Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information:

Mechanistic Implications of an Asymmetric Intermediate in Catalytic C—C Coupling by a Dinuclear Nickel Complex

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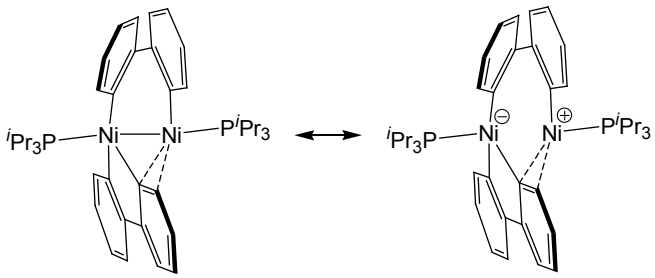
Contents:

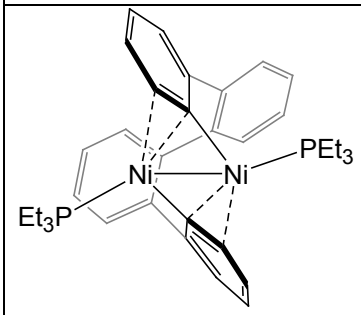
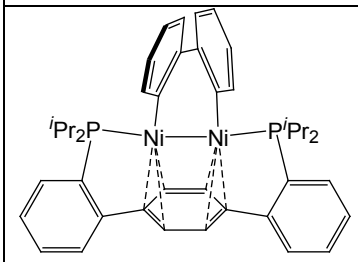
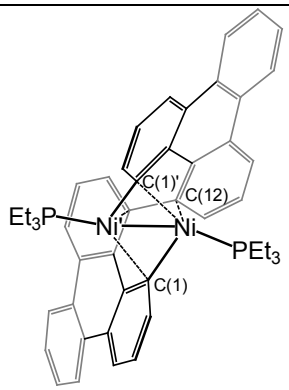
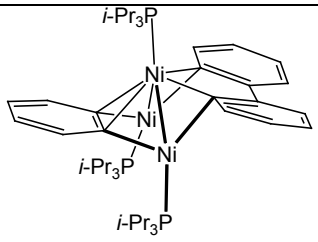
Lewis Structures of 4$^{i\text{-Pr}}$.



Ni(III)–Ni(I) Ni(II)–Ni(II)

These depictions of **4**$^{i\text{-Pr}}$ feature two extremes of electron assignment. The structure on the left displays the electrons in the Ni(III)-Ni(I) bond as covalently shared. The structure on the right shows the extreme limit of polarization of the nickel-nickel bond, where the electrons in this bond are assigned to the anionic nickel centre.

Table S1. Comparison of bond lengths to Ni(I) centres in $\mathbf{3}^{i\text{-Pr}}$ and $\mathbf{4}^{i\text{-Pr}}$ with related Ni(I) complexes

Compound	Ni-C σ-bond length(s) (Å)	Short Ni-C π-bond length(s) (Å)	Long Ni-C π-bond length(s) (Å)	Reference
	1.97(2) 1.89(2) 1.91(2) 1.87(1)	1.99(1) 1.93(1) 2.03(2) 2.01(2)	2.23(2) 2.25(2) 2.26(2) 2.27(2)	[a]
	1.9154(10) 1.9141(10)	1.9852(10) 2.0013(10) 2.0630(10) 2.0589(9)	2.2964(10) 2.2067(10)	[b]
	1.929(3)	2.055(3) Ni-C(1)′ 2.118(3) Ni-C(12)	2.234(3) 2.300(3)	
$\mathbf{3}^{i\text{-Pr}}$	1.930(3) 1.919(3)	1.970(3) 2.006(3)	2.265(3) 2.302(3)	[d]
$\mathbf{4}^{i\text{-Pr}}$	1.915(3)	1.941(3)	2.388(3)	[d]
	1.935(2) 1.918(2)	1.955(2) 1.952(2)		[e]

[a] J. J. Eisch, A. M. Piotrowski, K. I. Han, C. Kruger and Y. H. Tsay, *Organometallics*, 1985, **4**, 224-231; two molecules in asymmetric unit, and relatively large errors in bond lengths. [b] A. Velian, S. Lin, A. J. M. Miller, M. W. Day and T. Agapie, *J. Am. Chem. Soc.*, 2010, **132**, 6296-6297. [c] T. V. V. Ramakrishna and P. R. Sharp, *Organometallics*, 2004, **23**, 3079-3081. [d] this work. [e] M. A. Bennett, K. D. Griffiths, T. Okano, V. Parthasarathi and G. B. Robertson, *J. Am. Chem. Soc.*, 1990, **112**, 7047-7048.

General Procedures. Unless otherwise stated, all manipulations were performed under an inert atmosphere of nitrogen using either standard Schlenk techniques or an MBraun glovebox. Dry, oxygen-free solvents were employed throughout. Anhydrous pentane, toluene, and THF were purchased from Aldrich, sparged with dinitrogen, and passed through activated alumina under a positive pressure of nitrogen gas; toluene and hexanes were further deoxygenated using a Grubbs' type column system.[1] Benzene-d_6 was dried by heating at reflux with Na/K alloy in a sealed vessel under partial pressure then trap-to-trap distilled and freeze-pump-thaw degassed three times. Toluene-d_8 was purified in an analogous manner by heating at reflux over Na. THF-d_8 was purified in an analogous manner by heating at reflux over K. ^{1}H, ^{31}P{^{1}H} and ^{13}C{^{1}H}NMR spectra were recorded on a Bruker AMX Spectrometer operating at 300 MHz or 500 MHz with respect to proton nuclei. All chemical shifts are recorded in parts per million, and all coupling constants are reported in hertz. ^{1}H NMR spectra were referenced to residual protons (C_6D_5H, δ 7.16; C_7D_7H, δ 2.09; C_4D_7HO, δ 1.73) with respect to tetramethylsilane at δ 0.00. ^{31}P{^{1}H} NMR spectra were referenced to external 85% H_3PO_4 at δ 0.00. ^{13}C{^{1}H} NMR spectra were referenced relative to solvent resonances (C_6D_6, δ 128.0; C_7D_8, δ 20.4; C_4D_8O, δ 25.37). Infrared spectra (IR) were recorded on a Bruker *Tensor 27* operating from 4000 – 400 cm^{-1}. High Resolution Mass Spectroscopy (HRMS) was performed at McMaster University, Hamilton, Ontario, Canada. Elemental analyses were performed at the Center for Catalysis and Materials Research, Windsor, Ontario. The compounds benzene-d_6, toluene-d_8, and THF-d_8 were purchased from Cambridge Isotope Laboratory. Biphenylene[2] and Ni(COD)$_2$[3] (COD = 1,5 cyclooctadiene) were synthesized according literature methods. Triisopropylphosphine was purchased from STREM and *tert.*-Butyllithium from Aldrich. Both were used without further purification.

Synthesis of monodeuterated-Biphenylene (1-d_1). To a stirred solution of biphenylene (2.43 mmol, 370 mg) in the presence of (TMEDA) tetramethylethylenediamine (2.92 mmol, 340 mg) in 100 mL Et_2O at –80 °C, a solution *tert.*-Butyllithium (1.7 M) (3.16 mmol, 1.8 mL) was added dropwise over the

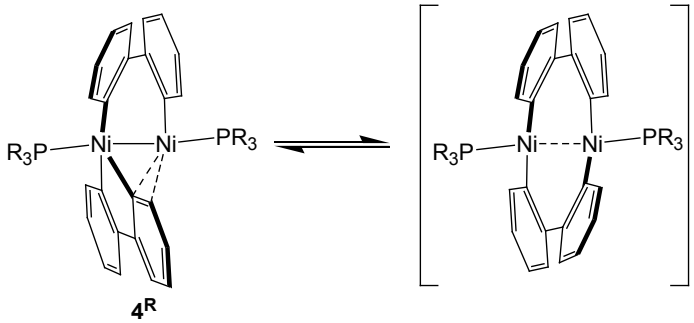
course of 30 min. The solution was then slowly warmed to room temperature and the progress of the reaction was monitored every 8 h by quenching an aliquot with D_2O and analyzing by mass spectrometry. Additional *tert.*-Butyllithium (1.7 M) (1.21 mmol, 0.71 mL) was added after 20 h. After 3 d the reaction mixture was quenched by D_2O and all volatiles were removed under vacuum, and the residue was extracted with 50 mL of pentane and filtered through silica gel (mesh 70-230, 60 Å). The pentane was removed under vacuum which afforded a yellow oil. The oil was taken up in 5 mL pentane and cooled to 5 °C to provide pale yellow crystals of deuterated biphenylene (127 mg, 34% yield). Mass spectrometry revealed a 85 % conversion to **1-*d*$_1$**, with 11.5 % **1** and 3.0 % **1-*d*$_2$**, as minor impurities, which is consistent with the observed integrals observed in the ^{1}H NMR spectrum. ^{1}H NMR (C_6D_6, 300 K, 300 MHz): δ 6.41 (m, 3.1H, 1-Ar-H), 6.50 (m, 4H, 2-Ar-H).

Synthesis of 4$^{i\text{-Pr}}$. To an ice cold suspension of $Ni(COD)_2$ (108 mg, 0.39 mmol) in 5 mL pentane, an excess of triisopropylphosphine (113 mg, 0.70 mmol) was added. After stirring for 5 minutes a cold solution of biphenylene (41 mg, 0.27 mmol) dissolved in 1 mL cold pentane was added dropwise, changing the color immediately from yellow to brown and stirred for additional 30 min. At –34 °C brown plates of **4$^{i\text{-Pr}}$** were isolated suitable for X-ray diffraction. Yield (49 mg, 30 - 34%). ^{1}H NMR (C_6D_6, 300 MHz, 298 K): δ 0.51 (dd, ^{3}J(H,H) = 11.4 Hz, ^{3}J(P,H) = 6.9 Hz, 18H, P(CH(C*H*$_3$)$_2$)$_3$); 0.79 (dd, ^{3}J(H,H) = 11.4 Hz, ^{3}J(P,H) = 6.9 Hz, 18H, P(CH(C*H*$_3$)$_2$)$_3$); 1.29 (6H, m, P(C*H*(CH$_3$)$_2$)$_3$), 6.75 (s(br), 4H, Ar-H), Ar-H), 7.02 (dd, apparent triplet, ^{3}J(H,H) = 7.5 Hz, 4H, Ar-H), 7.10 (m, 4H, Ar-H), 7.45 (dd, ^{3}J(H,H) = 7.5 Hz, ^{4}J(H,H) = 1.0 Hz, Ar-H). ^{31}P{^{1}H} NMR (C_6D_6, 121.5 MHz, 298 K): δ 30.6 (s(br), $W_{1/2}$ = 1200 Hz, 2P, NiP^{i}Pr$_3$). ^{13}C{^{1}H} NMR (C_7D_8, 75.5 MHz, 298 K): δ 20.4 (m, P(CH(*C*H$_3$)$_2$)$_3$), 23.2 (d, ^{1}J(P,C) = 16.0 Hz, P(*C*H(CH$_3$)$_2$)$_3$), 23.3 (119.8 (s, C-H), 123.9 (s, C-H), 126.2 (s, C-H), 151.5 (s, C-H); 154.2 (s, C); 162.2 (m(br), Ni-C). ^{31}P{^{1}H} NMR (C_7D_8, 121.5 MHz, 298 K): δ 20 – 35 (s(vbr), 2P, NiP^{i}Pr$_3$); ^{31}P{^{1}H} NMR (C_7D_8, 121.5 MHz, 233 K): δ 20.4 (d, ^{3}J(P,P) = 24.3 Hz, 1P, NiP^{i}Pr$_3$), 40.2 (d, ^{3}J(P,P) = 24.3 Hz, 1P, NiP^{i}Pr$_3$). IR (Nujol, KBr): 3034 m, 1924 w, 1889, 1570 m,

1557 m, 1278 s, 1236 m, 1154 m, 1092 s, 1060 m, 1028 m, 1010 m, 963 m, 929 m, 883 s, 850 w, 771 w, 735 vs, 653 vs, 600 m, 573 m, 525 s, 481 w, 433 w, cm^{-1}. Anal Calcd. for $C_{42}H_{58}Ni_2P_2$ (742.24): C, 67.96; H, 7.88; Found: C, 67.69; H, 7.51.

Variable Temperature $^{31}P\{^1H\}$ NMR study of $4^{i\text{-Pr}}$. The exchange of ^{31}P environments in $4^{i\text{-Pr}}$ is proposed to occur by the fluctional process depicted in Scheme S1. The π-interaction with the formally Ni(I) centre converts to a σ-bonding interaction. The symmetry of the intermediate is consistent with the observation of four aromatic proton environments in $4^{i\text{-Pr}}$ at room temperature, but two diastereotopic Me environments on the phosphine donors, even at temperatures where there is rapid exchange.

Scheme S1. Proposed intermediate in the fluxionality observed in the solution NMR spectrum of $4^{i\text{-Pr}}$.



4^R

Ni(III)–Ni(I) point group: D_2

The modeled variable-temperature $^{31}P\{^1H\}$ NMR spectra are shown in Figure S1, from 233 to 293 K. An Arrhenius plot, as shown in Figure S2, provided activation energy of E_a = 8.1 kcal·mol^{-1} (263 -293 K) for this process.

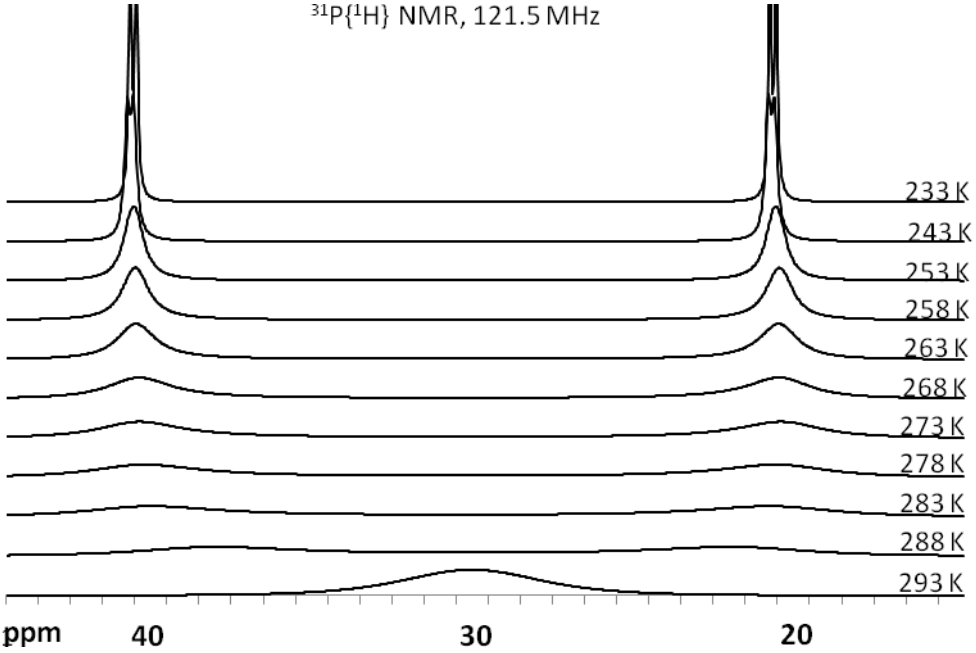


Figure S1. Stacked VT $^{31}P\{^{1}H\}$ NMR spectra of proposed fluxionality of $\mathbf{4}^{i\text{-Pr}}$.

Table S2. Sample rate constants at various temperatures measured for compound $\mathbf{4}^{i\text{-Pr}}$

$k_{ab}/(sec^{-1})$	T/(K)	ln(k/T)	lnk	$1/T\cdot(10^{-3}\ K^{-1})$
2777	293	2.25	7.93	3.41
2252	288	2.06	7.72	3.47
1815	283	1.86	7.50	3.53
1484	278	1.67	7.30	3.60
1129	273	1.42	7.02	3.66
765	268	1.04	6.63	3.73
562	263	0.75	6.33	3.80
379	258	0.38	5.93	3.88
212	253	-0.17	5.35	3.95
51	243	-1.56	3.93	4.11
7	233	-3.50	1.94	4.29

[a]Rate constants obtained by computer simulations using the program WINDMR[12]

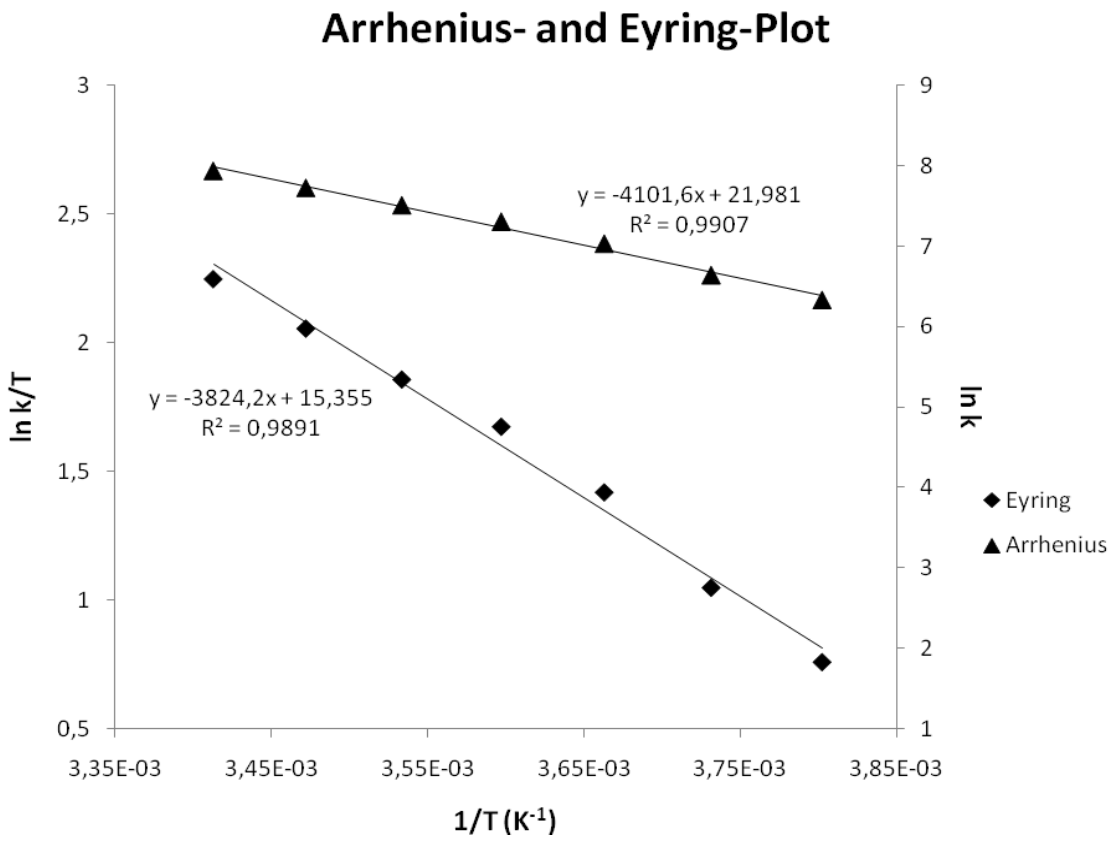
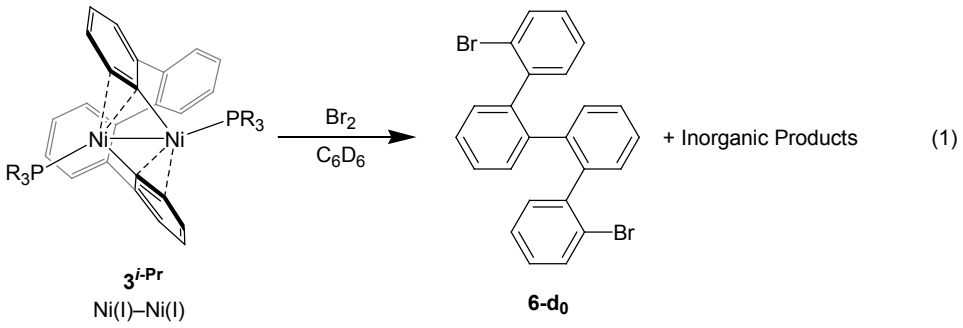


Figure S2. Standard Arrhenius- and Eyring-Plot of $\mathbf{4}^{\mathbf{i\text{-}Pr}}$; E_a = 8.1 kcal·mol^{-1}, $\Delta G^{\ddagger}_{293\ K}$ = 12.4 kcal·mol^{-1}, $\Delta H^{\ddagger}$ = 7.6 kcal·mol^{-1}, $\Delta S^{\ddagger}$ = -16.5 cal·mol^{-1}·K^{-1} (263 - 293 K)

Synthesis of $\mathbf{3}^{\mathbf{i\text{-}Pr}}$. One equivalent of triisopropylphosphine (65 mg 0.41 mmol) was added to a solution of Ni(COD)$_2$ (112 mg, 0.41 mmol) in 5 mL toluene at room temperature. After stirring for 5 minutes, biphenylene (62 mg, 0.41 mmol) dissolved in 1 mL toluene was added. Over the course of 20 h the solution turned green and the volatiles were removed in vacuum and the residue was extracted with pentane (2 × 10 mL). Cooling the solution to –34 °C afforded dark green needles suitable for X-ray diffraction. The combined yield from two recrystallizations was 129 mg (86%). ^{1}H NMR (C_6D_6, 300 MHz, 298 K): δ 0.86 (dd, ^{3}J(H,H) = 7.2 Hz, ^{3}J(P,H) = 3.6 Hz, 18H, P(CH(C*H*$_3$)$_2$)$_3$); 0.88 (dd, ^{3}J(H,H) = 7.2 Hz, ^{3}J(P,H) = 3.6 Hz, 18H, P(CH(C*H*$_3$)$_2$)$_3$), 1.70 (sept, ^{3}J(H,H) = 7.5 Hz, 6H, P(C*H*(CH$_3$)$_2$)$_3$); 6.22 (dd, ^{3}J(H,H) = 7.0 Hz, ^{4}J(H,H) = 1.5 Hz, 2H, Ar-H); 6.64 (dd, ^{3}J(H,H) = 7.0 Hz, ^{4}J(H,H) = 1.5 Hz, 2H, Ar-H); 6.87 (dd, ^{3}J(H,H) = 7.0 Hz, ^{4}J(H,H) = 1.0 Hz, 2H, Ar-H); 7.02 (dd, ^{3}J(H,H) = 7.0 Hz, ^{4}J(H,H) =

1.5 Hz, 2H, Ar-H); 7.08 (dd, ^{3}J(H,H) = 7.5 Hz, ^{4}J(H,H) = 1.5 Hz, 2H, Ar-H); 7.10 – 7.13 (m, 6H, Ar-H); 7.33 (dd, ^{3}J(H,H) = 7.5 Hz, ^{4}J(H,H) = 1.5 Hz, 2H, Ar-H). ^{13}C{^{1}H} NMR (C_6D_6, 75.5 MHz, 298 K): δ 19.9 (d, ^{2}J(P,C) = 13.3 Hz, P(CH(*C*H$_3$)$_2$)$_3$), 20.7 (d, ^{2}J(P,C) = 13.4 Hz, P(CH(*C*H$_3$)$_2$)$_3$), 21.7 (d, ^{2}J(P,C) = 18.5 Hz, P(CH(*C*H$_3$)$_2$)$_3$), 23.9 (dvt, ^{1}J(P,C) = 15.3 Hz, ^{3}J(P,C) = 5.8 Hz, P(*C*H(CH$_3$)$_2$)$_3$), 108.2 (s, C-H), 120.1 (s, C-H), 121.5 (s, C-H), 125.3 (s, C-H), 126.5 (s,C-H), 129.8 (s, C-H), 131.3 (s, C-H), 133.9 (s, C-H), 142.9 (s, C), 145.3 (s, C), 152.6 (s, C), 173.1 (vt, ^{2}J(P,C) = 10.5 Hz, Ni-C). ^{31}P{^{1}H} NMR (C_6D_6, 121.5 MHz, 298 K): δ 43.6 (s, Ni*P*^{i}Pr$_3$). IR (Nujol, KBr): 3061 w, 1884 vw, 1805 vw, 1557 m, 1524 m, 1494 w, 1414 w, 1238 m, 1197 w, 1155 w, 1085 w, 1025 m, 1005 m, 979 m, 943 w, 913 m ,883m , 800 m, 755 s, 746 vs, 722 vs, 660 m, 637 m, 590 s, 565 w, 522 m, 474 m cm^{-1}. Anal Calcd. for $C_{42}H_{58}Ni_2P_2$ (742.24): C, 67.96; H, 7.88; Found: C, 68.35, H, 8.27.

Product Analysis by High resolution Mass Spectra (HRMS): To demonstrate that HRMS provided suitable accuracy to distinguish between mixtures of deuterated and non-deuterated products a test reaction was performed with only non-deuterated reagents. Approximately equimolar amounts of Ni(COD)$_2$ (27 mg, 0.1 mmol) and biphenylene (15 mg, 0.1 mmol) and two equivalents triisopropylphosphine (32 mg, 0.2 mmol) were dissolved in 1 mL C_6D_6, to generate **4$^{i\text{-Pr}}$** in situ. After 20 h, the reaction mixture contained the dinuclear Ni(I)-Ni(I) complex **3$^{i\text{-Pr}}$** as the exclusive organometallic complex, as analyzed by ^{31}P{^{1}H} NMR spectroscopy. The reaction was quenched by the direct addition of Br_2, as shown in equation 1.



The solution was passed through a plug of silica gel (mesh 70-230, 60 Å) and the volatiles were removed in vacuum. The residue was dissolved in 1 mL CH_2Cl_2 and purified by TLC (silica F-254) with a mixture of hexane/CH_2Cl_2 (10:1) R_f = 0.34. The HRMS isotope pattern of the 1,1′-dibromoquaterphenyl (**6-d_0**) obtained was identified by HRMS, and is compared with the theoretical isotope pattern. (Figure S3). The maximum difference between the theoretical isotope pattern and the pattern observed experimentally is 0.3 %.

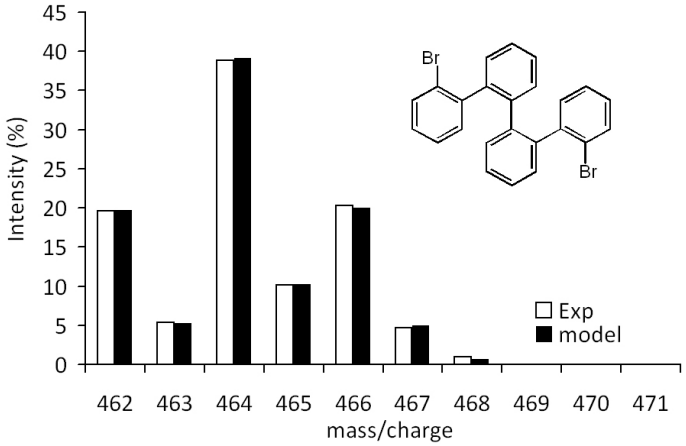


Figure S3. Experimental mass spectrum for 1,1′-Dibromoquaterphenyl **6-d_0** shown as white bars. Alongside in black bars is the theoretical mass spectrum, normalized so that the total intensity equals 100 %. Theoretical m/e: 462 (19.8%), 463 (5.3%), 464 (39.11%), 465 (10.3%), 466 (20.0%), 467 (5.0%), 468 (0.7%).

An additional experiment was performed in an identical manner, except after the in situ generation of **4$^{i\text{-Pr}}$** an equivalent of 85 % biphenylene-d_1 (15 mg, 0.1 mmol) was added. The mass spectrum obtained after bromination and workup was analogous to that shown in Figure S3, which confirms that **4$^{i\text{-Pr}}$** does not reversibly reductively-eliminate/oxidatively-add biphenylene.

An analogous experiment was performed using the primarily biphenylene-d_1 (**1-d_1**) sample to confirm the degree of deuteration. Approximately equimolar amounts of $Ni(COD)_2$ (27 mg, 0.1 mmol) and the biphenylene-d_1 (~85 % deuteration) (15 mg, 0.1 mmol) and two equivalents triisopropylphosphine (32 mg, 0.2 mmol) were dissolved in 1 mL C_6D_6, to generate **4$^{i\text{-Pr}}$-d_n** (n = 0-3) in

situ. After 20 h, the reaction mixture was quenched by the direct addition of Br_2. The sample of **6-d_n** (n = 0-3) was isolated in the same manner as **6-d_0**. The HRMS isotope pattern of (**6-d_n**) (n = 0-3) obtained was identified by HRMS, and is compared with a modeled isotope pattern. (Figure S4). The observed pattern corresponds to the sample of primarily **1-d_1** being composed of 11.5 % **1-d_0**, 85.5 % **1-d_1**, and 3.0 % **1-d_2**. The maximum difference between the theoretical isotope pattern and the experimental data is 0.3 %.

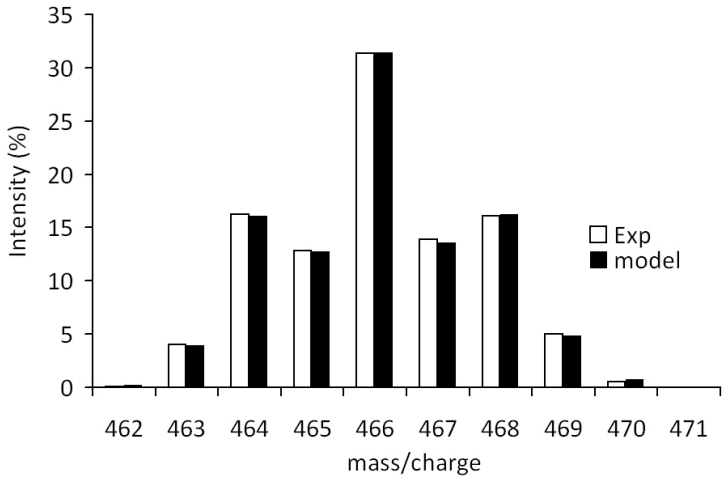


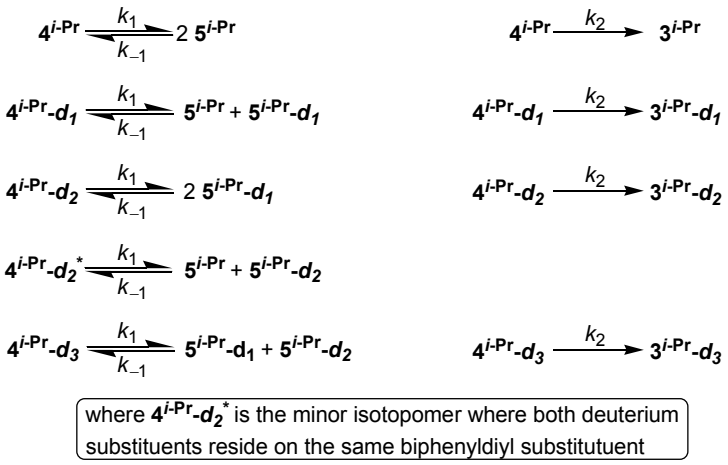
Figure S4. Experimental mass spectrum for 1,1´-Dibromoquaterphenyl **6-d_n** (n = 0-3) produced from **4$^{i\text{-}Pr}$-d_1** (~85% d_1) followed by bromination shown as white bars. The model spectrum shown as black bars was generated from the combination of theoretical spectra consistent with a mixture that is 1.3 % **6-d_0**, 19.7 % **6-d_1**, 74.0 % **6-d_2**, and 5.0 % **6-d_3**. This corresponds to the sample of primarily **1-d_1** being composed of 11.5 % **1-d_0**, 85.5 % **1-d_1**, and 3.0 % **1-d_2**.

Deuterium Labeling Cross-Over Experiment. Approximately equimolar amounts of $Ni(COD)_2$ (27 mg, 0.1 mmol) and biphenylene (15 mg, 0.1 mmol) and two equivalents triisopropylphosphine (32 mg, 0.2 mmol) were dissolved in 1 mL C_6D_6, to generate **4$^{i\text{-}Pr}$** in situ. At the same time a sample was prepared in the analogous manner except using the biphenylene-d_1 (~85% d_1). The samples were combined immediately. After 20 h, the reaction mixture was quenched by the direct addition of Br_2.

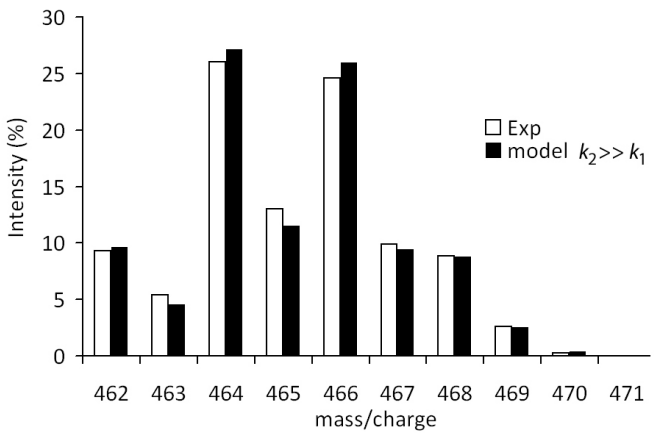
The sample of **6-d_n** (n = 0-3) was isolated in the same manner as **6-d_0**. The HRMS isotope pattern of (**6-d_n**) (n = 0-3) obtained was identified by HRMS.

The possible competing reactions in this cross-over experiment are the reversible equilibria between **4$^{i\text{-Pr}}$-d_n** (n = 0-3) and **5$^{i\text{-Pr}}$-d_n** (n = 0-2) shown on the left of Scheme S2, and the irreversible conversion of **4$^{i\text{-Pr}}$-d_n** to **3$^{i\text{-Pr}}$-d_n**.

Scheme S2.



The experimental isotope pattern can be compared to those predicted if k_2 is much larger than k_1 (i.e. conversion to **3$^{i\text{-Pr}}$** is much faster than to **5$^{i\text{-Pr}}$**), and conversely where k_1 is much larger than k_2. These model isotope patterns are compared to the experimental data in Figure S5. The assumption that k_2 is larger than k_1 provides a much better fit, which demonstrates that the dinuclear species **4$^{i\text{-Pr}}$** does not convert to **3$^{i\text{-Pr}}$** via a mononuclear intermediate such as **5$^{i\text{-Pr}}$**. The value of k_{-1} was assumed to be at least 100 times greater than k_1, but the exact value had no observable effect on the product ratios.



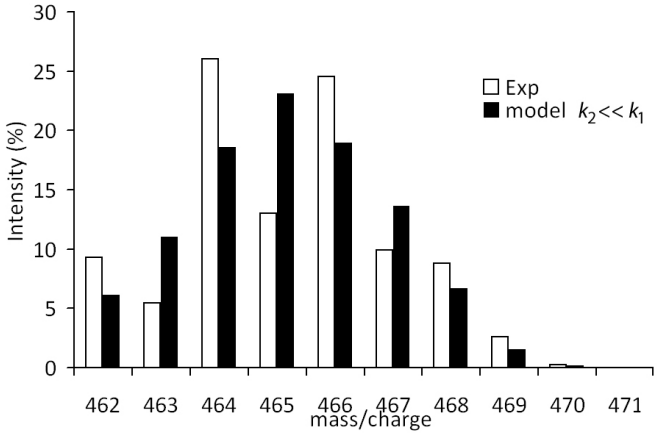


Figure S5. Experimental mass spectrum for the mixture of isotopomers of 1,1′-Dibromoquaterphenyl **6-d_n** (n= 0 to 3) shown as white bars obtained from the cross-over experiment performed with **4$^{i\text{-Pr}}$-d_0** and **4$^{i\text{-Pr}}$-d_1** (~85% d_1), followed by quenching with Br_2. The left spectrum includes a model where no exchange occurs from **4$^{i\text{-Pr}}$-d_n**. The model included on the right involves rapid scrambling *via* the mononuclear **5$^{i\text{-Pr}}$-d_n**. The largest error in the fit shown on the left of Figure S5 is 1.5 %.

Catalytic Conversion of Biphenylene to Tetraphenylene: Biphenylene (15 mg, 0.0986 mmol), $Ni(COD)_2$ (2 mg, 0.0072 mmol, 7.3 mol %) and *i*-Pr_3P (4 mg, 0.025 mmol) were dissolved in ca. 0.7 ml d_8-toluene. After heating at 90 °C for 16 h, the green solution was analyzed by ^{1}H NMR spectroscopy. An 80 % conversion to tetraphenylene was observed, relative to unreacted biphenylene. (TON ≅ 11; TOF ≅ 0.68 h^{-1}). ^{1}H NMR (C_7D_8, 300 K, 300 MHz): δ 7.03 (2nd order m, 8H, 1-Ar-H), 7.13 (2nd order m, 8H, 2-Ar-H).

X-ray Crystallography. The X-ray structures were obtained at low temperature, with the crystals covered in Paratone and placed rapidly into the cold N_2 stream of the Kryo-Flex low-temperature device. The data were collected using the SMART[4] software on a Bruker APEX CCD diffractometer using a graphite monochromator with Mo Kα radiation (λ = 0.71073 Å). A hemisphere of data was collected using a counting time of 10–30 s per frame. Data reductions were performed using the SAINT[5] software, and the data were corrected for absorption using SADABS.[6] The structures were solved by direct or Patterson's methods using SHELXS-97[7] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELX-97[7] and the WinGX[8] software package, and thermal ellipsoid plots were produced using ORTEP32.[9]

Complex **3$^{i\text{-Pr}}$** features disorder of two of the isopropyl groups attached to P(2), disordered with respect to rotation around the P–C bonds. The two arrangements of these groups are labeled A and B for C(34), C(35), C(36), C(41), C(42) and C(53). The population at these two sites was refined, with a 57 % occupation of the A sites.

Calculations. Ab initio DFT calculations were performed using the hybrid functional B3LYP[10] method with the Gaussian 09 package.[11] The basis functions used were the TZVP set, provided in the Gaussian 09 program. All geometries were optimized, and frequency calculations were performed to ensure that the geometries were local minima, and possessed no imaginary frequencies. Complex $\mathbf{5^{Me}}$ only exhibited zero imaginary frequencies with C_s, rather than C_1 symmetry.

Additional calculations using a solvent model were done using the polarizable continuum model (PCM) default parameters in Gaussian 09. Calculations for both $\mathbf{4^{Me}}$ **and** $\mathbf{5^{Me}}$ were done with PCM parameters appropriate for both n-pentane and toluene as the solvent. Species $\mathbf{5^{Me}}$ retained C_s symmetry with n-pentane as the model solvent, but was found to have no imaginary frequencies only in C_1 symmetry with toluene as the model solvent.

Optimized Coordinates and Energies for $\mathbf{4^{Me}}$ and $\mathbf{5^{Me}}$.

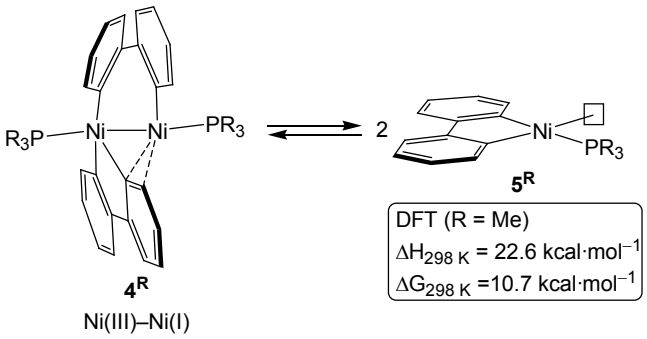


Table S3. Energies from DFT vibrational analyses of $\mathbf{5^{Me}}$ and $\mathbf{4^{Me}}$.

	$\mathbf{5^{Me}}$	$\mathbf{4^{Me}}$
Sum of electronic and zero-point Energies	–2431.512328	–4863.055356
Sum of electronic and thermal Energies	–2431.493733	–4863.018127
Sum of electronic and thermal Enthalpies	–2431.492788	–4863.017183
Sum of electronic and thermal Free Energies	–2431.560226	–4863.124837

	$\mathbf{5^{Me}}$ ***n*-pentane**	$\mathbf{4^{Me}}$ ***n*-pentane**
Sum of electronic and zero-point Energies	–2431.518317	–4863.059856
Sum of electronic and thermal Energies	–2431.499728	–4863.022639
Sum of electronic and thermal Enthalpies	–2431.498784	–4863.021694
Sum of electronic and thermal Free Energies	–2431.566882	–4863.128772

	$\mathbf{5^{Me}}$ **toluene**	$\mathbf{4^{Me}}$ **toluene**
Sum of electronic and zero-point Energies	–2431.520429	–4863.061556
Sum of electronic and thermal Energies	–2431.501919	–4863.024344
Sum of electronic and thermal Enthalpies	–2431.500975	–4863.023400
Sum of electronic and thermal Free Energies	–2431.568088	–4863.130341

Table S4. Optimized Cartesian Coordinates (Å) for 4^{Me}.

number	element	X	y	z	number	element	x	y	z
1	H	-4.7233	1.787807	2.275361	35	C	-0.01572	1.510076	-1.19255
2	C	-4.16294	-0.99238	1.20327	36	C	3.134355	3.799163	1.652282
3	H	-3.64962	-1.39111	2.076824	37	C	0.457007	2.806289	-0.83446
4	C	-3.65485	1.729022	2.058866	38	C	1.581112	2.783573	0.103098
5	C	-4.46816	1.194081	-0.65589	39	C	-0.09514	-1.46704	-1.21489
6	P	-3.33126	0.563386	0.661602	40	H	4.404987	2.422214	2.705536
7	H	-4.12886	2.173084	-0.99191	41	C	3.618463	2.534269	1.966791
8	H	-0.37134	-1.00262	4.826045	42	C	-0.7858	-2.91455	-3.07239
9	C	-0.46675	-1.31374	3.791906	43	C	3.093835	1.406526	1.332316
10	H	-0.16043	-3.39956	4.219079	44	C	2.078943	1.483848	0.371545
11	H	-0.81324	0.679625	3.085839	45	H	3.505111	0.447048	1.621459
12	C	-0.34416	-2.65711	3.451559	46	28	1.088058	0.019213	-0.52896
13	C	-0.7187	-0.36232	2.801442	47	H	-0.82652	-3.09743	-4.14089
14	H	-1.71339	-4.2925	-0.12441	48	C	-0.19149	-1.75039	-2.58615
15	C	-0.43035	-3.04222	2.116198	49	H	0.232594	-1.05512	-3.30494
16	C	-0.83066	-0.74012	1.464225	50	P	2.85684	-1.46568	-0.49688
17	Ni	-1.23884	0.395639	0.005008	51	C	3.244213	-2.31657	1.104879
18	H	-0.29614	-4.08462	1.84718	52	H	4.74572	0.09352	-0.3551
19	C	-0.65306	-2.09469	1.111952	53	H	1.928791	-3.55169	-1.38704
20	C	-1.26615	-3.58923	-0.81911	54	C	4.484864	-0.73883	-1.00446
21	H	-1.78652	-4.75062	-2.55349	55	H	4.108531	-2.97422	0.992223
22	C	-0.67411	-2.41824	-0.33274	56	C	2.782038	-2.9236	-1.63687
23	H	-2.44265	2.498081	-3.40585	57	H	-4.44647	0.514621	-1.50795
24	C	-1.31926	-3.84468	-2.18569	58	H	-5.49134	1.268758	-0.28199
25	H	-1.64259	4.733485	-2.69423	59	H	-4.09504	-1.7297	0.403397
26	C	-1.65695	2.589537	-2.66428	60	H	-5.21214	-0.81044	1.443202
27	C	-1.1994	3.835748	-2.27893	61	H	-3.2846	2.719772	1.795536
28	H	1.712159	4.903434	0.495933	62	H	-3.12785	1.386702	2.948213
29	H	0.219616	4.926081	-1.09618	63	H	5.274337	-1.49278	-0.9777
30	C	-1.06085	1.429453	-2.13445	64	H	4.392206	-0.35568	-2.02148
31	H	-1.37155	0.470868	-2.5318	65	H	2.376503	-2.90282	1.405672
32	C	-0.14456	3.941693	-1.36671	66	H	3.44452	-1.59083	1.890269
33	H	3.541017	4.679843	2.135354	67	H	3.70171	-3.50712	-1.5596
34	C	2.110319	3.920019	0.721113	68	H	2.657387	-2.58318	-2.66401

Stoichiometry: $C_{30}H_{34}Ni_2P_2$
Full point group: C_1

Item	Value	Threshold	Converged?
Maximum Force	0.000005	0.00045	YES
RMS Force	0.000001	0.0003	YES
Maximum Displacement	0.001541	0.0018	YES
RMS Displacement	0.000281	0.0012	YES

Table S5. Optimized Cartesian Coordinates (Å) for 4^{Me} with a *n*-pentane solvent model.

number	element	x	y	z	number	element	x	y	z
1	H	-4.76156	1.720001	2.265452	35	C	-0.03909	1.504617	-1.19461
2	C	-4.16372	-1.05192	1.191399	36	C	3.058275	3.854588	1.661866
3	H	-3.64748	-1.45022	2.063279	37	C	0.413646	2.809504	-0.84056
4	C	-3.69101	1.673961	2.057442	38	C	1.53296	2.808184	0.104239
5	C	-4.48546	1.135573	-0.66367	39	C	-0.0607	-1.47193	-1.21621
6	P	-3.35046	0.515906	0.659369	40	H	4.348161	2.502184	2.724413
7	H	-4.16007	2.1219	-0.99167	41	C	3.563811	2.598797	1.981088
8	H	-0.37304	-1.01213	4.827418	42	C	-0.72408	-2.93313	-3.07366
9	C	-0.45748	-1.32388	3.792459	43	C	3.063387	1.460554	1.344911
10	H	-0.10155	-3.40275	4.21693	44	C	2.052144	1.517486	0.378133
11	H	-0.85487	0.660605	3.089443	45	H	3.491306	0.509107	1.636501
12	C	-0.30177	-2.66358	3.45031	46	Ni	1.090758	0.034169	-0.527
13	C	-0.73018	-0.37734	2.80264	47	H	-0.75822	-3.1186	-4.14202
14	H	-1.64128	-4.3188	-0.12574	48	C	-0.1483	-1.75944	-2.58732
15	C	-0.37659	-3.04832	2.113967	49	H	0.268615	-1.06013	-3.30631
16	C	-0.829	-0.75481	1.464001	50	P	2.887734	-1.42058	-0.49031
17	Ni	-1.25046	0.376721	0.006632	51	C	3.281992	-2.2681	1.111093
18	H	-0.21712	-4.08685	1.843825	52	H	4.753168	0.164341	-0.32875
19	C	-0.61913	-2.10465	1.110519	53	H	1.998039	-3.5172	-1.39193
20	C	-1.20201	-3.61045	-0.82033	54	C	4.505542	-0.66492	-0.98722
21	H	-1.69963	-4.78313	-2.55427	55	H	4.157928	-2.91024	0.999949
22	C	-0.62914	-2.42965	-0.33431	56	C	2.84259	-2.87509	-1.63531
23	H	-2.47173	2.450773	-3.42061	57	H	-4.44871	0.459968	-1.51811
24	C	-1.2469	-3.86959	-2.18683	58	H	-5.51118	1.192588	-0.29409
25	H	-1.70164	4.700727	-2.72001	59	H	-4.09004	-1.78293	0.386426
26	C	-1.68771	2.556501	-2.67929	60	H	-5.2142	-0.8803	1.432375
27	C	-1.24803	3.810959	-2.29896	61	H	-3.32987	2.669078	1.798511
28	H	1.623429	4.931322	0.494442	62	H	-3.1673	1.335009	2.949901
29	H	0.151059	4.925403	-1.11504	63	H	5.304669	-1.40849	-0.9637
30	C	-1.07861	1.407301	-2.1413	64	H	4.410838	-0.27458	-2.00124
31	H	-1.37799	0.442843	-2.53297	65	H	2.423398	-2.87028	1.406345
32	C	-0.19879	3.934847	-1.38221	66	H	3.466875	-1.54084	1.898959
33	H	3.445732	4.743393	2.146075	67	H	3.770986	-3.44373	-1.55342
34	C	2.037696	3.955489	0.723719	68	H	2.719921	-2.53225	-2.66188

Table S6. Optimized Cartesian Coordinates (Å) for 4^{Me} with a toluene solvent model.

number	element	x	y	z	number	element	x	y	z
1	H	-4.77452	1.699358	2.259629	35	C	-0.04584	1.503384	-1.19464
2	C	-4.16432	-1.07037	1.187629	36	C	3.038259	3.870973	1.663085
3	H	-3.6479	-1.46679	2.060205	37	C	0.400556	2.81075	-0.84116
4	C	-3.70344	1.658024	2.053863	38	C	1.519286	2.815611	0.104801
5	C	-4.49146	1.115146	-0.66888	39	C	-0.05103	-1.473	-1.21549
6	P	-3.35738	0.500845	0.656934	40	H	4.33587	2.525882	2.725866
7	H	-4.17114	2.103737	-0.99492	41	C	3.551015	2.617983	1.982482
8	H	-0.37575	-1.01104	4.828706	42	C	-0.706	-2.93938	-3.07205
9	C	-0.45589	-1.3237	3.793664	43	C	3.057044	1.476756	1.346213
10	H	-0.08312	-3.39956	4.218992	44	C	2.045535	1.52763	0.379056
11	H	-0.87104	0.656806	3.090059	45	H	3.490703	0.527829	1.637494
12	C	-0.28872	-2.66223	3.452008	46	Ni	1.091887	0.03865	-0.52648
13	C	-0.73535	-0.3797	2.803192	47	H	-0.73862	-3.12599	-4.14029
14	H	-1.61714	-4.32727	-0.12317	48	C	-0.13653	-1.7622	-2.58642
15	C	-0.35941	-3.04794	2.115625	49	H	0.277386	-1.06171	-3.30596
16	C	-0.82924	-0.75805	1.46433	50	P	2.896826	-1.40813	-0.48891
17	Ni	-1.25442	0.370452	0.006241	51	C	3.294822	-2.25386	1.112375
18	H	-0.19149	-4.08529	1.846122	52	H	4.755995	0.184096	-0.32508
19	C	-0.60848	-2.10648	1.111661	53	H	2.017308	-3.5083	-1.39115
20	C	-1.18129	-3.61719	-0.81816	54	C	4.511123	-0.6447	-0.98516
21	H	-1.67192	-4.79423	-2.55129	55	H	4.173667	-2.89182	1.000652
22	C	-0.61508	-2.4328	-0.33299	56	C	2.85879	-2.86217	-1.63446
23	H	-2.48175	2.438016	-3.42227	57	H	-4.44921	0.440121	-1.52346
24	C	-1.2242	-3.87792	-2.18455	58	H	-5.51801	1.16609	-0.3009
25	H	-1.7214	4.692008	-2.72334	59	H	-4.08787	-1.8006	0.382251
26	C	-1.69778	2.547738	-2.68153	60	H	-5.21548	-0.90196	1.427562
27	C	-1.2639	3.804495	-2.30181	61	H	-3.34623	2.654446	1.794683
28	H	1.59779	4.939533	0.494819	62	H	-3.18007	1.321728	2.947486
29	H	0.129204	4.925626	-1.11725	63	H	5.312814	-1.38544	-0.96257
30	C	-1.0841	1.401606	-2.14236	64	H	4.414825	-0.25356	-1.9987
31	H	-1.3802	0.435735	-2.53304	65	H	2.439155	-2.86029	1.407357
32	C	-0.21586	3.93332	-1.38423	66	H	3.476777	-1.52593	1.900339
33	H	3.420452	4.762081	2.147306	67	H	3.78991	-3.42616	-1.55205
34	C	2.017321	3.966008	0.724386	68	H	2.735226	-2.51922	-2.66086

Table S7. Optimized Cartesian Coordinates (Å) for 5^{Me}.

number	element	x	y	z
1	H	3.542717	–3.76983	0
2	H	1.600744	–5.30116	0
3	C	2.535471	–3.36831	0
4	C	1.44394	–4.22887	0
5	H	–2.75229	–3.2187	0
6	H	–0.69857	–4.39876	0
7	C	2.334893	–1.98166	0
8	H	3.205678	–1.3298	0
9	C	0.145169	–3.71705	0
10	H	–4.71967	–1.72265	0
11	C	–2.60998	–2.1437	0
12	C	1.046512	–1.45746	0
13	C	–3.72162	–1.30077	0
14	C	–0.0521	–2.33953	0
15	C	–1.32448	–1.60894	0
16	H	–4.41135	0.734342	0
17	C	–3.54956	0.076554	0
18	C	–2.25801	0.621245	0
19	C	–1.14401	–0.20596	0
20	H	–2.15553	1.700852	0
21	Ni	0.645028	0.387271	0
22	P	0.678134	2.69984	0
23	C	–0.0521	3.589469	1.44954
24	H	–1.11816	3.372569	–1.51281
25	H	2.949103	2.955765	0.883482
26	C	–0.0521	3.589469	–1.44954
27	H	0.092665	4.6687	1.370405
28	C	2.426743	3.324917	0
29	H	0.092665	4.6687	–1.37041
30	H	0.417319	3.228955	–2.36513
31	H	0.417319	3.228955	2.365125
32	H	–1.11816	3.372569	1.512812
33	H	2.460992	4.416077	0
34	H	2.949103	2.955765	–0.88348

Stoichiometry: $C_{15}H_{17}NiP$
Full point group: C_S

Item	Value	Threshold	Converged?
Maximum Force	0.000003	0.00045	YES
RMS Force	0.000001	0.0003	YES
Maximum Displacement	0.000105	0.0018	YES
RMS Displacement	0.000024	0.0012	YES

Table S8. Optimized Cartesian Coordinates (Å) for 5^{Me} with a *n*-pentane solvent model.

number	element	x	y	z
1	H	3.542899	-3.77795	0
2	H	1.597227	-5.30627	0
3	C	2.536288	-3.37457	0
4	C	1.442894	-4.23357	0
5	H	-2.74528	-3.2252	0
6	H	-0.69998	-4.39837	0
7	C	2.337689	-1.98743	0
8	H	3.209529	-1.337	0
9	C	0.145141	-3.71828	0
10	H	-4.71811	-1.73625	0
11	C	-2.60654	-2.14965	0
12	C	1.050454	-1.4574	0
13	C	-3.7215	-1.31083	0
14	C	-0.04924	-2.33961	0
15	C	-1.32268	-1.60943	0
16	H	-4.41712	0.722589	0
17	C	-3.55319	0.067544	0
18	C	-2.2635	0.616798	0
19	C	-1.14427	-0.20521	0
20	H	-2.16485	1.696416	0
21	Ni	0.643931	0.390347	0
22	P	0.673164	2.709422	0
23	C	-0.04924	3.602552	1.450175
24	H	-1.11776	3.397981	-1.51335
25	H	2.94536	2.935665	0.883988
26	C	-0.04924	3.602552	-1.45018
27	H	0.106892	4.679886	1.369381
28	C	2.428533	3.310892	0
29	H	0.106892	4.679886	-1.36938
30	H	0.417746	3.238131	-2.36539
31	H	0.417746	3.238131	2.365387
32	H	-1.11776	3.397981	1.513354
33	H	2.460992	4.416077	0
34	H	2.949103	2.955765	–0.88348

Table S9. Optimized Cartesian Coordinates (Å) for 5^{Me} with a toluene solvent model.

number	element	x	y	z
1	H	-3.56015	-3.7788	-2.2E-05
2	H	-5.20212	-1.92779	0.000412
3	C	-3.21739	-2.74992	-0.00003
4	C	-4.14049	-1.70982	0.000234
5	H	-3.39006	2.527694	0.000336
6	H	-4.4323	0.419597	0.000466
7	C	-1.84441	-2.46878	-0.00024
8	H	-1.14342	-3.30019	-0.00047
9	C	-3.70331	-0.3837	0.000243
10	H	-2.02864	4.589885	0.000189
11	C	-2.30789	2.456368	0.000153
12	C	-1.39094	-1.15224	-0.0003
13	C	-1.54111	3.622123	0.000073
14	C	-2.33831	-0.10756	0.000012
15	C	-1.68775	1.208781	0.000001
16	H	0.444864	4.44411	-0.00023
17	C	-0.15468	3.540774	-0.00016
18	C	0.474194	2.288192	-0.00029
19	C	-0.27482	1.118279	-0.00024
20	H	1.55757	2.257547	-0.00045
21	Ni	0.430422	-0.62952	-0.0002
22	P	2.749708	-0.47949	0.000071
23	C	3.589577	0.300608	1.451932
24	H	3.31715	1.353981	-1.5151
25	H	3.130604	-2.73041	0.883799
26	C	3.590496	0.301085	-1.45102
27	H	4.674798	0.214132	1.372306
28	C	3.469865	-2.18911	-0.00011
29	H	4.675681	0.215061	-1.37041
30	H	3.256808	-0.19035	-2.36512
31	H	3.254855	-0.19068	2.365729
32	H	3.316616	1.353624	1.515757
33	H	4.560883	-2.15921	0.000308
34	H	3.131254	-2.72987	-0.8846

Tables of Crystallographic Data for $3^{i\text{-Pr}}$.

Table S10. Crystal data and structure refinement for $\mathbf{3}^{i\text{-Pr}}$.

Empirical formula	$C_{42}\ H_{58}\ Ni_2\ P_2$	
Formula weight	742.24	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.1261(14) Å	α= 90°.
	b = 24.900(4) Å	β= 100.710(2)°.
	c = 17.1650(17) Å	γ = 90°.
Volume	3832.7(9) $Å^3$	
Z	4	
Density (calculated)	1.286 Mg/m^3	
Absorption coefficient	1.094 mm^{-1}	
F(000)	1584	
Crystal size	0.45 x 0.4 x 0.25 mm^3	
Theta range for data collection	2.27 to 27.50°.	
Index ranges	-11<=h<=11, -32<=k<=32, -21<=l<=21	
Reflections collected	42451	
Independent reflections	8665 [R(int) = 0.0748]	
Completeness to theta = 27.50°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7716 and 0.6388	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8665 / 0 / 486	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0523, wR2 = 0.0980	
R indices (all data)	R1 = 0.0811, wR2 = 0.1123	
Largest diff. peak and hole	0.703 and -0.335 $e.Å^{-3}$	

Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**$^{i\text{-Pr}}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	2604(1)	3538(1)	7839(1)	23(1)
Ni(2)	2698(1)	4445(1)	7508(1)	23(1)
P(1)	3396(1)	2719(1)	8110(1)	24(1)
P(2)	3194(1)	5273(1)	7901(1)	34(1)
C(1)	3178(3)	3808(1)	6886(2)	22(1)
C(2)	4529(4)	4096(1)	6896(2)	26(1)
C(3)	5021(4)	4244(1)	6200(2)	32(1)
C(4)	4188(4)	4121(1)	5477(2)	34(1)
C(5)	2846(4)	3845(1)	5441(2)	29(1)
C(6)	2338(3)	3691(1)	6114(2)	23(1)
C(7)	954(3)	3362(1)	6044(2)	23(1)
C(8)	942(4)	2840(1)	5745(2)	30(1)
C(9)	-283(4)	2508(1)	5713(2)	36(1)
C(10)	-1517(4)	2689(2)	5988(2)	36(1)
C(11)	-1565(4)	3213(1)	6246(2)	32(1)
C(12)	-358(4)	3557(1)	6258(2)	25(1)
C(13)	-629(3)	4145(1)	6354(2)	26(1)
C(14)	-998(4)	4438(1)	5650(2)	32(1)
C(15)	-1497(4)	4960(1)	5643(2)	36(1)
C(16)	-1682(4)	5196(1)	6340(2)	35(1)
C(17)	-1291(4)	4921(1)	7044(2)	31(1)
C(18)	-725(3)	4398(1)	7070(2)	25(1)
C(19)	-187(4)	4135(1)	7854(2)	25(1)
C(20)	-1163(4)	3942(1)	8310(2)	33(1)
C(21)	-653(4)	3729(2)	9063(2)	36(1)
C(22)	838(4)	3713(1)	9358(2)	35(1)
C(23)	1861(4)	3907(1)	8907(2)	30(1)
C(24)	1388(4)	4131(1)	8136(2)	24(1)
C(25)	4070(4)	2602(1)	9190(2)	35(1)
C(26)	5038(5)	3065(2)	9591(2)	53(1)
C(27)	4878(5)	2075(2)	9421(2)	53(1)
C(28)	4900(4)	2437(1)	7647(2)	33(1)

C(29)	4442(4)	2401(2)	6747(2)	45(1)
C(30)	6320(4)	2774(2)	7862(3)	49(1)
C(31)	1810(4)	2252(1)	7805(2)	31(1)
C(32)	509(4)	2405(2)	8202(3)	51(1)
C(33)	2103(4)	1648(1)	7884(3)	48(1)
C(34A)	4772(9)	5320(3)	8739(5)	47(2)
C(35A)	5656(15)	5828(7)	8814(11)	59(4)
C(36A)	5760(30)	4833(9)	8796(16)	55(6)
C(34B)	5337(11)	5218(4)	8310(6)	36(3)
C(35B)	6190(20)	5713(12)	8672(17)	86(7)
C(36B)	5540(40)	4753(15)	8930(20)	63(9)
C(37)	3375(4)	5781(1)	7149(2)	38(1)
C(38)	1866(6)	5894(2)	6626(3)	74(2)
C(39)	4466(6)	5600(2)	6631(3)	81(2)
C(41A)	1633(9)	5639(3)	8335(4)	28(2)
C(42A)	1928(10)	6219(5)	8582(8)	47(3)
C(43A)	1340(20)	5350(7)	9087(11)	99(7)
C(41B)	2510(20)	5572(5)	8699(11)	71(5)
C(42B)	2700(20)	6199(7)	8771(12)	85(7)
C(43B)	1101(14)	5373(9)	8860(12)	56(7)

Table S12. Bond lengths [Å] and angles [°] for **3**$^{i\text{-Pr}}$.

Ni(1)-C(1)	1.930(3)	C(9)-H(9)	0.9300
Ni(1)-C(24)	1.970(3)	C(10)-C(11)	1.379(5)
Ni(1)-P(1)	2.1831(10)	C(10)-H(10)	0.9300
Ni(1)-C(23)	2.265(3)	C(11)-C(12)	1.394(5)
Ni(1)-Ni(2)	2.3352(6)	C(11)-H(11)	0.9300
Ni(2)-C(24)	1.919(3)	C(12)-C(13)	1.498(4)
Ni(2)-C(1)	2.006(3)	C(13)-C(14)	1.397(4)
Ni(2)-P(2)	2.1905(10)	C(13)-C(18)	1.400(4)
Ni(2)-C(2)	2.302(3)	C(14)-C(15)	1.378(5)
P(1)-C(28)	1.848(3)	C(14)-H(14)	0.9300
P(1)-C(31)	1.856(3)	C(15)-C(16)	1.371(5)
P(1)-C(25)	1.864(3)	C(15)-H(15)	0.9300
P(2)-C(41B)	1.773(11)	C(16)-C(17)	1.377(5)
P(2)-C(37)	1.838(4)	C(16)-H(16)	0.9300
P(2)-C(34A)	1.840(7)	C(17)-C(18)	1.397(4)
P(2)-C(41A)	1.952(8)	C(17)-H(17)	0.9300
P(2)-C(34B)	1.956(10)	C(18)-C(19)	1.495(4)
C(1)-C(2)	1.424(4)	C(19)-C(20)	1.377(4)
C(1)-C(6)	1.432(4)	C(19)-C(24)	1.429(4)
C(2)-C(3)	1.402(4)	C(20)-C(21)	1.396(5)
C(2)-H(2)	0.9300	C(20)-H(20)	0.9300
C(3)-C(4)	1.364(5)	C(21)-C(22)	1.361(5)
C(3)-H(3)	0.9300	C(21)-H(21)	0.9300
C(4)-C(5)	1.395(5)	C(22)-C(23)	1.405(5)
C(4)-H(4)	0.9300	C(22)-H(22)	0.9300
C(5)-C(6)	1.376(4)	C(23)-C(24)	1.426(4)
C(5)-H(5)	0.9300	C(23)-H(23)	0.9300
C(6)-C(7)	1.492(4)	C(25)-C(27)	1.520(5)
C(7)-C(8)	1.398(4)	C(25)-C(26)	1.536(5)
C(7)-C(12)	1.403(4)	C(25)-H(25)	0.9800
C(8)-C(9)	1.384(5)	C(26)-H(26A)	0.9600
C(8)-H(8)	0.9300	C(26)-H(26B)	0.9600
C(9)-C(10)	1.374(5)	C(26)-H(26C)	0.9600

C(27)-H(27A)	0.9600	C(35B)-H(35F)	0.9600
C(27)-H(27B)	0.9600	C(36B)-H(36D)	0.9600
C(27)-H(27C)	0.9600	C(36B)-H(36E)	0.9600
C(28)-C(29)	1.526(5)	C(36B)-H(36F)	0.9600
C(28)-C(30)	1.530(5)	C(37)-C(39)	1.521(5)
C(28)-H(28)	0.9800	C(37)-C(38)	1.524(6)
C(29)-H(29A)	0.9600	C(37)-H(37)	0.9800
C(29)-H(29B)	0.9600	C(38)-H(38A)	0.9600
C(29)-H(29C)	0.9600	C(38)-H(38B)	0.9600
C(30)-H(30A)	0.9600	C(38)-H(38C)	0.9600
C(30)-H(30B)	0.9600	C(39)-H(39A)	0.9600
C(30)-H(30C)	0.9600	C(39)-H(39B)	0.9600
C(31)-C(32)	1.524(5)	C(39)-H(39C)	0.9600
C(31)-C(33)	1.529(5)	C(41A)-C(42A)	1.517(13)
C(31)-H(31)	0.9800	C(41A)-C(43A)	1.543(19)
C(32)-H(32A)	0.9600	C(41A)-H(41A)	0.9800
C(32)-H(32B)	0.9600	C(42A)-H(42A)	0.9600
C(32)-H(32C)	0.9600	C(42A)-H(42B)	0.9600
C(33)-H(33A)	0.9600	C(42A)-H(42C)	0.9600
C(33)-H(33B)	0.9600	C(43A)-H(43A)	0.9600
C(33)-H(33C)	0.9600	C(43A)-H(43B)	0.9600
C(34A)-C(35A)	1.49(2)	C(43A)-H(43C)	0.9600
C(34A)-C(36A)	1.50(2)	C(41B)-C(43B)	1.45(2)
C(34A)-H(34A)	0.9800	C(41B)-C(42B)	1.57(2)
C(35A)-H(35A)	0.9600	C(41B)-H(41B)	0.9800
C(35A)-H(35B)	0.9600	C(42B)-H(42D)	0.9600
C(35A)-H(35C)	0.9600	C(42B)-H(42E)	0.9600
C(36A)-H(36A)	0.9600	C(42B)-H(42F)	0.9600
C(36A)-H(36B)	0.9600	C(43B)-H(43D)	0.9600
C(36A)-H(36C)	0.9600	C(43B)-H(43E)	0.9600
C(34B)-C(35B)	1.52(3)	C(43B)-H(43F)	0.9600
C(34B)-C(36B)	1.56(4)		
C(34B)-H(34B)	0.9800	C(1)-Ni(1)-C(24)	102.29(13)
C(35B)-H(35D)	0.9600	C(1)-Ni(1)-P(1)	112.02(9)
C(35B)-H(35E)	0.9600	C(24)-Ni(1)-P(1)	145.53(10)

C(1)-Ni(1)-C(23)	135.56(12)	C(34A)-P(2)-Ni(2)	112.8(2)
C(24)-Ni(1)-C(23)	38.57(12)	C(41A)-P(2)-Ni(2)	115.7(2)
P(1)-Ni(1)-C(23)	110.10(9)	C(34B)-P(2)-Ni(2)	100.4(3)
C(1)-Ni(1)-Ni(2)	55.12(9)	C(2)-C(1)-C(6)	115.3(3)
C(24)-Ni(1)-Ni(2)	52.11(9)	C(2)-C(1)-Ni(1)	122.4(2)
P(1)-Ni(1)-Ni(2)	158.31(3)	C(6)-C(1)-Ni(1)	122.1(2)
C(23)-Ni(1)-Ni(2)	80.44(8)	C(2)-C(1)-Ni(2)	82.44(19)
C(24)-Ni(2)-C(1)	101.36(13)	C(6)-C(1)-Ni(2)	121.4(2)
C(24)-Ni(2)-P(2)	108.98(10)	Ni(1)-C(1)-Ni(2)	72.77(11)
C(1)-Ni(2)-P(2)	148.83(9)	C(3)-C(2)-C(1)	122.4(3)
C(24)-Ni(2)-C(2)	133.10(12)	C(3)-C(2)-Ni(2)	131.7(2)
C(1)-Ni(2)-C(2)	37.83(11)	C(1)-C(2)-Ni(2)	59.73(16)
P(2)-Ni(2)-C(2)	111.69(9)	C(3)-C(2)-H(2)	118.8
C(24)-Ni(2)-Ni(1)	54.10(9)	C(1)-C(2)-H(2)	118.8
C(1)-Ni(2)-Ni(1)	52.11(9)	Ni(2)-C(2)-H(2)	80.4
P(2)-Ni(2)-Ni(1)	148.26(3)	C(4)-C(3)-C(2)	120.2(3)
C(2)-Ni(2)-Ni(1)	78.99(8)	C(4)-C(3)-H(3)	119.9
C(28)-P(1)-C(31)	104.01(16)	C(2)-C(3)-H(3)	119.9
C(28)-P(1)-C(25)	103.50(16)	C(3)-C(4)-C(5)	119.1(3)
C(31)-P(1)-C(25)	106.15(16)	C(3)-C(4)-H(4)	120.4
C(28)-P(1)-Ni(1)	120.43(12)	C(5)-C(4)-H(4)	120.4
C(31)-P(1)-Ni(1)	108.39(11)	C(6)-C(5)-C(4)	122.0(3)
C(25)-P(1)-Ni(1)	113.20(12)	C(6)-C(5)-H(5)	119.0
C(41B)-P(2)-C(37)	110.2(5)	C(4)-C(5)-H(5)	119.0
C(41B)-P(2)-C(34A)	73.0(7)	C(5)-C(6)-C(1)	120.9(3)
C(37)-P(2)-C(34A)	110.2(3)	C(5)-C(6)-C(7)	119.9(3)
C(41B)-P(2)-C(41A)	28.5(6)	C(1)-C(6)-C(7)	119.0(3)
C(37)-P(2)-C(41A)	96.5(3)	C(8)-C(7)-C(12)	118.1(3)
C(34A)-P(2)-C(41A)	101.1(3)	C(8)-C(7)-C(6)	119.3(3)
C(41B)-P(2)-C(34B)	103.1(7)	C(12)-C(7)-C(6)	122.7(3)
C(37)-P(2)-C(34B)	94.9(3)	C(9)-C(8)-C(7)	121.4(3)
C(34A)-P(2)-C(34B)	30.5(3)	C(9)-C(8)-H(8)	119.3
C(41A)-P(2)-C(34B)	130.4(4)	C(7)-C(8)-H(8)	119.3
C(41B)-P(2)-Ni(2)	123.4(4)	C(10)-C(9)-C(8)	119.8(3)
C(37)-P(2)-Ni(2)	118.18(12)	C(10)-C(9)-H(9)	120.1

C(8)-C(9)-H(9)	120.1	C(22)-C(21)-H(21)	120.2
C(9)-C(10)-C(11)	119.8(3)	C(20)-C(21)-H(21)	120.2
C(9)-C(10)-H(10)	120.1	C(21)-C(22)-C(23)	120.4(3)
C(11)-C(10)-H(10)	120.1	C(21)-C(22)-H(22)	119.8
C(10)-C(11)-C(12)	121.0(3)	C(23)-C(22)-H(22)	119.8
C(10)-C(11)-H(11)	119.5	C(22)-C(23)-C(24)	121.9(3)
C(12)-C(11)-H(11)	119.5	C(22)-C(23)-Ni(1)	129.4(2)
C(11)-C(12)-C(7)	119.5(3)	C(24)-C(23)-Ni(1)	59.45(17)
C(11)-C(12)-C(13)	117.2(3)	C(22)-C(23)-H(23)	119.1
C(7)-C(12)-C(13)	122.2(3)	C(24)-C(23)-H(23)	119.1
C(14)-C(13)-C(18)	118.7(3)	Ni(1)-C(23)-H(23)	82.5
C(14)-C(13)-C(12)	115.7(3)	C(23)-C(24)-C(19)	115.4(3)
C(18)-C(13)-C(12)	125.1(3)	C(23)-C(24)-Ni(2)	124.6(2)
C(15)-C(14)-C(13)	121.7(3)	C(19)-C(24)-Ni(2)	119.9(2)
C(15)-C(14)-H(14)	119.1	C(23)-C(24)-Ni(1)	81.98(19)
C(13)-C(14)-H(14)	119.1	C(19)-C(24)-Ni(1)	119.8(2)
C(16)-C(15)-C(14)	119.4(3)	Ni(2)-C(24)-Ni(1)	73.78(11)
C(16)-C(15)-H(15)	120.3	C(27)-C(25)-C(26)	108.7(3)
C(14)-C(15)-H(15)	120.3	C(27)-C(25)-P(1)	116.7(3)
C(15)-C(16)-C(17)	119.9(3)	C(26)-C(25)-P(1)	112.5(3)
C(15)-C(16)-H(16)	120.1	C(27)-C(25)-H(25)	106.1
C(17)-C(16)-H(16)	120.1	C(26)-C(25)-H(25)	106.1
C(16)-C(17)-C(18)	121.8(3)	P(1)-C(25)-H(25)	106.1
C(16)-C(17)-H(17)	119.1	C(25)-C(26)-H(26A)	109.5
C(18)-C(17)-H(17)	119.1	C(25)-C(26)-H(26B)	109.5
C(17)-C(18)-C(13)	118.3(3)	H(26A)-C(26)-H(26B)	109.5
C(17)-C(18)-C(19)	119.7(3)	C(25)-C(26)-H(26C)	109.5
C(13)-C(18)-C(19)	122.0(3)	H(26A)-C(26)-H(26C)	109.5
C(20)-C(19)-C(24)	121.4(3)	H(26B)-C(26)-H(26C)	109.5
C(20)-C(19)-C(18)	121.7(3)	C(25)-C(27)-H(27A)	109.5
C(24)-C(19)-C(18)	116.7(3)	C(25)-C(27)-H(27B)	109.5
C(19)-C(20)-C(21)	121.3(3)	H(27A)-C(27)-H(27B)	109.5
C(19)-C(20)-H(20)	119.3	C(25)-C(27)-H(27C)	109.5
C(21)-C(20)-H(20)	119.3	H(27A)-C(27)-H(27C)	109.5
C(22)-C(21)-C(20)	119.6(3)	H(27B)-C(27)-H(27C)	109.5

C(29)-C(28)-C(30)	109.6(3)	H(33B)-C(33)-H(33C)	109.5
C(29)-C(28)-P(1)	111.8(2)	C(35A)-C(34A)-C(36A)	111.7(13)
C(30)-C(28)-P(1)	110.6(3)	C(35A)-C(34A)-P(2)	116.9(9)
C(29)-C(28)-H(28)	108.2	C(36A)-C(34A)-P(2)	111.8(11)
C(30)-C(28)-H(28)	108.2	C(35A)-C(34A)-H(34A)	105.0
P(1)-C(28)-H(28)	108.2	C(36A)-C(34A)-H(34A)	105.0
C(28)-C(29)-H(29A)	109.5	P(2)-C(34A)-H(34A)	105.0
C(28)-C(29)-H(29B)	109.5	C(35B)-C(34B)-C(36B)	109.5(19)
H(29A)-C(29)-H(29B)	109.5	C(35B)-C(34B)-P(2)	119.3(11)
C(28)-C(29)-H(29C)	109.5	C(36B)-C(34B)-P(2)	106.5(14)
H(29A)-C(29)-H(29C)	109.5	C(35B)-C(34B)-H(34B)	107.0
H(29B)-C(29)-H(29C)	109.5	C(36B)-C(34B)-H(34B)	107.0
C(28)-C(30)-H(30A)	109.5	P(2)-C(34B)-H(34B)	107.0
C(28)-C(30)-H(30B)	109.5	C(34B)-C(35B)-H(35D)	109.5
H(30A)-C(30)-H(30B)	109.5	C(34B)-C(35B)-H(35E)	109.5
C(28)-C(30)-H(30C)	109.5	H(35D)-C(35B)-H(35E)	109.5
H(30A)-C(30)-H(30C)	109.5	C(34B)-C(35B)-H(35F)	109.5
H(30B)-C(30)-H(30C)	109.5	H(35D)-C(35B)-H(35F)	109.5
C(32)-C(31)-C(33)	110.1(3)	H(35E)-C(35B)-H(35F)	109.5
C(32)-C(31)-P(1)	110.4(2)	C(34B)-C(36B)-H(36D)	109.5
C(33)-C(31)-P(1)	118.5(3)	C(34B)-C(36B)-H(36E)	109.5
C(32)-C(31)-H(31)	105.6	H(36D)-C(36B)-H(36E)	109.5
C(33)-C(31)-H(31)	105.6	C(34B)-C(36B)-H(36F)	109.5
P(1)-C(31)-H(31)	105.6	H(36D)-C(36B)-H(36F)	109.5
C(31)-C(32)-H(32A)	109.5	H(36E)-C(36B)-H(36F)	109.5
C(31)-C(32)-H(32B)	109.5	C(39)-C(37)-C(38)	109.2(4)
H(32A)-C(32)-H(32B)	109.5	C(39)-C(37)-P(2)	111.1(3)
C(31)-C(32)-H(32C)	109.5	C(38)-C(37)-P(2)	110.6(3)
H(32A)-C(32)-H(32C)	109.5	C(39)-C(37)-H(37)	108.6
H(32B)-C(32)-H(32C)	109.5	C(38)-C(37)-H(37)	108.6
C(31)-C(33)-H(33A)	109.5	P(2)-C(37)-H(37)	108.6
C(31)-C(33)-H(33B)	109.5	C(37)-C(38)-H(38A)	109.5
H(33A)-C(33)-H(33B)	109.5	C(37)-C(38)-H(38B)	109.5
C(31)-C(33)-H(33C)	109.5	H(38A)-C(38)-H(38B)	109.5
H(33A)-C(33)-H(33C)	109.5	C(37)-C(38)-H(38C)	109.5

H(38A)-C(38)-H(38C)	109.5	C(42B)-C(41B)-P(2)	115.3(10)
H(38B)-C(38)-H(38C)	109.5	C(43B)-C(41B)-H(41B)	102.2
C(37)-C(39)-H(39A)	109.5	C(42B)-C(41B)-H(41B)	102.2
C(37)-C(39)-H(39B)	109.5	P(2)-C(41B)-H(41B)	102.2
H(39A)-C(39)-H(39B)	109.5	C(41B)-C(42B)-H(42D)	109.5
C(37)-C(39)-H(39C)	109.5	C(41B)-C(42B)-H(42E)	109.5
H(39A)-C(39)-H(39C)	109.5	H(42D)-C(42B)-H(42E)	109.5
H(39B)-C(39)-H(39C)	109.5	C(41B)-C(42B)-H(42F)	109.5
C(42A)-C(41A)-C(43A)	105.0(9)	H(42D)-C(42B)-H(42F)	109.5
C(42A)-C(41A)-P(2)	116.6(6)	H(42E)-C(42B)-H(42F)	109.5
C(43A)-C(41A)-P(2)	110.7(8)	C(41B)-C(43B)-H(43D)	109.5
C(42A)-C(41A)-H(41A)	108.1	C(41B)-C(43B)-H(43E)	109.5
C(43A)-C(41A)-H(41A)	108.1	H(43D)-C(43B)-H(43E)	109.5
P(2)-C(41A)-H(41A)	108.1	C(41B)-C(43B)-H(43F)	109.5
C(43B)-C(41B)-C(42B)	114.4(13)	H(43D)-C(43B)-H(43F)	109.5
C(43B)-C(41B)-P(2)	117.3(12)	H(43E)-C(43B)-H(43F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S13. Anisotropic displacement parameters ($Å^2$x 10^3)for **3**$^{i\text{-Pr}}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	25(1)	20(1)	24(1)	2(1)	6(1)	1(1)
Ni(2)	26(1)	19(1)	25(1)	0(1)	7(1)	-1(1)
P(1)	25(1)	21(1)	27(1)	4(1)	6(1)	1(1)
P(2)	45(1)	24(1)	32(1)	-4(1)	6(1)	-9(1)
C(1)	24(2)	18(2)	26(2)	2(1)	8(1)	4(1)
C(2)	26(2)	23(2)	30(2)	-4(1)	7(1)	0(1)
C(3)	32(2)	22(2)	46(2)	0(2)	17(2)	-3(1)
C(4)	41(2)	33(2)	34(2)	2(2)	21(2)	3(2)
C(5)	33(2)	31(2)	25(2)	1(1)	9(1)	4(2)
C(6)	23(2)	20(2)	26(2)	-1(1)	6(1)	5(1)
C(7)	26(2)	24(2)	20(2)	-2(1)	3(1)	0(1)
C(8)	33(2)	28(2)	30(2)	-6(1)	7(2)	5(2)
C(9)	43(2)	27(2)	35(2)	-7(2)	4(2)	-3(2)
C(10)	31(2)	37(2)	40(2)	-5(2)	2(2)	-11(2)
C(11)	30(2)	33(2)	33(2)	-1(2)	6(2)	2(2)
C(12)	29(2)	26(2)	20(2)	-1(1)	1(1)	0(1)
C(13)	20(2)	24(2)	33(2)	1(1)	5(1)	1(1)
C(14)	30(2)	37(2)	29(2)	3(2)	5(2)	2(2)
C(15)	34(2)	34(2)	40(2)	13(2)	9(2)	4(2)
C(16)	30(2)	23(2)	52(2)	6(2)	7(2)	3(2)
C(17)	25(2)	26(2)	41(2)	-2(2)	7(2)	2(1)
C(18)	18(2)	24(2)	33(2)	1(1)	7(1)	0(1)
C(19)	27(2)	19(2)	29(2)	-4(1)	7(1)	1(1)
C(20)	27(2)	36(2)	40(2)	-3(2)	11(2)	-1(2)
C(21)	38(2)	42(2)	32(2)	2(2)	18(2)	-5(2)
C(22)	48(2)	35(2)	24(2)	5(2)	10(2)	-1(2)
C(23)	29(2)	30(2)	30(2)	-1(1)	5(2)	2(1)
C(24)	27(2)	20(2)	26(2)	0(1)	9(1)	1(1)
C(25)	35(2)	40(2)	28(2)	11(2)	4(2)	2(2)
C(26)	60(3)	45(3)	44(2)	-2(2)	-17(2)	12(2)

C(27)	67(3)	42(2)	44(2)	15(2)	-4(2)	-1(2)
C(28)	32(2)	28(2)	42(2)	4(2)	12(2)	9(2)
C(29)	49(2)	45(2)	44(2)	0(2)	20(2)	12(2)
C(30)	34(2)	56(3)	61(3)	8(2)	18(2)	3(2)
C(31)	31(2)	25(2)	35(2)	3(2)	6(2)	-5(1)
C(32)	31(2)	47(3)	79(3)	-10(2)	19(2)	-9(2)
C(33)	42(2)	25(2)	76(3)	-1(2)	8(2)	-7(2)
C(34A)	45(5)	53(5)	37(5)	-8(4)	-6(4)	-1(4)
C(35A)	44(8)	53(6)	69(8)	-19(5)	-15(7)	-9(6)
C(36A)	43(8)	55(9)	66(13)	-22(10)	8(7)	-3(7)
C(34B)	41(6)	49(6)	17(5)	-11(4)	1(4)	-17(4)
C(35B)	58(14)	100(20)	93(14)	-11(12)	-2(13)	-37(12)
C(36B)	41(13)	87(15)	51(11)	18(9)	-16(11)	-4(10)
C(37)	49(2)	21(2)	48(2)	-3(2)	17(2)	-7(2)
C(38)	98(4)	51(3)	65(3)	12(2)	-9(3)	5(3)
C(39)	119(5)	45(3)	103(4)	-10(3)	83(4)	-17(3)
C(41A)	34(4)	28(4)	22(4)	-7(3)	4(3)	5(3)
C(42A)	36(5)	35(4)	71(6)	-18(4)	11(5)	-4(5)
C(43A)	205(19)	38(7)	77(11)	-18(6)	85(11)	-22(9)
C(41B)	118(14)	32(6)	80(11)	-17(7)	58(10)	-9(8)
C(42B)	100(14)	60(9)	120(16)	-52(10)	86(14)	-38(11)
C(43B)	12(5)	83(13)	73(13)	-56(10)	8(6)	5(5)

Tables of Crystallographic Data for $4^{i\text{-Pr}}$.

Table S14. Crystal data and structure refinement for $4^{i\text{-Pr}}$.

Empirical formula	$C_{42}H_{58}Ni_2P_2$	
Formula weight	742.24	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.0185(14) Å	α= 83.4740(10)°.
	b = 12.6516(17) Å	β= 70.9050(10)°.
	c = 15.558(2) Å	γ = 68.1500(10)°.
Volume	1902.2(4) $Å^3$	
Z	2	
Density (calculated)	1.296 Mg/m^3	
Absorption coefficient	1.102 mm^{-1}	
F(000)	792	
Crystal size	0.21 x 0.10 x 0.08 mm^3	
Theta range for data collection	2.23 to 26.37°.	
Index ranges	-13<=h<=13, -15<=k<=15, -19<=l<=19	
Reflections collected	20027	
Independent reflections	7736 [R(int) = 0.0371]	
Completeness to theta = 26.37°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9170 and 0.8016	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7736 / 0 / 427	
Goodness-of-fit on F^2	1.093	
Final R indices [I>2sigma(I)]	R1 = 0.0450, wR2 = 0.0889	
R indices (all data)	R1 = 0.0582, wR2 = 0.0960	
Largest diff. peak and hole	0.567 and -0.349 $e.Å^{-3}$	

Table S15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **4**$^{i\text{-Pr}}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	209(1)	8159(1)	2673(1)	23(1)
Ni(2)	1646(1)	6232(1)	2596(1)	25(1)
P(1)	-1459(1)	9893(1)	3017(1)	24(1)
P(2)	2898(1)	4460(1)	2178(1)	28(1)
C(1)	1460(3)	7387(2)	3399(2)	26(1)
C(2)	1264(3)	6652(2)	4141(2)	27(1)
C(3)	2135(3)	6328(3)	4686(2)	32(1)
C(4)	3190(3)	6727(3)	4508(2)	34(1)
C(5)	3420(3)	7449(3)	3772(2)	32(1)
C(6)	2580(3)	7781(2)	3219(2)	28(1)
C(7)	2732(3)	8504(3)	2412(2)	28(1)
C(8)	3850(3)	8855(3)	2017(2)	39(1)
C(9)	3925(4)	9506(3)	1234(2)	43(1)
C(10)	2891(3)	9779(3)	839(2)	38(1)
C(11)	1794(3)	9408(3)	1220(2)	31(1)
C(12)	1656(3)	8790(2)	2029(2)	27(1)
C(13)	1101(3)	6808(2)	1535(2)	25(1)
C(14)	2017(3)	6935(2)	690(2)	32(1)
C(15)	1642(3)	7138(3)	-95(2)	36(1)
C(16)	335(4)	7230(3)	-65(2)	44(1)
C(17)	-592(3)	7125(3)	753(2)	38(1)
C(18)	-229(3)	6915(2)	1550(2)	28(1)
C(19)	-1177(3)	6802(2)	2455(2)	29(1)
C(20)	-2100(3)	6233(3)	2604(2)	36(1)
C(21)	-2914(3)	6132(3)	3477(2)	40(1)
C(22)	-2795(3)	6590(3)	4194(2)	37(1)
C(23)	-1887(3)	7163(2)	4050(2)	31(1)
C(24)	-1058(3)	7298(2)	3177(2)	26(1)
C(25)	-794(3)	11078(3)	2852(2)	32(1)
C(26)	43(3)	10986(3)	3495(2)	41(1)

C(27)	-1791(4)	12295(3)	2833(2)	42(1)
C(28)	-2646(3)	9960(3)	4188(2)	29(1)
C(29)	-1906(4)	9665(3)	4913(2)	42(1)
C(30)	-3922(3)	11051(3)	4458(2)	42(1)
C(31)	-2639(3)	10327(3)	2315(2)	32(1)
C(32)	-3556(3)	9617(3)	2489(2)	40(1)
C(33)	-1831(4)	10288(3)	1307(2)	43(1)
C(34)	4707(3)	4213(3)	2052(2)	34(1)
C(35)	5195(4)	5048(3)	1362(3)	49(1)
C(36)	4894(4)	4353(3)	2957(3)	49(1)
C(37)	2430(4)	3484(3)	3093(3)	46(1)
C(38)	922(4)	3740(3)	3478(3)	54(1)
C(39)	3275(4)	2212(3)	2901(3)	51(1)
C(40)	2969(4)	4003(3)	1069(2)	37(1)
C(41)	1593(4)	3930(3)	1104(3)	61(1)
C(42)	4162(4)	2920(3)	622(2)	51(1)

Table S16. Bond lengths [Å] and angles [°] for **4**$^{i\text{-Pr}}$.

Ni(1)-C(1)	1.974(3)	C(10)-C(11)	1.386(4)
Ni(1)-C(12)	1.975(3)	C(10)-H(10)	0.9500
Ni(1)-C(24)	1.993(3)	C(11)-C(12)	1.400(4)
Ni(1)-P(1)	2.2581(8)	C(11)-H(11)	0.9500
Ni(1)-C(13)	2.306(3)	C(13)-C(14)	1.406(4)
Ni(1)-Ni(2)	2.3521(6)	C(13)-C(18)	1.414(4)
Ni(2)-C(13)	1.915(3)	C(14)-C(15)	1.381(4)
Ni(2)-C(1)	1.941(3)	C(14)-H(14)	0.9500
Ni(2)-P(2)	2.1897(9)	C(15)-C(16)	1.386(5)
Ni(2)-C(2)	2.388(3)	C(15)-H(15)	0.9500
P(1)-C(28)	1.852(3)	C(16)-C(17)	1.376(5)
P(1)-C(31)	1.857(3)	C(16)-H(16)	0.9500
P(1)-C(25)	1.860(3)	C(17)-C(18)	1.394(4)
P(2)-C(34)	1.845(3)	C(17)-H(17)	0.9500
P(2)-C(37)	1.847(3)	C(18)-C(19)	1.483(4)
P(2)-C(40)	1.849(3)	C(19)-C(20)	1.399(4)
C(1)-C(2)	1.410(4)	C(19)-C(24)	1.411(4)
C(1)-C(6)	1.432(4)	C(20)-C(21)	1.385(5)
C(2)-C(3)	1.403(4)	C(20)-H(20)	0.9500
C(2)-H(2)	0.9500	C(21)-C(22)	1.377(5)
C(3)-C(4)	1.371(4)	C(21)-H(21)	0.9500
C(3)-H(3)	0.9500	C(22)-C(23)	1.391(4)
C(4)-C(5)	1.397(4)	C(22)-H(22)	0.9500
C(4)-H(4)	0.9500	C(23)-C(24)	1.400(4)
C(5)-C(6)	1.387(4)	C(23)-H(23)	0.9500
C(5)-H(5)	0.9500	C(25)-C(27)	1.526(4)
C(6)-C(7)	1.469(4)	C(25)-C(26)	1.536(4)
C(7)-C(8)	1.394(4)	C(25)-H(25)	1.0000
C(7)-C(12)	1.409(4)	C(26)-H(26A)	0.9800
C(8)-C(9)	1.387(5)	C(26)-H(26B)	0.9800
C(8)-H(8)	0.9500	C(26)-H(26C)	0.9800
C(9)-C(10)	1.383(5)	C(27)-H(27A)	0.9800
C(9)-H(9)	0.9500	C(27)-H(27B)	0.9800

C(27)-H(27C)	0.9800	C(39)-H(39B)	0.9800
C(28)-C(29)	1.534(4)	C(39)-H(39C)	0.9800
C(28)-C(30)	1.537(4)	C(40)-C(41)	1.536(5)
C(28)-H(28)	1.0000	C(40)-C(42)	1.539(5)
C(29)-H(29A)	0.9800	C(40)-H(40)	1.0000
C(29)-H(29B)	0.9800	C(41)-H(41A)	0.9800
C(29)-H(29C)	0.9800	C(41)-H(41B)	0.9800
C(30)-H(30A)	0.9800	C(41)-H(41C)	0.9800
C(30)-H(30B)	0.9800	C(42)-H(42A)	0.9800
C(30)-H(30C)	0.9800	C(42)-H(42B)	0.9800
C(31)-C(33)	1.525(4)	C(42)-H(42C)	0.9800
C(31)-C(32)	1.530(4)		
C(31)-H(31)	1.0000	C(1)-Ni(1)-C(12)	83.12(12)
C(32)-H(32A)	0.9800	C(1)-Ni(1)-C(24)	96.04(12)
C(32)-H(32B)	0.9800	C(12)-Ni(1)-C(24)	170.23(12)
C(32)-H(32C)	0.9800	C(1)-Ni(1)-P(1)	123.97(8)
C(33)-H(33A)	0.9800	C(12)-Ni(1)-P(1)	93.61(9)
C(33)-H(33B)	0.9800	C(24)-Ni(1)-P(1)	94.91(8)
C(33)-H(33C)	0.9800	C(1)-Ni(1)-C(13)	98.47(11)
C(34)-C(36)	1.527(4)	C(12)-Ni(1)-C(13)	89.45(11)
C(34)-C(35)	1.533(5)	C(24)-Ni(1)-C(13)	81.04(11)
C(34)-H(34)	1.0000	P(1)-Ni(1)-C(13)	137.52(7)
C(35)-H(35A)	0.9800	C(1)-Ni(1)-Ni(2)	52.42(8)
C(35)-H(35B)	0.9800	C(12)-Ni(1)-Ni(2)	97.33(9)
C(35)-H(35C)	0.9800	C(24)-Ni(1)-Ni(2)	74.73(8)
C(36)-H(36A)	0.9800	P(1)-Ni(1)-Ni(2)	167.72(3)
C(36)-H(36B)	0.9800	C(13)-Ni(1)-Ni(2)	48.53(7)
C(36)-H(36C)	0.9800	C(13)-Ni(2)-C(1)	114.87(12)
C(37)-C(38)	1.489(5)	C(13)-Ni(2)-P(2)	100.48(9)
C(37)-C(39)	1.536(5)	C(1)-Ni(2)-P(2)	140.33(9)
C(37)-H(37)	1.0000	C(13)-Ni(2)-Ni(1)	64.49(8)
C(38)-H(38A)	0.9800	C(1)-Ni(2)-Ni(1)	53.73(8)
C(38)-H(38B)	0.9800	P(2)-Ni(2)-Ni(1)	164.95(3)
C(38)-H(38C)	0.9800	C(13)-Ni(2)-C(2)	144.19(11)
C(39)-H(39A)	0.9800	C(1)-Ni(2)-C(2)	36.19(11)

P(2)-Ni(2)-C(2)	114.75(7)	C(5)-C(6)-C(1)	120.1(3)
Ni(1)-Ni(2)-C(2)	80.11(7)	C(5)-C(6)-C(7)	126.2(3)
C(28)-P(1)-C(31)	102.69(14)	C(1)-C(6)-C(7)	113.7(2)
C(28)-P(1)-C(25)	109.53(14)	C(8)-C(7)-C(12)	121.3(3)
C(31)-P(1)-C(25)	103.06(14)	C(8)-C(7)-C(6)	124.7(3)
C(28)-P(1)-Ni(1)	112.11(10)	C(12)-C(7)-C(6)	113.9(3)
C(31)-P(1)-Ni(1)	114.83(10)	C(9)-C(8)-C(7)	120.5(3)
C(25)-P(1)-Ni(1)	113.72(10)	C(9)-C(8)-H(8)	119.7
C(34)-P(2)-C(37)	104.20(16)	C(7)-C(8)-H(8)	119.7
C(34)-P(2)-C(40)	103.92(15)	C(10)-C(9)-C(8)	119.1(3)
C(37)-P(2)-C(40)	111.10(17)	C(10)-C(9)-H(9)	120.5
C(34)-P(2)-Ni(2)	108.99(10)	C(8)-C(9)-H(9)	120.5
C(37)-P(2)-Ni(2)	110.37(12)	C(9)-C(10)-C(11)	120.5(3)
C(40)-P(2)-Ni(2)	117.24(11)	C(9)-C(10)-H(10)	119.7
C(2)-C(1)-C(6)	117.8(3)	C(11)-C(10)-H(10)	119.7
C(2)-C(1)-Ni(2)	89.45(19)	C(10)-C(11)-C(12)	122.0(3)
C(6)-C(1)-Ni(2)	118.1(2)	C(10)-C(11)-H(11)	119.0
C(2)-C(1)-Ni(1)	127.9(2)	C(12)-C(11)-H(11)	119.0
C(6)-C(1)-Ni(1)	113.6(2)	C(11)-C(12)-C(7)	116.6(3)
Ni(2)-C(1)-Ni(1)	73.85(10)	C(11)-C(12)-Ni(1)	128.6(2)
C(3)-C(2)-C(1)	120.8(3)	C(7)-C(12)-Ni(1)	114.6(2)
C(3)-C(2)-Ni(2)	132.1(2)	C(14)-C(13)-C(18)	117.2(3)
C(1)-C(2)-Ni(2)	54.36(15)	C(14)-C(13)-Ni(2)	123.7(2)
C(3)-C(2)-H(2)	119.6	C(18)-C(13)-Ni(2)	118.1(2)
C(1)-C(2)-H(2)	119.6	C(14)-C(13)-Ni(1)	121.2(2)
Ni(2)-C(2)-H(2)	84.9	C(18)-C(13)-Ni(1)	91.61(18)
C(4)-C(3)-C(2)	120.4(3)	Ni(2)-C(13)-Ni(1)	66.98(9)
C(4)-C(3)-H(3)	119.8	C(15)-C(14)-C(13)	121.5(3)
C(2)-C(3)-H(3)	119.8	C(15)-C(14)-H(14)	119.2
C(3)-C(4)-C(5)	120.2(3)	C(13)-C(14)-H(14)	119.2
C(3)-C(4)-H(4)	119.9	C(14)-C(15)-C(16)	120.3(3)
C(5)-C(4)-H(4)	119.9	C(14)-C(15)-H(15)	119.8
C(6)-C(5)-C(4)	120.7(3)	C(16)-C(15)-H(15)	119.8
C(6)-C(5)-H(5)	119.7	C(17)-C(16)-C(15)	119.6(3)
C(4)-C(5)-H(5)	119.7	C(17)-C(16)-H(16)	120.2

C(15)-C(16)-H(16)	120.2	H(26A)-C(26)-H(26C)	109.5
C(16)-C(17)-C(18)	120.8(3)	H(26B)-C(26)-H(26C)	109.5
C(16)-C(17)-H(17)	119.6	C(25)-C(27)-H(27A)	109.5
C(18)-C(17)-H(17)	119.6	C(25)-C(27)-H(27B)	109.5
C(17)-C(18)-C(13)	120.5(3)	H(27A)-C(27)-H(27B)	109.5
C(17)-C(18)-C(19)	123.7(3)	C(25)-C(27)-H(27C)	109.5
C(13)-C(18)-C(19)	115.7(3)	H(27A)-C(27)-H(27C)	109.5
C(20)-C(19)-C(24)	121.7(3)	H(27B)-C(27)-H(27C)	109.5
C(20)-C(19)-C(18)	123.9(3)	C(29)-C(28)-C(30)	110.4(3)
C(24)-C(19)-C(18)	114.3(3)	C(29)-C(28)-P(1)	112.8(2)
C(21)-C(20)-C(19)	120.1(3)	C(30)-C(28)-P(1)	116.7(2)
C(21)-C(20)-H(20)	119.9	C(29)-C(28)-H(28)	105.3
C(19)-C(20)-H(20)	119.9	C(30)-C(28)-H(28)	105.3
C(22)-C(21)-C(20)	119.1(3)	P(1)-C(28)-H(28)	105.3
C(22)-C(21)-H(21)	120.4	C(28)-C(29)-H(29A)	109.5
C(20)-C(21)-H(21)	120.4	C(28)-C(29)-H(29B)	109.5
C(21)-C(22)-C(23)	121.0(3)	H(29A)-C(29)-H(29B)	109.5
C(21)-C(22)-H(22)	119.5	C(28)-C(29)-H(29C)	109.5
C(23)-C(22)-H(22)	119.5	H(29A)-C(29)-H(29C)	109.5
C(22)-C(23)-C(24)	121.7(3)	H(29B)-C(29)-H(29C)	109.5
C(22)-C(23)-H(23)	119.1	C(28)-C(30)-H(30A)	109.5
C(24)-C(23)-H(23)	119.1	C(28)-C(30)-H(30B)	109.5
C(23)-C(24)-C(19)	116.3(3)	H(30A)-C(30)-H(30B)	109.5
C(23)-C(24)-Ni(1)	134.3(2)	C(28)-C(30)-H(30C)	109.5
C(19)-C(24)-Ni(1)	109.3(2)	H(30A)-C(30)-H(30C)	109.5
C(27)-C(25)-C(26)	111.0(3)	H(30B)-C(30)-H(30C)	109.5
C(27)-C(25)-P(1)	118.5(2)	C(33)-C(31)-C(32)	110.2(3)
C(26)-C(25)-P(1)	111.8(2)	C(33)-C(31)-P(1)	110.5(2)
C(27)-C(25)-H(25)	104.7	C(32)-C(31)-P(1)	113.4(2)
C(26)-C(25)-H(25)	104.7	C(33)-C(31)-H(31)	107.5
P(1)-C(25)-H(25)	104.7	C(32)-C(31)-H(31)	107.5
C(25)-C(26)-H(26A)	109.5	P(1)-C(31)-H(31)	107.5
C(25)-C(26)-H(26B)	109.5	C(31)-C(32)-H(32A)	109.5
H(26A)-C(26)-H(26B)	109.5	C(31)-C(32)-H(32B)	109.5
C(25)-C(26)-H(26C)	109.5	H(32A)-C(32)-H(32B)	109.5

C(31)-C(32)-H(32C)	109.5	H(36B)-C(36)-H(36C)	109.5
H(32A)-C(32)-H(32C)	109.5	C(38)-C(37)-C(39)	113.6(3)
H(32B)-C(32)-H(32C)	109.5	C(38)-C(37)-P(2)	113.7(3)
C(31)-C(33)-H(33A)	109.5	C(39)-C(37)-P(2)	115.7(2)
C(31)-C(33)-H(33B)	109.5	C(38)-C(37)-H(37)	104.0
H(33A)-C(33)-H(33B)	109.5	C(39)-C(37)-H(37)	104.0
C(31)-C(33)-H(33C)	109.5	P(2)-C(37)-H(37)	104.0
H(33A)-C(33)-H(33C)	109.5	C(41)-C(40)-C(42)	110.0(3)
H(33B)-C(33)-H(33C)	109.5	C(41)-C(40)-P(2)	111.4(2)
C(36)-C(34)-C(35)	109.3(3)	C(42)-C(40)-P(2)	117.9(2)
C(36)-C(34)-P(2)	111.7(2)	C(41)-C(40)-H(40)	105.5
C(35)-C(34)-P(2)	109.7(2)	C(42)-C(40)-H(40)	105.5
C(36)-C(34)-H(34)	108.7	P(2)-C(40)-H(40)	105.5
C(35)-C(34)-H(34)	108.7	C(40)-C(41)-H(41A)	109.5
P(2)-C(34)-H(34)	108.7	C(40)-C(41)-H(41B)	109.5
C(34)-C(35)-H(35A)	109.5	H(41A)-C(41)-H(41B)	109.5
C(34)-C(35)-H(35B)	109.5	C(40)-C(41)-H(41C)	109.5
H(35A)-C(35)-H(35B)	109.5	H(41A)-C(41)-H(41C)	109.5
C(34)-C(35)-H(35C)	109.5	H(41B)-C(41)-H(41C)	109.5
H(35A)-C(35)-H(35C)	109.5	C(40)-C(42)-H(42A)	109.5
H(35B)-C(35)-H(35C)	109.5	C(40)-C(42)-H(42B)	109.5
C(34)-C(36)-H(36A)	109.5	H(42A)-C(42)-H(42B)	109.5
C(34)-C(36)-H(36B)	109.5	C(40)-C(42)-H(42C)	109.5
H(36A)-C(36)-H(36B)	109.5	H(42A)-C(42)-H(42C)	109.5
C(34)-C(36)-H(36C)	109.5	H(42B)-C(42)-H(42C)	109.5
H(36A)-C(36)-H(36C)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table S17. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **4**$^{i\text{-Pr}}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	21(1)	22(1)	26(1)	1(1)	-7(1)	-8(1)
Ni(2)	25(1)	22(1)	24(1)	-1(1)	-6(1)	-7(1)
P(1)	24(1)	22(1)	27(1)	0(1)	-11(1)	-7(1)
P(2)	27(1)	23(1)	28(1)	0(1)	-2(1)	-9(1)
C(1)	21(1)	26(2)	27(2)	-2(1)	-7(1)	-5(1)
C(2)	22(2)	26(2)	27(2)	-3(1)	-6(1)	-3(1)
C(3)	33(2)	30(2)	27(2)	-3(1)	-7(1)	-4(1)
C(4)	31(2)	34(2)	34(2)	-6(1)	-15(1)	-3(1)
C(5)	27(2)	32(2)	40(2)	-6(1)	-12(1)	-9(1)
C(6)	24(2)	27(2)	33(2)	-4(1)	-11(1)	-8(1)
C(7)	27(2)	29(2)	30(2)	-2(1)	-7(1)	-13(1)
C(8)	37(2)	47(2)	42(2)	2(2)	-14(2)	-25(2)
C(9)	43(2)	54(2)	42(2)	2(2)	-6(2)	-34(2)
C(10)	43(2)	41(2)	32(2)	4(1)	-8(2)	-23(2)
C(11)	32(2)	33(2)	30(2)	1(1)	-8(1)	-14(1)
C(12)	27(2)	25(2)	30(2)	-4(1)	-6(1)	-11(1)
C(13)	30(2)	22(1)	25(2)	1(1)	-10(1)	-9(1)
C(14)	32(2)	28(2)	32(2)	-2(1)	-8(1)	-9(1)
C(15)	41(2)	34(2)	27(2)	0(1)	-6(1)	-9(2)
C(16)	55(2)	49(2)	31(2)	-1(2)	-17(2)	-20(2)
C(17)	38(2)	44(2)	42(2)	-3(2)	-19(2)	-17(2)
C(18)	29(2)	26(2)	33(2)	-3(1)	-11(1)	-11(1)
C(19)	25(2)	22(2)	39(2)	-1(1)	-10(1)	-7(1)
C(20)	30(2)	34(2)	49(2)	-4(2)	-15(2)	-15(1)
C(21)	26(2)	35(2)	60(2)	2(2)	-8(2)	-16(2)
C(22)	29(2)	32(2)	43(2)	5(2)	-1(2)	-12(1)
C(23)	28(2)	25(2)	35(2)	-1(1)	-6(1)	-7(1)
C(24)	22(1)	20(1)	32(2)	1(1)	-8(1)	-5(1)
C(25)	34(2)	29(2)	38(2)	1(1)	-14(1)	-13(1)
C(26)	41(2)	34(2)	58(2)	-3(2)	-26(2)	-14(2)
C(27)	54(2)	27(2)	50(2)	5(2)	-23(2)	-17(2)
C(28)	26(2)	27(2)	32(2)	1(1)	-7(1)	-8(1)
C(29)	48(2)	47(2)	28(2)	3(2)	-12(2)	-15(2)
C(30)	35(2)	40(2)	40(2)	-10(2)	-2(2)	-8(2)

C(31)	34(2)	28(2)	38(2)	3(1)	-21(2)	-9(1)
C(32)	35(2)	36(2)	56(2)	2(2)	-27(2)	-11(2)
C(33)	52(2)	47(2)	39(2)	8(2)	-29(2)	-17(2)
C(34)	27(2)	29(2)	40(2)	-6(1)	-4(1)	-6(1)
C(35)	31(2)	50(2)	59(2)	-2(2)	1(2)	-20(2)
C(36)	41(2)	44(2)	57(2)	-7(2)	-24(2)	-2(2)
C(37)	40(2)	37(2)	49(2)	9(2)	-2(2)	-13(2)
C(38)	44(2)	43(2)	59(2)	4(2)	7(2)	-20(2)
C(39)	45(2)	30(2)	66(3)	12(2)	-6(2)	-10(2)
C(40)	49(2)	29(2)	35(2)	-4(1)	-12(2)	-15(2)
C(41)	60(3)	56(3)	77(3)	-21(2)	-31(2)	-18(2)
C(42)	60(3)	44(2)	42(2)	-13(2)	-2(2)	-18(2)

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