	-0.8620619549	1.9656655197	-0.7154276177
C	-1.006408017	3.3267426403	-0.2773668287
C	-0.3148498097	4.1669672927	-1.1967369324
C	0.2504808667	3.3441704478	-2.2152778788

C	-0.0874938067	1.9914782366	-1.9275927151
C	2.8179265529	3.5448023638	0.1642951504
C	2.9542445174	2.2554655483	-0.4247713615
C	2.2037481618	1.3125879345	0.3592532665
C	1.6129420607	2.0525974587	1.4440162874
C	1.9958329531	3.4188178573	1.3210028028
P	-1.5053707901	0.425077171	0.0107240841
P	1.8908233333	-0.4518647667	-0.0303227082
C	-3.2431467253	0.4703831216	-0.5952925987
C	-1.6796785499	0.7464297918	1.809736397
C	2.9021481634	-1.3177485179	1.2451411472
C	2.8504443938	-0.6519526706	-1.5813468377
C	-3.5394112163	1.0428900377	-1.8396260203
C	-4.8440407018	1.0193330012	-2.3351029926
C	-5.8653950825	0.428768361	-1.5911433696
C	-5.5777718519	-0.1366446423	-0.3472742294
C	-4.2766246575	-0.1160713178	0.1490693916
C	-0.9311899525	-0.0356108577	2.7008928208
C	-1.0060437089	0.1882806373	4.0767738553
C	-1.8349375553	1.1949408729	4.5746508499
C	-2.6005756943	1.9654330731	3.6951753086
C	-2.5302218052	1.7376426586	2.3207951974
C	3.5407484557	-2.5301063463	0.9393330128
C	4.2409740735	-3.225731411	1.9242401923
C	4.3078716679	-2.7305564297	3.2278352713
C	3.6740491138	-1.5281234329	3.5410922251
C	2.9768307753	-0.8255610564	2.5563436311
C	4.2430052471	-0.4880030031	-1.6140551669
C	4.9372830333	-0.5974894876	-2.8189240819
C	4.2465674193	-0.8720356421	-4.0022679157
C	2.8622794709	-1.0469781731	-3.9751645062
C	2.1681466305	-0.94288007	-2.7688407613
H	-1.5037400211	3.6527682124	0.6247992973
H	-0.1997880728	5.2397976938	-1.1085847946
H	0.8689755336	3.6803259709	-3.0373657483
H	0.22335326	1.1220607592	-2.4904217947
H	3.2343923502	4.4648913707	-0.2252724071
H	3.4858018921	2.0301683775	-1.3376546055
H	0.9453928019	1.6573349382	2.1952392856
H	1.6745431491	4.2245277384	1.9685812653
H	-2.7552768798	1.5089210424	-2.4270955504
H	-5.0586764111	1.4648754209	-3.3026636466
H	-6.8802898475	0.4074040029	-1.9787855472
H	-6.3647181557	-0.6070930693	0.2350998286
H	-4.0618182015	-0.5843826942	1.1018500916
H	-0.2916391	-0.8244220407	2.3130226096

H	-0.4218385452	-0.4276766457	4.7545795719
H	-1.8961378377	1.3707476023	5.6450865323
H	-3.2606438139	2.7377164553	4.0805801326
H	-3.1526680268	2.3186509135	1.6471157085
H	3.4781911019	-2.9356103041	-0.0625275258
H	4.7284917842	-4.1628013467	1.6701588537
H	4.8520465906	-3.2771706891	3.9932383063
H	3.7256370697	-1.1282380551	4.5503720851
H	2.5037103732	0.113666724	2.81817973
H	4.7853941996	-0.281037184	-0.6959901648
H	6.0165950275	-0.472336326	-2.8329908544
H	4.7887474378	-0.9607953397	-4.9397799925
H	2.3225966873	-1.2819594367	-4.8882971257
H	1.0992557295	-1.1267001327	-2.739460852
Ni	-0.2486196541	-1.341769763	-0.2750135887
Cl	0.7482223035	-3.2871740464	-0.6544492418
C	-1.8974214416	-2.3012415084	-0.3695085792
C	-2.5401755596	-2.5327546698	-1.5993167515
C	-2.4416467383	-2.8334365549	0.8036228183
C	-3.733268178	-3.2639269422	-1.6144075161
C	-3.6316983316	-3.5690098067	0.7749055025
C	-4.2864468657	-3.7757452883	-0.4383350189
H	-4.2345381292	-3.4380160267	-2.5650016347
H	-4.0392803835	-3.9770828558	1.6973546038
H	-5.2149160988	-4.3400289059	-0.4743752886
H	-1.9364234197	-2.6838319867	1.7551471578
C	-1.9320450229	-2.037221643	-2.888649824
H	-1.0073326922	-2.5852622297	-3.1082224988
H	-2.6178211092	-2.1627670301	-3.7339265561
H	-1.6687525728	-0.9727843915	-2.8264859737

(dppf)Ni(*p*-OMePh)Cl



Zero-point correction= 0.645739 (Hartree/Particle)
Thermal correction to Energy= 0.688370
Thermal correction to Enthalpy= 0.689314
Thermal correction to Gibbs Free Energy= 0.567626
Sum of electronic and zero-point Energies= -5572.959563
Sum of electronic and thermal Energies= -5572.916932

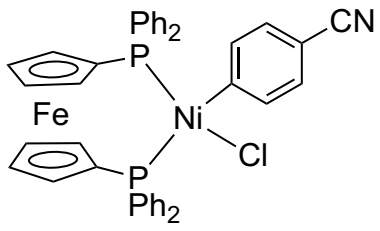
Sum of electronic and thermal Enthalpies= -5572.915988
Sum of electronic and thermal Free Energies= -5573.037676

Single-point energy (6-311+G(2d,2p)) = -5574.444894

Fe	1.8806510	2.5316660	-0.6840570
C	-0.1049660	2.2026210	-0.8859790
C	0.1289180	3.5941620	-0.6131150
C	0.9507840	4.1204270	-1.6509030
C	1.2229300	3.0728370	-2.5795640
C	0.5722170	1.8938360	-2.1176030
C	3.9026330	2.8618270	-0.3274670
C	3.6711990	1.5252620	-0.7612480
C	2.7580560	0.8984920	0.1554120
C	2.4429870	1.8786090	1.1621470
C	3.1499630	3.0780590	0.8626800
P	-1.0625980	0.9650860	0.0447530
P	1.9876290	-0.7583340	0.0004230
C	-2.7718560	1.3882960	-0.4899560
C	-1.0282700	1.5011770	1.8002310
C	2.8443110	-1.7062270	1.3292400
C	2.7475110	-1.3695280	-1.5537610
C	-3.0056800	1.8569350	-1.7897530
C	-4.3081220	2.1020830	-2.2277810
C	-5.3880660	1.8835880	-1.3722650
C	-5.1607440	1.4219430	-0.0739580
C	-3.8617210	1.1771100	0.3662420
C	-0.4701830	0.6318510	2.7484190
C	-0.3949760	1.0017220	4.0925300
C	-0.8826200	2.2439100	4.5015270
C	-1.4614100	3.1072880	3.5670850
C	-1.5419510	2.7352330	2.2252070
C	3.1603430	-3.0613190	1.1434290
C	3.7403400	-3.7975770	2.1758430
C	4.0046420	-3.1992550	3.4091670
C	3.6905240	-1.8541600	3.6035880
C	3.1152170	-1.1120540	2.5703590
C	4.1324370	-1.5562030	-1.6753280
C	4.6833950	-1.9770240	-2.8856480
C	3.8555760	-2.2165420	-3.9857260
C	2.4756310	-2.0449020	-3.8684530
C	1.9236860	-1.6285430	-2.6560020
H	-0.2096790	4.1351030	0.2587140
H	1.3394580	5.1297170	-1.6983890
H	1.8530020	3.1451370	-3.4565850
H	0.6174140	0.9169180	-2.5795220
H	4.5127080	3.5955200	-0.8386390

H	4.0694670	1.0736150	-1.6579330
H	1.7458350	1.7521690	1.9771890
H	3.0839890	4.0045820	1.4185110
H	-2.1742610	2.0312170	-2.4651420
H	-4.4751680	2.4653920	-3.2382250
H	-6.4020970	2.0719730	-1.7144810
H	-5.9955540	1.2419620	0.5973380
H	-3.7015820	0.7916040	1.3660010
H	-0.0987750	-0.3391290	2.4304470
H	0.0382420	0.3163690	4.8154930
H	-0.8262200	2.5341350	5.5470210
H	-1.8598200	4.0667340	3.8854640
H	-2.0237710	3.3972630	1.5122330
H	2.9407990	-3.5425460	0.1988110
H	3.9775900	-4.8455120	2.0150340
H	4.4539360	-3.7771690	4.2122250
H	3.8982320	-1.3751910	4.5568140
H	2.8911630	-0.0651260	2.7387030
H	4.7794370	-1.3793330	-0.8209330
H	5.7571470	-2.1219070	-2.9683000
H	4.2852840	-2.5482050	-4.9270700
H	1.8249170	-2.2518520	-4.7134180
H	0.8467420	-1.5432270	-2.5490350
Ni	-0.3183420	-1.0901030	-0.0642630
Cl	0.1394850	-3.2553330	-0.1570250
C	-2.1601110	-1.5880770	-0.0318090
C	-2.9196510	-1.6858170	-1.1988910
C	-2.7827150	-1.9064620	1.1839610
C	-4.2667920	-2.0643890	-1.1710080
H	-2.4725490	-1.4529660	-2.1631450
C	-4.1258850	-2.2765890	1.2333970
H	-2.2174550	-1.8768640	2.1124740
C	-4.8766050	-2.3449730	0.0550360
H	-4.8220330	-2.1213050	-2.1006240
H	-4.6082940	-2.5207220	2.1758280
O	-6.2026400	-2.6907010	0.2034210
C	-6.9931820	-2.7866590	-0.9681470
H	-6.6067910	-3.5539030	-1.6522470
H	-7.9930190	-3.0701900	-0.6345290
H	-7.0440150	-1.8254860	-1.4976430

(dppf)Ni(*p*-CNPh)Cl



Zero-point correction= 0.611722 (Hartree/Particle)
Thermal correction to Energy= 0.653510
Thermal correction to Enthalpy= 0.654454
Thermal correction to Gibbs Free Energy= 0.534817
Sum of electronic and zero-point Energies= -5550.720919
Sum of electronic and thermal Energies= -5550.679131
Sum of electronic and thermal Enthalpies= -5550.678187
Sum of electronic and thermal Free Energies= -5550.797824

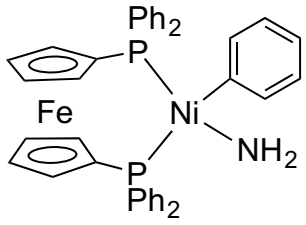
Single-point energy (6-311+G(2d,2p)) = -5552.157700

Fe	1.7582010	2.5825480	-0.5984400
C	-0.2121850	2.2078980	-0.8463320
C	-0.0214990	3.5976710	-0.5323110
C	0.8033020	4.1726600	-1.5410740
C	1.1199810	3.1581600	-2.4918390
C	0.4942150	1.9500170	-2.0736020
C	3.7659930	2.9536780	-0.1990700
C	3.5746450	1.6226810	-0.6671630
C	2.6614490	0.9532010	0.2191640
C	2.3055350	1.9020560	1.2423960
C	2.9883100	3.1243110	0.9821400
P	-1.1448000	0.9257600	0.0414670
P	1.9422640	-0.7191210	0.0050260
C	-2.8625560	1.3009500	-0.4920250
C	-1.1376050	1.3914730	1.8152570
C	2.7746920	-1.6795680	1.3389930
C	2.7603430	-1.2737060	-1.5396330
C	-3.1050050	1.7798300	-1.7867410
C	-4.4133430	1.9651270	-2.2355110
C	-5.4900480	1.6734250	-1.3975040
C	-5.2543980	1.2052680	-0.1031340
C	-3.9492060	1.0222880	0.3491870
C	-0.5788770	0.4936100	2.7362240
C	-0.5301690	0.8103980	4.0950830
C	-1.0451200	2.0270250	4.5452880
C	-1.6249610	2.9176890	3.6372670
C	-1.6794110	2.5988480	2.2806090

C	3.1269130	-3.0226230	1.1315720
C	3.6876290	-3.7714120	2.1656050
C	3.8966400	-3.1977540	3.4210550
C	3.5470640	-1.8646090	3.6364360
C	2.9907240	-1.1097010	2.6021940
C	4.1519390	-1.4317850	-1.6189960
C	4.7504050	-1.8086740	-2.8211220
C	3.9643010	-2.0316100	-3.9547850
C	2.5783200	-1.8869670	-3.8801630
C	1.9787480	-1.5147640	-2.6760990
H	-0.3904610	4.1065420	0.3464540
H	1.1645990	5.1929960	-1.5552400
H	1.7624300	3.2711110	-3.3554110
H	0.5734420	0.9880580	-2.5615270
H	4.3669130	3.7131840	-0.6825050
H	3.9999100	1.2012290	-1.5660780
H	1.5988020	1.7410810	2.0428740
H	2.8908490	4.0358010	1.5577810
H	-2.2756350	2.0067580	-2.4491270
H	-4.5885490	2.3358740	-3.2416850
H	-6.5086600	1.8081670	-1.7499640
H	-6.0879690	0.9715250	0.5526950
H	-3.7794560	0.6378280	1.3482600
H	-0.1835570	-0.4566440	2.3861690
H	-0.0952020	0.1043350	4.7966440
H	-1.0091590	2.2760840	5.6021390
H	-2.0447490	3.8565020	3.9876840
H	-2.1626500	3.2805650	1.5874490
H	2.9521050	-3.4850230	0.1683590
H	3.9539390	-4.8095490	1.9881230
H	4.3312780	-3.7853670	4.2250210
H	3.7128460	-1.4047030	4.6070260
H	2.7390930	-0.0720610	2.7874510
H	4.7668580	-1.2667700	-0.7389650
H	5.8287240	-1.9322390	-2.8713540
H	4.4311790	-2.3292480	-4.8896650
H	1.9603390	-2.0808130	-4.7522730
H	0.8974780	-1.4502000	-2.6048610
Ni	-0.3508110	-1.1137780	-0.1398100
Cl	0.1616390	-3.2591200	-0.2935060
C	-2.1628400	-1.6848570	-0.2068660
C	-2.8751650	-1.7337500	-1.4149680
C	-2.8135340	-2.0936700	0.9676550
C	-4.2047550	-2.1379400	-1.4524400
H	-2.3942530	-1.4345680	-2.3430340
C	-4.1459070	-2.4968790	0.9496770

H	-2.2759040	-2.1042670	1.9121800
C	-4.8568910	-2.5066330	-0.2623100
H	-4.7508450	-2.1570120	-2.3907940
H	-4.6436510	-2.8010890	1.8660240
C	-6.2421600	-2.8630650	-0.2827060
N	-7.3762120	-3.1318420	-0.2971390

(dppf)Ni(Ph)NH_2



Zero-point correction= 0.637745 (Hartree/Particle)
Thermal correction to Energy= 0.677816
Thermal correction to Enthalpy= 0.678760
Thermal correction to Gibbs Free Energy= 0.564237
Sum of electronic and zero-point Energies= -5054.144646
Sum of electronic and thermal Energies= -5054.104575
Sum of electronic and thermal Enthalpies= -5054.103631
Sum of electronic and thermal Free Energies= -5054.218154

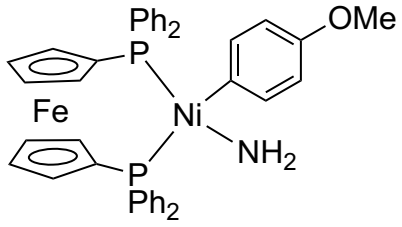
Single-point energy (6-311+G(2d,2p)) = -5055.577398506

Fe	-1.0782120	2.7243940	0.2061180
C	0.7591630	2.0002020	0.6938430
C	0.8833460	3.3393300	0.1885100
C	0.1249840	4.2078780	1.0250390
C	-0.4653720	3.4246670	2.0596880
C	-0.0791650	2.0681840	1.8610370
C	-2.9317460	3.4414120	-0.4019920
C	-3.0571400	2.1786240	0.2456270
C	-2.2636810	1.2196740	-0.4721950
C	-1.6620380	1.9180760	-1.5777450
C	-2.0744720	3.2800560	-1.5296580
P	1.4639570	0.4507510	0.0254490
P	-1.9049040	-0.5268360	-0.0851410
C	3.0350640	0.3531450	0.9883260
C	2.0218130	0.9591770	-1.6525130
C	-3.2004330	-1.3997560	-1.0592310
C	-2.4988980	-0.7211870	1.6426980
C	3.0739560	0.7711300	2.3258550
C	4.2375890	0.6206000	3.0828480
C	5.3769200	0.0528590	2.5122690

C	5.3459790	-0.3648960	1.1807000
C	4.1849930	-0.2189410	0.4243090
C	1.3693620	0.4085180	-2.7637820
C	1.7246370	0.7901360	-4.0584820
C	2.7448300	1.7223540	-4.2547660
C	3.4125640	2.2648470	-3.1537620
C	3.0555340	1.8836090	-1.8598560
C	-3.6766810	-2.6502530	-0.6296290
C	-4.6103010	-3.3479840	-1.3968120
C	-5.0796980	-2.8120580	-2.5975350
C	-4.6115930	-1.5702680	-3.0301540
C	-3.6768930	-0.8683480	-2.2668190
C	-3.8362070	-0.5063110	2.0068830
C	-4.2365340	-0.6420200	3.3365140
C	-3.3066330	-1.0045230	4.3145950
C	-1.9792050	-1.2449940	3.9565410
C	-1.5795540	-1.1099490	2.6259250
H	1.4142020	3.6270110	-0.7076090
H	-0.0147030	5.2705060	0.8721760
H	-1.1322250	3.7851010	2.8324240
H	-0.4043580	1.2255500	2.4550710
H	-3.3748350	4.3705500	-0.0666880
H	-3.6026530	1.9882560	1.1585310
H	-0.9705610	1.4927860	-2.2913140
H	-1.7515910	4.0628770	-2.2038860
H	2.2006480	1.2243650	2.7826970
H	4.2510010	0.9528890	4.1175190
H	6.2821090	-0.0652710	3.1018500
H	6.2226400	-0.8201480	0.7288210
H	4.1681300	-0.5778590	-0.5976680
H	0.5915450	-0.3349520	-2.6043900
H	1.2122910	0.3519270	-4.9106560
H	3.0272510	2.0176350	-5.2616440
H	4.2159610	2.9813420	-3.3023450
H	3.5902990	2.2966290	-1.0097160
H	-3.3001100	-3.0781760	0.2919510
H	-4.9683300	-4.3149280	-1.0538910
H	-5.8082030	-3.3575620	-3.1913610
H	-4.9762040	-1.1418490	-3.9599900
H	-3.3296490	0.1009290	-2.6101220
H	-4.5696290	-0.2494680	1.2479140
H	-5.2752940	-0.4729840	3.6074010
H	-3.6206480	-1.1138460	5.3491470
H	-1.2567640	-1.5506080	4.7083970
H	-0.5561540	-1.3316180	2.3354940
Ni	0.2177170	-1.3802580	-0.1779650

N	-0.6605250	-3.0383960	-0.2927900
C	1.8539190	-2.3704840	-0.2155600
C	2.3608040	-2.9164430	0.9770540
C	2.5594220	-2.6432530	-1.3998470
C	3.5296560	-3.6816720	0.9925570
H	1.8438370	-2.7329800	1.9175620
C	3.7337770	-3.4046910	-1.3914410
H	2.1966290	-2.2567540	-2.3492460
C	4.2276470	-3.9240660	-0.1931780
H	3.8992700	-4.0836640	1.9337100
H	4.2593820	-3.5950350	-2.3253880
H	5.1396450	-4.5158320	-0.1838650
H	-0.0060570	-3.8197010	-0.2756240
H	-1.1598590	-3.1263730	-1.1815640

(dppf)Ni(*p*-OMePh)NH_2



Zero-point correction= 0.670436 (Hartree/Particle)
Thermal correction to Energy= 0.713169
Thermal correction to Enthalpy= 0.714114
Thermal correction to Gibbs Free Energy= 0.593341
Sum of electronic and zero-point Energies= -5168.640320
Sum of electronic and thermal Energies= -5168.597586
Sum of electronic and thermal Enthalpies= -5168.596642
Sum of electronic and thermal Free Energies= -5168.717414

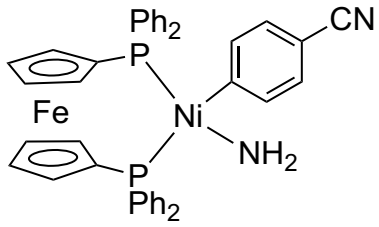
Single-point energy (6-311+G(2d,2p)) = -5170.142238

Fe	2.0712890	-2.4633190	0.0631310
C	0.1217590	-2.2867550	0.6183710
C	0.3498140	-3.5865740	0.0505080
C	1.3397420	-4.2509230	0.8303050
C	1.7270140	-3.3810680	1.8912870
C	0.9822270	-2.1735750	1.7656870
C	4.0302370	-2.6233880	-0.6126060
C	3.8292190	-1.4026390	0.0937600
C	2.7843740	-0.6656160	-0.5617480
C	2.3605840	-1.4536450	-1.6893890
C	3.1272280	-2.6532520	-1.7154390

P	-0.9899310	-0.9547860	0.0382460
P	1.9818620	0.9015870	-0.0830860
C	-2.5032430	-1.3226890	1.0270610
C	-1.4348260	-1.5157090	-1.6566010
C	2.9641410	2.1326620	-1.0363490
C	2.5559680	1.1759370	1.6407730
C	-2.3883180	-1.7329630	2.3624260
C	-3.5274250	-1.9182710	3.1483430
C	-4.7949330	-1.6974730	2.6094370
C	-4.9175050	-1.2917900	1.2793560
C	-3.7819080	-1.1042080	0.4939080
C	-0.9968910	-0.7482090	-2.7443590
C	-1.2703320	-1.1481330	-4.0533660
C	-1.9939350	-2.3186410	-4.2874850
C	-2.4490570	-3.0822170	-3.2094290
C	-2.1739540	-2.6819820	-1.9012730
C	3.0964440	3.4466060	-0.5555010
C	3.7836770	4.4028770	-1.3040620
C	4.3455180	4.0647950	-2.5366780
C	4.2182790	2.7616250	-3.0203550
C	3.5308960	1.8012450	-2.2759250
C	3.9126320	1.3153720	1.9682250
C	4.3036080	1.4986320	3.2949170
C	3.3419080	1.5553320	4.3072300
C	1.9880860	1.4429790	3.9869460
C	1.5975740	1.2604980	2.6592470
H	-0.1092810	-3.9698630	-0.8494060
H	1.7569530	-5.2282840	0.6234750
H	2.4894760	-3.5789540	2.6337270
H	1.0862970	-1.2994990	2.3932420
H	4.7181490	-3.4106050	-0.3313160
H	4.3306940	-1.1100360	1.0048490
H	1.5586040	-1.2022880	-2.3690240
H	3.0076230	-3.4650610	-2.4213570
H	-1.4107050	-1.9168370	2.7956380
H	-3.4201230	-2.2384380	4.1813430
H	-5.6813000	-1.8375470	3.2221280
H	-5.8990500	-1.1065650	0.8523300
H	-3.8925750	-0.7567160	-0.5260230
H	-0.4532560	0.1745690	-2.5536350
H	-0.9267320	-0.5411960	-4.8866360
H	-2.2123320	-2.6303510	-5.3052950
H	-3.0233920	-3.9875520	-3.3867130
H	-2.5461530	-3.2712610	-1.0684750
H	2.6453860	3.7176610	0.3918040
H	3.8765640	5.4156290	-0.9213530

H	4.8818620	4.8117330	-3.1157680
H	4.6580300	2.4872850	-3.9755800
H	3.4485530	0.7892240	-2.6593190
H	4.6636330	1.2981550	1.1836220
H	5.3575830	1.6054160	3.5372160
H	3.6475180	1.7022900	5.3396330
H	1.2342460	1.5106650	4.7665310
H	0.5436900	1.2095250	2.3994730
Ni	-0.2916050	1.1524670	-0.0931730
N	0.0930860	2.9899370	-0.1510930
C	-2.1420630	1.6431010	-0.0322000
C	-2.7334860	1.9641680	1.2055640
C	-2.9554520	1.7599990	-1.1653710
C	-4.0663390	2.3504790	1.3099470
H	-2.1453520	1.8986550	2.1191580
C	-4.3040160	2.1420850	-1.0848890
H	-2.5505690	1.5444790	-2.1512850
C	-4.8632780	2.4306490	0.1615630
H	-4.5127860	2.5841780	2.2724220
H	-4.8918990	2.2116200	-1.9941140
H	-0.7524460	3.5567300	-0.0991090
H	0.5348330	3.2457540	-1.0378070
O	-6.1770970	2.7984770	0.3631060
C	-7.0090460	2.9199160	-0.7762900
H	-7.1037100	1.9640060	-1.3098560
H	-7.9888250	3.2241160	-0.4036310
H	-6.6310950	3.6817660	-1.4712890

(dppf)Ni(*p*-CNPh)NH_2



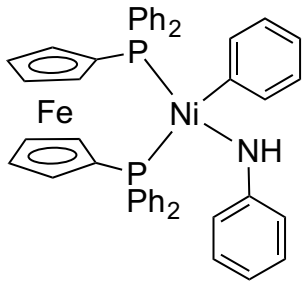
Zero-point correction= 0.636266 (Hartree/Particle)
Thermal correction to Energy= 0.678233
Thermal correction to Enthalpy= 0.679177
Thermal correction to Gibbs Free Energy= 0.559983
Sum of electronic and zero-point Energies= -5146.402373
Sum of electronic and thermal Energies= -5146.360406
Sum of electronic and thermal Enthalpies= -5146.359461
Sum of electronic and thermal Free Energies= -5146.478656

Single-point energy (6-311+G(2d,2p)) = -5147.855479

Fe	1.9039360	2.4920440	-0.3546880
C	-0.0599160	2.2054970	-0.7925980
C	0.1500460	3.5620920	-0.3676460
C	1.0782620	4.1724220	-1.2590680
C	1.4440400	3.2120640	-2.2469420
C	0.7476690	2.0022880	-1.9658310
C	3.8821840	2.7830360	0.2148270
C	3.6990050	1.4942210	-0.3635260
C	2.7110610	0.7883090	0.4051110
C	2.3036670	1.6664150	1.4704830
C	3.0248450	2.8880490	1.3487970
P	-1.0891320	0.9070020	-0.0277860
P	1.9518970	-0.8429470	0.1035180
C	-2.6760500	1.1257250	-0.9385870
C	-1.4456150	1.5758360	1.6461360
C	2.9833980	-1.9448840	1.1564080
C	2.4981920	-1.2645730	-1.5978500
C	-2.6578420	1.3464920	-2.3229520
C	-3.8491420	1.3897070	-3.0488340
C	-5.0723560	1.2113050	-2.4014110
C	-5.0990490	0.9966440	-1.0224330
C	-3.9103740	0.9550760	-0.2954070
C	-0.9473770	0.8820460	2.7576000
C	-1.1611360	1.3630330	4.0504490
C	-1.8837410	2.5413650	4.2444470
C	-2.3989050	3.2313480	3.1438750
C	-2.1848120	2.7500240	1.8520030
C	3.1738930	-3.2887140	0.7921160
C	3.8977850	-4.1456870	1.6220530
C	4.4389920	-3.6773390	2.8207420
C	4.2549840	-2.3433060	3.1881520
C	3.5307680	-1.4819130	2.3622560
C	3.8526870	-1.3955100	-1.9376410
C	4.2259600	-1.6908190	-3.2491490
C	3.2492070	-1.8674580	-4.2326600
C	1.8983040	-1.7624030	-3.8977320
C	1.5255390	-1.4689430	-2.5851410
H	-0.2774370	4.0209260	0.5121750
H	1.4710490	5.1774150	-1.1717940
H	2.1628420	3.3567490	-3.0431500
H	0.8508990	1.0733940	-2.5091450
H	4.5278960	3.5622510	-0.1696230
H	4.1739160	1.1324060	-1.2638940
H	1.5409530	1.4549910	2.2065330

H	2.9039830	3.7591500	1.9798120
H	-1.7149120	1.4901270	-2.8408890
H	-3.8183990	1.5641970	-4.1209820
H	-5.9993440	1.2379480	-2.9672610
H	-6.0457070	0.8500680	-0.5102790
H	-3.9461820	0.7631240	0.7701680
H	-0.4009120	-0.0454140	2.6007380
H	-0.7713070	0.8134480	4.9028020
H	-2.0556480	2.9159720	5.2497300
H	-2.9739820	4.1413100	3.2916820
H	-2.6066700	3.2803510	1.0033850
H	2.7411770	-3.6602480	-0.1293030
H	4.0360850	-5.1828600	1.3292290
H	5.0038930	-4.3471100	3.4633910
H	4.6791210	-1.9679160	4.1155630
H	3.4057040	-0.4444040	2.6551860
H	4.6163400	-1.2830920	-1.1733840
H	5.2782290	-1.7906080	-3.5012210
H	3.5411720	-2.1013140	-5.2528170
H	1.1338980	-1.9225690	-4.6530850
H	0.4751840	-1.4244240	-2.3109460
Ni	-0.3144950	-1.1714160	0.1943440
C	-2.1277930	-1.7502320	0.2198200
C	-2.7421280	-2.1608410	-0.9800390
C	-2.8995840	-1.8200240	1.3950200
C	-4.0680260	-2.5772600	-1.0218910
H	-2.1798370	-2.1336840	-1.9107910
C	-4.2294760	-2.2334090	1.3756880
H	-2.4623700	-1.5341140	2.3479760
C	-4.8297420	-2.6036780	0.1600900
H	-4.5275810	-2.8698540	-1.9614610
H	-4.8114230	-2.2679250	2.2925530
C	-6.2077350	-2.9854430	0.1217830
N	-7.3348880	-3.2806940	0.0876480
N	0.1560830	-2.9872160	0.3339770
H	0.5984130	-3.1745490	1.2374400
H	-0.6535120	-3.6060450	0.3014310

(dppf)Ni(Ph)PhNH



Zero-point correction= 0.718507 (Hartree/Particle)
Thermal correction to Energy= 0.763264
Thermal correction to Enthalpy= 0.764208
Thermal correction to Gibbs Free Energy= 0.637651
Sum of electronic and zero-point Energies= -5285.129003
Sum of electronic and thermal Energies= -5285.084245
Sum of electronic and thermal Enthalpies= -5285.083301
Sum of electronic and thermal Free Energies= -5285.209858

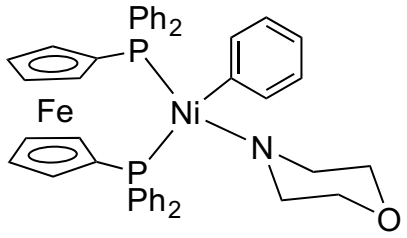
Single-point energy (6-311+G(2d,2p)) = -5286.717685

Fe	1.07367	-3.1653	-0.76041
C	2.07955	-1.42071	-1.04519
C	3.0117	-2.48688	-0.80241
C	2.83764	-3.4743	-1.81413
C	1.80983	-3.03055	-2.6971
C	1.34274	-1.76877	-2.23053
C	0.05056	-4.93341	-0.37484
C	-0.85417	-3.88897	-0.72069
C	-0.6844	-2.81133	0.21347
C	0.33774	-3.21995	1.14136
C	0.7814	-4.52389	0.7783
P	1.81387	0.11752	-0.09979
P	-1.44972	-1.14855	0.17446
C	3.08184	1.21478	-0.86146
C	2.52754	-0.2565	1.55309
C	-2.71915	-1.27156	1.50177
C	-2.42691	-1.22147	-1.37606
C	3.44854	1.05713	-2.20483
C	4.3618	1.93298	-2.79615
C	4.9204	2.97125	-2.05081
C	4.55939	3.13317	-0.7116
C	3.64411	2.26538	-0.12067
C	1.66658	-0.31588	2.65756
C	2.15756	-0.62637	3.92667
C	3.51947	-0.87509	4.10506

C	4.38867	-0.8011	3.01362
C	3.89707	-0.48809	1.74585
C	-3.90599	-0.52323	1.4113
C	-4.82746	-0.53492	2.45896
C	-4.58044	-1.2881	3.60872
C	-3.40911	-2.04047	3.70278
C	-2.48454	-2.03314	2.65579
C	-3.53542	-2.06815	-1.52252
C	-4.22595	-2.12205	-2.73341
C	-3.81784	-1.32962	-3.80975
C	-2.72071	-0.47891	-3.66994
C	-2.03256	-0.42501	-2.45723
H	3.6881	-2.55383	0.03772
H	3.36252	-4.41937	-1.87213
H	1.41674	-3.57617	-3.54524
H	0.53905	-1.19166	-2.66494
H	0.18729	-5.85848	-0.9203
H	-1.51853	-3.88105	-1.57297
H	0.74123	-2.62108	1.94542
H	1.57116	-5.08125	1.26559
H	3.03017	0.24774	-2.79405
H	4.63731	1.79745	-3.83857
H	5.63069	3.65261	-2.51131
H	4.97715	3.94721	-0.12629
H	3.34672	2.42474	0.90951
H	0.60888	-0.10694	2.51835
H	1.47809	-0.66455	4.77367
H	3.90537	-1.11322	5.09245
H	5.45185	-0.97891	3.15056
H	4.5827	-0.40793	0.90761
H	-4.09871	0.07496	0.52926
H	-5.73858	0.05078	2.37384
H	-5.2996	-1.29334	4.42336
H	-3.21296	-2.64001	4.58774
H	-1.58571	-2.63434	2.74039
H	-3.86345	-2.67877	-0.6863
H	-5.08554	-2.77895	-2.83509
H	-4.36084	-1.36833	-4.75006
H	-2.40903	0.1527	-4.49714
H	-1.19423	0.25501	-2.33588
Ni	-0.25665	0.84315	0.19963
N	-1.97703	1.55977	0.57803
C	0.46355	2.59328	0.42148
C	0.68553	3.46162	-0.65707
C	0.7454	3.06974	1.71165
C	1.17084	4.75617	-0.45832

H	0.48885	3.1292	-1.67332
C	1.24178	4.36184	1.91719
H	0.57431	2.43343	2.57795
C	1.45771	5.21115	0.83042
H	1.33057	5.40808	-1.31432
H	1.45144	4.70476	2.92853
H	1.83849	6.21741	0.98622
H	-2.10629	1.54232	1.58962
C	-2.57287	2.68879	0.05191
C	-3.32838	3.57321	0.85787
C	-2.51286	2.97229	-1.33188
C	-3.99465	4.66397	0.3071
H	-3.37621	3.39104	1.9303
C	-3.17642	4.06862	-1.87264
H	-1.93939	2.31248	-1.97342
C	-3.92707	4.92695	-1.06398
H	-4.56496	5.32203	0.95932
H	-3.10595	4.25588	-2.94232
H	-4.44359	5.78171	-1.4912

(dppf)Ni(Ph)Morpholine



Zero-point correction= 0.736274 (Hartree/Particle)
Thermal correction to Energy= 0.780595
Thermal correction to Enthalpy= 0.781539
Thermal correction to Gibbs Free Energy= 0.658244
Sum of electronic and zero-point Energies= -5285.296242
Sum of electronic and thermal Energies= -5285.251921
Sum of electronic and thermal Enthalpies= -5285.250976
Sum of electronic and thermal Free Energies= -5285.374271

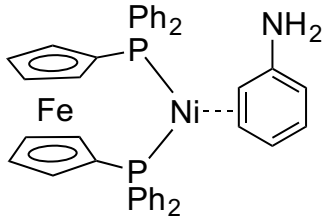
Single-point energy (6-311+G(2d,2p)) = -5286.900477

Fe	-0.79334	-3.25495	-0.04689
C	1.00479	-2.41024	-0.47958
C	1.20561	-3.6867	0.14968
C	0.58598	-4.68612	-0.65389
C	0.00656	-4.04774	-1.7891
C	0.26093	-2.65011	-1.68775

C	-2.62665	-4.07891	0.48026
C	-2.80024	-2.87235	-0.25783
C	-2.1378	-1.80897	0.44426
C	-1.56584	-2.3877	1.63208
C	-1.86838	-3.77924	1.64974
P	1.56282	-0.76227	0.07845
P	-1.87287	-0.05141	-0.0112
C	3.1904	-0.65648	-0.78077
C	2.00947	-1.04613	1.83892
C	-3.33571	0.72846	0.78646
C	-2.31883	-0.01899	-1.79641
C	3.32198	-1.1352	-2.09183
C	4.52025	-0.97287	-2.78908
C	5.60167	-0.33108	-2.18521
C	5.47911	0.14508	-0.87892
C	4.28402	-0.01606	-0.18085
C	1.24898	-0.40289	2.82547
C	1.52006	-0.60718	4.1793
C	2.56231	-1.45368	4.56068
C	3.33595	-2.08783	3.58508
C	3.06388	-1.88325	2.23193
C	-3.99595	1.80169	0.17104
C	-5.06537	2.43154	0.80613
C	-5.48876	2.00025	2.06549
C	-4.8394	0.93142	2.68373
C	-3.76974	0.29767	2.04707
C	-3.59807	-0.36277	-2.25844
C	-3.88364	-0.35886	-3.62441
C	-2.89702	-0.00189	-4.54685
C	-1.62611	0.35972	-4.09711
C	-1.34233	0.35344	-2.7305
H	1.69414	-3.85122	1.09926
H	0.52662	-5.74076	-0.41678
H	-0.57083	-4.52976	-2.56753
H	-0.09099	-1.89321	-2.37443
H	-2.97217	-5.06008	0.17982
H	-3.29122	-2.78454	-1.21634
H	-0.95902	-1.86472	2.3587
H	-1.53659	-4.49056	2.39524
H	2.49347	-1.64297	-2.57421
H	4.60599	-1.3523	-3.80382
H	6.53334	-0.20161	-2.72923
H	6.31092	0.65568	-0.40216
H	4.19597	0.38457	0.82141
H	0.44886	0.26929	2.52354
H	0.92364	-0.09924	4.93219

H	2.77886	-1.61142	5.61368
H	4.15604	-2.73796	3.87757
H	3.68152	-2.36496	1.47982
H	-3.65578	2.15889	-0.79408
H	-5.5617	3.26649	0.31927
H	-6.31997	2.49447	2.56102
H	-5.16421	0.58536	3.66134
H	-3.28064	-0.5392	2.53576
H	-4.3788	-0.61793	-1.54805
H	-4.87913	-0.62757	-3.96758
H	-3.1224	0.00563	-5.60978
H	-0.85772	0.65489	-4.80645
H	-0.3582	0.65264	-2.37754
Ni	0.1912	1.0105	0.03856
C	1.75894	2.07293	-0.13509
C	2.25307	2.4124	-1.40538
C	2.46889	2.54886	0.97887
C	3.39047	3.20808	-1.56044
H	1.74789	2.05096	-2.30026
C	3.60812	3.34846	0.83421
H	2.1308	2.30247	1.98333
C	4.07329	3.68443	-0.43812
H	3.74627	3.4536	-2.55881
H	4.12824	3.71204	1.71826
H	4.95697	4.30645	-0.55499
C	-0.90869	3.57359	-1.00519
C	-1.2771	3.122	1.31389
C	-0.13543	4.83962	-0.61122
H	-1.94622	3.88888	-1.23672
H	-0.48832	3.16719	-1.93238
C	-0.4617	4.36849	1.66658
H	-2.33764	3.43158	1.3297
H	-1.15765	2.36543	2.10254
H	-0.30218	5.63717	-1.34366
H	0.94031	4.638	-0.54448
H	-0.84227	4.83203	2.58379
H	0.60129	4.12894	1.80019
O	-0.60105	5.35326	0.64063
N	-0.95241	2.53881	0.01529

(dppf)Ni(η^2-PhNH$_2$)



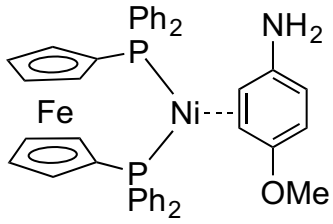
Zero-point correction= 0.638042 (Hartree/Particle)
Thermal correction to Energy= 0.678306
Thermal correction to Enthalpy= 0.679250
Thermal correction to Gibbs Free Energy= 0.563394
Sum of electronic and zero-point Energies= -5054.158280
Sum of electronic and thermal Energies= -5054.118016
Sum of electronic and thermal Enthalpies= -5054.117072
Sum of electronic and thermal Free Energies= -5054.232928
Single-point energy (6-311+G(2d,2p)) = -5055.590457

Fe	0.1905080	-1.2977900	2.4838790
C	-1.5099860	-0.4209440	1.7514380
C	-1.8492910	-1.5296740	2.5979550
C	-1.3250040	-1.2771350	3.8995000
C	-0.6630810	-0.0133140	3.8758070
C	-0.7750200	0.5149940	2.5581100
C	1.8718210	-2.2941080	3.1760950
C	2.2533190	-1.1374130	2.4346210
C	1.7230840	-1.2533650	1.1074650
C	1.0171660	-2.5027560	1.0440430
C	1.1152250	-3.1411540	2.3139990
P	-1.7524360	-0.1335790	-0.0338360
P	1.7582050	-0.0174240	-0.2521770
C	-3.4464940	0.5927970	-0.0934410
C	-2.0566650	-1.8083070	-0.7398460
C	2.5055230	-1.0084160	-1.6145770
C	3.1275730	1.0770690	0.3148390
C	-3.9321440	1.3962580	0.9477080
C	-5.1386280	2.0862420	0.8097080
C	-5.8768010	1.9867730	-0.3704270
C	-5.4050440	1.1832680	-1.4124960
C	-4.2008080	0.4935460	-1.2752720
C	-1.1880950	-2.2662460	-1.7393550
C	-1.3535660	-3.5342180	-2.3014640
C	-2.3970470	-4.3554660	-1.8725190
C	-3.2836640	-3.8991690	-0.8922840

C	-3.1191600	-2.6308220	-0.3352020
C	3.4352300	-2.0358830	-1.3945420
C	3.9399000	-2.7733560	-2.4660100
C	3.5202810	-2.4936410	-3.7695700
C	2.5929440	-1.4756970	-3.9982200
C	2.0856720	-0.7391610	-2.9257450
C	4.3869100	1.1281380	-0.2964270
C	5.3502730	2.0422150	0.1388230
C	5.0709960	2.9113530	1.1941590
C	3.8158110	2.8721560	1.8067350
C	2.8486600	1.9728410	1.3613150
H	-2.3611660	-2.4295870	2.2878940
H	-1.3786840	-1.9513830	4.7451130
H	-0.1312580	0.4428760	4.7009780
H	-0.3581690	1.4445180	2.1916200
H	2.0905720	-2.4772400	4.2205090
H	2.8170130	-0.2973050	2.8148220
H	0.4794180	-2.8800350	0.1862150
H	0.6547300	-4.0825420	2.5855850
H	-3.3638540	1.4878110	1.8681110
H	-5.5007900	2.7031110	1.6281210
H	-6.8142700	2.5255640	-0.4770370
H	-5.9777720	1.0905910	-2.3317860
H	-3.8466910	-0.1337830	-2.0899250
H	-0.3807840	-1.6227660	-2.0739710
H	-0.6680640	-3.8741030	-3.0730100
H	-2.5285250	-5.3430150	-2.3066950
H	-4.1076770	-4.5292820	-0.5676660
H	-3.8278920	-2.2733160	0.4064400
H	3.7563030	-2.2643380	-0.3822350
H	4.6581950	-3.5684360	-2.2837240
H	3.9116550	-3.0718960	-4.6023950
H	2.2564990	-1.2588800	-5.0085570
H	1.3447770	0.0379240	-3.0974610
H	4.6195030	0.4549530	-1.1152090
H	6.3216820	2.0703030	-0.3480340
H	5.8224220	3.6195230	1.5326950
H	3.5834160	3.5547440	2.6200310
H	1.8632810	1.9751450	1.8163990
Ni	-0.0748260	0.9933710	-0.8145340
N	-1.4187460	1.9506010	-3.0472350
C	-0.8783530	2.5598330	-1.8458950
C	-1.6897980	3.3815760	-0.9915500
C	-1.1248360	4.2294590	-0.0676680
C	0.2894000	4.3782270	0.0035300
C	1.0983730	3.6615670	-0.8469090

C	0.5511700	2.7035440	-1.7605280
H	-2.7707130	3.3160090	-1.0857250
H	-1.7638970	4.8188190	0.5851940
H	0.7233520	5.0873210	0.7037370
H	2.1733600	3.8154940	-0.8383860
H	1.1664660	2.3681820	-2.5932390
H	-2.3897610	1.6830560	-2.9003450
H	-1.4011330	2.6113100	-3.8265400

(dppf)Ni(η^2-*p*-OMePhNH$_2$)



Zero-point correction= 0.670415 (Hartree/Particle)
Thermal correction to Energy= 0.713523
Thermal correction to Enthalpy= 0.714467
Thermal correction to Gibbs Free Energy= 0.591282
Sum of electronic and zero-point Energies= -5168.652842
Sum of electronic and thermal Energies= -5168.609734
Sum of electronic and thermal Enthalpies= -5168.608790
Sum of electronic and thermal Free Energies= -5168.731975

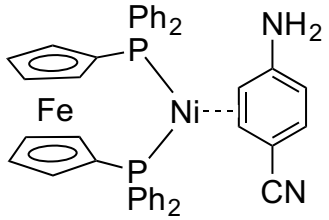
Single-point energy (6-311+G(2d,2p)) = -5170.153969

Fe	0.2335250	-1.1124200	2.6404690
C	-1.4871500	-0.4009120	1.7849150
C	-1.8012940	-1.3625660	2.8034260
C	-1.2780160	-0.8905270	4.0429140
C	-0.6415630	0.3649620	3.8087540
C	-0.7679310	0.6681380	2.4229570
C	1.9373950	-1.9467460	3.4756800
C	2.2924960	-0.9194640	2.5525110
C	1.7628530	-1.2624670	1.2651730
C	1.0823460	-2.5189210	1.4113700
C	1.1969200	-2.9389230	2.7681800
P	-1.7400060	-0.4162770	-0.0219770
P	1.7693230	-0.2610380	-0.2761010
C	-3.4410220	0.2755180	-0.1931360
C	-2.0296230	-2.1884230	-0.4366940
C	2.5151790	-1.4479750	-1.4723740
C	3.1276030	0.9266410	0.0964290
C	-3.9306940	1.2378380	0.7010050

C	-5.1375550	1.8942240	0.4487010
C	-5.8726860	1.6014590	-0.7007970
C	-5.3970820	0.6383650	-1.5957490
C	-4.1921500	-0.0165140	-1.3444460
C	-1.1555330	-2.7997300	-1.3454470
C	-1.3106920	-4.1448560	-1.6887300
C	-2.3488250	-4.8912050	-1.1295800
C	-3.2399270	-4.2852070	-0.2385950
C	-3.0857370	-2.9406060	0.0998490
C	3.4566940	-2.4211670	-1.1051060
C	3.9577090	-3.3130250	-2.0540380
C	3.5226500	-3.2432520	-3.3804420
C	2.5832260	-2.2808330	-3.7544620
C	2.0788820	-1.3899490	-2.8046890
C	4.3951800	0.8745720	-0.4977210
C	5.3501070	1.8561290	-0.2184030
C	5.0532170	2.8981930	0.6609120
C	3.7897150	2.9629680	1.2537150
C	2.8321790	1.9923830	0.9636400
H	-2.2963440	-2.3106080	2.6474800
H	-1.3153270	-1.4183370	4.9876900
H	-0.1156940	0.9599430	4.5445120
H	-0.3671720	1.5313660	1.9068730
H	2.1624680	-1.9519030	4.5347060
H	2.8383030	-0.0162940	2.7862860
H	0.5499460	-3.0422560	0.6302730
H	0.7574270	-3.8325840	3.1927900
H	-3.3649680	1.4788990	1.5956890
H	-5.5033030	2.6357440	1.1544670
H	-6.8106790	2.1137340	-0.8965140
H	-5.9672730	0.3952930	-2.4888130
H	-3.8337640	-0.7666180	-2.0457830
H	-0.3519240	-2.2147520	-1.7816440
H	-0.6213680	-4.6032520	-2.3926120
H	-2.4723070	-5.9381670	-1.3935630
H	-4.0590730	-4.8591600	0.1868880
H	-3.7972030	-2.4702990	0.7728260
H	3.7897300	-2.4866190	-0.0731660
H	4.6853490	-4.0642510	-1.7580800
H	3.9113970	-3.9412270	-4.1172890
H	2.2347140	-2.2270490	-4.7824210
H	1.3269540	-0.6565700	-3.0874120
H	4.6403980	0.0688290	-1.1821170
H	6.3280410	1.8024070	-0.6898830
H	5.7969420	3.6607560	0.8756200
H	3.5388880	3.7818050	1.9222510

H	1.8402170	2.0743240	1.3966760
Ni	-0.0879890	0.5933340	-0.9844330
N	-1.2720450	1.0877240	-3.4386000
C	-0.8817660	1.9326430	-2.3249520
C	-1.8072520	2.8130480	-1.6836840
C	-1.3921500	3.8143510	-0.8328720
C	-0.0003540	4.0490240	-0.6488550
C	0.9274550	3.2908990	-1.3293330
C	0.5214560	2.1873600	-2.1411310
H	-2.8698400	2.6712100	-1.8616420
H	-2.1333200	4.4274870	-0.3339160
H	1.9792350	3.5350250	-1.2334840
H	1.2323940	1.7866910	-2.8599840
H	-2.2164780	0.7340080	-3.3021330
H	-1.2669760	1.6128650	-4.3151130
O	0.4976640	5.0404550	0.1762010
C	-0.4230890	5.9205100	0.7950610
H	-1.0958270	5.3875320	1.4811870
H	0.1783560	6.6318020	1.3644040
H	-1.0236960	6.4660750	0.0548860

(dppf)Ni(η^2-*p*-CNPhNH$_2$)



Zero-point correction= 0.636608 (Hartree/Particle)
Thermal correction to Energy= 0.678758
Thermal correction to Enthalpy= 0.679702
Thermal correction to Gibbs Free Energy= 0.559003
Sum of electronic and zero-point Energies= -5146.419100
Sum of electronic and thermal Energies= -5146.376951
Sum of electronic and thermal Enthalpies= -5146.376007
Sum of electronic and thermal Free Energies= -5146.496706

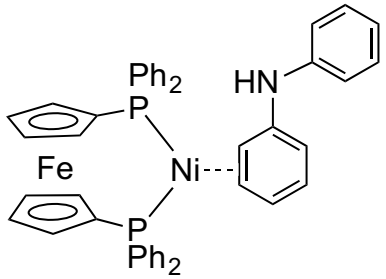
Single-point energy (6-311+G(2d,2p)) = -5147.872067

Fe	0.4192950	-2.5017770	-1.6461570
C	1.8277020	-1.0307100	-1.4196360
C	2.4677260	-2.2860600	-1.6954550
C	2.0066250	-2.7575730	-2.9592890
C	1.0866760	-1.8016070	-3.4816300

C	0.9692770	-0.7421980	-2.5372860
C	-0.8993290	-4.1009120	-1.7472460
C	-1.6064360	-2.8634550	-1.7120590
C	-1.2501430	-2.1713550	-0.5056050
C	-0.3149320	-3.0086900	0.1965570
C	-0.1060810	-4.1932360	-0.5659880
P	1.8616650	-0.0035870	0.0878750
P	-1.6844520	-0.4924220	0.0728260
C	3.0628930	1.3301960	-0.3236330
C	2.7896860	-1.0341080	1.2963130
C	-3.1239510	-0.8160150	1.1832450
C	-2.4445030	0.3028030	-1.3989650
C	3.1231610	1.8801530	-1.6122450
C	3.8875800	3.0214860	-1.8626600
C	4.6028190	3.6302230	-0.8303700
C	4.5538130	3.0870550	0.4560070
C	3.7877530	1.9492790	0.7085450
C	2.1414310	-1.3929610	2.4868050
C	2.7931790	-2.1827250	3.4370660
C	4.1007050	-2.6135960	3.2088480
C	4.7614710	-2.2440020	2.0333730
C	4.1113320	-1.4552560	1.0842980
C	-3.0153900	-1.8012450	2.1784560
C	-4.0167610	-1.9613780	3.1366860
C	-5.1442340	-1.1362380	3.1205680
C	-5.2626250	-0.1536760	2.1362200
C	-4.2606880	0.0074990	1.1770990
C	-3.5771560	-0.2016320	-2.0564810
C	-4.0924750	0.4525820	-3.1758530
C	-3.4892670	1.6237350	-3.6444670
C	-2.3726180	2.1433890	-2.9879990
C	-1.8557840	1.4843320	-1.8708890
H	3.1390770	-2.8109680	-1.0307920
H	2.2762390	-3.6996370	-3.4197330
H	0.5347110	-1.8862090	-4.4088750
H	0.3086650	0.1095430	-2.6207160
H	-0.9260390	-4.8219790	-2.5544530
H	-2.2519440	-2.4832260	-2.4906790
H	0.1871370	-2.7527960	1.1193320
H	0.5747740	-4.9964050	-0.3148690
H	2.5706470	1.4193960	-2.4250660
H	3.9203350	3.4357180	-2.8665910
H	5.1930350	4.5210060	-1.0256350
H	5.1104600	3.5515970	1.2657220
H	3.7537710	1.5392050	1.7141590
H	1.1300560	-1.0345290	2.6700530

H	2.2814300	-2.4536500	4.3567510
H	4.6098160	-3.2264030	3.9479330
H	5.7847230	-2.5662160	1.8593780
H	4.6357290	-1.1547570	0.1813840
H	-2.1421690	-2.4459280	2.2081790
H	-3.9161500	-2.7331480	3.8953350
H	-5.9245050	-1.2613360	3.8662140
H	-6.1377770	0.4904920	2.1110300
H	-4.3642130	0.7792960	0.4216830
H	-4.0664910	-1.0975580	-1.6846620
H	-4.9694450	0.0529750	-3.6783640
H	-3.8971700	2.1345280	-4.5125070
H	-1.9087110	3.0634320	-3.3321950
H	-0.9966150	1.8914030	-1.3449920
Ni	-0.0446340	0.6837070	0.8779330
C	-0.8857880	1.8640530	2.3082550
C	-2.0562610	2.5800360	1.8819600
C	-1.9791610	3.5900190	0.9597920
C	-0.7003200	3.9922820	0.4546850
C	0.4610070	3.4150000	0.9544440
C	0.4103210	2.3584620	1.9048470
H	-3.0187710	2.2869220	2.2917750
H	-2.8733470	4.0924430	0.6066790
H	1.4287600	3.7757420	0.6209300
H	1.2947470	2.1441780	2.5014400
C	-0.6210970	4.9852190	-0.5674890
N	-0.5718820	5.7776510	-1.4225850
N	-0.9251990	0.9416860	3.4109230
H	-0.5231710	1.3306980	4.2629400
H	-1.8690510	0.6182870	3.6053070

(dppf)Ni(η^2-Ph_2NH)



Zero-point correction= 0.719017 (Hartree/Particle)
Thermal correction to Energy= 0.763799
Thermal correction to Enthalpy= 0.764743
Thermal correction to Gibbs Free Energy= 0.636476
Sum of electronic and zero-point Energies= -5285.139303

Sum of electronic and thermal Energies= -5285.094521
Sum of electronic and thermal Enthalpies= -5285.093577
Sum of electronic and thermal Free Energies= -5285.221844

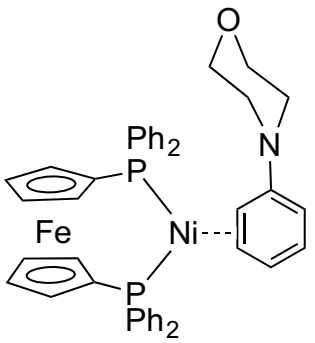
Single-point energy (6-311+G(2d,2p)) = -5286.727374

Fe	-2.90357	-1.70565	-0.81879
C	-0.97114	-2.32192	-1.10177
C	-1.82717	-3.45585	-0.89622
C	-2.81786	-3.46052	-1.92123
C	-2.58491	-2.3389	-2.77179
C	-1.4514	-1.63722	-2.27115
C	-4.85978	-1.13581	-0.43347
C	-4.06063	0.00747	-0.7285
C	-2.98895	0.06969	0.22204
C	-3.14706	-1.04911	1.1091
C	-4.29991	-1.78338	0.70678
P	0.40724	-1.65066	-0.11553
P	-1.56969	1.23497	0.26289
C	1.85882	-2.58769	-0.75748
C	0.19772	-2.39362	1.55613
C	-1.69792	1.89212	1.97948
C	-2.2142	2.59569	-0.79701
C	1.93939	-2.96018	-2.10698
C	3.11893	-3.49761	-2.62624
C	4.23762	-3.6653	-1.8086
C	4.16672	-3.30411	-0.46075
C	2.98729	-2.77174	0.05991
C	0.03611	-1.52508	2.64392
C	-0.14326	-2.02595	3.93547
C	-0.15576	-3.40445	4.15184
C	0.02682	-4.2797	3.07668
C	0.20993	-3.77763	1.78817
C	-2.91824	2.0146	2.66112
C	-2.95021	2.48828	3.97307
C	-1.76345	2.84397	4.61991
C	-0.5441	2.72363	3.95121
C	-0.5118	2.24717	2.63912
C	-2.63367	3.83666	-0.30139
C	-3.04509	4.8462	-1.1757
C	-3.04957	4.626	-2.5537
C	-2.62761	3.39318	-3.05774
C	-2.20024	2.39212	-2.18715
H	-1.76865	-4.15194	-0.07157
H	-3.63447	-4.16616	-2.00856
H	-3.1892	-2.04698	-3.62112
H	-1.02499	-0.72399	-2.66645

H	-5.71992	-1.47013	-0.99959
H	-4.21276	0.694	-1.54927
H	-2.48787	-1.30415	1.92633
H	-4.65742	-2.69823	1.16205
H	1.07961	-2.8257	-2.75595
H	3.16262	-3.78334	-3.67397
H	5.15652	-4.0776	-2.21578
H	5.0294	-3.43766	0.18641
H	2.94043	-2.51014	1.11466
H	0.04912	-0.45329	2.47233
H	-0.27042	-1.33772	4.76656
H	-0.29548	-3.79825	5.15497
H	0.03412	-5.35354	3.24414
H	0.37792	-4.46337	0.96253
H	-3.84268	1.72948	2.16728
H	-3.90114	2.57704	4.49179
H	-1.79034	3.20914	5.64309
H	0.38299	2.99263	4.45011
H	0.43821	2.13286	2.12394
H	-2.63903	4.01976	0.76823
H	-3.36514	5.80477	-0.77571
H	-3.37203	5.41172	-3.23144
H	-2.61331	3.21743	-4.13017
H	-1.83648	1.45099	-2.5873
Ni	0.41804	0.51716	-0.25035
N	3.14307	0.7416	0.35154
C	2.30021	1.03785	-0.78296
C	2.65051	0.52632	-2.08228
C	2.14334	1.08689	-3.22922
C	1.32979	2.25607	-3.16265
C	1.02806	2.81786	-1.94566
C	1.45593	2.20667	-0.72124
H	3.33518	-0.31547	-2.13399
H	2.40507	0.66786	-4.19768
H	0.98257	2.72306	-4.08066
H	0.46026	3.74234	-1.89532
H	1.46864	2.81296	0.18189
H	3.15908	-0.24246	0.58937
C	4.39806	1.35463	0.49861
C	4.75939	2.51323	-0.2104
C	5.31508	0.81717	1.4221
C	5.99891	3.11224	0.01333
H	4.07471	2.93616	-0.93671
C	6.55022	1.4218	1.63135
H	5.04344	-0.0777	1.97912
C	6.9045	2.57866	0.93114

H	6.25813	4.00762	-0.54668
H	7.24115	0.98514	2.34858
H	7.86834	3.05115	1.0967

(dppf)Ni(η^2-4-phenylmorpholine)



Zero-point correction= 0.737608 (Hartree/Particle)
Thermal correction to Energy= 0.781784
Thermal correction to Enthalpy= 0.782728
Thermal correction to Gibbs Free Energy= 0.658547
Sum of electronic and zero-point Energies= -5285.322468
Sum of electronic and thermal Energies= -5285.278292
Sum of electronic and thermal Enthalpies= -5285.277348
Sum of electronic and thermal Free Energies= -5285.401529

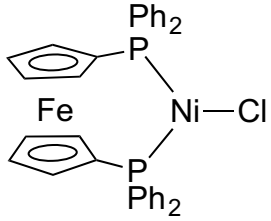
Single-point energy (6-311+G(2d,2p)) = -5286.924838

Fe	1.87957	2.79278	-0.27114
C	-0.08658	2.52043	-0.77064
C	0.11268	3.84358	-0.24981
C	1.05667	4.5179	-1.07829
C	1.4489	3.62822	-2.12158
C	0.74831	2.40219	-1.93493
C	3.83779	3.07681	0.34989
C	3.69339	1.80035	-0.26946
C	2.70465	1.05484	0.45337
C	2.25004	1.8901	1.5304
C	2.95234	3.12839	1.4665
P	-1.09442	1.11204	-0.17208
P	1.98544	-0.58137	0.02889
C	-2.74228	1.54916	-0.88762
C	-1.325	1.44821	1.62494
C	2.22444	-1.49742	1.61084
C	3.30446	-1.24711	-1.07845
C	-2.82175	1.79642	-2.26915
C	-4.05351	2.00278	-2.88806

C	-5.23292	1.96163	-2.13867
C	-5.16764	1.70781	-0.76878
C	-3.93319	1.49824	-0.14904
C	-0.88638	0.46233	2.51962
C	-0.9845	0.65217	3.89964
C	-1.53207	1.83347	4.40178
C	-1.99241	2.81569	3.51978
C	-1.89493	2.62212	2.14147
C	3.23843	-1.19112	2.53043
C	3.33789	-1.89343	3.73265
C	2.42686	-2.91059	4.02821
C	1.4171	-3.22452	3.11629
C	1.31419	-2.51976	1.91602
C	4.2642	-2.18186	-0.67154
C	5.19368	-2.68717	-1.58488
C	5.18178	-2.25888	-2.9125
C	4.22867	-1.32517	-3.32844
C	3.29277	-0.83299	-2.42037
H	-0.32859	4.24418	0.65117
H	1.4441	5.51548	-0.91336
H	2.18263	3.8313	-2.89111
H	0.84882	1.50352	-2.52985
H	4.48273	3.87681	0.00904
H	4.21277	1.46069	-1.15468
H	1.48529	1.63132	2.24842
H	2.80259	3.97481	2.12464
H	-1.9131	1.83026	-2.8643
H	-4.09256	2.19796	-3.95664
H	-6.19318	2.12237	-2.62113
H	-6.07591	1.65419	-0.17556
H	-3.909	1.27826	0.91246
H	-0.45508	-0.45267	2.12699
H	-0.63056	-0.12192	4.57502
H	-1.6094	1.98717	5.47477
H	-2.4334	3.7308	3.90624
H	-2.27953	3.38061	1.46635
H	3.94338	-0.39443	2.31224
H	4.12482	-1.64387	4.43961
H	2.50338	-3.45371	4.96649
H	0.705	-4.01478	3.33925
H	0.52564	-2.75978	1.20877
H	4.28338	-2.52484	0.35774
H	5.92718	-3.41826	-1.25493
H	5.90469	-2.65381	-3.62104
H	4.20623	-0.99139	-4.36261
H	2.53673	-0.12813	-2.75568

Ni	-0.05285	-0.72312	-0.72576
C	-1.94568	-2.87953	-0.85082
C	-1.30938	-1.95567	-1.75708
C	0.04496	-2.22577	-2.14571
C	0.68278	-3.44166	-1.7507
C	0.04568	-4.30165	-0.88786
C	-1.25851	-4.00227	-0.41771
H	-1.92602	-1.28768	-2.35053
H	0.46848	-1.68079	-2.98879
H	0.52638	-5.22367	-0.57202
H	-1.77184	-4.70106	0.23752
H	1.67313	-3.66839	-2.13424
C	-3.39969	-2.24888	0.9954
C	-4.16703	-1.91645	-1.27434
C	-4.85449	-2.32196	1.44533
H	-3.02653	-1.21734	1.11756
H	-2.7893	-2.90075	1.62705
C	-5.60023	-2.00485	-0.75794
H	-3.87595	-0.859	-1.33313
H	-4.12336	-2.34135	-2.28325
H	-4.96994	-1.90274	2.44902
H	-5.18912	-3.37192	1.45438
H	-6.25512	-1.35472	-1.34371
H	-5.96389	-3.04232	-0.82881
O	-5.70214	-1.55763	0.59292
N	-3.28575	-2.69131	-0.40042

(dppf)NiCl



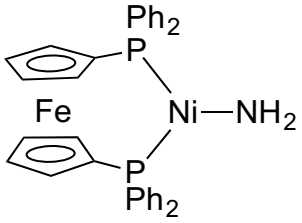
Zero-point correction= 0.521357 (Hartree/Particle)
Thermal correction to Energy= 0.556663
Thermal correction to Enthalpy= 0.557607
Thermal correction to Gibbs Free Energy= 0.448437
Sum of electronic and zero-point Energies= -5226.924780
Sum of electronic and thermal Energies= -5226.889473
Sum of electronic and thermal Enthalpies= -5226.888529
Sum of electronic and thermal Free Energies= -5226.997699

Single-point energy (6-311+G(2d,2p)) = -5228.170414

Fe	0.0579135252	2.3153537959	1.0815495236
Ni	-0.0515605268	-1.6218863535	-0.4068739086
P	1.7765388877	-0.4584662427	0.1547938092
P	-1.8103674004	-0.291014768	-0.0246371113
Cl	-0.1075593364	-3.6620352573	-1.1791187256
C	-1.5511957358	1.5027944502	0.1109688185
C	2.1165563786	2.3190977306	1.0768547172
H	2.7153480544	2.6630564529	0.2450161986
C	-1.9978630069	2.4151802689	1.125273631
H	-2.5944254542	2.1522579042	1.9877139042
C	1.6400522693	3.1171923538	2.1573135863
H	1.81757143	4.1771622146	2.2875448264
C	-0.7398674916	2.2529693999	-0.8080154797
H	-0.2245105127	1.8484527497	-1.6683768766
C	-3.9500299812	0.6572033794	-1.6560539645
H	-3.7870103119	1.6354004413	-1.2131643647
C	3.0787255509	-1.4545195081	0.9816296807
C	-3.1446732887	-0.4271180981	-1.2786348094
C	-2.6366730432	-0.7271535062	1.557963035
C	-3.9233054496	-0.2795219011	1.8902666135
H	-4.4838905213	0.3293483026	1.1865071623
C	-3.346325043	-1.6800184087	-1.8792887662
H	-2.7021958332	-2.5156469331	-1.6175698652
C	0.8423364515	2.2902263468	3.0027536052
H	0.3083655132	2.6104971305	3.8881801766
C	0.8169676371	0.9812682897	2.4435082027
H	0.2668718422	0.1348421435	2.8313176355
C	-0.6912708504	3.6041586998	-0.3622491356
H	-0.1260989907	4.4031252863	-0.824754421
C	1.6075375473	0.9871886963	1.243291719
C	-1.4632913091	3.7037204549	0.833187787
H	-1.5866578282	4.5923187258	1.439143602
C	4.1903320544	-3.5997844598	1.1836159036
H	4.2819526836	-4.6399129225	0.8835547242
C	-4.3557747412	-1.8459588303	-2.8274303332
H	-4.503313383	-2.8186402568	-3.2883213218
C	-1.9455567783	-1.5526955419	2.4557769404
H	-0.9661180272	-1.9370937172	2.1798298491
C	3.2081945195	-2.7994874119	0.6001624403
H	2.529505283	-3.2206629632	-0.1371741924
C	5.0389140946	-3.0723303254	2.1596918673
H	5.7976620544	-3.7004898289	2.6186711067
C	-4.4950545999	-0.6284823974	3.1138802964
H	-5.4931251658	-0.2781729934	3.3629246743
C	3.9282662222	-0.9315049081	1.9672880147
H	3.8211424038	0.1016147469	2.284750875

C	-4.9530869004	0.4871675318	-2.6121552014
H	-5.5701078913	1.33344312	-2.9025758034
C	-5.1601244487	-0.7647007976	-3.1947377045
H	-5.9403030015	-0.8948482406	-3.9399408442
C	4.9036764981	-1.7398262445	2.5541191785
H	5.5552784553	-1.3283187118	3.3204861747
C	-2.5181258294	-1.9014380232	3.6803848055
H	-1.9752181709	-2.5460159421	4.3660543457
C	-3.7907045465	-1.4346922445	4.0126079113
H	-4.2402875416	-1.7091446837	4.962986506
C	2.6105514184	0.22040217	-1.3355655127
C	3.9233905004	0.7124695538	-1.3119425136
H	4.4993315334	0.6760753492	-0.3914943805
C	1.8974494407	0.2291252343	-2.5424747717
H	0.8955249363	-0.1933438121	-2.5720656655
C	4.5006669704	1.2317958056	-2.4707953126
H	5.5190426787	1.6100434442	-2.4438860858
C	2.4755812391	0.7492258339	-3.7019513537
H	1.9152229985	0.7460497002	-4.6327359152
C	3.7753011405	1.2562384326	-3.6653879225
H	4.2290067289	1.6567710933	-4.5678255853

(dppf)NiNH$_2$



Zero-point correction= 0.544110 (Hartree/Particle)
Thermal correction to Energy= 0.580042
Thermal correction to Enthalpy= 0.580987
Thermal correction to Gibbs Free Energy= 0.472921
Sum of electronic and zero-point Energies= -4822.592883
Sum of electronic and thermal Energies= -4822.556950
Sum of electronic and thermal Enthalpies= -4822.556006
Sum of electronic and thermal Free Energies= -4822.664072

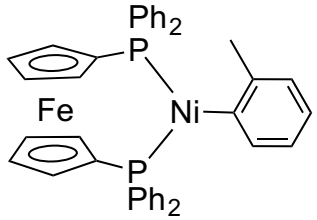
Single-point energy (6-311+G(2d,2p)) = -4823.854787

Fe	0.0000000	-0.0005320	2.5004300
Ni	0.0000530	0.0002590	-1.7647320
P	1.7647760	-0.0138870	-0.4058170
P	-1.7647070	0.0139480	-0.4058560
C	-1.6213210	0.5006720	1.3444540

C	2.0516280	0.1952810	2.5228050
H	2.5660640	1.1462230	2.5359430
C	-2.0516190	-0.1964600	2.5226760
H	-2.5659860	-1.1474450	2.5353870
C	1.6268660	-0.5472050	3.6632530
H	1.7650600	-0.2553990	4.6966910
C	-0.9294680	1.6821260	1.7811980
H	-0.4515180	2.4068910	1.1364120
C	-4.0545160	1.7100250	-0.1341820
H	-3.9283170	1.6299010	0.9416650
C	3.1641150	-1.0519490	-0.9954660
C	-3.1639240	1.0524400	-0.9950790
C	-2.4935980	-1.6736410	-0.2939420
C	-3.8060280	-1.9135190	0.1361070
H	-4.4509400	-1.0789140	0.3962440
C	-3.3202840	1.1881680	-2.3839850
H	-2.6015720	0.7110470	-3.0476420
C	0.9389270	-1.7096940	3.2045110
H	0.4637900	-2.4570070	3.8271120
C	0.9293900	-1.6829330	1.7805180
H	0.4514310	-2.4074090	1.1354140
C	-0.9390420	1.7082920	3.2052030
H	-0.4639690	2.4553800	3.8281240
C	1.6213110	-0.5013270	1.3442770
C	-1.6269280	0.5455750	3.6634440
H	-1.7651070	0.2533360	4.6967620
C	4.3699360	-1.9481480	-2.8995390
H	4.4853780	-2.0463700	-3.9757690
C	-4.3693540	1.9501040	-2.8987030
H	-4.4845450	2.0492040	-3.9748800
C	-1.6889770	-2.7595360	-0.6675300
H	-0.6846200	-2.5703840	-1.0405020
C	3.3207820	-1.1865870	-2.3844490
H	2.6022490	-0.7089380	-3.0479140
C	5.2585790	-2.5959240	-2.0378240
H	6.0697010	-3.1961580	-2.4416390
C	-4.2947840	-3.2182890	0.2153100
H	-5.3143310	-3.3934300	0.5484870
C	4.0544690	-1.7102680	-0.1348950
H	3.9280500	-1.6309570	0.9409860
C	-5.0959720	2.4809900	-0.6548040
H	-5.7787590	2.9911750	0.0197600
C	-5.2582360	2.5971300	-2.0366770
H	-6.0692930	3.1976470	-2.4402010
C	5.0959930	-2.4808920	-0.6558990
H	5.7785930	-2.9916600	0.0184120

C	-2.1763760	-4.0650910	-0.5855250
H	-1.5435530	-4.8979890	-0.8799830
C	-3.4788420	-4.2959060	-0.1393320
H	-3.8625200	-5.3108530	-0.0796630
C	2.4935030	1.6737190	-0.2931770
C	3.8058760	1.9134890	0.1371070
H	4.4508080	1.0788060	0.3969510
C	1.6888450	2.7597170	-0.6663810
H	0.6845470	2.5706510	-1.0395530
C	4.2945390	3.2182570	0.2169340
H	5.3140390	3.3933200	0.5502930
C	2.1761570	4.0652650	-0.5837640
H	1.5433210	4.8982550	-0.8779340
C	3.4785620	4.2959710	-0.1373290
H	3.8621620	5.3109190	-0.0771790
N	-0.0003690	0.0007630	-3.6070350
H	-0.1295400	-0.8124510	-4.2058590
H	0.1281690	0.8138250	-4.2061810

(dppf)Ni(*ortho*-tolyl)



Zero-point correction= 0.637487 (Hartree/Particle)
Thermal correction to Energy= 0.678105
Thermal correction to Enthalpy= 0.679049
Thermal correction to Gibbs Free Energy= 0.559696
Sum of electronic and zero-point Energies= -5037.502460
Sum of electronic and thermal Energies= -5037.461842
Sum of electronic and thermal Enthalpies= -5037.460898
Sum of electronic and thermal Free Energies= -5037.580250

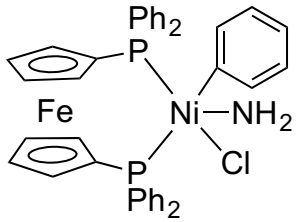
Single-point energy (6-311+G(2d,2p)) = -5038.925188

Fe	1.27047	-2.74143	0.0006
Ni	-0.28001	1.19839	-0.08791
P	-1.45018	-0.70243	0.0213
P	1.87093	0.59166	-0.04401
C	2.34976	-1.08888	-0.55155
C	-0.63007	-3.53723	-0.10854
H	-1.13119	-3.77605	-1.03621

C	3.20093	-2.03221	0.11651
H	3.7227	-1.85781	1.04732
C	0.21448	-4.40932	0.63807
H	0.46485	-5.42882	0.37309
C	1.81375	-1.74726	-1.71126
H	1.10778	-1.31954	-2.4093
C	4.04735	1.18893	-1.80135
H	4.32156	0.1398	-1.73987
C	-2.99223	-0.67376	1.0232
C	2.9297	1.6618	-1.09962
C	2.61608	0.75201	1.62973
C	4.	0.81163	1.84652
H	4.68226	0.78848	1.00141
C	2.57141	3.01471	-1.21015
H	1.68791	3.38056	-0.69113
C	0.718	-3.68677	1.75993
H	1.41571	-4.05983	2.49875
C	0.19315	-2.36376	1.70202
H	0.42056	-1.56145	2.39019
C	2.33073	-3.07319	-1.75236
H	2.08	-3.8274	-2.48721
C	-0.65146	-2.25897	0.54296
C	3.18233	-3.25132	-0.62191
H	3.69177	-4.16601	-0.34638
C	-5.11952	0.39981	1.48577
H	-5.85752	1.15757	1.23813
C	3.33172	3.8833	-1.99257
H	3.04496	4.92829	-2.07115
C	1.74796	0.82655	2.72798
H	0.6746	0.82014	2.55783
C	-3.96482	0.29255	0.71332
H	-3.81021	0.96992	-0.11915
C	-5.31855	-0.44765	2.57881
H	-6.21726	-0.35739	3.18312
C	4.50522	0.91694	3.14279
H	5.57929	0.96368	3.30138
C	-3.20036	-1.52486	2.11755
H	-2.46188	-2.27957	2.36847
C	4.80111	2.05904	-2.592
H	5.6635	1.68273	-3.13596
C	4.44741	3.40642	-2.68509
H	5.03432	4.08128	-3.30225
C	-4.35781	-1.4095	2.89198
H	-4.50663	-2.07615	3.73748
C	2.2535	0.93066	4.02494
H	1.57039	0.99068	4.86777

C	3.63307	0.97097	4.23357
H	4.02912	1.05697	5.24177
C	-2.06639	-1.11212	-1.6628
C	-3.1018	-2.03152	-1.88291
H	-3.58925	-2.50789	-1.03682
C	-1.47496	-0.47541	-2.76191
H	-0.69974	0.26742	-2.5884
C	-3.51906	-2.32555	-3.18145
H	-4.32322	-3.03877	-3.34163
C	-1.89053	-0.76984	-4.0615
H	-1.42673	-0.26581	-4.90508
C	-2.91067	-1.69887	-4.27245
H	-3.24053	-1.92563	-5.28271
C	-1.66872	2.56114	-0.20024
C	-2.19723	3.18409	0.96101
C	-2.20916	2.9731	-1.4357
C	-3.20373	4.15131	0.86265
C	-3.2145	3.94218	-1.53751
H	-1.85062	2.51241	-2.35632
C	-3.71764	4.53355	-0.37981
H	-3.59869	4.60932	1.7689
H	-3.60466	4.22734	-2.5129
H	-4.5035	5.2833	-0.43833
C	-1.68427	2.78351	2.32847
H	-1.7919	1.70145	2.48375
H	-0.61861	3.02198	2.44272
H	-2.22734	3.29157	3.13451

(dppf)Ni(Ph)(NH_2)Cl



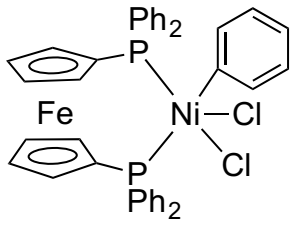
Zero-point correction= 0.614397 (Hartree/Particle)
Thermal correction to Energy= 0.656451
Thermal correction to Enthalpy= 0.657395
Thermal correction to Gibbs Free Energy= 0.537791
Sum of electronic and zero-point Energies= -5918.673472
Sum of electronic and thermal Energies= -5918.631418
Sum of electronic and thermal Enthalpies= -5918.630474
Sum of electronic and thermal Free Energies= -5918.750078

Single-point energy (6-311+G(2d,2p)) = -5515.828615

Fe	-0.5242160	-1.8099270	-2.2498530
C	1.3061440	-1.4087640	-1.4242770
C	1.2128600	-2.8019120	-1.7628980
C	0.9801300	-2.9055790	-3.1635820
C	0.9310690	-1.5863360	-3.7048420
C	1.1208520	-0.6614170	-2.6412500
C	-2.3408400	-1.9936430	-3.2046870
C	-2.2172590	-0.7003520	-2.6161800
C	-2.0484340	-0.8616990	-1.2010810
C	-2.0278200	-2.2764080	-0.9351200
C	-2.2270880	-2.9657610	-2.1664790
P	1.5218210	-0.6411980	0.2072850
P	-1.8918140	0.4660350	0.0432640
C	3.3332120	-0.5240420	0.4391480
C	1.0748370	-1.9768470	1.3860370
C	-2.9324230	-0.1718930	1.4403890
C	-3.0413050	1.7960090	-0.5234720
C	4.2517050	-1.0655450	-0.4664590
C	5.6229610	-0.9160730	-0.2445710
C	6.0784070	-0.2259610	0.8788500
C	5.1614400	0.3152800	1.7846840
C	3.7933160	0.1700200	1.5689720
C	-0.0326130	-1.8243770	2.2246580
C	-0.4154770	-2.8511790	3.0903370
C	0.3193950	-4.0355170	3.1353690
C	1.4521610	-4.1817340	2.3283490
C	1.8337940	-3.1562080	1.4642060
C	-2.7559590	0.3689610	2.7222330
C	-3.5825410	-0.0288910	3.7748910
C	-4.5999200	-0.9591520	3.5614400
C	-4.7960280	-1.4836450	2.2822650
C	-3.9733290	-1.0894460	1.2271740
C	-4.1623940	1.5619890	-1.3313180
C	-5.0445470	2.6016800	-1.6293630
C	-4.8248830	3.8802950	-1.1126250
C	-3.7200130	4.1168110	-0.2931380
C	-2.8310510	3.0819850	0.0002410
H	1.2590710	-3.6253790	-1.0651020
H	0.8182790	-3.8257350	-3.7107970
H	0.7208890	-1.3292480	-4.7352050
H	1.0276570	0.4140950	-2.7023760
H	-2.4523740	-2.1988420	-4.2616700
H	-2.2197040	0.2438480	-3.1430230
H	-1.8782730	-2.7317640	0.0339890
H	-2.2385180	-4.0405350	-2.2945280

H	3.9008150	-1.5887490	-1.3509760
H	6.3322530	-1.3354050	-0.9533200
H	7.1451390	-0.1037470	1.0464040
H	5.5121900	0.8644390	2.6538560
H	3.0788880	0.6156330	2.2556390
H	-0.5700240	-0.8888960	2.2327400
H	-1.2793790	-2.7097640	3.7336450
H	0.0268220	-4.8354670	3.8102330
H	2.0449160	-5.0911630	2.3797350
H	2.7307310	-3.2669270	0.8619570
H	-1.9564720	1.0791620	2.9008970
H	-3.4235180	0.3920590	4.7638870
H	-5.2403820	-1.2694970	4.3826820
H	-5.5935630	-2.1993540	2.1007510
H	-4.1477550	-1.5028010	0.2404760
H	-4.3529130	0.5698520	-1.7267570
H	-5.9068140	2.4096160	-2.2622400
H	-5.5136290	4.6874790	-1.3461770
H	-3.5434730	5.1075520	0.1160080
H	-1.9683150	3.2720870	0.6330960
Ni	0.3877020	1.4329760	0.1038910
C	2.0500900	2.4423220	-0.0933130
C	2.3636700	3.4629340	0.8073110
C	2.9192750	2.1738870	-1.1539540
C	3.5653330	4.1672740	0.6710090
H	1.6949060	3.6978790	1.6252750
C	4.1249470	2.8721220	-1.2777180
H	2.6875980	1.4081800	-1.8854470
C	4.4552510	3.8696630	-0.3612770
H	3.7996070	4.9537440	1.3849510
H	4.8014510	2.6263500	-2.0927960
H	5.3913750	4.4138230	-0.4550000
N	-0.0542420	2.2714050	-1.4883570
H	-1.0139850	2.5867880	-1.6064650
H	0.5665580	2.9865210	-1.8553970
Cl	0.3648190	1.6766740	2.4505170

(dppf)Ni(Ph)Cl$_2$



Zero-point correction= 0.614397 (Hartree/Particle)

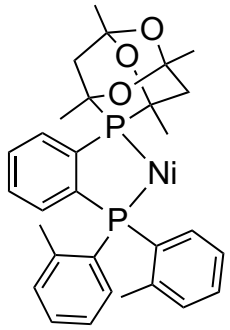
Thermal correction to Energy= 0.656450
Thermal correction to Enthalpy= 0.657395
Thermal correction to Gibbs Free Energy= 0.537791
Sum of electronic and zero-point Energies= -5918.673472
Sum of electronic and thermal Energies= -5918.631418
Sum of electronic and thermal Enthalpies= -5918.630474
Sum of electronic and thermal Free Energies= -5918.750078

Single-point energy (6-311+G(2d,2p)) = -5920.124913

Fe	-0.5327	-1.79762	-2.28843
C	1.30494	-1.48827	-1.44052
C	1.10959	-2.88768	-1.70974
C	0.90395	-3.04394	-3.10904
C	0.97373	-1.75488	-3.71633
C	1.21588	-0.79373	-2.6976
C	-2.32452	-1.79293	-3.31026
C	-2.1534	-0.55518	-2.6256
C	-2.04319	-0.82774	-1.22257
C	-2.10566	-2.25679	-1.05938
C	-2.29954	-2.84352	-2.34427
P	1.5383	-0.69553	0.17013
P	-1.90198	0.41383	0.10808
C	3.34914	-0.57434	0.39724
C	1.10755	-2.02087	1.3666
C	-2.9463	-0.30766	1.46269
C	-3.02861	1.78595	-0.37297
C	4.25957	-1.06377	-0.54496
C	5.63241	-0.92178	-0.32703
C	6.09575	-0.29297	0.82856
C	5.18576	0.19344	1.7721
C	3.81677	0.05612	1.56046
C	-0.024	-1.91424	2.17751
C	-0.37729	-2.94838	3.04651
C	0.41099	-4.09603	3.12083
C	1.56398	-4.19868	2.33621
C	1.91594	-3.16578	1.46857
C	-2.76974	0.16692	2.77128
C	-3.59444	-0.28204	3.80429
C	-4.61315	-1.19944	3.54523
C	-4.81194	-1.65655	2.24114
C	-3.98993	-1.21059	1.20596
C	-4.17926	1.58282	-1.1436
C	-5.04827	2.64474	-1.39946
C	-4.78185	3.91107	-0.87591
C	-3.6427	4.11386	-0.09448

C	-2.76759	3.05749	0.15416
H	1.07827	-3.67428	-0.97003
H	0.68324	-3.97548	-3.61454
H	0.81419	-1.53484	-4.76405
H	1.25032	0.27731	-2.82988
H	-2.41067	-1.91483	-4.38238
H	-2.08839	0.42684	-3.07183
H	-2.01499	-2.78904	-0.12274
H	-2.36448	-3.90393	-2.55192
H	3.90151	-1.54099	-1.45218
H	6.33629	-1.29965	-1.06369
H	7.16349	-0.17657	0.99305
H	5.54305	0.69335	2.6678
H	3.10854	0.46042	2.27826
H	-0.61002	-1.01034	2.16209
H	-1.26106	-2.8399	3.66871
H	0.14214	-4.90146	3.79888
H	2.19542	-5.08022	2.40641
H	2.82445	-3.24539	0.87933
H	-1.97563	0.87298	2.98525
H	-3.4356	0.09016	4.81269
H	-5.25345	-1.54967	4.35031
H	-5.61248	-2.35888	2.02408
H	-4.17082	-1.56904	0.19932
H	-4.39953	0.60081	-1.55
H	-5.93446	2.47973	-2.00642
H	-5.45898	4.73669	-1.07685
H	-3.42599	5.09744	0.31249
H	-1.87463	3.22645	0.74885
Ni	0.39111	1.36462	0.25762
C	2.05	2.42254	0.09363
C	2.2729	3.47026	0.98436
C	2.95201	2.17795	-0.94124
C	3.43744	4.24097	0.8611
H	1.5755	3.68499	1.78297
C	4.11726	2.94017	-1.04628
H	2.76607	1.40644	-1.6776
C	4.36702	3.97264	-0.14092
H	3.60825	5.05025	1.56711
H	4.82012	2.72662	-1.84764
H	5.27236	4.56792	-0.22441
Cl	0.37314	1.54288	2.52955
Cl	-0.11931	2.21508	-1.7517

(PAd-DalPhos)Ni$^{(0)}$



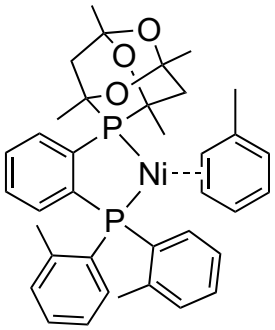
Zero-point correction= 0.575791 (Hartree/Particle)
Thermal correction to Energy= 0.610190
Thermal correction to Enthalpy= 0.611135
Thermal correction to Gibbs Free Energy= 0.511577
Sum of electronic and zero-point Energies= -3579.792858
Sum of electronic and thermal Energies= -3579.758458
Sum of electronic and thermal Enthalpies= -3579.757514
Sum of electronic and thermal Free Energies= -3579.857072

Single-point energy (6-311+G(2d,2p)) = -3581.014408

Ni	0.2736600	0.0216600	-1.7063280
P	-1.3529430	-0.3304910	-0.4509620
P	1.8321280	0.0372710	-0.3084960
C	-0.4498920	-1.0078010	1.0383950
C	0.9607650	-0.8490810	1.0821130
C	-2.9342590	-1.3828100	-0.6143610
C	-2.3393040	1.1896970	0.1496360
C	2.2610960	1.6849250	0.4024540
C	3.4504660	-0.8507400	-0.3731610
O	-3.7491340	-1.4000760	0.5835440
O	-3.2032180	1.5599520	-0.9505150
C	1.6867600	-1.4089360	2.1414400
C	-1.0747250	-1.7299580	2.0687210
C	-3.2117060	0.8605470	1.3629260
C	-3.7415460	-0.7010410	-1.7298720
C	-2.6159360	-2.8337800	-0.9378860
C	-1.4273240	2.3784700	0.3899740
C	2.7385640	2.7007330	-0.4619250
C	2.0374620	1.9846380	1.7545440
C	3.4946940	-2.1513530	-0.9338420
C	4.6419580	-0.2421710	0.0484790
H	2.7670820	-1.2971540	2.1624670
C	1.0478730	-2.1197730	3.1575040
C	-0.3359530	-2.2813080	3.1169600

H	-2.1468210	-1.8816370	2.0358830
C	-4.3076410	-0.1451730	0.9809060
H	-2.6026900	0.4705590	2.1830810
H	-3.7015860	1.7792780	1.7080240
H	-4.5995020	-1.3338000	-1.9871860
H	-3.1237860	-0.5651020	-2.6228660
C	-4.2708140	0.6582610	-1.2466000
H	-3.5461560	-3.3962710	-1.0801180
H	-2.0471380	-3.3038820	-0.1302720
H	-2.0224080	-2.8907960	-1.8563210
H	-2.0277120	3.2610230	0.6411710
H	-0.8363770	2.5936040	-0.5053020
H	-0.7353330	2.1766150	1.2127580
C	2.9799160	3.9728650	0.0700040
C	2.2797130	3.2607910	2.2633390
H	1.6658970	1.2126360	2.4194950
C	2.9919760	2.4522520	-1.9294770
C	4.7353340	-2.7889610	-1.0431540
H	4.6094780	0.7539110	0.4788370
C	2.2493650	-2.8667520	-1.4005130
C	5.8693590	-0.8941250	-0.0755900
O	-5.0687950	0.4236490	-0.0832760
H	1.6296610	-2.5497350	3.9685090
H	-0.8451220	-2.8440520	3.8951070
C	-5.2716150	-0.4462850	2.1109220
C	-5.1512580	1.3577420	-2.2619710
H	3.3484260	4.7542800	-0.5904390
C	2.7541560	4.2602860	1.4162980
H	2.0981430	3.4680840	3.3145200
H	3.7625780	1.6883460	-2.0876560
H	3.3195840	3.3699460	-2.4279170
H	2.0839570	2.0882380	-2.4298870
H	4.7741320	-3.7877800	-1.4719710
H	1.6444860	-2.2298990	-2.0624390
H	1.5988970	-3.1386860	-0.5600420
H	2.5057080	-3.7846980	-1.9388830
C	5.9157950	-2.1747780	-0.6228860
H	6.7796700	-0.4026430	0.2574300
H	-6.0311520	-1.1511440	1.7628840
H	-5.7611810	0.4745460	2.4393620
H	-4.7346500	-0.8878300	2.9558490
H	-5.5134950	2.2991910	-1.8409050
H	-6.0070660	0.7259460	-2.5150770
H	-4.5771580	1.5696800	-3.1684840
H	2.9466210	5.2596230	1.7972710
H	6.8642630	-2.6950740	-0.7261260

(PAd-DalPhos)Ni(η^2-PhCH$_3$)



Zero-point correction= 0.706137 (Hartree/Particle)
Thermal correction to Energy= 0.747644
Thermal correction to Enthalpy= 0.748588
Thermal correction to Gibbs Free Energy= 0.635228
Sum of electronic and zero-point Energies= -3851.279479
Sum of electronic and thermal Energies= -3851.237972
Sum of electronic and thermal Enthalpies= -3851.237028
Sum of electronic and thermal Free Energies= -3851.350388

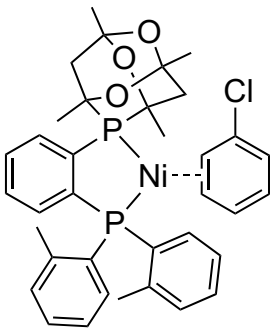
Single-point energy (6-311+G(2d,2p)) = -3852.724250

Ni	0.2485680	1.3144450	-0.1226080
P	-1.3183510	-0.1641440	-0.3719960
P	1.7422370	-0.2848330	0.0624600
C	-0.4497540	-1.6581750	-1.0466450
C	0.9531460	-1.6733340	-0.8846580
C	-2.9111240	-0.0086440	-1.3965440
C	-2.2791880	-0.7311550	1.1781100
C	2.1657700	-1.1110690	1.6735530
C	3.3809590	-0.1559260	-0.7889950
O	-3.7113110	-1.2169480	-1.3899580
O	-3.1485790	0.3638850	1.5393830
C	1.7093060	-2.7047440	-1.4567760
C	-1.0577350	-2.6920980	-1.7790980
C	-3.1406260	-1.9599220	0.8761410
C	-3.7201210	1.1040090	-0.7183430
C	-2.6131440	0.3055820	-2.8543170
C	-1.3576720	-0.9374530	2.3653590
C	2.6415260	-0.3397640	2.7612120
C	1.9411610	-2.4837440	1.8674930
C	3.4362350	0.2907880	-2.1327970
C	4.5788870	-0.4129030	-0.1053920
H	2.7891670	-2.7033780	-1.3382880
C	1.0935140	-3.7202540	-2.1868920
C	-0.2930380	-3.7119400	-2.3458030

H	-2.1308440	-2.6809070	-1.9260060
C	-4.2522570	-1.6040160	-0.1227010
H	-2.5271030	-2.7792940	0.4913110
H	-3.6165320	-2.2961000	1.8054300
H	-4.5856190	1.3466500	-1.3472270
H	-3.1107120	2.0008480	-0.5925530
C	-4.2315240	0.6336680	0.6481070
H	-3.5522720	0.4355950	-3.4047130
H	-2.0437570	-0.5000020	-3.3271040
H	-2.0296020	1.2288380	-2.9234820
H	-1.9553560	-1.1591710	3.2573880
H	-0.7667760	-0.0360790	2.5516210
H	-0.6706940	-1.7688650	2.1870980
C	2.8738410	-0.9719350	3.9890870
C	2.1739900	-3.0947400	3.0995450
H	1.5719600	-3.0895700	1.0487740
C	2.9157350	1.1363940	2.6324490
C	4.6909310	0.4799270	-2.7239410
H	4.5438120	-0.7785690	0.9154850
C	2.1959700	0.5315330	-2.9614380
C	5.8188830	-0.2168780	-0.7137420
O	-5.0192590	-0.5428180	0.4422230
H	1.6931850	-4.5096070	-2.6322750
H	-0.7820060	-4.4945840	-2.9200310
C	-5.2047140	-2.7499520	-0.3989710
C	-5.1106720	1.6522610	1.3437080
H	3.2393620	-0.3749420	4.8212550
C	2.6428880	-2.3346940	4.1685950
H	1.9866210	-4.1585950	3.2177950
H	3.7828660	1.3320300	1.9894290
H	3.1174420	1.5846370	3.6103620
H	2.0620600	1.6481930	2.1819690
H	4.7347140	0.8272670	-3.7538250
H	1.3960290	0.9989170	-2.3742440
H	1.7872590	-0.4108670	-3.3470450
H	2.4202780	1.1746320	-3.8187650
C	5.8758620	0.2370780	-2.0297290
H	6.7311070	-0.4219760	-0.1598510
H	-5.9758780	-2.4206710	-1.1002190
H	-5.6806120	-3.0720500	0.5312280
H	-4.6619020	-3.5940960	-0.8349280
H	-5.4580800	1.2436060	2.2962290
H	-5.9760130	1.8904240	0.7190700
H	-4.5374260	2.5641290	1.5327020
H	2.8261600	-2.7951390	5.1356280
H	6.8338580	0.3994120	-2.5162320

C	-0.0529700	3.1659680	-1.0974530
C	0.9598480	3.1985310	-0.0735920
C	0.4788080	3.5412590	1.2363460
C	-0.8246480	3.9452410	1.4669950
C	-1.7341220	4.1096740	0.3937160
C	-1.3425460	3.7255310	-0.8711300
H	0.2601890	3.0273590	-2.1314500
H	1.1862120	3.5542850	2.0620600
H	-1.1326290	4.1991070	2.4780970
H	-2.7239170	4.5196960	0.5731180
H	-2.0176890	3.8403110	-1.7165950
C	2.4250560	3.3832520	-0.4115660
H	3.0732090	3.0014860	0.3829790
H	2.6583400	4.4504300	-0.5435670
H	2.6978350	2.8697380	-1.3370800

(PAd-DalPhos)Ni(η^2-PhCl)



Zero-point correction= 0.668556 (Hartree/Particle)
Thermal correction to Energy= 0.709736
Thermal correction to Enthalpy= 0.710680
Thermal correction to Gibbs Free Energy= 0.597119
Sum of electronic and zero-point Energies= -4271.600069
Sum of electronic and thermal Energies= -4271.558889
Sum of electronic and thermal Enthalpies= -4271.557944
Sum of electronic and thermal Free Energies= -4271.671505

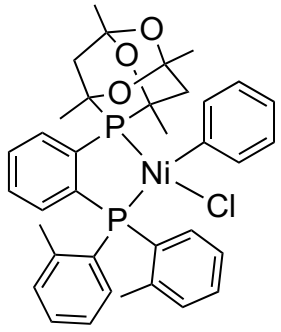
Single-point energy (6-311+G(2d,2p)) = -4273.022227

Ni	0.2392290	1.2183100	-0.1290980
P	-1.3972010	-0.2076750	-0.3846030
P	1.6453790	-0.4821740	0.0860850
C	-0.6002800	-1.7368190	-1.0534130
C	0.7977950	-1.8239080	-0.8734540
C	-2.9638270	0.0622000	-1.4161100
C	-2.3917690	-0.7153080	1.1608690

C	1.9950430	-1.3097850	1.7073850
C	3.2992000	-0.4157120	-0.7288600
O	-3.8352010	-1.0936390	-1.4181030
O	-3.1869980	0.4329270	1.5221790
C	1.5065760	-2.8902790	-1.4417890
C	-1.2544320	-2.7346050	-1.7955730
C	-3.3291070	-1.8843850	0.8473750
C	-3.7013750	1.2213040	-0.7332430
C	-2.6365760	0.3645200	-2.8701150
C	-1.4878060	-0.9876000	2.3485510
C	2.4269320	-0.5303070	2.8054940
C	1.7960520	-2.6873790	1.8845160
C	3.3995550	0.0196920	-2.0720570
C	4.4658530	-0.7205130	-0.0135110
H	2.5843710	-2.9413780	-1.3163140
C	0.8461630	-3.8707310	-2.1808740
C	-0.5365120	-3.7914240	-2.3552580
H	-2.3238020	-2.6660910	-1.9553170
C	-4.4094060	-1.4510280	-0.1550950
H	-2.7677760	-2.7400470	0.4617320
H	-3.8304330	-2.1931700	1.7725610
H	-4.5458630	1.5236560	-1.3643830
H	-3.0363400	2.0764490	-0.5983990
C	-4.2482270	0.7769990	0.6282640
H	-3.5622320	0.5564910	-3.4247640
H	-2.1164530	-0.4728370	-3.3442710
H	-1.9958070	1.2496490	-2.9317300
H	-2.1011020	-1.1811040	3.2362940
H	-0.8456730	-0.1247920	2.5470700
H	-0.8509180	-1.8570230	2.1648250
C	2.6540620	-1.1652820	4.0326160
C	2.0166140	-3.2997200	3.1184120
H	1.4585330	-3.2950310	1.0533220
C	2.6236330	0.9596930	2.6957470
C	4.6734190	0.1372840	-2.6389080
H	4.3921390	-1.0630830	1.0131290
C	2.1907340	0.3367890	-2.9187200
C	5.7258910	-0.5913770	-0.5975830
O	-5.1079190	-0.3450740	0.4114770
H	1.4092410	-4.6879880	-2.6233590
H	-1.0577790	-4.5467320	-2.9373810
C	-5.4328450	-2.5303740	-0.4443260
C	-5.0609180	1.8469420	1.3269270
H	2.9914150	-0.5662440	4.8749420
C	2.4505930	-2.5345800	4.1985740
H	1.8507240	-4.3678950	3.2285150

H	3.2923320	1.2379010	1.8736620
H	3.0398580	1.3663680	3.6228380
H	1.6669800	1.4546790	2.5030420
H	4.7559540	0.4789750	-3.6679180
H	1.4363480	0.8938810	-2.3515080
H	1.7055530	-0.5766310	-3.2849050
H	2.4753330	0.9397970	-3.7862380
C	5.8299240	-0.1578990	-1.9173210
H	6.6158660	-0.8289460	-0.0213120
H	-6.1765060	-2.1470090	-1.1477060
H	-5.9345030	-2.8261630	0.4810180
H	-4.9438380	-3.4055540	-0.8826230
H	-5.4371070	1.4568140	2.2762270
H	-5.9069810	2.1441490	0.7012420
H	-4.4296910	2.7183510	1.5222440
H	2.6290260	-2.9970630	5.1655420
H	6.8042990	-0.0469190	-2.3853450
C	-0.0844330	3.0398720	-0.9930530
C	1.0291370	2.9946540	-0.0703830
C	0.8205050	3.5581430	1.2355880
C	-0.3826070	4.1327010	1.5794910
C	-1.4220090	4.2918510	0.6228620
C	-1.2545130	3.7848950	-0.6432460
H	0.1075690	2.8681180	-2.0505270
H	1.6495830	3.5676060	1.9348720
H	-0.5118800	4.5300000	2.5830320
H	-2.3210570	4.8408340	0.8878690
H	-2.0033750	3.9645430	-1.4116960
Cl	2.7263320	3.1619790	-0.7134630

(PAd-DalPhos)Ni(Ph)Cl



Zero-point correction= 0.669717 (Hartree/Particle)
Thermal correction to Energy= 0.710944
Thermal correction to Enthalpy= 0.711888
Thermal correction to Gibbs Free Energy= 0.598366

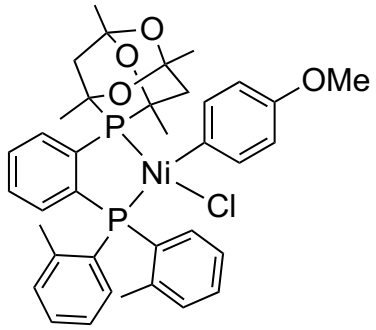
Sum of electronic and zero-point Energies= -4271.640752
Sum of electronic and thermal Energies= -4271.599524
Sum of electronic and thermal Enthalpies= -4271.598580
Sum of electronic and thermal Free Energies= -4271.712102

Single-point energy (6-311+G(2d,2p)) = -4273.065005

Ni	0.2294730	1.3238010	-0.0238930
Cl	1.5796940	3.0840710	-0.0861570
P	-1.0733230	-0.4083730	-0.3699090
P	1.9523770	-0.1514150	0.0447110
C	-1.2222190	2.5557740	0.0584700
C	-1.6089680	3.3445740	-1.0342010
C	-1.8751380	2.7528450	1.2828260
C	-0.0040300	-1.7062170	-1.1656490
C	1.3867900	-1.5651200	-0.9803140
C	-2.6618430	-0.3610970	-1.4214430
C	-1.9688990	-1.2172520	1.1124110
C	2.3412400	-0.9214100	1.6775040
C	3.5723840	0.3115180	-0.6720770
C	-2.6428770	4.2784630	-0.9182310
C	-2.8971920	3.7012700	1.4086680
H	-1.6053140	2.1555960	2.1503380
O	-3.2103740	-1.6957620	-1.5369910
O	-3.0126300	-0.3117460	1.5055660
C	2.2772150	-2.4468400	-1.6054010
C	-0.4687010	-2.7533590	-1.9804740
C	-2.5947470	-2.5460570	0.6788920
C	-3.6975320	0.5035730	-0.6978570
C	-2.3807440	0.1263060	-2.8336650
C	-1.0606040	-1.3626890	2.3189290
C	2.3935550	-0.1310480	2.8499620
C	2.5455330	-2.3073280	1.7682090
C	3.6411600	0.8278800	-1.9884630
C	4.7359330	0.2031820	0.1007460
H	-2.9283450	4.8770590	-1.7806590
C	-3.2955070	4.4577980	0.3045530
H	-3.3829370	3.8440830	2.3719100
H	3.3464390	-2.3076240	-1.4735640
C	1.8014680	-3.4771180	-2.4138050
C	0.4264760	-3.6267790	-2.5981190
H	-1.5302320	-2.8646470	-2.1550530
C	-3.7207880	-2.2938350	-0.3343420
H	-1.8395380	-3.2186360	0.2638730
H	-3.0341990	-3.0276940	1.5602470
H	-4.5794460	0.5797400	-1.3447340
H	-3.3169420	1.5041600	-0.5075090

C	-4.1244870	-0.1653930	0.6108310
H	-3.3100460	0.1113800	-3.4139690
H	-1.6462690	-0.5068600	-3.3397720
H	-2.0019810	1.1515100	-2.8009000
H	-1.6434290	-1.7493710	3.1625180
H	-0.6372540	-0.3959990	2.6032060
H	-0.2392260	-2.0535700	2.1117310
C	2.6497300	-0.7737440	4.0689760
C	2.7948670	-2.9244460	2.9929440
H	2.5007190	-2.9189400	0.8745980
C	2.1774250	1.3604280	2.8405080
C	4.8954130	1.2087080	-2.4771210
H	4.6763510	-0.1880490	1.1107810
C	2.4273640	0.9749760	-2.8737050
H	-4.0954480	5.1876010	0.3982910
C	5.9733920	0.5976420	-0.4078130
O	-4.6759000	-1.4463680	0.2884900
H	2.4988370	-4.1512190	-2.9032220
H	0.0443890	-4.4184360	-3.2367860
C	-4.4420270	-3.5552020	-0.7642330
C	-5.1817490	0.6095830	1.3662640
H	2.6911960	-0.1719820	4.9732230
C	2.8452930	-2.1510480	4.1510840
H	2.9467950	-3.9992400	3.0367960
H	2.8353820	1.8778270	2.1361160
H	2.3446840	1.7791700	3.8374340
H	1.1581220	1.6214300	2.5320450
H	4.9605960	1.6110520	-3.4848430
H	1.6420440	1.5454410	-2.3658760
H	2.0091530	0.0024910	-3.1598940
H	2.6872520	1.5096150	-3.7921970
C	6.0514800	1.1015320	-1.7037050
H	6.8640110	0.5121150	0.2082060
H	-5.2358620	-3.2970750	-1.4697310
H	-4.8839940	-4.0455680	0.1072830
H	-3.7437670	-4.2453240	-1.2473630
H	-5.4419970	0.0744570	2.2833510
H	-6.0764850	0.7141620	0.7463670
H	-4.7988800	1.6015390	1.6167340
H	3.0358650	-2.6151860	5.1149060
H	7.0072200	1.4165350	-2.1136260
H	-1.0840820	3.2502400	-1.9820930

(PAd-DalPhos)Ni(*p*-OMePh)Cl



Zero-point correction= 0.702510 (Hartree/Particle)
Thermal correction to Energy= 0.746362
Thermal correction to Enthalpy= 0.747307
Thermal correction to Gibbs Free Energy= 0.627584
Sum of electronic and zero-point Energies= -4386.136079
Sum of electronic and thermal Energies= -4386.092227
Sum of electronic and thermal Enthalpies= -4386.091282
Sum of electronic and thermal Free Energies= -4386.211005

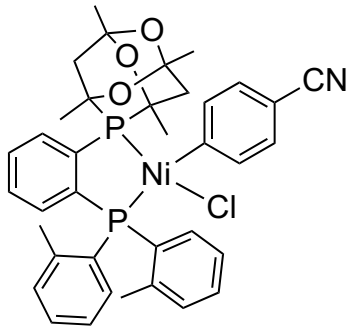
Single-point energy (6-311+G(2d,2p)) = -4387.629963

Ni	-0.1128100	-1.1471060	-0.0223890
Cl	-0.9145180	-3.2161850	-0.1055560
P	0.6514040	0.8804160	-0.3682240
P	-2.1794060	-0.2167220	0.0423250
C	1.6311850	-1.9126970	0.0806090
C	2.2345020	-2.5824660	-0.9870600
C	2.3118130	-1.9030380	1.3082170
C	-0.7384620	1.8255880	-1.1667780
C	-2.0339880	1.3006850	-0.9800310
C	2.1886090	1.2732740	-1.4237030
C	1.2873220	1.9156240	1.1072880
C	-2.7640200	0.4094840	1.6780130
C	-3.6066420	-1.1126260	-0.6736850
C	3.4900680	-3.1931570	-0.8639880
C	3.5527830	-2.5223510	1.4575480
H	1.8860730	-1.3930940	2.1686190
O	2.3408090	2.7073270	-1.5481800
O	2.5437640	1.3416380	1.5018200
C	-3.1364910	1.8974380	-1.6040480
C	-0.5865870	2.9595610	-1.9837410
C	1.5155220	3.3641920	0.6657150
C	3.4267690	0.7383160	-0.6991610
C	2.0521920	0.7177160	-2.8321090
C	0.3756570	1.8072630	2.3153130

C	-2.5852280	-0.3648150	2.8486890
C	-3.3524330	1.6805170	1.7724800
C	-3.5310400	-1.6244730	-1.9914920
C	-4.7522500	-1.3362400	0.1011570
H	3.9206430	-3.7008630	-1.7202260
C	4.1540610	-3.1604310	0.3663370
H	4.0705610	-2.5214410	2.4128170
H	-4.1237010	1.4641400	-1.4711880
C	-2.9692480	3.0190420	-2.4135690
C	-1.6912220	3.5468600	-2.6006410
H	0.4011760	3.3627570	-2.1608660
C	2.6652700	3.4317430	-0.3501410
H	0.6015610	3.7969960	0.2507760
H	1.8049530	3.9537020	1.5435420
H	4.2934940	0.9094740	-1.3484370
H	3.3417300	-0.3276100	-0.5024420
C	3.6512710	1.5076140	0.6049060
H	2.9410460	0.9836410	-3.4150800
H	1.1714850	1.1209180	-3.3403400
H	1.9692910	-0.3719020	-2.7915120
H	0.8266300	2.3474300	3.1553570
H	0.2409190	0.7623940	2.6062940
H	-0.6070840	2.2378670	2.1058610
C	-3.0080590	0.1774520	4.0701020
C	-3.7616740	2.2000560	2.9994990
H	-3.4862060	2.2808540	0.8800420
C	-1.9552180	-1.7338870	2.8346470
C	-4.6297650	-2.3397410	-2.4794900
H	-4.8021840	-0.9464400	1.1122670
C	-2.3261290	-1.4245850	-2.8785840
C	-5.8310380	-2.0599830	-0.4067730
O	3.8206450	2.8899810	0.2736100
H	-3.8280740	3.4706770	-2.9021570
H	-1.5466800	4.4128290	-3.2408200
C	3.0028840	4.8422060	-0.7891550
C	4.8844110	1.0650550	1.3614200
H	-2.8734560	-0.4123540	4.9731550
C	-3.5859350	1.4426370	4.1559950
H	-4.2119140	3.1876130	3.0464610
H	-2.4421240	-2.4155060	2.1310190
H	-1.9929170	-2.1844010	3.8310350
H	-0.9048330	-1.6945940	2.5223400
H	-4.5820160	-2.7417740	-3.4883240
H	-1.4121110	-1.7548750	-2.3730620
H	-2.1962610	-0.3733430	-3.1623620
H	-2.4285280	-2.0080520	-3.7984530

C	-5.7679310	-2.5622650	-1.7040950
H	-6.7086220	-2.2286740	0.2107960
H	3.8360290	4.8128830	-1.4959450
H	3.2911560	5.4420010	0.0782940
H	2.1382420	5.3059680	-1.2735040
H	4.9882190	1.6612640	2.2718900
H	5.7713980	1.2068250	0.7377950
H	4.7939130	0.0085690	1.6240480
H	-3.8963360	1.8325350	5.1215650
H	-6.5982980	-3.1310300	-2.1136220
H	1.7169660	-2.6601240	-1.9403870
O	5.3883460	-3.7229920	0.6019650
C	6.0125990	-4.4186140	-0.4638050
H	6.2137390	-3.7536760	-1.3146980
H	6.9576290	-4.7921730	-0.0659280
H	5.4001640	-5.2640400	-0.8038300

(PAd-DalPhos)Ni(*p*-CNPh)Cl



Zero-point correction= 0.668288 (Hartree/Particle)
Thermal correction to Energy= 0.711405
Thermal correction to Enthalpy= 0.712349
Thermal correction to Gibbs Free Energy= 0.594046
Sum of electronic and zero-point Energies= -4363.896229
Sum of electronic and thermal Energies= -4363.853113
Sum of electronic and thermal Enthalpies= -4363.852169
Sum of electronic and thermal Free Energies= -4363.970471

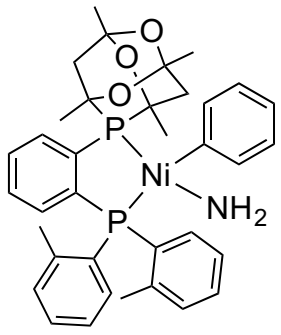
Single-point energy (6-311+G(2d,2p)) = -4365.341341

Ni	0.1238030	1.1804420	-0.0798950
Cl	1.0365690	3.1967400	-0.1765050
P	-0.7458930	-0.8170960	-0.3741500
P	2.1335600	0.1379820	0.0521940
C	-1.5575380	2.0691240	-0.0472090
C	-2.0946290	2.7212950	-1.1699250

C	-2.2545320	2.1657940	1.1683100
C	0.6012690	-1.8620890	-1.1131000
C	1.9194390	-1.3963310	-0.9305760
C	-2.2863530	-1.1634380	-1.4412820
C	-1.4650560	-1.7414750	1.1349390
C	2.6553620	-0.4748170	1.7135070
C	3.6132810	0.9417880	-0.6636560
C	-3.3028240	3.4086570	-1.1009850
C	-3.4556350	2.8655440	1.2614820
H	-1.8717170	1.6751520	2.0587740
O	-2.5194110	-2.5890990	-1.5027530
O	-2.6893810	-1.0714560	1.4761600
C	2.9963190	-2.0695450	-1.5200870
C	0.3989540	-3.0184680	-1.8863590
C	-1.7722820	-3.1924180	0.7535570
C	-3.5022110	-0.5236440	-0.7648060
C	-2.0948480	-0.6828830	-2.8710380
C	-0.5700970	-1.6316210	2.3551340
C	2.5231860	0.3454120	2.8588210
C	3.1498770	-1.7815860	1.8516420
C	3.5832880	1.4227560	-1.9947890
C	4.7580550	1.1234000	0.1235160
H	-3.7103830	3.9010620	-1.9790800
C	-3.9990970	3.4787700	0.1193400
H	-3.9817050	2.9353480	2.2093460
H	4.0029880	-1.6823880	-1.3909130
C	2.7795480	-3.2109870	-2.2893430
C	1.4785820	-3.6826650	-2.4686530
H	-0.6060370	-3.3793040	-2.0581550
C	-2.9072810	-3.2381650	-0.2796030
H	-0.8786450	-3.6957080	0.3751500
H	-2.1097200	-3.7241920	1.6507470
H	-4.3671330	-0.6711690	-1.4218840
H	-3.3586200	0.5435820	-0.6155170
C	-3.7927440	-1.2171700	0.5685300
H	-2.9882010	-0.9244050	-3.4573730
H	-1.2313370	-1.1593520	-3.3437950
H	-1.9493980	0.4009720	-2.8818330
H	-1.0692100	-2.1030030	3.2091090
H	-0.3768400	-0.5842470	2.6010030
H	0.3878260	-2.1304570	2.1869820
C	2.8943500	-0.1890240	4.1002290
C	3.5092030	-2.2918790	3.0979550
H	3.2490690	-2.4166890	0.9791430
C	1.9963400	1.7560040	2.7981440
C	4.7249740	2.0670980	-2.4828860

H	4.7733280	0.7565120	1.1442560
C	2.3832340	1.2618470	-2.8963260
C	5.8805840	1.7761400	-0.3854760
O	-4.0370000	-2.5994950	0.2974990
H	3.6186580	-3.7226870	-2.7520900
H	1.2969350	-4.5647430	-3.0763850
C	-3.3231810	-4.6438330	-0.6621350
C	-5.0098050	-0.6705600	1.2820240
H	2.7953270	0.4360310	4.9838850
C	3.3778630	-1.4895600	4.2297570
H	3.8869470	-3.3071620	3.1787290
H	2.5380370	2.3778840	2.0794000
H	2.0607160	2.2328620	3.7806660
H	0.9481960	1.7848980	2.4780410
H	4.7132710	2.4453130	-3.5018500
H	1.4790130	1.6507100	-2.4154390
H	2.2041630	0.2116480	-3.1562160
H	2.5289890	1.8155730	-3.8285050
C	5.8620740	2.2487470	-1.6953560
H	6.7572720	1.9135030	0.2409020
H	-4.1412980	-4.5963610	-1.3852130
H	-3.6618630	-5.1850820	0.2253050
H	-2.4807040	-5.1804080	-1.1087960
H	-5.1638180	-1.2196180	2.2145890
H	-5.8935560	-0.7855120	0.6487130
H	-4.8631730	0.3889580	1.5037260
H	3.6504280	-1.8715680	5.2096960
H	6.7269840	2.7626870	-2.1056020
H	-1.5517310	2.7108290	-2.1113640
C	-5.2531970	4.1638660	0.1977570
N	-6.2809560	4.7094510	0.2607510

(PAd-DalPhos)Ni(Ph)NH_2



Zero-point correction= 0.694116 (Hartree/Particle)
Thermal correction to Energy= 0.735520

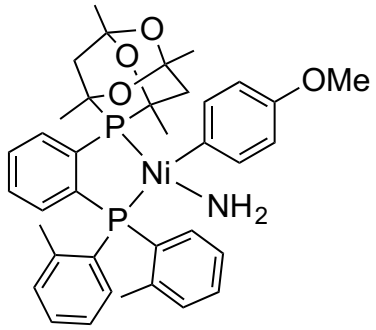
Thermal correction to Enthalpy= 0.736464
Thermal correction to Gibbs Free Energy= 0.623431
Sum of electronic and zero-point Energies= -3867.319599
Sum of electronic and thermal Energies= -3867.278195
Sum of electronic and thermal Enthalpies= -3867.277251
Sum of electronic and thermal Free Energies= -3867.390284

Single-point energy (6-311+G(2d,2p)) = -3868.761114

Ni	0.2415260	1.3881780	0.1030070
P	-1.0338000	-0.3688870	-0.3535920
P	1.9652350	-0.0411700	0.0423580
C	-1.1953020	2.6429360	0.1751240
C	-1.5872750	3.4413730	-0.9126230
C	-1.8714690	2.8360030	1.3930510
C	0.0558790	-1.5658750	-1.2678590
C	1.4447780	-1.3831100	-1.1004980
C	-2.6377500	-0.2826370	-1.3748490
C	-1.8811540	-1.3332930	1.0600260
C	2.4617820	-0.9346880	1.5829750
C	3.5390040	0.5806610	-0.6689660
C	-2.6381690	4.3603510	-0.8064320
C	-2.9130170	3.7624620	1.5112740
H	-1.5990690	2.2409540	2.2617360
O	-3.1821660	-1.6083850	-1.5873660
O	-2.9217800	-0.4713320	1.5579610
C	2.3523650	-2.1648270	-1.8257940
C	-0.3885880	-2.5573670	-2.1588710
C	-2.5097220	-2.6260670	0.5343920
C	-3.6593960	0.5159850	-0.5605540
C	-2.3966330	0.3144930	-2.7519110
C	-0.9401660	-1.5790000	2.2243150
C	2.4076930	-0.3010990	2.8478470
C	2.8838950	-2.2718880	1.4972090
C	3.5434480	1.2025130	-1.9431290
C	4.7225180	0.5209600	0.0805240
H	-2.9252700	4.9560040	-1.6708340
C	-3.3107190	4.5210470	0.4067780
H	-3.4154820	3.8904570	2.4682860
H	3.4188540	-1.9898750	-1.7137110
C	1.8960640	-3.1393680	-2.7116470
C	0.5238630	-3.3348030	-2.8727900
H	-1.4501410	-2.6963120	-2.3168890
C	-3.6614080	-2.3018330	-0.4261310
H	-1.7600550	-3.2536570	0.0449070
H	-2.9222980	-3.1850710	1.3826820
H	-4.5584050	0.6435170	-1.1750720

H	-3.2731410	1.4984250	-0.2973910
C	-4.0519460	-0.2588640	0.7004710
H	-3.3401090	0.3323860	-3.3091520
H	-1.6696400	-0.2715120	-3.3218520
H	-2.0271630	1.3381560	-2.6509540
H	-1.4886550	-2.0692220	3.0367930
H	-0.5361150	-0.6357380	2.5981680
H	-0.1065000	-2.2208650	1.9250540
C	2.7972340	-1.0458810	3.9717260
C	3.2560420	-2.9922630	2.6298830
H	2.9154240	-2.7658540	0.5332130
C	1.9212540	1.1105650	3.0565930
C	4.7526010	1.7265490	-2.4154600
H	4.7123210	0.0561100	1.0604210
C	2.3073580	1.3144310	-2.8052410
H	-4.1257400	5.2349940	0.4939860
C	5.9132290	1.0554110	-0.4112730
O	-4.6058630	-1.5125060	0.2868260
H	2.6065330	-3.7347490	-3.2784210
H	0.1578150	-4.0847730	-3.5687180
C	-4.3891400	-3.5291040	-0.9366050
C	-5.0942260	0.4490280	1.5386690
H	2.7612350	-0.5653130	4.9461200
C	3.2142510	-2.3711140	3.8770280
H	3.5754320	-4.0262540	2.5344030
H	2.2789090	1.8260950	2.3112400
H	2.1975380	1.4619220	4.0560900
H	0.8271620	1.1629800	2.9775900
H	4.7660540	2.2066220	-3.3908720
H	1.4532500	1.6978470	-2.2326110
H	2.0112210	0.3425460	-3.2175260
H	2.4867720	1.9933440	-3.6445310
C	5.9275580	1.6581060	-1.6670350
H	6.8181000	1.0019060	0.1873570
H	-5.2017890	-3.2202050	-1.5990530
H	-4.8065410	-4.0903320	-0.0962320
H	-3.7006780	-4.1739350	-1.4911730
H	-5.3335700	-0.1584290	2.4155060
H	-6.0025410	0.6017490	0.9492800
H	-4.7067850	1.4189020	1.8601270
H	3.5019660	-2.9148290	4.7728880
H	6.8466360	2.0815220	-2.0628650
H	-1.0656650	3.3502830	-1.8641150
N	1.3870700	2.8447620	0.4153680
H	2.2090860	2.8404280	-0.1918820
H	0.9373580	3.7473330	0.2740890

(PAd-DalPhos)Ni(*p*-OMePh)NH_2



Zero-point correction= 0.726827 (Hartree/Particle)
Thermal correction to Energy= 0.770897
Thermal correction to Enthalpy= 0.771841
Thermal correction to Gibbs Free Energy= 0.652395
Sum of electronic and zero-point Energies= -3981.815032
Sum of electronic and thermal Energies= -3981.770962
Sum of electronic and thermal Enthalpies= -3981.770018
Sum of electronic and thermal Free Energies= -3981.889464

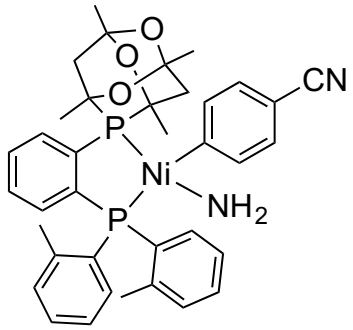
Single-point energy (6-311+G(2d,2p)) = -3983.325936

Ni	-0.1351000	-1.2211880	-0.0617200
P	0.6051970	0.8514170	-0.3490780
P	-2.1755810	-0.3110870	0.0646040
C	1.5905800	-2.0393320	-0.1439050
C	2.1384380	-2.5973270	-1.3139210
C	2.3533510	-2.1608860	1.0252290
C	-0.8062330	1.7992590	-1.1016510
C	-2.0867830	1.2331090	-0.9282800
C	2.1194500	1.2959750	-1.4134900
C	1.2431620	1.8645680	1.1384880
C	-2.8163610	0.2500230	1.7055700
C	-3.5591600	-1.2560460	-0.6847940
C	3.3977710	-3.1975130	-1.3299720
C	3.6160540	-2.7725890	1.0379950
H	1.9795560	-1.7526850	1.9614370
O	2.2833420	2.7332750	-1.4954970
O	2.4992120	1.2681790	1.5135890
C	-3.2040410	1.8120740	-1.5426970
C	-0.6856440	2.9596940	-1.8849270
C	1.4807630	3.3232980	0.7405330
C	3.3577160	0.7252080	-0.7167810
C	1.9700860	0.7925370	-2.8399870
C	0.3331100	1.7340640	2.3453350
C	-2.5263430	-0.4675510	2.8910900

C	-3.5919770	1.4190920	1.7776940
C	-3.4576560	-1.7194280	-2.0209250
C	-4.6790950	-1.5968010	0.0868990
H	3.8133350	-3.6153200	-2.2429580
C	4.1467810	-3.2826330	-0.1506850
H	4.1633910	-2.8431470	1.9721490
H	-4.1788600	1.3454550	-1.4306260
C	-3.0673950	2.9597210	-2.3216600
C	-1.8059260	3.5325670	-2.4877030
H	0.2919300	3.3936130	-2.0494560
C	2.6238530	3.4137180	-0.2791780
H	0.5672740	3.7727340	0.3418900
H	1.7772060	3.8863950	1.6335040
H	4.2243170	0.9035030	-1.3642900
H	3.2582580	-0.3454020	-0.5511630
C	3.5982640	1.4506730	0.6099860
H	2.8543790	1.0790160	-3.4203680
H	1.0857820	1.2167620	-3.3245910
H	1.8863980	-0.2972020	-2.8395980
H	0.7733180	2.2726320	3.1923890
H	0.2135260	0.6851400	2.6251660
H	-0.6554890	2.1536940	2.1369840
C	-3.0471060	0.0228040	4.0985330
C	-4.0889760	1.8901060	2.9907570
H	-3.8067600	1.9792320	0.8752590
C	-1.6627350	-1.7026590	2.9314770
C	-4.5043890	-2.4980180	-2.5287360
H	-4.7470090	-1.2515060	1.1128500
C	-2.2782790	-1.4032430	-2.9113380
C	-5.7062210	-2.3784340	-0.4417520
O	3.7796740	2.8407110	0.3205900
H	-3.9376400	3.3970710	-2.8031990
H	-1.6868340	4.4208090	-3.1022000
C	2.9743700	4.8344560	-0.6728730
C	4.8335790	0.9698230	1.3401710
H	-2.8314490	-0.5243790	5.0127330
C	-3.8154410	1.1825860	4.1601390
H	-4.6836020	2.7989400	3.0171550
H	-1.8593180	-2.4163140	2.1266770
H	-1.7701390	-2.2079540	3.8968420
H	-0.6027620	-1.4433100	2.8083510
H	-4.4353080	-2.8592980	-3.5518610
H	-1.3269770	-1.6011250	-2.4011600
H	-2.2703940	-0.3496760	-3.2148810
H	-2.3106840	-2.0129450	-3.8194740
C	-5.6185660	-2.8279180	-1.7572890

H	-6.5634190	-2.6341330	0.1745620
H	3.8031670	4.8199440	-1.3852790
H	3.2733370	5.4026270	0.2121360
H	2.1118830	5.3223170	-1.1370310
H	4.9509850	1.5310580	2.2710040
H	5.7170430	1.1237140	0.7144090
H	4.7325490	-0.0948840	1.5647370
H	-4.1951440	1.5317890	5.1166240
H	-6.4091920	-3.4399440	-2.1827340
H	1.5724320	-2.5662130	-2.2434110
O	5.3814300	-3.8844640	-0.2601500
C	6.1591290	-4.0144960	0.9170160
H	5.6442630	-4.6207550	1.6741600
H	7.0799160	-4.5168010	0.6155240
H	6.4042510	-3.0339470	1.3476400
N	-0.8375090	-2.9559140	0.1020770
H	-1.6564460	-3.1119720	-0.4891030
H	-0.1679880	-3.6823170	-0.1445340

(PAd-DalPhos)Ni(*p*-CNPh)NH_2



Zero-point correction= 0.692648 (Hartree/Particle)
Thermal correction to Energy= 0.736009
Thermal correction to Enthalpy= 0.736953
Thermal correction to Gibbs Free Energy= 0.618746
Sum of electronic and zero-point Energies= -3959.575816
Sum of electronic and thermal Energies= -3959.532455
Sum of electronic and thermal Enthalpies= -3959.531511
Sum of electronic and thermal Free Energies= -3959.649718

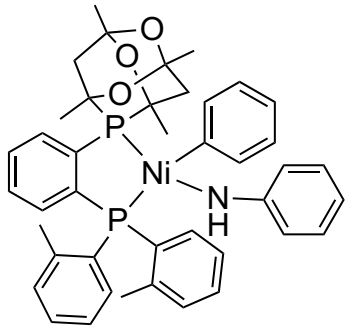
Single-point energy (6-311+G(2d,2p)) = -3961.037961

Ni	0.1188270	1.2479530	0.0295050
P	-0.7098330	-0.7775980	-0.3565620
P	2.1264870	0.2503710	0.0483260
C	-1.5558870	2.1515910	0.0363890

C	-2.1007970	2.7947700	-1.0914210
C	-2.2736700	2.2552390	1.2447850
C	0.6421970	-1.7305200	-1.2004550
C	1.9474310	-1.2216250	-1.0362330
C	-2.2700440	-1.1050670	-1.3971350
C	-1.3482300	-1.8324470	1.0999160
C	2.7824690	-0.4401370	1.6323030
C	3.5242970	1.1915180	-0.6767500
C	-3.3216640	3.4646690	-1.0403160
C	-3.4889140	2.9305170	1.3219210
H	-1.8878960	1.7811420	2.1433760
O	-2.4937830	-2.5274260	-1.5420630
O	-2.5659190	-1.2002680	1.5361210
C	3.0232900	-1.8042300	-1.7171930
C	0.4538630	-2.8412510	-2.0402340
C	-1.6565530	-3.2589250	0.6386940
C	-3.4647260	-0.5198990	-0.6380450
C	-2.1391000	-0.5400020	-2.8026990
C	-0.4023260	-1.7978030	2.2854870
C	2.5711890	0.2196540	2.8668920
C	3.4918580	-1.6527070	1.6091130
C	3.4094630	1.7421470	-1.9781120
C	4.6747860	1.4386790	0.0857880
H	-3.7300950	3.9420440	-1.9266030
C	-4.0321210	3.5299640	0.1708400
H	-4.0269170	2.9962820	2.2635650
H	4.0182150	-1.3812280	-1.6091090
C	2.8197080	-2.9004430	-2.5536190
C	1.5334760	-3.4187560	-2.7091480
H	-0.5435830	-3.2313150	-2.1953340
C	-2.8299990	-3.2534360	-0.3496800
H	-0.7732070	-3.7234950	0.1921250
H	-1.9507510	-3.8533810	1.5116580
H	-4.3551990	-0.6302140	-1.2678220
H	-3.3188460	0.5366340	-0.4244170
C	-3.6989980	-1.2985660	0.6598900
H	-3.0510880	-0.7608470	-3.3684550
H	-1.2887350	-0.9779030	-3.3332910
H	-2.0071170	0.5441550	-2.7570620
H	-0.8444890	-2.3562810	3.1183050
H	-0.2296740	-0.7694370	2.6105050
H	0.5611090	-2.2489570	2.0310530
C	3.0993610	-0.3708050	4.0251500
C	3.9978840	-2.2225390	2.7750720
H	3.6468460	-2.1688820	0.6691240
C	1.7828080	1.4966720	3.0093860

C	4.4735640	2.5118660	-2.4627610
H	4.7533670	1.0255360	1.0855470
C	2.1990860	1.5258330	-2.8566880
C	5.7189650	2.2130360	-0.4193160
O	-3.9431070	-2.6633040	0.3100480
H	3.6578090	-3.3408210	-3.0864750
H	1.3631720	-4.2670580	-3.3663540
C	-3.2508250	-4.6370620	-0.8012970
C	-4.8927220	-0.8069100	1.4492600
H	2.9438900	0.1314910	4.9764860
C	3.8011050	-1.5731400	3.9925750
H	4.5401850	-3.1626270	2.7278860
H	1.9931270	2.2436790	2.2396380
H	1.9533750	1.9386730	3.9962640
H	0.7058710	1.3047070	2.9137850
H	4.3950850	2.9400640	-3.4589570
H	1.2671550	1.7163970	-2.3094280
H	2.1498640	0.4970610	-3.2327780
H	2.2288060	2.1966410	-3.7206680
C	5.6175950	2.7491710	-1.7010410
H	6.6000720	2.3958750	0.1889770
H	-4.0975790	-4.5533550	-1.4872430
H	-3.5493650	-5.2354760	0.0636160
H	-2.4228590	-5.1363310	-1.3136040
H	-5.0100940	-1.4133900	2.3510880
H	-5.7985800	-0.8876900	0.8424370
H	-4.7425730	0.2381050	1.7312290
H	4.1890670	-2.0000800	4.9134280
H	6.4213600	3.3568980	-2.1073700
H	-1.5616110	2.7740000	-2.0360650
C	-5.2956730	4.1989280	0.2324770
N	-6.3291380	4.7353880	0.2811810
N	0.9011580	2.9362510	0.2915520
H	1.7186070	3.0887370	-0.3022730
H	0.2717800	3.7149780	0.1058710

(PAd-DalPhos)Ni(Ph)PhNH



Zero-point correction= 0.775069 (Hartree/Particle)
Thermal correction to Energy= 0.821095
Thermal correction to Enthalpy= 0.822039
Thermal correction to Gibbs Free Energy= 0.697053
Sum of electronic and zero-point Energies= -4098.300984
Sum of electronic and thermal Energies= -4098.254957
Sum of electronic and thermal Enthalpies= -4098.254013
Sum of electronic and thermal Free Energies= -4098.379000

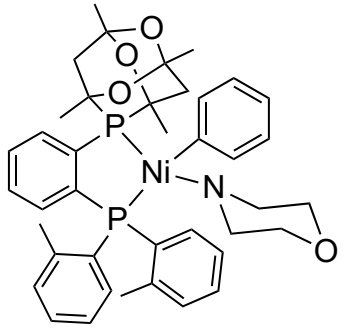
Single-point energy (6-311+G(2d,2p)) = -4099.898781

Ni	0.4696160	0.6674850	-0.1174210
P	-1.4920040	-0.3585770	-0.3182230
P	1.3513530	-1.4088470	0.0320840
C	-0.2754660	2.4127480	-0.2547920
C	-0.2502520	3.1354860	-1.4562580
C	-0.8218620	3.0433060	0.8742650
C	-1.1323460	-2.0470560	-1.0155940
C	0.1890560	-2.5142350	-0.8580160
C	-2.9572910	0.2896490	-1.3488050
C	-2.5750240	-0.6057870	1.2343740
C	1.5415840	-2.1879880	1.6955460
C	2.9578050	-1.6666970	-0.8133650
C	-0.7700020	4.4317540	-1.5369110
C	-1.3250280	4.3463330	0.8061100
H	-0.8742310	2.5119840	1.8216470
O	-4.0380920	-0.6745530	-1.3412080
O	-3.0973070	0.6921310	1.5701090
C	0.5824410	-3.7316670	-1.4286720
C	-2.0397280	-2.8383460	-1.7414630
C	-3.7396340	-1.5510200	0.9286520
C	-3.4744360	1.5691460	-0.6878090
C	-2.5676490	0.5061810	-2.8023440
C	-1.7522770	-1.0550910	2.4279750
C	1.9440930	-1.4210180	2.8149340

C	1.2572440	-3.5535640	1.8596210
C	3.1014160	-1.3166230	-2.1789510
C	4.0696640	-2.1165340	-0.0886690
H	-0.7360670	4.9697680	-2.4819530
C	-1.3116740	5.0432240	-0.4043410
H	-1.7285690	4.8166410	1.7008480
H	1.6128360	-4.0613210	-1.3282500
C	-0.3275330	-4.5019530	-2.1495890
C	-1.6395580	-4.0516520	-2.3014730
H	-3.0519630	-2.4881540	-1.8921250
C	-4.6938710	-0.9017250	-0.0838770
H	-3.3762070	-2.5139010	0.5599460
H	-4.2988600	-1.7284460	1.8549090
H	-4.2698750	1.9777780	-1.3220750
H	-2.6854510	2.3113720	-0.5919630
C	-4.0787370	1.2486780	0.6823790
H	-3.4437940	0.8479120	-3.3648420
H	-2.1987310	-0.4148460	-3.2632420
H	-1.7894540	1.2720090	-2.8631900
H	-2.3962840	-1.1107740	3.3129780
H	-0.9462010	-0.3447190	2.6288680
H	-1.3110460	-2.0403640	2.2512510
C	2.0584510	-2.0714600	4.0522010
C	1.3686460	-4.1745480	3.1019690
H	0.9351020	-4.1433790	1.0096630
C	2.2228980	0.0585770	2.7466630
C	4.3678140	-1.4446320	-2.7618880
H	3.9579130	-2.3708050	0.9599500
C	1.9502560	-0.8305630	-3.0319250
H	-1.7071790	6.0539670	-0.4615320
C	5.3212630	-2.2336200	-0.6923870
O	-5.1494960	0.3205520	0.4806410
H	-0.0123690	-5.4403820	-2.5972590
H	-2.3550880	-4.6382080	-2.8712480
C	-5.9152060	-1.7444030	-0.3912680
C	-4.6518960	2.4597630	1.3852960
H	2.3713740	-1.4890450	4.9149900
C	1.7756010	-3.4267550	4.2054780
H	1.1401810	-5.2319330	3.2015580
H	2.8395770	0.3459920	1.8906970
H	2.7038110	0.4001460	3.6682950
H	1.2899690	0.6247620	2.6266590
H	4.4899130	-1.1743120	-3.8079050
H	1.3291530	-0.0930990	-2.5084580
H	1.2884780	-1.6553730	-3.3222540
H	2.3245630	-0.3639240	-3.9482210

C	5.4695020	-1.8966060	-2.0358610
H	6.1717050	-2.5792740	-0.1117980
H	-6.5529640	-1.2137360	-1.1027680
H	-6.4799830	-1.9288510	0.5265500
H	-5.6146790	-2.7028620	-0.8252650
H	-5.0690500	2.1597370	2.3502160
H	-5.4438830	2.9010550	0.7739660
H	-3.8637910	3.2000190	1.5407050
H	1.8700750	-3.8935510	5.1821840
H	6.4396170	-1.9762110	-2.5184830
H	0.2011340	2.6944870	-2.3433860
N	2.2362610	1.3886930	-0.1713470
H	2.6907960	1.0034450	-0.9975320
C	2.7118910	2.6726530	0.0384870
C	2.3989030	3.3917520	1.2144750
C	3.5981750	3.2903740	-0.8749060
C	2.9336920	4.6537040	1.4503370
H	1.7265770	2.9433130	1.9371090
C	4.1414990	4.5476600	-0.6240290
H	3.8536330	2.7625420	-1.7931080
C	3.8114450	5.2483910	0.5384550
H	2.6636310	5.1798760	2.3636380
H	4.8208370	4.9880530	-1.3510920
H	4.2274640	6.2334580	0.7301260

(PAd-DalPhos)Ni(Ph)Morpholine



Zero-point correction= 0.793385 (Hartree/Particle)
Thermal correction to Energy= 0.838830
Thermal correction to Enthalpy= 0.839774
Thermal correction to Gibbs Free Energy= 0.718101
Sum of electronic and zero-point Energies= -4098.472490
Sum of electronic and thermal Energies= -4098.427045
Sum of electronic and thermal Enthalpies= -4098.426101
Sum of electronic and thermal Free Energies= -4098.547773

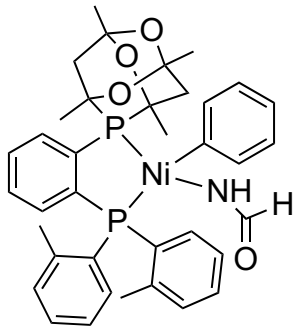
Single-point energy (6-311+G(2d,2p)) = -4100.085994

Ni	0.2828060	0.9505660	0.0259090
P	-1.4586810	-0.4164110	-0.3169680
P	1.5514870	-0.9901920	-0.0317230
C	-0.7552320	2.5298710	-0.1612690
C	-0.9029380	3.1500230	-1.4129550
C	-1.4007200	3.1296570	0.9339590
C	-0.8261110	-1.9724770	-1.1073670
C	0.5643210	-2.1844960	-1.0219530
C	-3.0759110	-0.0338990	-1.2500770
C	-2.3859150	-0.8909260	1.2806270
C	1.9744760	-1.9773550	1.4794960
C	3.1030440	-0.8577030	-1.0070680
C	-1.6755420	4.3064130	-1.5731750
C	-2.1664710	4.2902840	0.7843920
H	-1.3207700	2.6801420	1.9208490
O	-3.9579070	-1.1830130	-1.2147420
O	-3.1215220	0.2804010	1.6797580
C	1.1574150	-3.2638990	-1.6903910
C	-1.5983260	-2.8782110	-1.8576220
C	-3.3670530	-2.0331740	1.0079650
C	-3.7831530	1.1133740	-0.5253290
C	-2.8236210	0.2811960	-2.7162850
C	-1.4274460	-1.1903640	2.4190170
C	2.6751540	-1.3880470	2.5551750
C	1.5134940	-3.3010690	1.6082900
C	3.0572630	-0.3121250	-2.3127470
C	4.3336680	-1.2396690	-0.4580640
H	-1.7704290	4.7606690	-2.5574230
C	-2.3156870	4.8808360	-0.4735580
H	-2.6485420	4.7338180	1.6535920
H	2.2328430	-3.4037420	-1.6279770
C	0.3819060	-4.1450840	-2.4395340
C	-0.9986920	-3.9507770	-2.5161310
H	-2.6660280	-2.7266850	-1.9433410
C	-4.4836670	-1.5551200	0.0680030
H	-2.8494930	-2.8991640	0.5857230
H	-3.8279070	-2.3370460	1.9552940
H	-4.6744140	1.3804940	-1.1052300
H	-3.1412420	1.9877410	-0.4461540
C	-4.2388150	0.6579280	0.8638530
H	-3.7822540	0.4544720	-3.2182000
H	-2.3104350	-0.5395050	-3.2254160
H	-2.2157800	1.1862450	-2.7977290
H	-1.9991860	-1.3512260	3.3401310

H	-0.7405920	-0.3528390	2.5742800
H	-0.8375370	-2.0868840	2.2108840
C	2.8904480	-2.1510580	3.7130940
C	1.7331180	-4.0367880	2.7701080
H	0.9688840	-3.7663210	0.7962360
C	3.2271060	0.0138660	2.5076560
C	4.2630060	-0.1519380	-3.0053800
H	4.3655520	-1.6741510	0.5347560
C	1.7655140	0.0658580	-3.0015340
H	-2.9147270	5.7798030	-0.5926440
C	5.5223120	-1.0721230	-1.1680780
O	-5.1268900	-0.4513600	0.6921050
H	0.8504970	-4.9749500	-2.9612640
H	-1.6135410	-4.6299430	-3.1005590
C	-5.5414580	-2.6069240	-0.1984820
C	-4.9873930	1.7252840	1.6321920
H	3.4332960	-1.6952730	4.5380780
C	2.4270700	-3.4573460	3.8322520
H	1.3614470	-5.0551780	2.8418560
H	2.8628580	0.5976770	1.6554680
H	4.3238870	-0.0048110	2.4524290
H	2.9651820	0.5580440	3.4225330
H	4.2372920	0.2751260	-4.0050300
H	1.0647970	0.5677740	-2.3222370
H	1.2503770	-0.8189780	-3.3951140
H	1.9603200	0.7406110	-3.8407970
C	5.4864340	-0.5194220	-2.4461790
H	6.4663980	-1.3698010	-0.7205660
H	-6.3076610	-2.1923580	-0.8585420
H	-6.0072750	-2.9124450	0.7423090
H	-5.0921900	-3.4825940	-0.6766420
H	-5.2881250	1.3314320	2.6066230
H	-5.8796600	2.0247600	1.0755120
H	-4.3426830	2.5958910	1.7725840
H	2.6039750	-4.0175650	4.7463350
H	6.4045980	-0.3741840	-3.0086390
H	-0.4052180	2.7322500	-2.2871930
C	2.3498990	2.8251770	-0.7216640
C	1.7313810	2.9505340	1.5499690
C	3.7340960	3.3765780	-0.3712050
H	1.7047010	3.6796050	-1.0022000
H	2.4550670	2.1862200	-1.6036010
C	3.1153280	3.5197380	1.8896070
H	1.0532310	3.8061390	1.3848970
H	1.3530400	2.4011120	2.4232590
H	4.1266640	4.0001430	-1.1813430

H	4.4326100	2.5427940	-0.1899920
H	3.0451350	4.2503920	2.7023520
H	3.8006870	2.7139390	2.1963890
N	1.8153470	2.0575710	0.3973110
O	3.6788740	4.2163210	0.7805710

(PAd-DalPhos)Ni(Ph)HCONH



Zero-point correction= 0.705575 (Hartree/Particle)
Thermal correction to Energy= 0.748628
Thermal correction to Enthalpy= 0.749572
Thermal correction to Gibbs Free Energy= 0.632361
Sum of electronic and zero-point Energies= -3980.670481
Sum of electronic and thermal Energies= -3980.627428
Sum of electronic and thermal Enthalpies= -3980.626484
Sum of electronic and thermal Free Energies= -3980.743695

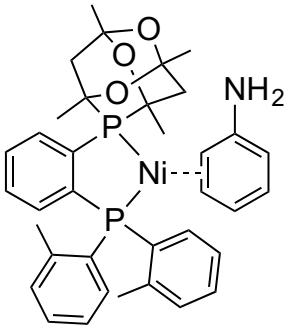
Single-point energy (6-311+G(2d,2p)) = -3982.153867

Ni	0.24406	1.2817	-0.06565
P	-1.15432	-0.41552	-0.37
P	1.88637	-0.28796	0.04418
C	-1.18179	2.55218	-0.00453
C	-1.5325	3.33117	-1.1185
C	-1.83229	2.81429	1.21088
C	-0.15077	-1.76759	-1.15278
C	1.24477	-1.67662	-0.97864
C	-2.73752	-0.30902	-1.43156
C	-2.09851	-1.17046	1.11269
C	2.19167	-1.07243	1.69231
C	3.55165	0.00185	-0.67123
C	-2.52744	4.31221	-1.03482
C	-2.81631	3.80434	1.30374
H	-1.58827	2.23449	2.09722
O	-3.34579	-1.61839	-1.53675
O	-3.10195	-0.21282	1.48951
C	2.09583	-2.59422	-1.60781

C	-0.66093	-2.8031	-1.95541
C	-2.78152	-2.47368	0.68853
C	-3.74161	0.60645	-0.72578
C	-2.42956	0.14454	-2.84973
C	-1.21074	-1.34937	2.32937
C	2.11493	-0.33556	2.89848
C	2.46486	-2.45041	1.74572
C	3.66924	0.54573	-1.97361
C	4.7022	-0.26854	0.08299
H	-2.7858	4.89619	-1.91543
C	-3.17787	4.54893	0.1777
H	-3.30011	3.9937	2.25972
H	3.17074	-2.49298	-1.49157
C	1.57549	-3.61271	-2.4034
C	0.19472	-3.71454	-2.57351
H	-1.72689	-2.87413	-2.12243
C	-3.88942	-2.182	-0.33269
H	-2.05505	-3.18368	0.28488
H	-3.24653	-2.92607	1.57221
H	-4.61587	0.70921	-1.3793
H	-3.32425	1.59361	-0.545
C	-4.20324	-0.02863	0.58826
H	-3.35683	0.16249	-3.43317
H	-1.72389	-0.52996	-3.34311
H	-2.00425	1.15138	-2.8335
H	-1.81682	-1.71683	3.16515
H	-0.75943	-0.3984	2.62069
H	-0.41172	-2.06855	2.13027
C	2.31262	-1.02378	4.10554
C	2.66057	-3.11008	2.9562
H	2.51368	-3.02438	0.82786
C	1.83734	1.14578	2.96928
C	4.95537	0.79544	-2.46473
H	4.60634	-0.67643	1.08348
C	2.47166	0.87207	-2.83309
H	-3.94737	5.313	0.24842
C	5.97207	-0.0055	-0.42947
O	-4.80901	-1.28677	0.2773
H	2.24418	-4.31406	-2.8945
H	-0.22228	-4.49641	-3.20224
C	-4.66434	-3.41353	-0.75544
C	-5.22908	0.79944	1.33079
H	2.24576	-0.46471	5.03525
C	2.58215	-2.38884	4.14653
H	2.86638	-4.17666	2.96526
H	2.72835	1.73479	2.72507

H	1.52812	1.42656	3.98062
H	1.05722	1.46546	2.27148
H	5.05845	1.22197	-3.45907
H	1.79408	1.55892	-2.31216
H	1.89954	-0.02594	-3.09619
H	2.78887	1.34987	-3.76469
C	6.09728	0.52954	-1.70949
H	6.85202	-0.21216	0.17282
H	-5.44173	-3.12667	-1.46812
H	-5.1329	-3.87528	0.11781
H	-3.99524	-4.139	-1.22791
H	-5.51944	0.2833	2.24968
H	-6.11411	0.94024	0.70419
H	-4.80373	1.77481	1.57772
H	2.72386	-2.88552	5.10243
H	7.07934	0.74805	-2.11933
H	-1.02098	3.18056	-2.06773
N	1.36086	2.81079	-0.13461
H	0.90342	3.69162	-0.36439
C	2.63469	3.05761	0.23241
H	3.19399	2.16845	0.56594
O	3.19883	4.15953	0.2147

(PAd-DalPhos)Ni(η^2-PhNH$_2$)



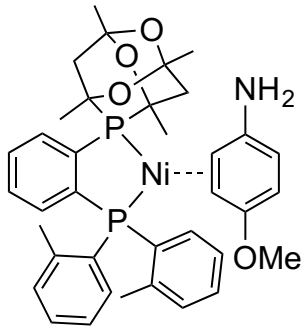
Zero-point correction= 0.694667 (Hartree/Particle)
Thermal correction to Energy= 0.736016
Thermal correction to Enthalpy= 0.736960
Thermal correction to Gibbs Free Energy= 0.623424
Sum of electronic and zero-point Energies= -3867.325456
Sum of electronic and thermal Energies= -3867.284108
Sum of electronic and thermal Enthalpies= -3867.283164
Sum of electronic and thermal Free Energies= -3867.396700

Single-point energy (6-311+G(2d,2p)) = -3868.766029

Ni	0.2981260	1.1833050	-0.4182980
P	-1.3630890	-0.2032110	-0.3404540
P	1.6685890	-0.4240150	0.1010920
C	-0.6108480	-1.8725970	-0.6439680
C	0.7899440	-1.9497120	-0.4793630
C	-2.8910700	-0.1358200	-1.4648860
C	-2.4235040	-0.3337250	1.2369850
C	1.9816690	-0.8235760	1.8887850
C	3.3315100	-0.5663130	-0.6850890
O	-3.8107190	-1.2322520	-1.2379280
O	-3.1807880	0.8970020	1.3010270
C	1.4630440	-3.1394030	-0.7847960
C	-1.3004270	-3.0044630	-1.1106910
C	-3.4032420	-1.5063310	1.1650590
C	-3.6086760	1.1699120	-1.0965820
C	-2.5060730	-0.1898000	-2.9349390
C	-1.5588420	-0.3628820	2.4837880
C	2.2252330	0.2192290	2.8124470
C	1.9237940	-2.1457830	2.3566360
C	3.4522260	-0.5726120	-2.0987480
C	4.4905710	-0.5190880	0.1050590
H	2.5437900	-3.1835840	-0.6787620
C	0.7658550	-4.2546040	-1.2474240
C	-0.6185030	-4.1842570	-1.4094780
H	-2.3701790	-2.9489010	-1.2712790
C	-4.4339040	-1.2750520	0.0495980
H	-2.8698690	-2.4477940	1.0072980
H	-3.9449900	-1.5760280	2.1162610
H	-4.4301660	1.3352390	-1.8039100
H	-2.9207360	2.0159140	-1.1543350
C	-4.2020040	1.0663160	0.3163460
H	-3.4030000	-0.0917580	-3.5575440
H	-2.0163820	-1.1366440	-3.1801710
H	-1.8154680	0.6255690	-3.1734020
H	-2.1963750	-0.3528330	3.3756890
H	-0.9007890	0.5097660	2.5120980
H	-0.9374670	-1.2633450	2.5044200
C	2.4061970	-0.1061960	4.1630850
C	2.1022240	-2.4496920	3.7058890
H	1.7268590	-2.9548400	1.6638460
C	2.2783380	1.6629740	2.3909160
C	4.7373730	-0.5216620	-2.6539090
H	4.3995640	-0.5232810	1.1866590
C	2.2589100	-0.6613770	-3.0237190
C	5.7593150	-0.4664960	-0.4723910
O	-5.1016440	-0.0451950	0.3257870

H	1.3015230	-5.1688290	-1.4887590
H	-1.1694200	-5.0441520	-1.7813080
C	-5.4942800	-2.3550200	-0.0261520
C	-4.9942680	2.2895630	0.7300030
H	2.5923180	0.6973170	4.8715440
C	2.3449360	-1.4226640	4.6157340
H	2.0493890	-3.4828130	4.0385220
H	3.0475790	1.8447890	1.6328180
H	2.4888850	2.3122770	3.2466180
H	1.3318040	1.9834620	1.9427280
H	4.8357290	-0.5258770	-3.7371390
H	1.4382140	-0.0128710	-2.6997980
H	1.8730760	-1.6861130	-3.0773960
H	2.5378000	-0.3544030	-4.0365350
C	5.8834670	-0.4650060	-1.8603410
H	6.6410650	-0.4284060	0.1615750
H	-6.2013130	-2.1152100	-0.8245160
H	-6.0331390	-2.4160740	0.9232610
H	-5.0309930	-3.3233620	-0.2380820
H	-5.4135820	2.1304390	1.7268070
H	-5.8088470	2.4663400	0.0223620
H	-4.3402620	3.1658050	0.7550120
H	2.4830610	-1.6419210	5.6711170
H	6.8644120	-0.4209910	-2.3257870
C	-0.2790760	2.9717560	-1.1314660
C	1.1605790	2.9064930	-1.1827700
C	1.9036990	3.6997330	-0.2404040
C	1.2803860	4.4237790	0.7442390
C	-0.1424110	4.4368650	0.8295270
C	-0.8930960	3.7574380	-0.0989450
H	-0.8451830	2.7455330	-2.0336570
H	2.9881350	3.7186930	-0.3361990
H	1.8679160	5.0025070	1.4523080
H	-0.6308660	5.0193070	1.6060380
H	-1.9776130	3.8282050	-0.0705730
N	1.7678500	2.5248110	-2.4476640
H	1.9450400	3.3539680	-3.0179570
H	2.6664370	2.0710580	-2.2927690

(PAd-DalPhos)Ni(η^2-*p*-OMePhNH$_2$)



Zero-point correction= 0.727398 (Hartree/Particle)
Thermal correction to Energy= 0.771544
Thermal correction to Enthalpy= 0.772488
Thermal correction to Gibbs Free Energy= 0.652356
Sum of electronic and zero-point Energies= -3981.818790
Sum of electronic and thermal Energies= -3981.774644
Sum of electronic and thermal Enthalpies= -3981.773700
Sum of electronic and thermal Free Energies= -3981.893832

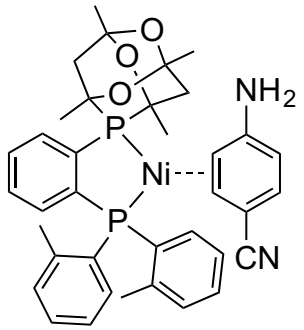
Single-point energy (6-311+G(2d,2p)) = -3983.329228

Ni	0.2068220	1.0293080	-0.5064370
P	-1.0975010	-0.7027680	-0.4162800
P	1.8995910	-0.2156440	0.1208450
C	0.0319560	-2.1463090	-0.6969920
C	1.4084970	-1.8893130	-0.5102530
C	-2.6329680	-1.0478390	-1.4784500
C	-2.0464050	-1.0332110	1.2066690
C	2.3123070	-0.5800160	1.8965400
C	3.5609640	0.0255400	-0.6532900
O	-3.2436980	-2.3305990	-1.1931980
O	-3.0844110	-0.0315960	1.2747090
C	2.3506090	-2.8782620	-0.8201950
C	-0.3625650	-3.4062690	-1.1777340
C	-2.6991470	-2.4177250	1.1945080
C	-3.6346610	0.0515970	-1.1061250
C	-2.3010720	-1.0435880	-2.9625260
C	-1.1728830	-0.8094530	2.4266900
C	2.4548470	0.4854950	2.8158970
C	2.4267630	-1.8982410	2.3644610
C	3.6646110	0.1559610	-2.0619270
C	4.7098780	0.1829630	0.1382890
H	3.4085690	-2.6659370	-0.6928300
C	1.9453120	-4.1208910	-1.3058810
C	0.5857560	-4.3838320	-1.4803220

H	-1.4143550	-3.6092930	-1.3399300
C	-3.7940210	-2.4848720	0.1194480
H	-1.9505960	-3.1978100	1.0291930
H	-3.1702500	-2.5962970	2.1687960
H	-4.4902430	-0.0000190	-1.7904270
H	-3.1745440	1.0369020	-1.1899040
C	-4.1457770	-0.1523020	0.3242180
H	-3.2159450	-1.1951370	-3.5470270
H	-1.5929470	-1.8379940	-3.2155320
H	-1.8563010	-0.0831170	-3.2416440
H	-1.7800930	-0.9114070	3.3338670
H	-0.7369590	0.1933340	2.4061160
H	-0.3591500	-1.5387070	2.4642690
C	2.7143890	0.1886090	4.1594350
C	2.6769460	-2.1751000	3.7086870
H	2.3115900	-2.7261960	1.6754200
C	2.3196130	1.9256570	2.3938720
C	4.9192830	0.4474170	-2.6111320
H	4.6369760	0.0695610	1.2149630
C	2.4834640	-0.0247710	-2.9844260
C	5.9483150	0.4772010	-0.4323310
O	-4.7381730	-1.4528110	0.3969480
H	2.6868740	-4.8765580	-1.5508500
H	0.2607410	-5.3473430	-1.8641040
C	-4.5519470	-3.7971900	0.1108700
C	-5.1978180	0.8582580	0.7306470
H	2.8257370	1.0101540	4.8630260
C	2.8228930	-1.1253370	4.6124740
H	2.7558760	-3.2064530	4.0416600
H	3.0543650	2.2014710	1.6276230
H	2.4591980	2.5967050	3.2475340
H	1.3312100	2.1131180	1.9636240
H	5.0013760	0.5538500	-3.6901320
H	1.6011790	0.5075130	-2.6111590
H	2.2113890	-1.0823870	-3.0849960
H	2.7115980	0.3655590	-3.9805000
C	6.0530200	0.6120230	-1.8153630
H	6.8221030	0.5953520	0.2028400
H	-5.3224800	-3.7666150	-0.6638350
H	-5.0270770	-3.9599030	1.0821000
H	-3.8682540	-4.6257600	-0.0972420
H	-5.5183020	0.6582500	1.7567080
H	-6.0625030	0.7842650	0.0652540
H	-4.7802210	1.8671980	0.6685650
H	3.0172240	-1.3241320	5.6629590
H	7.0097710	0.8443470	-2.2752970

C	-0.4912100	2.5403120	-1.7298410
C	0.6770200	2.9377870	-0.9755370
C	0.4114220	3.7244460	0.1959820
C	-0.8616310	4.0950840	0.5800780
C	-1.9750650	3.7782500	-0.2453440
C	-1.7777300	3.0613810	-1.4039850
H	-0.3333080	2.1670370	-2.7400170
H	1.2599050	4.0814120	0.7748620
H	-0.9915880	4.6833020	1.4814150
H	-2.6164870	2.9041490	-2.0751770
N	1.9490150	3.0436720	-1.6679190
H	2.2010410	4.0201140	-1.8208270
H	2.7074670	2.5963370	-1.1599850
O	-3.2677500	4.1753030	0.0308320
C	-3.5056250	4.9001060	1.2258970
H	-4.5808660	5.0855360	1.2536540
H	-3.2144920	4.3203800	2.1118150
H	-2.9745040	5.8612970	1.2299520

(PAd-DalPhos)Ni(η^2-*p*-CNPhNH$_2$)



Zero-point correction= 0.693526 (Hartree/Particle)
Thermal correction to Energy= 0.736757
Thermal correction to Enthalpy= 0.737701
Thermal correction to Gibbs Free Energy= 0.620177
Sum of electronic and zero-point Energies= -3959.583185
Sum of electronic and thermal Energies= -3959.539954
Sum of electronic and thermal Enthalpies= -3959.539010
Sum of electronic and thermal Free Energies= -3959.656534

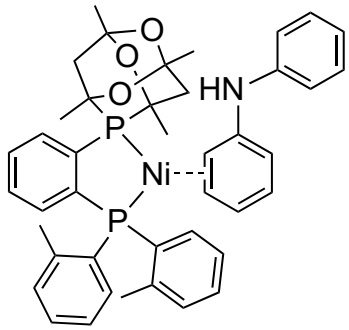
Single-point energy (6-311+G(2d,2p)) = -3961.044964

Ni	0.2331680	1.1391690	-0.3715980
P	-1.1674470	-0.5455390	-0.4082080
P	1.8669330	-0.2525090	0.1052220
C	-0.1040600	-1.9802560	-0.9001560
C	1.2857310	-1.8106840	-0.7095360

C	-2.7357410	-0.6716730	-1.4699680
C	-2.0993350	-1.0407300	1.1825280
C	2.2496120	-0.8254310	1.8287820
C	3.5373670	0.0050060	-0.6377710
O	-3.3830420	-1.9586330	-1.3428220
O	-3.0909100	-0.0182650	1.4005250
C	2.1759430	-2.7966000	-1.1537460
C	-0.5635810	-3.1507580	-1.5267880
C	-2.8042950	-2.3875840	1.0007020
C	-3.6891320	0.4023610	-0.9284230
C	-2.4315950	-0.4809370	-2.9479770
C	-1.1976530	-1.0127980	2.4022130
C	2.3814810	0.1192270	2.8722290
C	2.3641170	-2.1915890	2.1284980
C	3.6622370	0.2622930	-2.0267480
C	4.6802220	0.0475480	0.1772000
H	3.2444750	-2.6503380	-1.0220890
C	1.7058280	-3.9498100	-1.7807240
C	0.3335820	-4.1254020	-1.9641950
H	-1.6255050	-3.2833060	-1.6945100
C	-3.9187380	-2.2706450	-0.0494520
H	-2.0894820	-3.1664060	0.7204870
H	-3.2665310	-2.6744660	1.9528060
H	-4.5569950	0.4735900	-1.5945980
H	-3.1961750	1.3746930	-0.8907860
C	-4.1815070	0.0247860	0.4734190
H	-3.3629680	-0.5218010	-3.5240880
H	-1.7596750	-1.2594000	-3.3209230
H	-1.9568570	0.4918010	-3.1099220
H	-1.7958110	-1.2097460	3.2992810
H	-0.7247350	-0.0325850	2.5071050
H	-0.4136860	-1.7711030	2.3280170
C	2.6262780	-0.3419510	4.1715710
C	2.6015600	-2.6323510	3.4302530
H	2.2567510	-2.9275490	1.3408670
C	2.2500620	1.6004060	2.6298310
C	4.9341440	0.5551320	-2.5346780
H	4.5889950	-0.1596220	1.2383110
C	2.4880250	0.2159420	-2.9744270
C	5.9354660	0.3460670	-0.3522690
O	-4.8157500	-1.2543850	0.3832030
H	2.4074790	-4.7028970	-2.1288530
H	-0.0415070	-5.0173500	-2.4588190
C	-4.7242410	-3.5426350	-0.2204470
C	-5.1921710	0.9969750	1.0427860
H	2.7270990	0.3856250	4.9730670

C	2.7332190	-1.7017820	4.4586040
H	2.6805300	-3.6966410	3.6339850
H	2.9771720	1.9629000	1.8932110
H	2.4045350	2.1622890	3.5563120
H	1.2572380	1.8469690	2.2404400
H	5.0340360	0.7585610	-3.5979940
H	1.6115510	0.7176190	-2.5503120
H	2.1973740	-0.8165130	-3.2025430
H	2.7350290	0.7169470	-3.9146670
C	6.0624530	0.6019710	-1.7163240
H	6.8044870	0.3740980	0.2992580
H	-5.5061880	-3.3798310	-0.9665840
H	-5.1889130	-3.8195800	0.7296640
H	-4.0756000	-4.3583940	-0.5537570
H	-5.5071400	0.6535100	2.0316770
H	-6.0667690	1.0498160	0.3886250
H	-4.7525230	1.9937650	1.1320230
H	2.9157620	-2.0290250	5.4784680
H	7.0328600	0.8389850	-2.1438110
C	-0.3282690	2.7510600	-1.4902890
C	0.8526820	3.0052110	-0.6817990
C	0.6125150	3.7074920	0.5599250
C	-0.6355170	4.1194520	0.9538620
C	-1.7628770	3.9388160	0.0883810
C	-1.5863670	3.2948150	-1.1265360
H	-0.1772910	2.4567840	-2.5269870
H	1.4727490	3.9485800	1.1792860
H	-0.7727180	4.6392310	1.8969290
H	-2.4177680	3.2246250	-1.8220270
N	2.1260200	3.1434860	-1.3610950
H	2.4270280	4.1176510	-1.3773200
H	2.8621690	2.5914950	-0.9293870
C	-3.0505650	4.4217110	0.4644030
N	-4.1098970	4.8001370	0.7746430

(PAd-DalPhos)Ni(η^2-Ph_2NH)



Zero-point correction= 0.775750 (Hartree/Particle)
Thermal correction to Energy= 0.821610
Thermal correction to Enthalpy= 0.822554
Thermal correction to Gibbs Free Energy= 0.696530
Sum of electronic and zero-point Energies= -4098.307723
Sum of electronic and thermal Energies= -4098.261863
Sum of electronic and thermal Enthalpies= -4098.260918
Sum of electronic and thermal Free Energies= -4098.386943

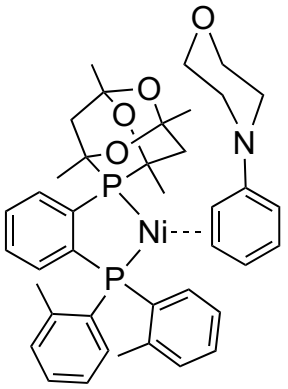
Single-point energy (6-311+G(2d,2p)) = -4099.904390

Ni	-0.3017340	-0.4849240	0.4547830
P	1.6861000	-0.3921100	-0.4087350
P	-0.5793870	1.6363980	0.0393490
C	1.6541390	1.0672310	-1.5534010
C	0.5795710	1.9643170	-1.3687940
C	2.5473880	-1.7708810	-1.3894670
C	3.1738730	-0.1706530	0.7581620
C	-0.0692450	2.9289050	1.2723600
C	-2.1955880	2.2433390	-0.6127580
O	3.8575310	-1.3848070	-1.8710150
O	3.3121860	-1.4284140	1.4569230
C	0.4028440	3.0331470	-2.2566920
C	2.5351160	1.2784730	-2.6276360
C	4.4633600	0.1029760	-0.0179760
C	2.7273970	-2.9250560	-0.3951430
C	1.7391040	-2.1814390	-2.6104880
C	2.8889170	0.8749510	1.8208930
C	-0.4116040	2.7752700	2.6360990
C	0.7083200	4.0324850	0.8871890
C	-2.7683000	1.6448930	-1.7651260
C	-2.9295920	3.2039150	0.1010420
H	-0.4418340	3.7039240	-2.1240530
C	1.2825740	3.2287290	-3.3203080
C	2.3510290	2.3493710	-3.5023450

H	3.3475870	0.5822950	-2.7959570
C	4.8444770	-1.1183000	-0.8685800
H	4.3566690	0.9914930	-0.6465210
H	5.2761040	0.2848870	0.6956630
H	3.1031590	-3.8027280	-0.9344060
H	1.7739460	-3.1811430	0.0703660
C	3.7563500	-2.5420710	0.6793700
H	2.2397810	-3.0096970	-3.1250400
H	1.6333320	-1.3506130	-3.3139740
H	0.7381340	-2.5056050	-2.3076050
H	3.7262280	0.9220180	2.5269750
H	1.9787700	0.6200310	2.3709420
H	2.7531470	1.8620690	1.3684060
C	0.0290710	3.7379350	3.5534560
C	1.1428830	4.9770600	1.8165300
H	0.9911850	4.1577470	-0.1507020
C	-1.2170210	1.6038710	3.1311730
C	-4.0583340	2.0402010	-2.1453500
H	-2.4888470	3.6685790	0.9773970
C	-2.0414660	0.6233010	-2.6125040
C	-4.2139410	3.5759030	-0.2952480
O	4.9817680	-2.2328290	0.0104360
H	1.1295530	4.0569420	-4.0069570
H	3.0362070	2.4873600	-4.3345600
C	6.1616670	-0.9576380	-1.6002880
C	4.0472160	-3.6576850	1.6618960
H	-0.2358960	3.6180820	4.6010610
C	0.8000310	4.8296040	3.1588420
H	1.7460300	5.8192870	1.4886110
H	-2.1996580	1.5452240	2.6503170
H	-1.3760310	1.6681410	4.2121360
H	-0.7163690	0.6546720	2.9146820
H	-4.5008790	1.5863530	-3.0291490
H	-1.4798250	-0.0920170	-2.0019970
H	-1.3295530	1.1051230	-3.2927860
H	-2.7535400	0.0532800	-3.2169810
C	-4.7825160	2.9897150	-1.4246680
H	-4.7620270	4.3199120	0.2762200
H	6.3765830	-1.8676370	-2.1663770
H	6.9680090	-0.7834210	-0.8827250
H	6.1079190	-0.1110630	-2.2913930
H	4.8129420	-3.3281340	2.3688660
H	4.4073140	-4.5425550	1.1300490
H	3.1385250	-3.9118440	2.2148060
H	1.1323860	5.5555270	3.8960110
H	-5.7832200	3.2664600	-1.7445910

C	-0.8762700	-2.3789990	0.7832290
C	-2.0159300	-1.5075030	0.9646240
C	-2.5075460	-1.3126550	2.3042670
C	-1.8637050	-1.8404060	3.3932430
C	-0.7161930	-2.6671080	3.2135130
C	-0.2659270	-2.9542290	1.9486520
H	-0.7396940	-2.8722870	-0.1779270
H	-3.4241750	-0.7400890	2.4258800
H	-2.2473060	-1.6621770	4.3944240
H	-0.2283750	-3.1070290	4.0789950
H	0.5574190	-3.6516910	1.8183890
N	-2.9358580	-1.3236670	-0.1295170
H	-3.1899580	-0.3586420	-0.3005190
C	-3.9762510	-2.2283880	-0.3762540
C	-3.9750410	-3.5359580	0.1409610
C	-5.0421780	-1.8343770	-1.2088190
C	-5.0053820	-4.4177060	-0.1837430
H	-3.1744700	-3.8548550	0.7989030
C	-6.0640790	-2.7247170	-1.5220700
H	-5.0596980	-0.8201220	-1.6020600
C	-6.0553480	-4.0278320	-1.0163940
H	-4.9847050	-5.4240000	0.2279490
H	-6.8770910	-2.3948130	-2.1645640
H	-6.8540160	-4.7215650	-1.2621520

(PAd-DalPhos)Ni(η^2-PhMorpholine)



Zero-point correction= 0.794979 (Hartree/Particle)
Thermal correction to Energy= 0.840204
Thermal correction to Enthalpy= 0.841148
Thermal correction to Gibbs Free Energy= 0.719518
Sum of electronic and zero-point Energies= -4098.496934
Sum of electronic and thermal Energies= -4098.451709
Sum of electronic and thermal Enthalpies= -4098.450765

Sum of electronic and thermal Free Energies= -4098.572396

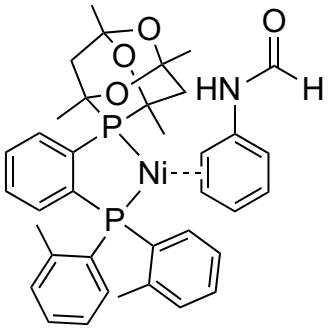
Single-point energy (6-311+G(2d,2p)) = -4100.109716

Ni	0.0212430	-0.8298700	-0.5640800
P	-1.9115100	-0.2306850	0.2050450
P	0.8669270	1.0879160	0.0478170
C	-1.5148350	1.0053720	1.5308870
C	-0.2281420	1.5863790	1.4639400
C	-3.1705420	-1.4198810	0.9823240
C	-3.2388210	0.5688440	-0.9132910
C	0.6689310	2.5231750	-1.1181260
C	2.5466770	1.3649210	0.7664350
O	-4.3322360	-0.7439470	1.5253900
O	-3.7141820	-0.4846740	-1.7818140
C	0.1905190	2.4638350	2.4726980
C	-2.3464450	1.3247490	2.6174050
C	-4.4185950	1.0948840	-0.0919370
C	-3.6423550	-2.3202140	-0.1678120
C	-2.5513260	-2.2111960	2.1231670
C	-2.6521870	1.6288810	-1.8255660
C	0.8171700	2.3499310	-2.5137500
C	0.3208580	3.7910690	-0.6259320
C	2.9823460	0.5535390	1.8427260
C	3.4130790	2.3349810	0.2407620
H	1.1887550	2.8903520	2.4309650
C	-0.6465370	2.7725390	3.5442420
C	-1.9164080	2.1992580	3.6155390
H	-3.3215910	0.8601500	2.6961680
C	-5.1649800	-0.0654810	0.5817460
H	-4.0797580	1.8198220	0.6530330
H	-5.1202110	1.6012340	-0.7659540
H	-4.2617490	-3.1261410	0.2439200
H	-2.7877530	-2.7613520	-0.6819820
C	-4.4886390	-1.5157720	-1.1619770
H	-3.2875290	-2.9181620	2.5238930
H	-2.2317470	-1.5497080	2.9339290
H	-1.6803780	-2.7666310	1.7615540
H	-3.4318920	2.0061370	-2.4976770
H	-1.8443010	1.2092400	-2.4292780
H	-2.2514240	2.4651870	-1.2456470
C	0.6122550	3.4530250	-3.3539130
C	0.1192790	4.8766170	-1.4768470
H	0.1912670	3.9342430	0.4404590
C	1.1673340	1.0230080	-3.1403030
C	4.2606480	0.7770310	2.3678800
H	3.0827400	2.9557990	-0.5855170

C	2.1084460	-0.5121940	2.4589760
C	4.6910380	2.5280670	0.7689350
O	-5.5924620	-0.9572000	-0.4471050
H	-0.3038070	3.4483820	4.3232080
H	-2.5708140	2.4216000	4.4542760
C	-6.4023640	0.3709850	1.3399720
C	-5.0579000	-2.3550700	-2.2873140
H	0.7200780	3.3176960	-4.4272860
C	0.2661850	4.7058270	-2.8519870
H	-0.1535290	5.8443490	-1.0648960
H	2.1691720	0.6887350	-2.8495490
H	1.1433110	1.0921970	-4.2323650
H	0.4677100	0.2385580	-2.8251370
H	4.5937300	0.1659760	3.2038300
H	1.5792700	-1.0954010	1.6980510
H	1.3486430	-0.0760300	3.1189740
H	2.7103080	-1.2049090	3.0553740
C	5.1133790	1.7512220	1.8457560
H	5.3439590	3.2854420	0.3438490
H	-6.8906900	-0.5054190	1.7738430
H	-7.0993760	0.8701840	0.6613730
H	-6.1278330	1.0612960	2.1433040
H	-5.6658190	-1.7236770	-2.9405350
H	-5.6824830	-3.1544880	-1.8794440
H	-4.2444530	-2.7947640	-2.8715590
H	0.1081260	5.5387300	-3.5317220
H	6.1017260	1.8941290	2.2740310
C	2.3155960	-2.6779910	-0.3726290
C	1.3431270	-2.1736280	-1.3223750
C	0.0144760	-2.7222110	-1.3394220
C	-0.3157590	-3.7960700	-0.4492770
C	0.6139320	-4.2316200	0.4597690
C	1.9194810	-3.6764430	0.5097820
H	1.7056140	-1.7054180	-2.2301390
H	-0.5873560	-2.5962410	-2.2395830
H	0.3744390	-5.0470080	1.1382320
H	2.6120830	-4.0886110	1.2319200
H	-1.2820840	-4.2859460	-0.5244130
C	4.6597350	-2.9107280	0.3170180
C	4.0866580	-1.4442820	-1.5480810
C	5.9452970	-2.1039140	0.4734570
H	4.8670240	-3.8467240	-0.2308720
H	4.3258800	-3.1794250	1.3222440
C	5.3940760	-0.7047760	-1.2904380
H	4.2204820	-2.1485210	-2.3889530
H	3.3458400	-0.6997150	-1.8420190

H	6.7446630	-2.7504690	0.8457200
H	5.7856660	-1.2841570	1.1893290
H	5.7866970	-0.3086060	-2.2309060
H	5.2232870	0.1291570	-0.5960480
O	6.3961360	-1.5683850	-0.7635120
N	3.6134130	-2.1356490	-0.3495690

(PAd-DalPhos)Ni(η^2-PhHCONH)



Zero-point correction= 0.705036 (Hartree/Particle)
Thermal correction to Energy= 0.748000
Thermal correction to Enthalpy= 0.748944
Thermal correction to Gibbs Free Energy= 0.631172
Sum of electronic and zero-point Energies= -3980.670163
Sum of electronic and thermal Energies= -3980.627200
Sum of electronic and thermal Enthalpies= -3980.626256
Sum of electronic and thermal Free Energies= -3980.744028

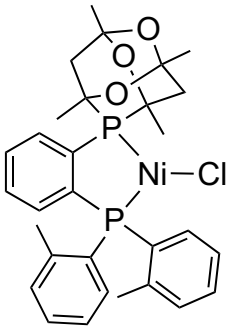
Single-point energy (6-311+G(2d,2p)) = -3982.151553

Ni	0.30744	1.04572	0.26308
P	-1.45081	-0.06725	-0.3675
P	1.5127	-0.7668	0.07059
C	-0.79221	-1.50168	-1.34037
C	0.58195	-1.77843	-1.16875
C	-2.89132	0.61616	-1.39797
C	-2.61645	-0.76305	0.96696
C	1.69747	-1.9489	1.48872
C	3.20012	-0.64711	-0.65819
O	-3.89263	-0.38628	-1.69479
O	-3.28981	0.38397	1.53264
C	1.19882	-2.76304	-1.95044
C	-1.51742	-2.23996	-2.29081
C	-3.66423	-1.70001	0.36324
C	-3.54328	1.69497	-0.52291
C	-2.41716	1.16468	-2.73487
C	-1.83862	-1.40065	2.1037

C	1.9794	-1.4563	2.78408
C	1.50166	-3.32773	1.31244
C	3.38625	-0.00587	-1.91
C	4.32072	-1.05025	0.08553
H	2.26285	-2.94997	-1.83245
C	0.46774	-3.48519	-2.89262
C	-0.89297	-3.22306	-3.0587
H	-2.56599	-2.02066	-2.45075
C	-4.60203	-0.92195	-0.57211
H	-3.1848	-2.5247	-0.17151
H	-4.26998	-2.12429	1.17308
H	-4.30441	2.21818	-1.11378
H	-2.79931	2.42101	-0.18918
C	-4.23252	1.0485	0.68823
H	-3.26585	1.58992	-3.28271
H	-1.96713	0.37982	-3.34931
H	-1.66932	1.94861	-2.57731
H	-2.53122	-1.71906	2.89154
H	-1.12869	-0.68569	2.52854
H	-1.28035	-2.27324	1.75123
C	2.0635	-2.3656	3.84619
C	1.5837	-4.21667	2.38375
H	1.27199	-3.71889	0.32886
C	2.1741	0.0116	3.05509
C	4.69786	0.22059	-2.35041
H	4.17784	-1.55048	1.03824
C	2.24082	0.41647	-2.80513
C	5.61532	-0.81966	-0.37834
O	-5.20192	0.12444	0.18892
H	0.95944	-4.24101	-3.49898
H	-1.46886	-3.7738	-3.79762
C	-5.72479	-1.76546	-1.14103
C	-4.96539	2.04104	1.56707
H	2.28108	-1.98535	4.84122
C	1.86739	-3.73257	3.65909
H	1.42512	-5.27865	2.2176
H	2.9989	0.43332	2.47025
H	2.38843	0.18865	4.11366
H	1.28382	0.58905	2.78506
H	4.8453	0.72855	-3.29991
H	1.36934	0.75215	-2.2324
H	1.90748	-0.41649	-3.43636
H	2.54798	1.2409	-3.45466
C	5.8046	-0.17549	-1.6002
H	6.46737	-1.13952	0.21525
H	-6.35953	-1.14428	-1.77815

H	-6.32843	-2.17945	-0.32885
H	-5.31448	-2.58629	-1.73685
H	-5.4597	1.50756	2.38299
H	-5.71742	2.57727	0.98195
H	-4.25611	2.75834	1.98962
H	1.93278	-4.41186	4.50471
H	6.80726	0.02214	-1.96879
C	-0.03704	3.01395	0.31275
C	1.38842	2.78836	0.43196
C	2.01443	3.03545	1.70583
C	1.27776	3.35991	2.81337
C	-0.13482	3.5341	2.70989
C	-0.75635	3.40549	1.49382
H	-0.46932	3.24925	-0.65826
H	3.09826	2.96826	1.7571
H	1.77182	3.52254	3.76732
H	-0.70835	3.8166	3.58809
H	-1.81855	3.61799	1.40731
N	2.2329	2.89986	-0.73167
H	2.92851	2.17872	-0.89747
C	2.17846	3.89484	-1.65271
H	1.43552	4.67299	-1.40338
O	2.86638	3.94394	-2.6696

(PAd-DalPhos)NiCl



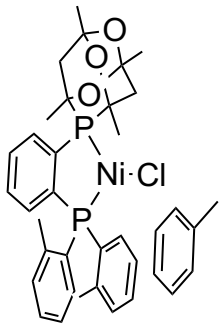
Zero-point correction= 0.577585 (Hartree/Particle)
Thermal correction to Energy= 0.614113
Thermal correction to Enthalpy= 0.615057
Thermal correction to Gibbs Free Energy= 0.508903
Sum of electronic and zero-point Energies= -4040.097886
Sum of electronic and thermal Energies= -4040.061359
Sum of electronic and thermal Enthalpies= -4040.060415
Sum of electronic and thermal Free Energies= -4040.166568

Single-point energy (6-311+G(2d,2p)) = -4041.351185

Ni	0.2460210	0.0241620	-1.5905020
P	-1.2842830	-0.2763970	-0.0379810
P	1.7824250	0.0170440	0.0170030
C	-0.4237660	-0.9967980	1.4219400
C	0.9849040	-0.8654010	1.4313130
C	-2.7730650	-1.3650630	-0.4258710
C	-2.3448140	1.1917460	0.5279160
C	2.1920280	1.6874030	0.6599500
C	3.3955630	-0.8370960	-0.1770680
O	-3.6779610	-1.4632980	0.6964810
O	-3.0965960	1.5855870	-0.6350950
C	1.7307770	-1.4495770	2.4622540
C	-1.0485680	-1.7226780	2.4481110
C	-3.3214970	0.7749490	1.6297090
C	-3.4796580	-0.6455220	-1.5850940
C	-2.3574980	-2.7811660	-0.7889240
C	-1.4856360	2.3837300	0.9093970
C	2.5714660	2.6957320	-0.2591320
C	2.0649630	1.9966900	2.0215520
C	3.4314320	-2.0982360	-0.8195210
C	4.5860430	-0.2411580	0.2629370
H	2.8136120	-1.3634330	2.4558970
C	1.0956340	-2.1590110	3.4816800
C	-0.2933480	-2.2979260	3.4706630
H	-2.1227320	-1.8660850	2.4238380
C	-4.3324580	-0.2476750	1.0861160
H	-2.7867480	0.3685560	2.4929680
H	-3.8777460	1.6604860	1.9593860
H	-4.2871480	-1.2870060	-1.9569140
H	-2.7789400	-0.4521940	-2.4037100
C	-4.0999610	0.6678540	-1.0887520
H	-3.2453530	-3.3684180	-1.0488710
H	-1.8508230	-3.2725640	0.0473410
H	-1.6810920	-2.7614270	-1.6494970
H	-2.1290890	3.2360560	1.1558840
H	-0.8326810	2.6667620	0.0789160
H	-0.8607470	2.1511140	1.7771250
C	2.8107600	3.9831150	0.2363320
C	2.3035050	3.2885040	2.4905790
H	1.7705790	1.2234190	2.7232750
C	2.7246350	2.4263370	-1.7373120
C	4.6757070	-2.7164620	-0.9873370
H	4.5515750	0.7287450	0.7491940
C	2.1834260	-2.7861000	-1.3208940
C	5.8151200	-0.8745160	0.0779860
O	-4.9990730	0.3470210	-0.0219710

H	1.6846880	-2.6121050	4.2742330
H	-0.7906110	-2.8657080	4.2523250
C	-5.3935180	-0.6413150	2.0935730
C	-4.8911350	1.3990490	-2.1518330
H	3.1039440	4.7638940	-0.4609170
C	2.6766470	4.2857480	1.5916660
H	2.1974550	3.5094640	3.5489910
H	3.4439810	1.6231230	-1.9358000
H	3.0745220	3.3226510	-2.2580300
H	1.7762000	2.1199900	-2.1973580
H	4.7155970	-3.6847360	-1.4799880
H	1.6606600	-2.1791240	-2.0716480
H	1.4696200	-2.9783470	-0.5104560
H	2.4318690	-3.7480520	-1.7794660
C	5.8576730	-2.1181550	-0.5493320
H	6.7283160	-0.3973630	0.4224940
H	-6.0855560	-1.3509270	1.6330530
H	-5.9494690	0.2436710	2.4146540
H	-4.9297180	-1.1101800	2.9666900
H	-5.3248040	2.3066330	-1.7238340
H	-5.6950560	0.7593060	-2.5258040
H	-4.2305800	1.6712640	-2.9795430
H	2.8638000	5.2974980	1.9409160
H	6.8076530	-2.6229690	-0.7022260
Cl	-0.0552360	0.0061930	-3.7397260

(PAd-DalPhos)NiCl–toluene post-reaction complex



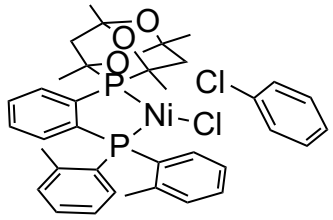
Zero-point correction= 0.707184 (Hartree/Particle)
Thermal correction to Energy= 0.751806
Thermal correction to Enthalpy= 0.752750
Thermal correction to Gibbs Free Energy= 0.626829
Sum of electronic and zero-point Energies= -4311.552021
Sum of electronic and thermal Energies= -4311.507399
Sum of electronic and thermal Enthalpies= -4311.506455
Sum of electronic and thermal Free Energies= -4311.632376

Single-point energy (6-311+G(2d,2p)) = -4.313010095233E+03

Ni	-0.0019030	-0.7258610	-0.8300510
P	-1.8672510	-0.2265650	0.2384140
P	0.9278150	1.0833150	0.0751030
C	-1.4282450	0.9283380	1.6016860
C	-0.1484060	1.5227810	1.5136070
C	-2.9438070	-1.5959250	0.9569840
C	-3.2841310	0.5294740	-0.7734070
C	0.8533620	2.5378860	-1.0448590
C	2.6127560	1.1038030	0.7983720
O	-4.1353630	-1.0723030	1.5841640
O	-3.6710190	-0.4922170	-1.7096790
C	0.2976440	2.3661540	2.5388120
C	-2.2259670	1.1863110	2.7279830
C	-4.4831700	0.8610340	0.1177010
C	-3.3425170	-2.4455770	-0.2595850
C	-2.2048160	-2.4019460	2.0128490
C	-2.8042780	1.7105440	-1.5980070
C	1.3806860	2.4189100	-2.3537150
C	0.2216910	3.7270690	-0.6542630
C	2.9997450	0.0491060	1.6584120
C	3.5207620	2.1255420	0.4887780
H	1.2894070	2.8050000	2.4779470
C	-0.5102790	2.6245340	3.6458420
C	-1.7695620	2.0292940	3.7414050
H	-3.1894080	0.6989170	2.8239620
C	-5.0753890	-0.4270210	0.7124100
H	-4.2010200	1.5593650	0.9107170
H	-5.2558080	1.3377360	-0.4971620
H	-3.8649970	-3.3420340	0.0943590
H	-2.4570550	-2.7525480	-0.8253210
C	-4.3015810	-1.6561120	-1.1614340
H	-2.8494920	-3.2110390	2.3740760
H	-1.9244070	-1.7761500	2.8656460
H	-1.2974010	-2.8378260	1.5825090
H	-3.6239000	2.0769870	-2.2266390
H	-1.9735610	1.4126850	-2.2442480
H	-2.4650870	2.5250650	-0.9505390
C	1.2528910	3.5119170	-3.2190720
C	0.1003170	4.8004900	-1.5366980
H	-0.1848570	3.8160950	0.3475010
C	2.0678280	1.1638420	-2.8371920
C	4.2945210	0.0697550	2.1850050
H	3.2189440	2.9290750	-0.1757410
C	2.0603180	-1.0709560	2.0341060

C	4.8097240	2.1204000	1.0216420
O	-5.4331860	-1.2811340	-0.3680000
H	-0.1518020	3.2769230	4.4372420
H	-2.3942080	2.2115060	4.6116350
C	-6.3251490	-0.1924770	1.5363430
C	-4.8104700	-2.4552440	-2.3415750
H	1.6569820	3.4305520	-4.2249680
C	0.6180150	4.6902380	-2.8256360
H	-0.3945120	5.7128480	-1.2156870
H	2.8895060	0.8666010	-2.1761360
H	2.4813460	1.3129310	-3.8392640
H	1.3746980	0.3138330	-2.8849940
H	4.6078330	-0.7439180	2.8324430
H	1.5906780	-1.5193590	1.1499470
H	1.2500970	-0.7170360	2.6844800
H	2.5974010	-1.8618330	2.5643360
C	5.1949060	1.0880920	1.8740450
H	5.5036650	2.9173180	0.7689470
H	-6.7000440	-1.1497330	1.9073810
H	-7.0952490	0.2784860	0.9194670
H	-6.1000770	0.4572160	2.3875250
H	-5.5060380	-1.8441920	-2.9227710
H	-5.3279150	-3.3523350	-1.9909290
H	-3.9692960	-2.7463620	-2.9765400
H	0.5302470	5.5169760	-3.5252160
H	6.1980850	1.0666830	2.2906930
Cl	0.1683360	-2.4645650	-2.1320500
C	6.2109840	-2.3993560	0.4275650
C	5.1544700	-3.2762880	0.6760120
C	3.9705700	-3.2130510	-0.0725070
C	3.8678310	-2.2367510	-1.0736300
C	4.9237520	-1.3570800	-1.3230050
C	6.0994020	-1.4346270	-0.5757400
H	7.1215990	-2.4693940	1.0178270
H	5.2512970	-4.0280850	1.4572390
H	2.9531530	-2.1717700	-1.6567380
H	4.8277480	-0.6116200	-2.1083080
H	6.9190700	-0.7481260	-0.7697940
C	2.8453180	-4.1919130	0.1713470
H	2.7052290	-4.3835010	1.2422740
H	1.9024390	-3.8276150	-0.2467640
H	3.0580110	-5.1597810	-0.3022450

(PAd-DalPhos)NiCl–chlorobenzene pre-reaction complex



Zero-point correction= 0.669680 (Hartree/Particle)
Thermal correction to Energy= 0.713908
Thermal correction to Enthalpy= 0.714852
Thermal correction to Gibbs Free Energy= 0.588385
Sum of electronic and zero-point Energies= -4731.869021
Sum of electronic and thermal Energies= -4731.824793
Sum of electronic and thermal Enthalpies= -4731.823849
Sum of electronic and thermal Free Energies= -4731.950316

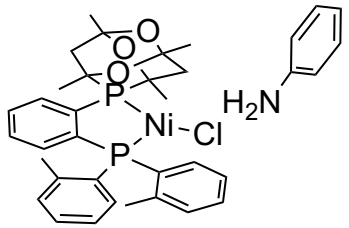
Single-point energy (6-311+G(2d,2p)) = -4.733303470830E+03

Ni1	0.0274528348	0.5764171972	-1.2422991097
Cl2	-0.3495380535	0.8621364117	-3.3693474546
Cl3	-0.3705495599	5.4143345361	0.3553833121
P4	-1.3683577412	-0.0531199571	0.3520481744
P5	1.7096978245	0.1834698790	0.1659941035
O6	-3.7089275604	-1.4150976316	0.9405281187
O7	-3.1743372184	1.9007677884	0.5675915616
O8	-5.0396099534	0.5246182500	0.9773138159
C9	-0.3905709316	-1.1795163789	1.4340152933
C10	1.0161281785	-1.0490731123	1.3541303377
C11	-2.9264249706	-0.9674891578	-0.1879524461
C12	-2.3155649742	1.1660403208	1.4580799064
C13	2.2166750063	1.6214899134	1.1869686248
C14	3.2797698934	-0.5892273163	-0.3921935641
C15	1.8372951447	-1.8975691781	2.1066881229
C16	-0.9366390623	-2.1779085882	2.2559626307
C17	-3.1813698206	0.4208469266	2.4769833653
C18	-3.7314808911	0.0783666658	-0.9770972638
C19	-2.5976370369	-2.1959039299	-1.0203667544
C20	-1.3844481843	2.1760683586	2.1015758866
C21	2.5666531589	2.8297391475	0.5382195197
C22	2.1970711607	1.5619249331	2.5879914451
C23	3.2342520147	-1.6548577009	-1.3235227365
C24	4.5167090769	-0.1105789912	0.0631796578
C25	1.2801573100	-2.8743945946	2.9318486026
C26	-0.1067041920	-3.0179614137	2.9990865812
C27	-4.2768906324	-0.3843517859	1.7617465963

C28	-4.2521136958	1.1691703822	-0.0298177752
C29	2.8835759341	3.9380072930	1.3329571338
C30	2.5116858256	2.6806136110	3.3586774426
C31	2.6234894830	2.9524322286	-0.9652876080
C32	4.4473385589	-2.2023427288	-1.7567591069
C33	1.9350442258	-2.2131684527	-1.8542746571
C34	5.7123975260	-0.6687540354	-0.3889732925
C35	-5.2341431871	-1.0776093997	2.7098516185
C36	-5.1339751894	2.1943868922	-0.7084173722
C37	2.8546507235	3.8744344207	2.7261654226
C38	5.6752698097	-1.7198934819	-1.3029879947
C39	-3.4952926875	5.8879232895	-2.1386207623
C40	-2.5855769533	6.0796439295	-1.0971599465
C41	-1.5424826277	5.1680135824	-0.9421726687
C42	-1.3954551223	4.0731889606	-1.7893826623
C43	-2.3100818933	3.8966389333	-2.8293376331
C44	-3.3568063805	4.8035457483	-3.0083403099
H45	2.9168117345	-1.8051693690	2.0296114547
H46	-2.0110606102	-2.3170129301	2.2850969608
H47	-2.5699259336	-0.2303847036	3.1075451544
H48	-3.6701313710	1.1590728559	3.1237551167
H49	-4.5939444428	-0.4177803331	-1.4372087832
H50	-3.1184084968	0.5185710682	-1.7697733153
H51	-3.5266380908	-2.6740278279	-1.3508285098
H52	-2.0219265106	-2.9238722112	-0.4403618320
H53	-2.0147800680	-1.9048268866	-1.9002521598
H54	-1.9737403369	2.9175671193	2.6526513746
H55	-0.7925325307	2.7003515183	1.3484797487
H56	-0.7009833235	1.6805298120	2.7979230472
H57	1.9267984305	0.6348692019	3.0828103011
H58	4.5449544718	0.7089538363	0.7743169003
H59	1.9271365688	-3.5300214853	3.5080093073
H60	-0.5451472609	-3.7922638834	3.6226805344
H61	3.1496071003	4.8711033147	0.8435879599
H62	2.4868424959	2.6167539154	4.4428958214
H63	3.3930289912	2.3007368712	-1.3972516424
H64	2.8478193226	3.9808250626	-1.2614751738
H65	1.6746359707	2.6675897103	-1.4359643718
H66	4.4242895596	-3.0205124493	-2.4722260580
H67	1.3513813076	-1.4489199984	-2.3827901053
H68	1.3003238198	-2.6046726683	-1.0499189775
H69	2.1263436145	-3.0325002415	-2.5539449963
H70	6.6615539331	-0.2829312781	-0.0276933777
H71	-5.9950456968	-1.6092321408	2.1327925974
H72	-5.7225808406	-0.3396946697	3.3519390695
H73	-4.6936701903	-1.7951775266	3.3346038178

H74	-5.5006071758	2.9052845446	0.0366911394
H75	-5.9866461771	1.6989756764	-1.1811095731
H76	-4.5596221336	2.7363650626	-1.4630039109
H77	3.0986439279	4.7560380786	3.3124265595
H78	6.5980774260	-2.1639976482	-1.6661583070
H79	-4.3098489650	6.5949151024	-2.2703676578
H80	-2.6805202214	6.9212903319	-0.4191676580
H81	-0.5894739000	3.3615839815	-1.6527391118
H82	-2.1829580316	3.0424543723	-3.4871128044
H83	-4.0628918671	4.6662453798	-3.8225748047

(PAd-DalPhos)NiCl–aniline post-reaction complex



Zero-point correction= 0.696234 (Hartree/Particle)
Thermal correction to Energy= 0.740590
Thermal correction to Enthalpy= 0.741534
Thermal correction to Gibbs Free Energy= 0.614739
Sum of electronic and zero-point Energies= -4327.605689
Sum of electronic and thermal Energies= -4327.561333
Sum of electronic and thermal Enthalpies= -4327.560388
Sum of electronic and thermal Free Energies= -4327.687184

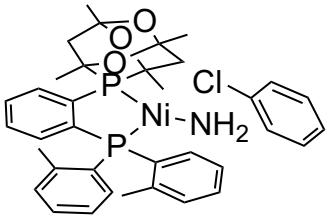
Single-point energy (6-311+G(2d,2p)) = -4.329061399370E+03

Ni	-0.4067270	-0.6186060	-1.1295360
P	0.3684630	1.2198520	-0.1844550
P	-2.2819370	-0.3513160	0.0395240
C	-1.1150430	2.1848670	0.3240110
C	-2.3211940	1.4529410	0.4342640
C	1.4669760	2.3332530	-1.2362130
C	1.5915480	1.1724100	1.2671660
C	-2.2600890	-1.2090820	1.6616890
C	-3.9404520	-0.6824100	-0.6715630
O	1.8561310	3.5299120	-0.5283290
O	2.7707890	0.5359980	0.7468160
C	-3.5094830	2.1164100	0.7630170
C	-1.1379330	3.5730290	0.5303170
C	1.9495990	2.5868120	1.7304700
C	2.7150400	1.4814780	-1.5180420

C	0.7643850	2.7753210	-2.5094480
C	1.0855740	0.3002790	2.4023290
C	-1.9683980	-2.5947510	1.6965970
C	-2.4428540	-0.5034390	2.8593490
C	-4.2087580	-0.2900740	-2.0051050
C	-4.9224310	-1.3506350	0.0736210
H	-4.4365700	1.5542980	0.8297860
C	-3.5145110	3.4944730	0.9798410
C	-2.3294470	4.2217750	0.8564910
H	-0.2278800	4.1473470	0.4005200
C	2.6980800	3.3374000	0.6186820
H	1.0549520	3.1361850	2.0365900
H	2.6164940	2.5114630	2.5975340
H	3.3479820	2.0149060	-2.2366080
H	2.4362160	0.5153550	-1.9501730
C	3.5220200	1.2788360	-0.2281180
H	1.4479870	3.3839720	-3.1117840
H	-0.1240870	3.3735450	-2.2846210
H	0.4627600	1.8991070	-3.0925030
H	1.8670370	0.2029820	3.1643120
H	0.8181400	-0.6976150	2.0442070
H	0.1967430	0.7419170	2.8625640
C	-1.8615470	-3.2143390	2.9476620
C	-2.3312750	-1.1430630	4.0938720
H	-2.6663610	0.5579400	2.8290050
C	-1.7839940	-3.4148390	0.4419910
C	-5.4697760	-0.5838370	-2.5362440
H	-4.7072070	-1.6535530	1.0936200
C	-3.1896940	0.4286870	-2.8577690
C	-6.1698520	-1.6378440	-0.4805940
O	3.8498550	2.5758300	0.2829450
H	-4.4432180	3.9997270	1.2299400
H	-2.3327640	5.2983620	1.0031250
C	3.1708440	4.7161050	1.0327370
C	4.8175850	0.5287480	-0.4393540
H	-1.6340610	-4.2764730	2.9852070
C	-2.0341330	-2.5039980	4.1361570
H	-2.4737400	-0.5794690	5.0116490
H	-2.6734670	-3.3838990	-0.1986670
H	-1.5836340	-4.4607830	0.6897340
H	-0.9449910	-3.0543820	-0.1651500
H	-5.6872260	-0.2882980	-3.5595420
H	-2.2766810	-0.1667190	-2.9869910
H	-2.8894490	1.3860930	-2.4145010
H	-3.5974530	0.6370160	-3.8515420
C	-6.4427530	-1.2511160	-1.7913370

H	-6.9183610	-2.1592070	0.1093920
H	3.7105830	5.1784520	0.2024290
H	3.8394860	4.6376240	1.8941870
H	2.3158390	5.3454830	1.2976920
H	5.3418310	0.4280330	0.5136250
H	5.4498200	1.0808720	-1.1404430
H	4.6168970	-0.4680500	-0.8371770
H	-1.9379180	-3.0152100	5.0900460
H	-7.4090230	-1.4697860	-2.2375330
Cl	0.4633900	-1.7601070	-2.7716070
C	5.6626040	-2.8778760	0.9467980
C	4.2772340	-2.8337250	1.0846590
C	3.4425730	-2.9955670	-0.0348950
C	4.0354240	-3.2048360	-1.2930900
C	5.4231770	-3.2486520	-1.4188030
C	6.2498200	-3.0845250	-0.3042020
H	6.2883050	-2.7465940	1.8263810
H	3.8292760	-2.6645450	2.0612780
H	3.3975900	-3.3271880	-2.1647050
H	5.8606160	-3.4086800	-2.4012940
H	7.3304100	-3.1179660	-0.4080990
N	2.0498310	-2.9969650	0.1021710
H	1.5527330	-2.7561580	-0.7529890
H	1.7190200	-2.4258160	0.8714720

(PAd-DalPhos)NiNH_2–chlorobenzene pre-reaction complex



Zero-point correction= 0.692974 (Hartree/Particle)
Thermal correction to Energy= 0.737672
Thermal correction to Enthalpy= 0.738616
Thermal correction to Gibbs Free Energy= 0.613938
Sum of electronic and zero-point Energies= -4327.537188
Sum of electronic and thermal Energies= -4327.492491
Sum of electronic and thermal Enthalpies= -4327.491546
Sum of electronic and thermal Free Energies= -4327.616224

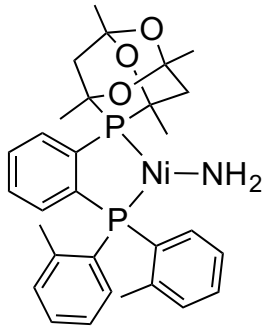
Single-point energy (6-311+G(2d,2p)) = -4.328987104964E+03

Ni 0.3617930 -0.0838900 -1.5313520

P	-1.0035390	-1.2096870	-0.2198420
P	1.9460660	-0.4522560	0.0085220
C	0.0538380	-2.3865300	0.7264350
C	1.4171050	-2.0221700	0.8333330
C	-2.3315500	-2.2206640	-1.1051300
C	-2.2450010	-0.4345740	0.9921610
C	2.0011170	0.7881880	1.3655520
C	3.7119560	-0.7634060	-0.4044410
O	-3.1361490	-3.0119600	-0.2006590
O	-3.1338560	0.3485900	0.1627630
C	2.3144930	-2.8770470	1.4843230
C	-0.3705710	-3.6122640	1.2619690
C	-3.0701380	-1.4982110	1.7199760
C	-3.2250650	-1.1635700	-1.7731810
C	-1.7239000	-3.1843090	-2.1109670
C	-1.5747120	0.5278510	1.9556580
C	2.0627830	2.1617540	1.0296960
C	1.9062890	0.4054710	2.7109930
C	4.0279770	-1.5989320	-1.5035320
C	4.7432820	-0.1418070	0.3144970
H	3.3631440	-2.6017610	1.5521740
C	1.8763130	-4.0868150	2.0241610
C	0.5351600	-4.4557700	1.9069580
H	-1.4034890	-3.9191660	1.1427470
C	-3.9424250	-2.2773210	0.7264520
H	-2.4197390	-2.1779430	2.2773300
H	-3.7328890	-0.9977890	2.4362510
H	-3.9469970	-1.6697810	-2.4250250
H	-2.6180650	-0.4836290	-2.3796890
C	-4.0087050	-0.3877130	-0.7044050
H	-2.5222500	-3.7098270	-2.6473870
H	-1.0932500	-3.9276880	-1.6138230
H	-1.1130150	-2.6311040	-2.8314690
H	-2.3390610	1.0633400	2.5302940
H	-0.9567060	1.2592250	1.4309230
H	-0.9325640	-0.0195420	2.6516780
C	2.0048480	3.1004730	2.0665750
C	1.8518630	1.3583160	3.7283720
H	1.8624250	-0.6480060	2.9675130
C	2.1954110	2.6350590	-0.3969530
C	5.3764000	-1.7804890	-1.8311010
H	4.4977540	0.4999370	1.1546410
C	2.9623790	-2.2909050	-2.3193480
C	6.0805900	-0.3324260	-0.0349800
O	-4.7702780	-1.3356070	0.0461890
H	2.5827700	-4.7441120	2.5237970

H	0.1937990	-5.4060860	2.3085650
C	-4.8599150	-3.2860240	1.3872110
C	-4.9790090	0.6228220	-1.2795860
H	2.0391110	4.1573890	1.8163390
C	1.8936540	2.7125000	3.4021170
H	1.7724200	1.0416620	4.7646940
H	3.1021570	2.2418200	-0.8725370
H	2.2343520	3.7264990	-0.4396100
H	1.3490150	2.3058650	-1.0103390
H	5.6274090	-2.4203200	-2.6737160
H	2.2448520	-1.5665550	-2.7258570
H	2.3890850	-3.0062110	-1.7165730
H	3.4105510	-2.8414090	-3.1525480
C	6.3971870	-1.1571020	-1.1126240
H	6.8647210	0.1602200	0.5334130
H	-5.4623810	-3.7838730	0.6230930
H	-5.5238000	-2.7805010	2.0936800
H	-4.2708520	-4.0368620	1.9224220
H	-5.5187290	1.1140340	-0.4657640
H	-5.6967460	0.1212850	-1.9342580
H	-4.4341680	1.3772770	-1.8541730
H	1.8409040	3.4677460	4.1813620
H	7.4339520	-1.3146170	-1.3976880
N	0.2657930	0.4455990	-3.2960460
H	0.3623170	1.4043640	-3.6231640
H	0.3914280	-0.1665740	-4.0996940
C	-1.6648110	3.2830480	-0.5759670
C	-1.3396700	3.1321900	-1.9259570
C	-0.5907500	4.1086490	-2.5864270
C	-0.1560790	5.2399980	-1.8930380
C	-0.4627370	5.4006870	-0.5400920
C	-1.2157510	4.4162940	0.0988890
H	-2.2526490	2.5270280	-0.0700120
H	-1.6512200	2.2343410	-2.4505210
H	-0.3448890	3.9865030	-3.6375290
H	0.4258930	6.0038190	-2.4015470
H	-0.1290400	6.2748840	0.0091940
Cl	-1.6084170	4.6132530	1.8076990

(PAd-DalPhos)NiNH$_2$



Zero-point correction= 0.600330 (Hartree/Particle)
Thermal correction to Energy= 0.637566
Thermal correction to Enthalpy= 0.638510
Thermal correction to Gibbs Free Energy= 0.532344
Sum of electronic and zero-point Energies= -3635.765878
Sum of electronic and thermal Energies= -3635.728642
Sum of electronic and thermal Enthalpies= -3635.727697
Sum of electronic and thermal Free Energies= -3635.833864

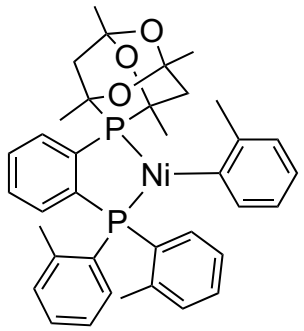
Single-point energy (6-311+G(2d,2p)) = -3637.035467

Ni	0.2280560	0.1405980	-1.7153370
P	-1.2878490	-0.2753540	-0.1843230
P	1.7539720	0.0233390	-0.0914980
C	-0.4526480	-1.0331970	1.2764210
C	0.9540150	-0.8939840	1.3044200
C	-2.7945250	-1.3436200	-0.5764640
C	-2.3435940	1.1830720	0.4251250
C	2.2290210	1.6502420	0.6221500
C	3.3428490	-0.8815060	-0.2988600
O	-3.6976840	-1.4638440	0.5471310
O	-3.1093000	1.6121540	-0.7196670
C	1.6923070	-1.4974140	2.3303250
C	-1.0840820	-1.7875870	2.2785030
C	-3.3135990	0.7501780	1.5262710
C	-3.5061220	-0.5952640	-1.7140940
C	-2.3964830	-2.7562370	-0.9717610
C	-1.4757500	2.3625400	0.8245800
C	2.7376620	2.6546250	-0.2388420
C	2.0103720	1.9437400	1.9761860
C	3.3357290	-2.1294920	-0.9669600
C	4.5551870	-0.3432690	0.1551500
H	2.7744670	-1.4026910	2.3387070
C	1.0514740	-2.2347830	3.3255360
C	-0.3367350	-2.3825480	3.2952130

H	-2.1572930	-1.9348500	2.2406720
C	-4.3366750	-0.2538140	0.9713020
H	-2.7738730	0.3205850	2.3749220
H	-3.8611830	1.6316730	1.8809950
H	-4.3175990	-1.2239030	-2.0996250
H	-2.8038410	-0.3803340	-2.5261990
C	-4.1180540	0.7092650	-1.1834030
H	-3.2904370	-3.3301390	-1.2415090
H	-1.8912340	-3.2699530	-0.1481910
H	-1.7208290	-2.7250660	-1.8326790
H	-2.1115380	3.2154840	1.0890900
H	-0.8219090	2.6536540	-0.0027110
H	-0.8493870	2.1096240	1.6852970
C	3.0035540	3.9176720	0.3044190
C	2.2795450	3.2110780	2.4930760
H	1.6203890	1.1757310	2.6355630
C	3.0164480	2.4010200	-1.7009860
C	4.5557570	-2.7900720	-1.1508510
H	4.5567260	0.6152120	0.6650680
C	2.0607580	-2.7644670	-1.4693770
C	5.7603880	-1.0174840	-0.0433210
O	-5.0114620	0.3690710	-0.1178520
H	1.6345630	-2.7021000	4.1144450
H	-0.8389770	-2.9715020	4.0580560
C	-5.3909010	-0.6609920	1.9808080
C	-4.9179630	1.4652690	-2.2232440
H	3.3940720	4.6935270	-0.3495630
C	2.7768100	4.2034190	1.6508620
H	2.0999600	3.4168560	3.5447500
H	3.8221860	1.6681480	-1.8339760
H	3.3216320	3.3256530	-2.2005310
H	2.1415510	1.9954950	-2.2242550
H	4.5592320	-3.7485420	-1.6643990
H	1.5004230	-2.0793510	-2.1200190
H	1.3908020	-3.0352170	-0.6435700
H	2.2782420	-3.6761900	-2.0344830
C	5.7590690	-2.2469370	-0.6995380
H	6.6899660	-0.5825800	0.3136130
H	-6.0927510	-1.3559490	1.5126970
H	-5.9370260	0.2209530	2.3263120
H	-4.9215870	-1.1513450	2.8390460
H	-5.3433800	2.3654610	-1.7719810
H	-5.7285780	0.8367470	-2.6019250
H	-4.2655850	1.7531940	-3.0522910
H	2.9886570	5.1968780	2.0369150
H	6.6900720	-2.7828060	-0.8636220

N	0.1777510	0.4046640	-3.5320460
H	-0.0833820	1.2775560	-3.9863130
H	0.3504600	-0.2848510	-4.2599890

(PAd-DalPhos)Ni(*ortho*-tolyl)



Zero-point correction= 0.693796 (Hartree/Particle)
Thermal correction to Energy= 0.735664
Thermal correction to Enthalpy= 0.736608
Thermal correction to Gibbs Free Energy= 0.619357
Sum of electronic and zero-point Energies= -3850.677344
Sum of electronic and thermal Energies= -3850.635477
Sum of electronic and thermal Enthalpies= -3850.634532
Sum of electronic and thermal Free Energies= -3850.751783

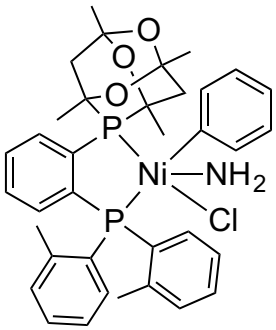
Single-point energy (6-311+G(2d,2p)) = -3852.108025

Ni	0.1935570	1.2450150	-0.0763340
P	-1.0087070	-0.6046040	-0.3024760
P	1.9990800	-0.0627090	0.0144330
C	0.1251880	-1.9337280	-0.9058220
C	1.5061590	-1.6717510	-0.7526030
C	-2.5483240	-0.6502570	-1.3968960
C	-1.9339130	-1.2779720	1.2159940
C	2.5678490	-0.4847680	1.7103460
C	3.5308290	0.3763310	-0.9044100
O	-3.1800390	-1.9528960	-1.3953470
O	-2.9323680	-0.2872200	1.5273300
C	2.4491410	-2.5868690	-1.2372180
C	-0.2738330	-3.1116000	-1.5582860
C	-2.6369960	-2.6004050	0.9030000
C	-3.5096790	0.3668670	-0.7692170
C	-2.2210760	-0.3188810	-2.8435460
C	-1.0209630	-1.3674330	2.4261120
C	2.8280110	0.5662250	2.6235660
C	2.6647270	-1.8162330	2.1386860
C	3.4160440	0.8915160	-2.2179840

C	4.7965010	0.2408090	-0.3169940
H	3.5087570	-2.3712580	-1.1328280
C	2.0375930	-3.7579810	-1.8726620
C	0.6752280	-4.0153160	-2.0368920
H	-1.3288480	-3.3017130	-1.7174830
C	-3.7381600	-2.3812530	-0.1459010
H	-1.9206730	-3.3521270	0.5598620
H	-3.1097990	-2.9726380	1.8198460
H	-4.3779650	0.4805750	-1.4289740
H	-3.0244000	1.3388370	-0.6562460
C	-4.0065820	-0.1443130	0.5876550
H	-3.1408300	-0.3330750	-3.4392700
H	-1.5209220	-1.0434730	-3.2708680
H	-1.7789920	0.6803140	-2.9014630
H	-1.6045720	-1.6631380	3.3056330
H	-0.5481020	-0.4022480	2.6273560
H	-0.2329340	-2.1087000	2.2617150
C	3.1783690	0.2311030	3.9366880
C	3.0113820	-2.1261390	3.4539200
H	2.4615150	-2.6210180	1.4402000
C	2.7505810	2.0202040	2.2226460
C	4.5885120	1.2486620	-2.8932500
H	4.8791500	-0.1520670	0.6916660
C	2.0806940	1.0548270	-2.9042490
C	5.9514650	0.6088090	-1.0076900
O	-4.6419940	-1.4089820	0.3704330
H	2.7770600	-4.4592140	-2.2495340
H	0.3488340	-4.9168060	-2.5484920
C	-4.5429280	-3.6296120	-0.4463770
C	-5.0146770	0.7797060	1.2363710
H	3.3801390	1.0319890	4.6436480
C	3.2678660	-1.0963460	4.3567300
H	3.0778770	-3.1645130	3.7665430
H	3.4882280	2.2683740	1.4497920
H	2.9356160	2.6700680	3.0831050
H	1.7653920	2.2737250	1.8098340
H	4.5104090	1.6461590	-3.9022180
H	1.3923870	1.6662840	-2.3043820
H	1.5864090	0.0888640	-3.0658240
H	2.2015830	1.5359180	-3.8795910
C	5.8451860	1.1141920	-2.3019900
H	6.9236910	0.4993860	-0.5351940
H	-5.3159620	-3.3943620	-1.1823810
H	-5.0185540	-3.9955970	0.4675910
H	-3.8915680	-4.4109310	-0.8496260
H	-5.3222490	0.3690760	2.2017120

H	-5.8928410	0.8813520	0.5929490
H	-4.5636500	1.7646230	1.3857750
H	3.5358780	-1.3215530	5.3853540
H	6.7356110	1.4067220	-2.8517700
C	-0.9836830	2.7931770	-0.2481980
C	-1.6825510	3.3704660	0.8454920
C	-1.2611440	3.3328670	-1.5220250
C	-2.6054270	4.4046480	0.6422120
C	-2.1793280	4.3694980	-1.7278960
H	-0.7526870	2.9245060	-2.3971540
C	-2.8623520	4.9050430	-0.6375260
H	-2.3606140	4.7516320	-2.7308650
H	-3.5851330	5.7058400	-0.7759460
H	-3.1315150	4.8285790	1.4969340
C	-1.4466430	2.8561220	2.2505030
H	-0.3939530	2.9631080	2.5426930
H	-2.0506680	3.3970600	2.9891820
H	-1.6994550	1.7922120	2.3236410

(PAd-DalPhos)Ni(Ph)(NH_2)Cl



Zero-point correction= 0.695730 (Hartree/Particle)
Thermal correction to Energy= 0.739188
Thermal correction to Enthalpy= 0.740132
Thermal correction to Gibbs Free Energy= 0.621156
Sum of electronic and zero-point Energies= -4327.527525
Sum of electronic and thermal Energies= -4327.484067
Sum of electronic and thermal Enthalpies= -4327.483123
Sum of electronic and thermal Free Energies= -4327.602099

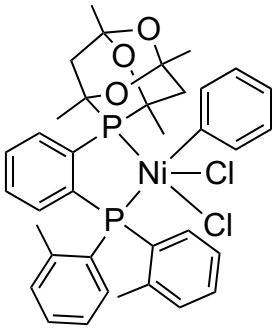
Single-point energy (6-311+G(2d,2p)) = -4329.003895

Ni	0.3108970	1.4308270	-0.2576220
P	-1.6136250	-0.0359810	-0.3817710
P	1.4785570	-0.7415500	0.0426280
C	-0.9941480	-1.6344740	-1.0457100

C	0.3694290	-1.9448270	-0.8321520
C	-3.0824950	0.5146170	-1.4657720
C	-2.7432720	-0.4192060	1.1219240
C	1.5563760	-1.3838290	1.7692700
C	3.1447080	-1.2028520	-0.6381820
O	-4.1231890	-0.4858330	-1.5086500
O	-3.3421500	0.8305390	1.4894810
C	0.8813710	-3.1560500	-1.3209580
C	-1.7934790	-2.5315330	-1.7760030
C	-3.8570110	-1.3976280	0.7292540
C	-3.6168160	1.7687710	-0.7561920
C	-2.7316510	0.7875060	-2.9195530
C	-1.9778610	-0.9161600	2.3336880
C	2.2221270	-0.6433430	2.7765990
C	0.9612570	-2.6126050	2.0909090
C	3.4767160	-0.9760780	-1.9970580
C	4.1036370	-1.7799740	0.2098910
H	1.9254120	-3.4006080	-1.1544230
C	0.0743110	-4.0406280	-2.0337450
C	-1.2630200	-3.7213790	-2.2712570
H	-2.8295440	-2.2803020	-1.9699400
C	-4.8108780	-0.7552680	-0.2811960
H	-3.4420200	-2.3268390	0.3290840
H	-4.4247310	-1.6419840	1.6346950
H	-4.3719840	2.2382650	-1.3971420
H	-2.8077770	2.4859130	-0.5866310
C	-4.2823200	1.3890170	0.5745550
H	-3.6578510	1.0173010	-3.4579960
H	-2.2720580	-0.0863110	-3.3936010
H	-2.0486760	1.6362250	-2.9857430
H	-2.6741340	-0.9867660	3.1774670
H	-1.1706400	-0.2335600	2.5994540
H	-1.5668170	-1.9097900	2.1402120
C	2.2204030	-1.1588360	4.0794070
C	0.9797100	-3.1069340	3.3939960
H	0.4690110	-3.1918980	1.3180560
C	2.9649650	0.6373970	2.4956270
C	4.7577200	-1.3270740	-2.4397810
H	3.8562980	-1.9743790	1.2464710
C	2.5052310	-0.3817720	-2.9828320
C	5.3751170	-2.1172450	-0.2526080
O	-5.3213790	0.4456670	0.2837770
H	0.4927130	-4.9702680	-2.4093310
H	-1.8946470	-4.3961650	-2.8424540
C	-5.9973400	-1.6272330	-0.6390600
C	-4.9169850	2.5650120	1.2858240

H	2.7207270	-0.5916100	4.8597530
C	1.6031910	-2.3676560	4.3965180
H	0.5057410	-4.0582180	3.6191130
H	3.7765990	0.4851940	1.7748150
H	3.4088960	1.0307030	3.4147790
H	2.2983390	1.4036390	2.0936250
H	5.0121570	-1.1511230	-3.4819160
H	2.1146810	0.5737670	-2.6246080
H	1.6438530	-1.0399010	-3.1502630
H	2.9892530	-0.2126560	-3.9492500
C	5.7060040	-1.8869900	-1.5853330
H	6.0964260	-2.5583660	0.4294540
H	-6.6331980	-1.0998450	-1.3547930
H	-6.5790240	-1.8505410	0.2593730
H	-5.6555880	-2.5650610	-1.0874120
H	-5.3993310	2.2167010	2.2027470
H	-5.6658320	3.0346880	0.6421730
H	-4.1458330	3.2957600	1.5442410
H	1.6187860	-2.7319130	5.4201130
H	6.6929940	-2.1419830	-1.9612680
N	0.1065340	1.8548640	-2.0650070
H	-0.0301040	1.0644790	-2.6948000
H	0.8523000	2.4211880	-2.4653550
Cl	-0.1647080	2.0343900	1.8793790
C	1.7549560	2.7191270	-0.2965830
C	1.3878210	4.0601260	-0.1423030
C	3.0903920	2.3953500	-0.5348110
C	2.3568920	5.0646700	-0.2075710
H	0.3533830	4.3240180	0.0536420
C	4.0602750	3.4053550	-0.5928910
H	3.4040610	1.3673710	-0.6709600
C	3.6976930	4.7411600	-0.4307730
H	2.0596310	6.1024030	-0.0755830
H	5.0991790	3.1354450	-0.7693700
H	4.4501520	5.5239570	-0.4779760

(PAd-DalPhos)Ni(Ph)Cl_2



Zero-point correction= 0.670853 (Hartree/Particle)
Thermal correction to Energy= 0.714263
Thermal correction to Enthalpy= 0.715207
Thermal correction to Gibbs Free Energy= 0.595893
Sum of electronic and zero-point Energies= -4731.840913
Sum of electronic and thermal Energies= -4731.797503
Sum of electronic and thermal Enthalpies= -4731.796559
Sum of electronic and thermal Free Energies= -4731.915873

Single-point energy (6-311+G(2d,2p)) = -4733.300804

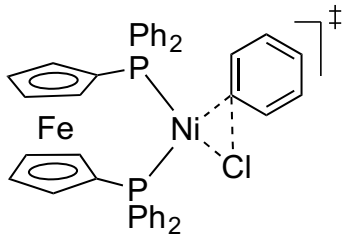
Ni	0.3784240	1.3428010	-0.2170070
P	-1.6705670	-0.0653330	-0.3117770
P	1.4090410	-0.7979270	0.1060340
C	-1.1155650	-1.7509440	-0.7752780
C	0.2363370	-2.0735290	-0.5432850
C	-3.1204370	0.3953560	-1.4687070
C	-2.8155000	-0.2417300	1.2177170
C	1.6307220	-1.2481100	1.8814860
C	2.9783450	-1.3192710	-0.7177040
O	-4.2054050	-0.5535940	-1.3749530
O	-3.3390720	1.0773990	1.4325500
C	0.7037090	-3.3605940	-0.8498620
C	-1.9586140	-2.7152550	-1.3557940
C	-3.9857240	-1.1950990	0.9466150
C	-3.5907940	1.7518240	-0.9237710
C	-2.7694830	0.4181060	-2.9474660
C	-2.0793960	-0.6658210	2.4768900
C	2.4373170	-0.4712660	2.7489910
C	0.9676080	-2.3793560	2.3833660
C	3.0952210	-1.3069160	-2.1304060
C	4.0679350	-1.7325600	0.0635100
H	1.7437820	-3.6110500	-0.6678390
C	-0.1462330	-4.3125700	-1.4070610
C	-1.4764780	-3.9829110	-1.6738870
H	-2.9876520	-2.4573600	-1.5752460

C	-4.9078060	-0.6280200	-0.1309450
H	-3.6262080	-2.1875070	0.6612840
H	-4.5558090	-1.2962010	1.8774640
H	-4.3367090	2.1683860	-1.6102880
H	-2.7515800	2.4510570	-0.8588440
C	-4.2558660	1.5720380	0.4525270
H	-3.6819000	0.6458960	-3.5100070
H	-2.3994170	-0.5576460	-3.2772710
H	-2.0090550	1.1681710	-3.1574010
H	-2.7785300	-0.6206930	3.3200650
H	-1.2313120	-0.0174050	2.6886140
H	-1.7313630	-1.6978370	2.3726800
C	2.5315430	-0.8701410	4.0893150
C	1.0730220	-2.7491420	3.7223760
H	0.3553350	-2.9829650	1.7248580
C	3.1921370	0.7586350	2.3157040
C	4.3196320	-1.6892320	-2.6931640
H	3.9744840	-1.7666560	1.1423450
C	1.9609240	-0.9334110	-3.0533080
C	5.2747060	-2.1109050	-0.5226990
O	-5.3464330	0.6597330	0.2838540
H	0.2331730	-5.3022530	-1.6451130
H	-2.1394920	-4.7116530	-2.1318860
C	-6.1439700	-1.4666850	-0.3848130
C	-4.8178800	2.8595120	1.0166940
H	3.1502210	-0.2791970	4.7594570
C	1.8575200	-1.9849410	4.5823920
H	0.5448230	-3.6267880	4.0838420
H	3.6874730	0.6408310	1.3491630
H	3.9587840	1.0124540	3.0542970
H	2.5105560	1.6088950	2.2261770
H	4.4185510	-1.6736540	-3.7755670
H	1.4041840	-0.0559920	-2.7150280
H	1.2426460	-1.7568590	-3.1493950
H	2.3423550	-0.7094520	-4.0540110
C	5.4029880	-2.0827970	-1.9093370
H	6.1045080	-2.4230740	0.1048160
H	-6.7510520	-0.9934280	-1.1608060
H	-6.7339890	-1.5461510	0.5322760
H	-5.8588420	-2.4697760	-0.7161250
H	-5.3090770	2.6534770	1.9711230
H	-5.5463050	3.2875950	0.3226830
H	-4.0061420	3.5735580	1.1801240
H	1.9509500	-2.2556710	5.6304810
H	6.3389920	-2.3677610	-2.3817420
Cl	-0.0743340	2.0127360	1.8912890

C	1.9976280	2.4753600	-0.2939280
C	1.9513470	3.7430560	0.2829510
C	3.1281730	2.0546630	-0.9862930
C	3.0807650	4.5669890	0.2129510
H	1.0655160	4.0906890	0.7980950
C	4.2569230	2.8805730	-1.0378740
H	3.1572940	1.1053790	-1.5008380
C	4.2395970	4.1368250	-0.4334860
H	3.0423010	5.5512750	0.6734330
H	5.1401670	2.5346430	-1.5695350
H	5.1141200	4.7802470	-0.4789740
Cl	0.0864740	2.1005730	-2.3050030

Transition States

(dppf)Ni(Ph)Cl oxidative addition



Zero-point correction= 0.610601 (Hartree/Particle)
Thermal correction to Energy= 0.650532
Thermal correction to Enthalpy= 0.651476
Thermal correction to Gibbs Free Energy= 0.535888
Sum of electronic and zero-point Energies= -5458.419435
Sum of electronic and thermal Energies= -5458.379504
Sum of electronic and thermal Enthalpies= -5458.378560
Sum of electronic and thermal Free Energies= -5458.494148

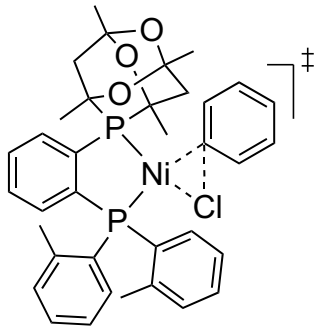
Single-point energy (6-311+G(2d,2p)) = -5459.833083689

Fe	0.3318580	-2.1224080	-1.9481420
C	1.8539060	-0.8188730	-1.5309630
C	2.3884930	-2.0982830	-1.9016440
C	1.9445760	-2.4021630	-3.2217470
C	1.1408010	-1.3168560	-3.6825900
C	1.0803780	-0.3435080	-2.6455040
C	-1.1721410	-3.4960400	-2.3222510
C	-1.7310810	-2.2182210	-2.0253620
C	-1.2941130	-1.8251990	-0.7175390
C	-0.4612150	-2.8817620	-0.2150690
C	-0.3942100	-3.9089920	-1.2002020

P	1.9254370	0.0839240	0.0430120
P	-1.6614840	-0.2674290	0.1777850
C	3.3914910	1.1775930	-0.1571450
C	2.5313980	-1.1569020	1.2581410
C	-2.6522220	-0.9298190	1.5882070
C	-2.9276950	0.4634800	-0.9487670
C	4.1631230	1.2260320	-1.3251020
C	5.2306700	2.1227120	-1.4282780
C	5.5388320	2.9738390	-0.3667580
C	4.7720540	2.9317330	0.8016530
C	3.7015860	2.0451490	0.9046270
C	1.6859530	-1.5095430	2.3190220
C	2.0915940	-2.4562200	3.2622150
C	3.3492020	-3.0520810	3.1566220
C	4.2075060	-2.6891440	2.1145660
C	3.8036170	-1.7414710	1.1739480
C	-3.3720100	-2.1334730	1.5163200
C	-4.0996460	-2.5901600	2.6158510
C	-4.1174950	-1.8512140	3.8012590
C	-3.3974930	-0.6584620	3.8852420
C	-2.6640600	-0.2037010	2.7878930
C	-4.2973350	0.1777690	-0.8783300
C	-5.1872990	0.7560580	-1.7861530
C	-4.7176760	1.6191890	-2.7781290
C	-3.3551700	1.9159240	-2.8491240
C	-2.4695780	1.3496710	-1.9331320
H	2.9772240	-2.7432210	-1.2642510
H	2.1439230	-3.3197670	-3.7608120
H	0.6260910	-1.2638950	-4.6333640
H	0.5204810	0.5815730	-2.6627760
H	-1.2872820	-4.0376470	-3.2526460
H	-2.3481950	-1.6224900	-2.6836210
H	0.0496830	-2.8839110	0.7374940
H	0.1870780	-4.8193490	-1.1265310
H	3.9298030	0.5669370	-2.1557630
H	5.8215420	2.1521460	-2.3401130
H	6.3689000	3.6701720	-0.4491760
H	5.0020950	3.5961590	1.6301330
H	3.0963010	2.0290530	1.8078180
H	0.7160530	-1.0274640	2.4069300
H	1.4276430	-2.7200780	4.0808720
H	3.6673430	-3.7872540	3.8909410
H	5.1943710	-3.1382700	2.0399910
H	4.4837770	-1.4453730	0.3798600
H	-3.3554310	-2.7196340	0.6024060
H	-4.6503930	-3.5247460	2.5473230

H	-4.6826120	-2.2094050	4.6576640
H	-3.3942490	-0.0853670	4.8085650
H	-2.0761530	0.7040520	2.8699230
H	-4.6739660	-0.4904960	-0.1105760
H	-6.2484590	0.5313340	-1.7164970
H	-5.4119480	2.0678040	-3.4837060
H	-2.9835910	2.6058660	-3.6018190
H	-1.4181180	1.6194690	-1.9561360
Ni	0.0229070	1.0717570	0.6035660
Cl	0.1708270	2.1672160	2.7692420
C	-0.7115220	2.7529250	1.0111190
C	0.2322590	3.3287850	0.1272770
C	-0.2414640	4.2235100	-0.8560320
C	-1.5736470	4.6096450	-0.8751850
C	-2.4635970	4.1181860	0.1044280
C	-2.0431800	3.2171250	1.0665820
H	1.2978180	3.1965270	0.2717210
H	0.4676350	4.6609210	-1.5551070
H	-1.9269330	5.3226380	-1.6143980
H	-3.5043450	4.4314460	0.0917340
H	-2.7306820	2.8221680	1.8068710

(PAd-DalPhos)Ni(Ph)Cl oxidative addition



Zero-point correction= 0.667304 (Hartree/Particle)
Thermal correction to Energy= 0.708285
Thermal correction to Enthalpy= 0.709229
Thermal correction to Gibbs Free Energy= 0.596476
Sum of electronic and zero-point Energies= -4271.587154
Sum of electronic and thermal Energies= -4271.546174
Sum of electronic and thermal Enthalpies= -4271.545230
Sum of electronic and thermal Free Energies= -4271.657983

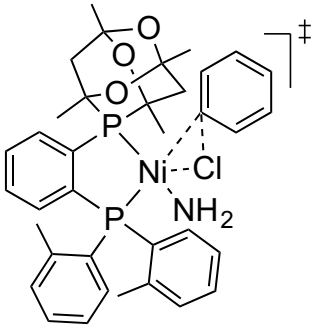
Single-point energy (6-311+G(2d,2p)) = -4273.019837

28 0.19236 1.13168 0.01325

17	1.1313	2.74983	2.53577
15	-1.45246	-0.25454	-0.31286
15	1.63031	-0.53122	-0.01431
6	0.87348	2.84665	0.55483
6	-0.50037	3.00642	0.14936
6	1.93117	3.50128	-0.14737
6	-0.72779	-1.88773	-0.78165
6	0.67463	-1.99063	-0.66063
6	-2.99766	-0.04124	-1.38746
6	-2.4667	-0.48725	1.27901
6	2.32182	-1.1428	1.58144
6	3.04433	-0.52384	-1.1981
6	-0.73028	3.7396	-1.06645
6	1.65183	4.13818	-1.33152
1	2.94195	3.45943	0.24311
8	-3.93224	-1.13398	-1.22822
8	-3.18546	0.75268	1.46457
6	1.32196	-3.16511	-1.06665
6	-1.44789	-2.97154	-1.31403
6	-3.47882	-1.62449	1.13336
6	-3.66965	1.24418	-0.88592
6	-2.65064	0.02806	-2.86625
6	-1.56288	-0.63924	2.48977
6	3.26828	-0.37307	2.29838
6	1.80136	-2.30934	2.16689
6	2.87246	0.06648	-2.47243
6	4.27453	-1.10845	-0.86576
1	-1.7559	3.93546	-1.37268
6	0.30968	4.25307	-1.80197
1	2.46178	4.57817	-1.90725
1	2.40263	-3.23544	-0.98718
6	0.59639	-4.23545	-1.58512
6	-0.79077	-4.13499	-1.71119
1	-2.52039	-2.88867	-1.44192
6	-4.5288	-1.27201	0.06831
1	-2.9753	-2.5623	0.8823
1	-3.99863	-1.76127	2.08913
1	-4.50394	1.4904	-1.55341
1	-2.9592	2.07295	-0.89074
6	-4.22929	1.03167	0.52819
1	-3.56203	0.19117	-3.45286
1	-2.18196	-0.89969	-3.20741
1	-1.95793	0.85615	-3.04935
1	-2.17213	-0.68403	3.40004
1	-0.87472	0.20804	2.56811
1	-0.97213	-1.55765	2.41799

6	3.65189	-0.80759	3.57367
6	2.19698	-2.72135	3.4379
1	1.07712	-2.90623	1.62417
6	3.91221	0.86957	1.73493
6	3.95995	0.06645	-3.35493
1	4.39853	-1.57401	0.10709
6	1.55847	0.65956	-2.92085
1	0.1111	4.80466	-2.71672
6	5.34328	-1.09971	-1.76146
8	-5.15583	-0.05508	0.4651
1	1.11185	-5.13881	-1.89961
1	-1.36229	-4.95952	-2.12898
6	-5.61858	-2.3148	-0.07504
6	-4.97588	2.23327	1.06934
1	4.37528	-0.21406	4.12756
6	3.12766	-1.96388	4.14715
1	1.77718	-3.62657	3.86796
1	4.84251	0.62609	1.20633
1	4.1504	1.57566	2.53496
1	3.25948	1.37992	1.02665
1	3.83677	0.52205	-4.3345
1	1.20764	1.44131	-2.23595
1	0.7703	-0.10199	-2.97008
1	1.65456	1.10303	-3.91695
6	5.18566	-0.5026	-3.01078
1	6.28919	-1.55536	-1.48159
1	-6.33751	-1.98824	-0.83082
1	-6.13658	-2.44593	0.87882
1	-5.18639	-3.27175	-0.38266
1	-5.37085	1.99879	2.06108
1	-5.80501	2.49055	0.40458
1	-4.29812	3.08799	1.14968
1	3.4424	-2.26803	5.14168
1	6.01025	-0.48206	-3.71821
1	-1.29965	2.93889	0.88274

(PAd-DalPhos)Ni(Ph)(NH_2)Cl oxidative addition



Zero-point correction= 0.693144 (Hartree/Particle)
Thermal correction to Energy= 0.736469
Thermal correction to Enthalpy= 0.737413
Thermal correction to Gibbs Free Energy= 0.618864
Sum of electronic and zero-point Energies= -4327.487426
Sum of electronic and thermal Energies= -4327.444102
Sum of electronic and thermal Enthalpies= -4327.443158
Sum of electronic and thermal Free Energies= -4327.561707

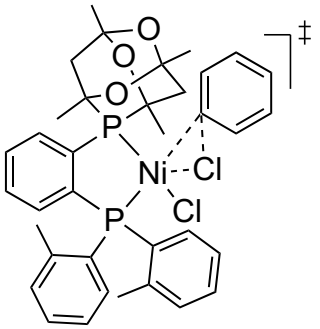
Single-point energy (6-311+G(2d,2p)) = -4328.993040

Ni	0.2819695857	1.3398337736	-0.3955176704
P	-1.6222684605	-0.0411526456	-0.3069928535
P	1.4450373462	-0.7590520667	0.0761742168
C	-1.009062787	-1.6269954534	-1.0250310424
C	0.3883678397	-1.8572077909	-0.9751612759
C	-3.1653793078	0.4130558283	-1.3224207704
C	-2.6474260222	-0.3569820726	1.2752958004
C	1.387128142	-1.7021620318	1.6865365477
C	3.1765005966	-1.0912706779	-0.5025035884
O	-4.1918858302	-0.6058761865	-1.2467115346
O	-3.240507655	0.9210370822	1.5913247261
C	0.9347294517	-2.9497878458	-1.6594853009
C	-1.8169650239	-2.5254664765	-1.7419678811
C	-3.7594610767	-1.3778240335	1.0310403563
C	-3.7015463118	1.6988912759	-0.6766911832
C	-2.879390099	0.6113536206	-2.8021425531
C	-1.7871160944	-0.7041322031	2.4745760323
C	1.8997433333	-1.1487988708	2.8846181654
C	0.8069407353	-2.981065485	1.7301680024
C	3.6290818124	-0.636739289	-1.7666579598
C	4.0855072525	-1.7330804421	0.3558473103
H	2.0058843371	-3.1229409709	-1.6175516171
C	0.1204242986	-3.8193392394	-2.3848936216
C	-1.2584166043	-3.6116412712	-2.4163307342
H	-2.8850770101	-2.3512355485	-1.7957760923

C	-4.7860599191	-0.818441521	0.0366021686
H	-3.3434472432	-2.3205511844	0.6619413125
H	-4.2740106323	-1.5779807866	1.9788185409
H	-4.5108501375	2.0962273402	-1.300584534
H	-2.9079931082	2.4495943433	-0.6114281863
C	-4.2659765668	1.3923813032	0.7151950167
H	-3.8269620434	0.7964346655	-3.3206846999
H	-2.4086828911	-0.2688871148	-3.2492655982
H	-2.2249728348	1.4755060208	-2.9346991038
H	-2.4164962532	-0.7026517433	3.3720984295
H	-0.9904754971	0.0317837452	2.6075074368
H	-1.3379682537	-1.6923459047	2.3620736751
C	1.77356333	-1.8816753976	4.0725053356
C	0.6973077618	-3.6967807864	2.9219907958
H	0.4216557423	-3.4306168491	0.8240623098
C	2.6129336347	0.1776738005	2.9312153901
C	4.9790884363	-0.8209676655	-2.095145539
H	3.7459251452	-2.1109330854	1.3128652487
C	2.714520796	-0.0126004547	-2.7857587294
C	5.423838519	-1.9051873636	0.0056183125
O	-5.2901687831	0.4048067337	0.5665097323
H	0.5624027088	-4.6576225764	-2.9165085059
H	-1.9015187029	-4.2874271028	-2.9736291052
C	-5.9722346693	-1.7343658535	-0.1877519426
C	-4.8889114607	2.5937088644	1.3949320405
H	2.1625027755	-1.4495601094	4.9910268901
C	1.1734979577	-3.1385139232	4.1053625578
H	0.2378911481	-4.6813721797	2.9186247577
H	3.5300598718	0.1578889442	2.3297375017
H	2.8992370038	0.4275963669	3.9571921528
H	1.983694665	0.9865622369	2.5557686189
H	5.326703977	-0.4684136996	-3.0630843841
H	2.0665978073	0.7590616203	-2.3572008525
H	2.0466164199	-0.764374703	-3.2274475455
H	3.2931869171	0.435597015	-3.5995408162
C	5.8762176885	-1.4378188531	-1.2259290145
H	6.1016189433	-2.4032259359	0.6934175345
H	-6.6646191899	-1.2663343492	-0.8922174086
H	-6.4901197824	-1.9123477428	0.7586166179
H	-5.6366755276	-2.691356666	-0.598642181
H	-5.2929655467	2.2938398794	2.365341476
H	-5.6977940925	2.9952530889	0.7784183724
H	-4.1307821333	3.3671256845	1.5467262629
H	1.0881966056	-3.6767682966	5.0453252281
H	6.9174050634	-1.5573965116	-1.5133342704
N	0.1402134073	2.021847506	-2.1313288909

H	-0.2132229549	1.515360473	-2.9402950891
H	0.7658509379	2.7539720759	-2.4635891647
Cl	0.3509391246	2.6588666555	1.605645362
C	1.5812403357	3.0456835587	0.1186799913
C	1.2680368833	4.2344059507	-0.5656637819
C	2.9172603033	2.6293487589	0.2391608695
C	2.277312715	4.9131132555	-1.243509182
H	0.2430473739	4.5863214056	-0.5935933724
C	3.9083363712	3.3195872844	-0.4569873756
H	3.1750129622	1.7593568644	0.825699778
C	3.600213639	4.4572620435	-1.2080953255
H	2.0250740004	5.8143466324	-1.7971597538
H	4.9326879149	2.959291465	-0.4030817811
H	4.3814391889	4.9966848981	-1.7350950612

(PAd-DalPhos)Ni(Ph)Cl_2 oxidative addition



Zero-point correction= 0.668928 (Hartree/Particle)
Thermal correction to Energy= 0.712168
Thermal correction to Enthalpy= 0.713112
Thermal correction to Gibbs Free Energy= 0.594100
Sum of electronic and zero-point Energies= -4731.821052
Sum of electronic and thermal Energies= -4731.777811
Sum of electronic and thermal Enthalpies= -4731.776867
Sum of electronic and thermal Free Energies= -4731.895879

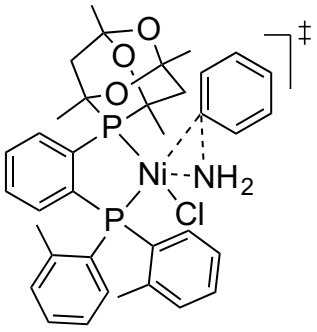
Single-point energy (6-311+G(2d,2p)) = -4733.281273

Ni	0.3174170443	1.233831965	-0.1143475519
P	-1.7018405542	-0.1203252314	-0.2179914669
P	1.3900420708	-0.834612478	0.115695691
C	-1.1746326746	-1.8445366877	-0.5787091749
C	0.186170241	-2.1563141661	-0.3685647653
C	-3.0918239362	0.2963273927	-1.4338212092
C	-2.8816720614	-0.1813551066	1.2782679767
C	1.7728090748	-1.1862658441	1.8811620038
C	2.8776169626	-1.3741905538	-0.8339094412

O	-4.2064783532	-0.6190449559	-1.3511162941
O	-3.3967830391	1.1557184305	1.399927943
C	0.6427417375	-3.4608536512	-0.6106568838
C	-2.0299259827	-2.8417096197	-1.0817446602
C	-4.0572644133	-1.1317658327	1.0331908489
C	-3.5637065106	1.6908221447	-0.9921546572
C	-2.6255162995	0.2562020099	-2.880349658
C	-2.1435850181	-0.5002863949	2.5662861616
C	2.6395502754	-0.3353803002	2.609436138
C	1.1484068498	-2.2618485176	2.5309900533
C	2.8523464028	-1.3664906839	-2.2500267309
C	4.0465967802	-1.7641178343	-0.1658153004
H	1.6890087236	-3.7001891868	-0.4478383076
C	-0.2223691898	-4.4450574128	-1.0820116669
C	-1.5584898556	-4.1281028798	-1.3342383101
H	-3.0618413774	-2.5949086873	-1.2997567933
C	-4.935851027	-0.6221721663	-0.1162427444
H	-3.7068050366	-2.1475994492	0.8326168571
H	-4.668630813	-1.1584838874	1.9429121478
H	-4.2788911187	2.0725338096	-1.730125458
H	-2.7203524778	2.3856807837	-0.9317794634
C	-4.2772515431	1.6003844752	0.3677079486
H	-3.4592496085	0.5295717614	-3.5370346864
H	-2.2855758094	-0.746853654	-3.1557946926
H	-1.8038673431	0.9596918973	-3.0382383315
H	-2.8475001191	-0.4526930231	3.4054798463
H	-1.338266058	0.2166100041	2.7376043983
H	-1.7245197172	-1.5111269541	2.5208835631
C	2.8493695534	-0.6169264018	3.965305749
C	1.3642690399	-2.5120344044	3.8850947813
H	0.4812554848	-2.9129694451	1.9784607512
C	3.3245973228	0.8590452357	1.9976234535
C	4.0178377124	-1.728128315	-2.9364050646
H	4.0601232861	-1.7907488386	0.918234557
C	1.6145364613	-1.025001911	-3.0473620804
C	5.1950110877	-2.1232433263	-0.8712679703
O	-5.3734357543	0.6911809648	0.2128345593
H	0.149275508	-5.4489026549	-1.2678360496
H	-2.2343609026	-4.8814060394	-1.7298085368
C	-6.1726521212	-1.4641557862	-0.3551661718
C	-4.8426870795	2.9240023785	0.8370711907
H	3.5147288324	0.0305400303	4.530323914
C	2.2207089393	-1.6832490201	4.6057179168
H	0.8652119455	-3.3479836733	4.367057804
H	3.8276905247	0.6250434292	1.0558092734
H	4.0754417963	1.262311413	2.683809427

H	2.5947034995	1.649083929	1.7967914249
H	4.0066852748	-1.7172561002	-4.0236413556
H	1.0639956618	-0.1771808037	-2.6303123124
H	0.9198789199	-1.8732504952	-3.0797757156
H	1.8788029988	-0.7724982495	-4.0789117524
C	5.1820780788	-2.0991828131	-2.2640760897
H	6.0902605654	-2.4184032321	-0.3312967729
H	-6.7543540134	-1.0318782235	-1.1734143949
H	-6.7877784707	-1.4862780861	0.5484674676
H	-5.8882260009	-2.4869774279	-0.6202947345
H	-5.3695954938	2.7775751926	1.7834156122
H	-5.5410022663	3.3197688134	0.0944714584
H	-4.0280608288	3.6371011934	0.990105132
H	2.4000528713	-1.8626255519	5.6622937078
H	6.0705621288	-2.3701531014	-2.8277281899
Cl	0.0553719455	2.2300527196	1.9221783095
C	1.8603026514	2.62971375	-0.8868379019
C	1.9083465811	3.8161539051	-0.1479915507
C	3.016231426	2.0450298795	-1.4093200267
C	3.1573071249	4.3307119006	0.1934872921
H	0.9982870892	4.2885069839	0.1985902839
C	4.25650427	2.5783416573	-1.0537229559
H	2.9608446972	1.1880723964	-2.0659969881
C	4.3343429617	3.7145575398	-0.2463622964
H	3.2049143834	5.2260454531	0.8075877393
H	5.1598238089	2.1029031323	-1.4271573248
H	5.3010491483	4.1326155643	0.0183973001
Cl	0.239373125	2.4371869238	-2.1278961984

(PAd-DalPhos)Ni(Ph)(NH_2)Cl Reductive Elimination



Zero-point correction= 0.694354 (Hartree/Particle)
Thermal correction to Energy= 0.737502
Thermal correction to Enthalpy= 0.738447
Thermal correction to Gibbs Free Energy= 0.620413
Sum of electronic and zero-point Energies= -4327.517772

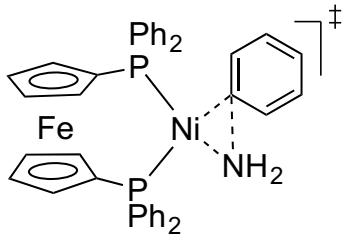
Sum of electronic and thermal Energies= -4327.474624
Sum of electronic and thermal Enthalpies= -4327.473680
Sum of electronic and thermal Free Energies= -4327.591713

Single-point energy (6-311+G(2d,2p)) = -4328.963319

Ni	0.3494794025	1.3573397814	-0.020175506
P	-1.6573594624	-0.14419795	-0.3036478572
P	1.4383338822	-0.7660651677	0.092268364
C	-1.031819702	-1.7755528282	-0.8828457892
C	0.3295763427	-2.0583148007	-0.6364348825
C	-2.9756959111	0.3967719592	-1.5464431736
C	-2.9371024849	-0.4743132276	1.0717316164
C	1.6608591815	-1.2901649597	1.8439160339
C	3.0355690676	-1.1685774922	-0.7411991442
O	-4.0499341574	-0.5615875489	-1.6860870714
O	-3.52886111	0.8075529121	1.3485855376
C	0.8606251073	-3.2987854845	-1.0219522421
C	-1.8068199604	-2.7260622117	-1.571668873
C	-4.0453246929	-1.4214487133	0.6039934894
C	-3.5474917014	1.6892361884	-0.9425505461
C	-2.3967901674	0.5946892544	-2.9372706475
C	-2.2733055176	-0.9419897413	2.3547005608
C	2.390098877	-0.4829863364	2.750633036
C	1.0585272947	-2.4736468552	2.2982293453
C	3.1560054132	-1.0249797363	-2.1445910892
C	4.1506023317	-1.5667825523	0.010139292
H	1.9056650695	-3.518032108	-0.8266622123
C	0.0712982887	-4.2421434498	-1.6751436791
C	-1.261152681	-3.9454132935	-1.9673100161
H	-2.8346122816	-2.4915875786	-1.820047883
C	-4.86278657	-0.7792015899	-0.5258883856
H	-3.6340115192	-2.3830823481	0.2864405357
H	-4.7192758797	-1.6043436565	1.4494871907
H	-4.2239291291	2.1525427588	-1.6703267856
H	-2.7452494067	2.395990803	-0.708121632
C	-4.352520598	1.3685396162	0.328652854
H	-3.1709945596	0.9924383526	-3.6039718086
H	-2.0458467214	-0.3570836287	-3.3488248703
H	-1.5502302218	1.287296521	-2.8924367606
H	-3.0316020245	-1.0349368623	3.1410801327
H	-1.5147257742	-0.2254209182	2.6764604257
H	-1.8052930688	-1.920355125	2.2045535649
C	2.4834040438	-0.9106822364	4.0814949805
C	1.1578795437	-2.8709120061	3.6303808139
H	0.5003235781	-3.0943318112	1.6071458797

C	3.0525475477	0.8122587528	2.3562342456
C	4.403100098	-1.2668075988	-2.7335421703
H	4.0554416097	-1.6932504509	1.0829179101
C	1.9895585226	-0.6654950228	-3.0360915824
C	5.3820865252	-1.8059130355	-0.5987727517
O	-5.3891073248	0.4524529452	-0.0437195072
H	0.500002961	-5.1960216231	-1.9697790224
H	-1.8765346383	-4.6622434001	-2.5042454239
C	-6.0359292614	-1.6239470238	-0.9801858974
C	-5.0140492927	2.5845816383	0.941916409
H	3.0425117599	-0.2969901489	4.7829217783
C	1.8738248664	-2.0817426975	4.5274575678
H	0.6782932003	-3.788752311	3.9586038244
H	2.3010432059	1.5972879716	2.2250591379
H	3.6137865669	0.7375352049	1.4210803776
H	3.7479811432	1.1373135746	3.1362456737
H	4.5026341643	-1.1506639292	-3.8102451379
H	1.2765255991	0.0059380976	-2.5519002578
H	1.4268405416	-1.5620151889	-3.3250609717
H	2.340692559	-0.1863896831	-3.9560883792
C	5.5102454724	-1.6496122462	-1.9774898435
H	6.232767074	-2.1101030757	0.0044791929
H	-6.5790294226	-1.0975754357	-1.7693381773
H	-6.7117679652	-1.8049900834	-0.1399578002
H	-5.6824248583	-2.583791961	-1.3689822985
H	-5.6016839404	2.2776158079	1.8109080881
H	-5.6742249496	3.0625988054	0.2128387804
H	-4.2474983827	3.294679829	1.2641077339
H	1.9604118289	-2.3744383885	5.5703135159
H	6.4652598807	-1.8253549891	-2.4648913983
N	0.3752977513	2.2201839553	-1.7636417868
H	1.1049128863	2.1672798802	-2.4675301381
H	0.0117613627	3.1710805205	-1.7994804978
Cl	-0.2897310537	2.0663941997	2.0595847837
C	1.7880899634	2.7179062136	-0.3856686279
C	1.612017782	3.9696114206	0.2262136616
C	3.0665929152	2.3388955515	-0.8177434176
C	2.7192582057	4.7784551771	0.4820329282
H	0.6278074649	4.2838216716	0.5573841044
C	4.1680225141	3.155864454	-0.5521989144
H	3.2193353696	1.4023913661	-1.3413445649
C	4.003846108	4.3769915789	0.1033428456
H	2.5716920775	5.7297426463	0.9875887875
H	5.1564203406	2.8305814064	-0.8686091856
H	4.8606251006	5.0136066962	0.3047886085

(dppf)Ni(Ph)NH_2 reductive elimination



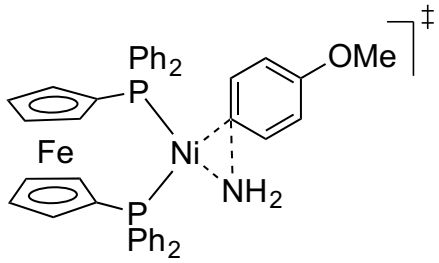
Zero-point correction= 0.635907 (Hartree/Particle)
Thermal correction to Energy= 0.675726
Thermal correction to Enthalpy= 0.676670
Thermal correction to Gibbs Free Energy= 0.562321
Sum of electronic and zero-point Energies= -5054.114134
Sum of electronic and thermal Energies= -5054.074315
Sum of electronic and thermal Enthalpies= -5054.073371
Sum of electronic and thermal Free Energies= -5054.187721
Single-point energy (6-311+G(2d,2p)) = -5055.545971

Fe	-1.0834560	-2.7876410	0.0870420
C	0.7716530	-2.1374020	-0.4828270
C	0.8800080	-3.3941560	0.2028230
C	0.1233910	-4.3650100	-0.5149830
C	-0.4537640	-3.7261070	-1.6522660
C	-0.0582490	-2.3577860	-1.6357550
C	-2.9433110	-3.4383190	0.7420000
C	-3.0689390	-2.2426170	-0.0225200
C	-2.2897500	-1.2152040	0.6094140
C	-1.6857020	-1.8045490	1.7756820
C	-2.0959140	-3.1662330	1.8557980
P	1.4906950	-0.5152160	-0.0563240
P	-1.8951480	0.4549360	-0.0075040
C	3.1294150	-0.6041570	-0.8825770
C	1.9342640	-0.7068830	1.7208140
C	-2.9099510	1.5631070	1.0471110
C	-2.7789580	0.5032540	-1.6192440
C	3.4032750	-1.5235720	-1.9056150
C	4.6432560	-1.5168000	-2.5482600
C	5.6208560	-0.5922460	-2.1764770
C	5.3517150	0.3290500	-1.1627040
C	4.1138200	0.3292170	-0.5220890
C	1.2164390	0.0332130	2.6702960
C	1.4983220	-0.0914920	4.0316830
C	2.5098840	-0.9544170	4.4570740

C	3.2436710	-1.6827910	3.5171010
C	2.9614580	-1.5557280	2.1563110
C	-3.2138180	2.8533150	0.5743300
C	-3.8677730	3.7715580	1.3963310
C	-4.2277130	3.4208310	2.6991540
C	-3.9331990	2.1414690	3.1750380
C	-3.2774470	1.2195240	2.3571720
C	-4.1765020	0.4329370	-1.7162270
C	-4.7990320	0.4486350	-2.9645800
C	-4.0316260	0.5405570	-4.1294210
C	-2.6414240	0.6257880	-4.0419850
C	-2.0195710	0.6117740	-2.7917890
H	1.4045330	-3.5581820	1.1337440
H	-0.0255410	-5.3962420	-0.2206580
H	-1.1157060	-4.1855370	-2.3751440
H	-0.3609160	-1.6001300	-2.3452110
H	-3.3821020	-4.3966840	0.4947190
H	-3.6136980	-2.1356910	-0.9498370
H	-0.9969130	-1.3144080	2.4490880
H	-1.7771230	-3.8792270	2.6053390
H	2.6540760	-2.2520970	-2.1981170
H	4.8442090	-2.2390240	-3.3353360
H	6.5857270	-0.5881100	-2.6767630
H	6.0969960	1.0655370	-0.8764350
H	3.9139480	1.0624970	0.2516360
H	0.4417430	0.7165860	2.3316980
H	0.9359000	0.4917960	4.7558520
H	2.7352610	-1.0502500	5.5157860
H	4.0418310	-2.3444130	3.8430660
H	3.5500960	-2.1074270	1.4289950
H	-2.9383970	3.1311060	-0.4372600
H	-4.0990410	4.7628530	1.0151990
H	-4.7396090	4.1366130	3.3365180
H	-4.2203190	1.8548820	4.1834120
H	-3.0640110	0.2258360	2.7379010
H	-4.7771300	0.3735270	-0.8127680
H	-5.8824350	0.3924340	-3.0288160
H	-4.5183800	0.5551630	-5.1009010
H	-2.0413600	0.7122390	-4.9438470
H	-0.9388390	0.7048690	-2.7149670
Ni	0.2437070	1.2558950	-0.3273190
N	-0.2001550	3.0554790	-0.7036850
C	1.5688930	2.6351940	-0.4448540
C	2.3717160	2.8420930	-1.6040880
C	2.0975590	3.1050470	0.7927960
C	3.6003950	3.4860960	-1.5236060

H	2.0205300	2.4773990	-2.5678820
C	3.3427790	3.7264150	0.8558340
H	1.5189410	2.9764100	1.7055260
C	4.1096350	3.9340730	-0.2968310
H	4.1847140	3.6190200	-2.4322760
H	3.7163880	4.0589010	1.8228660
H	5.0737260	4.4308690	-0.2421820
H	-0.1062080	3.5418700	-1.5862640
H	-0.4254990	3.7204020	0.0299840

(dppf)Ni(*p*-OMePh)NH_2 reductive elimination



Zero-point correction= 0.668484 (Hartree/Particle)
Thermal correction to Energy= 0.711039
Thermal correction to Enthalpy= 0.711983
Thermal correction to Gibbs Free Energy= 0.590828
Sum of electronic and zero-point Energies= -5168.607192
Sum of electronic and thermal Energies= -5168.564637
Sum of electronic and thermal Enthalpies= -5168.563693
Sum of electronic and thermal Free Energies= -5168.684849

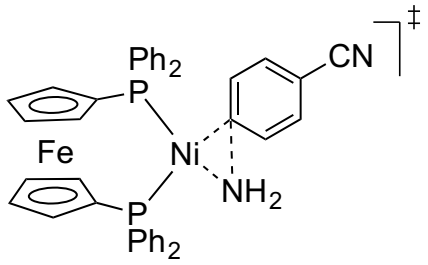
Single-point energy (6-311+G(2d,2p)) = -5170.107433

Fe	-2.13787	-2.46721	-0.10586
C	-0.15072	-2.36072	-0.58952
C	-0.44395	-3.63024	0.01375
C	-1.42092	-4.29275	-0.78429
C	-1.73882	-3.44842	-1.8892
C	-0.96113	-2.26073	-1.7727
C	-4.13076	-2.58261	0.46455
C	-3.87475	-1.36149	-0.22348
C	-2.85846	-0.64136	0.49122
C	-2.49722	-1.44508	1.62932
C	-3.28614	-2.63093	1.61213
P	0.9791	-1.03849	-0.03683
P	-1.97277	0.87284	-0.01
C	2.57014	-1.55605	-0.7972
C	1.25438	-1.43249	1.7418
C	-2.65281	2.17009	1.09544

C	-2.7536	1.26698	-1.62797
C	2.62386	-2.41221	-1.90627
C	3.84963	-2.72799	-2.49681
C	5.03346	-2.1939	-1.98483
C	4.98586	-1.33622	-0.88409
C	3.76349	-1.01169	-0.29794
C	0.75271	-0.54647	2.70518
C	0.91722	-0.80665	4.0668
C	1.59404	-1.95568	4.47936
C	2.11394	-2.83615	3.52691
C	1.95026	-2.5733	2.16623
C	-2.54909	3.51637	0.69761
C	-2.92469	4.54147	1.56635
C	-3.40804	4.24349	2.84206
C	-3.51785	2.91029	3.24348
C	-3.14105	1.88097	2.37919
C	-4.10752	1.61341	-1.74794
C	-4.6602	1.87791	-3.00126
C	-3.86409	1.80436	-4.14802
C	-2.51259	1.47472	-4.03681
C	-1.96018	1.21221	-2.78146
H	-0.03098	-3.99424	0.94403
H	-1.87686	-5.24949	-0.56283
H	-2.47629	-3.65042	-2.65543
H	-1.00069	-1.40686	-2.43477
H	-4.81777	-3.35654	0.14636
H	-4.32781	-1.04923	-1.15374
H	-1.72354	-1.21435	2.34769
H	-3.21742	-3.44606	2.32113
H	1.7111	-2.84268	-2.30597
H	3.87706	-3.39854	-3.35184
H	5.98713	-2.44449	-2.44204
H	5.89971	-0.90832	-0.48119
H	3.74035	-0.32772	0.54384
H	0.23994	0.35461	2.37808
H	0.52597	-0.10816	4.80164
H	1.72807	-2.15891	5.5384
H	2.65468	-3.72402	3.84371
H	2.37743	-3.24943	1.43123
H	-2.17864	3.75447	-0.29374
H	-2.84262	5.57585	1.24262
H	-3.70325	5.04327	3.51569
H	-3.90491	2.66773	4.22978
H	-3.24056	0.84956	2.70216
H	-4.72686	1.6824	-0.8579
H	-5.71067	2.1441	-3.08333

H	-4.29571	2.01282	-5.12332
H	-1.88622	1.43034	-4.92377
H	-0.902	0.98169	-2.68387
Ni	0.31657	1.02775	-0.24995
N	0.44774	2.89034	-0.55783
C	1.9936	1.97082	-0.26299
C	2.8783	1.95224	-1.37358
C	2.58497	2.22605	1.00862
C	4.24642	2.18104	-1.2319
H	2.48688	1.7391	-2.36641
C	3.95374	2.424	1.1492
H	1.95551	2.26402	1.89529
C	4.79903	2.41041	0.03291
H	4.87387	2.14209	-2.11605
H	4.38789	2.59942	2.13003
H	0.71155	3.36416	-1.41209
H	0.37695	3.56551	0.19773
O	6.14695	2.61841	0.28055
C	7.02303	2.58334	-0.82797
H	8.02437	2.76009	-0.43035
H	6.99879	1.60586	-1.3313
H	6.78077	3.36555	-1.56124

(dppf)Ni(*p*-CNPh)NH_2 reductive elimination



Zero-point correction= 0.634601 (Hartree/Particle)
Thermal correction to Energy= 0.676327
Thermal correction to Enthalpy= 0.677271
Thermal correction to Gibbs Free Energy= 0.557183
Sum of electronic and zero-point Energies= -5146.378876
Sum of electronic and thermal Energies= -5146.337150
Sum of electronic and thermal Enthalpies= -5146.336206
Sum of electronic and thermal Free Energies= -5146.456294

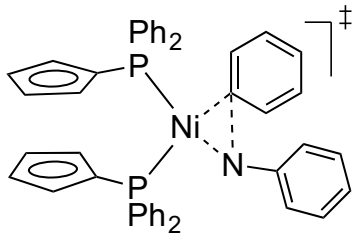
Single-point energy (6-311+G(2d,2p)) = -5147.830393

Fe	1.90204	2.49087	-0.55634
C	-0.10291	2.22727	-0.84109
C	0.16469	3.58933	-0.47395

C	1.0356	4.154	-1.44974
C	1.31067	3.157	-2.43148
C	0.61356	1.97165	-2.06169
C	3.92255	2.78051	-0.16774
C	3.68602	1.45934	-0.64529
C	2.76181	0.81463	0.24464
C	2.43903	1.76436	1.27723
C	3.15958	2.96621	1.02217
P	-1.09824	0.96171	0.01033
P	1.95101	-0.80512	0.04795
C	-2.77974	1.25664	-0.66103
C	-1.22275	1.55418	1.74407
C	2.75963	-1.85777	1.31771
C	2.66459	-1.42462	-1.52721
C	-2.9613	1.72417	-1.9699
C	-4.24432	1.81957	-2.51198
C	-5.3556	1.44436	-1.75573
C	-5.1814	0.9792	-0.4509
C	-3.90205	0.88699	0.09451
C	-0.64615	0.77248	2.75518
C	-0.69842	1.18351	4.08844
C	-1.33507	2.37978	4.42321
C	-1.9299	3.156	3.42465
C	-1.88019	2.74287	2.09302
C	2.62667	-3.25381	1.20862
C	3.14043	-4.09068	2.19836
C	3.79008	-3.55042	3.31089
C	3.92747	-2.16637	3.4254
C	3.41603	-1.32341	2.43591
C	4.02199	-1.75144	-1.6595
C	4.52367	-2.19599	-2.88291
C	3.67343	-2.3231	-3.98513
C	2.31873	-2.01215	-3.85922
C	1.81733	-1.56902	-2.63389
H	-0.18962	4.08265	0.42005
H	1.45298	5.15253	-1.42274
H	1.97075	3.2642	-3.28255
H	0.64841	1.02493	-2.58283
H	4.54272	3.52575	-0.64931
H	4.09077	1.02762	-1.54978
H	1.7356	1.60939	2.08306
H	3.09726	3.87589	1.60549
H	-2.1042	2.01858	-2.56772
H	-4.37273	2.18774	-3.5264
H	-6.35318	1.50953	-2.18084
H	-6.04039	0.67319	0.13871

H	-3.77752	0.50219	1.1002
H	-0.16155	-0.1645	2.4906
H	-0.25003	0.56637	4.86211
H	-1.3806	2.70093	5.46017
H	-2.44141	4.07876	3.68449
H	-2.36954	3.33573	1.32571
H	2.11518	-3.67521	0.34993
H	3.0334	-5.16763	2.09943
H	4.19091	-4.20448	4.08034
H	4.44046	-1.7377	4.28226
H	3.53993	-0.24992	2.53303
H	4.68383	-1.66516	-0.80224
H	5.57696	-2.44641	-2.97566
H	4.06564	-2.67256	-4.93625
H	1.65109	-2.12281	-4.70931
H	0.75812	-1.34882	-2.52382
Ni	-0.33473	-1.08646	-0.04124
N	-0.3828	-2.9795	-0.13905
C	-1.98535	-1.9967	-0.09571
C	-2.73245	-2.0793	-1.31268
C	-2.71388	-2.20401	1.11788
C	-4.086	-2.3465	-1.31309
H	-2.22987	-1.89862	-2.26086
C	-4.06982	-2.47243	1.11055
H	-2.19061	-2.14598	2.07045
C	-4.78965	-2.54765	-0.1026
H	-4.63088	-2.37746	-2.25254
H	-4.5982	-2.61342	2.04997
H	-0.53528	-3.51831	-0.98384
H	-0.48406	-3.58008	0.6722
C	-6.19336	-2.76537	-0.10521
N	-7.35091	-2.92869	-0.10737

(dppf)Ni(Ph)PhNH reductive elimination



Zero-point correction= 0.718146 (Hartree/Particle)
Thermal correction to Energy= 0.762190
Thermal correction to Enthalpy= 0.763135
Thermal correction to Gibbs Free Energy= 0.639301

Sum of electronic and zero-point Energies= -5285.102232
Sum of electronic and thermal Energies= -5285.058188
Sum of electronic and thermal Enthalpies= -5285.057244
Sum of electronic and thermal Free Energies= -5285.181077

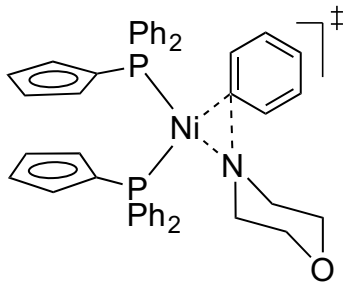
Single-point energy (6-311+G(2d,2p)) = -5286.690115

Fe	-1.03292	-3.24165	0.18102
C	-2.14043	-1.62008	0.75006
C	-3.00167	-2.63532	0.21172
C	-2.85473	-3.81532	0.996
C	-1.91389	-3.54453	2.03218
C	-1.47049	-2.19889	1.88356
C	0.08816	-4.86689	-0.46328
C	0.91997	-3.89369	0.16187
C	0.78041	-2.65457	-0.54959
C	-0.14523	-2.889	-1.62597
C	-0.56479	-4.24898	-1.57041
P	-1.87589	0.08127	0.13038
P	1.4956	-1.02251	-0.16865
C	-2.98829	1.04755	1.23299
C	-2.80321	0.03956	-1.46061
C	2.98542	-0.98941	-1.24941
C	2.2085	-1.27202	1.50964
C	-3.38239	0.57868	2.49517
C	-4.17177	1.37244	3.32998
C	-4.57702	2.64173	2.91397
C	-4.18715	3.11405	1.65989
C	-3.39445	2.32741	0.82579
C	-2.07378	0.02895	-2.65681
C	-2.72495	-0.04068	-3.88894
C	-4.11927	-0.08834	-3.93688
C	-4.85681	-0.06223	-2.75056
C	-4.20306	0.00237	-1.51919
C	4.01486	-0.07765	-0.96419
C	5.10635	0.04993	-1.8223
C	5.18733	-0.72826	-2.97896
C	4.17028	-1.6389	-3.26977
C	3.07538	-1.76899	-2.41237
C	3.32824	-2.08124	1.74937
C	3.82087	-2.23874	3.04551
C	3.20296	-1.58676	4.11597
C	2.09459	-0.76977	3.88617
C	1.60503	-0.61147	2.58886
H	-3.61671	-2.5318	-0.67092
H	-3.34016	-4.76466	0.80842
H	-1.55808	-4.24921	2.77289

H	-0.72574	-1.71228	2.49599
H	-0.05628	-5.88592	-0.12731
H	1.51336	-4.04202	1.05325
H	-0.49818	-2.14703	-2.32788
H	-1.29061	-4.71454	-2.22473
H	-3.0873	-0.41084	2.82716
H	-4.47417	0.99263	4.30248
H	-5.19195	3.25849	3.5641
H	-4.48251	4.10509	1.32791
H	-3.09147	2.71491	-0.13981
H	-0.98885	0.09313	-2.61272
H	-2.14556	-0.04538	-4.80834
H	-4.6305	-0.1353	-4.89459
H	-5.94269	-0.08903	-2.78347
H	-4.78235	0.03255	-0.60114
H	3.96495	0.53888	-0.07409
H	5.88726	0.76696	-1.58556
H	6.0374	-0.62677	-3.64826
H	4.22813	-2.25576	-4.16284
H	2.29666	-2.48727	-2.64753
H	3.82249	-2.5782	0.91955
H	4.69047	-2.86687	3.21926
H	3.59115	-1.7077	5.12361
H	1.61789	-0.2484	4.71181
H	0.75453	0.0402	2.40186
Ni	0.15223	0.84044	-0.27652
N	1.35352	2.18185	-0.90462
C	-0.24439	2.7424	-0.5042
C	-0.37443	3.54239	0.66948
C	-0.93366	3.20064	-1.66971
C	-1.1114	4.72245	0.65309
H	0.10494	3.23333	1.59167
C	-1.66824	4.37978	-1.65891
H	-0.881	2.61654	-2.58617
C	-1.76584	5.16537	-0.50127
H	-1.18785	5.29945	1.57269
H	-2.17745	4.68863	-2.5701
H	-2.33567	6.08955	-0.50106
H	1.40005	2.30451	-1.91031
C	2.4636	2.72077	-0.26317
C	3.40625	3.48139	-0.98407
C	2.67735	2.52425	1.1137
C	4.5357	3.99251	-0.35453
H	3.24971	3.64954	-2.04745
C	3.80721	3.05126	1.73855
H	1.97034	1.92633	1.67659

C	4.74936	3.78227	1.01317
H	5.25442	4.56541	-0.93538
H	3.95386	2.87532	2.80144
H	5.63173	4.18496	1.50161

(dppf)Ni(Ph)Morpholine reductive elimination



Zero-point correction= 0.735439 (Hartree/Particle)
Thermal correction to Energy= 0.779333
Thermal correction to Enthalpy= 0.780277
Thermal correction to Gibbs Free Energy= 0.657388
Sum of electronic and zero-point Energies= -5285.274147
Sum of electronic and thermal Energies= -5285.230253
Sum of electronic and thermal Enthalpies= -5285.229309
Sum of electronic and thermal Free Energies= -5285.352198

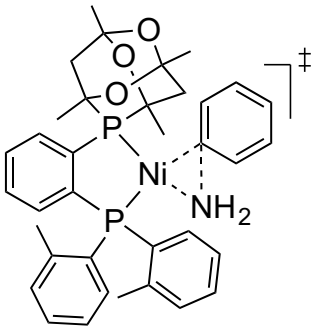
Single-point energy (6-311+G(2d,2p)) = -5286.878808

Fe	0.45085	-3.36154	-0.13635
C	-1.24496	-2.38257	0.44406
C	-1.59277	-3.58758	-0.25475
C	-1.03221	-4.69338	0.4471
C	-0.34301	-4.19064	1.58961
C	-0.46931	-2.77166	1.59115
C	2.16008	-4.33226	-0.80971
C	2.49719	-3.20343	-0.00845
C	1.92247	-2.03267	-0.61002
C	1.23398	-2.46614	-1.79754
C	1.38528	-3.87706	-1.91658
P	-1.64995	-0.65306	0.01287
P	1.87356	-0.31286	-0.00524
C	-3.18416	-0.39199	0.99554
C	-2.27629	-0.81172	-1.71003
C	3.31964	0.43627	-0.86926
C	2.46222	-0.44865	1.7325
C	-3.46321	-1.14836	2.14353
C	-4.60212	-0.88243	2.90668

C	-5.47472	0.14041	2.5318
C	-5.20118	0.89826	1.39235
C	-4.06249	0.64001	0.63104
C	-1.49241	-0.29703	-2.75164
C	-1.90374	-0.41774	-4.07962
C	-3.11302	-1.04806	-4.37857
C	-3.90982	-1.5496	-3.34633
C	-3.49562	-1.42993	-2.01889
C	4.07146	1.44991	-0.25643
C	5.07399	2.11728	-0.95935
C	5.34329	1.78097	-2.28735
C	4.60889	0.76599	-2.90337
C	3.6039	0.09911	-2.20113
C	3.74357	-0.90526	2.07641
C	4.12473	-0.99816	3.41518
C	3.23322	-0.62797	4.42625
C	1.96206	-0.1571	4.09456
C	1.58144	-0.06579	2.75424
H	-2.14229	-3.63744	-1.18417
H	-1.0832	-5.73012	0.13943
H	0.22082	-4.77632	2.30436
H	-0.02193	-2.09829	2.30852
H	2.41149	-5.36204	-0.58939
H	3.04011	-3.22979	0.92557
H	0.65281	-1.83673	-2.4566
H	0.94491	-4.49776	-2.68627
H	-2.80126	-1.95431	2.44155
H	-4.80769	-1.48127	3.79016
H	-6.36117	0.34627	3.12601
H	-5.8613	1.70906	1.0986
H	-3.8525	1.25301	-0.23759
H	-0.56354	0.21476	-2.5096
H	-1.28746	-0.01035	-4.87657
H	-3.43987	-1.13826	-5.41091
H	-4.85768	-2.02978	-3.57409
H	-4.12703	-1.80717	-1.2198
H	3.86878	1.72833	0.77236
H	5.63905	2.90516	-0.46914
H	6.12153	2.30341	-2.83656
H	4.81812	0.48902	-3.93325
H	3.04545	-0.69146	-2.69284
H	4.4492	-1.1739	1.29541
H	5.11941	-1.35415	3.6697
H	3.5339	-0.6976	5.46807
H	1.26902	0.14488	4.87496
H	0.59604	0.31263	2.4891

Ni	-0.08905	0.90305	0.03022
C	-1.24187	2.43279	0.09624
C	-1.80674	2.8362	1.34486
C	-1.95046	2.85166	-1.07212
C	-2.89029	3.70501	1.40488
H	-1.39165	2.45617	2.27555
C	-3.03833	3.7166	-0.99037
H	-1.63907	2.50106	-2.05196
C	-3.51255	4.17966	0.24317
H	-3.27681	3.99271	2.38128
H	-3.53472	4.02115	-1.91067
H	-4.35921	4.85721	0.29869
C	1.16834	3.33034	1.14319
C	1.06146	3.2284	-1.27929
C	1.05432	4.85245	1.04105
H	2.23149	3.05909	1.2501
H	0.66157	2.9922	2.05088
C	0.95175	4.75439	-1.29711
H	2.10876	2.93957	-1.45372
H	0.4733	2.81561	-2.10476
H	1.60491	5.34087	1.85143
H	-0.00302	5.1517	1.09056
H	1.43013	5.16938	-2.18992
H	-0.10553	5.05643	-1.2787
O	1.62992	5.32661	-0.17711
N	0.58313	2.67809	-0.01703

(PAd-DalPhos)Ni(Ph)NH_2 reductive elimination



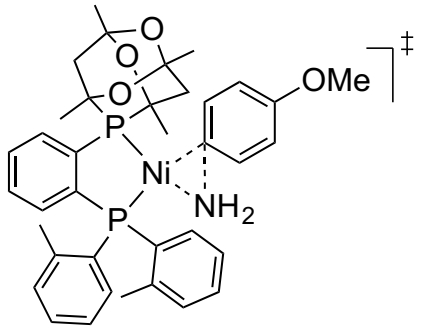
Zero-point correction= 0.692220 (Hartree/Particle)
Thermal correction to Energy= 0.733340
Thermal correction to Enthalpy= 0.734284
Thermal correction to Gibbs Free Energy= 0.621423
Sum of electronic and zero-point Energies= -3867.289495
Sum of electronic and thermal Energies= -3867.248376
Sum of electronic and thermal Enthalpies= -3867.247432
Sum of electronic and thermal Free Energies= -3867.360292

Single-point energy (6-311+G(2d,2p)) = -3868.729506

Ni	0.1747930	1.3235040	0.1935760
P	-1.0455170	-0.3878590	-0.3766190
P	1.9900360	-0.0815900	0.0354830
C	-1.0033390	2.8188530	0.3367260
C	-1.5169650	3.4662040	-0.8261870
C	-1.7682760	2.9544950	1.5333300
C	0.0472550	-1.5435750	-1.3269590
C	1.4406270	-1.3665050	-1.1616290
C	-2.6700570	-0.2812910	-1.3444520
C	-1.8389460	-1.3859030	1.0393430
C	2.5721980	-1.0405450	1.4967160
C	3.5254610	0.5970290	-0.7093510
C	-2.7049080	4.1905620	-0.7857610
C	-2.9526530	3.6849380	1.5519630
H	-1.4331250	2.4575390	2.4416920
O	-3.2485460	-1.5899180	-1.5726410
O	-2.8541080	-0.5368120	1.6061300
C	2.3386390	-2.1159270	-1.9323840
C	-0.4059720	-2.4945750	-2.2571530
C	-2.4980750	-2.6584190	0.5010280
C	-3.6290590	0.5248960	-0.4604330
C	-2.4744280	0.3580490	-2.7096880
C	-0.8508820	-1.6654940	2.1568040
C	2.7285750	-0.3669530	2.7309930
C	2.8028910	-2.4226540	1.4308620
C	3.4354720	1.3726430	-1.8916310
C	4.7677580	0.4407310	-0.0774000
H	-3.0644720	4.6636920	-1.6980820
C	-3.4430880	4.3121410	0.3984330
H	-3.5081330	3.7607330	2.4854860
H	3.4066700	-1.9521870	-1.8171710
C	1.8732280	-3.0517670	-2.8548570
C	0.4989730	-3.2406910	-3.0123240
H	-1.4704590	-2.6288940	-2.4060300
C	-3.6847130	-2.3001470	-0.4064290
H	-1.7730940	-3.2753440	-0.0374970
H	-2.8820260	-3.2409800	1.3470480
H	-4.5456300	0.7165640	-1.0306960
H	-3.1904620	1.4817210	-0.1767130
C	-4.0024960	-0.2799150	0.7882550
H	-3.4356630	0.3916110	-3.2353060
H	-1.7648310	-0.2063150	-3.3221100
H	-2.1057450	1.3803610	-2.5857060
H	-1.3702450	-2.1585500	2.9866730

H	-0.4126980	-0.7330960	2.5234050
H	-0.0421690	-2.3158670	1.8118700
C	3.1275530	-1.1076650	3.8498620
C	3.1873210	-3.1443530	2.5609220
H	2.6759320	-2.9449040	0.4889870
C	2.4530530	1.1102150	2.8763360
C	4.6049400	1.9538810	-2.3944900
H	4.8361600	-0.1512730	0.8294540
C	2.1357110	1.5663850	-2.6364380
H	-4.3686130	4.8789910	0.4226660
C	5.9192650	1.0344760	-0.5946830
O	-4.5909510	-1.5130460	0.3577670
H	2.5782340	-3.6255800	-3.4501730
H	0.1271150	-3.9625590	-3.7345860
C	-4.4474470	-3.5100350	-0.9075920
C	-5.0090440	0.4198210	1.6754350
H	3.2540250	-0.5932680	4.7993860
C	3.3528030	-2.4821590	3.7760600
H	3.3578010	-4.2149120	2.4875330
H	2.9706950	1.7140030	2.1230090
H	2.7563400	1.4641190	3.8666720
H	1.3834840	1.3197130	2.7506490
H	4.5430230	2.5496970	-3.3020860
H	1.3190290	1.8467640	-1.9581700
H	1.8213880	0.6474500	-3.1467520
H	2.2362250	2.3508750	-3.3930260
C	5.8369220	1.7940330	-1.7598550
H	6.8711140	0.9007380	-0.0880550
H	-5.2834360	-3.1798150	-1.5295140
H	-4.8357970	-4.0827560	-0.0610150
H	-3.7900010	-4.1509840	-1.5028460
H	-5.2340810	-0.2102340	2.5401580
H	-5.9305150	0.6049480	1.1166500
H	-4.5959150	1.3729400	2.0133500
H	3.6532920	-3.0306580	4.6646270
H	6.7246940	2.2646270	-2.1735480
H	-0.9670150	3.3933110	-1.7635880
N	0.8062360	3.0700550	0.5695780
H	0.8502750	3.4791790	1.4960690
H	0.9920510	3.7853830	-0.1231110

(PAd-DalPhos)Ni(*p*-OMePh)NH_2 reductive elimination



Zero-point correction= 0.724850 (Hartree/Particle)
Thermal correction to Energy= 0.768662
Thermal correction to Enthalpy= 0.769606
Thermal correction to Gibbs Free Energy= 0.650259
Sum of electronic and zero-point Energies= -3981.781719
Sum of electronic and thermal Energies= -3981.737907
Sum of electronic and thermal Enthalpies= -3981.736962
Sum of electronic and thermal Free Energies= -3981.856310

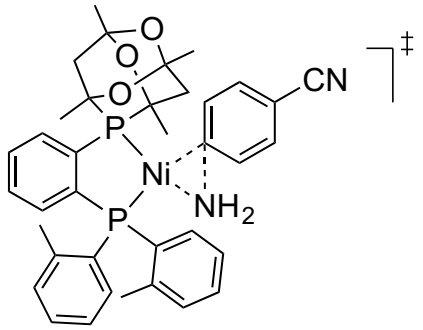
Single-point energy (6-311+G(2d,2p)) = -3983.290405

Ni	-0.1054870	-1.1577190	0.1906120
P	0.6350850	0.8099680	-0.3791840
P	-2.2225860	-0.2600520	0.0299720
C	1.4161280	-2.3128340	0.3580160
C	2.1121270	-2.7986050	-0.7815780
C	2.1690830	-2.2391780	1.5681840
C	-0.7143020	1.6471580	-1.3330250
C	-2.0167180	1.1198860	-1.1696730
C	2.2349970	1.1232540	-1.3441870
C	1.1449660	1.9813150	1.0352400
C	-3.0306640	0.5238460	1.4879520
C	-3.5362800	-1.3065290	-0.7131540
C	3.4572420	-3.1761010	-0.7247480
C	3.5047910	-2.6132960	1.6186240
H	1.6972500	-1.8564410	2.4707220
O	2.4625800	2.5351260	-1.5754250
O	2.3426630	1.4210530	1.6059430
C	-3.0742910	1.6126270	-1.9448570
C	-0.5172230	2.6799780	-2.2657060
C	1.4581410	3.3790160	0.4947990
C	3.3667040	0.5900900	-0.4571100
C	2.2113850	0.4520020	-2.7079650
C	0.1168050	2.0020910	2.1512240
C	-3.0151020	-0.1663500	2.7229940

C	-3.5987460	1.8047540	1.4212030
C	-3.2522430	-2.0367240	-1.8938120
C	-4.7767600	-1.4721870	-0.0796910
H	3.9368870	-3.5320260	-1.6309010
C	4.1675220	-3.0843190	0.4759230
H	4.0621870	-2.5413690	2.5491410
H	-4.0653420	1.1818800	-1.8306520
C	-2.8614230	2.6337550	-2.8696930
C	-1.5807210	3.1675470	-3.0252920
H	0.4777580	3.0822820	-2.4125010
C	2.6990830	3.3350200	-0.4096110
H	0.6005470	3.7886080	-0.0464680
H	1.6783510	4.0423600	1.3398380
H	4.3033370	0.6375250	-1.0252150
H	3.1853180	-0.4463240	-0.1724430
C	3.5202430	1.4653310	0.7907710
H	3.1517680	0.6596370	-3.2315230
H	1.3845220	0.8180820	-3.3238450
H	2.1098450	-0.6298050	-2.5815820
H	0.4926220	2.6122060	2.9807310
H	-0.0705120	0.9894550	2.5189250
H	-0.8302360	2.4248840	1.8044430
C	-3.5872550	0.4517150	3.8410620
C	-4.1518770	2.4083880	2.5505540
H	-3.6052440	2.3416360	0.4790080
C	-2.3795760	-1.5279810	2.8689590
C	-4.2344880	-2.8991260	-2.3935980
H	-4.9937550	-0.9148530	0.8257730
C	-1.9470090	-1.8928360	-2.6404380
C	-5.7383660	-2.3423420	-0.5936450
O	3.7747290	2.8069780	0.3577430
H	-3.6883190	3.0067230	-3.4679090
H	-1.4040360	3.9587990	-3.7490320
C	3.1282460	4.6990260	-0.9116730
C	4.6713990	1.0481480	1.6799690
H	-3.5820340	-0.0773770	4.7909370
C	-4.1482100	1.7266080	3.7661280
H	-4.5838640	3.4025980	2.4762150
H	-2.7382690	-2.2442550	2.1215500
H	-2.5770970	-1.9423020	3.8626010
H	-1.2926400	-1.4651680	2.7334420
H	-4.0230340	-3.4614230	-3.3001050
H	-1.0853840	-1.9486670	-1.9619550
H	-1.8810230	-0.9268990	-3.1564980
H	-1.8422770	-2.6812050	-3.3925130
C	-5.4657070	-3.0585220	-1.7573570

H	-6.6922730	-2.4552570	-0.0857730
H	4.0223970	4.5926390	-1.5312850
H	3.3552490	5.3532030	-0.0654960
H	2.3301810	5.1496660	-1.5094910
H	4.7282050	1.7182570	2.5420350
H	5.6101350	1.1015200	1.1218100
H	4.5161900	0.0226010	2.0226020
H	-4.5766480	2.1833980	4.6540890
H	-6.2038830	-3.7417470	-2.1685220
H	1.5894980	-2.8814420	-1.7331920
N	-0.2605900	-3.0111250	0.5615610
H	-0.2318410	-3.4147720	1.4912640
H	-0.2491600	-3.7536020	-0.1270060
O	5.5014700	-3.4213660	0.6382350
C	6.2013790	-3.8701580	-0.5048060
H	6.2181310	-3.1048030	-1.2941650
H	7.2228050	-4.0719730	-0.1765550
H	5.7627640	-4.7920910	-0.9122310

(PAd-DalPhos)Ni(*p*-CNPh)NH_2 reductive elimination



Zero-point correction= 0.691120 (Hartree/Particle)
Thermal correction to Energy= 0.734074
Thermal correction to Enthalpy= 0.735018
Thermal correction to Gibbs Free Energy= 0.617748
Sum of electronic and zero-point Energies= -3959.552536
Sum of electronic and thermal Energies= -3959.509581
Sum of electronic and thermal Enthalpies= -3959.508637
Sum of electronic and thermal Free Energies= -3959.625908

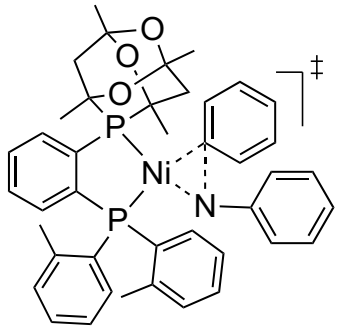
Single-point energy (6-311+G(2d,2p)) = -3961.012524

Ni	0.1050510	1.1838250	0.1277860
P	-0.7232940	-0.7699860	-0.3803590
P	2.1692200	0.1951820	0.0395140
C	-1.3650320	2.3599800	0.2059100
C	-1.9779140	2.8813960	-0.9775720

C	-2.1544770	2.3931950	1.3994300
C	0.6063850	-1.7019250	-1.2706200
C	1.9260980	-1.2231000	-1.1053150
C	-2.3160130	-1.0369080	-1.3712820
C	-1.3235360	-1.8411450	1.0754510
C	2.9056280	-0.5561200	1.5507190
C	3.5292080	1.1681800	-0.7152660
C	-3.2634550	3.3887420	-0.9672050
C	-3.4380920	2.9037560	1.4041120
H	-1.7482330	1.9793860	2.3194650
O	-2.5942010	-2.4461260	-1.5419640
O	-2.5034450	-1.1933210	1.5826140
C	2.9766840	-1.7961590	-1.8328840
C	0.3813260	-2.7697730	-2.1557000
C	-1.6895680	-3.2460500	0.5896780
C	-3.4450690	-0.4162040	-0.5400660
C	-2.2265540	-0.4339890	-2.7642350
C	-0.3239700	-1.8568810	2.2174930
C	2.8854610	0.1780050	2.7595070
C	3.4344490	-1.8554340	1.5394490
C	3.2956930	1.8597210	-1.9290480
C	4.7639300	1.3040790	-0.0647840
H	-3.7040300	3.7665940	-1.8860840
C	-4.0282930	3.4086290	0.2215490
H	-4.0154180	2.9055550	2.3250880
H	3.9828820	-1.4020600	-1.7191400
C	2.7366660	-2.8509610	-2.7122740
C	1.4376420	-3.3376700	-2.8683800
H	-0.6271580	-3.1354700	-2.3051170
C	-2.9031340	-3.1834180	-0.3497510
H	-0.8389240	-3.7206660	0.0922330
H	-1.9632920	-3.8574380	1.4576190
H	-4.3675060	-0.4507440	-1.1311550
H	-3.2288670	0.6238970	-0.2976990
C	-3.6668290	-1.2251690	0.7417590
H	-3.1631700	-0.6227180	-3.3006970
H	-1.4044910	-0.8692110	-3.3401130
H	-2.0770300	0.6468880	-2.6900130
H	-0.7479170	-2.4107950	3.0627860
H	-0.0994290	-0.8383510	2.5460150
H	0.6106230	-2.3376050	1.9149330
C	3.4135810	-0.4190930	3.9104820
C	3.9445980	-2.4358070	2.7004550
H	3.4437300	-2.4255210	0.6171940
C	2.2914050	1.5628020	2.8484350
C	4.3226320	2.6587960	-2.4438070

H	4.9400460	0.7763260	0.8668210
C	1.9983400	1.7417280	-2.6934930
C	5.7709850	2.1106040	-0.5952620
O	-3.9696740	-2.5716210	0.3639770
H	3.5572360	-3.2860610	-3.2759600
H	1.2407280	-4.1543090	-3.5575760
C	-3.3851150	-4.5450390	-0.8073370
C	-4.8167490	-0.7170370	1.5833490
H	3.4053950	0.1426470	4.8412200
C	3.9357230	-1.7120650	3.8914840
H	4.3468700	-3.4444970	2.6697090
H	2.6539980	2.2324140	2.0615180
H	2.5175810	2.0182300	3.8174990
H	1.2003210	1.5244490	2.7381080
H	4.1516610	3.1930510	-3.3752370
H	1.1284080	1.8780280	-2.0377670
H	1.8919870	0.7545360	-3.1599390
H	1.9469260	2.4931040	-3.4874320
C	5.5484260	2.7902610	-1.7909150
H	6.7199340	2.2038110	-0.0746690
H	-4.2564190	-4.4221810	-1.4555990
H	-3.6663940	-5.1506000	0.0584100
H	-2.5949140	-5.0589030	-1.3630620
H	-4.9265580	-1.3467230	2.4702260
H	-5.7435800	-0.7475250	1.0044080
H	-4.6205580	0.3130360	1.8893680
H	4.3309480	-2.1502200	4.8037740
H	6.3222430	3.4242590	-2.2148710
H	-1.4197930	2.8772980	-1.9121130
N	0.3864370	3.0275040	0.4538720
H	0.3059360	3.4660630	1.3645070
H	0.4074400	3.7422090	-0.2642490
C	-5.3606290	3.9031850	0.2249730
N	-6.4586600	4.3031630	0.2277030

(PAd-DalPhos)Ni(Ph)PhNH reductive elimination



Zero-point correction= 0.774185 (Hartree/Particle)
Thermal correction to Energy= 0.819562
Thermal correction to Enthalpy= 0.820506
Thermal correction to Gibbs Free Energy= 0.698039
Sum of electronic and zero-point Energies= -4098.277309
Sum of electronic and thermal Energies= -4098.231932
Sum of electronic and thermal Enthalpies= -4098.230987
Sum of electronic and thermal Free Energies= -4098.353454

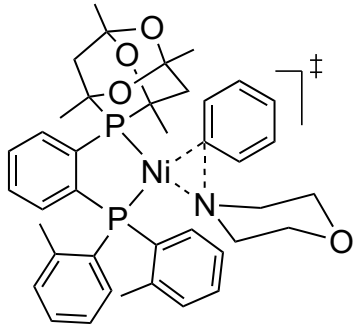
Single-point energy (6-311+G(2d,2p)) = -4099.873157

Ni	0.1895250	0.6869280	-0.5649140
P	-1.4155590	-0.7026620	-0.0690030
P	1.6929340	-0.9779120	-0.0685020
C	-0.6434290	2.2885560	-1.2921720
C	-0.9402830	2.2003370	-2.6874260
C	-1.4297710	3.2004490	-0.5271110
C	-0.7207410	-2.4204320	-0.0923740
C	0.6863410	-2.5274850	-0.0575350
C	-3.0815000	-0.8029750	-0.9658600
C	-2.2377120	-0.4696990	1.6350800
C	2.5144940	-0.9390530	1.5780390
C	3.0200510	-1.4501230	-1.2589630
C	-1.9585090	2.9574840	-3.2610740
C	-2.4220950	3.9641900	-1.1301980
H	-1.2571310	3.2979340	0.5382850
O	-3.9394230	-1.8203100	-0.3939760
O	-2.9828280	0.7592880	1.5527370
C	1.2936590	-3.7901710	-0.1059470
C	-1.4839020	-3.5972050	-0.1990520
C	-3.2064080	-1.6155530	1.9382850
C	-3.7501800	0.5608520	-0.7657910
C	-2.9059130	-1.1472060	-2.4360900
C	-1.2053040	-0.2727330	2.7301470
C	3.4425270	0.0862620	1.8813860

C	2.1252790	-1.8361930	2.5868190
C	2.7278560	-1.4666080	-2.6438370
C	4.3091570	-1.7877190	-0.8222960
H	-2.1590060	2.8469930	-4.3253230
C	-2.7143800	3.8530640	-2.4971180
H	-2.9921550	4.6565520	-0.5130790
H	2.3771660	-3.8627490	-0.0927700
C	0.5240360	-4.9474300	-0.1942390
C	-0.8674640	-4.8462880	-0.2503360
H	-2.5620380	-3.5274870	-0.2679180
C	-4.3829220	-1.5925340	0.9505490
H	-2.6928180	-2.5800780	1.9090760
H	-3.6109950	-1.4743490	2.9477100
H	-4.6656310	0.5893320	-1.3683060
H	-3.0955980	1.3699890	-1.0883700
C	-4.1395620	0.7495310	0.7045370
H	-3.8889040	-1.2004400	-2.9178780
H	-2.4047300	-2.1114370	-2.5658740
H	-2.3150940	-0.3676830	-2.9268980
H	-1.7114180	-0.0533420	3.6773500
H	-0.5403210	0.5605250	2.4879060
H	-0.5959550	-1.1720980	2.8568620
C	3.9300290	0.1759800	3.1915500
C	2.6248340	-1.7274220	3.8833400
H	1.4229650	-2.6299830	2.3570040
C	3.9642390	1.0550970	0.8472600
C	3.7537690	-1.7965460	-3.5377130
H	4.5285290	-1.7932180	0.2405730
C	1.3436810	-1.1894460	-3.1790740
H	-3.4999440	4.4494600	-2.9502610
C	5.3153100	-2.1180090	-1.7297130
O	-5.0151110	-0.3241640	1.0677440
H	1.0069810	-5.9199670	-0.2339280
H	-1.4767880	-5.7414690	-0.3422160
C	-5.4308930	-2.6496320	1.2352930
C	-4.8775770	2.0420440	0.9765580
H	4.6374000	0.9672160	3.4283800
C	3.5295440	-0.7114530	4.1887430
H	2.3058430	-2.4315000	4.6469600
H	4.9072220	0.6927560	0.4178120
H	4.1511370	2.0357800	1.2928530
H	3.2661100	1.1982540	0.0211590
H	3.5356610	-1.8055710	-4.6030190
H	0.9054150	-0.2875810	-2.7329160
H	0.6554910	-2.0134020	-2.9510870
H	1.3624990	-1.0614200	-4.2658750

C	5.0372280	-2.1157810	-3.0954610
H	6.3075810	-2.3739440	-1.3683740
H	-6.2433790	-2.5595840	0.5097350
H	-5.8339210	-2.5130590	2.2424860
H	-4.9912010	-3.6486700	1.1576360
H	-5.1381040	2.0958000	2.0369870
H	-5.7930230	2.0792140	0.3797710
H	-4.2414350	2.8888680	0.7123290
H	3.9226290	-0.6094100	5.1966050
H	5.8125730	-2.3640830	-3.8150670
H	-0.3603180	1.5270460	-3.3167280
N	1.0799730	2.3163280	-1.0037810
H	1.4760730	2.4596370	-1.9261780
C	1.5862700	3.2036470	-0.0563950
C	1.2749040	3.0498340	1.3076200
C	2.4192770	4.2720170	-0.4382450
C	1.7947940	3.9265400	2.2562040
H	0.6466360	2.2167440	1.6096640
C	2.9484490	5.1330670	0.5192480
H	2.6568800	4.4123390	-1.4907780
C	2.6423660	4.9698750	1.8742950
H	1.5450990	3.7830670	3.3045720
H	3.6002160	5.9436130	0.2028230
H	3.0542460	5.6464190	2.6173010

(PAd-DalPhos)Ni(Ph)Morpholine reductive elimination



Zero-point correction= 0.792625 (Hartree/Particle)
Thermal correction to Energy= 0.837586
Thermal correction to Enthalpy= 0.838531
Thermal correction to Gibbs Free Energy= 0.717835
Sum of electronic and zero-point Energies= -4098.449280
Sum of electronic and thermal Energies= -4098.404318
Sum of electronic and thermal Enthalpies= -4098.403374
Sum of electronic and thermal Free Energies= -4098.524070

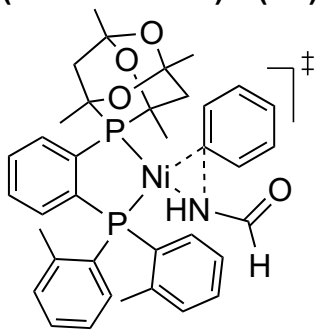
Single-point energy (6-311+G(2d,2p)) = -4100.062715765

Ni	0.2420740	0.9579910	0.0166520
P	-1.3965950	-0.4469350	-0.3914410
P	1.6188830	-0.9240430	0.0516960
C	-0.5875600	2.6829420	0.0881050
C	-1.1123960	3.3983120	-1.0258850
C	-1.1500840	3.0004370	1.3591290
C	-0.6431950	-1.8986330	-1.2607400
C	0.7471320	-2.0810460	-1.0862790
C	-2.9559080	-0.0031880	-1.3780500
C	-2.4145970	-1.1337710	1.0736730
C	1.8470580	-1.9521160	1.5764000
C	3.3120090	-0.8087580	-0.6559550
C	-2.1135870	4.3551920	-0.8724420
C	-2.1577640	3.9513720	1.4931990
H	-0.8168090	2.4662210	2.2457150
O	-3.8358850	-1.1422680	-1.5389670
O	-3.1932580	-0.0334990	1.5767370
C	1.4159180	-3.0850790	-1.7989970
C	-1.3295420	-2.7518490	-2.1426510
C	-3.3620560	-2.2389690	0.5981780
C	-3.6913450	1.0592110	-0.5531690
C	-2.6165900	0.4845060	-2.7774040
C	-1.5352720	-1.5822600	2.2252750
C	2.0158770	-1.3186010	2.8285040
C	1.8056820	-3.3537390	1.5208320
C	3.4979480	-0.2878830	-1.9594440
C	4.4331040	-1.1161130	0.1304450
H	-2.4843960	4.8718310	-1.7559950
C	-2.6547610	4.6469370	0.3839760
H	-2.5644190	4.1477530	2.4838160
H	2.4899420	-3.1992980	-1.6801140
C	0.7224810	-3.9195230	-2.6736220
C	-0.6531390	-3.7513750	-2.8411730
H	-2.3923740	-2.6136890	-2.2973770
C	-4.4292460	-1.6591520	-0.3412020
H	-2.8083930	-3.0427500	0.1049640
H	-3.8731650	-2.6614770	1.4715400
H	-4.5333290	1.4345690	-1.1467720
H	-3.0353820	1.8960650	-0.3169290
C	-4.2485010	0.4430650	0.7326090
H	-3.5426060	0.7248860	-3.3121570
H	-2.0745590	-0.2751590	-3.3484370
H	-2.0033050	1.3871270	-2.7134630
H	-2.1687560	-1.8868050	3.0663190
H	-0.8908410	-0.7641490	2.5555840

H	-0.9065120	-2.4278880	1.9343920
C	2.1422110	-2.1134090	3.9744400
C	1.9287980	-4.1291320	2.6732570
H	1.6641700	-3.8512790	0.5686610
C	2.0438270	0.1814310	2.9637010
C	4.8067000	-0.1116960	-2.4249590
H	4.2928210	-1.5163660	1.1292850
C	2.3452680	0.0641370	-2.8719060
H	-3.4343150	5.3940970	0.4966470
C	5.7274310	-0.9203410	-0.3501440
O	-5.1176050	-0.6351480	0.3668430
H	1.2532730	-4.6913610	-3.2242700
H	-1.2019850	-4.3919010	-3.5263250
C	-5.4613480	-2.6767400	-0.7837960
C	-5.0553950	1.4155070	1.5651290
H	2.2690400	-1.6253440	4.9375520
C	2.0986610	-3.5049100	3.9076720
H	1.8901990	-5.2126100	2.6024570
H	1.1112290	0.6245660	2.5940720
H	2.8550510	0.6288250	2.3804540
H	2.1755540	0.4793060	4.0084090
H	4.9548220	0.2880180	-3.4254900
H	1.4974480	0.4845020	-2.3187750
H	1.9694150	-0.8181540	-3.4039580
H	2.6589670	0.7970540	-3.6220660
C	5.9152680	-0.4183540	-1.6366810
H	6.5799580	-1.1617600	0.2784940
H	-6.1936930	-2.1915340	-1.4341480
H	-5.9756130	-3.0892320	0.0884760
H	-4.9782890	-3.4904420	-1.3332690
H	-5.4192180	0.9116200	2.4646530
H	-5.9096970	1.7777970	0.9866960
H	-4.4269630	2.2632480	1.8473200
H	2.1928000	-4.0951790	4.8150160
H	6.9174590	-0.2587510	-2.0244520
H	-0.7394720	3.1926680	-2.0250240
C	1.7752700	3.2321990	-1.1153940
C	1.7899660	3.2441820	1.2666590
C	3.3029280	3.3022120	-1.1066280
H	1.3713370	4.2590820	-1.1893670
H	1.4553960	2.6892730	-2.0085080
C	3.3176170	3.3074040	1.2346990
H	1.3920000	4.2735740	1.3279220
H	1.4745920	2.7231660	2.1720320
H	3.6638660	3.8885020	-1.9579370
H	3.7325630	2.2918790	-1.1603330

H	3.6987700	3.8871350	2.0815530
H	3.7426430	2.2912880	1.2772240
N	1.2770140	2.5716190	0.0822420
O	3.7850100	3.9629410	0.0608840

(PAd-DalPhos)Ni(Ph)HCONH reductive elimination



Zero-point correction= 0.702891 (Hartree/Particle)
Thermal correction to Energy= 0.745650
Thermal correction to Enthalpy= 0.746594
Thermal correction to Gibbs Free Energy= 0.629569
Sum of electronic and zero-point Energies= -3980.632343
Sum of electronic and thermal Energies= -3980.589584
Sum of electronic and thermal Enthalpies= -3980.588640
Sum of electronic and thermal Free Energies= -3980.705665

Single-point energy (6-311+G(2d,2p)) = -3982.112809

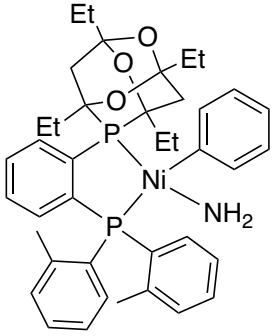
Ni	0.2138560	1.1079910	0.2224950
P	-1.2031990	-0.4444120	-0.3576370
P	1.8645080	-0.4434980	0.0261780
C	-0.7166560	2.8186830	0.3483340
C	-1.1415210	3.4458120	-0.8630290
C	-1.5093180	3.0547620	1.5120120
C	-0.2424100	-1.7127080	-1.3027430
C	1.1622140	-1.6775550	-1.1481960
C	-2.8200220	-0.1821620	-1.3050940
C	-2.0706000	-1.3447570	1.0784820
C	2.4238210	-1.4491070	1.4664090
C	3.4131320	0.1057480	-0.7949840
C	-2.2940220	4.2210970	-0.8964700
C	-2.6541460	3.8416450	1.4508980
H	-1.2270060	2.5879800	2.4533480
O	-3.5381370	-1.4221490	-1.5111370
O	-2.9818990	-0.3895540	1.6544750
C	1.9721400	-2.5215960	-1.9189780
C	-0.7990330	-2.6191340	-2.2212630
C	-2.8686380	-2.5451320	0.5626930

C	-3.6700060	0.7308670	-0.4125900
C	-2.5786800	0.4226850	-2.6789970
C	-1.0951290	-1.7175110	2.1802260
C	2.7376870	-0.7938690	2.6809340
C	2.4853580	-2.8493750	1.4047340
C	3.3319590	0.8435560	-2.0016910
C	4.6626410	-0.0996820	-0.1917650
H	-2.5958530	4.6673320	-1.8420160
C	-3.0688970	4.4352090	0.2522500
H	-3.2350640	3.9911550	2.3588550
H	3.0523730	-2.4662160	-1.8149640
C	1.4058330	-3.4125620	-2.8293100
C	0.0181960	-3.4607040	-2.9758550
H	-1.8730930	-2.6447370	-2.3604980
C	-4.0260040	-2.0720510	-0.3304100
H	-2.2209000	-3.2388180	0.0191220
H	-3.2979280	-3.0776440	1.4197700
H	-4.5691960	1.0208620	-0.9687000
H	-3.1234950	1.6351650	-0.1434810
C	-4.1089060	-0.0196920	0.8497350
H	-3.5386290	0.5587470	-3.1901740
H	-1.9457180	-0.2205810	-3.2974890
H	-2.0966050	1.3988220	-2.5707500
H	-1.6445000	-2.1548390	3.0218810
H	-0.5601650	-0.8315360	2.5343530
H	-0.3603610	-2.4452130	1.8238050
C	3.1206310	-1.5714880	3.7802550
C	2.8559580	-3.6061470	2.5162900
H	2.2362280	-3.3589470	0.4809580
C	2.6460430	0.7054650	2.8350800
C	4.5150290	1.3526270	-2.5489080
H	4.7254290	-0.6676470	0.7307560
C	2.0295540	1.0674070	-2.7355480
H	-3.9609010	5.0519100	0.2146370
C	5.8276730	0.4184480	-0.7558830
O	-4.8309640	-1.1855000	0.4391560
H	2.0436770	-4.0598880	-3.4248570
H	-0.4312670	-4.1463250	-3.6891820
C	-4.9209370	-3.1989110	-0.8053250
C	-5.0234030	0.7889810	1.7442220
H	3.3694200	-1.0708110	4.7126490
C	3.1791680	-2.9630810	3.7093230
H	2.8935250	-4.6896070	2.4446260
H	3.1840050	1.2494700	2.0515590
H	3.0525240	1.0212150	3.8005040
H	1.5984630	1.0280540	2.7881540

H	4.4594750	1.9263000	-3.4709020
H	1.2048120	1.3123130	-2.0519060
H	1.7199250	0.1704830	-3.2863050
H	2.1278700	1.8849760	-3.4566150
C	5.7525540	1.1510220	-1.9386300
H	6.7843820	0.2523040	-0.2687880
H	-5.7280300	-2.7880260	-1.4172400
H	-5.3528110	-3.7193470	0.0537910
H	-4.3453060	-3.9113110	-1.4039920
H	-5.3040220	0.1907190	2.6151460
H	-5.9266110	1.0698030	1.1957350
H	-4.5068730	1.6935010	2.0734280
H	3.4731100	-3.5386190	4.5827420
H	6.6505480	1.5696480	-2.3841380
H	-0.5649080	3.3066560	-1.7740040
N	0.9305640	2.8278730	0.7006390
H	1.0775070	2.9593570	1.7011430
C	1.8705550	3.5216890	-0.0209270
H	1.6834010	3.5336710	-1.1048010
O	2.8310170	4.0970250	0.4812210

CHAPTER 5 COMPOUNDS

(L32)Ni(Ph)NH_2



Zero-point correction= 0.808895 (Hartree/Particle)
Thermal correction to Energy= 0.856213
Thermal correction to Enthalpy= 0.857158
Thermal correction to Gibbs Free Energy= 0.730214
Sum of electronic and zero-point Energies= -4024.464546
Sum of electronic and thermal Energies= -4024.417228
Sum of electronic and thermal Enthalpies= -4024.416284
Sum of electronic and thermal Free Energies= -4024.543228

Single-point energy (6-311+G(2d,2p)) = -4.026080081287E+03

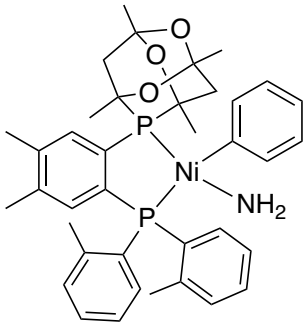
Ni 0.2256837 1.3748468 0.1150659

P	-1.0398037	-0.3920342	-0.3557680
P	1.9616941	-0.0395903	0.0493859
C	-1.2163889	2.6227021	0.1918152
C	-1.6153768	3.4217343	-0.8930939
C	-1.8891994	2.8113990	1.4122372
C	0.0655204	-1.5755844	-1.2673813
C	1.4526093	-1.3825981	-1.0971739
C	-2.6432679	-0.3067159	-1.3820954
C	-1.8785685	-1.3646759	1.0585631
C	2.4680559	-0.9347155	1.5870063
C	3.5279899	0.5987635	-0.6636073
C	-2.6701835	4.3355333	-0.7821498
C	-2.9345727	3.7329062	1.5354767
H	-1.6112794	2.2161019	2.2791198
O	-3.1828182	-1.6342948	-1.5923839
O	-2.9113596	-0.4975152	1.5553720
C	2.3671466	-2.1568834	-1.8218867
C	-0.3689148	-2.5712662	-2.1576506
C	-2.5062769	-2.6566539	0.5262034
C	-3.6610777	0.4889201	-0.5582187
C	-2.3584251	0.2909690	-2.7639767
C	-0.8928741	-1.5826223	2.2056499
C	2.4065934	-0.3082673	2.8550019
C	2.8909253	-2.2713984	1.4971574
C	3.5231087	1.2247643	-1.9357286
C	4.7140437	0.5478942	0.0823802
H	-2.9626849	4.9312361	-1.6447368
C	-3.3396422	4.4912629	0.4335204
H	-3.4346751	3.8567739	2.4942546
H	3.4320948	-1.9731692	-1.7089017
C	1.9199816	-3.1362174	-2.7072053
C	0.5495865	-3.3436352	-2.8688265
H	-1.4282406	-2.7190386	-2.3144169
C	-3.6587707	-2.3290051	-0.4332697
H	-1.7481108	-3.2749672	0.0394830
H	-2.9253773	-3.2262282	1.3618773
H	-4.5705033	0.6160880	-1.1532547
H	-3.2731198	1.4713164	-0.2979849
C	-4.0443805	-0.2869206	0.7050822
H	-1.6050514	-0.3320255	-3.2600128
H	-1.9022453	1.2734642	-2.6026671
H	-0.4788855	-0.6045023	2.4697081
H	-0.0576972	-2.1846620	1.8296126
C	2.7841312	-1.0609619	3.9780251
C	3.2523681	-2.9993066	2.6283975
H	2.9289146	-2.7603986	0.5309585

C	1.9240595	1.1039131	3.0693652
C	4.7258767	1.7618923	-2.4096068
H	4.7108670	0.0794457	1.0606730
C	2.2837017	1.3275962	-2.7942104
H	-4.1577383	5.2012166	0.5245347
C	5.8983024	1.0953512	-0.4108042
O	-4.5960454	-1.5387628	0.2891927
H	2.6360694	-3.7262836	-3.2724907
H	0.1897483	-4.0986618	-3.5625481
C	-4.4349440	-3.5457023	-0.9299605
C	-5.0944872	0.4371716	1.5383144
H	2.7416884	-0.5855312	4.9547238
C	3.1987953	-2.3866897	3.8792722
H	3.5718695	-4.0328927	2.5290077
H	2.2730299	1.8190099	2.3197142
H	2.2126068	1.4549309	4.0655698
H	0.8291254	1.1571110	3.0038069
H	4.7320223	2.2453104	-3.3834529
H	1.4266004	1.6982091	-2.2175864
H	1.9975245	0.3546602	-3.2109729
H	2.4535925	2.0130445	-3.6301900
C	5.9034761	1.7023180	-1.6645829
H	6.8052824	1.0485655	0.1852060
H	-5.2915432	-3.1597745	-1.4934457
H	-4.8372287	-4.0517662	-0.0449211
H	-5.9611953	0.6058574	0.8884019
H	-4.6823772	1.4204627	1.7890225
H	3.4769623	-2.9366087	4.7743744
H	6.8173690	2.1358647	-2.0614691
H	-1.0971689	3.3344170	-1.8467444
N	1.3627677	2.8373342	0.4361202
H	2.1816252	2.8427007	-0.1755101
H	0.9061051	3.7375366	0.3017765
C	-3.6388630	-4.5296074	-1.7904359
H	-3.2812567	-4.0533350	-2.7084933
H	-2.7739910	-4.9404585	-1.2572710
H	-4.2750891	-5.3729131	-2.0793479
C	-3.5813529	0.4246063	-3.6788418
H	-3.2663481	0.7749239	-4.6678389
H	-4.0898298	-0.5360250	-3.8036409
H	-4.3058329	1.1481213	-3.2915133
C	-5.5189214	-0.3108348	2.8038173
H	-6.2909757	0.2561763	3.3355152
H	-5.9266294	-1.2968368	2.5609573
H	-4.6708851	-0.4485686	3.4808070
C	-1.4784577	-2.2350710	3.4624481

H	-0.7116831	-2.2701325	4.2437358
H	-2.3298845	-1.6633129	3.8421007
H	-1.8099159	-3.2637117	3.2831420

(L33)Ni(Ph)NH_2



Zero-point correction= 0.749647 (Hartree/Particle)
Thermal correction to Energy= 0.794488
Thermal correction to Enthalpy= 0.795433
Thermal correction to Gibbs Free Energy= 0.675079
Sum of electronic and zero-point Energies= -3945.906373
Sum of electronic and thermal Energies= -3945.861532
Sum of electronic and thermal Enthalpies= -3945.860587
Sum of electronic and thermal Free Energies= -3945.980941

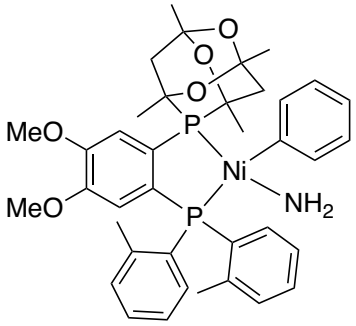
Single-point energy (6-311+G(2d,2p)) = -3.947431048360E+03

Ni	-0.0295650	-1.5763680	-0.3415390
P	1.0701910	0.3395160	-0.1241390
P	-1.8669010	-0.4009840	0.1776590
C	1.5072160	-2.6188000	-0.7831450
C	1.9020880	-2.9036150	-2.1013270
C	2.2652510	-3.1913120	0.2540190
C	-0.1627670	1.6772420	-0.4881110
C	-1.5172070	1.3126400	-0.3769720
C	2.6144710	0.8009250	-1.1358390
C	1.9157950	0.7750010	1.5306610
C	-2.3575530	-0.2087320	1.9500850
C	-3.4184560	-0.8568690	-0.6915430
C	3.0299620	-3.6861690	-2.3764020
C	3.3852510	-3.9861180	-0.0124780
H	1.9940420	-2.9997190	1.2897400
O	3.0355650	2.1556190	-0.8393650
O	3.0516890	-0.1036580	1.6404410
C	-2.5149290	2.2257830	-0.7331400
C	0.1392150	2.9711170	-0.9405410
C	2.4035490	2.2258550	1.5242450

C	3.7443780	-0.1407730	-0.7106020
C	2.3432170	0.7481040	-2.6306720
C	1.0249350	0.4684230	2.7197100
C	-2.1870760	-1.2635490	2.8786430
C	-2.8931830	1.0150150	2.3850420
C	-3.4372590	-0.9454580	-2.1064500
C	-4.5633530	-1.1990090	0.0419040
H	3.3160950	-3.8787690	-3.4086440
C	3.7814240	-4.2270490	-1.3310370
H	3.9501370	-4.4166680	0.8123310
H	-3.5570370	1.9204970	-0.6762930
C	-2.2116520	3.5091400	-1.1921160
C	-0.8560110	3.8872680	-1.2927210
H	1.1761880	3.2616850	-1.0527360
C	3.5209070	2.4030730	0.4876280
H	1.5771490	2.9137350	1.3258530
H	2.8163310	2.4618870	2.5123190
H	4.6139890	0.0629020	-1.3466200
H	3.4576200	-1.1830530	-0.8336930
C	4.1435030	0.1353350	0.7419510
H	3.2510940	1.0331050	-3.1744070
H	1.5392220	1.4329170	-2.9160300
H	2.0634790	-0.2682710	-2.9193780
H	1.5749480	0.6665680	3.6468510
H	0.7225060	-0.5811110	2.7128500
H	0.1250450	1.0901740	2.7042750
C	-2.5808050	-1.0384590	4.2068720
C	-3.2669860	1.2161540	3.7117270
H	-3.0133920	1.8296590	1.6805350
C	-1.5733980	-2.5955730	2.5287820
C	-4.6219060	-1.3630820	-2.7244420
H	-4.5415000	-1.1421490	1.1248170
C	-2.2416120	-0.6034340	-2.9648590
H	4.6566770	-4.8367940	-1.5402700
C	-5.7299860	-1.6170950	-0.5981740
O	4.5674080	1.5005480	0.8254290
C	4.1133130	3.7978120	0.4678500
C	5.2875980	-0.7302900	1.2234980
H	-2.4559750	-1.8448760	4.9251110
C	-3.1113960	0.1778970	4.6287620
H	-3.6759460	2.1740060	4.0210300
H	-1.8996410	-3.0053380	1.5689980
H	-1.7753690	-3.3247440	3.3202370
H	-0.4831360	-2.5090400	2.4287820
H	-4.6455080	-1.4357250	-3.8090360
H	-1.3316360	-1.0948930	-2.5976120

H	-2.0453210	0.4752430	-2.9742150
H	-2.4084860	-0.9234650	-3.9979930
C	-5.7590390	-1.6960290	-1.9885880
H	-6.6045290	-1.8812520	-0.0104000
H	4.9088640	3.8441850	-0.2802440
H	4.5307290	4.0387890	1.4492480
H	3.3421850	4.5324440	0.2166300
H	5.5261630	-0.4786240	2.2602820
H	6.1698370	-0.5588860	0.6005680
H	5.0008570	-1.7827950	1.1591640
H	-3.3985180	0.3134490	5.6681020
H	-6.6593640	-2.0226870	-2.5018520
H	1.3217980	-2.5106910	-2.9348110
N	-1.0334110	-3.1470730	-0.5825250
H	-1.8855660	-2.9928220	-1.1253520
H	-0.5202190	-3.8811560	-1.0669870
C	-0.4705450	5.2582900	-1.7916760
H	-0.8825110	6.0506320	-1.1534050
H	0.6164320	5.3772190	-1.8158580
H	-0.8505660	5.4412350	-2.8049580
C	-3.3169830	4.4594500	-1.5791760
H	-3.2899600	5.3762250	-0.9762650
H	-3.2324560	4.7702320	-2.6283060
H	-4.2995150	3.9978480	-1.4446690

(L34)Ni(Ph)NH_2



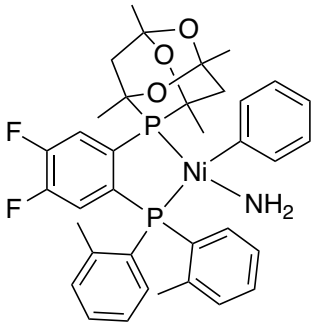
Zero-point correction= 0.759845 (Hartree/Particle)
Thermal correction to Energy= 0.806571
Thermal correction to Enthalpy= 0.807515
Thermal correction to Gibbs Free Energy= 0.682742
Sum of electronic and zero-point Energies= -4096.311319
Sum of electronic and thermal Energies= -4096.264593
Sum of electronic and thermal Enthalpies= -4096.263649
Sum of electronic and thermal Free Energies= -4096.388422

Single-point energy (6-311+G(2d,2p)) = -4.097894642836E+03

Ni	0.2092080	-1.7183340	-0.4786470
P	1.1264410	0.2556510	-0.0458380
P	-1.7157280	-0.7922750	0.2025710
C	1.8255590	-2.5432850	-1.0696600
C	2.2085150	-2.6239760	-2.4193260
C	2.6639610	-3.1613100	-0.1244780
C	-0.2334230	1.4976470	-0.2334540
C	-1.5392380	0.9951820	-0.1527500
C	2.5929570	0.9841430	-1.0144070
C	1.9696970	0.5661890	1.6374300
C	-2.1835880	-0.8577470	1.9904640
C	-3.2407420	-1.2809130	-0.6969560
C	3.3978380	-3.2519670	-2.8082950
C	3.8470120	-3.8030220	-0.5063400
H	2.4048470	-3.1267510	0.9313180
O	2.8878410	2.3301130	-0.5578450
O	3.1883580	-0.2020330	1.6221540
C	-2.6383980	1.8365120	-0.3889340
C	-0.0535450	2.8623470	-0.5345860
C	2.3149290	2.0478830	1.8057910
C	3.8199850	0.1158650	-0.7244950
C	2.2912110	1.0860450	-2.5007560
C	1.1438060	0.0281830	2.7906840
C	-1.9084210	-1.9994340	2.7806310
C	-2.8013720	0.2578520	2.5800540
C	-3.2850750	-1.2002520	-2.1119940
C	-4.3375980	-1.8019050	0.0042270
H	3.6715750	-3.2876520	-3.8610470
C	4.2269870	-3.8401820	-1.8509140
H	4.4736080	-4.2738480	0.2489670
H	-3.6365330	1.4161970	-0.3567780
C	-2.4582680	3.1795670	-0.7007660
C	-1.1395610	3.6992860	-0.7689640
H	0.9510290	3.2487710	-0.6212990
C	3.3827170	2.4598720	0.7836310
H	1.4206590	2.6691190	1.7061230
H	2.7288700	2.2010160	2.8096150
H	4.6492010	0.4804490	-1.3423550
H	3.6321780	-0.9270540	-0.9714600
C	4.2276250	0.2507990	0.7452940
H	3.1517490	1.5270510	-3.0167720
H	1.4141710	1.7117830	-2.6902760
H	2.1091600	0.0884200	-2.9084960
H	1.6961520	0.1628710	3.7277880
H	0.9439200	-1.0372250	2.6552410
H	0.1880410	0.5548060	2.8661150

C	-2.2875800	-1.9698690	4.1316340
C	-3.1585290	0.2658940	3.9264600
H	-2.9987100	1.1406410	1.9831090
C	-1.1971470	-3.2231920	2.2614980
C	-4.4467080	-1.6365180	-2.7603600
H	-4.2951130	-1.8737310	1.0856750
C	-2.1411080	-0.6605340	-2.9386740
H	5.1502860	-4.3305120	-2.1487800
C	-5.4816170	-2.2347740	-0.6664000
O	4.5197380	1.6318340	0.9902790
C	3.8390330	3.8978010	0.9295900
C	5.4625990	-0.5485090	1.1002720
H	-2.0826190	-2.8445290	4.7437950
C	-2.9018720	-0.8603820	4.7067690
H	-3.6319850	1.1438520	4.3571220
H	-1.5124310	-3.5404860	1.2639350
H	-1.3187430	-4.0570280	2.9606320
H	-0.1207280	-3.0332020	2.1556500
H	-4.4892700	-1.5803700	-3.8453750
H	-1.1866700	-1.1167440	-2.6468480
H	-2.0309020	0.4236690	-2.8182900
H	-2.3069450	-0.8656040	-4.0007800
C	-5.5364140	-2.1478790	-2.0556070
H	-6.3181490	-2.6392970	-0.1036480
H	4.6025740	4.1153600	0.1783480
H	4.2621840	4.0541710	1.9254650
H	2.9944080	4.5795960	0.7902960
H	5.7027330	-0.4018470	2.1566680
H	6.3074580	-0.2162990	0.4906750
H	5.2773960	-1.6087130	0.9110550
H	-3.1743690	-0.8753040	5.7586940
H	-6.4191970	-2.4835820	-2.5929670
H	1.5696660	-2.1911040	-3.1876830
N	-0.6467370	-3.3395080	-0.8932630
H	-1.5237640	-3.2054790	-1.4008650
H	-0.0792540	-3.9567430	-1.4711760
O	-3.4608910	4.0564430	-0.9622510
O	-1.0396390	5.0165120	-1.0874610
C	0.2617360	5.5815310	-1.1970260
H	0.7993900	5.5257820	-0.2421290
H	0.8494190	5.0807770	-1.9758310
H	0.1059930	6.6260560	-1.4678700
C	-4.7977100	3.5680180	-0.9409290
H	-4.9424910	2.7762110	-1.6862350
H	-5.0662690	3.1894850	0.0532910
H	-5.4266560	4.4235550	-1.1878070

(L35)Ni(Ph)NH_2



Zero-point correction= 0.677398 (Hartree/Particle)
Thermal correction to Energy= 0.720684
Thermal correction to Enthalpy= 0.721628
Thermal correction to Gibbs Free Energy= 0.604195
Sum of electronic and zero-point Energies= -4065.814241
Sum of electronic and thermal Energies= -4065.770955
Sum of electronic and thermal Enthalpies= -4065.770010
Sum of electronic and thermal Free Energies= -4065.887444

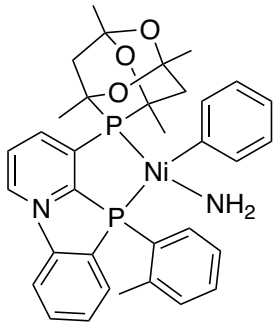
Single-point energy (6-311+G(2d,2p)) = -4.067295921418E+03

Ni	-0.0522490	-1.5750590	-0.3088920
P	1.0716090	0.3267440	-0.1308720
P	-1.8799660	-0.3748480	0.1786530
C	1.4765870	-2.6407270	-0.7220900
C	1.8694160	-2.9599930	-2.0326260
C	2.2290190	-3.1912960	0.3303900
C	-0.1474000	1.6722600	-0.5333110
C	-1.5094680	1.3242610	-0.4210610
C	2.6152040	0.7582180	-1.1574360
C	1.9202050	0.8016680	1.5133480
C	-2.3593010	-0.1226390	1.9454120
C	-3.4392680	-0.8224560	-0.6780590
C	2.9923510	-3.7565910	-2.2867440
C	3.3439290	-3.9999030	0.0845870
H	1.9579180	-2.9727120	1.3607360
O	3.0367700	2.1181150	-0.8912580
O	3.0488690	-0.0822920	1.6379650
C	-2.5082280	2.2281690	-0.8039800
C	0.1883230	2.9484610	-1.0154070
C	2.4178130	2.2485140	1.4731230
C	3.7405460	-0.1790140	-0.7108960
C	2.3432610	0.6695610	-2.6506360
C	1.0299560	0.5268590	2.7106320
C	-2.1921270	-1.1536100	2.9012540

C	-2.8830140	1.1169030	2.3494560
C	-3.4609830	-0.9513130	-2.0899040
C	-4.5894770	-1.1202170	0.0670610
H	3.2777900	-3.9771550	-3.3134200
C	3.7391820	-4.2760160	-1.2272630
H	3.9051170	-4.4137170	0.9202620
H	-3.5595310	1.9612290	-0.7586530
C	-2.1539920	3.4780950	-1.2828900
C	-0.8111350	3.8342610	-1.3822520
H	1.2218130	3.2452500	-1.1416070
C	3.5323240	2.3954180	0.4287600
H	1.5962680	2.9400380	1.2669580
H	2.8367170	2.5015530	2.4542140
H	4.6098620	0.0046120	-1.3531520
H	3.4474740	-1.2223310	-0.8090820
C	4.1430130	0.1301640	0.7336110
H	3.2515330	0.9406710	-3.2003540
H	1.5410310	1.3478680	-2.9559980
H	2.0629970	-0.3533260	-2.9145800
H	1.5840910	0.7421100	3.6313160
H	0.7215930	-0.5207320	2.7281480
H	0.1338830	1.1538060	2.6847660
C	-2.5739350	-0.8878060	4.2252870
C	-3.2452530	1.3581790	3.6725480
H	-3.0061370	1.9136810	1.6254220
C	-1.5967730	-2.5019170	2.5835410
C	-4.6546920	-1.3630970	-2.6942180
H	-4.5648810	-1.0326090	1.1478170
C	-2.2615340	-0.6551460	-2.9603120
H	4.6102770	-4.8967440	-1.4204200
C	-5.7647110	-1.5331770	-0.5599360
O	4.5730690	1.4942800	0.7829510
C	4.1323960	3.7854370	0.3713920
C	5.2823750	-0.7293670	1.2361740
H	-2.4516600	-1.6751500	4.9646560
C	-3.0905060	0.3446180	4.6168920
H	-3.6450620	2.3272380	3.9572520
H	-1.9434210	-2.9376240	1.6426360
H	-1.7942190	-3.2040400	3.3999730
H	-0.5075070	-2.4309630	2.4638000
H	-4.6820430	-1.4656180	-3.7761580
H	-1.3535970	-1.1323020	-2.5703810
H	-2.0621750	0.4215080	-3.0231540
H	-2.4278590	-1.0216290	-3.9777640
C	-5.7967660	-1.6517100	-1.9475800
H	-6.6437970	-1.7620660	0.0355410

H	4.9266900	3.8073960	-0.3790310
H	4.5534290	4.0487400	1.3454460
H	3.3663220	4.5190440	0.1025820
H	5.5231750	-0.4528510	2.2660290
H	6.1650370	-0.5785200	0.6086390
H	4.9898710	-1.7815780	1.1987340
H	-3.3685130	0.5116400	5.6539940
H	-6.7042990	-1.9742030	-2.4503910
H	1.2917490	-2.5847140	-2.8758620
N	-1.0685510	-3.1404430	-0.5150000
H	-1.9152380	-2.9934390	-1.0683130
H	-0.5599520	-3.8940280	-0.9734980
F	-0.4888500	5.0548700	-1.8603630
F	-3.1033970	4.3570000	-1.6638940

(L36)Ni(Ph)NH_2



Zero-point correction= 0.682081 (Hartree/Particle)
Thermal correction to Energy= 0.723340
Thermal correction to Enthalpy= 0.724285
Thermal correction to Gibbs Free Energy= 0.611502
Sum of electronic and zero-point Energies= -3883.368414
Sum of electronic and thermal Energies= -3883.327155
Sum of electronic and thermal Enthalpies= -3883.326210
Sum of electronic and thermal Free Energies= -3883.438993

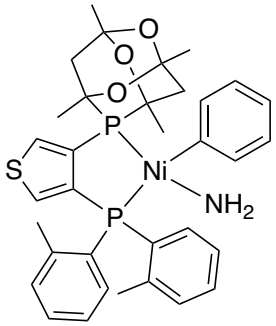
Single-point energy (6-311+G(2d,2p)) = -3.884798011753E+03

Ni	0.2347400	1.3802600	0.1117000
P	-1.0355600	-0.3780700	-0.3270700
P	1.9827800	-0.0177200	0.0659100
C	-1.2103800	2.6285500	0.1823500
C	-1.5972200	3.4306800	-0.9047500
C	-1.9002800	2.8112500	1.3943700
C	0.0581700	-1.5946900	-1.1985300
C	1.4441700	-1.4436300	-0.9912400
C	-2.6190200	-0.3041200	-1.3780400
C	-1.8996000	-1.3574100	1.0681000

C	2.5625200	-0.8237000	1.6184600
C	3.4976000	0.6020900	-0.7569100
C	-2.6549600	4.3424000	-0.8042600
C	-2.9481600	3.7312500	1.5076500
H	-1.6335200	2.2138800	2.2632100
O	-3.1476900	-1.6343700	-1.6025000
O	-2.9522000	-0.5036000	1.5518900
C	-0.3486200	-2.6096400	-2.0795300
C	-2.5155900	-2.6517500	0.5306500
C	-3.6579200	0.4874300	-0.5788000
C	-2.3557600	0.2966400	-2.7493100
C	-0.9697900	-1.6077500	2.2406100
C	2.3646300	-0.2275300	2.8867300
C	3.2145600	-2.0654400	1.5203600
C	3.4274400	1.1209500	-2.0724300
C	4.7052900	0.6571900	-0.0489900
H	-2.9371900	4.9408800	-1.6682800
C	-3.3400300	4.4929400	0.4032700
H	-3.4599800	3.8516300	2.4606600
C	1.9572900	-3.1899400	-2.3919900
C	0.6122500	-3.4108300	-2.6901300
H	-1.4004200	-2.7473900	-2.2973000
C	-3.6493400	-2.3312400	-0.4512500
H	-1.7568400	-3.2823200	0.0596800
H	-2.9435200	-3.2084400	1.3727300
H	-4.5476300	0.6128300	-1.2070500
H	-3.2797200	1.4709500	-0.3074100
C	-4.0680900	-0.2925100	0.6738000
H	-3.2876900	0.3070000	-3.3257000
H	-1.6124300	-0.2820900	-3.3062600
H	-1.9964000	1.3229600	-2.6402500
H	-1.5119100	-2.1405600	3.0301800
H	-0.6036500	-0.6643700	2.6487800
H	-0.1098300	-2.2123000	1.9354800
C	2.8252200	-0.9273700	4.0129800
C	3.6571600	-2.7387100	2.6563400
H	3.3866100	-2.4990800	0.5410600
C	1.6873700	1.1044800	3.0923100
C	4.5918300	1.6588400	-2.6318000
H	4.7516100	0.2709400	0.9631800
C	2.1550700	1.1126300	-2.8866200
H	-4.1599000	5.2017600	0.4863600
C	5.8509400	1.2042300	-0.6264200
O	-4.6091800	-1.5467500	0.2446500
H	2.7383500	-3.8000400	-2.8408900
H	0.3251100	-4.1913300	-3.3883200

C	-4.3632200	-3.5597600	-0.9778900
C	-5.1279500	0.4080700	1.4956200
H	2.6795900	-0.4808800	4.9933300
C	3.4566600	-2.1646900	3.9113600
H	4.1573700	-3.6981600	2.5583600
H	2.0577100	1.8900500	2.4263200
H	1.7984700	1.4275500	4.1324600
H	0.6131300	1.0474300	2.8752700
H	4.5487100	2.0581300	-3.6422300
H	1.3076500	1.5057300	-2.3096700
H	1.8904500	0.0992500	-3.2121000
H	2.2688700	1.7294500	-3.7833900
C	5.7938500	1.7028400	-1.9257600
H	6.7771200	1.2404200	-0.0599800
H	-5.1645100	-3.2521300	-1.6545500
H	-4.7942100	-4.1241600	-0.1466100
H	-3.6630400	-4.2018200	-1.5210000
H	-5.3797200	-0.2028800	2.3665000
H	-6.0265200	0.5583800	0.8909400
H	-4.7505400	1.3787600	1.8264300
H	3.7951300	-2.6745700	4.8095400
H	6.6778300	2.1331200	-2.3885300
H	-1.0650700	3.3487200	-1.8512600
N	1.3814900	2.8414600	0.3939000
H	2.1930900	2.8296400	-0.2271100
H	0.9266300	3.7406300	0.2470600
N	2.3707500	-2.2272900	-1.5616200

(L37)Ni(Ph)NH_2



Zero-point correction= 0.660176 (Hartree/Particle)
Thermal correction to Energy= 0.701383
Thermal correction to Enthalpy= 0.702327
Thermal correction to Gibbs Free Energy= 0.589091
Sum of electronic and zero-point Energies= -4188.112411
Sum of electronic and thermal Energies= -4188.071204
Sum of electronic and thermal Enthalpies= -4188.070260

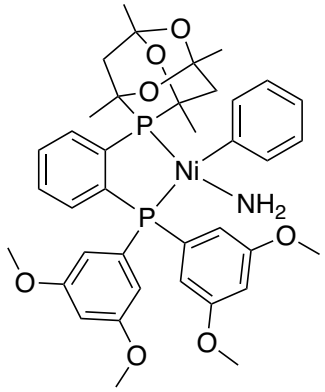
Sum of electronic and thermal Free Energies= -4188.183496

Single-point energy (6-311+G(2d,2p)) = -4.189525980631E+03

Ni	0.2397190	1.4223820	0.0743130
P	-1.0611160	-0.3421050	-0.2860560
P	1.9967470	0.0033480	0.0742150
C	-1.2168340	2.6554970	0.0996150
C	-1.6090280	3.4140060	-1.0162550
C	-1.9168960	2.8650990	1.3008570
C	1.4446710	-1.3874500	-0.9701410
C	-1.9308470	-1.2439310	1.1520710
C	2.5034130	-0.8051360	1.6552040
C	3.5595840	0.5740100	-0.6988340
C	-2.6804810	4.3128270	-0.9510470
C	-2.9789750	3.7724700	1.3780940
H	-1.6477160	2.2986750	2.1893840
O	-3.1066100	-1.6884880	-1.5246390
O	-3.0118340	-0.3886660	1.5682980
C	-2.5043990	-2.5801350	0.6753840
C	-3.6954940	0.4748440	-0.6212170
C	-1.0155220	-1.3945940	2.3529660
C	2.4226690	-0.1205750	2.8913050
C	2.9649000	-2.1315250	1.6251240
C	3.5448250	1.1193050	-2.0073810
C	4.7549230	0.5512900	0.0339110
H	-2.9667720	4.8781630	-1.8357690
C	-3.3745750	4.4925500	0.2473950
H	-3.4993360	3.9145730	2.3233850
C	-3.6201290	-2.3361550	-0.3492320
H	-1.7194890	-3.2119420	0.2518120
H	-2.9399400	-3.1025070	1.5354370
H	-4.5752020	0.5529640	-1.2708320
H	-3.3400330	1.4780300	-0.3914020
C	-4.1136590	-0.2517630	0.6598300
H	-3.2706970	0.1673140	-3.3455270
H	-1.5830920	-0.3833390	-3.2655270
H	-2.0145480	1.2447910	-2.6886660
H	-1.5660010	-1.8646070	3.1759630
H	-0.6576950	-0.4177820	2.6870030
H	-0.1494210	-2.0170080	2.1080570
C	2.8238940	-0.8080320	4.0472640
C	3.3502790	-2.7937680	2.7881290
H	3.0150210	-2.6594230	0.6794920
C	1.9018740	1.2871600	3.0353240
C	4.7493030	1.6047970	-2.5304540

H	4.7580270	0.1463060	1.0401170
C	2.2943420	1.1914350	-2.8528400
H	-4.2053020	5.1913730	0.3027680
C	5.9403660	1.0460830	-0.5094150
O	-4.6148400	-1.5386370	0.2820540
C	-4.2940290	-3.6065500	-0.8267040
C	-5.2078270	0.4610870	1.4244300
H	2.7676040	-0.2898260	5.0011660
C	3.2798190	-2.1233400	4.0085820
H	3.7011760	-3.8206610	2.7376520
H	2.2602420	1.9790790	2.2680960
H	2.1524550	1.6838940	4.0245010
H	0.8088470	1.3131700	2.9344470
H	4.7491070	2.0256770	-3.5329150
H	1.4532930	1.6166660	-2.2905700
H	1.9823950	0.1990590	-3.1991770
H	2.4646270	1.8165170	-3.7347270
C	5.9366210	1.5719350	-1.7993990
H	6.8551590	1.0218440	0.0758390
H	-5.0858400	-3.3536690	-1.5364230
H	-4.7315300	-4.1374240	0.0230880
H	-3.5666850	-4.2590460	-1.3193030
H	-5.4644950	-0.1136470	2.3182400
H	-6.0961970	0.5607720	0.7947060
H	-4.8603060	1.4551470	1.7167460
H	3.5761010	-2.6216680	4.9277390
H	6.8514970	1.9634440	-2.2356860
H	-1.0713530	3.3068770	-1.9569420
N	1.3770920	2.8990550	0.2999030
H	2.1870470	2.8744740	-0.3232270
H	0.9182780	3.7922650	0.1302230
C	2.1759430	-2.2664770	-1.7216340
C	-0.2766040	-2.6069170	-1.9659070
S	1.1518450	-3.3438610	-2.6124420
C	-2.6248440	-0.3323920	-1.3595260
C	-2.3491080	0.2062540	-2.7537840
C	0.0224360	-1.5742200	-1.1122980
H	3.2517390	-2.3222250	-1.8257450
H	-1.2541300	-2.9430490	-2.2790530

(L38)Ni(Ph)NH_2



Zero-point correction= 0.769462 (Hartree/Particle)
Thermal correction to Energy= 0.818315
Thermal correction to Enthalpy= 0.819259
Thermal correction to Gibbs Free Energy= 0.687754
Sum of electronic and zero-point Energies= -4246.732265
Sum of electronic and thermal Energies= -4246.683412
Sum of electronic and thermal Enthalpies= -4246.682468
Sum of electronic and thermal Free Energies= -4246.813973

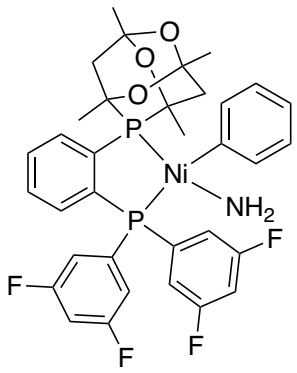
Single-point energy (6-311+G(2d,2p)) = -4.248369413872E+03

Ni	0.4052130	-1.0024880	0.8646900
P	1.6820870	-0.0320430	-0.6522370
P	-1.3081550	-0.0692150	-0.1949490
C	1.8138190	-1.9673980	1.7195230
C	2.1624760	-3.2640010	1.3013360
C	2.5049860	-1.4397910	2.8243460
C	0.6208120	0.3936460	-2.1174110
C	-0.7725520	0.3595550	-1.8936470
C	3.3137910	-0.6824070	-1.3766090
C	2.4851190	1.5911430	-0.0518550
C	-1.9087470	1.4826970	0.5670810
C	-2.8036110	-1.0992430	-0.4320930
C	3.1789570	-3.9908500	1.9321890
C	3.5199920	-2.1613200	3.4624820
H	2.2622010	-0.4423360	3.1827860
O	3.8660140	0.2698390	-2.3174860
O	3.5104070	1.2108380	0.8844940
C	-1.6658610	0.6038350	-2.9432340
C	1.0861600	0.6834390	-3.4106580
C	3.1316060	2.3362630	-1.2216930
C	4.3042970	-0.8279800	-0.2171470
C	3.1143600	-1.9840730	-2.1363590
C	1.4986660	2.4468250	0.7214830

C	-1.9258960	1.4838460	1.9725550
C	-2.2881220	2.6039850	-0.1650380
C	-2.5880030	-2.4792350	-0.5979630
C	-4.0866880	-0.5644780	-0.4607250
H	3.4285730	-4.9902960	1.5807360
C	3.8689620	-3.4380410	3.0134630
H	4.0401760	-1.7242480	4.3129710
H	-2.7354170	0.5455660	-2.7627410
C	-1.1880120	0.8907710	-4.2208720
C	0.1880090	0.9285210	-4.4501770
H	2.1506120	0.6919490	-3.6067290
C	4.3103910	1.5245710	-1.7777230
H	2.3988260	2.5444750	-2.0057810
H	3.5215720	3.2932080	-0.8552090
H	5.2210850	-1.2843000	-0.6090360
H	3.9022800	-1.4665690	0.5673810
C	4.6627690	0.5495730	0.3486320
H	4.0733280	-2.3129240	-2.5526240
H	2.4027160	-1.8641270	-2.9586960
H	2.7430820	-2.7547180	-1.4549680
H	2.0156820	3.3277510	1.1190290
H	1.0708970	1.8830930	1.5548200
H	0.6806470	2.7807860	0.0759130
C	-2.3469020	2.6378080	2.6321620
C	-2.7044080	3.7575210	0.5216340
H	-2.2620900	2.6253740	-1.2484160
C	-3.6857010	-3.3131390	-0.8057490
H	-4.2686930	0.4939330	-0.3108770
H	4.6608600	-3.9973890	3.5050390
C	-5.1819820	-1.4208790	-0.6708050
O	5.2327940	1.3216510	-0.7145800
H	-1.8854770	1.0730560	-5.0336460
H	0.5684220	1.1384810	-5.4462040
C	5.0537110	2.2252630	-2.8969360
C	5.6797650	0.4912610	1.4678220
C	-2.7378940	3.7800100	1.9136340
C	-4.9877160	-2.7887520	-0.8461520
H	5.8856440	1.5988400	-3.2288600
H	5.4460390	3.1816310	-2.5407560
H	4.3822180	2.4061470	-3.7417070
H	5.8938000	1.5037190	1.8203340
H	6.6048420	0.0348750	1.1048400
H	5.2819150	-0.1063290	2.2915560
H	1.6362540	-3.7202430	0.4635130
N	-0.7085130	-1.5171990	2.2869190
H	-1.5859520	-1.9486400	1.9876200

H	-0.2687910	-2.1921940	2.9108920
H	-1.5793430	-2.8683390	-0.5325240
H	-1.5836520	0.5961030	2.4996390
H	-3.0479210	4.6536050	2.4729240
H	-5.8086030	-3.4774250	-1.0003720
O	-2.3964230	2.7580830	3.9900010
O	-3.0577310	4.8169410	-0.2693490
O	-6.4065340	-0.8156520	-0.6864500
O	-3.5999810	-4.6665080	-0.9677400
C	-2.3113900	-5.2682590	-0.8923270
H	-2.4767250	-6.3376940	-1.0270940
H	-1.6533620	-4.8954020	-1.6871680
H	-1.8457490	-5.0867640	0.0839330
C	-7.5580030	-1.6301050	-0.8670050
H	-7.5334590	-2.1441320	-1.8360920
H	-7.6502710	-2.3701380	-0.0623810
H	-8.4098770	-0.9498910	-0.8366950
C	-3.4909670	6.0127940	0.3653240
H	-2.7015080	6.4345750	1.0000170
H	-3.7219950	6.7100990	-0.4409250
H	-4.3905900	5.8389290	0.9688550
C	-1.9931330	1.6304060	4.7677630
H	-2.1056470	1.9371790	5.8082460
H	-2.6291750	0.7618620	4.5630750
H	-0.9494440	1.3635730	4.5667610

(L39)Ni(Ph)NH_2



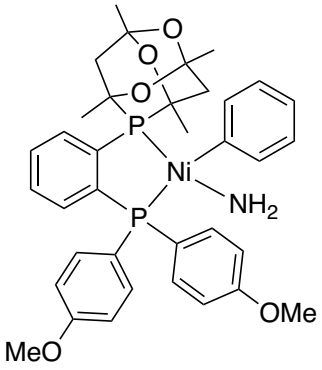
Zero-point correction= 0.604894 (Hartree/Particle)
Thermal correction to Energy= 0.646687
Thermal correction to Enthalpy= 0.647631
Thermal correction to Gibbs Free Energy= 0.531438
Sum of electronic and zero-point Energies= -4185.742417
Sum of electronic and thermal Energies= -4185.700624
Sum of electronic and thermal Enthalpies= -4185.699680
Sum of electronic and thermal Free Energies= -4185.815873

Single-point energy (6-311+G(2d,2p)) = -4.187177321281E+03

Ni	-0.0812040	1.2478090	0.5570120
P	-1.3521030	-0.1790820	-0.5557720
P	1.6331780	0.0328580	-0.1183210
C	-1.4958240	2.4292300	1.0498070
C	-1.8396920	3.5186930	0.2309440
C	-2.1947080	2.2791400	2.2593620
C	-0.2704100	-1.0814260	-1.7714160
C	1.1220950	-0.9722220	-1.5600070
C	-2.9684870	0.1892430	-1.4824720
C	-2.1707920	-1.5003370	0.5503200
C	2.2562730	-1.1502520	1.1397530
C	3.1402910	0.9117950	-0.6911910
C	-2.8652910	4.4030500	0.5847980
C	-3.2178150	3.1628460	2.6210060
H	-1.9523750	1.4533290	2.9236960
O	-3.5111290	-1.0265550	-2.0489750
O	-3.2018140	-0.8209120	1.2865700
C	2.0258220	-1.5665130	-2.4491450
C	-0.7214070	-1.8013620	-2.8898560
C	-2.8083570	-2.5987590	-0.3034130
C	-3.9703700	0.7232650	-0.4535730
C	-2.7497210	1.1554990	-2.6355890
C	-1.1962650	-2.0407360	1.5814180
C	2.3143860	-0.6734120	2.4585710
C	2.6175970	-2.4699270	0.8365690
C	2.9446130	2.0909570	-1.4256330
C	4.4361290	0.4518550	-0.4269310
H	-3.1121070	5.2354400	-0.0711960
C	-3.5651320	4.2236030	1.7802150
H	-3.7440420	3.0216680	3.5631530
H	3.0945650	-1.4512330	-2.2909010
C	1.5604270	-2.2792190	-3.5529890
C	0.1865460	-2.3920380	-3.7698620
H	-1.7837860	-1.8760280	-3.0832140
C	-3.9739630	-2.0210010	-1.1195300
H	-2.0687290	-3.0667100	-0.9585710
H	-3.2108920	-3.3706850	0.3629170
H	-4.8793150	1.0212700	-0.9893220
H	-3.5726470	1.5904540	0.0709230
C	-4.3452270	-0.3785550	0.5422650
H	-3.7014110	1.3286110	-3.1503420
H	-2.0314590	0.7610670	-3.3606060
H	-2.3784310	2.1100050	-2.2515910

H	-1.7207810	-2.7307790	2.2519310
H	-0.7747470	-1.2252840	2.1759170
H	-0.3765160	-2.5798440	1.0960600
C	2.7568940	-1.5434110	3.4448070
C	3.0419940	-3.2896280	1.8746300
H	2.5630650	-2.8684870	-0.1696370
C	4.0582310	2.7726660	-1.8944910
H	4.6194330	-0.4456640	0.1521380
H	-4.3627550	4.9075880	2.0583040
C	5.5110340	1.1846190	-0.9162270
O	-4.9062490	-1.4648700	-0.2026800
H	2.2651570	-2.7321230	-4.2444200
H	-0.1844770	-2.9332520	-4.6358270
C	-4.7091400	-3.0582400	-1.9437820
C	-5.3747020	0.0577300	1.5615800
C	3.1271780	-2.8599320	3.1915410
C	5.3605080	2.3490140	-1.6566400
H	-5.5317340	-2.5792240	-2.4808220
H	-5.1138400	-3.8345220	-1.2888560
H	-4.0294100	-3.5188590	-2.6670190
H	-5.5996420	-0.7748920	2.2332790
H	-6.2922490	0.3655660	1.0526220
H	-4.9832600	0.8983330	2.1393390
H	-1.3016870	3.6865290	-0.7009890
N	1.0397480	2.2027130	1.7207900
H	1.8663880	2.5928200	1.2612680
H	0.5724940	2.9975690	2.1545620
H	1.9495220	2.4805460	-1.6135150
H	1.9926180	0.3437260	2.6898740
F	2.8216040	-1.1054100	4.7258460
F	3.3900070	-4.5719800	1.5907590
H	3.4596260	-3.5196820	3.9839830
H	6.2150910	2.9048610	-2.0229890
F	6.7681260	0.7425960	-0.6632450
F	3.8763700	3.9108940	-2.6076940

(L40)Ni(Ph)NH_2



Zero-point correction= 0.703977 (Hartree/Particle)
Thermal correction to Energy= 0.747522
Thermal correction to Enthalpy= 0.748466
Thermal correction to Gibbs Free Energy= 0.628542
Sum of electronic and zero-point Energies= -4017.735581
Sum of electronic and thermal Energies= -4017.692036
Sum of electronic and thermal Enthalpies= -4017.691092
Sum of electronic and thermal Free Energies= -4017.811015

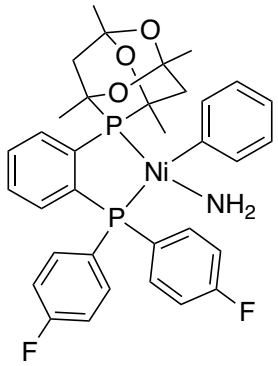
Single-point energy (6-311+G(2d,2p)) = -4.019232425829E+03

Ni	-0.0875960	-0.9814390	-0.9764640
P	-1.4069300	-0.1469420	0.5813030
P	1.5790260	0.0180940	0.0918040
C	-1.4425550	-1.9941370	-1.8639460
C	-1.7045090	-3.3273280	-1.5011330
C	-2.1780500	-1.4621810	-2.9374340
C	-0.3561390	0.3051990	2.0481450
C	1.0341920	0.3603230	1.8098510
C	-2.9735710	-0.9390040	1.3084050
C	-2.3385990	1.4308380	0.0493580
C	2.0512180	1.6363110	-0.6116790
C	3.1445890	-0.9035670	0.2735320
C	-2.6829250	-4.0868530	-2.1532210
C	-3.1548010	-2.2165370	-3.5970690
H	-1.9993650	-0.4379910	-3.2557760
O	-3.5790290	-0.0618590	2.2894900
O	-3.3494860	1.0070650	-0.8833820
C	1.9225250	0.6191290	2.8604560
C	-0.8226860	0.5245690	3.3549640
C	-3.0184120	2.0878890	1.2527940
C	-3.9709040	-1.1205060	0.1599800
C	-2.6643450	-2.2463460	2.0199380
C	-1.4326390	2.3814140	-0.7118530

C	2.0726340	1.7374870	-2.0171440
C	2.3455480	2.7681470	0.1537270
C	3.0728540	-2.2900860	0.4584330
C	4.4102130	-0.2952000	0.2367300
H	-2.8652100	-5.1147550	-1.8451200
C	-3.4198070	-3.5304990	-3.2013150
H	-3.7102030	-1.7759940	-4.4231640
H	2.9921360	0.6249330	2.6696090
C	1.4439690	0.8358880	4.1517170
C	0.0705800	0.7874810	4.3943930
H	-1.8831950	0.4602130	3.5615880
C	-4.1242200	1.1726250	1.7985760
H	-2.2900470	2.3246660	2.0329410
H	-3.4849160	3.0242160	0.9243110
H	-4.8445010	-1.6560330	0.5503360
H	-3.5365860	-1.7023360	-0.6510880
C	-4.4400310	0.2439970	-0.3539210
H	-3.5892010	-2.6631250	2.4346390
H	-1.9530720	-2.0995470	2.8382440
H	-2.2431440	-2.9618820	1.3080930
H	-2.0196380	3.2356180	-1.0685260
H	-0.9846400	1.8780310	-1.5727810
H	-0.6265810	2.7508610	-0.0707030
C	2.3984230	2.9394090	-2.6275850
C	2.6657430	3.9855250	-0.4540980
H	2.3157780	2.7201700	1.2380760
C	4.2243870	-3.0587640	0.6261200
H	4.4911470	0.7742740	0.0675440
H	-4.1820930	-4.1156440	-3.7095260
C	5.5653200	-1.0496570	0.3965080
O	-5.0473580	0.9367110	0.7433830
H	2.1388760	1.0282520	4.9645500
H	-0.3105210	0.9403240	5.4005390
C	-4.8980420	1.7795920	2.9516100
C	-5.4688900	0.1467020	-1.4593200
H	2.4162280	3.0317200	-3.7090920
C	2.6954500	4.0702320	-1.8510550
H	2.8828420	4.8479040	0.1652310
H	4.1338970	-4.1299500	0.7615350
C	5.4784490	-2.4351340	0.5964320
H	6.5477380	-0.5894890	0.3614330
H	-5.6755130	1.0824100	3.2743170
H	-5.3662410	2.7150750	2.6335860
H	-4.2276140	1.9823990	3.7923080
H	-5.7638640	1.1513710	-1.7736820
H	-6.3509180	-0.3897000	-1.0985530

H	-5.0415160	-0.3917010	-2.3086120
H	-1.1375040	-3.7876350	-0.6928730
N	1.0475060	-1.3741230	-2.4152060
H	1.9480050	-1.7705470	-2.1371880
H	0.6444740	-2.0377650	-3.0747810
H	2.1022550	-2.7795870	0.4559160
H	1.8095030	0.8622550	-2.6108700
O	6.6673350	-3.0891550	0.7419680
O	2.9939590	5.2069850	-2.5463760
C	6.6456010	-4.5006060	0.9200500
H	7.6894390	-4.8038960	1.0068450
H	6.1065190	-4.7776070	1.8345110
H	6.1887060	-5.0022780	0.0581880
C	3.2884080	6.3896960	-1.8149900
H	3.4895960	7.1582720	-2.5620600
H	2.4366610	6.6963550	-1.1948380
H	4.1737340	6.2557670	-1.1806680

(L41)Ni(Ph)NH_2



Zero-point correction= 0.703902 (Hartree/Particle)
Thermal correction to Energy= 0.747686
Thermal correction to Enthalpy= 0.748631
Thermal correction to Gibbs Free Energy= 0.627046
Sum of electronic and zero-point Energies= -4017.739545
Sum of electronic and thermal Energies= -4017.695760
Sum of electronic and thermal Enthalpies= -4017.694816
Sum of electronic and thermal Free Energies= -4017.816401

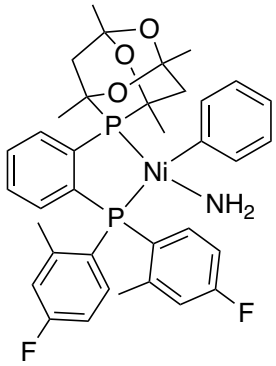
Single-point energy (6-311+G(2d,2p)) = -3.988639746714E+03

Ni	0.1074260	1.2521990	0.5444340
P	-1.1821980	-0.1747660	-0.5401510
P	1.8069780	-0.0250200	-0.0723850
C	-1.2857220	2.4810010	0.9842270
C	-1.5946910	3.5558360	0.1321640

C	-2.0030270	2.3834960	2.1888270
C	-0.1118550	-1.1344670	-1.7213310
C	1.2800850	-1.0462400	-1.5000040
C	-2.7788280	0.2071910	-1.4962190
C	-2.0479450	-1.4455100	0.5891110
C	2.3663270	-1.1997920	1.2160970
C	3.3331820	0.8102360	-0.6425870
C	-2.6019910	4.4748420	0.4484590
C	-3.0081300	3.3014210	2.5136690
H	-1.7889550	1.5707050	2.8785330
O	-3.3460300	-1.0093140	-2.0385200
O	-3.0726930	-0.7230730	1.2940350
C	2.1780750	-1.6750440	-2.3708700
C	-0.5687760	-1.8713680	-2.8265310
C	-2.7014400	-2.5506020	-0.2437000
C	-3.7811860	0.7922900	-0.4960940
C	-2.5223500	1.1366090	-2.6715980
C	-1.1016280	-1.9812760	1.6480960
C	2.3917490	-0.7157140	2.5360920
C	2.7182320	-2.5320100	0.9581400
C	3.1836410	1.9768950	-1.4108880
C	4.6221050	0.3476290	-0.3448490
H	-2.8211110	5.2939870	-0.2337340
C	-3.3198360	4.3464740	1.6397750
H	-3.5487950	3.1994210	3.4528160
H	3.2474270	-1.5718430	-2.2081450
C	1.7081100	-2.4037230	-3.4623500
C	0.3339890	-2.4984090	-3.6863900
H	-1.6307810	-1.9295090	-3.0272600
C	-3.8428700	-1.9673610	-1.0896100
H	-1.9651490	-3.0524390	-0.8772170
H	-3.1304940	-3.2952010	0.4371340
H	-4.6759610	1.0967700	-1.0518090
H	-3.3698850	1.6637510	0.0104230
C	-4.1946730	-0.2731840	0.5235620
H	-3.4629840	1.3193840	-3.2032050
H	-1.8049230	0.7052670	-3.3761520
H	-2.1320870	2.0913240	-2.3075300
H	-1.6517800	-2.6421260	2.3275620
H	-0.6705590	-1.1602250	2.2274880
H	-0.2857220	-2.5490740	1.1903260
C	2.7824190	-1.5499830	3.5821250
C	3.1021830	-3.3778180	1.9999950
H	2.6829120	-2.9243090	-0.0532470
C	4.2968140	2.6595600	-1.8953200
H	4.7534160	-0.5390150	0.2671180

H	-4.1037810	5.0570370	1.8888730
C	5.7480320	1.0250230	-0.8160970
O	-4.7732620	-1.3655280	-0.1996870
H	2.4095380	-2.8826860	-4.1397170
H	-0.0408500	-3.0518280	-4.5430660
C	-4.5925250	-3.0088250	-1.8955170
C	-5.2261290	0.2149900	1.5172260
H	2.8076930	-1.1994970	4.6086620
C	3.1281410	-2.8635020	3.2898280
H	3.3731020	-4.4135780	1.8248520
H	4.2004860	3.5636890	-2.4867670
C	5.5581080	2.1641670	-1.5862130
H	6.7535320	0.6860780	-0.5905710
H	-5.3968910	-2.5251360	-2.4555340
H	-5.0235290	-3.7576880	-1.2255740
H	-3.9150950	-3.5042550	-2.5976260
H	-5.4793250	-0.5935060	2.2081090
H	-6.1296540	0.5306330	0.9882870
H	-4.8216260	1.0615080	2.0771280
H	-1.0427880	3.6838110	-0.7981360
N	1.2314350	2.2191110	1.6945150
H	2.0973400	2.5358040	1.2517120
H	0.7911690	3.0598650	2.0652320
H	2.1872950	2.3589190	-1.6163110
H	2.0819090	0.3129700	2.7248300
F	6.6499060	2.8280380	-2.0488350
F	3.5009350	-3.6848440	4.3078160

(L42)Ni(Ph)NH_2



Zero-point correction= 0.677515 (Hartree/Particle)
Thermal correction to Energy= 0.720679
Thermal correction to Enthalpy= 0.721623
Thermal correction to Gibbs Free Energy= 0.604321
Sum of electronic and zero-point Energies= -4065.823744
Sum of electronic and thermal Energies= -4065.780581

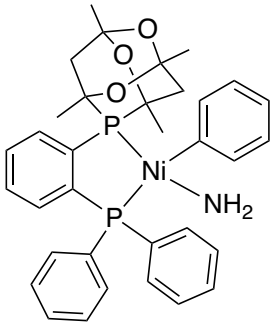
Sum of electronic and thermal Enthalpies= -4065.779637
Sum of electronic and thermal Free Energies= -4065.896939

Single-point energy (6-311+G(2d,2p)) = -4.067303852855E+03

Ni	0.0330400	-1.2759740	-0.5851770
P	-1.2807260	0.1451760	0.5028470
P	1.7270510	0.0398320	0.0494000
C	-1.3784760	-2.4240730	-1.1608930
C	-1.7600940	-3.5894600	-0.4751670
C	-2.0432940	-2.1372000	-2.3662980
C	-0.2177440	0.9145170	1.8201110
C	1.1755790	0.8359100	1.6114980
C	-2.8859630	-0.3590100	1.3921640
C	-2.1417690	1.5675770	-0.4360020
C	2.2269870	1.4578510	-1.0243100
C	3.3043900	-0.7872430	0.4917730
C	-2.7918680	-4.4109550	-0.9447950
C	-3.0654120	-2.9611580	-2.8497250
H	-1.7787620	-1.2460930	-2.9310640
O	-3.4563020	0.7710810	2.0956300
O	-3.1612970	0.9482390	-1.2409490
C	2.0637210	1.2949910	2.5921740
C	-0.6860590	1.4783750	3.0189090
C	-2.7987740	2.5446220	0.5421770
C	-3.8876830	-0.7963790	0.3197830
C	-2.6373650	-1.4395570	2.4322390
C	-1.1994580	2.2607420	-1.4021310
C	2.1892280	1.3615870	-2.4382010
C	2.6362670	2.6616570	-0.4264060
C	3.3065080	-1.8531710	1.4286320
C	4.4958910	-0.4316340	-0.1563940
H	-3.0718970	-5.3010460	-0.3848560
C	-3.4539670	-4.0965890	-2.1334400
H	-3.5597030	-2.7140260	-3.7873460
H	3.1343800	1.1953450	2.4355010
C	1.5836140	1.8462170	3.7789990
C	0.2069610	1.9388390	3.9870250
H	-1.7509360	1.5255230	3.2059080
C	-3.9467620	1.8526890	1.2890970
H	-2.0642080	2.9477450	1.2445450
H	-3.2202540	3.3806310	-0.0284350
H	-4.7861600	-1.1677990	0.8265420
H	-3.4810450	-1.5930800	-0.2995880
C	-4.2913110	0.4003940	-0.5460120
H	-3.5821870	-1.6893370	2.9279710

H	-1.9251780	-1.1078540	3.1935800
H	-2.2462070	-2.3370100	1.9461630
H	-1.7524590	3.0177060	-1.9697620
H	-0.7739760	1.5415960	-2.1055130
H	-0.3818350	2.7511560	-0.8655640
C	2.5811930	2.4786540	-3.1896410
C	3.0142980	3.7703200	-1.1794490
H	2.6548410	2.7486220	0.6532380
C	1.7153830	0.1406670	-3.1841910
C	4.5143810	-2.5078680	1.6903360
H	4.4915190	0.3731730	-0.8829250
C	2.0640780	-2.3040460	2.1603030
H	-4.2538210	-4.7332080	-2.5027180
C	5.6954310	-1.0926640	0.1051910
O	-4.8716150	1.3851660	0.3150960
H	2.2791410	2.1909970	4.5390410
H	-0.1775140	2.3566740	4.9134050
C	-4.7015820	2.7720100	2.2277080
C	-5.3153400	0.0558600	-1.6054340
H	2.5671490	2.4419940	-4.2741300
C	2.9787480	3.6462360	-2.5595050
H	3.3276020	4.6995510	-0.7164270
H	2.0521810	-0.8079270	-2.7562760
H	2.0198250	0.1952990	-4.2340700
H	0.6194580	0.0749500	-3.1594970
H	4.5573250	-3.3276640	2.4002050
H	1.2239680	-2.4438720	1.4683810
H	1.7497810	-1.5677580	2.9091480
H	2.2443650	-3.2520060	2.6755090
C	5.6734290	-2.1204360	1.0332450
H	6.6186690	-0.8239500	-0.3961780
H	-5.5100530	2.2155990	2.7087170
H	-5.1275280	3.6080420	1.6664760
H	-4.0289550	3.1630260	2.9971180
H	-5.5630260	0.9517950	-2.1807750
H	-6.2229690	-0.3286400	-1.1321080
H	-4.9073690	-0.7067140	-2.2733380
H	-1.2455460	-3.8683790	0.4430490
N	1.2119010	-2.4764890	-1.4241320
H	2.0191130	-2.7121290	-0.8432740
H	0.7753520	-3.3628710	-1.6703510
F	6.8287270	-2.7812100	1.3122320
F	3.3433080	4.7094290	-3.3242910

(L23)Ni(Ph)NH_2



Zero-point correction= 0.638329 (Hartree/Particle)
Thermal correction to Energy= 0.676646
Thermal correction to Enthalpy= 0.677590
Thermal correction to Gibbs Free Energy= 0.569745
Sum of electronic and zero-point Energies= -3788.741135
Sum of electronic and thermal Energies= -3788.702818
Sum of electronic and thermal Enthalpies= -3788.701874
Sum of electronic and thermal Free Energies= -3788.809720

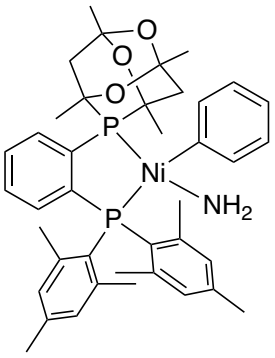
Single Point Energy (SCF+ XDM) = -3.790097368592E+03

Ni	0.3061710	1.3825060	0.0896240
P	-0.9205460	-0.3935270	-0.3709290
P	2.0558460	0.0257160	0.0031440
C	-1.1329910	2.6364730	0.0364020
C	-1.4733690	3.3017700	-1.1546700
C	-1.8579290	2.9721070	1.1930280
C	0.1933960	-1.6864670	-1.1111740
C	1.5783980	-1.4704030	-0.9427080
C	-2.5167690	-0.4520610	-1.3998990
C	-1.7607570	-1.1813190	1.1505380
C	2.6301550	-0.5680910	1.6383470
C	3.5632740	0.6348790	-0.8396190
C	-2.5164760	4.2340400	-1.2012540
C	-2.8986450	3.9068120	1.1552280
H	-1.6204920	2.4855900	2.1359540
O	-3.0385790	-1.8020320	-1.4504920
O	-2.8192160	-0.2855790	1.5353620
C	2.5074660	-2.3445410	-1.5195770
C	-0.2255540	-2.7979870	-1.8611700
C	-2.3665780	-2.5395350	0.7892780
C	-3.5511200	0.4275030	-0.6906680
C	-2.2750070	-0.0195160	-2.8370650
C	-0.8129540	-1.2506850	2.3340150
C	2.6323280	0.3741480	2.6804270

C	3.0192410	-1.8901410	1.8937630
C	3.3876920	1.4074130	-1.9989120
C	4.8597150	0.3705560	-0.3795190
H	-2.7590530	4.7286100	-2.1399520
C	-3.2404060	4.5353920	-0.0453180
H	-3.4439110	4.1444410	2.0669020
H	3.5703130	-2.1482430	-1.4089730
C	2.0754600	-3.4436660	-2.2600690
C	0.7081530	-3.6660440	-2.4286470
H	-1.2825100	-2.9656240	-2.0231450
C	-3.5151650	-2.3546220	-0.2133060
H	-1.6052910	-3.2139930	0.3882590
H	-2.7798960	-2.9922080	1.6983660
H	-4.4475150	0.4727590	-1.3205070
H	-3.1745220	1.4381370	-0.5434900
C	-3.9439420	-0.1953150	0.6522270
H	-3.2140400	-0.0802190	-3.3987650
H	-1.5349790	-0.6575250	-3.3294420
H	-1.9195530	1.0146550	-2.8549770
H	-1.3508600	-1.6334430	3.2089520
H	-0.4191880	-0.2581630	2.5691770
H	0.0298730	-1.9154210	2.1214340
C	3.0380610	-0.0089270	3.9589760
C	3.4154240	-2.2669100	3.1787970
H	3.0026510	-2.6297950	1.0991340
C	4.4932990	1.8887300	-2.6977650
H	5.0053010	-0.2069460	0.5281600
H	-4.0522210	5.2576400	-0.0770600
C	5.9655630	0.8612550	-1.0778940
O	-4.4773460	-1.4983490	0.3884550
H	2.8008950	-4.1140440	-2.7125810
H	0.3625240	-4.5119660	-3.0166980
C	-4.2191540	-3.6475410	-0.5726790
C	-5.0042130	0.5920190	1.3909890
H	3.0373320	0.7221960	4.7629200
C	3.4280430	-1.3266390	4.2110690
H	3.7110240	-3.2946950	3.3721230
H	4.3476560	2.4882080	-3.5920600
C	5.7843570	1.6155890	-2.2379930
H	6.9677280	0.6568930	-0.7109610
H	-5.0317170	-3.4363690	-1.2725310
H	-4.6337290	-4.1079050	0.3282290
H	-3.5163330	-4.3441580	-1.0397070
H	-5.2406090	0.0916400	2.3338110
H	-5.9101530	0.6557370	0.7818680
H	-4.6345910	1.5999040	1.5942690

H	3.7347200	-1.6225790	5.2107840
H	6.6460280	1.9991240	-2.7774040
H	-0.9175770	3.0922770	-2.0677210
N	1.3846330	2.7571810	0.7703600
H	2.2502230	2.8971180	0.2439650
H	0.9180140	3.6628520	0.7772640
H	2.3817110	1.6407720	-2.3384080
H	2.2951940	1.3894950	2.4719320

(L43)Ni(Ph)NH_2



Zero-point correction= 0.806546 (Hartree/Particle)
Thermal correction to Energy= 0.854195
Thermal correction to Enthalpy= 0.855140
Thermal correction to Gibbs Free Energy= 0.729278
Sum of electronic and zero-point Energies= -4024.465255
Sum of electronic and thermal Energies= -4024.417606
Sum of electronic and thermal Enthalpies= -4024.416662
Sum of electronic and thermal Free Energies= -4024.542524

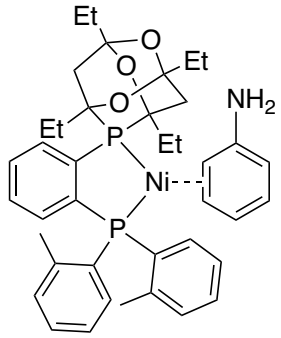
Single-point energy (6-311+G(2d,2p)) = -4.026074812260E+03

Ni	-0.0516820	-1.1185610	-0.8539690
P	-1.3726450	0.0550690	0.5114260
P	1.6693780	0.0571960	0.0087590
C	-1.4397610	-2.1655690	-1.6492730
C	-1.7430870	-3.4733250	-1.2304550
C	-2.1745250	-1.6586520	-2.7373110
C	-0.2863570	0.5287480	1.9412320
C	1.1093490	0.4769140	1.7258930
C	-2.9095410	-0.7474980	1.3109980
C	-2.3611880	1.6107220	-0.0062360
C	2.0347190	1.6830920	-0.8241280
C	3.2063480	-0.9395100	0.2679850
C	-2.7612610	-4.2225920	-1.8311400
C	-3.1817910	-2.4073330	-3.3560470
H	-1.9810520	-0.6521260	-3.1010550

O	-3.5226640	0.1294830	2.2877570
O	-3.3793810	1.1429730	-0.9109330
C	1.9750020	0.5944720	2.8210310
C	-0.7635480	0.7734360	3.2411970
C	-3.0311460	2.2635670	1.2066650
C	-3.9319270	-0.9769460	0.1946750
C	-2.5517830	-2.0270610	2.0492920
C	-1.5216370	2.6086920	-0.7807040
C	1.5258740	1.8816860	-2.1362060
C	2.7462170	2.7456240	-0.2060660
C	3.0985740	-2.0606570	1.1373330
C	4.4253980	-0.7295840	-0.4289180
H	-2.9778870	-5.2267150	-1.4715280
C	-3.4907250	-3.6899960	-2.8961970
H	-3.7282290	-1.9845910	-4.1972140
H	3.0402270	0.4630150	2.6763190
C	1.4885930	0.8209700	4.1060060
C	0.1142820	0.9286870	4.3123260
H	-1.8292200	0.7823130	3.4241220
C	-4.1060120	1.3390960	1.7881420
H	-2.2903020	2.5299660	1.9649060
H	-3.5231710	3.1851660	0.8738690
H	-4.7846150	-1.5177770	0.6219870
H	-3.5106220	-1.5716810	-0.6123340
C	-4.4422950	0.3642990	-0.3400000
H	-3.4582760	-2.4538690	2.4933870
H	-1.8308680	-1.8376370	2.8499430
H	-2.1267490	-2.7512390	1.3505770
H	-2.1351940	3.4807770	-1.0349230
H	-1.1543580	2.1677590	-1.7065430
H	-0.6641740	2.9427970	-0.1885660
C	1.6601450	3.1390830	-2.7380980
C	2.8383270	3.9825950	-0.8507410
C	0.8614730	0.8110350	-2.9667400
C	4.2333760	-2.8376150	1.3948320
C	1.8057130	-2.5247710	1.7798890
H	-4.2802570	-4.2693760	-3.3679670
C	5.5251510	-1.5402230	-0.1274150
O	-5.0430990	1.0679900	0.7519160
H	2.1801890	0.8983100	4.9405310
H	-0.2804900	1.0980660	5.3104040
C	-4.8729830	1.9496380	2.9439080
C	-5.4890970	0.2178840	-1.4230300
H	1.2572270	3.2747700	-3.7388970
C	2.2875520	4.2118660	-2.1109410
H	3.3815450	4.7847990	-0.3552790

H	1.4171370	-0.1314160	-2.9917700
H	0.7159760	1.1708920	-3.9904790
H	-0.1256120	0.5402150	-2.5712560
H	4.1350890	-3.6879860	2.0661160
H	0.9454670	-2.3858580	1.1147640
H	1.5876120	-2.0013960	2.7163830
H	1.8771150	-3.5931490	2.0068930
C	5.4669200	-2.5783720	0.8023610
H	6.4552650	-1.3651090	-0.6637580
H	-5.6270830	1.2401470	3.2941250
H	-5.3696170	2.8674270	2.6176080
H	-4.1926290	2.1842310	3.7682530
H	-5.8150460	1.2075250	-1.7540140
H	-6.3503870	-0.3320950	-1.0339200
H	-5.0657870	-0.3299240	-2.2685640
H	-1.1726560	-3.9235770	-0.4196250
N	1.1721150	-2.1454860	-1.8668340
H	1.9142540	-2.5278760	-1.2769870
H	0.7297330	-2.9515040	-2.3059600
C	4.6202850	0.2723320	-1.5486730
H	3.8198340	0.2073710	-2.2897500
H	4.6611540	1.3078510	-1.2017730
H	5.5625670	0.0597850	-2.0626040
C	6.6858880	-3.4075170	1.1240740
H	7.2523260	-3.6560060	0.2195720
H	7.3674760	-2.8657540	1.7934320
H	6.4125290	-4.3434710	1.6218490
C	3.4992070	2.6245390	1.0980690
H	2.8477810	2.7441550	1.9684230
H	4.0030790	1.6587260	1.1895930
H	4.2668830	3.4026220	1.1537050
C	2.4193540	5.5535010	-2.7882530
H	2.2679600	6.3758240	-2.0799830
H	3.4202630	5.6804090	-3.2217390
H	1.6935270	5.6642390	-3.6000120

(L32)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.809750 (Hartree/Particle)
Thermal correction to Energy= 0.856798
Thermal correction to Enthalpy= 0.857742
Thermal correction to Gibbs Free Energy= 0.731243
Sum of electronic and zero-point Energies= -4024.469372
Sum of electronic and thermal Energies= -4024.422323
Sum of electronic and thermal Enthalpies= -4024.421379
Sum of electronic and thermal Free Energies= -4024.547878

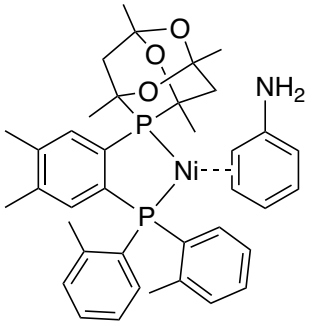
Single-point energy (6-311+G(2d,2p)) = -4.026084173881E+03

Ni	0.6662150	1.2053440	-0.4305400
P	-1.0076390	-0.1668610	-0.2999930
P	2.0367300	-0.4135720	0.0496420
C	-0.2765700	-1.8411070	-0.6258150
C	1.1282300	-1.9307120	-0.5067580
C	-2.5677910	-0.0753820	-1.3785470
C	-2.0130550	-0.2851000	1.3147080
C	2.3870080	-0.8172320	1.8305970
C	3.6787610	-0.5704500	-0.7753370
O	-3.4952700	-1.1567370	-1.1178010
O	-2.7396160	0.9594390	1.3985840
C	1.7800900	-3.1266020	-0.8333920
C	-0.9906900	-2.9683230	-1.0646640
C	-3.0125230	-1.4438030	1.2695260
C	-3.2488930	1.2432520	-0.9813430
C	-2.1944230	-0.1504780	-2.8631980
C	-1.0628020	-0.3207550	2.5116760
C	2.6162490	0.2241690	2.7592490
C	2.3578190	-2.1431060	2.2906200
C	3.7672890	-0.5820100	-2.1913840
C	4.8557550	-0.5254740	-0.0118520
H	2.8634870	-3.1799380	-0.7647590
C	1.0580070	-4.2368860	-1.2691170
C	-0.3305720	-4.1554140	-1.3822750

H	-2.0641690	-2.9043480	-1.1857670
C	-4.0741220	-1.1920900	0.1875010
H	-2.4892370	-2.3871030	1.0950670
H	-3.5341230	-1.5163340	2.2297640
H	-4.0915820	1.4268650	-1.6529730
H	-2.5473650	2.0760990	-1.0633910
C	-3.7926870	1.1482250	0.4517120
H	-1.6753270	-1.1003290	-3.0358680
H	-1.4600030	0.6410280	-3.0586700
H	-0.3839800	0.5331930	2.4108490
H	-0.4424340	-1.2208180	2.4274190
C	2.8040810	-0.1057260	4.1081360
C	2.5453670	-2.4519620	3.6373710
H	2.1726490	-2.9515200	1.5938470
C	2.6460870	1.6711180	2.3468110
C	5.0398080	-0.5399320	-2.7756820
H	4.7888370	-0.5246040	1.0715710
C	2.5525940	-0.6654480	-3.0886970
C	6.1112950	-0.4814680	-0.6180630
O	-4.7055980	0.0515580	0.4931890
H	1.5773920	-5.1561020	-1.5266140
H	-0.9020270	-5.0118850	-1.7303020
C	-5.1935990	-2.2285970	0.1498290
C	-4.5389930	2.3904950	0.9291520
H	2.9767860	0.6969950	4.8208890
C	2.7675650	-1.4256620	4.5533680
H	2.5137910	-3.4879550	3.9636790
H	3.4088030	1.8684560	1.5863120
H	2.8513560	2.3180000	3.2056360
H	1.6929610	1.9816040	1.9048400
H	5.1135480	-0.5482020	-3.8608490
H	1.7434450	-0.0115340	-2.7471540
H	2.1593800	-1.6878490	-3.1317180
H	2.8101820	-0.3617100	-4.1081320
C	6.2038870	-0.4863480	-2.0085340
H	7.0074280	-0.4450250	-0.0044870
H	-5.9315690	-1.8652070	-0.5739150
H	-5.6772230	-2.2176740	1.1332990
H	-4.8513500	2.1849320	1.9590270
H	-3.8112320	3.2091350	0.9742520
H	2.9103690	-1.6483360	5.6074300
H	7.1742320	-0.4492530	-2.4962770
C	0.0903380	2.9977170	-1.1362920
C	1.5281250	2.9137540	-1.2175720
C	2.3002940	3.7020200	-0.2940190
C	1.7065390	4.4413540	0.6973730

C	0.2858040	4.4772020	0.8089870
C	-0.4921760	3.8016250	-0.0993990
H	-0.4970100	2.7724350	-2.0251250
H	3.3828990	3.7048970	-0.4107940
H	2.3159940	5.0159340	1.3902030
H	-0.1790350	5.0735870	1.5894390
H	-1.5747530	3.8900060	-0.0517220
N	2.1043250	2.5233540	-2.4945950
H	2.2843400	3.3503770	-3.0671710
H	2.9982190	2.0549060	-2.3572310
C	-4.7549440	-3.6491250	-0.2140740
H	-4.3055140	-3.6801120	-1.2113610
H	-4.0302270	-4.0534920	0.5015410
H	-5.6208360	-4.3197890	-0.2166660
C	-1.7323880	-0.2766170	3.8890270
H	-2.3379040	-1.1681670	4.0870070
H	-0.9629240	-0.2250290	4.6669680
H	-2.3766960	0.6021670	3.9846880
C	-5.7495710	2.7889830	0.0813280
H	-6.4561010	1.9584740	-0.0093560
H	-6.2725100	3.6305550	0.5482100
H	-5.4609370	3.1036480	-0.9276890
C	-3.3702170	-0.0372790	-3.8405080
H	-3.8514130	0.9457420	-3.7976160
H	-3.0155290	-0.1820350	-4.8668020
H	-4.1297330	-0.7963470	-3.6314510

(L33)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.750285 (Hartree/Particle)
Thermal correction to Energy= 0.795025
Thermal correction to Enthalpy= 0.795969
Thermal correction to Gibbs Free Energy= 0.675119
Sum of electronic and zero-point Energies= -3945.911853
Sum of electronic and thermal Energies= -3945.867113
Sum of electronic and thermal Enthalpies= -3945.866168
Sum of electronic and thermal Free Energies= -3945.987019

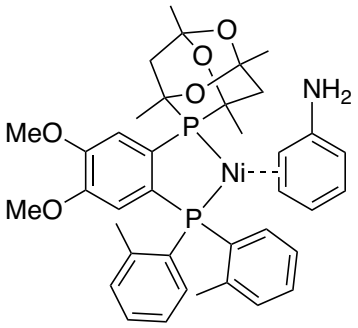
Single-point energy (6-311+G(2d,2p)) = -3.947435530618E+03

Ni	-0.2826440	-1.3501010	-0.5979740
P	1.3668370	0.0132240	-0.2597430
P	-1.6682190	0.1239500	0.2064240
C	0.5985870	1.6991390	-0.2478920
C	-0.7994610	1.7330790	-0.0773460
C	2.8953080	0.1704990	-1.3736250
C	2.4259980	-0.1444240	1.3157100
C	-1.9895830	0.1804300	2.0362260
C	-3.3314680	0.3974130	-0.5446300
O	3.8042370	1.2145870	-0.9444870
O	3.1975290	-1.3572210	1.1517570
C	-1.4716570	2.9571190	-0.1590280
C	1.2695420	2.9075420	-0.4916870
C	3.3926070	1.0313820	1.4664960
C	3.6264770	-1.1735620	-1.2542690
C	2.5100180	0.4954850	-2.8082250
C	1.5600440	-0.3587820	2.5433640
C	-2.2196340	-1.0175770	2.7513080
C	-1.9494480	1.3945510	2.7395510
C	-3.4515930	0.6720860	-1.9315200
C	-4.4910030	0.1925490	0.2192730
H	-2.5537780	2.9733590	-0.0502420
C	-0.8025720	4.1584170	-0.4037380
C	0.5978400	4.1304220	-0.5727400
H	2.3406790	2.8919120	-0.6559610
C	4.4260370	1.0230490	0.3296400
H	2.8485830	1.9797750	1.4845460
H	3.9332590	0.9288450	2.4153990
H	4.4492250	-1.1965950	-1.9789240
H	2.9467050	-2.0007190	-1.4689530
C	4.2193310	-1.3292460	0.1542520
H	3.4077500	0.5240860	-3.4367990
H	2.0115180	1.4670860	-2.8714010
H	1.8267130	-0.2666230	-3.1966550
H	2.1964580	-0.5255970	3.4204470
H	0.9149090	-1.2308170	2.4061100
H	0.9255430	0.5133590	2.7281310
C	-2.4057170	-0.9488520	4.1382930
C	-2.1329380	1.4425880	4.1210600
H	-1.7619790	2.3190580	2.2069180
C	-2.2526270	-2.3593920	2.0706340
C	-4.7360800	0.7194190	-2.4886340
H	-4.4007650	-0.0088320	1.2820210

C	-2.2586130	0.9418800	-2.8211990
C	-5.7590560	0.2424380	-0.3599540
O	5.1074630	-0.2295390	0.3726440
C	5.4744610	2.1095910	0.4595240
C	5.0245200	-2.6000100	0.3332290
H	-2.5811130	-1.8714610	4.6862580
C	-2.3626250	0.2625010	4.8256130
H	-2.0940770	2.3973320	4.6386100
H	-3.0206710	-2.4092690	1.2914690
H	-2.4517730	-3.1586640	2.7915240
H	-1.3025790	-2.5773530	1.5711410
H	-4.8336500	0.9291770	-3.5514650
H	-1.4386220	0.2411230	-2.6328240
H	-1.8712580	1.9561500	-2.6698770
H	-2.5387390	0.8422810	-3.8745640
C	-5.8824330	0.5050480	-1.7228810
H	-6.6408660	0.0781050	0.2534890
H	6.1838190	2.0316970	-0.3684740
H	6.0130030	1.9975590	1.4044730
H	5.0000010	3.0952070	0.4323110
H	5.4426940	-2.6255990	1.3428150
H	5.8404510	-2.6333640	-0.3938980
H	4.3793060	-3.4719660	0.1933420
H	-2.5043500	0.2819280	5.9029140
H	-6.8627280	0.5441520	-2.1901810
C	0.3081980	-2.9652460	-1.6374440
C	-1.1326430	-2.9032730	-1.6696760
C	-1.8640690	-3.8675020	-0.8913660
C	-1.2298360	-4.7603410	-0.0651730
C	0.1936840	-4.7786380	0.0088030
C	0.9337430	-3.9290340	-0.7769740
H	0.8675190	-2.5671980	-2.4826650
H	-2.9489770	-3.8764870	-0.9837440
H	-1.8090490	-5.4676740	0.5228330
H	0.6909230	-5.4948690	0.6573430
H	2.0188610	-3.9965350	-0.7686490
N	-1.7509290	-2.2975510	-2.8386730
H	-1.9391670	-3.0100090	-3.5466170
H	-2.6453070	-1.8760740	-2.5940140
C	1.3698240	5.3965330	-0.8533290
H	2.4377870	5.1889000	-0.9675560
H	1.0236140	5.8865550	-1.7725150
H	1.2539870	6.1291270	-0.0439290
C	-1.5724820	5.4525740	-0.4947220
H	-1.2360800	6.1768300	0.2584840
H	-1.4412580	5.9328080	-1.4729620

H	-2.6432090	5.2856350	-0.3447700

(L34)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.760350 (Hartree/Particle)
Thermal correction to Energy= 0.807079
Thermal correction to Enthalpy= 0.808023
Thermal correction to Gibbs Free Energy= 0.681984
Sum of electronic and zero-point Energies= -4096.316683
Sum of electronic and thermal Energies= -4096.269954
Sum of electronic and thermal Enthalpies= -4096.269010
Sum of electronic and thermal Free Energies= -4096.395049

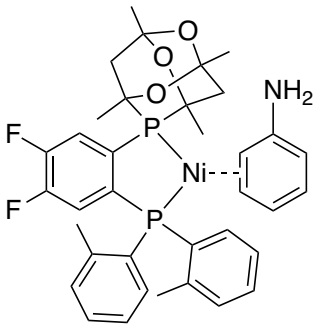
Single-point energy (6-311+G(2d,2p)) = -4.097898760310E+03

Ni	-0.2400330	-1.5560440	-0.6342060
P	1.3788290	-0.1745270	-0.2227260
P	-1.6602120	-0.1418140	0.2177570
C	0.5782920	1.4897630	-0.1392710
C	-0.8151600	1.4887080	0.0208170
C	2.9122510	0.0718820	-1.3128190
C	2.4281450	-0.3897530	1.3519980
C	-2.0267420	-0.1747280	2.0394260
C	-3.3077430	0.1572250	-0.5613250
O	3.7908930	1.1174170	-0.8212220
O	3.2320160	-1.5733020	1.1343320
C	-1.5238150	2.7010120	-0.0056570
C	1.2395030	2.7205620	-0.3230980
C	3.3644900	0.7993290	1.5743990
C	3.6775010	-1.2566150	-1.2541880
C	2.5327880	0.4581520	-2.7337010
C	1.5548640	-0.6892430	2.5564420
C	-2.3355200	-1.3988920	2.6764940
C	-1.9369960	0.9911720	2.8161220
C	-3.3909300	0.4872610	-1.9390990
C	-4.4878430	-0.0612430	0.1662930

H	-2.6023320	2.6775140	0.0970760
C	-0.8710780	3.9143410	-0.1935500
C	0.5380420	3.9210710	-0.3546040
H	2.3084430	2.7191510	-0.4809600
C	4.4070430	0.8751950	0.4484070
H	2.7967040	1.7317520	1.6377380
H	3.9001380	0.6597740	2.5214440
H	4.5069790	-1.2221690	-1.9707100
H	3.0208840	-2.0883790	-1.5177230
C	4.2610800	-1.4692370	0.1504900
H	3.4359060	0.5464850	-3.3489740
H	2.0027140	1.4146950	-2.7548620
H	1.8788920	-0.3047590	-3.1685210
H	2.1854130	-0.8882240	3.4310760
H	0.9312120	-1.5670040	2.3647760
H	0.8981480	0.1570700	2.7793960
C	-2.5533940	-1.4024860	4.0603470
C	-2.1510260	0.9667610	4.1940820
H	-1.6865990	1.9337920	2.3445460
C	-2.4142660	-2.6947820	1.9150990
C	-4.6609010	0.5714180	-2.5245640
H	-4.4259920	-0.3021850	1.2228320
C	-2.1739440	0.7802360	-2.7879020
C	-5.7409780	0.0264220	-0.4407660
O	5.1194340	-0.3594700	0.4325890
C	5.4273580	1.9788290	0.6440970
C	5.0979100	-2.7261530	0.2731010
H	-2.7912360	-2.3450780	4.5474170
C	-2.4626980	-0.2380750	4.8206840
H	-2.0715180	1.8851700	4.7695260
H	-3.1578990	-2.6588750	1.1111950
H	-2.6773790	-3.5235750	2.5799950
H	-1.4599400	-2.9308470	1.4339870
H	-4.7301140	0.8225970	-3.5806150
H	-1.3657840	0.0634890	-2.6088970
H	-1.7802330	1.7830000	-2.5844970
H	-2.4292030	0.7277690	-3.8508800
C	-5.8280210	0.3418500	-1.7952530
H	-6.6393060	-0.1501960	0.1446860
H	6.1435420	1.9637330	-0.1815310
H	5.9625900	1.8293290	1.5856510
H	4.9292400	2.9529740	0.6677690
H	5.5072480	-2.7923430	1.2844480
H	5.9210700	-2.7012670	-0.4461690
H	4.4773400	-3.6063040	0.0824280
H	-2.6303590	-0.2746980	5.8937860

H	-6.7961040	0.4102510	-2.2841690
C	0.3990640	-3.1085590	-1.7365630
C	-1.0429610	-3.0881930	-1.7727440
C	-1.7468740	-4.1040160	-1.0358350
C	-1.0888550	-5.0064570	-0.2390860
C	0.3342300	-4.9834130	-0.1578910
C	1.0507300	-4.0840390	-0.9092730
H	0.9486220	-2.6621440	-2.5638810
H	-2.8305330	-4.1433920	-1.1339470
H	-1.6483820	-5.7530150	0.3186950
H	0.8507870	-5.7071090	0.4667750
H	2.1373190	-4.1188860	-0.8983350
N	-1.6752930	-2.4586320	-2.9217010
H	-1.8529090	-3.1525810	-3.6504040
H	-2.5760570	-2.0596330	-2.6632370
O	1.1075960	5.1418910	-0.5480980
O	-1.4859590	5.1258480	-0.2477550
C	2.5152900	5.1966500	-0.7406170
H	3.0513980	4.8182470	0.1391950
H	2.8199830	4.6244080	-1.6253860
H	2.7515230	6.2512330	-0.8857190
C	-2.9029350	5.1584900	-0.1256100
H	-3.3843280	4.5858070	-0.9280570
H	-3.2275060	4.7678720	0.8470920
H	-3.1809350	6.2095680	-0.2079360

(L35)Ni(η^2-PhNH$_2$)



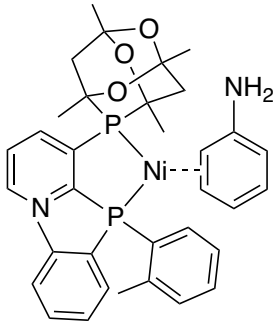
Zero-point correction= 0.678015 (Hartree/Particle)
Thermal correction to Energy= 0.721237
Thermal correction to Enthalpy= 0.722181
Thermal correction to Gibbs Free Energy= 0.604020
Sum of electronic and zero-point Energies= -4065.821353
Sum of electronic and thermal Energies= -4065.778132
Sum of electronic and thermal Enthalpies= -4065.777187
Sum of electronic and thermal Free Energies= -4065.895348

Single-point energy (6-311+G(2d,2p)) = -4.067301849484E+03

Ni	-0.2849690	-1.3402800	-0.5960720
P	1.3646980	0.0148470	-0.2645330
P	-1.6753910	0.1271490	0.2016670
C	0.5949650	1.7050680	-0.2648880
C	-0.8067960	1.7400040	-0.0963130
C	2.8893410	0.1822890	-1.3830090
C	2.4286170	-0.1243670	1.3115850
C	-1.9676730	0.1959840	2.0350610
C	-3.3464210	0.4134230	-0.5258370
O	3.7856750	1.2371810	-0.9566210
O	3.2054460	-1.3324820	1.1464130
C	-1.4946450	2.9567300	-0.1877260
C	1.2818880	2.9040340	-0.5190760
C	3.3886690	1.0574160	1.4567330
C	3.6311000	-1.1556980	-1.2595300
C	2.5002890	0.4967520	-2.8191960
C	1.5680140	-0.3413580	2.5425040
C	-2.1683780	-1.0015270	2.7597860
C	-1.9394150	1.4150800	2.7304370
C	-3.4872970	0.6816470	-1.9118850
C	-4.4941090	0.2209740	0.2594510
H	-2.5748750	3.0018350	-0.0871200
C	-0.7978010	4.1264770	-0.4399120
C	0.5847400	4.0976880	-0.6028820
H	2.3517270	2.9115530	-0.6889130
C	4.4176920	1.0540220	0.3160960
H	2.8410160	2.0036860	1.4799810
H	3.9336130	0.9576540	2.4032760
H	4.4519210	-1.1750900	-1.9862360
H	2.9574570	-1.9893050	-1.4697440
C	4.2278900	-1.3006510	0.1479240
H	3.3976640	0.5290580	-3.4477240
H	1.9950710	1.4643230	-2.8907470
H	1.8230200	-0.2727790	-3.2034660
H	2.2093930	-0.5036150	3.4166370
H	0.9271450	-1.2170220	2.4097200
H	0.9300630	0.5277220	2.7297640
C	-2.3338320	-0.9272550	4.1490480
C	-2.1025050	1.4686330	4.1141920
H	-1.7794820	2.3414950	2.1923680
C	-2.1940970	-2.3478470	2.0875640
C	-4.7806930	0.7376330	-2.4470290
H	-4.3875420	0.0232650	1.3212980
C	-2.3082650	0.9384720	-2.8238830

C	-5.7710700	0.2787020	-0.2985920
O	5.1067270	-0.1933470	0.3595150
C	5.4580140	2.1489480	0.4362910
C	5.0426820	-2.5643260	0.3320320
H	-2.4864240	-1.8490780	4.7049130
C	-2.3000210	0.2887090	4.8286660
H	-2.0737610	2.4271810	4.6249090
H	-2.9712940	-2.4118230	1.3186730
H	-2.3749820	-3.1445120	2.8159550
H	-1.2474980	-2.5588780	1.5780890
H	-4.8950780	0.9446280	-3.5086000
H	-1.4804110	0.2479260	-2.6331340
H	-1.9283260	1.9602750	-2.7053920
H	-2.6021520	0.8140850	-3.8707220
C	-5.9150800	0.5365980	-1.6604570
H	-6.6436890	0.1249320	0.3302920
H	6.1652520	2.0712960	-0.3934390
H	6.0003080	2.0456840	1.3800530
H	4.9775800	3.1314790	0.4050110
H	5.4616030	-2.5823450	1.3414150
H	5.8585170	-2.5942450	-0.3952680
H	4.4044870	-3.4420600	0.1960020
H	-2.4254080	0.3122100	5.9077890
H	-6.9028140	0.5830330	-2.1108400
C	0.3127830	-2.9706730	-1.6198660
C	-1.1246560	-2.9037630	-1.6786930
C	-1.8763820	-3.8538360	-0.9047830
C	-1.2608440	-4.7429870	-0.0598080
C	0.1602740	-4.7684350	0.0387880
C	0.9190670	-3.9283770	-0.7401940
H	0.8899030	-2.5759510	-2.4543570
H	-2.9594960	-3.8572070	-1.0153680
H	-1.8541840	-5.4411470	0.5248200
H	0.6421730	-5.4812720	0.7023140
H	2.0035620	-3.9981280	-0.7103540
N	-1.7171490	-2.2856820	-2.8522540
H	-1.8343140	-2.9769640	-3.5955260
H	-2.6420030	-1.9178010	-2.6363860
F	1.2423050	5.2504880	-0.8604330
F	-1.4531100	5.3036980	-0.5385910

(**L36**)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.682459 (Hartree/Particle)
Thermal correction to Energy= 0.723703
Thermal correction to Enthalpy= 0.724648
Thermal correction to Gibbs Free Energy= 0.611335
Sum of electronic and zero-point Energies= -3883.375612
Sum of electronic and thermal Energies= -3883.334367
Sum of electronic and thermal Enthalpies= -3883.333423
Sum of electronic and thermal Free Energies= -3883.446736

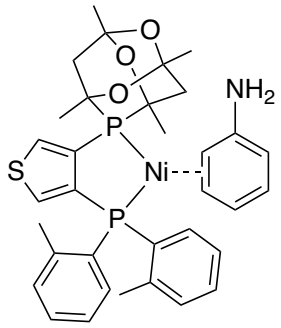
Single-point energy (6-311+G(2d,2p)) = -3.884803985410E+03

Ni	0.2709700	1.1973100	-0.3543100
P	-1.3652000	-0.2037400	-0.2879700
P	1.7045500	-0.3661000	0.1199500
C	-0.5837500	-1.8550700	-0.5946200
C	0.8131200	-1.9306200	-0.3952300
C	-2.8575300	-0.1387100	-1.4582900
C	-2.4735400	-0.4229800	1.2497000
C	2.1366200	-0.7707300	1.8755300
C	3.3066300	-0.4756100	-0.7775400
O	-3.7570300	-1.2631200	-1.2971000
O	-3.2566500	0.7887600	1.3350300
C	-1.2263100	-3.0069100	-1.0734200
C	-3.4297800	-1.6085500	1.1062600
C	-3.6107700	1.1403400	-1.0674800
C	-2.4247500	-0.1382600	-2.9158800
C	-1.6469800	-0.4920700	2.5205300
C	1.9877400	0.1867500	2.9035800
C	2.5833900	-2.0650000	2.1927200
C	3.3366800	-0.5599200	-2.1916200
C	4.5060500	-0.2997800	-0.0710800
C	0.8849900	-4.1374400	-1.0429100
C	-0.4843300	-4.1622600	-1.3058300
H	-2.2886000	-2.9845100	-1.2866300
C	-4.4261400	-1.3588800	-0.0349500

H	-2.8782600	-2.5382400	0.9426400
H	-4.0014500	-1.7139500	2.0363400
H	-4.4122800	1.3182300	-1.7943200
H	-2.9356500	1.9988000	-1.0717300
C	-4.2474000	0.9757900	0.3208100
H	-3.3026100	-0.0348500	-3.5641600
H	-1.9128300	-1.0699300	-3.1752300
H	-1.7391900	0.6932800	-3.1071300
H	-2.3081900	-0.5817900	3.3904100
H	-1.0452300	0.4120800	2.6319400
H	-0.9742800	-1.3557700	2.4989200
C	2.2683800	-0.2052200	4.2212400
C	2.8639000	-2.4294900	3.5076000
H	2.7126800	-2.7886700	1.3950800
C	1.5772600	1.6130400	2.6428600
C	4.5779300	-0.4711800	-2.8345900
H	4.4831900	-0.2333500	1.0119500
C	2.0908200	-0.7492800	-3.0265200
C	5.7297000	-0.2096600	-0.7344500
O	-5.1252300	-0.1515000	0.2589400
H	1.5015400	-5.0201200	-1.2014600
H	-0.9555500	-5.0630400	-1.6878900
C	-5.4633800	-2.4535900	-0.1836700
C	-5.0745300	2.1697700	0.7504100
H	2.1479100	0.5245600	5.0182300
C	2.6980000	-1.4938800	4.5290000
H	3.2074300	-3.4361600	3.7298700
H	2.3689300	2.1709300	2.1330700
H	1.3548200	2.1318600	3.5809600
H	0.6962600	1.6861000	1.9937300
H	4.6070000	-0.5377600	-3.9198100
H	1.2784600	-0.0921300	-2.6971600
H	1.7350100	-1.7848000	-2.9789500
H	2.2949300	-0.5132900	-4.0755200
C	5.7661800	-0.2972500	-2.1247800
H	6.6449600	-0.0736900	-0.1647200
H	-6.1473900	-2.1983900	-0.9971300
H	-6.0327100	-2.5564500	0.7440700
H	-4.9765100	-3.4065100	-0.4122600
H	-5.5235900	1.9685400	1.7264200
H	-5.8683400	2.3582200	0.0225100
H	-4.4365000	3.0547200	0.8276600
H	2.9049300	-1.7638200	5.5613400
H	6.7112100	-0.2280500	-2.6567300
C	-0.2978900	2.9907200	-1.0894200
C	1.1403600	2.8966900	-1.1272900

C	1.8885800	3.6719500	-0.1728500
C	1.2665200	4.4251500	0.7908700
C	-0.1566700	4.4874600	0.8453600
C	-0.9096500	3.8129900	-0.0842900
H	-0.8572500	2.7582800	-1.9940100
H	2.9748600	3.6553500	-0.2456700
H	1.8572100	4.9930200	1.5052300
H	-0.6405500	5.0995700	1.6016500
H	-1.9924300	3.9158300	-0.0801600
N	1.7512100	2.4940800	-2.3831600
H	1.9713000	3.3160100	-2.9485600
H	2.6256900	1.9983300	-2.2197700
N	1.5242700	-3.0481400	-0.6033600

(L37)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.661474 (Hartree/Particle)
Thermal correction to Energy= 0.702312
Thermal correction to Enthalpy= 0.703256
Thermal correction to Gibbs Free Energy= 0.590267
Sum of electronic and zero-point Energies= -4188.133919
Sum of electronic and thermal Energies= -4188.093082
Sum of electronic and thermal Enthalpies= -4188.092138
Sum of electronic and thermal Free Energies= -4188.205127

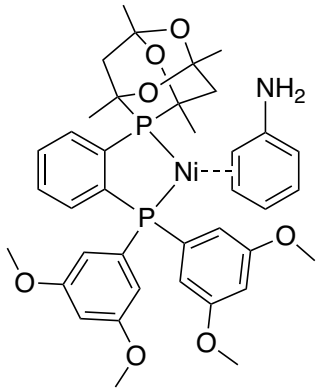
Single-point energy (6-311+G(2d,2p)) = -4.189546700323E+03

Ni	-0.2939590	1.0058550	-0.7844840
P	1.4547370	0.1068940	0.1138390
P	-1.5941790	-0.5686310	-0.0092850
C	-0.6470280	-1.1760060	1.4445540
C	2.5734920	-1.0583120	-0.8923580
C	-1.8946360	-2.1176640	-0.9837740
C	-3.2423720	-0.1547620	0.7016880
O	3.8468000	0.1015640	1.5298650
O	3.3246030	-0.2114270	-1.7919330
C	3.5549170	-1.8037970	0.0141490

C	3.6453630	1.6941140	-0.2866550
C	1.7533330	-1.9899790	-1.7664670
C	-2.1455120	-2.0485120	-2.3743920
C	-1.8273190	-3.3754740	-0.3652690
C	-3.3469680	0.8790870	1.6668530
C	-4.4092150	-0.7433720	0.1894310
C	4.5309440	-0.8149110	0.6683590
H	3.0189810	-2.3753330	0.7766500
H	4.1390370	-2.5053440	-0.5937600
H	4.4299640	2.3498910	0.1091160
H	2.9428080	2.2978500	-0.8662690
C	4.3033340	0.6406960	-1.1880600
H	3.3436350	2.5396150	2.3440470
H	1.9717570	1.4945410	2.7718730
H	1.7771130	2.7284330	1.5085250
H	2.4200010	-2.5978020	-2.3894210
H	1.0892250	-1.4151870	-2.4183270
H	1.1394620	-2.6568550	-1.1527240
C	-2.3263390	-3.2430200	-3.0836890
C	-2.0050830	-4.5537670	-1.0892910
H	-1.6199490	-3.4374230	0.6967380
C	-2.2091230	-0.7406530	-3.1240080
C	-4.6262830	1.2741040	2.0772670
H	-4.3278910	-1.5397240	-0.5439460
C	-2.1390110	1.5549740	2.2722230
C	-5.6734100	-0.3234440	0.6054540
O	5.2046760	-0.1180180	-0.3788040
C	5.5929260	-1.4857340	1.5159350
C	5.1084980	1.2356580	-2.3247850
H	-2.5187300	-3.1909410	-4.1524910
C	-2.2575120	-4.4865740	-2.4579330
H	-1.9440500	-5.5138910	-0.5842920
H	-3.0024110	-0.0850170	-2.7466170
H	-2.3987800	-0.9132640	-4.1879070
H	-1.2688450	-0.1861830	-3.0236920
H	-4.7134260	2.0642920	2.8197040
H	-1.3809350	1.7877230	1.5153860
H	-1.6605890	0.9183380	3.0259880
H	-2.4256310	2.4938780	2.7546920
C	-5.7823880	0.6911670	1.5550590
H	-6.5625970	-0.7918650	0.1925480
H	6.2619230	-0.7265820	1.9292950
H	6.1743990	-2.1810560	0.9044760
H	5.1262180	-2.0365980	2.3381350
H	5.5682890	0.4313530	-2.9048880
H	5.8935860	1.8851010	-1.9281080

H	4.4538290	1.8185800	-2.9789820
H	-2.3962530	-5.3946950	-3.0382720
H	-6.7593150	1.0283590	1.8906630
C	-1.0995890	-1.8025220	2.5739270
C	1.3432100	-1.3397990	2.6566900
S	0.1797740	-2.0744450	3.7129020
C	2.9240480	1.0131880	0.8847030
C	2.4733990	2.0052850	1.9447990
C	0.7703410	-0.9004700	1.4902870
C	0.5012630	3.8590800	-0.7669660
C	0.1063090	2.8100580	-1.6653830
C	-1.2857360	2.4767070	-1.7705250
C	-2.2420790	3.1795930	-0.9554740
C	-1.8136020	4.1453550	-0.0656050
C	-0.4369280	4.4895100	0.0147960
H	1.5413320	4.1728100	-0.7348560
H	0.7797720	2.5452470	-2.4798180
H	-1.6657400	2.0075280	-2.6759940
H	-2.5383380	4.6643120	0.5581080
H	-0.1342610	5.2824900	0.6945410
N	-3.6018780	2.8934330	-1.1534420
H	-3.7874840	1.9072360	-1.3040880
H	-4.2010080	3.2387710	-0.4115600
H	-2.1145480	-2.0907980	2.8155900
H	2.3726030	-1.2343690	2.9685500

(L38)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.769560 (Hartree/Particle)
Thermal correction to Energy= 0.818528
Thermal correction to Enthalpy= 0.819472
Thermal correction to Gibbs Free Energy= 0.687058
Sum of electronic and zero-point Energies= -4246.735921
Sum of electronic and thermal Energies= -4246.686954
Sum of electronic and thermal Enthalpies= -4246.686009
Sum of electronic and thermal Free Energies= -4246.818423

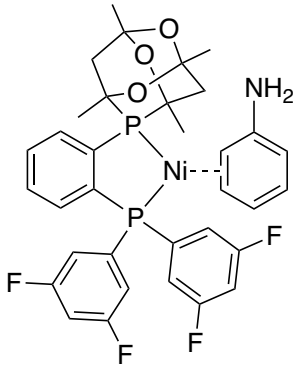
Single-point energy (6-311+G(2d,2p)) = -4.187184286460E+03

Ni	0.3893190	-0.7853980	1.1767950
P	1.9280890	-0.5418700	-0.3215110
P	-1.1066180	-0.1323890	-0.2307420
C	1.0410280	-0.6293850	-1.9501830
C	-0.3630100	-0.4662490	-1.8923340
C	3.4473820	-1.6608830	-0.5043930
C	2.9822260	1.0440600	-0.3365390
C	-1.4489520	1.6759320	-0.2492570
C	-2.7623900	-0.9166260	-0.3739820
O	4.2859580	-1.2992260	-1.6280670
O	3.8271700	0.9631030	0.8343860
C	-1.1302300	-0.5960210	-3.0566030
C	1.6367090	-0.9212740	-3.1880210
C	3.8755310	1.1182000	-1.5759830
C	4.2538640	-1.4505010	0.7853020
C	3.0498920	-3.1141230	-0.7083170
C	2.1204920	2.2797700	-0.1540150
C	-1.4394860	2.3208000	1.0013040
C	-1.6551740	2.3977410	-1.4206890
C	-2.7705910	-2.3261530	-0.4173120
C	-3.9547870	-0.2027030	-0.3513540
H	-2.2102410	-0.4922200	-3.0006950
C	-0.5228120	-0.8800780	-4.2794080
C	0.8614520	-1.0445980	-4.3418650
H	2.7064200	-1.0844140	-3.2410140
C	4.9130860	-0.0145580	-1.5568370
H	3.2762810	1.0765900	-2.4895120
H	4.4166410	2.0722130	-1.5661760
H	5.0792290	-2.1720210	0.8108280
H	3.6209140	-1.6076300	1.6620600
C	4.8492990	-0.0345330	0.8106240
H	3.9469580	-3.7429000	-0.7495620
H	2.4936510	-3.2427240	-1.6415510
H	2.4165650	-3.4489470	0.1198420
H	2.7583170	3.1693890	-0.0916530
H	1.5316530	2.2018140	0.7635370
H	1.4304690	2.3985700	-0.9955510
C	-1.6457970	3.7002990	1.0507100
C	-1.8612120	3.7853800	-1.3518590
H	-1.6483260	1.9245990	-2.3953760
C	-3.9897420	-2.9986360	-0.4473020
H	-3.9715390	0.8806220	-0.3185210
C	-5.1775570	-0.8992960	-0.3729580

O	5.6683110	0.1094710	-0.3530440
H	-1.1286960	-0.9820030	-5.1757080
H	1.3407310	-1.2812090	-5.2882090
C	5.8937150	0.0451120	-2.7105730
C	5.7291070	0.2285360	2.0155440
C	-1.8583000	4.4398960	-0.1232310
C	-5.2033730	-2.2900240	-0.4227030
H	6.6112210	-0.7746200	-2.6208610
H	6.4324790	0.9963850	-2.6934320
H	5.3616270	-0.0481950	-3.6620830
H	6.1420920	1.2384480	1.9499750
H	6.5498740	-0.4932340	2.0462240
H	5.1386960	0.1443590	2.9323360
H	-2.0047090	5.5085850	-0.0317780
H	-6.1254570	-2.8567110	-0.4383520
C	1.0221100	-1.5689560	2.9166260
C	-0.4215430	-1.5439470	2.8672720
C	-1.1012420	-0.5488420	3.6596070
C	-0.4108730	0.3937210	4.3794150
C	1.0169940	0.3849430	4.3970970
C	1.7035360	-0.5861210	3.7113300
H	1.5373690	-2.4929570	2.6588160
H	-2.1896730	-0.5738740	3.6821580
H	-0.9510810	1.1281470	4.9714800
H	1.5541870	1.1225920	4.9870590
H	2.7881840	-0.6292940	3.7763040
N	-1.1041270	-2.7711940	2.4852120
H	-1.3259200	-3.3248570	3.3152260
H	-1.9834950	-2.5600740	2.0170730
H	-1.8299250	-2.8634710	-0.4128510
H	-1.2453140	1.7404100	1.8956150
O	-2.0525650	4.4133740	-2.5518210
O	-1.6442190	4.4381960	2.2006000
O	-4.1135420	-4.3596790	-0.4866160
O	-6.2983770	-0.1166680	-0.3463050
C	-7.5663900	-0.7577100	-0.3741660
H	-7.7023000	-1.4082060	0.4990160
H	-8.3053250	0.0441340	-0.3497930
H	-7.6941160	-1.3465980	-1.2912300
C	-1.3998810	3.7579030	3.4267930
H	-1.4254100	4.5258580	4.2010530
H	-2.1757540	3.0084830	3.6236510
H	-0.4198390	3.2674090	3.4207300
C	-2.2646130	5.8187660	-2.5477010
H	-1.4006840	6.3500410	-2.1288140
H	-2.3952980	6.1025810	-3.5926840

H	-3.1659230	6.0831820	-1.9805770
C	-2.9199890	-5.1375260	-0.4960060
H	-3.2464880	-6.1780780	-0.5075460
H	-2.3212060	-4.9304880	-1.3918240
H	-2.3137090	-4.9487750	0.3981890

(L39)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.604721 (Hartree/Particle)
Thermal correction to Energy= 0.646916
Thermal correction to Enthalpy= 0.647860
Thermal correction to Gibbs Free Energy= 0.529508
Sum of electronic and zero-point Energies= -4185.751361
Sum of electronic and thermal Energies= -4185.709166
Sum of electronic and thermal Enthalpies= -4185.708222
Sum of electronic and thermal Free Energies= -4185.826574

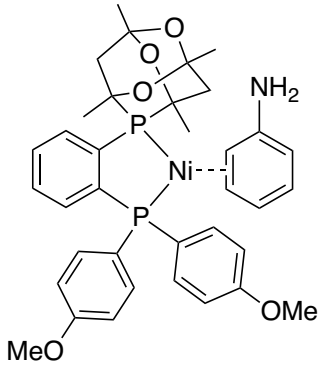
Single-point energy (6-311+G(2d,2p)) = -4.187184286460E+03

Ni	0.0916160	-1.3446910	0.2793930
P	1.7005690	-0.1549870	-0.5182220
P	-1.3423420	0.1423650	-0.2575160
C	0.8905750	1.0763580	-1.6514690
C	-0.5187190	1.1792260	-1.5539330
C	3.2710340	-0.7234020	-1.4241540
C	2.7029310	0.8342200	0.7670260
C	-1.7746310	1.3614820	1.0610280
C	-2.9924190	-0.2250910	-0.9975750
O	4.1514410	0.3661580	-1.7893930
O	3.4913090	-0.1473020	1.4811190
C	-1.2200570	2.0139670	-2.4323930
C	1.5542180	1.8288520	-2.6337410
C	3.6519910	1.8360440	0.1079700
C	4.0065410	-1.6154210	-0.4122660
C	2.9424840	-1.4610460	-2.7125850
C	1.7925370	1.4750800	1.7985870

C	-2.1346030	0.8200030	2.3045520
C	-1.7095520	2.7511480	0.8961220
C	-3.0973300	-1.4382650	-1.6956100
C	-4.1093650	0.6132050	-0.8711450
H	-2.3029230	2.0732100	-2.3702870
C	-0.5447710	2.7548610	-3.4027200
C	0.8433870	2.6601910	-3.5009100
H	2.6290410	1.7399560	-2.7376330
C	4.7278590	1.1002310	-0.7040770
H	3.0990420	2.5320740	-0.5289440
H	4.1563400	2.4165690	0.8900080
H	4.8544150	-2.0983380	-0.9126240
H	3.3393290	-2.3907530	-0.0252270
C	4.5500020	-0.7645000	0.7458560
H	3.8651740	-1.8259970	-3.1784240
H	2.4305090	-0.8066620	-3.4239740
H	2.2898250	-2.3144160	-2.5001640
H	2.3963180	1.9525440	2.5792270
H	1.1477720	0.7214160	2.2595160
H	1.1580380	2.2350370	1.3319710
C	-2.4340470	1.6846120	3.3457760
C	-2.0101560	3.5647720	1.9821870
H	-1.4226980	3.2039320	-0.0457020
C	-4.3166980	-1.7659190	-2.2700540
H	-4.0671040	1.5463140	-0.3207120
C	-5.3035210	0.2221260	-1.4621900
O	5.4175760	0.2225170	0.1847530
H	-1.1015840	3.3940380	-4.0823560
H	1.3764440	3.2250140	-4.2610600
C	5.7618710	2.0237440	-1.3153910
C	5.3599470	-1.5591180	1.7497140
C	-2.3795640	3.0687970	3.2242410
C	-5.4454770	-0.9609070	-2.1751180
H	6.5027860	1.4315570	-1.8586330
H	6.2649040	2.5929560	-0.5290440
H	5.2815120	2.7195060	-2.0098420
H	5.7337490	-0.8880680	2.5272860
H	6.2076140	-2.0385520	1.2526420
H	4.7320220	-2.3262140	2.2121460
H	-2.6067750	3.7242740	4.0561150
H	-6.3895920	-1.2461870	-2.6230820
C	0.6061680	-3.0598410	1.1720510
C	-0.7151180	-3.2891060	0.6611150
C	-1.8352780	-3.1983600	1.5395100
C	-1.6767520	-2.8067750	2.8523060
C	-0.3900870	-2.4600680	3.3365670

C	0.7188300	-2.5945610	2.5216950
H	1.4720380	-3.5042100	0.6829890
H	-2.8192820	-3.4534060	1.1515200
H	-2.5397060	-2.7484480	3.5095670
H	-0.2708830	-2.1189090	4.3609870
H	1.7107940	-2.3851050	2.9128720
N	-0.9045190	-3.8673950	-0.6314050
H	-0.0311900	-4.1422960	-1.0691230
H	-1.5452670	-4.6571510	-0.6294720
H	-2.2604690	-2.1294140	-1.7528540
H	-2.1525600	-0.2525500	2.4672820
F	-4.4289300	-2.9412740	-2.9454550
F	-6.3882620	1.0333940	-1.3429040
F	-2.7824580	1.1635680	4.5510120
F	-1.9404210	4.9132590	1.8240420

(L40)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.703902 (Hartree/Particle)
Thermal correction to Energy= 0.747686
Thermal correction to Enthalpy= 0.748631
Thermal correction to Gibbs Free Energy= 0.627046
Sum of electronic and zero-point Energies= -4017.739545
Sum of electronic and thermal Energies= -4017.695760
Sum of electronic and thermal Enthalpies= -4017.694816
Sum of electronic and thermal Free Energies= -4017.816401

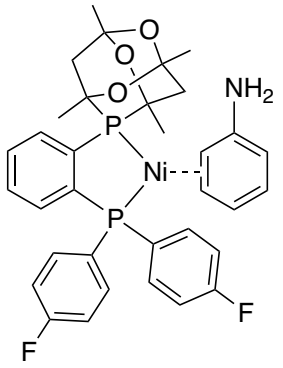
Single-point energy (6-311+G(2d,2p)) = -4.019234299087E+03

Ni	0.1021390	-0.7738860	1.1766710
P	1.6562400	-0.6187150	-0.3092800
P	-1.3480990	-0.0068190	-0.2172730
C	0.7810990	-0.5576350	-1.9479750
C	-0.6106430	-0.3086150	-1.8902250
C	3.0940890	-1.8325940	-0.5472720
C	2.8233860	0.8848290	-0.2323150

C	-1.5788880	1.8134520	-0.1618070
C	-3.0470160	-0.6786580	-0.3930750
O	3.9657000	-1.4717150	-1.6466110
O	3.6533610	0.6799220	0.9343270
C	-1.3731910	-0.3354750	-3.0645780
C	1.3681030	-0.8248180	-3.1956760
C	3.7286840	0.9632500	-1.4626540
C	3.9035520	-1.7510680	0.7553250
C	2.5962320	-3.2405890	-0.8316230
C	2.0492450	2.1655550	0.0202780
C	-1.5551760	2.4257480	1.1051160
C	-1.7201170	2.6279910	-1.2895940
C	-3.1910620	-2.0736980	-0.4221940
C	-4.2092170	0.1093090	-0.4199480
H	-2.4462400	-0.1730580	-3.0093210
C	-0.7742670	-0.5964680	-4.2969030
C	0.5978130	-0.8422760	-4.3593800
H	2.4254490	-1.0543970	-3.2501890
C	4.6820910	-0.2413250	-1.5029550
H	3.1347140	1.0146980	-2.3792180
H	4.3373100	1.8735350	-1.3985020
H	4.6736720	-2.5316710	0.7453760
H	3.2538760	-1.9080390	1.6203090
C	4.6002920	-0.3859120	0.8593860
H	3.4466790	-3.9286240	-0.9039400
H	2.0388990	-3.2788310	-1.7722490
H	1.9348690	-3.5737030	-0.0249200
H	2.7463800	3.0048470	0.1292630
H	1.4571640	2.0764760	0.9348300
H	1.3687030	2.3767500	-0.8107970
C	-1.6842170	3.8010380	1.2364430
C	-1.8420370	4.0154450	-1.1732700
H	-1.7213520	2.1884510	-2.2821660
C	-4.4480390	-2.6749160	-0.4945880
H	-4.1285960	1.1914370	-0.3881610
C	-5.4689470	-0.4769760	-0.4808360
O	5.4361120	-0.2384590	-0.2923690
H	-1.3778310	-0.6199770	-5.2004210
H	1.0701650	-1.0630050	-5.3130670
C	5.6723300	-0.1890670	-2.6489870
C	5.4898520	-0.2533790	2.0785740
H	-1.6612470	4.2776300	2.2114890
C	-1.8269320	4.6050760	0.0961920
H	-1.9419360	4.6169290	-2.0693300
H	-4.5191050	-3.7560990	-0.5186510
C	-5.5957900	-1.8715200	-0.5223330

H	-6.3699980	0.1283910	-0.4977490
H	6.3283610	-1.0621700	-2.6027740
H	6.2780680	0.7184250	-2.5777720
H	5.1413530	-0.1914030	-3.6057180
H	5.9721340	0.7274970	2.0710780
H	6.2583110	-1.0311480	2.0687820
H	4.8910590	-0.3485210	2.9887760
C	0.6834190	-1.5198490	2.9519660
C	-0.7556050	-1.4197840	2.8986820
C	-1.3844410	-0.3588420	3.6437880
C	-0.6462610	0.5901690	4.3064850
C	0.7786940	0.5106530	4.3223270
C	1.4143480	-0.5313940	3.6931120
H	1.1524640	-2.4784320	2.7350770
H	-2.4727760	-0.3271750	3.6655330
H	-1.1467570	1.3914070	4.8448650
H	1.3544060	1.2563710	4.8635250
H	2.4960000	-0.6218290	3.7542560
N	-1.4983830	-2.6139480	2.5325700
H	-1.6688100	-3.1977040	3.3539060
H	-2.4045650	-2.3665720	2.1402830
H	-2.3071640	-2.7052540	-0.3755100
H	-1.4134680	1.8137940	1.9912260
O	-1.9359650	5.9479970	0.3241760
O	-6.8744000	-2.3535230	-0.5831120
C	-2.0639920	6.8142280	-0.7954180
H	-2.1299770	7.8224320	-0.3848170
H	-1.1896480	6.7441750	-1.4547280
H	-2.9730380	6.5927930	-1.3687490
C	-7.0617910	-3.7620280	-0.6191330
H	-8.1403690	-3.9170280	-0.6656820
H	-6.5901460	-4.2044840	-1.5056340
H	-6.6624010	-4.2403740	0.2840920

(L41)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.621521 (Hartree/Particle)
Thermal correction to Energy= 0.661895
Thermal correction to Enthalpy= 0.662840
Thermal correction to Gibbs Free Energy= 0.548653
Sum of electronic and zero-point Energies= -3987.250025
Sum of electronic and thermal Energies= -3987.209651
Sum of electronic and thermal Enthalpies= -3987.208707
Sum of electronic and thermal Free Energies= -3987.322894

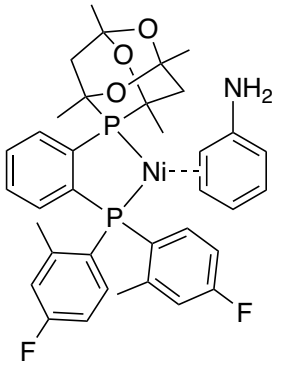
Single-point energy (6-311+G(2d,2p)) = -3.988642958593E+03

Ni	0.1035610	0.7989700	-1.0677990
P	-1.4943510	-0.4416940	-0.3238020
P	1.5390390	-0.2925040	0.0924490
C	-0.6748070	-1.9868770	0.3053960
C	0.7298940	-1.9173140	0.4634100
C	-3.0062650	-1.0300360	-1.3060010
C	-2.5697350	0.2457020	1.0900840
C	1.8972200	0.4124810	1.7549480
C	3.1892700	-0.8012320	-0.5395570
O	-3.8953610	-1.8687870	-0.5296620
O	-3.3639680	1.3005020	0.5002640
C	1.4467730	-3.0579260	0.8463160
C	-1.3201760	-3.2115320	0.5422900
C	-3.5152130	-0.8164610	1.6533740
C	-3.7606810	0.2545680	-1.6801010
C	-2.6007070	-1.8397050	-2.5272150
C	-1.7144740	0.9064980	2.1556210
C	1.9573200	1.8124950	1.8465110
C	2.0579150	-0.3519400	2.9197690
C	3.2305430	-1.3678020	-1.8272730
C	4.3946590	-0.5807760	0.1407940
H	2.5284030	-3.0064650	0.9376910
C	0.7899930	-4.2655020	1.0828380

C	-0.5947090	-4.3395280	0.9286470
H	-2.3899560	-3.2894660	0.3900130
C	-4.5359310	-1.2430820	0.5871450
H	-2.9548410	-1.6816090	2.0180830
H	-4.0681740	-0.3875310	2.4978760
H	-4.5739790	0.0011200	-2.3705130
H	-3.0901900	0.9643680	-2.1717300
C	-4.3739420	0.8919680	-0.4241570
H	-3.4911360	-2.1109420	-3.1062160
H	-2.0838760	-2.7590830	-2.2365450
H	-1.9284020	-1.2514600	-3.1605670
H	-2.3572450	1.3587290	2.9200150
H	-1.0913920	1.6865540	1.7101920
H	-1.0595920	0.1720130	2.6356370
C	2.1895850	2.4413800	3.0691370
C	2.2819660	0.2616650	4.1531910
H	1.9938080	-1.4342100	2.8751230
C	4.4415900	-1.7255530	-2.4150470
H	4.3857450	-0.1367020	1.1309480
C	5.6189710	-0.9225350	-0.4402720
O	-5.2417410	-0.0756380	0.1713940
H	1.3579860	-5.1451940	1.3732970
H	-1.1127770	-5.2802560	1.0952220
C	-5.5645360	-2.2321140	1.0971830
C	-5.2071460	2.1227670	-0.7174550
H	2.2339570	3.5219640	3.1551620
C	2.3458980	1.6482040	4.1980620
H	2.4012140	-0.3146970	5.0646550
H	4.4875240	-2.1673990	-3.4049390
C	5.6141130	-1.4921240	-1.7046980
H	6.5595860	-0.7552810	0.0740520
H	-6.2666520	-2.4728630	0.2948030
H	-6.1148180	-1.7985160	1.9366050
H	-5.0716970	-3.1511710	1.4283220
H	-5.6296550	2.5060240	0.2148970
H	-6.0207920	1.8702740	-1.4027990
H	-4.5816490	2.8975110	-1.1700570
C	-0.4581180	2.2546260	-2.3433910
C	0.9742150	2.1002440	-2.3822660
C	1.7847140	3.0980580	-1.7392480
C	1.2206660	4.1175640	-1.0104820
C	-0.1970500	4.2379910	-0.9250290
C	-1.0043350	3.3524430	-1.5992580
H	-1.0672700	1.7710310	-3.1055380
H	2.8661620	3.0248580	-1.8427520
H	1.8556220	4.8498490	-0.5179900

H	-0.6362780	5.0531870	-0.3568480
H	-2.0836740	3.4783950	-1.5777630
N	1.5252100	1.2232700	-3.3942730
H	1.4668390	1.6465480	-4.3217060
H	2.5042800	1.0208930	-3.2057220
H	2.3055720	-1.5154220	-2.3783520
H	1.8012350	2.4139960	0.9556810
F	6.8027680	-1.8308340	-2.2767160
F	2.5620410	2.2521200	5.3983570

(L42)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.678142 (Hartree/Particle)
Thermal correction to Energy= 0.721235
Thermal correction to Enthalpy= 0.722179
Thermal correction to Gibbs Free Energy= 0.604485
Sum of electronic and zero-point Energies= -4065.830095
Sum of electronic and thermal Energies= -4065.787002
Sum of electronic and thermal Enthalpies= -4065.786058
Sum of electronic and thermal Free Energies= -4065.903752

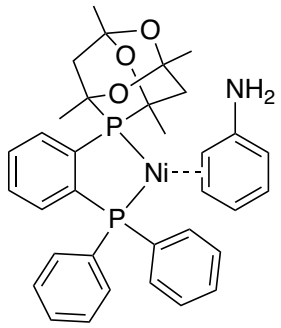
Single-point energy (6-311+G(2d,2p)) = -4.067309088764E+03

Ni	-0.0533480	-1.3021710	0.2745900
P	1.5651210	-0.0720820	-0.4728530
P	-1.4680420	0.2887880	-0.1520120
C	0.7552660	1.1269940	-1.6355240
C	-0.6452080	1.2573750	-1.5023510
C	3.0773110	-0.7324420	-1.4107830
C	2.6443740	0.9410630	0.7271560
C	-1.7621070	1.6027540	1.1279000
C	-3.1522360	-0.0367780	-0.8345880
O	3.9644130	0.3183880	-1.8656450
O	3.4394150	-0.0278640	1.4478690

C	-1.3579490	2.0668340	-2.3960710
C	1.4030850	1.8206060	-2.6716120
C	3.5856870	1.8877800	-0.0196730
C	3.8415930	-1.5928830	-0.3947570
C	2.6686240	-1.5196740	-2.6459530
C	1.7985400	1.6509450	1.7682210
C	-1.9398290	1.2411360	2.4847980
C	-1.7520110	2.9639460	0.7847000
C	-3.3063600	-0.8133620	-2.0132370
C	-4.2928930	0.3539100	-0.1161900
H	-2.4380800	2.1441660	-2.3026560
C	-0.7012860	2.7504950	-3.4185830
C	0.6818640	2.6245950	-3.5546870
H	2.4715200	1.7031940	-2.8051120
C	4.6061980	1.0879440	-0.8433040
H	3.0211960	2.5690420	-0.6622150
H	4.1389980	2.4889000	0.7120910
H	4.6574820	-2.1115540	-0.9121130
H	3.1814620	-2.3383930	0.0534000
C	4.4520940	-0.7029130	0.6981460
H	3.5582190	-1.9383270	-3.1306460
H	2.1505540	-0.8808000	-3.3670520
H	1.9962060	-2.3373200	-2.3667270
H	2.4493020	2.1562680	2.4913450
H	1.1703780	0.9332740	2.3027470
H	1.1494180	2.3956090	1.2974960
C	-2.1054660	2.2491670	3.4421010
C	-1.9124010	3.9678880	1.7387460
H	-1.6054580	3.2596980	-0.2467510
C	-1.9400400	-0.1941400	2.9361890
C	-4.5985580	-1.1694190	-2.4172040
H	-4.1808790	0.9542700	0.7805780
C	-2.1378470	-1.2473660	-2.8685150
C	-5.5778180	-0.0078110	-0.5216130
O	5.3156870	0.2375610	0.0554570
H	-1.2675590	3.3685530	-4.1100730
H	1.2012060	3.1425700	-4.3565530
C	5.6311400	1.9567190	-1.5439050
C	5.2879470	-1.4678060	1.7036930
H	-2.2418860	2.0007060	4.4897170
C	-2.0866650	3.5804290	3.0572740
H	-1.9014500	5.0189480	1.4711160
H	-2.7133990	-0.7835840	2.4331290
H	-2.1074000	-0.2661140	4.0150400
H	-0.9882000	-0.6829210	2.7019270
H	-4.7537010	-1.7598670	-3.3149510

H	-1.3050130	-1.6193940	-2.2631050
H	-1.7654780	-0.4165080	-3.4785940
H	-2.4377740	-2.0531170	-3.5453560
C	-5.6983150	-0.7690300	-1.6722180
H	-6.4596050	0.2919100	0.0344010
H	6.3325500	1.3220330	-2.0915560
H	6.1828200	2.5490640	-0.8089270
H	5.1349450	2.6313880	-2.2480430
H	5.7158160	-0.7686190	2.4267140
H	6.0977960	-1.9966300	1.1938300
H	4.6623920	-2.1905850	2.2351780
C	0.5832910	-3.1694140	0.6734960
C	-0.8551570	-3.1917860	0.5976690
C	-1.5936990	-3.3523280	1.8206980
C	-0.9676380	-3.3867050	3.0413210
C	0.4528710	-3.3030970	3.1180180
C	1.2007430	-3.2282410	1.9677030
H	1.1593380	-3.4614610	-0.2030160
H	-2.6752120	-3.4588040	1.7524950
H	-1.5512290	-3.4945190	3.9518610
H	0.9437780	-3.3397550	4.0866660
H	2.2860980	-3.2328900	2.0291460
N	-1.4499470	-3.5803470	-0.6696020
H	-1.5116600	-4.5983390	-0.7341630
H	-2.3990340	-3.2185960	-0.7448670
F	-2.2430330	4.5383810	4.0114080
F	-6.9403310	-1.1390300	-2.0934670

(L23)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.638186 (Hartree/Particle)
Thermal correction to Energy= 0.676779
Thermal correction to Enthalpy= 0.677723
Thermal correction to Gibbs Free Energy= 0.568021
Sum of electronic and zero-point Energies= -3788.745981
Sum of electronic and thermal Energies= -3788.707388
Sum of electronic and thermal Enthalpies= -3788.706444

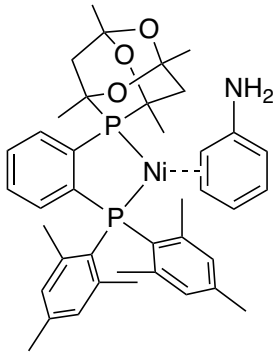
Sum of electronic and thermal Free Energies= -3788.816145

Single-point energy (6-311+G(2d,2p)) = -3.790100365729E+03

Ni	0.3609170	1.0998070	-0.6359420
P	-1.2768020	-0.2731700	-0.3611610
P	1.7595140	-0.3842930	0.0408620
C	-0.5114510	-1.9668470	-0.3540870
C	0.8947440	-2.0042300	-0.1998280
C	-2.8068110	-0.4107210	-1.4729100
C	-2.3295280	-0.1191640	1.2187170
C	2.1333530	-0.3396640	1.8428860
C	3.3924050	-0.6743510	-0.7522850
O	-3.7253810	-1.4473460	-1.0489960
O	-3.0880240	1.1029720	1.0671810
C	1.5723050	-3.2278970	-0.2699860
C	-1.1984490	-3.1716130	-0.5753540
C	-3.3107630	-1.2834230	1.3632450
C	-3.5166380	0.9448550	-1.3407470
C	-2.4269340	-0.7273380	-2.9105250
C	-1.4541390	0.0761420	2.4429900
C	2.2452320	0.9290010	2.4326670
C	2.2633200	-1.4799060	2.6481900
C	3.4126830	-0.7855100	-2.1548130
C	4.6068100	-0.6922910	-0.0532710
H	2.6548530	-3.2469670	-0.1783430
C	0.8746290	-4.4163710	-0.4846580
C	-0.5117780	-4.3849620	-0.6387470
H	-2.2700850	-3.1538580	-0.7331640
C	-4.3447500	-1.2556300	0.2268420
H	-2.7800670	-2.2392870	1.3775940
H	-3.8495490	-1.1780290	2.3128250
H	-4.3375140	0.9892020	-2.0664640
H	-2.8210530	1.7629150	-1.5453550
C	-4.1090000	1.0955780	0.0686390
H	-3.3250000	-0.7379220	-3.5391490
H	-1.9418220	-1.7052000	-2.9834420
H	-1.7337190	0.0305140	-3.2903180
H	-2.0831680	0.2318340	3.3274650
H	-0.8070160	0.9472770	2.3114310
H	-0.8212760	-0.8013010	2.6105310
C	2.4974640	1.0532940	3.7992440
C	2.5064860	-1.3532370	4.0172670
H	2.1605370	-2.4685920	2.2121260
C	4.6194190	-0.9295150	-2.8366140
H	4.6097150	-0.5998470	1.0283540

C	5.8166190	-0.8254360	-0.7411380
O	-5.0105400	0.0047860	0.2770260
H	1.4122620	-5.3589780	-0.5433740
H	-1.0614880	-5.3043160	-0.8228240
C	-5.4066080	-2.3297150	0.3505210
C	-4.8996990	2.3739970	0.2574870
H	2.5784720	2.0415360	4.2440350
C	2.6267450	-0.0872190	4.5945490
H	2.5987630	-2.2441990	4.6329270
H	4.6190840	-1.0186700	-3.9197640
C	5.8267130	-0.9476010	-2.1307150
H	6.7512080	-0.8359110	-0.1862750
H	-6.1160670	-2.2366320	-0.4758000
H	-5.9423150	-2.2175850	1.2970740
H	-4.9451230	-3.3211910	0.3152170
H	-5.3125900	2.3995060	1.2692350
H	-5.7187470	2.4190460	-0.4654640
H	-4.2464620	3.2399800	0.1176370
H	2.8128530	0.0090870	5.6608780
H	6.7682350	-1.0519120	-2.6629340
C	-0.1429510	2.9119280	-1.3566000
C	1.2883960	2.7394050	-1.4035530
C	2.0855740	3.4382350	-0.4294360
C	1.5082320	4.1680710	0.5805260
C	0.0892460	4.2985440	0.6514820
C	-0.7028870	3.7154090	-0.3077200
H	-0.7263960	2.7267540	-2.2570400
H	3.1690900	3.3698630	-0.5129750
H	2.1329610	4.6706480	1.3149360
H	-0.3589260	4.8902280	1.4449340
H	-1.7797470	3.8626280	-0.2838740
N	1.8654000	2.2788290	-2.6531010
H	2.0062330	3.0585860	-3.2979970
H	2.7709410	1.8418250	-2.4953470
H	2.4782670	-0.7456960	-2.7093090
H	2.1141130	1.8160110	1.8192790

(L43)Ni(η^2-PhNH$_2$)



Zero-point correction= 0.806905 (Hartree/Particle)
Thermal correction to Energy= 0.854448
Thermal correction to Enthalpy= 0.855393
Thermal correction to Gibbs Free Energy= 0.729584
Sum of electronic and zero-point Energies= -4024.471923
Sum of electronic and thermal Energies= -4024.424380
Sum of electronic and thermal Enthalpies= -4024.423436
Sum of electronic and thermal Free Energies= -4024.549244

Single Point Energy (SCF+ XDM) = -4.026081177686E+03

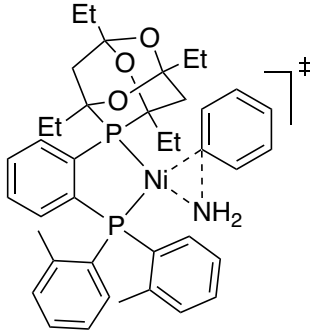
Ni	0.3850979	1.1090133	-0.2295029
P	-1.3369429	-0.2050790	-0.1507134
P	1.7302638	-0.5506005	0.2146511
C	-0.6416921	-1.8899100	-0.4988787
C	0.7614178	-2.0387673	-0.3735095
C	-2.7400323	0.0320659	-1.4120198
C	-2.5725311	-0.3857934	1.2983225
C	1.9962244	-0.9384342	2.0285964
C	3.3327591	-0.6374177	-0.7160584
O	-3.7536946	-1.0019385	-1.3609557
O	-3.2455993	0.8910625	1.3867269
C	1.3536837	-3.2344018	-0.7996137
C	-1.3975843	-2.9570252	-1.0134112
C	-3.6234491	-1.4673734	1.0368819
C	-3.4002831	1.3612707	-1.0180773
C	-2.2099689	0.0367166	-2.8370814
C	-1.8703602	-0.5962251	2.6267525
C	1.5527465	0.0360903	2.9633459
C	2.5413046	-2.1475082	2.5304643
C	3.2846482	-0.8345015	-2.1255204
C	4.5791418	-0.3006116	-0.1224801
H	2.4318552	-3.3257602	-0.8001917
C	0.5902943	-4.2894992	-1.2960296

C	-0.7926209	-4.1529751	-1.3963445
H	-2.4606410	-2.8294689	-1.1699047
C	-4.5120360	-1.0820209	-0.1522951
H	-3.1502984	-2.4385377	0.8730370
H	-4.2650224	-1.5491125	1.9227516
H	-4.1317280	1.6365422	-1.7873264
H	-2.6542107	2.1538749	-0.9420649
C	-4.1428139	1.2084741	0.3177781
H	-3.0251432	0.2587450	-3.5356740
H	-1.7884104	-0.9388040	-3.0970363
H	-1.4248526	0.7903935	-2.9500940
H	-2.6134876	-0.7085802	3.4251699
H	-1.2365318	0.2576608	2.8651488
H	-1.2465277	-1.4954311	2.5968415
C	1.5611771	-0.2618640	4.3301344
C	2.5301150	-2.3932338	3.9087285
C	1.1318231	1.4341692	2.5852055
C	4.4786370	-0.8359716	-2.8572812
C	2.0048244	-0.9725454	-2.9288484
C	5.7379662	-0.3152828	-0.9055887
O	-5.1161240	0.1745575	0.1527151
H	1.0800854	-5.2018408	-1.6262142
H	-1.3981804	-4.9593751	-1.8013581
C	-5.6339424	-2.0664079	-0.4151266
C	-4.8810378	2.4609843	0.7431297
H	1.2099147	0.4959564	5.0267829
C	2.0175799	-1.4809494	4.8279695
H	2.9544349	-3.3280180	4.2701988
H	1.9512228	1.9976133	2.1316160
H	0.8020572	1.9874910	3.4704506
H	0.3042305	1.4584031	1.8598533
H	4.4220139	-0.9944191	-3.9324458
H	1.1970690	-0.3584225	-2.5215102
H	1.6496079	-2.0059862	-2.9822392
H	2.1832080	-0.6280968	-3.9520364
C	5.7219976	-0.6134863	-2.2685406
H	6.6843003	-0.0635854	-0.4310354
H	-6.2349676	-1.7158268	-1.2581393
H	-6.2716262	-2.1506322	0.4690821
H	-5.2225333	-3.0514293	-0.6555605
H	-5.4135612	2.2693245	1.6783203
H	-5.6012593	2.7520317	-0.0263515
H	-4.1687700	3.2762274	0.8992191
C	-0.0543927	2.9289716	-0.9820446
C	1.3679249	2.7009190	-1.0726493
C	2.2218297	3.4290757	-0.1677955

C	1.7110776	4.2668546	0.7909670
C	0.3017530	4.4681011	0.8924368
C	-0.5459653	3.8387797	0.0151582
H	-0.6631156	2.7401792	-1.8642550
H	3.2984474	3.3104860	-0.2809880
H	2.3795568	4.7992620	1.4631924
H	-0.0920743	5.1487752	1.6424276
H	-1.6134215	4.0460360	0.0524452
N	1.8912575	2.2486436	-2.3519618
H	2.1959747	3.0500404	-2.9075510
H	2.7046123	1.6504296	-2.2200275
C	3.2181015	-3.2022163	1.6849277
H	2.5113185	-3.9657258	1.3450282
H	3.7071912	-2.7797358	0.8052902
H	3.9849026	-3.7113128	2.2781618
C	1.9696912	-1.7933400	6.3030658
H	2.0872297	-0.8883612	6.9086771
H	1.0073385	-2.2453860	6.5783278
H	2.7548679	-2.5010466	6.5894928
C	4.7412807	0.1498636	1.3150113
H	3.9975147	0.9024318	1.5925895
H	4.6511267	-0.6685272	2.0343451
H	5.7299696	0.6001794	1.4471508
C	6.9959407	-0.6661224	-3.0754674
H	7.7472845	0.0293248	-2.6858488
H	7.4398858	-1.6705339	-3.0499553
H	6.8150600	-0.4181588	-4.1267840

C-N Reductive Elimination Transition States

(L32)Ni(Ph)NH_2



Zero-point correction= 0.807061 (Hartree/Particle)
Thermal correction to Energy= 0.854046
Thermal correction to Enthalpy= 0.854991
Thermal correction to Gibbs Free Energy= 0.728489

Sum of electronic and zero-point Energies= -4024.434338
Sum of electronic and thermal Energies= -4024.387352
Sum of electronic and thermal Enthalpies= -4024.386408
Sum of electronic and thermal Free Energies= -4024.512909

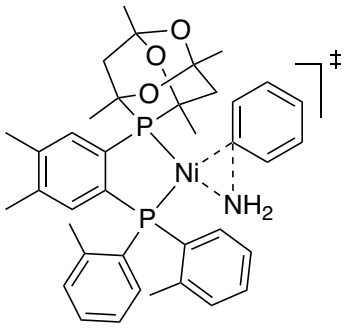
Single-point energy (6-311+G(2d,2p)) = -4.026048432629E+03

Ni	0.5993410	1.4055220	0.2515230
P	-0.7611820	-0.1619430	-0.4166980
P	2.2917390	-0.1335410	0.0114860
C	-0.4451250	2.9858920	0.4873620
C	-0.9061850	3.7431360	-0.6305920
C	-1.1895570	3.1174830	1.6974420
C	0.2383670	-1.3479650	-1.4302250
C	1.6408840	-1.2999060	-1.2542650
C	-2.3675730	0.1468100	-1.3747280
C	-1.6362110	-1.1712910	0.9443340
C	2.7857250	-1.2178030	1.4175060
C	3.8793790	0.4569590	-0.6970440
C	-2.0264230	4.5636960	-0.5367130
C	-2.3056690	3.9455650	1.7701840
H	-0.8946170	2.5414430	2.5725130
O	-3.0561950	-1.0911420	-1.6736800
O	-2.5643670	-0.2644570	1.5611510
C	2.4758000	-2.0811290	-2.0634940
C	-0.2882990	-2.2068650	-2.4093530
C	-2.4049370	-2.3451790	0.3292160
C	-3.2473840	0.9799790	-0.4328900
C	-2.0711580	0.8406160	-2.7083990
C	-0.6343910	-1.5806700	2.0240820
C	2.9811760	-0.6309890	2.6898420
C	2.8962840	-2.6089870	1.2756180
C	3.8565340	1.2993760	-1.8360690
C	5.1024810	0.1682710	-0.0743790
H	-2.3476320	5.1189160	-1.4165300
C	-2.7456270	4.6791270	0.6598840
H	-2.8478760	4.0142990	2.7119940
H	3.5533010	-2.0149620	-1.9392430
C	1.9374920	-2.9246250	-3.0341860
C	0.5529460	-2.9877850	-3.2017440
H	-1.3588430	-2.2432550	-2.5637890
C	-3.5528720	-1.8271540	-0.5514700
H	-1.7274620	-2.9844950	-0.2424850
H	-2.8497620	-2.9473940	1.1281270
H	-4.1507530	1.2874550	-0.9682940
H	-2.7218990	1.8743030	-0.0981410

C	-3.6862770	0.1386420	0.7695990
H	-1.3802200	0.2114640	-3.2820080
H	-1.5390900	1.7696060	-2.4741570
H	-0.1038520	-0.6747780	2.3390900
H	0.1145960	-2.2356380	1.5651660
C	3.2922470	-1.4658000	3.7698430
C	3.1953000	-3.4242530	2.3671400
H	2.7380360	-3.0647470	0.3044630
C	2.8356450	0.8543860	2.9163090
C	5.0708200	1.8111260	-2.3071590
H	5.1192610	-0.4751760	0.7993280
C	2.5794620	1.6359540	-2.5691670
H	-3.6183860	5.3213210	0.7261570
C	6.2999250	0.6948530	-0.5591340
O	-4.3796140	-1.0083460	0.2680280
H	2.5943510	-3.5244670	-3.6582370
H	0.1241150	-3.6377540	-3.9598370
C	-4.4624660	-2.9202910	-1.1054510
C	-4.6345780	0.8903330	1.6952040
H	3.4471660	-1.0183650	4.7486370
C	3.3953300	-2.8488230	3.6207040
H	3.2719320	-4.4999290	2.2345450
H	3.4115320	1.4501440	2.1998680
H	3.1599950	1.1248150	3.9261110
H	1.7899210	1.1644720	2.7980310
H	5.0605290	2.4575670	-3.1815710
H	1.7845330	1.9423920	-1.8765520
H	2.1956510	0.7741020	-3.1290970
H	2.7450810	2.4503230	-3.2814710
C	6.2834010	1.5196250	-1.6820230
H	7.2359450	0.4586330	-0.0604820
H	-5.2931840	-2.4105030	-1.6057460
H	-4.8854580	-3.4537090	-0.2464760
H	-5.4951660	1.2015850	1.0915650
H	-4.1166000	1.8010430	2.0128290
H	3.6293590	-3.4708720	4.4803610
H	7.2076740	1.9390810	-2.0700090
H	-0.3692440	3.6784710	-1.5760430
N	1.3801580	3.0682110	0.7165490
H	1.4646910	3.4206770	1.6633090
H	1.6231310	3.8018000	0.0617050
C	-3.7915880	-3.9038310	-2.0672780
H	-3.4040200	-3.3890310	-2.9517550
H	-2.9634420	-4.4441860	-1.5947590
H	-4.5174550	-4.6504300	-2.4068000
C	-3.3031030	1.1467580	-3.5681730

H	-2.9887960	1.5734710	-4.5270670
H	-3.8799310	0.2396190	-3.7707750
H	-3.9665660	1.8735740	-3.0885720
C	-5.1019670	0.0815510	2.9070790
H	-5.7968770	0.6752980	3.5113290
H	-5.6161310	-0.8330810	2.5964310
H	-4.2555550	-0.2004080	3.5400580
C	-1.2375140	-2.2664280	3.2545480
H	-0.4481300	-2.4557490	3.9900100
H	-1.9994360	-1.6362420	3.7216830
H	-1.6957750	-3.2311720	3.0105270

(L33)Ni(Ph)NH_2



Zero-point correction= 0.747722 (Hartree/Particle)
Thermal correction to Energy= 0.792284
Thermal correction to Enthalpy= 0.793229
Thermal correction to Gibbs Free Energy= 0.673008
Sum of electronic and zero-point Energies= -3945.876058
Sum of electronic and thermal Energies= -3945.831496
Sum of electronic and thermal Enthalpies= -3945.830552
Sum of electronic and thermal Free Energies= -3945.950772

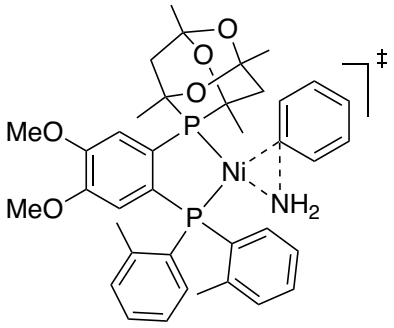
Single-point energy (6-311+G(2d,2p)) = -3.947399158186E+03

Ni	0.0266590	-1.5395120	-0.2370270
P	1.0782440	0.3660060	-0.1280240
P	-1.8983440	-0.3543570	0.1994580
C	1.3224110	-2.8581690	-0.7103160
C	1.8188880	-2.9597230	-2.0442280
C	2.1619330	-3.3710490	0.3233410
C	-0.1524750	1.6867820	-0.5307210
C	-1.5130470	1.3332000	-0.4159790
C	2.6472910	0.7879760	-1.1007260
C	1.8738910	0.8165660	1.5431060
C	-2.4756390	-0.0908220	1.9291440
C	-3.4131420	-0.8348430	-0.7214790

C	3.0590930	-3.5314250	-2.3134220
C	3.3978470	-3.9401940	0.0316990
H	1.8414800	-3.2931710	1.3604870
O	3.1094660	2.1328250	-0.8217430
O	2.9838600	-0.0844860	1.7159950
C	-2.4986280	2.2419290	-0.8163670
C	0.1632380	2.9603230	-1.0292830
C	2.3996550	2.2542680	1.5204150
C	3.7152930	-0.2007720	-0.6188620
C	2.4216430	0.7034760	-2.6015670
C	0.9333950	0.5552420	2.7052170
C	-2.5135810	-1.1980180	2.8090010
C	-2.8146270	1.1831280	2.4085660
C	-3.3257550	-1.0817160	-2.1139620
C	-4.6285110	-1.0514210	-0.0559880
H	3.4022440	-3.5829550	-3.3454860
C	3.8696890	-4.0292270	-1.2851930
H	4.0090760	-4.3161000	0.8508160
H	-3.5441050	1.9501920	-0.7492820
C	-2.1812310	3.5058520	-1.3185040
C	-0.8216070	3.8705150	-1.4228410
H	1.2048550	3.2393180	-1.1380050
C	3.5558250	2.3820500	0.5169010
H	1.5985190	2.9578750	1.2767770
H	2.7854100	2.5044790	2.5160100
H	4.6092510	-0.0749250	-1.2410390
H	3.3681530	-1.2298150	-0.7140100
C	4.0980420	0.0984500	0.8340540
H	3.3498210	0.9640310	-3.1232080
H	1.6351560	1.3896360	-2.9299080
H	2.1411600	-0.3184520	-2.8724660
H	1.4583660	0.7452770	3.6485780
H	0.5940480	-0.4842920	2.6976370
H	0.0560460	1.2061050	2.6534040
C	-2.9083300	-0.9841090	4.1349770
C	-3.1931020	1.3767270	3.7370760
H	-2.7771840	2.0359340	1.7396730
C	-2.1170530	-2.5853120	2.3650620
C	-4.4708460	-1.5301350	-2.7817750
H	-4.6949510	-0.8645530	1.0109100
C	-2.0561740	-0.8509640	-2.8990680
H	4.8359410	-4.4738070	-1.5025500
C	-5.7556430	-1.5042410	-0.7421760
O	4.5636590	1.4520940	0.8972940
C	4.1917040	3.7577180	0.5022860
C	5.2059730	-0.7892540	1.3579200

H	-2.9437240	-1.8330700	4.8133990
C	-3.2426780	0.2862940	4.6037220
H	-3.4488940	2.3728580	4.0877360
H	-2.6311380	-2.9003780	1.4504550
H	-2.3322500	-3.3182460	3.1489840
H	-1.0441750	-2.6287810	2.1401700
H	-4.4104950	-1.7207820	-3.8507290
H	-1.1862880	-1.2998960	-2.4016190
H	-1.8388410	0.2185980	-3.0101000
H	-2.1371290	-1.2823010	-3.9017890
C	-5.6760740	-1.7437000	-2.1124230
H	-6.6866360	-1.6661850	-0.2058230
H	5.0129770	3.7702490	-0.2188980
H	4.5831830	3.9981880	1.4944840
H	3.4524380	4.5120230	0.2159990
H	5.4310810	-0.5200830	2.3934210
H	6.1050510	-0.6586870	0.7494370
H	4.8885640	-1.8334810	1.3108300
H	-3.5369300	0.4212500	5.6410060
H	-6.5447210	-2.0989380	-2.6601990
H	1.2135700	-2.5836690	-2.8680860
N	-0.4451610	-3.3470250	-0.5542240
H	-0.4072490	-4.0830830	0.1418010
H	-0.6161040	-3.7542380	-1.4658190
C	-0.4224370	5.2208120	-1.9657830
H	-0.8339380	6.0380150	-1.3592680
H	0.6655790	5.3313210	-1.9846800
H	-0.7927380	5.3708850	-2.9880830
C	-3.2763160	4.4523670	-1.7430460
H	-3.2463430	5.3881110	-1.1699440
H	-3.1830700	4.7285980	-2.8011240
H	-4.2632740	4.0027690	-1.6001300

(L34)Ni(Ph)NH_2



Zero-point correction= 0.757854 (Hartree/Particle)
Thermal correction to Energy= 0.804347

Thermal correction to Enthalpy= 0.805292
Thermal correction to Gibbs Free Energy= 0.680268
Sum of electronic and zero-point Energies= -4096.281070
Sum of electronic and thermal Energies= -4096.234577
Sum of electronic and thermal Enthalpies= -4096.233632
Sum of electronic and thermal Free Energies= -4096.358656

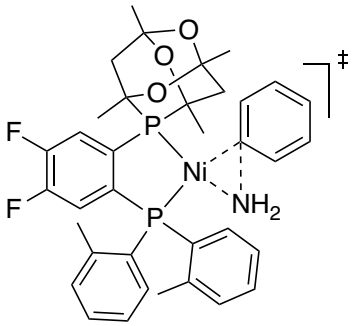
Single-point energy (6-311+G(2d,2p)) = -4.097862700266E+03

Ni	0.2616310	-1.6914300	-0.3755110
P	1.1321580	0.2773400	-0.0379310
P	-1.7552160	-0.7539130	0.2288400
C	1.6647960	-2.8037080	-1.0343280
C	2.1261390	-2.6853100	-2.3794950
C	2.5827720	-3.3562180	-0.0917200
C	-0.2226870	1.5130220	-0.2498370
C	-1.5362850	1.0227640	-0.1679850
C	2.6246560	0.9710510	-0.9734960
C	1.9318150	0.5823850	1.6635060
C	-2.3197710	-0.7694410	1.9828100
C	-3.2449750	-1.2367370	-0.7331840
C	3.4065460	-3.0919410	-2.7441070
C	3.8575100	-3.7584890	-0.4783300
H	2.2898640	-3.4413870	0.9529360
O	2.9612510	2.3104050	-0.5272300
O	3.1290400	-0.2180050	1.6976950
C	-2.6221760	1.8733030	-0.4347050
C	-0.0250570	2.8679420	-0.5822050
C	2.3155950	2.0556640	1.8242490
C	3.7987410	0.0425780	-0.6438000
C	2.3651710	1.0579000	-2.4687070
C	1.0544080	0.0778650	2.7943910
C	-2.2701460	-1.9859350	2.7032710
C	-2.7284750	0.4027670	2.6360970
C	-3.1660680	-1.2914510	-2.1469350
C	-4.4293800	-1.6279540	-0.0917460
H	3.7198930	-2.9781530	-3.7806610
C	4.2935590	-3.6328880	-1.8046770
H	4.5279290	-4.1722140	0.2734930
H	-3.6260530	1.4677350	-0.3918370
C	-2.4241680	3.2073330	-0.7737480
C	-1.0993640	3.7116040	-0.8440290
H	0.9857910	3.2412660	-0.6636740
C	3.4225380	2.4274240	0.8257930
H	1.4426990	2.7011950	1.6918110
H	2.7068120	2.2106360	2.8369810

H	4.6573040	0.3378200	-1.2585270
H	3.5518340	-0.9952160	-0.8684540
C	4.1929460	0.1877310	0.8292190
H	3.2464070	1.4788180	-2.9666190
H	1.5026910	1.6927990	-2.6926550
H	2.1827090	0.0552740	-2.8661400
H	1.5844870	0.1926360	3.7470240
H	0.8168220	-0.9801270	2.6515030
H	0.1170050	0.6390240	2.8428830
C	-2.6531930	-1.9809760	4.0497660
C	-3.0935330	0.3885480	3.9823310
H	-2.7560230	1.3395410	2.0902350
C	-1.7929810	-3.2699300	2.0688490
C	-4.2880340	-1.7318630	-2.8581310
H	-4.4890800	-1.5887220	0.9911370
C	-1.9315710	-0.8654630	-2.9057730
H	5.2906030	-3.9482400	-2.0962050
C	-5.5336660	-2.0686980	-0.8218320
O	4.5266820	1.5626770	1.0612470
C	3.9220410	3.8500240	0.9815440
C	5.3978710	-0.6432680	1.2132690
H	-2.6217600	-2.9148840	4.6057350
C	-3.0586460	-0.8107860	4.6915660
H	-3.4037860	1.3091140	4.4691600
H	-2.3076100	-3.4940650	1.1280510
H	-1.9392060	-4.1151070	2.7487420
H	-0.7260790	-3.2076660	1.8226250
H	-4.2336750	-1.7758560	-3.9433810
H	-1.0223640	-1.3096470	-2.4798520
H	-1.7944920	0.2225520	-2.8750500
H	-1.9999040	-1.1653540	-3.9562060
C	-5.4624030	-2.1196280	-2.2124310
H	-6.4402860	-2.3685990	-0.3033740
H	4.7128290	4.0396340	0.2511730
H	4.3221680	3.9964310	1.9884380
H	3.1041630	4.5582310	0.8160300
H	5.6263570	-0.4883280	2.2711680
H	6.2611820	-0.3451710	0.6120360
H	5.1832330	-1.6994430	1.0351100
H	-3.3414960	-0.8378160	5.7403800
H	-6.3130580	-2.4632930	-2.7947440
H	1.4612880	-2.2707280	-3.1362540
N	-0.0406670	-3.4840860	-0.9087420
H	0.0935170	-4.2938150	-0.3138210
H	-0.2016980	-3.7893030	-1.8611800
O	-3.4159960	4.0920230	-1.0555480

O	-0.9821240	5.0217200	-1.1872710
C	0.3269930	5.5685850	-1.2956180
H	0.8565210	5.5229650	-0.3356230
H	0.9149650	5.0467600	-2.0602650
H	0.1867830	6.6099940	-1.5863530
C	-4.7575590	3.6183280	-1.0328870
H	-4.9069080	2.8147420	-1.7646090
H	-5.0357080	3.2600170	-0.0337530
H	-5.3763680	4.4757760	-1.2983920

(L35)Ni(Ph)NH_2



Zero-point correction= 0.675561 (Hartree/Particle)
Thermal correction to Energy= 0.718547
Thermal correction to Enthalpy= 0.719491
Thermal correction to Gibbs Free Energy= 0.602249
Sum of electronic and zero-point Energies= -4065.784600
Sum of electronic and thermal Energies= -4065.741614
Sum of electronic and thermal Enthalpies= -4065.740670
Sum of electronic and thermal Free Energies= -4065.857912

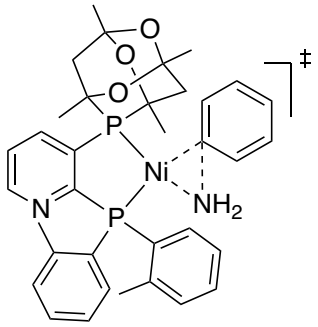
Single-point energy (6-311+G(2d,2p)) = -4.067264597948E+03

Ni	0.0072650	-1.5366720	-0.2265020
P	1.0788120	0.3552030	-0.1417320
P	-1.9088260	-0.3338580	0.1947390
C	1.2983950	-2.8756370	-0.6623410
C	1.8088160	-3.0056900	-1.9871100
C	2.1203360	-3.3694660	0.3924190
C	-0.1411180	1.6840740	-0.5682170
C	-1.5084050	1.3435890	-0.4509170
C	2.6453220	0.7625100	-1.1254980
C	1.8778270	0.8329140	1.5222270
C	-2.4654160	-0.0283540	1.9234070
C	-3.4387290	-0.7969280	-0.7082480
C	3.0513730	-3.5848800	-2.2290110
C	3.3597650	-3.9453940	0.1287070
H	1.7850240	-3.2729990	1.4232200

O	3.1034020	2.1116570	-0.8659090
O	2.9848090	-0.0686610	1.7016050
C	-2.4981340	2.2428390	-0.8688830
C	0.2043770	2.9432560	-1.0878810
C	2.4070630	2.2687950	1.4783960
C	3.7132480	-0.2200610	-0.6308010
C	2.4177390	0.6537650	-2.6247340
C	0.9407350	0.5886590	2.6907600
C	-2.5019130	-1.1200850	2.8225200
C	-2.7940750	1.2557050	2.3828330
C	-3.3649790	-1.0747270	-2.0956680
C	-4.6545290	-0.9697180	-0.0302280
H	3.4070160	-3.6597390	-3.2551960
C	3.8475420	-4.0615940	-1.1798950
H	3.9591890	-4.3065080	0.9628230
H	-3.5517080	1.9869660	-0.8126290
C	-2.1338700	3.4757960	-1.3830210
C	-0.7882440	3.8224210	-1.4869270
H	1.2414890	3.2321210	-1.2101420
C	3.5589330	2.3811070	0.4681770
H	1.6073680	2.9736620	1.2334600
H	2.7987400	2.5291180	2.4688960
H	4.6053750	-0.1047660	-1.2574470
H	3.3644860	-1.2499910	-0.7100100
C	4.0995680	0.1011200	0.8159900
H	3.3452250	0.9063910	-3.1510410
H	1.6317150	1.3338930	-2.9665730
H	2.1372930	-0.3724540	-2.8788810
H	1.4710950	0.7877190	3.6290700
H	0.5977010	-0.4495820	2.6972890
H	0.0658320	1.2425240	2.6361780
C	-2.8825470	-0.8800620	4.1480750
C	-3.1586090	1.4751260	3.7111320
H	-2.7614520	2.0980250	1.7006960
C	-2.1201030	-2.5181600	2.3996110
C	-4.5249330	-1.5085460	-2.7472210
H	-4.7094870	-0.7600370	1.0330200
C	-2.0954230	-0.8909260	-2.8933260
H	4.8152630	-4.5127720	-1.3757500
C	-5.7962780	-1.4086410	-0.7007120
O	4.5654340	1.4546370	0.8569110
C	4.1963480	3.7551650	0.4284620
C	5.2073290	-0.7789510	1.3524400
H	-2.9170390	-1.7166190	4.8416270
C	-3.2049800	0.4004010	4.5972880
H	-3.4067460	2.4784950	4.0457040

H	-2.6420890	-2.8442010	1.4933260
H	-2.3383220	-3.2357130	3.1966500
H	-1.0484470	-2.5758280	2.1715210
H	-4.4765530	-1.7221650	-3.8122770
H	-1.2299010	-1.3355700	-2.3849270
H	-1.8634510	0.1706810	-3.0460260
H	-2.1876860	-1.3551910	-3.8800450
C	-5.7304910	-1.6780780	-2.0662080
H	-6.7278040	-1.5361010	-0.1563550
H	5.0157200	3.7540710	-0.2948710
H	4.5909590	4.0112230	1.4154650
H	3.4585200	4.5066030	0.1313830
H	5.4339490	-0.4934420	2.3831620
H	6.1056950	-0.6582840	0.7409480
H	4.8895190	-1.8236640	1.3224700
H	-3.4886190	0.5554000	5.6346030
H	-6.6111210	-2.0221300	-2.6015950
H	1.2134750	-2.6473160	-2.8258720
N	-0.4812100	-3.3437020	-0.5203560
H	-0.4572710	-4.0657010	0.1910760
H	-0.6291850	-3.7717920	-1.4262960
F	-0.4585830	5.0288820	-1.9967160
F	-3.0768970	4.3521280	-1.7890250

(L36)Ni(Ph)NH_2



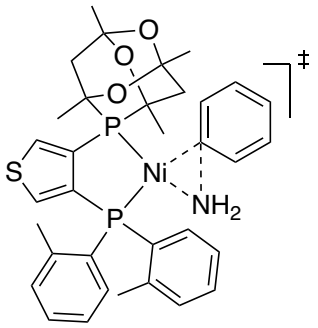
Zero-point correction= 0.680012 (Hartree/Particle)
Thermal correction to Energy= 0.721046
Thermal correction to Enthalpy= 0.721990
Thermal correction to Gibbs Free Energy= 0.609105
Sum of electronic and zero-point Energies= -3883.337578
Sum of electronic and thermal Energies= -3883.296545
Sum of electronic and thermal Enthalpies= -3883.295601
Sum of electronic and thermal Free Energies= -3883.408485

Single-point energy (6-311+G(2d,2p)) = -3.884765555592E+03

Ni	0.1739670	1.3221030	0.2202520
P	-1.0433270	-0.3706380	-0.3825130
P	2.0068560	-0.0661000	0.0467950
C	-1.0116380	2.8073810	0.3871600
C	-1.5276200	3.4745910	-0.7630820
C	-1.7793360	2.9129160	1.5847910
C	0.0501690	-1.5073840	-1.3463720
C	1.4435990	-1.3573670	-1.1614280
C	-2.6646970	-0.2632410	-1.3546470
C	-1.8263550	-1.4173600	1.0048190
C	2.6129850	-1.0472150	1.4805900
C	3.5137490	0.6444860	-0.7139230
C	-2.7208940	4.1894500	-0.7100270
C	-2.9695740	3.6336840	1.6162860
H	-1.4411800	2.4015340	2.4839810
O	-3.2222140	-1.5749880	-1.6161930
O	-2.8520230	-0.5944330	1.5892140
C	-0.3727100	-2.4425700	-2.3046950
C	-2.4707420	-2.6837990	0.4350270
C	-3.6349580	0.5098390	-0.4537660
C	-2.4728780	0.4113130	-2.7032850
C	-0.8342770	-1.7136830	2.1144900
C	2.6239340	-0.4502960	2.7623760
C	3.0214040	-2.3812000	1.3298290
C	3.3998960	1.4029740	-1.9030960
C	4.7549520	0.5420970	-0.0716680
H	-3.0817120	4.6796480	-1.6127630
C	-3.4624920	4.2806270	0.4748910
H	-3.5270370	3.6864120	2.5501940
C	1.9291130	-2.9361680	-2.7601580
C	0.5771320	-3.1627560	-3.0234430
H	-1.4310490	-2.5820620	-2.4924310
C	-3.6575970	-2.3171980	-0.4683530
H	-1.7384840	-3.2838750	-0.1127390
H	-2.8516870	-3.2881420	1.2669030
H	-4.5528770	0.7046780	-1.0207330
H	-3.2077720	1.4648880	-0.1465240
C	-4.0013520	-0.3296980	0.7741340
H	-3.4321280	0.4429760	-3.2325350
H	-1.7525180	-0.1265820	-3.3273860
H	-2.1196530	1.4355050	-2.5534860
H	-1.3425460	-2.2484270	2.9251280
H	-0.4206850	-0.7846960	2.5148880
H	-0.0086400	-2.3315970	1.7491860
C	3.0370720	-1.2254850	3.8528180
C	3.4201820	-3.1372570	2.4318520

H	3.0437370	-2.8239180	0.3402930
C	2.1985420	0.9810560	2.9866690
C	4.5480830	2.0238410	-2.4064720
H	4.8408050	-0.0416920	0.8387650
C	2.0964740	1.5376360	-2.6540660
H	-4.3920070	4.8403690	0.5089590
C	5.8852000	1.1754280	-0.5884060
O	-4.5744060	-1.5580830	0.3101590
H	2.7026760	-3.4770740	-3.3015050
H	0.2777870	-3.8828060	-3.7792950
C	-4.4058560	-3.5223590	-1.0015500
C	-5.0176040	0.3365490	1.6756840
H	3.0496100	-0.7734530	4.8415900
C	3.4244550	-2.5564640	3.6992860
H	3.7319060	-4.1693220	2.2966890
H	2.7164780	1.6804930	2.3212390
H	2.3931680	1.2831410	4.0206030
H	1.1265490	1.1112820	2.7894460
H	4.4691760	2.6056740	-3.3218840
H	1.2652290	1.7929940	-1.9825730
H	1.8248350	0.6020470	-3.1592230
H	2.1670580	2.3182850	-3.4180670
C	5.7809530	1.9184910	-1.7624580
H	6.8386060	1.0834190	-0.0754910
H	-5.2431040	-3.1858580	-1.6183370
H	-4.7911190	-4.1193560	-0.1705280
H	-3.7401570	-4.1424590	-1.6096750
H	-5.2373230	-0.3166930	2.5243780
H	-5.9399070	0.5249750	1.1194420
H	-4.6158130	1.2857440	2.0377110
H	3.7327380	-3.1336980	4.5668570
H	6.6527000	2.4183760	-2.1759690
H	-0.9747370	3.4258910	-1.7003280
N	0.8017020	3.0627430	0.6281890
H	0.8396260	3.4562380	1.5616350
H	0.9850740	3.7898700	-0.0527260
N	2.3591040	-2.0564090	-1.8495090

(L37)Ni(Ph)NH_2



Zero-point correction= 0.658213 (Hartree/Particle)
Thermal correction to Energy= 0.699221
Thermal correction to Enthalpy= 0.700165
Thermal correction to Gibbs Free Energy= 0.586537
Sum of electronic and zero-point Energies= -4188.082372
Sum of electronic and thermal Energies= -4188.041364
Sum of electronic and thermal Enthalpies= -4188.040420
Sum of electronic and thermal Free Energies= -4188.154048

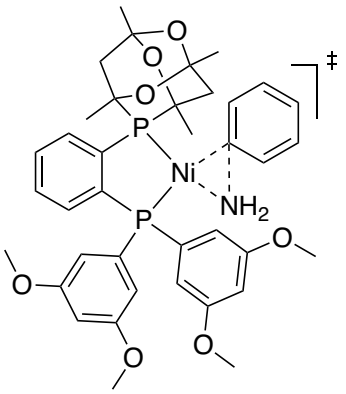
Single-point energy (6-311+G(2d,2p)) = -4.189494361825E+03

Ni	0.1648410	1.3693200	0.1718480
P	-1.0733740	-0.3587210	-0.3141660
P	2.0254760	-0.0342160	0.0681960
C	-1.0361970	2.8486440	0.2591560
C	-1.5544600	3.4419740	-0.9295400
C	-1.8118910	3.0093400	1.4449150
C	1.4424840	-1.3594900	-1.0464030
C	-1.8803710	-1.3097750	1.1235260
C	2.6011470	-0.9270160	1.5724890
C	3.5612090	0.5819120	-0.7272130
C	-2.7589930	4.1400470	-0.9233830
C	-3.0135720	3.7111470	1.4291340
H	-1.4725690	2.5532130	2.3728710
O	-3.1795240	-1.6633750	-1.5216760
O	-2.9372480	-0.4679430	1.6212910
C	-2.4842010	-2.6239800	0.6235200
C	-3.6756170	0.4867550	-0.5096240
C	-0.9119000	-1.5038750	2.2763090
C	2.7520580	-0.2003880	2.7765990
C	2.8318390	-2.3102410	1.5651430
C	3.4669070	1.3042210	-1.9423750
C	4.8091610	0.4299290	-0.1055710
H	-3.1215250	4.5731090	-1.8541710
C	-3.5090230	4.2856670	0.2504780

H	-3.5782390	3.8059510	2.3552810
C	-3.6433820	-2.3377180	-0.3427240
H	-1.7233420	-3.2427340	0.1400390
H	-2.8847200	-3.1776710	1.4811410
H	-4.5788380	0.6318440	-1.1138560
H	-3.2707080	1.4657940	-0.2503190
C	-4.0650910	-0.2807430	0.7569900
H	-3.3867720	0.2446520	-3.2707430
H	-1.6945750	-0.2987920	-3.2748010
H	-2.1134770	1.3051440	-2.6196920
H	-1.4319190	-1.9806260	3.1152760
H	-0.5180150	-0.5397600	2.6107380
H	-0.0705490	-2.1365450	1.9785340
C	3.1451080	-0.8929160	3.9279110
C	3.2111270	-2.9832450	2.7265210
H	2.7070230	-2.8684370	0.6434770
C	2.4787570	1.2823920	2.8547890
C	4.6397110	1.8364390	-2.4895130
H	4.8790550	-0.1200040	0.8273550
C	2.1576490	1.4924280	-2.6714890
H	-4.4474070	4.8314900	0.2481170
C	5.9639210	0.9749420	-0.6677380
O	-4.6002480	-1.5467510	0.3532400
C	-4.3530830	-3.5881530	-0.8213800
C	-5.1219360	0.4197330	1.5830920
H	3.2679510	-0.3388700	4.8553360
C	3.3703900	-2.2694330	3.9131180
H	3.3824320	-4.0558290	2.6999180
H	3.0030970	1.8512370	2.0790310
H	2.7769400	1.6795300	3.8301250
H	1.4107700	1.4885580	2.7126950
H	4.5755460	2.3905770	-3.4229630
H	1.3648750	1.8377660	-1.9949400
H	1.8056880	0.5538670	-3.1174270
H	2.2641270	2.2264230	-3.4763310
C	5.8781540	1.6802700	-1.8663140
H	6.9208710	0.8457110	-0.1696840
H	-5.1744580	-3.3079680	-1.4858480
H	-4.7560820	-4.1381710	0.0333470
H	-3.6564840	-4.2330260	-1.3657090
H	-5.3559710	-0.1829770	2.4647140
H	-6.0297300	0.5535560	0.9884500
H	-4.7496700	1.3979910	1.8965060
H	3.6664050	-2.7796640	4.8256590
H	6.7686150	2.1120060	-2.3150560
H	-0.9948470	3.3492760	-1.8593810

N	0.7708380	3.1368180	0.4845360
H	0.8037820	3.5802800	1.3956610
H	0.9450290	3.8313750	-0.2321670
C	2.1683710	-2.1964880	-1.8504860
C	-0.2857450	-2.5312930	-2.0946450
S	1.1407870	-3.2278960	-2.7919310
C	-2.6653510	-0.3230370	-1.3295230
C	-2.4436540	0.2665420	-2.7126640
C	0.0164950	-1.5439210	-1.1907410
H	3.2440060	-2.2495940	-1.9577730
H	-1.2658270	-2.8564630	-2.4134660

(L38)Ni(Ph)NH_2



Zero-point correction= 0.767234 (Hartree/Particle)
Thermal correction to Energy= 0.815980
Thermal correction to Enthalpy= 0.816924
Thermal correction to Gibbs Free Energy= 0.683785
Sum of electronic and zero-point Energies= -4246.693999
Sum of electronic and thermal Energies= -4246.645253
Sum of electronic and thermal Enthalpies= -4246.644309
Sum of electronic and thermal Free Energies= -4246.777448

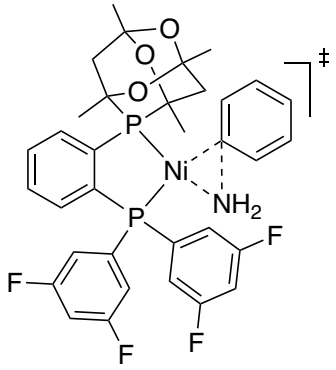
Single-point energy (6-311+G(2d,2p)) = -4.248329440420E+03

Ni	0.4580070	-0.8322830	0.9560970
P	1.7278680	0.0785710	-0.5600160
P	-1.3110900	-0.0336980	-0.1900670
C	1.5168580	-2.0475720	1.9815270
C	1.6459530	-3.3296590	1.3711730
C	2.5291570	-1.6761950	2.9168120
C	0.6901510	0.4352290	-2.0571250
C	-0.7112510	0.3724150	-1.8772030
C	3.3593740	-0.6227430	-1.2128790
C	2.5238900	1.7208390	-0.0245940
C	-2.0072060	1.5173060	0.4874670

C	-2.7640530	-1.1105800	-0.4843280
C	2.7315090	-4.1574200	1.6547730
C	3.5851150	-2.5309750	3.2080470
H	2.4840290	-0.6951850	3.3856940
O	3.9890550	0.2692200	-2.1653880
O	3.4951170	1.3721680	0.9829860
C	-1.5703390	0.5575290	-2.9680120
C	1.1920120	0.6880060	-3.3446740
C	3.2463070	2.3944820	-1.1931160
C	4.2700190	-0.7451910	0.0124310
C	3.1590780	-1.9547890	-1.9171070
C	1.5111200	2.6289700	0.6497150
C	-2.1780040	1.5244750	1.8850720
C	-2.2990000	2.6430320	-0.2749360
C	-2.4738910	-2.4692060	-0.7147760
C	-4.0780150	-0.6572470	-0.4568030
H	2.8056110	-5.1204920	1.1520680
C	3.7124820	-3.7781710	2.5768040
H	4.3388020	-2.2110360	3.9258610
H	-2.6444070	0.4818990	-2.8225620
C	-1.0557550	0.8140330	-4.2377010
C	0.3264980	0.8764340	-4.4226410
H	2.2629280	0.7085100	-3.5051270
C	4.4323850	1.5322730	-1.6521900
H	2.5578500	2.5787720	-2.0223790
H	3.6404590	3.3603430	-0.8548440
H	5.1915560	-1.2576840	-0.2880900
H	3.7900170	-1.3255080	0.8014630
C	4.6469140	0.6467410	0.5332620
H	4.1263370	-2.3288180	-2.2720650
H	2.4890290	-1.8566430	-2.7767680
H	2.7359760	-2.6797490	-1.2146930
H	2.0142880	3.5281020	1.0240800
H	1.0364980	2.1134080	1.4900250
H	0.7291300	2.9301840	-0.0546870
C	-2.6667430	2.6766380	2.4980680
C	-2.7803540	3.7997230	0.3632090
H	-2.1601170	2.6613980	-1.3497150
C	-3.5234570	-3.3580780	-0.9375860
H	-4.3195290	0.3828770	-0.2682470
H	4.5472860	-4.4339870	2.8036630
C	-5.1256120	-1.5704050	-0.6728150
O	5.2932110	1.3517620	-0.5323730
H	-1.7290880	0.9545170	-5.0788280
H	0.7359930	1.0613250	-5.4121960
C	5.2527630	2.1726250	-2.7538480

C	5.6068800	0.6085240	1.7029900
C	-2.9696090	3.8214210	1.7423480
C	-4.8560630	-2.9147210	-0.9165500
H	6.0866120	1.5156540	-3.0142530
H	5.6471860	3.1341280	-2.4139870
H	4.6331210	2.3329620	-3.6413500
H	5.8404720	1.6289410	2.0182300
H	6.5308050	0.1027480	1.4096100
H	5.1486530	0.0658930	2.5334590
H	0.8873250	-3.6623160	0.6636000
N	-0.1603230	-1.6251370	2.5543980
H	0.0847980	-1.4017740	3.5094710
H	-0.7311940	-2.4660320	2.5361650
H	-1.4412520	-2.7986730	-0.7051360
H	-1.9005590	0.6445480	2.4539880
H	-3.3366510	4.6949050	2.2658970
H	-5.6379370	-3.6445240	-1.0833160
O	-2.8736060	2.8005980	3.8430960
O	-3.0378240	4.8609030	-0.4598880
O	-6.3849150	-1.0407820	-0.6299890
O	-3.3617960	-4.6949870	-1.1737910
C	-2.0374470	-5.2143930	-1.1990150
H	-2.1409350	-6.2798420	-1.4073810
H	-1.4405340	-4.7416170	-1.9888320
H	-1.5382180	-5.0770580	-0.2315060
C	-7.4887900	-1.9118690	-0.8382490
H	-7.4493750	-2.3727850	-1.8332410
H	-7.5248770	-2.6972450	-0.0729270
H	-8.3789930	-1.2865270	-0.7611860
C	-3.5278420	6.0607850	0.1242010
H	-2.8094570	6.4749490	0.8427280
H	-3.6616710	6.7601180	-0.7019500
H	-4.4904120	5.8950830	0.6240050
C	-2.5651780	1.6834450	4.6697570
H	-2.8033630	1.9941960	5.6876750
H	-3.1712220	0.8103310	4.3987980
H	-1.5016460	1.4231740	4.6022670

(L39)Ni(Ph)NH_2



Zero-point correction= 0.603094 (Hartree/Particle)
Thermal correction to Energy= 0.644725
Thermal correction to Enthalpy= 0.645669
Thermal correction to Gibbs Free Energy= 0.528058
Sum of electronic and zero-point Energies= -4185.706893
Sum of electronic and thermal Energies= -4185.665262
Sum of electronic and thermal Enthalpies= -4185.664318
Sum of electronic and thermal Free Energies= -4185.781929

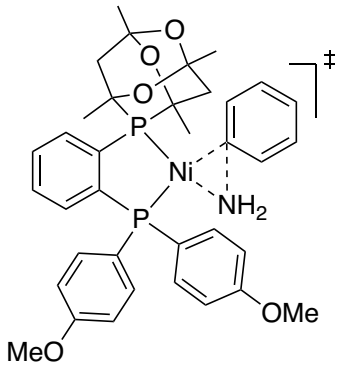
Single-point energy (6-311+G(2d,2p)) = -4.187140375438E+03

Ni	-0.1208720	1.0781460	0.7615840
P	-1.3752460	-0.1943890	-0.4879760
P	1.6598720	0.0350110	-0.1253100
C	-1.2037920	2.4945250	1.4674900
C	-1.2874340	3.5928360	0.5699580
C	-2.2432010	2.3536260	2.4280660
C	-0.3120150	-0.9622140	-1.8039970
C	1.0870100	-0.8570220	-1.6226700
C	-2.9711240	0.3319890	-1.3602160
C	-2.2294360	-1.6173600	0.4442900
C	2.2898390	-1.2628420	1.0115890
C	3.1847270	0.8876570	-0.6955140
C	-2.3799310	4.4609600	0.6011550
C	-3.3043370	3.2505800	2.4656710
H	-2.2172920	1.5169450	3.1228520
O	-3.5906720	-0.7761150	-2.0561980
O	-3.2168250	-0.9888390	1.2847860
C	1.9648820	-1.3666650	-2.5890630
C	-0.7904030	-1.5744730	-2.9743200
C	-2.9367340	-2.5722030	-0.5193890
C	-3.9153280	0.7962950	-0.2473000
C	-2.7168830	1.4184970	-2.3924550
C	-1.2605510	-2.3246980	1.3752130

C	2.4207280	-0.8844940	2.3573560
C	2.5735680	-2.5763420	0.6159510
C	3.0064060	1.9707530	-1.5737520
C	4.4699440	0.5645840	-0.2403980
H	-2.4249350	5.2787060	-0.1155840
C	-3.3973260	4.3072790	1.5470460
H	-4.0842410	3.1149610	3.2127300
H	3.0375850	-1.2650030	-2.4492000
C	1.4716270	-1.9807320	-3.7387870
C	0.0924650	-2.0777300	-3.9303280
H	-1.8578150	-1.6288490	-3.1479630
C	-4.0845720	-1.8455990	-1.2374090
H	-2.2313280	-2.9930940	-1.2409510
H	-3.3683550	-3.3989100	0.0573930
H	-4.8147140	1.2203230	-0.7090960
H	-3.4467840	1.5631160	0.3702610
C	-4.3404340	-0.3964710	0.6174670
H	-3.6640400	1.7002830	-2.8663510
H	-2.0286500	1.0775920	-3.1720330
H	-2.2918050	2.2997420	-1.9019170
H	-1.7971020	-3.0775980	1.9639030
H	-0.7965830	-1.6067800	2.0583660
H	-0.4700670	-2.8231240	0.8044990
C	2.8558120	-1.8333660	3.2713280
C	2.9913560	-3.4822860	1.5826180
H	2.4687320	-2.9013370	-0.4125440
C	4.1191850	2.6846130	-1.9882970
H	4.6469530	-0.2596480	0.4401370
H	-4.2346920	4.9974080	1.5790660
C	5.5442630	1.3280270	-0.6825900
O	-4.9715200	-1.3532400	-0.2395430
H	2.1589610	-2.3697690	-4.4847060
H	-0.3008730	-2.5383930	-4.8324120
C	-4.8888840	-2.7445720	-2.1544780
C	-5.3334590	-0.0324130	1.7000120
C	3.1478280	-3.1465090	2.9207950
C	5.4103140	2.3947930	-1.5599310
H	-5.6965900	-2.1673630	-2.6116710
H	-5.3190500	-3.5711280	-1.5824550
H	-4.2483810	-3.1502150	-2.9434900
H	-5.6016020	-0.9283420	2.2660960
H	-6.2353810	0.3907590	1.2495530
H	-4.8883640	0.7044150	2.3725530
H	-0.4919790	3.7554020	-0.1555940
N	0.4720880	2.1772550	2.1749380
H	0.1710420	2.1817270	3.1407380

H	1.0280500	3.0099300	1.9970770
H	2.0207430	2.2581730	-1.9261090
H	2.1577990	0.1180390	2.6833810
F	2.9898030	-1.4768490	4.5734350
F	3.2636880	-4.7582660	1.2051090
H	3.4749420	-3.8725430	3.6551950
H	6.2640060	2.9745260	-1.8888250
F	6.7894970	1.0105110	-0.2445230
F	3.9480890	3.7249670	-2.8435270

(L40)Ni(Ph)NH_2



Zero-point correction= 0.701924 (Hartree/Particle)
Thermal correction to Energy= 0.745319
Thermal correction to Enthalpy= 0.746263
Thermal correction to Gibbs Free Energy= 0.625348
Sum of electronic and zero-point Energies= -4017.698334
Sum of electronic and thermal Energies= -4017.654940
Sum of electronic and thermal Enthalpies= -4017.653995
Sum of electronic and thermal Free Energies= -4017.774911

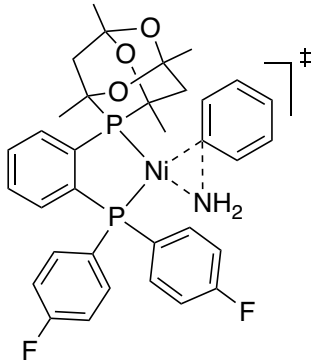
Single-point energy (6-311+G(2d,2p)) = -4.019193659277E+03

Ni	-0.1515680	-0.8623360	-1.0255700
P	-1.4315860	-0.0583480	0.5413570
P	1.6021300	0.0335750	0.0811070
C	-1.1875950	-2.0804030	-2.0711540
C	-1.2569630	-3.3884990	-1.5092320
C	-2.2291960	-1.7118360	-2.9739710
C	-0.3745750	0.3525100	2.0121460
C	1.0224430	0.3822580	1.7908140
C	-2.9818760	-0.8923970	1.2372950
C	-2.3728930	1.5247520	0.0618030
C	2.1108710	1.6531580	-0.5952380
C	3.1674430	-0.8839060	0.3083770
C	-2.3141500	-4.2468750	-1.8090750

C	-3.2561110	-2.5955220	-3.2829490
H	-2.2297950	-0.7127360	-3.4049420
O	-3.6419530	-0.0657560	2.2278890
O	-3.3517900	1.1177340	-0.9150330
C	1.8977230	0.6076180	2.8613560
C	-0.8533190	0.5545610	3.3175340
C	-3.1004530	2.1244830	1.2668330
C	-3.9260980	-1.0662680	0.0437820
C	-2.6552400	-2.2157060	1.9098180
C	-1.4613570	2.5187540	-0.6351950
C	2.2481820	1.7355730	-1.9951540
C	2.3072760	2.8099710	0.1636670
C	3.0783210	-2.2689010	0.4998900
C	4.4433050	-0.2964990	0.2700870
H	-2.3417480	-5.2311280	-1.3442400
C	-3.3244420	-3.8705970	-2.7001770
H	-4.0326930	-2.2781910	-3.9771950
H	2.9701150	0.6004100	2.6864270
C	1.4056950	0.8137520	4.1491240
C	0.0283900	0.7845040	4.3741060
H	-1.9178070	0.4996210	3.5090750
C	-4.1993210	1.1667730	1.7538580
H	-2.3980580	2.3500210	2.0739410
H	-3.5803160	3.0613730	0.9589990
H	-4.7933040	-1.6532780	0.3685600
H	-3.4327920	-1.5952520	-0.7723930
C	-4.4277790	0.3000310	-0.4376550
H	-3.5777440	-2.6690440	2.2905360
H	-1.9644140	-2.0800750	2.7476380
H	-2.2030630	-2.8944990	1.1799960
H	-2.0477020	3.3806080	-0.9746630
H	-0.9817370	2.0539880	-1.5016570
H	-0.6779920	2.8698990	0.0437770
C	2.5910480	2.9319450	-2.6066510
C	2.6409410	4.0254310	-0.4419350
H	2.1918880	2.7786560	1.2428540
C	4.2173990	-3.0543010	0.6785810
H	4.5409480	0.7716620	0.1004220
H	-4.1368830	-4.5494000	-2.9405170
C	5.5870810	-1.0672410	0.4359400
O	-5.0853160	0.9378170	0.6636760
H	2.0932080	0.9841720	4.9732680
H	-0.3635140	0.9274300	5.3776550
C	-5.0235570	1.7259840	2.8961700
C	-5.4260700	0.2075190	-1.5714570
H	2.6989280	3.0037290	-3.6843930

C	2.7872480	4.0862030	-1.8321550
H	2.7808140	4.9054430	0.1749760
H	4.1107680	-4.1226100	0.8255750
C	5.4803010	-2.4496270	0.6465160
H	6.5762120	-0.6210420	0.4042630
H	-5.7945550	1.0031800	3.1751530
H	-5.5026470	2.6593650	2.5881480
H	-4.3848170	1.9199690	3.7632320
H	-5.7482990	1.2122140	-1.8578510
H	-6.2969630	-0.3720350	-1.2532810
H	-4.9601770	-0.2852380	-2.4279760
H	-0.4731700	-3.7196010	-0.8289830
N	0.4699960	-1.5748670	-2.6581990
H	0.2013170	-1.3170270	-3.5983390
H	1.0613460	-2.4008270	-2.6859330
H	2.0998870	-2.7445710	0.5080580
H	2.0652670	0.8505150	-2.5997070
O	6.6606190	-3.1201470	0.8002230
O	3.1116770	5.2176730	-2.5253590
C	6.6160830	-4.5265600	1.0058980
H	7.6545800	-4.8450400	1.1027530
H	6.0692210	-4.7773820	1.9234300
H	6.1543640	-5.0388230	0.1526130
C	3.3012300	6.4240080	-1.7976100
H	3.5406360	7.1848440	-2.5413120
H	2.3887550	6.7115680	-1.2602970
H	4.1319130	6.3337500	-1.0863640

(L41)Ni(Ph)NH_2



Zero-point correction= 0.621739 (Hartree/Particle)
Thermal correction to Energy= 0.661781
Thermal correction to Enthalpy= 0.662725
Thermal correction to Gibbs Free Energy= 0.550434
Sum of electronic and zero-point Energies= -3987.243391
Sum of electronic and thermal Energies= -3987.203349

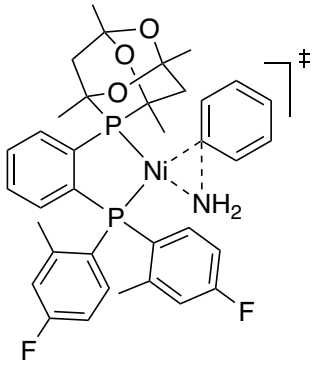
Sum of electronic and thermal Enthalpies= -3987.202405
Sum of electronic and thermal Free Energies= -3987.314697

Single-point energy (6-311+G(2d,2p)) = -3.988638214708E+03

Ni	0.0473420	1.0978350	0.7398750
P	-1.2047860	-0.2032470	-0.4798860
P	1.8307880	-0.0193860	-0.0660250
C	-1.0276690	2.5523710	1.3660240
C	-1.1078340	3.6147080	0.4221320
C	-2.0743240	2.4598150	2.3284630
C	-0.1332750	-1.0254130	-1.7556220
C	1.2643440	-0.9314940	-1.5568150
C	-2.7827760	0.3118440	-1.3903490
C	-2.0893760	-1.5831930	0.4880210
C	2.4146120	-1.3043690	1.1021890
C	3.3664180	0.8172980	-0.6187820
C	-2.1912200	4.4936200	0.4196630
C	-3.1267020	3.3673650	2.3294020
H	-2.0594890	1.6494960	3.0543450
O	-3.4093140	-0.8105890	-2.0579990
O	-3.0810470	-0.9169290	1.2940260
C	2.1472920	-1.4646520	-2.5053230
C	-0.6043070	-1.6580590	-2.9182570
C	-2.7947390	-2.5608790	-0.4540020
C	-3.7351480	0.8246960	-0.3060770
C	-2.5032040	1.3611560	-2.4540150
C	-1.1426650	-2.2710830	1.4552890
C	2.5295530	-0.9128200	2.4476540
C	2.6875900	-2.6335320	0.7509390
C	3.2123020	2.0005110	-1.3623630
C	4.6601530	0.3778630	-0.3042050
H	-2.2296230	5.2811820	-0.3308550
C	-3.2107130	4.3889080	1.3707020
H	-3.9091550	3.2665520	3.0796230
H	3.2190650	-1.3652720	-2.3563790
C	1.6622340	-2.0966110	-3.6490370
C	0.2846330	-2.1885670	-3.8537260
H	-1.6701220	-1.7058510	-3.1037740
C	-3.9251600	-1.8459220	-1.2104750
H	-2.0844110	-3.0111090	-1.1527930
H	-3.2427290	-3.3644910	0.1427460
H	-4.6229110	1.2447610	-0.7933710
H	-3.2643490	1.6052550	0.2923450
C	-4.1870300	-0.3329470	0.5919810
H	-3.4408420	1.6351900	-2.9510040

H	-1.8063180	0.9890820	-3.2113120
H	-2.0781080	2.2541820	-1.9853110
H	-1.6969290	-2.9980800	2.0600730
H	-0.6793460	-1.5370230	2.1212380
H	-0.3491980	-2.7960090	0.9136480
C	2.9318780	-1.8234760	3.4228070
C	3.0794440	-3.5603000	1.7188480
H	2.5870050	-2.9564730	-0.2803600
C	4.3197080	2.7180300	-1.8077700
H	4.7992750	-0.5252020	0.2814880
H	-4.0421670	5.0868630	1.3742230
C	5.7811730	1.0921870	-0.7319340
O	-4.8192400	-1.3107350	-0.2411370
H	2.3548010	-2.5031930	-4.3809030
H	-0.1025330	-2.6638970	-4.7509720
C	-4.7283060	-2.7665820	-2.1070320
C	-5.1893130	0.0807830	1.6478080
H	3.0263130	-1.5395960	4.4656590
C	3.1964740	-3.1311350	3.0340580
H	3.2905080	-4.5942730	1.4670890
H	4.2163060	3.6309890	-2.3845070
C	5.5847510	2.2447260	-1.4796670
H	6.7887330	0.7668180	-0.4951220
H	-5.5234370	-2.1961660	-2.5938930
H	-5.1752720	-3.5684290	-1.5130850
H	-4.0825710	-3.2057000	-2.8735710
H	-5.4760550	-0.7913160	2.2414070
H	-6.0798790	0.4990470	1.1709110
H	-4.7430320	0.8354880	2.2995050
H	-0.3134970	3.7389650	-0.3125980
N	0.6325980	2.2766170	2.0927650
H	0.3407040	2.3235380	3.0598860
H	1.2027710	3.0894030	1.8740210
H	2.2129420	2.3631890	-1.5910630
H	2.2801390	0.1080160	2.7270690
F	6.6726360	2.9442900	-1.9013650
F	3.5799920	-4.0293120	3.9809340

(L42)Ni(Ph)NH_2



Zero-point correction= 0.675575 (Hartree/Particle)
Thermal correction to Energy= 0.718488
Thermal correction to Enthalpy= 0.719432
Thermal correction to Gibbs Free Energy= 0.602046
Sum of electronic and zero-point Energies= -4065.793626
Sum of electronic and thermal Energies= -4065.750713
Sum of electronic and thermal Enthalpies= -4065.749769
Sum of electronic and thermal Free Energies= -4065.867155

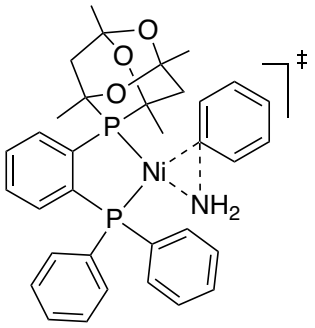
Single-point energy (6-311+G(2d,2p)) = -4.067271917168E+03

Ni	-0.0282240	-1.2032550	-0.6096610
P	-1.2924950	0.1636100	0.5239740
P	1.7514690	0.0831050	0.0667870
C	-1.1718140	-2.5664050	-1.3059850
C	-1.6887530	-3.5980690	-0.4681860
C	-1.9167000	-2.2648900	-2.4839130
C	-0.2284660	0.9174440	1.8407840
C	1.1695200	0.8428830	1.6382380
C	-2.9182450	-0.3186770	1.3674240
C	-2.1019860	1.5943000	-0.4407000
C	2.3236960	1.5119880	-0.9438280
C	3.2991070	-0.7868970	0.5362740
C	-2.8645390	-4.2697250	-0.7908370
C	-3.0897690	-2.9493320	-2.7881040
H	-1.5761420	-1.4694890	-3.1439970
O	-3.5246640	0.8056350	2.0496140
O	-3.0951060	0.9909210	-1.2895520
C	2.0473160	1.2829300	2.6374270
C	-0.7063270	1.4571430	3.0471490
C	-2.7907720	2.5707110	0.5166010
C	-3.8562680	-0.7649350	0.2394140
C	-2.7130160	-1.4073310	2.4084780
C	-1.1158640	2.2809810	-1.3678150

C	2.4960650	1.3321000	-2.3379640
C	2.5274930	2.7819260	-0.3835920
C	3.2212990	-1.9416940	1.3558560
C	4.5415000	-0.3905630	0.0200180
H	-3.2281030	-5.0468300	-0.1206710
C	-3.5850480	-3.9580790	-1.9508040
H	-3.6312420	-2.6859210	-3.6952420
H	3.1195420	1.1950170	2.4839000
C	1.5571980	1.8121610	3.8304380
C	0.1783530	1.9001050	4.0305850
H	-1.7741410	1.5046460	3.2228440
C	-3.9727890	1.8839850	1.2175610
H	-2.0814370	2.9630990	1.2507890
H	-3.1842400	3.4138160	-0.0637210
H	-4.7708670	-1.1671580	0.6907410
H	-3.3977780	-1.5454740	-0.3678980
C	-4.2418620	0.4325170	-0.6346410
H	-3.6751950	-1.6505600	2.8735210
H	-2.0202000	-1.0897280	3.1935460
H	-2.3186700	-2.3060980	1.9257080
H	-1.6423440	3.0323520	-1.9674460
H	-0.6559790	1.5545400	-2.0435910
H	-0.3242510	2.7770140	-0.7990530
C	2.8831010	2.4270480	-3.1176050
C	2.9002160	3.8752750	-1.1649150
H	2.3879170	2.9298540	0.6812460
C	2.2495280	0.0031800	-3.0095250
C	4.3953490	-2.6488660	1.6330500
H	4.6046370	0.4910770	-0.6088080
C	1.9240750	-2.4159040	1.9660190
H	-4.5008410	-4.4865560	-2.1965750
C	5.7089310	-1.1031720	0.2937230
O	-4.8579770	1.4124570	0.2084630
H	2.2466050	2.1476860	4.6002760
H	-0.2126960	2.3035060	4.9607540
C	-4.7639630	2.8126730	2.1164010
C	-5.2293600	0.0861680	-1.7276040
H	3.0280390	2.3237300	-4.1882400
C	3.0722990	3.6667020	-2.5239860
H	3.0563220	4.8594580	-0.7367000
H	2.7768510	-0.8211990	-2.5177070
H	2.5607360	0.0342720	-4.0579370
H	1.1836490	-0.2534820	-2.9741890
H	4.3744830	-3.5358350	2.2583460
H	1.1161220	-2.4380480	1.2231330
H	1.5949060	-1.7504450	2.7734600

H	2.0350370	-3.4210550	2.3835970
C	5.6043200	-2.2234060	1.1015350
H	6.6713770	-0.8008600	-0.1045430
H	-5.5949690	2.2623510	2.5649880
H	-5.1614700	3.6472210	1.5324780
H	-4.1234750	3.2047640	2.9122580
H	-5.4637860	0.9838300	-2.3059820
H	-6.1492500	-0.3062030	-1.2855440
H	-4.7950840	-0.6706690	-2.3847710
H	-1.1516630	-3.8668100	0.4405210
N	0.6444710	-2.6901230	-1.5741060
H	0.7098590	-2.7377650	-2.5847850
H	0.8279290	-3.6070660	-1.1847700
F	6.7273420	-2.9379420	1.3871030
F	3.4385690	4.7148930	-3.3095620

(L23)Ni(Ph)NH_2



Zero-point correction= 0.636362 (Hartree/Particle)
Thermal correction to Energy= 0.674537
Thermal correction to Enthalpy= 0.675482
Thermal correction to Gibbs Free Energy= 0.566513
Sum of electronic and zero-point Energies= -3788.704483
Sum of electronic and thermal Energies= -3788.666308
Sum of electronic and thermal Enthalpies= -3788.665364
Sum of electronic and thermal Free Energies= -3788.774332

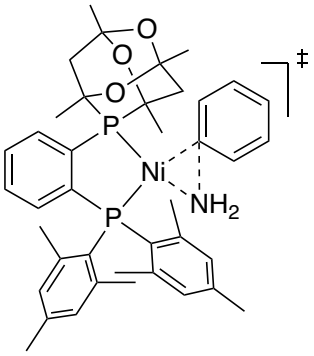
Single-point energy (6-311+G(2d,2p)) = -3.790059326991E+03

Ni	0.2564660	1.2978680	0.3272710
P	-0.9406490	-0.4026350	-0.3222680
P	2.0815580	0.0055200	0.0120360
C	-0.8775350	2.8257120	0.3663950
C	-1.0271300	3.4674620	-0.8958030
C	-1.8990410	3.0604100	1.3325560

C	0.1680690	-1.6023700	-1.2049460
C	1.5595280	-1.3997670	-1.0502250
C	-2.5263570	-0.3095460	-1.3515470
C	-1.7894850	-1.3519710	1.0915130
C	2.6982910	-0.7476600	1.5633890
C	3.5837490	0.6523580	-0.8153040
C	-2.1362680	4.2665320	-1.1724740
C	-2.9811380	3.8853250	1.0471370
H	-1.8405360	2.5648110	2.2994950
O	-3.1133260	-1.6186290	-1.5551430
O	-2.8094080	-0.4680970	1.5979240
C	2.4691390	-2.2135180	-1.7382790
C	-0.2708420	-2.6294050	-2.0573330
C	-2.4550550	-2.6307980	0.5793640
C	-3.5025210	0.5376530	-0.5293410
C	-2.2707970	0.2812520	-2.7284960
C	-0.8303010	-1.6020920	2.2414610
C	2.8187510	0.1173270	2.6643970
C	2.9899780	-2.1086810	1.7244880
C	3.3857300	1.4873800	-1.9279430
C	4.8905760	0.3990950	-0.3770530
H	-2.2226640	4.7269060	-2.1553140
C	-3.1247580	4.4927280	-0.2093650
H	-3.7400780	4.0427850	1.8119190
H	3.5353740	-2.0329940	-1.6326160
C	2.0166020	-3.2325810	-2.5745460
C	0.6448220	-3.4360380	-2.7336690
H	-1.3325530	-2.7752180	-2.2133600
C	-3.6019770	-2.2831470	-0.3825490
H	-1.7247830	-3.2823520	0.0916440
H	-2.8811310	-3.1727920	1.4322240
H	-4.3983900	0.7211970	-1.1341350
H	-3.0594400	1.4975710	-0.2617250
C	-3.9262680	-0.2203220	0.7339250
H	-3.2123270	0.3219480	-3.2881650
H	-1.5556510	-0.3209580	-3.2972220
H	-1.8784180	1.2975310	-2.6235000
H	-1.3674040	-2.0727910	3.0731210
H	-0.3970270	-0.6595050	2.5889250
H	-0.0143370	-2.2622490	1.9307150
C	3.2450480	-0.3716320	3.8986130
C	3.4051880	-2.5964820	2.9657970
H	2.8860760	-2.7901030	0.8856360
C	4.4738420	2.0365140	-2.6034940
H	5.0576750	-0.2312890	0.4909780
H	-3.9788930	5.1268960	-0.4261680

C	5.9794350	0.9602660	-1.0487490
O	-4.5209040	-1.4570630	0.3236300
H	2.7296350	-3.8559360	-3.1072300
H	0.2829260	-4.2175420	-3.3964860
C	-4.3678010	-3.4961540	-0.8713900
C	-4.9498960	0.5223820	1.5652480
H	3.3366360	0.3047040	4.7442320
C	3.5368720	-1.7296940	4.0522390
H	3.6253980	-3.6543350	3.0825540
H	4.3077650	2.6786070	-3.4642330
C	5.7743450	1.7743740	-2.1637150
H	6.9886460	0.7588120	-0.6993400
H	-5.1766050	-3.1728470	-1.5316920
H	-4.7939260	-4.0355000	-0.0210450
H	-3.7017380	-4.1662040	-1.4234760
H	-5.2130790	-0.0761210	2.4414660
H	-5.8496240	0.7041330	0.9710900
H	-4.5330590	1.4793130	1.8876360
H	3.8596350	-2.1118210	5.0168730
H	6.6231220	2.2101230	-2.6835460
H	-0.2622340	3.3296310	-1.6590140
N	0.8194140	2.9208840	1.0970160
H	0.5246880	3.3455330	1.9658130
H	1.3479830	3.5980560	0.5535340
H	2.3726330	1.7066870	-2.2582760
H	2.5574700	1.1663940	2.5463670

(L43)Ni(Ph)NH_2



Zero-point correction= 0.803995 (Hartree/Particle)
Thermal correction to Energy= 0.851641
Thermal correction to Enthalpy= 0.852585
Thermal correction to Gibbs Free Energy= 0.725516
Sum of electronic and zero-point Energies= -4024.436646
Sum of electronic and thermal Energies= -4024.389001
Sum of electronic and thermal Enthalpies= -4024.388056
Sum of electronic and thermal Free Energies= -4024.515125

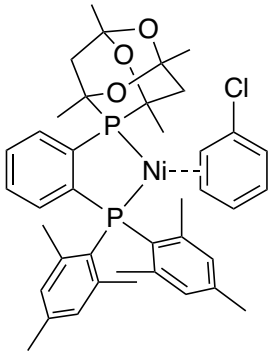
Single-point energy (6-311+G(2d,2p)) = -4.026044961457E+03

Ni	-0.0705380	-1.1720380	-0.7124540
P	-1.3707800	0.0338360	0.5508240
P	1.7075340	0.1104710	0.1247340
C	-1.1774940	-2.4549110	-1.5913220
C	-1.7211820	-3.5899400	-0.9196840
C	-1.8767090	-2.0065300	-2.7509930
C	-0.3256910	0.5831820	1.9801260
C	1.0776680	0.5138740	1.8063750
C	-2.9661520	-0.6440380	1.3280280
C	-2.2703170	1.5469260	-0.1881510
C	2.0084210	1.6907570	-0.8002320
C	3.2950510	-0.7839670	0.4471070
C	-2.8784080	-4.2155020	-1.3729060
C	-3.0356200	-2.6434670	-3.1857520
H	-1.5158720	-1.1322280	-3.2894430
O	-3.6202400	0.3359500	2.1724520
O	-3.2486680	1.0214300	-1.1045440
C	1.9216160	0.6418830	2.9168440
C	-0.8312060	0.8790360	3.2593350
C	-2.9873940	2.3353580	0.9115320
C	-3.9019250	-0.9682080	0.1579320
C	-2.6989260	-1.8604740	2.1998090
C	-1.3536900	2.4205930	-1.0217920
C	2.0534700	1.5435350	-2.2111740
C	2.0986060	2.9962020	-0.2529720
C	3.1444450	-2.0808450	1.0189990
C	4.5952070	-0.3471770	0.0839820
H	-3.2614390	-5.0755190	-0.8260630
C	-3.5576640	-3.7531460	-2.5077380
H	-3.5444710	-2.2618490	-4.0695820
H	2.9941500	0.5333710	2.7831970
C	1.4043290	0.9035520	4.1822210
C	0.0247820	1.0452930	4.3470670
H	-1.9024240	0.9312950	3.4087110
C	-4.1279590	1.5004050	1.5118430
H	-2.2837690	2.6422630	1.6910040
H	-3.4243210	3.2387360	0.4691630
H	-4.7879750	-1.4770730	0.5556040
H	-3.4178630	-1.6280150	-0.5614760
C	-4.3575740	0.3214170	-0.5288800
H	-3.6444950	-2.2120780	2.6284730
H	-2.0126960	-1.6282870	3.0191860
H	-2.2705460	-2.6605970	1.5904470

H	-1.9478710	3.2058740	-1.5034730
H	-0.8568800	1.8328690	-1.7973650
H	-0.5874150	2.8911260	-0.4015540
C	2.1702950	2.6708800	-3.0280460
C	2.1916070	4.0930930	-1.1181780
C	1.9698440	0.2008110	-2.8987320
C	4.2634230	-2.9031530	1.1684710
C	1.8325310	-2.6154460	1.5503780
H	-4.4611540	-4.2445290	-2.8553330
C	5.6784230	-1.2198970	0.2538910
O	-5.0061800	1.1407740	0.4511190
H	2.0726660	1.0005810	5.0335250
H	-0.3898800	1.2577010	5.3288680
C	-4.9474080	2.2508750	2.5425460
C	-5.3436480	0.0872680	-1.6527340
H	2.2153930	2.5295610	-4.1058100
C	2.2207760	3.9623330	-2.5058330
H	2.2594990	5.0880020	-0.6834720
H	2.5686770	-0.5784700	-2.4185450
H	2.2962980	0.2894100	-3.9400650
H	0.9354800	-0.1636770	-2.8993390
H	4.1266480	-3.8891040	1.6077660
H	0.9962120	-2.4386720	0.8624770
H	1.5640350	-2.1442750	2.5034150
H	1.9049450	-3.6940360	1.7209810
C	5.5405490	-2.5036430	0.7768550
H	6.6693760	-0.8710510	-0.0286890
H	-5.7450050	1.6022740	2.9138900
H	-5.3921360	3.1409250	2.0891480
H	-4.3134570	2.5542120	3.3813330
H	-5.6269420	1.0456260	-2.0962650
H	-6.2383120	-0.4069660	-1.2641610
H	-4.8841010	-0.5479020	-2.4136380
H	-1.2150440	-3.9777490	-0.0365760
N	0.6535830	-2.5651350	-1.7806470
H	0.7725550	-2.5203440	-2.7867420
H	0.8047700	-3.5179850	-1.4719700
C	4.9326530	1.0278600	-0.4543520
H	4.5646080	1.1876750	-1.4718870
H	4.5162180	1.8284650	0.1612270
H	6.0192620	1.1554930	-0.4733470
C	6.7240910	-3.4307450	0.9053200
H	7.6653700	-2.8740690	0.9619490
H	6.6457990	-4.0602530	1.7985360
H	6.7938580	-4.1037950	0.0402550
C	2.1388600	3.3155260	1.2245620

H	1.1949620	3.0946910	1.7312560
H	2.9176510	2.7521320	1.7456400
H	2.3501930	4.3795330	1.3666670
C	2.2915890	5.1706200	-3.4062270
H	2.7720070	6.0172050	-2.9046350
H	2.8501200	4.9548240	-4.3233310
H	1.2870960	5.4967180	-3.7074460

(L43)Ni(η^2-PhCl)



Zero-point correction= 0.780698 (Hartree/Particle)
Thermal correction to Energy= 0.828177
Thermal correction to Enthalpy= 0.829121
Thermal correction to Gibbs Free Energy= 0.702411
Sum of electronic and zero-point Energies= -4428.748484
Sum of electronic and thermal Energies= -4428.701005
Sum of electronic and thermal Enthalpies= -4428.700061
Sum of electronic and thermal Free Energies= -4428.826771

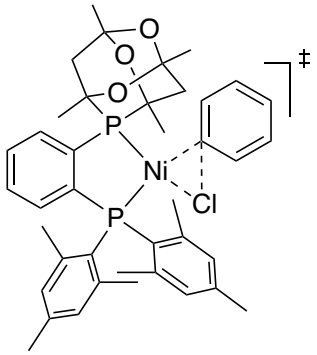
Single-point energy (6-311+G(2d,2p)) = -4.430340073844E+03

Ni -0.1756960 0.6119750 -1.0150280
P -1.7491020 -0.4559710 0.0366340
P 1.4012390 -0.3373930 0.2324420
C -0.9270900 -1.6554860 1.1911590
C 0.4840730 -1.5900230 1.2733410
C -3.1209850 -1.4855100 -0.7939880
C -3.0266380 0.5943990 1.0020280
C 2.1681380 0.9970830 1.2651970
C 2.7848860 -1.4377800 -0.3496900
O -4.0248350 -2.0707000 0.1739690
O -3.8211090 1.2710960 0.0014820
C 1.1698810 -2.5509680 2.0295150
C -1.5977730 -2.6778380 1.8868380
C -3.9638940 -0.2716490 1.8433560
C -3.9194880 -0.5086040 -1.6666610
C -2.5570410 -2.6433230 -1.6005400

C -2.3531020 1.6951500 1.8029000
C 3.1075680 1.8273720 0.5949530
C 1.7721540 1.3415950 2.5813370
C 2.5319060 -2.1578450 -1.5455040
C 4.0257920 -1.6188810 0.3111390
H 2.2521050 -2.5395560 2.0573290
C 0.4894860 -3.5419170 2.7316720
C -0.9015240 -3.6046260 2.6594070
H -2.6686220 -2.7807260 1.7808450
C -4.8275010 -1.1599180 0.9327440
H -3.4008930 -0.8762000 2.5586320
H -4.6365080 0.3846170 2.4089280
H -4.6337370 -1.0773670 -2.2738390
H -3.2534700 0.0439550 -2.3342990
C -4.7040600 0.4662950 -0.7789030
H -3.3787720 -3.2014970 -2.0635520
H -1.9892210 -3.3292850 -0.9652260
H -1.8971330 -2.2667490 -2.3880110
H -3.1186750 2.3703660 2.2030770
H -1.6706700 2.2712330 1.1723780
H -1.7930200 1.2721030 2.6409320
C 3.5926390 2.9723940 1.2330270
C 2.2839760 2.5062300 3.1657050
C 3.6828050 1.5138110 -0.7687520
C 3.5300210 -2.9702980 -2.0876670
C 1.1913770 -2.1343300 -2.2427480
C 4.9908350 -2.4481680 -0.2771070
O -5.5637250 -0.3042690 0.0644710
H 1.0451510 -4.2712920 3.3148760
H -1.4451310 -4.3872850 3.1817700
C -5.8311800 -2.0057340 1.6902030
C -5.5882000 1.4187970 -1.5582600
H 4.3122580 3.5930680 0.7027600
C 3.1852450 3.3450720 2.5124080
H 1.9679360 2.7576420 4.1760250
H 4.4799220 0.7649140 -0.7047100
H 4.1202360 2.4148950 -1.2095010
H 2.9429670 1.1259270 -1.4696890
H 3.3189030 -3.5111380 -3.0076620
H 0.8922640 -1.1219470 -2.5340330
H 0.4032810 -2.5340720 -1.5952360
H 1.2210820 -2.7507290 -3.1468910
C 4.7786390 -3.1148270 -1.4819410
H 5.9418440 -2.5779930 0.2357530
H -6.4228850 -2.5904110 0.9812040
H -6.4990020 -1.3620300 2.2691220

H -5.3130920 -2.6880690 2.3709100
H -6.1084540 2.0830060 -0.8633820
H -6.3262860 0.8530200 -2.1332020
H -4.9859380 2.0204400 -2.2445030
C -1.0114490 1.8848870 -2.3167580
C 0.4264420 2.0249810 -2.2608450
C 0.9847740 3.1991600 -1.6482860
C 0.1719570 4.1221390 -1.0422280
C -1.2469780 4.0007990 -1.1070000
C -1.8144980 2.9368770 -1.7588240
H -1.4494890 1.2609200 -3.0942980
H 2.0562470 3.3478710 -1.6787960
H 0.6179270 4.9791130 -0.5444740
H -1.8742850 4.7769710 -0.6775640
H -2.8916840 2.8795650 -1.8667930
Cl 1.3801670 1.3538730 -3.6678890
C 0.8726240 0.4983970 3.4588600
H -0.0604150 0.2141810 2.9739680
H 1.3611280 -0.4349230 3.7612400
H 0.6218410 1.0483200 4.3709780
C 3.6834600 4.6158090 3.1558090
H 4.7016200 4.8569970 2.8316540
H 3.0470250 5.4702210 2.8888090
H 3.6829710 4.5395190 4.2484280
C 4.4173500 -0.9902510 1.6355480
H 4.8007460 0.0282770 1.5130970
H 3.5915190 -0.9226210 2.3449410
H 5.2101700 -1.5853460 2.1003480
C 5.8571390 -3.9632560 -2.1098520
H 6.3998310 -3.4025420 -2.8825370
H 6.5921010 -4.2921090 -1.3677740
H 5.4376490 -4.8530570 -2.5921760

(L43)Ni(Ph)Cl Oxidative Addition Transition State



Zero-point correction= 0.779114 (Hartree/Particle)
Thermal correction to Energy= 0.826746
Thermal correction to Enthalpy= 0.827690
Thermal correction to Gibbs Free Energy= 0.700059
Sum of electronic and zero-point Energies= -4428.734116
Sum of electronic and thermal Energies= -4428.686484
Sum of electronic and thermal Enthalpies= -4428.685539
Sum of electronic and thermal Free Energies= -4428.813171

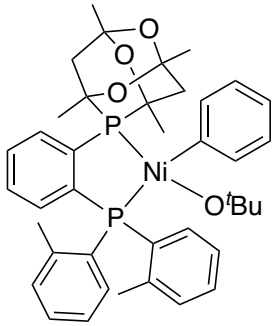
Single-point energy (6-311+G(2d,2p)) = -4430.325197

Ni -0.1480090 0.5670090 -1.0466770
P -1.6158220 -0.5555820 0.0966230
P 1.5670060 -0.2974070 0.1061490
C -0.6471190 -1.6362020 1.2666460
C 0.7602080 -1.4757020 1.3008910
C -2.9094490 -1.7397200 -0.6522340
C -2.9593670 0.3874190 1.0859690
C 2.3045540 1.2012490 0.9066610
C 3.0105530 -1.3523920 -0.4193940
O -3.7293350 -2.3787400 0.3569350
O -3.8385730 0.9618680 0.0928080
C 1.5307680 -2.3257210 2.1070330
C -1.2202830 -2.6599290 2.0432490
C -3.7956510 -0.5330650 1.9748830
C -3.8153170 -0.8647510 -1.5287090
C -2.2607200 -2.8609820 -1.4454300
C -2.3699060 1.5621120 1.8460250
C 3.1130920 2.0044470 0.0569930
C 1.9889830 1.6765650 2.2005450
C 2.7826030 -2.2039240 -1.5309190
C 4.2817140 -1.3706480 0.2086690
H 2.6100810 -2.2360620 2.1018160
C 0.9407640 -3.3073470 2.8980310
C -0.4420550 -3.4785220 2.8589970

H -2.2807570 -2.8531870 1.9686930
C -4.5933610 -1.5246470 1.1122030
H -3.1678670 -1.0578320 2.6985020
H -4.5150530 0.0785410 2.5331230
H -4.4908110 -1.5129670 -2.0997640
H -3.2148830 -0.2802280 -2.2316270
C -4.6628310 0.0587320 -0.6432290
H -3.0380390 -3.5039100 -1.8741130
H -1.6187100 -3.4759820 -0.8076600
H -1.6578890 -2.4434510 -2.2572400
H -3.1826570 2.1797210 2.2456670
H -1.7480070 2.1798780 1.1933540
H -1.7621230 1.2060830 2.6832160
C 3.5696420 3.2434930 0.5139900
C 2.4671770 2.9292440 2.6032170
C 3.5340460 1.5904250 -1.3388120
C 3.8213180 -3.0008880 -2.0171620
C 1.4345270 -2.3194020 -2.2025210
C 5.2884760 -2.1888760 -0.3224810
O -5.4266600 -0.7650900 0.2424270
H 1.5601690 -3.9484220 3.5194300
H -0.9164270 -4.2621710 3.4436660
C -5.4963180 -2.4362570 1.9189010
C -5.6563280 0.9040260 -1.4148800
H 4.1819850 3.8477570 -0.1524700
C 3.2590730 3.7320100 1.7837050
H 2.2082640 3.2847450 3.5983820
H 2.7274840 1.1114530 -1.9040030
H 4.3633590 0.8747050 -1.3150940
H 3.8667050 2.4652370 -1.9059130
H 3.6258220 -3.6473300 -2.8700590
H 1.0952620 -1.3685400 -2.6233070
H 0.6636900 -2.6459240 -1.4966600
H 1.4747460 -3.0560890 -3.0110950
C 5.0916380 -2.9972280 -1.4399290
H 6.2605010 -2.1950280 0.1667360
H -6.0508620 -3.0908800 1.2416940
H -6.2044340 -1.8398570 2.5006960
H -4.9010530 -3.0509100 2.6010770
H -6.2227090 1.5252010 -0.7162160
H -6.3481870 0.2565770 -1.9603270
H -5.1365410 1.5508470 -2.1259920
C -2.2049780 2.6192830 -1.9484510
C -0.9121150 2.0710030 -1.8845160
C 0.1706290 2.8150530 -1.3667420
C -0.1119590 4.0017960 -0.6620040

C -1.4098030 4.4922390 -0.6111010
C -2.4442270 3.8121910 -1.2872130
H -3.0011500 2.0841890 -2.4493580
H 1.1930750 2.5493170 -1.5888900
H 0.7097290 4.5555250 -0.2155160
H -1.6237320 5.4240580 -0.0956770
H -3.4549400 4.2114800 -1.2681200
Cl -0.3180510 0.8272240 -3.4401970
C 1.1845320 0.8979170 3.2166670
H 0.2280070 0.5547290 2.8220350
H 1.7179650 0.0060840 3.5641870
H 0.9813140 1.5230340 4.0913930
C 3.7809080 5.0662550 2.2587530
H 3.1188160 5.5109790 3.0091220
H 4.7730860 4.9645840 2.7189520
H 3.8804870 5.7754800 1.4299290
C 4.6663840 -0.5692700 1.4375610
H 4.9491680 0.4585930 1.1862600
H 3.8664370 -0.4968730 2.1760350
H 5.5279370 -1.0381740 1.9239240
C 6.2095990 -3.8366780 -2.0081620
H 6.6831810 -3.3366110 -2.8635110
H 6.9909240 -4.0213360 -1.2636590
H 5.8421470 -4.8053760 -2.3644970

(L18)Ni(Ph)(O^{t}Bu)



Zero-point correction= 0.794502 (Hartree/Particle)
Thermal correction to Energy= 0.841460
Thermal correction to Enthalpy= 0.842404
Thermal correction to Gibbs Free Energy= 0.716909
Sum of electronic and zero-point Energies= -4044.358344
Sum of electronic and thermal Energies= -4044.311386
Sum of electronic and thermal Enthalpies= -4044.310441
Sum of electronic and thermal Free Energies= -4044.435936

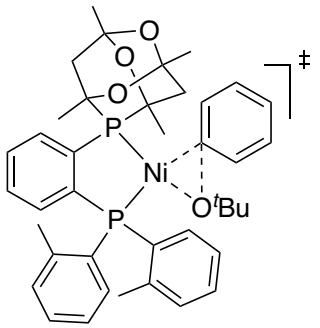
Single-point energy (6-311+G(2d,2p)) = -4.045962525877E+03

Ni 0.2920430 1.0226070 -0.0110670
P -1.3191730 -0.4521340 -0.3824800
P 1.6902530 -0.8000130 0.0104630
C -0.9067260 2.4972220 0.0334950
C -1.2350930 3.2625220 -1.0963770
C -1.4987750 2.8619840 1.2545130
C -0.5220390 -1.9043810 -1.2337000
C 0.8740610 -2.0330760 -1.0727320
C -2.9207740 -0.1299120 -1.3686850
C -2.2850670 -1.1291030 1.1235740
C 1.9909840 -1.7274390 1.5803490
C 3.3507820 -0.5581270 -0.7228120
C -2.1192590 4.3450840 -1.0175290
C -2.3776690 3.9462610 1.3445070
H -1.2801430 2.2910550 2.1537130
O -3.6986690 -1.3471390 -1.4721820
O -3.1422780 -0.0638060 1.5706990
C 1.5775630 -3.0287400 -1.7622090
C -1.1843560 -2.8122240 -2.0787270
C -3.1457100 -2.3243370 0.7045850
C -3.7621660 0.8891450 -0.5949040
C -2.6268760 0.3180400 -2.7917700
C -1.3752700 -1.4507790 2.2937730
C 2.1940790 -1.0288900 2.7932320
C 1.9845630 -3.1315970 1.5849410
C 3.4767660 0.0287480 -2.0048770
C 4.4975900 -0.8940020 0.0069970
H -2.3520080 4.9191810 -1.9120250
C -2.6971270 4.6910800 0.2055070
H -2.8123000 4.2097630 2.3067630
H 2.6563870 -3.0929420 -1.6510030
C 0.9080480 -3.9135220 -2.6048430
C -0.4748760 -3.8040680 -2.7560970
H -2.2524080 -2.7251980 -2.2259800
C -4.2528040 -1.8681310 -0.2551800
H -2.5328340 -3.1060250 0.2477680
H -3.6231260 -2.7421890 1.5987550
H -4.6421910 1.1293580 -1.2031870
H -3.2059970 1.8044810 -0.4089010
C -4.2462930 0.2830700 0.7246040
H -3.5720350 0.4611410 -3.3275640
H -2.0315290 -0.4229510 -3.3327590
H -2.0834260 1.2657620 -2.7772090
H -1.9880300 -1.7408730 3.1548350
H -0.7788240 -0.5778690 2.5698190

H -0.6979460 -2.2734500 2.0510350
C 2.3950950 -1.7766000 3.9621020
C 2.1758350 -3.8535080 2.7616290
H 1.8205510 -3.6732970 0.6606400
C 2.1706900 0.4753740 2.8850600
C 4.7651390 0.2436070 -2.5053940
H 4.3970700 -1.3340610 0.9932560
C 2.2837700 0.4341570 -2.8348650
H -3.3837300 5.5310000 0.2718470
C 5.7724770 -0.6604920 -0.5098740
O -5.0226300 -0.8790460 0.4160090
H 1.4617530 -4.6776310 -3.1433360
H -1.0069720 -4.4839670 -3.4159450
C -5.1973480 -2.9805620 -0.6633390
C -5.1243810 1.2164720 1.5294710
H 2.5567360 -1.2442140 4.8961580
C 2.3843230 -3.1696320 3.9583160
H 2.1643840 -4.9396430 2.7386300
H 2.6417390 0.9673070 2.0313980
H 2.6545390 0.8109400 3.8081100
H 1.1384650 0.8504980 2.8953150
H 4.8731930 0.6968640 -3.4876960
H 1.6243210 1.0907320 -2.2563900
H 1.6959470 -0.4324860 -3.1601670
H 2.6045210 0.9742160 -3.7310830
C 5.9053220 -0.0907310 -1.7732310
H 6.6497840 -0.9213520 0.0752890
H -5.9633740 -2.5797140 -1.3320390
H -5.6807770 -3.4012500 0.2224990
H -4.6480390 -3.7723900 -1.1815170
H -5.4396680 0.7183050 2.4501070
H -6.0095610 1.4862840 0.9468550
H -4.5658650 2.1222770 1.7764710
H 2.5374840 -3.7161930 4.8849550
H 6.8908120 0.0999510 -2.1894890
H -0.7919600 3.0206470 -2.0600960
O 1.8671110 1.9816020 0.1289330
C 2.3594980 3.3038420 0.1721310
C 2.1170130 4.0492690 -1.1541120
H 2.5105160 3.4600010 -1.9906290
H 1.0513450 4.2190930 -1.3178830
H 2.6205960 5.0247980 -1.1581860
C 1.7734100 4.1081420 1.3468730
H 1.9116350 3.5555640 2.2837510
H 2.2731900 5.0805050 1.4472300
H 0.7050360 4.2841340 1.2108100

C 3.8848150 3.1582060 0.3762320
H 4.3168850 2.5595630 -0.4323030
H 4.3826850 4.1363180 0.3941120
H 4.0961870 2.6500810 1.3239240

(L18)Ni(Ph)(O^{t}Bu) C-O reductive elimination transition state



Zero-point correction= 0.793473 (Hartree/Particle)
Thermal correction to Energy= 0.839592
Thermal correction to Enthalpy= 0.840536
Thermal correction to Gibbs Free Energy= 0.717968
Sum of electronic and zero-point Energies= -4044.315149
Sum of electronic and thermal Energies= -4044.269030
Sum of electronic and thermal Enthalpies= -4044.268086
Sum of electronic and thermal Free Energies= -4044.390654

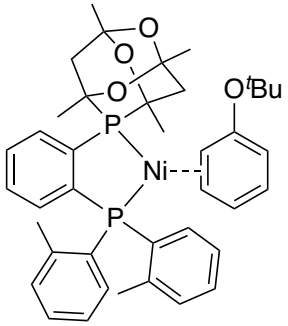
Single-point energy (6-311+G(2d,2p)) = -4.045919005106E+03

Ni 0.2352760 0.9365360 0.0961330
P -1.2772930 -0.5428550 -0.3647230
P 1.7758720 -0.7677960 0.0268480
C -0.6765460 2.6629810 0.1874330
C -1.0723810 3.2582340 -1.0458850
C -1.4445540 2.9940660 1.3455320
C -0.4226610 -1.9413630 -1.2315160
C 0.9797390 -2.0090320 -1.0760890
C -2.8608160 -0.2171060 -1.3561110
C -2.2398970 -1.2866260 1.1062400
C 2.1195560 -1.7366560 1.5655590
C 3.4225670 -0.4971710 -0.7399480
C -2.1575030 4.1348690 -1.0997840
C -2.5154390 3.8700680 1.2627880
H -1.1711260 2.5519820 2.2991010
O -3.6573090 -1.4182550 -1.5051970
O -3.0936460 -0.2374040 1.5989110
C 1.7180130 -2.9680780 -1.7818390
C -1.0495780 -2.8593750 -2.0919510

C -3.1094550 -2.4595190 0.6452040
C -3.6688940 0.7988670 -0.5415120
C -2.5551100 0.2826980 -2.7588230
C -1.3229470 -1.6547650 2.2576350
C 2.3391070 -1.0630050 2.7905690
C 2.0814430 -3.1403230 1.5543930
C 3.5044570 0.0651450 -2.0385420
C 4.5982320 -0.7176450 -0.0061180
H -2.4365690 4.5597300 -2.0627290
C -2.8898040 4.4629940 0.0434640
H -3.0713030 4.1040250 2.1692140
H 2.7988660 -2.9956590 -1.6729430
C 1.0824570 -3.8681440 -2.6351520
C -0.3040630 -3.8116800 -2.7865590
H -2.1215470 -2.8073960 -2.2358340
C -4.2128520 -1.9639770 -0.3018220
H -2.5017090 -3.2295130 0.1617900
H -3.5921930 -2.9056680 1.5230080
H -4.5361510 1.1078090 -1.1368940
H -3.0733260 1.6823800 -0.3143890
C -4.1796320 0.1561960 0.7514950
H -3.4949280 0.4487190 -3.2978700
H -1.9556170 -0.4385560 -3.3223400
H -2.0115520 1.2297470 -2.6990210
H -1.9272140 -1.9866270 3.1098710
H -0.7291130 -0.7900550 2.5659080
H -0.6411200 -2.4613230 1.9745850
C 2.5066440 -1.8269680 3.9531660
C 2.2503930 -3.8812470 2.7231470
H 1.9034590 -3.6667300 0.6241320
C 2.4172800 0.4391970 2.8841270
C 4.7697810 0.3835190 -2.5449420
H 4.5348460 -1.1544130 0.9855590
C 2.2854910 0.3054400 -2.9005600
H -3.7264830 5.1525110 -0.0072100
C 5.8475210 -0.3877950 -0.5309760
O -4.9714840 -0.9835390 0.3954740
H 1.6659210 -4.6038130 -3.1820530
H -0.8085940 -4.5029410 -3.4563380
C -5.1713090 -3.0553830 -0.7344890
C -5.0545390 1.0737580 1.5775460
H 2.6704530 -1.3104170 4.8956760
C 2.4613250 -3.2195440 3.9313350
H 2.2117230 -4.9664330 2.6857600
H 3.3185670 0.8213190 2.3919020
H 2.4505480 0.7613610 3.9295480

H 1.5690960 0.9331610 2.3986130
H 4.8391940 0.8173410 -3.5397980
H 1.4404700 0.6956760 -2.3193720
H 1.9422330 -0.6213930 -3.3756140
H 2.5104320 1.0252150 -3.6937230
C 5.9335030 0.1663250 -1.8070650
H 6.7447450 -0.5656450 0.0554690
H -5.9356550 -2.6286490 -1.3890070
H -5.6555500 -3.4947990 0.1418420
H -4.6324700 -3.8384420 -1.2766170
H -5.3899960 0.5467900 2.4748590
H -5.9270100 1.3793190 0.9935140
H -4.4848720 1.9602630 1.8640210
H 2.5873110 -3.7815540 4.8527540
H 6.8995590 0.4316670 -2.2275950
H -0.5478370 3.0032590 -1.9608630
O 0.9308180 2.6252600 0.6031960
C 1.8759990 3.6429150 0.1870620
C 2.2188030 3.5797830 -1.3050570
H 2.6021470 2.5906970 -1.5658030
H 1.3557180 3.8082060 -1.9318570
H 3.0020880 4.3131620 -1.5327280
C 1.3033760 5.0147490 0.5704070
H 1.0537720 5.0344410 1.6359510
H 2.0433710 5.7988050 0.3711600
H 0.3977430 5.2404300 0.0031300
C 3.1438760 3.3502340 0.9997520
H 3.5585210 2.3750140 0.7258800
H 3.9062790 4.1131120 0.8008550
H 2.9219370 3.3523040 2.0711410

(L18)Ni(η^2-PhO^{t}Bu)



Zero-point correction= 0.795019 (Hartree/Particle)
Thermal correction to Energy= 0.841631
Thermal correction to Enthalpy= 0.842575
Thermal correction to Gibbs Free Energy= 0.718760

Sum of electronic and zero-point Energies= -4044.353989
Sum of electronic and thermal Energies= -4044.307377
Sum of electronic and thermal Enthalpies= -4044.306433
Sum of electronic and thermal Free Energies= -4044.430248

Single-point energy (6-311+G(2d,2p)) = -4.045956831762E+03

Ni 0.2274010 0.7594860 -0.5656630
P -1.4945620 -0.4928460 -0.1400900
P 1.5813990 -0.7634020 0.2301440
C -0.8412600 -2.2130250 0.0524120
C 0.5497950 -2.3157900 0.2667640
C -3.0125030 -0.6261750 -1.2711810
C -2.5724970 -0.1701460 1.4006370
C 2.1863370 -0.6031430 1.9697290
C 3.0308670 -1.4084330 -0.7199490
O -4.0143970 -1.5601180 -0.7982170
O -3.2348920 1.0915470 1.1459210
C 1.1380230 -3.5805050 0.4037990
C -1.6031050 -3.3894900 -0.0556440
C -3.6409260 -1.2481480 1.5979520
C -3.6326400 0.7791760 -1.2577910
C -2.6250550 -1.0844010 -2.6679180
C -1.7314280 0.0148550 2.6503790
C 3.0934620 0.4276860 2.3266560
C 1.6494190 -1.4174770 2.9799150
C 2.8834740 -1.6546240 -2.1066980
C 4.2682980 -1.6524150 -0.1067790
H 2.2104050 -3.6571930 0.5574840
C 0.3684680 -4.7389340 0.3171140
C -1.0031180 -4.6413160 0.0742310
H -2.6627720 -3.3217170 -0.2707950
C -4.6464400 -1.2309820 0.4408730
H -3.1811020 -2.2348980 1.6946840
H -4.1871150 -1.0349120 2.5249740
H -4.4382550 0.8202890 -2.0006760
H -2.8836550 1.5317390 -1.5101100
C -4.2369540 1.0795570 0.1222820
H -3.5088190 -1.0861250 -3.3168640
H -2.2118740 -2.0973070 -2.6453160
H -1.8716150 -0.4124140 -3.0890560
H -2.3743760 0.3154190 3.4861020
H -0.9647720 0.7764810 2.5043230
H -1.2336390 -0.9237590 2.9118190
C 3.4177400 0.5902740 3.6799900
C 1.9819380 -1.2318440 4.3214570

H 0.9602290 -2.2117170 2.7167390
C 3.7273240 1.3436370 1.3093820
C 4.0023850 -2.0890480 -2.8281750
H 4.3732290 -1.5028390 0.9630990
C 1.5560190 -1.5333350 -2.8133350
C 5.3677980 -2.0930130 -0.8432950
O -5.2183830 0.0767100 0.3884300
H 0.8396840 -5.7127190 0.4203080
H -1.6064850 -5.5401890 -0.0221820
C -5.7880490 -2.2123060 0.6134130
C -4.9318630 2.4237670 0.1955240
H 4.1167320 1.3768420 3.9543230
C 2.8712320 -0.2197700 4.6747350
H 1.5479600 -1.8773060 5.0803460
H 4.3990470 0.8011350 0.6352550
H 4.3163180 2.1200210 1.8079570
H 2.9770770 1.8405750 0.6892230
H 3.8950670 -2.2713250 -3.8950030
H 1.0276270 -0.6132180 -2.5415310
H 0.8970550 -2.3724320 -2.5554960
H 1.6918910 -1.5357670 -3.8990990
C 5.2365390 -2.3012930 -2.2150010
H 6.3170330 -2.2709720 -0.3450140
H -6.4717050 -2.1277120 -0.2352770
H -6.3329560 -1.9930300 1.5356450
H -5.4014500 -3.2348350 0.6596780
H -5.3628230 2.5566720 1.1912100
H -5.7299440 2.4747160 -0.5500620
H -4.2120050 3.2259750 0.0085440
H 3.1415100 -0.0603920 5.7151360
H 6.0856900 -2.6360700 -2.8048250
C -0.2724900 2.3955990 -1.6539490
C 1.1060700 2.5145310 -1.2510210
C 2.1269630 2.2062420 -2.2117290
C 1.8220020 1.8283410 -3.4946720
C 0.4645200 1.7681710 -3.9182040
C -0.5388310 2.0614640 -3.0281260
H -1.0606200 2.8984040 -1.1075750
H 3.1576780 2.3262920 -1.8916510
H 2.6209320 1.5963540 -4.1931860
H 0.2277910 1.5176310 -4.9486190
H -1.5725020 2.0789910 -3.3659550
O 1.6055420 3.3069750 -0.2145340
C 0.8164290 4.0587830 0.7407070
C 1.8905120 4.6783590 1.6457770
H 2.5826670 5.2856730 1.0540420

H 1.4260550 5.3162370 2.4053660
H 2.4628110 3.8962720 2.1526890
C 0.0359870 5.1868540 0.0473170
H 0.7143870 5.7834660 -0.5713600
H -0.7691070 4.8190420 -0.5912320
H -0.4102420 5.8445670 0.8019450
C -0.0819450 3.1403370 1.5768140
H -0.8755960 2.6670180 0.9945900
H 0.5250240 2.3510900 2.0323290
H -0.5582100 3.7130200 2.3816640

APPENDIX C. Copyright Information for Published Work

Reference: Lavoie, C.M.; MacQueen, P.M.; Rotta-Loria, N.L.; Sawatzky, R.S.; Chisholm, A.J.; Hargreaves, B.K.V.; McDonald, R.; Ferguson, M.J.; Stradiotto, M., Challenging Nickel-catalysed Amine Arylations Enabled by Tailored Ancillary Ligand Design *Nat*. *Commun*. **2016**, *7*, 11073.

Reference: Lavoie, C.M.; MacQueen, P.M.; M.J.; Stradiotto, M., Nickel-Catalyzed *N*-Arylation of Primary Amides and Lactams with Activated (Hetero)aryl Electrophiles. *Chem. Eur. J.* **2016**, *22*, 18572-18575.

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Reference: Lavoie, C.M.; Tassone, J.P.; Ferguson, M.J.; Zhou, Y.; Johnson, E.R.; Stradiotto, M. Probing the Influence of PAd-DalPhos Ancillary Ligand Structure on Nickel-Catalyzed Ammonia Cross-Coupling. *ACS Catalysis.* **2018**, 4015-4023.

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