

Supporting Information

A Useful Method for the Preparation of Low-coordinate Ni(I) Complexes *via* Transformations of the Ni(I) bis(amido) Complex $\text{K}\{\text{Ni}[\text{N}(\text{SiMe}_3)(2,6\text{-}i\text{Pr-C}_6\text{H}_3)]_2\}$

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1. Experimental Details, Synthetic Procedures, Spectroscopic Characterization

General Considerations. Unless otherwise stated, all reactions and manipulations were carried out in a MBraun Lab Master DP glovebox or using standard Schlenk techniques under a nitrogen atmosphere. Pentane, toluene, and 1,2-difluorobenzene were purchased from Sigma Aldrich. Diethyl ether was purchased from Honeywell and tetrahydrofuran was purchased from Macron Chemicals. Pentane, toluene, tetrahydrofuran, diethyl ether and 1,2-difluorobenzene were dried and degassed using a JC Meyers Phoenix SDS solvent purification system. C₆D₆ was purchased from Cambridge Isotope Laboratories, dried over Na/K alloy and then degassed by four freeze-pump-thaw cycles. All NMR spectra were collected at ambient temperature (ca. 22°C) on Bruker AVB-400, AV-500, AV-600 or AVQ-400 NMR spectrometers, each equipped with a 5 mm BB probe, and referenced to the residual proteo solvent signals. Solution magnetic susceptibilities were determined by ¹H NMR spectroscopy using Evans' method¹ and the values given are the average of 3 measurements for each compound. Elemental analyses were performed by the UC Berkeley College of Chemistry Microanalytical facility. The abbreviation "DIPP" refers to a 2,6-diisopropylphenyl moiety. The abbreviation "DPPE" refers to 1,2-(bisdiphenylphosphino)ethane. The abbreviation "IPr" refers to the N-heterocyclic carbene N,N'-1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene. DPPE and PtBu₃ were purchased from Sigma Aldrich and used as received. NEt₃•HCl was purchased from Sigma Aldrich and sublimed before use. PiPr₃ was purchased from STREM chemical and used as received. 2,6-di-*tert*-butyl-4-methyl-phenol was purchased from Pfaltz and Bauer and used as received. IPr was prepared according to the standard literature procedure.²

X-ray Diffraction Experiments. Single crystal X-ray diffraction experiments were carried out at UC Berkeley CHEXRAY crystallographic facility. Measurements of compounds **3**, **4**, **5**, **6**, **7** and **8** were performed on a Bruker APEX-II CCD area detector using Mo K α radiation (λ = 0.71073 Å) monochromated using QUAZAR multilayer mirrors. Specific details of each experiment can be found below, in section 5 at the end of this document and in the included crystallographic information files.

Table S1: Experimental Details

	Detector Distance	Image Width	Exposure Time
Compound 3	40mm	0.5°	5 seconds
Compound 4	40mm	0.5°	5 seconds
Compound 5	40mm	0.5°	5 seconds
Compound 6	40mm	0.5°	10 seconds
Compound 7	40mm	0.5°	10 seconds
Compound 8	40mm	0.5°	5 seconds

¹ Evans, D. F. *J. Chem. Soc.*, **1959**, 2003

² Jafarpour, L.; Stevens, E. D.; Nolan, S. P. *J. Organomet. Chem.*, **2000**, 606, 49

K{Ni[N(SiMe₃)DIPP]₂} (2). Full preparation and characterization data for **2** is available in a prior publication.³

(IPr)Ni-N(SiMe₃)DIPP (3). To a 20 mL scintillation vial was added **2** (0.100 g, 0.168 mmol), IPr (0.066 g, 0.170 mmol) and 6 mL Et₂O, forming a yellow solution. To a separate 20 mL scintillation vial was added NEt₃•HCl (0.023 g, 0.168 mmol) and a magnetic stir bar and both vials were cooled to -30 °C. The chilled solution of **2** and IPr was then transferred to the vial containing the NEt₃•HCl and the resulting suspension was stirred while warming to room temperature for 1 hour, during which the color of the mixture changed from yellow to dark orange/brown. The mixture was then filtered and the volatile components were removed under reduced pressure. The resulting residue was dissolved in 1.5 mL dimethoxyethane upon which was layered 6 mL of pentane. The layered solution was then placed in the -30 °C freezer overnight, yielding 0.106 g of **3** (91%) as yellow/orange plates which were isolated by decantation, washed with 4 aliquots of 2 mL of -30 °C pentane and dried in vacuo. Full characterization data for **3** is available in a prior publication. For convenience, its spectroscopic properties are reproduced here.³ ¹H NMR (400 MHz, C₆D₆, 21°C) δ 22.20 (2H), 10.93 (4H), 9.37 (2H), 8.37 (*p*-Ar-*H*, 1H), 4.17 (4H), 3.99 (2H), 3.82 (-Si(CH₃)₃, 9H), 3.56 (Ar-CH(CH₃)₂, 12H), 1.88 (Ar-CH(CH₃)₂, 12H), -0.65 (Ar-CH(CH₃)₂, 6H), -6.27 (Ar-CH(CH₃)₂, 6H), -11.69 (2H). Assignment of shifts to particular protons is given where integration allows unambiguous assignment. μ_{eff} = 2.12 μ_B (C₆D₆, 21°C, Evans' method).

(*t*Bu₃P)Ni-N(SiMe₃)DIPP (4). To a 20 mL scintillation vial was added **2** (0.138 g, 0.232 mmol), PtBu₃ (0.047 g, 0.232 mmol) and 8 mL Et₂O, forming a yellow solution. To a separate 20 mL scintillation vial was added NEt₃•HCl (0.032 g, 0.232 mmol) and a magnetic stir bar and both vials were cooled to -30 °C. The chilled solution of **2** and PtBu₃ was then transferred to the vial containing the NEt₃•HCl, resulting in an immediate color change from yellow to dark yellow/orange. The resulting suspension was stirred while warming to room temperature for 1.5 hours, at which point the color of the mixture was dark orange. The mixture was then filtered and the volatile components were removed under reduced pressure. The resulting residue was dissolved in 8 mL Et₂O upon which was layered 12 mL of pentane. The layered solution was placed in the -30 °C freezer overnight, yielding 0.081 g of **4** as orange blocks which were collected by decantation and dried in vacuo. The volatile components of the supernatant were removed under reduced pressure, the resulting residue was washed with 2 mL of -30 °C pentane, and a second crystallization was set up in an identical fashion to the first using 3 mL of Et₂O and 6 mL pentane, yielding an additional 0.020 g of **4**. Total yield: 0.101 g (85%). ¹H NMR (500 MHz, C₆D₆, 20 °C) δ 24.97 (2H, Ar-CH(CH₃)₂ or *m*-Ar-*H*), 10.94 (1H, *p*-Ar-*H*), 3.30 (27H, P(C(CH₃)₃)₃, overlaps with -SiMe₃ signal), 3.21 (9H, Si(CH₃)₃, overlaps with -PtBu₃ signal), -0.51 (6H, Ar-CH(CH₃)₂), -6.14 (6H, Ar-CH(CH₃)₂), -20.73 (2H, Ar-CH(CH₃)₂ or *m*-Ar-*H*). μ_{eff} = 2.35 μ_B (C₆D₆, 20°C, Evans' method). Anal. Calcd. for C₂₇H₅₃NNiPSi: C, 63.65%; H, 10.49%; N, 2.75%. Found: C, 63.73%; H, 10.45%; N, 2.82%. Crystals suitable for single crystal X-ray diffraction studies were obtained from the workup described above.

(*i*Pr₃P)Ni-N(SiMe₃)DIPP (5). To a 20 mL scintillation vial was added **2** (0.150 g, 0.252 mmol), PiPr₃ (0.041 g, 0.256 mmol) and 6 mL Et₂O, forming a yellow solution. To a separate 20 mL scintillation vial was added NEt₃•HCl (0.035 g, 0.255 mmol) and a magnetic stir bar and both

³ Lipschutz, M. I.; Yang, X.; Chatterjee, R.; Tilley, T. D. *J. Am. Chem. Soc.* **2013**, *135*, 15298

vials were cooled to -30 °C. The chilled solution of **2** and $\text{P}(\text{iPr})_3$ was then transferred to the vial containing the $\text{NEt}_3 \cdot \text{HCl}$, resulting in an immediate color change from yellow to dark orange. The resulting suspension was stirred while warming to room temperature for 30 minutes. The mixture was then filtered and the volatile components were removed under reduced pressure. The resulting gooeey residue was dissolved in 1.5 mL of pentane and placed in the -30 °C freezer. Over 3 days, large, light orange blocks crystallized out of solution. These were collected by decantation and dried in vacuo, yielding 0.079 g of **5** (69%). Analysis of the mother liquor by ^1H NMR indicates that additional **5** is present in the mother liquor, but due to its extreme solubility, no further product could be crystallized. ^1H NMR (500 MHz, C_6D_6 , 20 °C) δ 26.80 (2H, $\text{Ar-CH}(\text{CH}_3)_2$ or *m*-Ar-H), 15.28 (3H, $\text{P}(\text{CH}(\text{CH}_3)_2)_3$), 11.68 (1H, *p*-Ar-H), 1.94 (6H, $\text{Ar-CH}(\text{CH}_3)_2$, overlaps with $\text{P}(\text{CH}(\text{CH}_3)_2)_3$), 1.82 (18H, $\text{P}(\text{CH}(\text{CH}_3)_2)_3$, overlaps with $\text{Ar-CH}(\text{CH}_3)_2$), -0.61 (9H, $\text{Si}(\text{CH}_3)_3$), -10.62 (6H, $\text{Ar-CH}(\text{CH}_3)_2$), -11.97 (2H, $\text{Ar-CH}(\text{CH}_3)_2$ or *m*-Ar-H). $\mu_{\text{eff}} = 2.55 \mu_{\text{B}}$ (C_6D_6 , 20°C, Evans' method). Anal. Calcd. for $\text{C}_{24}\text{H}_{47}\text{NNiPSi}$: C, 61.67%; H, 10.14%; N, 3.00%. Found: C, 61.33%; H, 10.46%; N, 2.96%. Crystals suitable for single crystal X-ray diffraction studies were obtained from the workup described above.

(DPPE)Ni-N(SiMe₃)DIPP (6). To a 20 mL scintillation vial was added **2** (0.100 g, 0.168 mmol), 1,2-(diphenylphosphino)-ethane (DPPE) (0.068 g, 0.171 mmol) and 8 mL Et_2O which, after several minutes of swirling, formed an orange solution. To a separate 20 mL scintillation vial was added $\text{NEt}_3 \cdot \text{HCl}$ (0.024 g, 0.174 mmol) and a magnetic stirbar and both vials were cooled to -30 °C. The chilled solution of **2** and DPPE was then transferred to the vial containing the $\text{NEt}_3 \cdot \text{HCl}$, resulting in an immediate darkening of the orange color. The resulting suspension was stirred while warming to room temperature for 3 hours, at which point the color of the solution was red. The mixture was then filtered and the volatile components were removed under reduced pressure. The resulting residue was dissolved in 2.5 mL of toluene upon which was layered 8 mL of pentane. The layered solution was placed in the -30 °C freezer overnight, yielding 0.085 g of **6** (77%) as red plates, which were isolated by decantation, washed with 2 mL of -30 °C pentane and dried in vacuo. The ^1H NMR spectrum of **5** reveals only a wavy, uneven baseline with no characteristic peaks. We attribute this to the paramagnetism of **5**. $\mu_{\text{eff}} = 1.53 \mu_{\text{B}}$ (C_6D_6 , 21°C, Evans' method). Anal. Calcd. for $\text{C}_{41}\text{H}_{50}\text{NNiP}_2\text{Si}$: C, 69.79%; H, 7.14%; N, 1.99%. Found: C, 70.15%; H, 6.94%; N, 2.26%. Crystals suitable for single crystal X-ray diffraction studies were obtained from the workup described above.

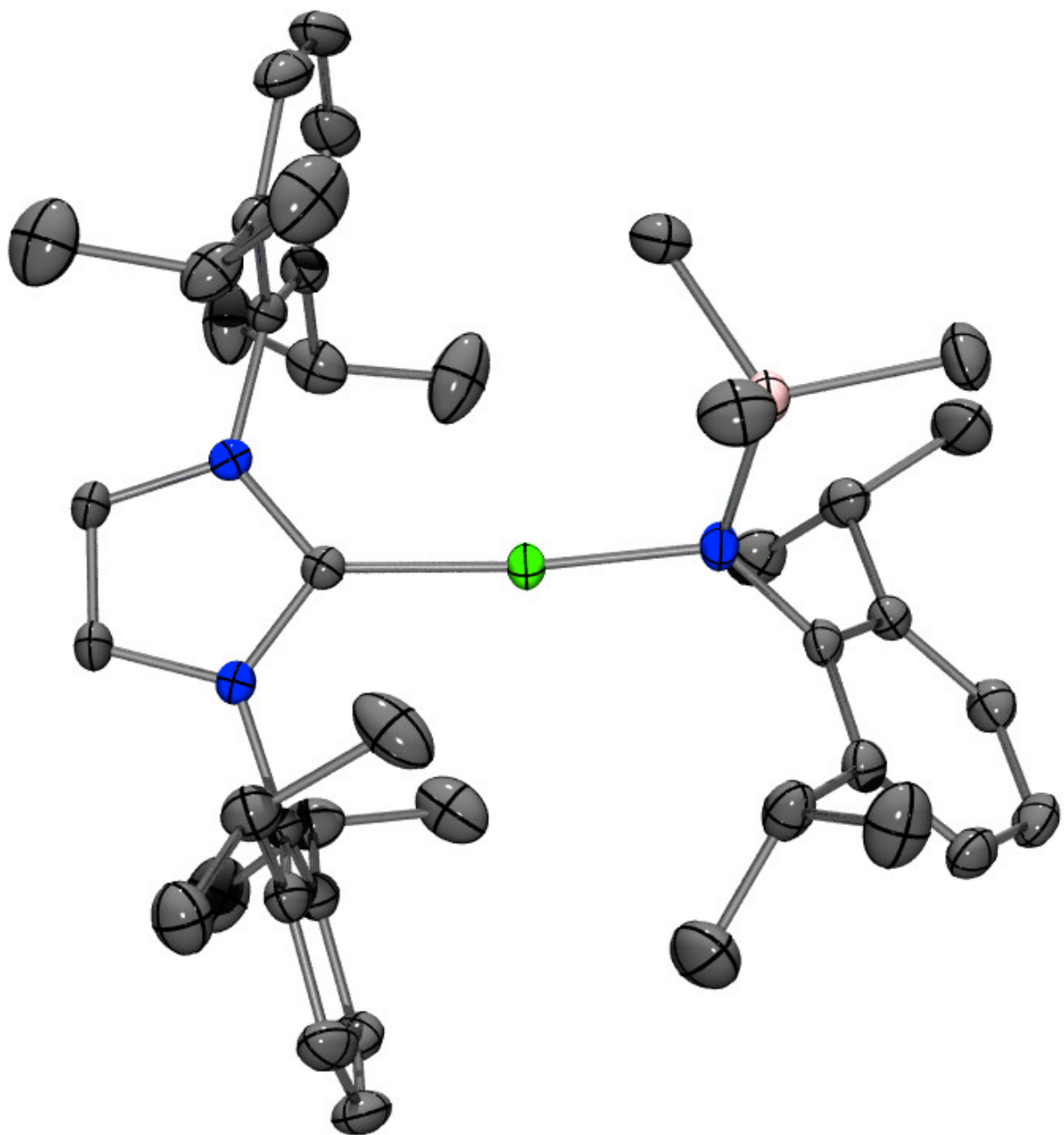
(IPr)Ni[(2,6-di-*tert*-butyl-4-methyl) C_6H_2]O (7). To a 20 mL scintillation vial was added **3** (0.135 g, 0.194 mmol) and 6 mL of THF, forming a yellow/orange solution. To this stirring solution at ambient temperature was added a solution of 2,6-di-*tert*-butyl-4-methylphenol (0.043 g, 0.194 mmol) in 4 mL of THF resulting in an immediate color change from yellow/orange to red. Stirring was continued for 30 minutes, then the mixture was filtered and the volatile components removed under reduced pressure. The resulting residue was dissolved in 2.5 mL toluene upon which was layered 8 mL of pentane. The layered solution was placed in the -30 °C freezer overnight, yielding 0.107 g of **7** (80%) as large red blocks, which were isolated by decantation and dried in vacuo. After extensive drying in this manner (>8 hours), approximately 0.25 eq. of toluene of crystallization remained in the sample (quantified by ^1H NMR spectroscopy using an internal standard). The yield listed above accounts for the presence of this toluene. ^1H NMR (400 MHz, C_6D_6 , 24 °C) δ 21.38 (12H), 18.82 (4H), 16.69 (2H), 11.18 (2H), 6.80 (3H), 2.84 (12H), -0.94 (4H), -3.49 (2H), -7.09 (18H). $\mu_{\text{eff}} = 1.80 \mu_{\text{B}}$ (C_6D_6 , 20°C, Evans'

method). Anal. Calcd. for $C_{42}H_{59}N_2NiO + 0.25(C_7H_8)$: C, 76.19%; H, 8.92%; N, 4.06%. Found: C, 76.54%; H, 9.12%; N, 3.72%. Crystals suitable for single crystal X-ray diffraction studies were obtained from the workup described above.

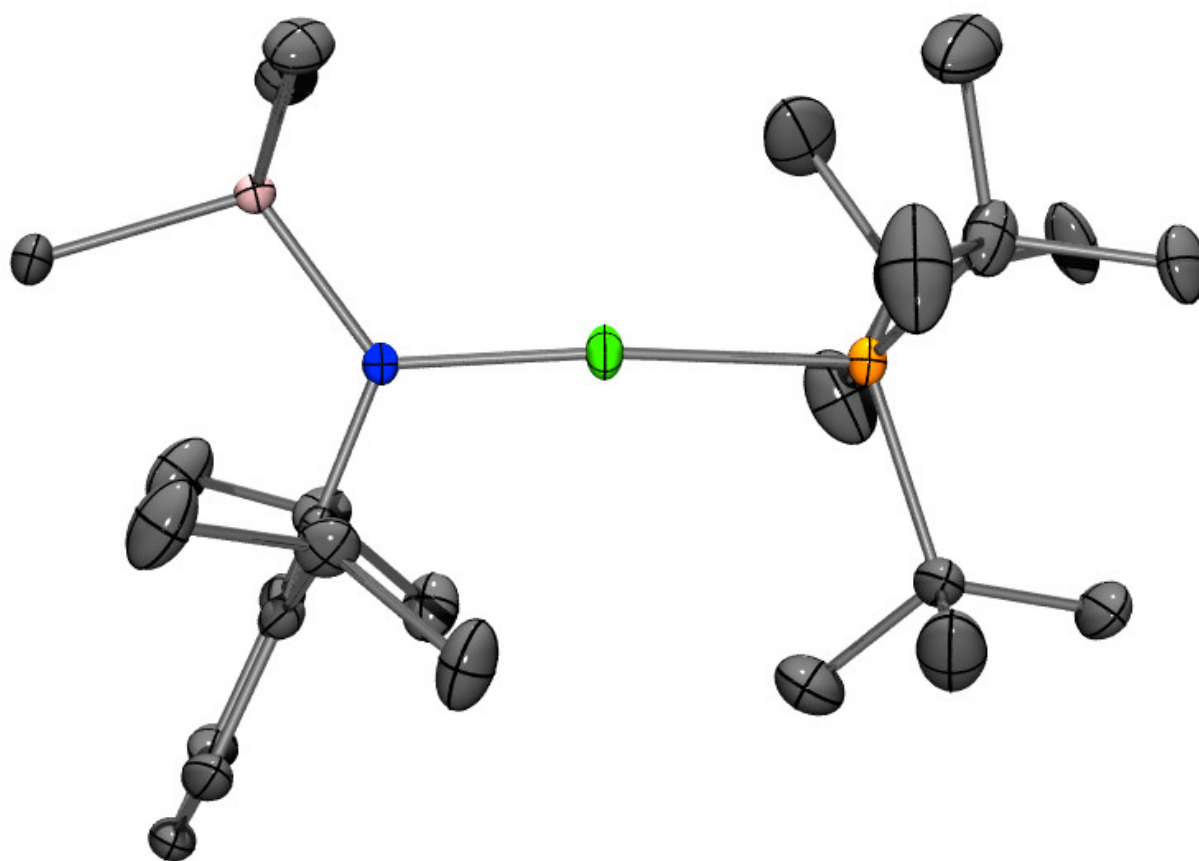
(*t*Bu₃P)Ni[η^5 -(2,6-di-*tert*-butyl-4-methyl)C₆H₂O] (8). To a 20 mL scintillation vial was added **4** (0.094 g, 0.185 mmol) and 5 mL of THF which, after several minutes of stirring, formed an orange solution which was cooled to -30 °C. To this chilled, stirring solution was added a -30 °C solution of 2,6-di-*tert*-butyl-4-methylphenol (0.041 g, 0.186 mmol) in 2 mL of THF. The solution was allowed to warm to ambient temperature and stirred for 3 hours, at which point the solution was green. The volatile components were then removed under reduced pressure, resulting in a royal blue residue. The residue was extracted with 2 aliquots of 2 mL of 1,2-difluorobenzene, the extracts were filtered and the volatile components removed under reduced pressure. The resulting residue was washed with 3 aliquots of 2 mL of -30 °C pentane, dried in vacuo, then redissolved in 3 mL of 1,2-difluorobenzene, upon which was layered 8 mL of pentane. The layered solution was then placed in the -30 °C freezer for 2 days, yielding 0.063 g of **8** (72%) as clusters of dark blue plates, which were isolated by decantation and dried in vacuo. The ¹H NMR spectrum of **7** reveals only a single, extremely broad peak. ¹H NMR (500 MHz, C₆D₆, 20 °C) δ 4.90. $\mu_{\text{eff}} = 2.29 \mu_B$ (C₆D₆, 20°C, Evans' method). Anal. Calcd. for C₂₇H₅₀NiOP: C, 67.51%; H, 10.49%. Found: C, 67.49%; H, 10.46%. Crystals suitable for single crystal X-ray diffraction studies were obtained from the workup described above.

2. Enlarged ORTEP Diagrams

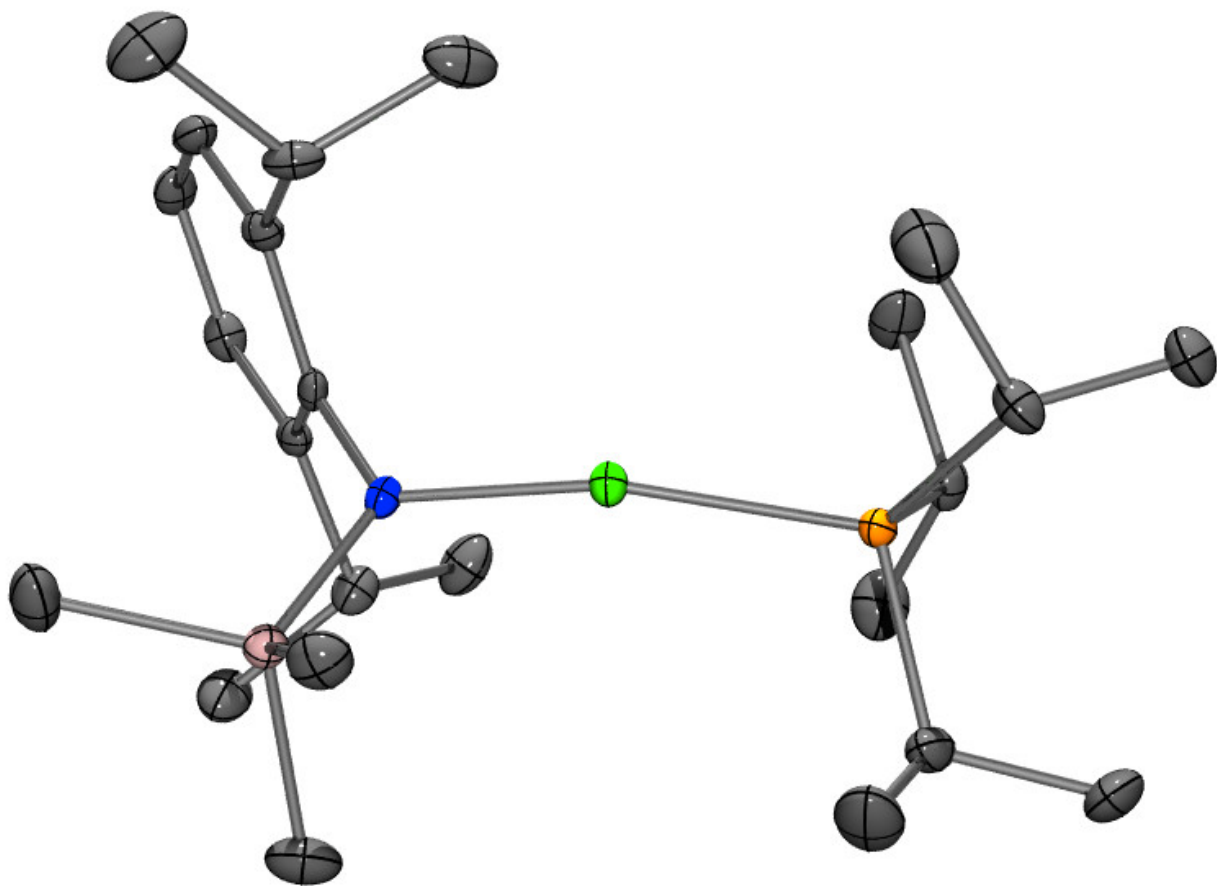
Carbon atoms are shown in dark grey, Nickel in green, Silicon in pink, Nitrogen in blue, Phosphorous in orange and Oxygen in red in all of the following diagrams. All thermal ellipsoids are shown at 50% probability. Full bond length and angle tables for each compound are provided as separate documents.



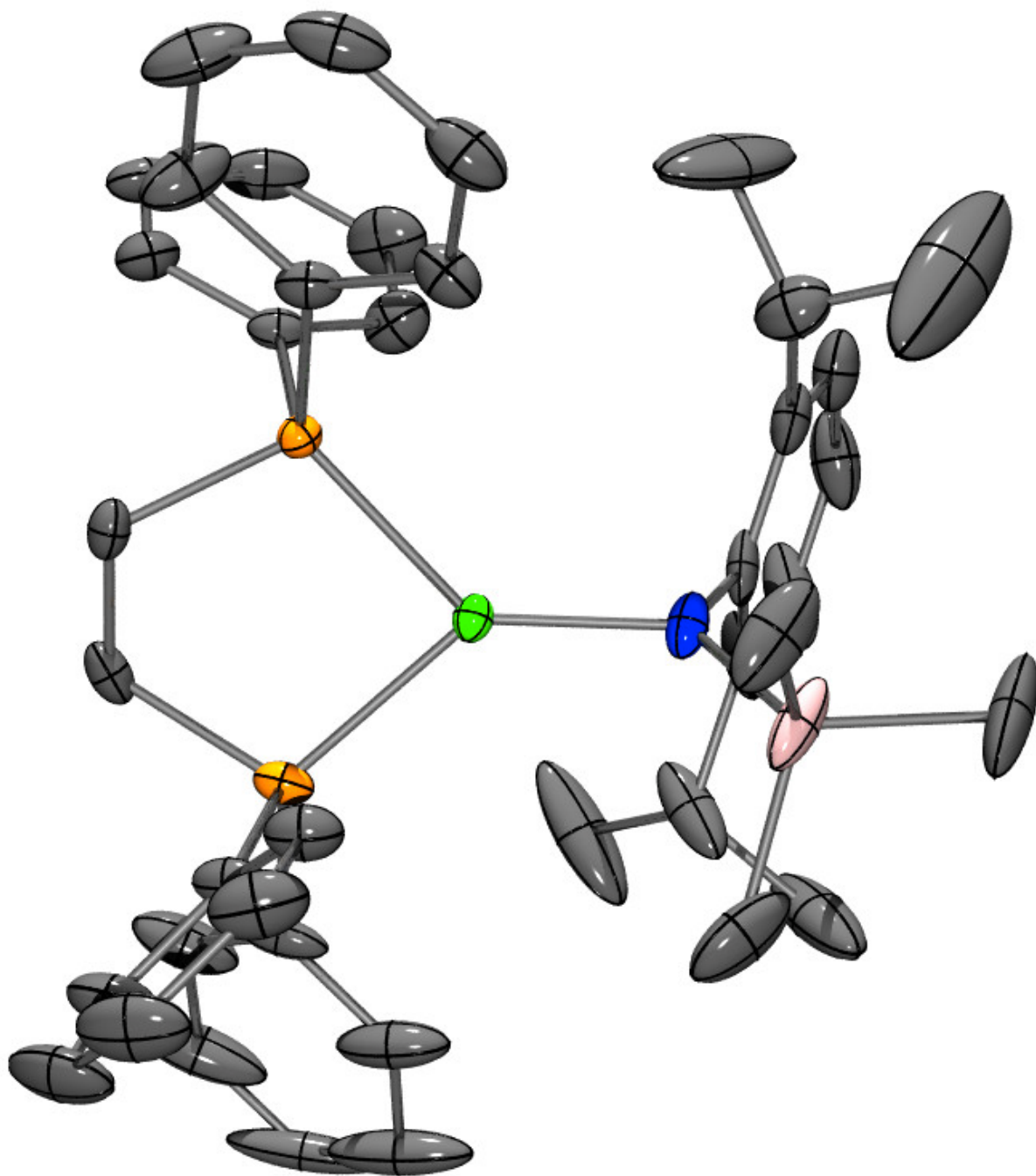
ORTEP diagram for compound 3.



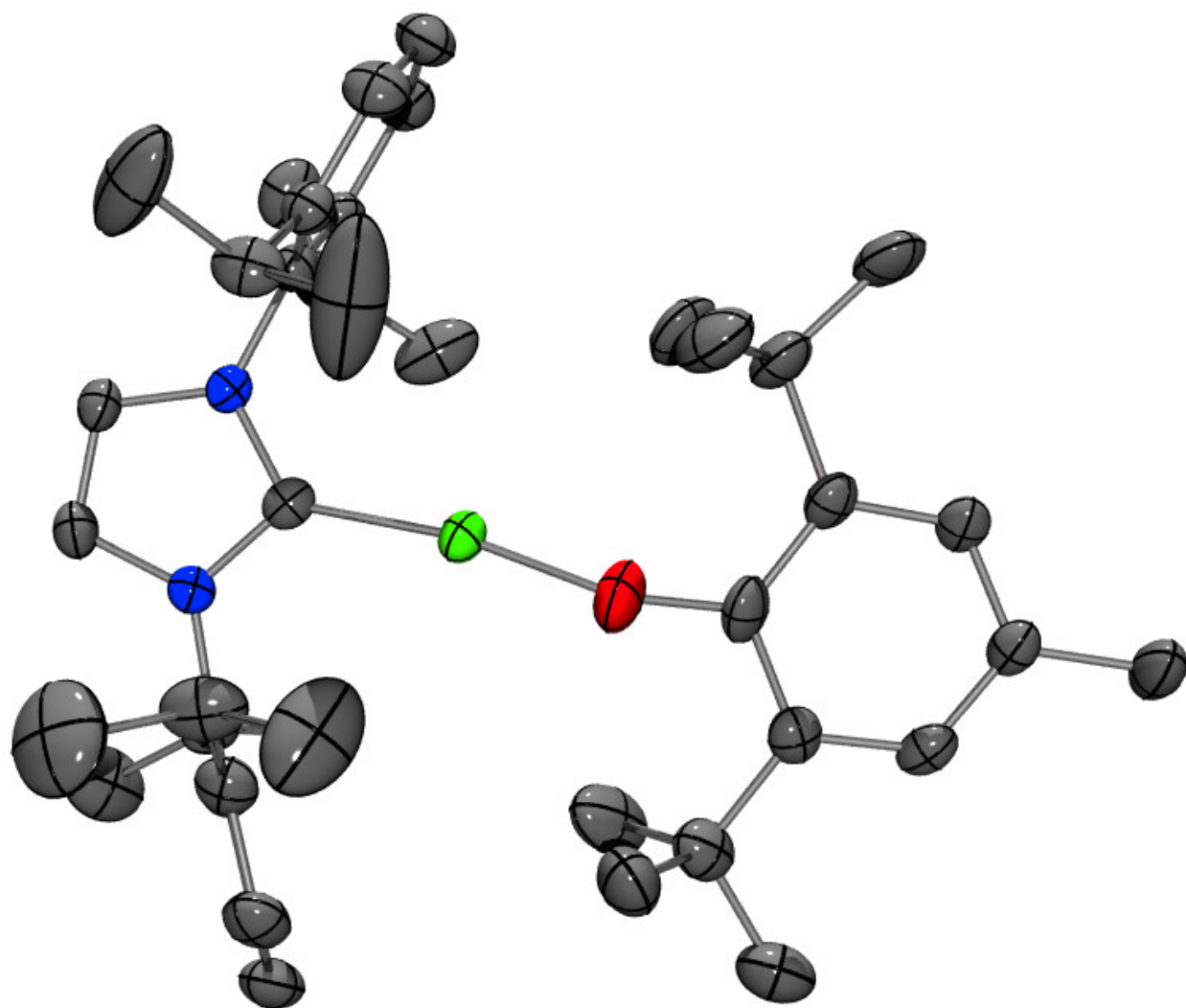
ORTEP diagram for compound 4.



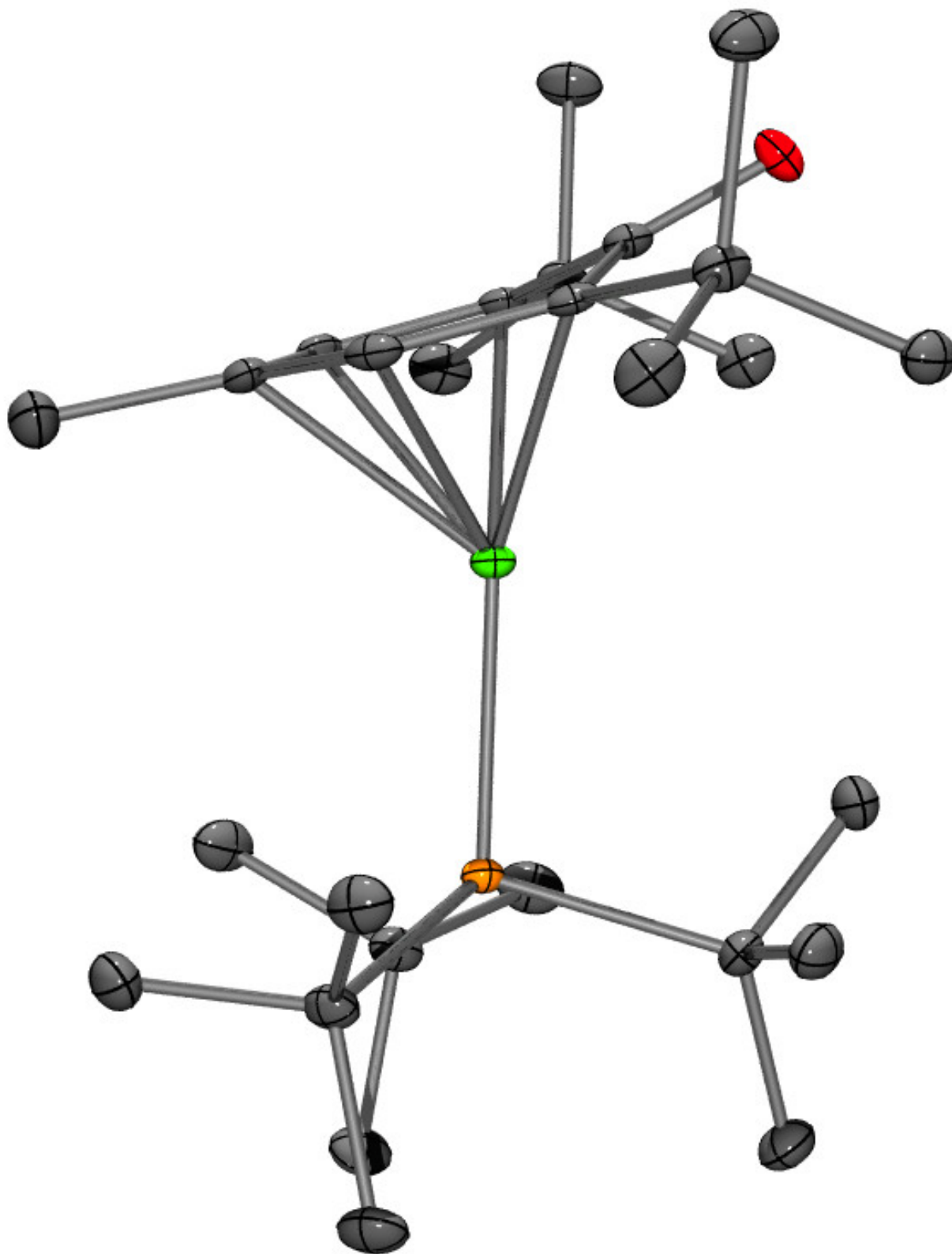
ORTEP diagram for compound **5**.



ORTEP diagram for compound **6**.



ORTEP diagram for compound 7.



ORTEP diagram for compound **8**.

3. X-ray Data Tables

General X-ray Data

Table S2: Compound 3

Empirical formula	C ₄₂ H ₆₂ N ₃ Ni Si	
Formula weight	695.75	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.4100(4) Å	a = 90°.
	b = 18.0926(7) Å	b = 99.612(2)°.
	c = 22.1319(8) Å	g = 90°.
Volume	4109.9(3) Å ³	
Z	4	
Density (calculated)	1.124 Mg/m ³	
Absorption coefficient	0.531 mm ⁻¹	
F(000)	1508	
Crystal size	0.19 x 0.15 x 0.07 mm ³	
Theta range for data collection	1.46 to 27.55°.	
Index ranges	-13 ≤ h ≤ 13, -23 ≤ k ≤ 23, -28 ≤ l ≤ 28	
Reflections collected	62759	
Independent reflections	9320 [R(int) = 0.0439]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9637 and 0.9058	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9320 / 0 / 439	
Goodness-of-fit on F ²	1.024	
Final R indices [I > 2σ(I)]	R1 = 0.0374, wR2 = 0.0837	
R indices (all data)	R1 = 0.0559, wR2 = 0.0922	
Largest diff. peak and hole	0.363 and -0.314 e.Å ⁻³	

Table S3: Compound 4

Empirical formula	C ₂₇ H ₅₃ N Ni P Si	
Formula weight	509.47	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 8.6401(5) Å	a = 90°.
	b = 14.7417(9) Å	b = 92.321(3)°.

	$c = 23.2643(14) \text{ \AA}$	$g = 90^\circ$.
Volume	$2960.7(3) \text{ \AA}^3$	
Z	4	
Density (calculated)	1.143 Mg/m^3	
Absorption coefficient	0.764 mm^{-1}	
F(000)	1116	
Crystal size	$0.13 \times 0.12 \times 0.12 \text{ mm}^3$	
Theta range for data collection	1.64 to 31.50° .	
Index ranges	$-12 \leq h \leq 10$, $-17 \leq k \leq 21$, $-33 \leq l \leq 31$	
Reflections collected	40981	
Independent reflections	8851 [$R(\text{int}) = 0.0297$]	
Completeness to $\theta = 25.00^\circ$	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9139 and 0.9072	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8851 / 0 / 306	
Goodness-of-fit on F^2	1.046	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0462$, $wR2 = 0.1300$	
R indices (all data)	$R1 = 0.0579$, $wR2 = 0.1385$	
Largest diff. peak and hole	0.894 and $-0.428 \text{ e.\AA}^{-3}$	

Table S4: Compound **5**

Empirical formula	$\text{C}_{24} \text{H}_{47} \text{N Ni P Si}$	
Formula weight	467.40	
Temperature	$100(2) \text{ K}$	
Wavelength	$0.71073 \text{ \AA}$	
Crystal system	Monoclinic	
Space group	$P2(1)/n$	
Unit cell dimensions	$a = 11.9515(5) \text{ \AA}$	$a = 90^\circ$.
	$b = 13.9669(5) \text{ \AA}$	$b = 102.4770(10)^\circ$.
	$c = 16.9287(7) \text{ \AA}$	$g = 90^\circ$.
Volume	$2759.09(19) \text{ \AA}^3$	
Z	4	
Density (calculated)	1.125 Mg/m^3	
Absorption coefficient	0.814 mm^{-1}	
F(000)	1020	
Crystal size	$0.10 \times 0.08 \times 0.01 \text{ mm}^3$	
Theta range for data collection	1.91 to 25.37° .	
Index ranges	$-14 \leq h \leq 14$, $-16 \leq k \leq 12$, $-20 \leq l \leq 18$	
Reflections collected	13644	
Independent reflections	4989 [$R(\text{int}) = 0.0423$]	
Completeness to $\theta = 25.00^\circ$	98.7 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.9919 and 0.9230
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4989 / 0 / 266
Goodness-of-fit on F ²	0.991
Final R indices [I>2sigma(I)]	R1 = 0.0383, wR2 = 0.0751
R indices (all data)	R1 = 0.0573, wR2 = 0.0829
Largest diff. peak and hole	0.415 and -0.299 e.Å ⁻³

Table S5: Compound 6

Empirical formula	C41 H50 N Ni P2 Si
Formula weight	705.56
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.2622(5) Å a = 95.201(2)°. b = 10.9582(5) Å b = 102.210(2)°. c = 18.1585(8) Å g = 108.057(2)°.
Volume	1870.53(15) Å ³
Z	2
Density (calculated)	1.253 Mg/m ³
Absorption coefficient	0.665 mm ⁻¹
F(000)	750
Crystal size	0.09 x 0.06 x 0.06 mm ³
Theta range for data collection	1.98 to 25.41°.
Index ranges	-12<=h<=12, -12<=k<=13, -21<=l<=21
Reflections collected	52301
Independent reflections	6884 [R(int) = 0.0321]
Completeness to theta = 25.00°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9612 and 0.9425
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6884 / 7 / 422
Goodness-of-fit on F ²	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.1072
R indices (all data)	R1 = 0.0551, wR2 = 0.1119
Largest diff. peak and hole	1.678 and -1.856 e.Å ⁻³

Table S6: Compound 7

Empirical formula	C42 H59 N2 Ni O
Formula weight	666.60
Temperature	100(2) K
Wavelength	0.71073 Å

Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 18.329(5) Å b = 19.847(5) Å c = 20.428(5) Å	a = 109.439(5)°. b = 106.744(5)°. g = 96.811(5)°.
Volume	6518(3) Å ³	
Z	6	
Density (calculated)	1.019 Mg/m ³	
Absorption coefficient	0.475 mm ⁻¹	
F(000)	2166	
Crystal size	0.08 x 0.06 x 0.06 mm ³	
Theta range for data collection	1.43 to 26.44°.	
Index ranges	-22<=h<=22, -24<=k<=24, -25<=l<=25	
Reflections collected	157318	
Independent reflections	26731 [R(int) = 0.0625]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9721 and 0.9630	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	26731 / 0 / 1288	
Goodness-of-fit on F ²	1.094	
Final R indices [I>2sigma(I)]	R1 = 0.0552, wR2 = 0.1287	
R indices (all data)	R1 = 0.0924, wR2 = 0.1395	
Largest diff. peak and hole	0.937 and -0.652 e.Å ⁻³	

Table S7: Compound 8

Empirical formula	C27 H50 Ni O P	
Formula weight	480.353	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.7648(7) Å b = 16.4415(12) Å c = 16.7346(12) Å	a = 90°. b = 103.794(3)°. g = 90°.
Volume	2609.2(3) Å ³	
Z	4	
Density (calculated)	1.223 Mg/m ³	
Absorption coefficient	0.821 mm ⁻¹	
F(000)	1052	
Crystal size	0.10 x 0.10 x 0.08 mm ³	
Theta range for data collection	1.76 to 25.41°.	
Index ranges	-11<=h<=11, -19<=k<=19, -20<=l<=20	

Reflections collected	50067
Independent reflections	4796 [R(int) = 0.0313]
Completeness to theta = 25.00°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9372 and 0.9224
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4796 / 0 / 287
Goodness-of-fit on F ²	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0231, wR2 = 0.0571
R indices (all data)	R1 = 0.0264, wR2 = 0.0590
Largest diff. peak and hole	0.340 and -0.208 e.Å ⁻³

Full Bond Lengths and Angles Tables

Table S8. Bond lengths [Å] and angles [°] for Compound 3.

C(1)-N(3)	1.363(2)
C(1)-N(2)	1.365(2)
C(1)-Ni(1)	1.9123(16)
C(2)-C(3)	1.346(2)
C(2)-N(2)	1.385(2)
C(2)-H(2)	0.9500
C(3)-N(3)	1.388(2)
C(3)-H(3)	0.9500
C(4)-C(9)	1.393(2)
C(4)-C(5)	1.402(2)
C(4)-N(3)	1.443(2)
C(5)-C(6)	1.390(3)
C(5)-C(13)	1.525(2)
C(6)-C(7)	1.384(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.374(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.397(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.514(3)
C(10)-C(12)	1.527(3)
C(10)-C(11)	1.528(3)
C(10)-H(10)	1.0000

C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.522(3)
C(13)-C(15)	1.531(3)
C(13)-H(13)	1.0000
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(21)	1.396(2)
C(16)-C(17)	1.397(2)
C(16)-N(2)	1.445(2)
C(17)-C(18)	1.395(3)
C(17)-C(25)	1.520(3)
C(18)-C(19)	1.378(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.374(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.395(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.514(3)
C(22)-C(24)	1.519(3)
C(22)-C(23)	1.527(3)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800

C(25)-C(27)	1.526(3)
C(25)-C(26)	1.529(3)
C(25)-H(25)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(33)	1.416(2)
C(28)-C(29)	1.419(2)
C(28)-N(1)	1.424(2)
C(29)-C(30)	1.394(2)
C(29)-C(37)	1.521(2)
C(30)-C(31)	1.378(3)
C(30)-H(30)	0.9500
C(31)-C(32)	1.382(3)
C(31)-H(31)	0.9500
C(32)-C(33)	1.397(2)
C(32)-H(32)	0.9500
C(33)-C(34)	1.517(2)
C(34)-C(36)	1.526(3)
C(34)-C(35)	1.530(3)
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.529(3)
C(37)-C(39)	1.533(3)
C(37)-H(37)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800

C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-Si(1)	1.8756(19)
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-Si(1)	1.871(2)
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-Si(1)	1.868(2)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
N(1)-Si(1)	1.7183(15)
N(1)-Ni(1)	1.8271(14)
Si(1)-Ni(1)	2.9051(5)
N(3)-C(1)-N(2)	103.08(13)
N(3)-C(1)-Ni(1)	127.15(12)
N(2)-C(1)-Ni(1)	129.74(12)
C(3)-C(2)-N(2)	106.48(14)
C(3)-C(2)-H(2)	126.8
N(2)-C(2)-H(2)	126.8
C(2)-C(3)-N(3)	106.63(14)
C(2)-C(3)-H(3)	126.7
N(3)-C(3)-H(3)	126.7
C(9)-C(4)-C(5)	123.29(15)
C(9)-C(4)-N(3)	117.63(15)
C(5)-C(4)-N(3)	119.00(15)
C(6)-C(5)-C(4)	116.66(16)
C(6)-C(5)-C(13)	121.54(16)
C(4)-C(5)-C(13)	121.78(15)
C(7)-C(6)-C(5)	121.43(18)
C(7)-C(6)-H(6)	119.3

C(5)-C(6)-H(6)	119.3
C(8)-C(7)-C(6)	120.43(17)
C(8)-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8
C(7)-C(8)-C(9)	120.86(17)
C(7)-C(8)-H(8)	119.6
C(9)-C(8)-H(8)	119.6
C(4)-C(9)-C(8)	117.32(16)
C(4)-C(9)-C(10)	122.37(16)
C(8)-C(9)-C(10)	120.31(16)
C(9)-C(10)-C(12)	111.47(17)
C(9)-C(10)-C(11)	110.46(17)
C(12)-C(10)-C(11)	112.08(17)
C(9)-C(10)-H(10)	107.5
C(12)-C(10)-H(10)	107.5
C(11)-C(10)-H(10)	107.5
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(5)	110.62(15)
C(14)-C(13)-C(15)	109.70(16)
C(5)-C(13)-C(15)	113.14(15)
C(14)-C(13)-H(13)	107.7
C(5)-C(13)-H(13)	107.7
C(15)-C(13)-H(13)	107.7
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5

H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(21)-C(16)-C(17)	123.19(16)
C(21)-C(16)-N(2)	118.89(15)
C(17)-C(16)-N(2)	117.85(15)
C(18)-C(17)-C(16)	116.88(17)
C(18)-C(17)-C(25)	121.38(17)
C(16)-C(17)-C(25)	121.73(16)
C(19)-C(18)-C(17)	121.16(18)
C(19)-C(18)-H(18)	119.4
C(17)-C(18)-H(18)	119.4
C(20)-C(19)-C(18)	120.65(18)
C(20)-C(19)-H(19)	119.7
C(18)-C(19)-H(19)	119.7
C(19)-C(20)-C(21)	120.88(19)
C(19)-C(20)-H(20)	119.6
C(21)-C(20)-H(20)	119.6
C(20)-C(21)-C(16)	117.23(17)
C(20)-C(21)-C(22)	120.43(17)
C(16)-C(21)-C(22)	122.34(16)
C(21)-C(22)-C(24)	111.15(17)
C(21)-C(22)-C(23)	111.29(17)
C(24)-C(22)-C(23)	110.35(17)
C(21)-C(22)-H(22)	108.0
C(24)-C(22)-H(22)	108.0
C(23)-C(22)-H(22)	108.0
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5

H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(17)-C(25)-C(27)	110.75(16)
C(17)-C(25)-C(26)	112.21(18)
C(27)-C(25)-C(26)	110.22(17)
C(17)-C(25)-H(25)	107.8
C(27)-C(25)-H(25)	107.8
C(26)-C(25)-H(25)	107.8
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(33)-C(28)-C(29)	118.40(15)
C(33)-C(28)-N(1)	121.24(15)
C(29)-C(28)-N(1)	120.34(15)
C(30)-C(29)-C(28)	119.39(16)
C(30)-C(29)-C(37)	119.25(16)
C(28)-C(29)-C(37)	121.30(15)
C(31)-C(30)-C(29)	122.23(17)
C(31)-C(30)-H(30)	118.9

C(29)-C(30)-H(30)	118.9
C(30)-C(31)-C(32)	118.48(17)
C(30)-C(31)-H(31)	120.8
C(32)-C(31)-H(31)	120.8
C(31)-C(32)-C(33)	121.88(17)
C(31)-C(32)-H(32)	119.1
C(33)-C(32)-H(32)	119.1
C(32)-C(33)-C(28)	119.58(16)
C(32)-C(33)-C(34)	118.92(16)
C(28)-C(33)-C(34)	121.48(15)
C(33)-C(34)-C(36)	112.82(16)
C(33)-C(34)-C(35)	110.27(17)
C(36)-C(34)-C(35)	110.46(18)
C(33)-C(34)-H(34)	107.7
C(36)-C(34)-H(34)	107.7
C(35)-C(34)-H(34)	107.7
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(29)-C(37)-C(38)	109.95(15)
C(29)-C(37)-C(39)	113.52(16)
C(38)-C(37)-C(39)	109.51(17)
C(29)-C(37)-H(37)	107.9
C(38)-C(37)-H(37)	107.9
C(39)-C(37)-H(37)	107.9
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5

H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
Si(1)-C(40)-H(40A)	109.5
Si(1)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
Si(1)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
Si(1)-C(41)-H(41A)	109.5
Si(1)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
Si(1)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
Si(1)-C(42)-H(42A)	109.5
Si(1)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
Si(1)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(28)-N(1)-Si(1)	120.66(11)
C(28)-N(1)-Ni(1)	128.51(11)
Si(1)-N(1)-Ni(1)	110.01(7)
C(1)-N(2)-C(2)	112.00(13)
C(1)-N(2)-C(16)	125.76(13)
C(2)-N(2)-C(16)	122.13(13)
C(1)-N(3)-C(3)	111.81(14)
C(1)-N(3)-C(4)	124.89(13)

C(3)-N(3)-C(4)	123.05(14)
N(1)-Si(1)-C(42)	113.93(9)
N(1)-Si(1)-C(41)	110.24(8)
C(42)-Si(1)-C(41)	106.63(10)
N(1)-Si(1)-C(40)	110.46(8)
C(42)-Si(1)-C(40)	106.68(10)
C(41)-Si(1)-C(40)	108.68(10)
N(1)-Si(1)-Ni(1)	36.23(5)
C(42)-Si(1)-Ni(1)	98.04(7)
C(41)-Si(1)-Ni(1)	85.62(6)
C(40)-Si(1)-Ni(1)	145.86(7)
N(1)-Ni(1)-C(1)	173.01(7)
N(1)-Ni(1)-Si(1)	33.76(4)
C(1)-Ni(1)-Si(1)	139.25(5)

Table S9. Bond lengths [Å] and angles [°] for Compound 4.

C(1)-C(2)	1.415(2)
C(1)-C(6)	1.416(2)
C(1)-N(1)	1.423(2)
C(2)-C(3)	1.401(2)
C(2)-C(7)	1.517(3)
C(3)-C(4)	1.385(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.386(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.399(2)
C(5)-H(5)	0.9500
C(6)-C(10)	1.516(3)
C(7)-C(8)	1.532(3)
C(7)-C(9)	1.534(3)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800

C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(12)	1.531(3)
C(10)-C(11)	1.533(3)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-Si(1)	1.8771(19)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-Si(1)	1.8718(18)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-Si(1)	1.8732(18)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(18)	1.523(3)
C(16)-C(19)	1.544(3)
C(16)-C(17)	1.561(3)
C(16)-P(1)	1.8889(19)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(20)-C(21)	1.522(3)
C(20)-C(23)	1.527(3)
C(20)-C(22)	1.558(3)
C(20)-P(1)	1.9093(19)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.523(3)
C(24)-C(27)	1.534(3)
C(24)-C(26)	1.565(3)
C(24)-P(1)	1.8978(19)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
N(1)-Si(1)	1.7209(14)
N(1)-Ni(1A)	1.824(5)
N(1)-Ni(1)	1.8250(16)
P(1)-Ni(1)	2.2006(11)
P(1)-Ni(1A)	2.210(6)
C(2)-C(1)-C(6)	119.38(15)
C(2)-C(1)-N(1)	120.30(14)
C(6)-C(1)-N(1)	120.31(14)
C(3)-C(2)-C(1)	119.08(17)

C(3)-C(2)-C(7)	119.30(16)
C(1)-C(2)-C(7)	121.62(15)
C(4)-C(3)-C(2)	121.54(18)
C(4)-C(3)-H(3)	119.2
C(2)-C(3)-H(3)	119.2
C(3)-C(4)-C(5)	119.23(18)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
C(4)-C(5)-C(6)	121.37(18)
C(4)-C(5)-H(5)	119.3
C(6)-C(5)-H(5)	119.3
C(5)-C(6)-C(1)	119.32(17)
C(5)-C(6)-C(10)	119.14(16)
C(1)-C(6)-C(10)	121.53(15)
C(2)-C(7)-C(8)	112.27(16)
C(2)-C(7)-C(9)	111.75(15)
C(8)-C(7)-C(9)	109.96(15)
C(2)-C(7)-H(7)	107.5
C(8)-C(7)-H(7)	107.5
C(9)-C(7)-H(7)	107.5
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(12)	111.32(16)
C(6)-C(10)-C(11)	112.52(16)
C(12)-C(10)-C(11)	109.98(16)
C(6)-C(10)-H(10)	107.6

C(12)-C(10)-H(10)	107.6
C(11)-C(10)-H(10)	107.6
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(1)-C(13)-H(13A)	109.5
Si(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
Si(1)-C(14)-H(14A)	109.5
Si(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
Si(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
Si(1)-C(15)-H(15A)	109.5
Si(1)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
Si(1)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(18)-C(16)-C(19)	110.91(18)
C(18)-C(16)-C(17)	104.83(19)
C(19)-C(16)-C(17)	107.33(18)
C(18)-C(16)-P(1)	109.33(16)

C(19)-C(16)-P(1)	115.62(13)
C(17)-C(16)-P(1)	108.22(14)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-C(23)	111.59(19)
C(21)-C(20)-C(22)	104.15(18)
C(23)-C(20)-C(22)	106.88(17)
C(21)-C(20)-P(1)	109.14(14)
C(23)-C(20)-P(1)	115.34(14)
C(22)-C(20)-P(1)	109.10(15)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5

H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(25)-C(24)-C(27)	110.52(18)
C(25)-C(24)-C(26)	106.2(2)
C(27)-C(24)-C(26)	106.07(19)
C(25)-C(24)-P(1)	108.81(16)
C(27)-C(24)-P(1)	116.71(13)
C(26)-C(24)-P(1)	107.94(15)
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(24)-C(27)-H(27A)	109.5
C(24)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(24)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(1)-N(1)-Si(1)	121.63(11)
C(1)-N(1)-Ni(1A)	115.5(2)
Si(1)-N(1)-Ni(1A)	121.9(2)
C(1)-N(1)-Ni(1)	114.90(11)

Si(1)-N(1)-Ni(1)	123.37(9)
Ni(1A)-N(1)-Ni(1)	13.2(6)
N(1)-Si(1)-C(14)	111.29(8)
N(1)-Si(1)-C(15)	111.22(8)
C(14)-Si(1)-C(15)	107.10(10)
N(1)-Si(1)-C(13)	109.74(8)
C(14)-Si(1)-C(13)	108.66(9)
C(15)-Si(1)-C(13)	108.74(9)
C(16)-P(1)-C(24)	110.40(10)
C(16)-P(1)-C(20)	109.59(9)
C(24)-P(1)-C(20)	108.42(9)
C(16)-P(1)-Ni(1)	111.06(12)
C(24)-P(1)-Ni(1)	108.19(10)
C(20)-P(1)-Ni(1)	109.13(7)
C(16)-P(1)-Ni(1A)	100.8(6)
C(24)-P(1)-Ni(1A)	116.5(5)
C(20)-P(1)-Ni(1A)	110.86(16)
Ni(1)-P(1)-Ni(1A)	10.9(5)
N(1)-Ni(1)-P(1)	167.6(2)
N(1)-Ni(1A)-P(1)	165.6(12)

Table S10. Bond lengths [Å] and angles [°] for Compound 5.

C(1)-C(6)	1.413(3)
C(1)-C(2)	1.419(3)
C(1)-N(1)	1.426(3)
C(2)-C(3)	1.394(3)
C(2)-C(10)	1.522(3)
C(3)-C(4)	1.384(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.383(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.396(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.519(3)
C(7)-C(9)	1.530(3)

C(7)-C(8)	1.535(3)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.532(3)
C(10)-C(12)	1.534(4)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-Si(1)	1.872(3)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-Si(1)	1.879(3)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-Si(1)	1.869(2)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.527(3)
C(16)-C(18)	1.539(3)
C(16)-P(1)	1.841(3)
C(16)-H(16)	1.0000
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800

C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(21)	1.520(4)
C(19)-C(20)	1.528(3)
C(19)-P(1)	1.843(3)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.532(3)
C(22)-C(24)	1.532(4)
C(22)-P(1)	1.862(2)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
N(1)-Si(1)	1.721(2)
N(1)-Ni(1)	1.8407(18)
P(1)-Ni(1)	2.1992(7)

C(6)-C(1)-C(2)	118.8(2)
C(6)-C(1)-N(1)	121.2(2)
C(2)-C(1)-N(1)	119.94(19)
C(3)-C(2)-C(1)	119.5(2)
C(3)-C(2)-C(10)	120.1(2)
C(1)-C(2)-C(10)	120.3(2)
C(4)-C(3)-C(2)	121.8(2)
C(4)-C(3)-H(3)	119.1
C(2)-C(3)-H(3)	119.1

C(5)-C(4)-C(3)	118.6(2)
C(5)-C(4)-H(4)	120.7
C(3)-C(4)-H(4)	120.7
C(4)-C(5)-C(6)	122.0(2)
C(4)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0
C(5)-C(6)-C(1)	119.3(2)
C(5)-C(6)-C(7)	119.5(2)
C(1)-C(6)-C(7)	121.1(2)
C(6)-C(7)-C(9)	111.1(2)
C(6)-C(7)-C(8)	111.8(2)
C(9)-C(7)-C(8)	110.6(2)
C(6)-C(7)-H(7)	107.7
C(9)-C(7)-H(7)	107.7
C(8)-C(7)-H(7)	107.7
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(2)-C(10)-C(11)	108.86(19)
C(2)-C(10)-C(12)	114.1(2)
C(11)-C(10)-C(12)	110.6(2)
C(2)-C(10)-H(10)	107.7
C(11)-C(10)-H(10)	107.7
C(12)-C(10)-H(10)	107.7
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5

C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(1)-C(13)-H(13A)	109.5
Si(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
Si(1)-C(14)-H(14A)	109.5
Si(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
Si(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
Si(1)-C(15)-H(15A)	109.5
Si(1)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
Si(1)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(18)	110.2(2)
C(17)-C(16)-P(1)	109.17(18)
C(18)-C(16)-P(1)	110.33(17)
C(17)-C(16)-H(16)	109.0
C(18)-C(16)-H(16)	109.0
P(1)-C(16)-H(16)	109.0
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5

C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(21)-C(19)-C(20)	110.9(2)
C(21)-C(19)-P(1)	111.20(19)
C(20)-C(19)-P(1)	115.41(18)
C(21)-C(19)-H(19)	106.2
C(20)-C(19)-H(19)	106.2
P(1)-C(19)-H(19)	106.2
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-C(24)	110.7(2)
C(23)-C(22)-P(1)	115.44(17)
C(24)-C(22)-P(1)	110.77(18)
C(23)-C(22)-H(22)	106.5
C(24)-C(22)-H(22)	106.5
P(1)-C(22)-H(22)	106.5
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5

C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(1)-N(1)-Si(1)	122.08(15)
C(1)-N(1)-Ni(1)	118.73(14)
Si(1)-N(1)-Ni(1)	119.19(11)
N(1)-Si(1)-C(15)	110.91(10)
N(1)-Si(1)-C(13)	110.65(11)
C(15)-Si(1)-C(13)	107.94(12)
N(1)-Si(1)-C(14)	113.00(11)
C(15)-Si(1)-C(14)	105.40(12)
C(13)-Si(1)-C(14)	108.69(13)
C(19)-P(1)-C(16)	105.01(12)
C(19)-P(1)-C(22)	105.24(12)
C(16)-P(1)-C(22)	106.86(11)
C(19)-P(1)-Ni(1)	111.12(8)
C(16)-P(1)-Ni(1)	112.22(8)
C(22)-P(1)-Ni(1)	115.61(8)
N(1)-Ni(1)-P(1)	164.09(6)

Table S11. Bond lengths [Å] and angles [°] for Compound 6.

C(1)-C(6)	1.416(4)
C(1)-N(1)	1.419(4)
C(1)-C(2)	1.419(5)
C(2)-C(3)	1.393(5)
C(2)-C(10)	1.519(5)
C(3)-C(4)	1.386(5)
C(3)-H(20)	0.9500
C(4)-C(5)	1.367(6)

C(4)-H(37)	0.9500
C(5)-C(6)	1.400(6)
C(5)-H(32)	0.9500
C(6)-C(7)	1.513(6)
C(7)-C(8)	1.527(7)
C(7)-C(9)	1.535(6)
C(7)-H(40)	1.0000
C(8)-H(17A)	0.9800
C(8)-H(17B)	0.9800
C(8)-H(17C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(12)	1.451(5)
C(10)-C(11)	1.461(6)
C(10)-H(10A)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-Si(1)	1.881(4)
C(13)-H(48A)	0.9800
C(13)-H(48B)	0.9800
C(13)-H(48C)	0.9800
C(14)-Si(1)	1.872(5)
C(14)-H(41A)	0.9800
C(14)-H(41B)	0.9800
C(14)-H(41C)	0.9800
C(15)-Si(1)	1.880(4)
C(15)-H(46A)	0.9800
C(15)-H(46B)	0.9800
C(15)-H(46C)	0.9800
C(16)-C(21)	1.380(6)
C(16)-C(17)	1.392(6)

C(16)-P(1)	1.830(3)
C(17)-C(18)	1.397(5)
C(17)-H(35)	0.9500
C(18)-C(19)	1.356(9)
C(18)-H(7)	0.9500
C(19)-C(20)	1.363(9)
C(19)-H(19)	0.9500
C(20)-C(21)	1.405(6)
C(20)-H(45)	0.9500
C(21)-H(42)	0.9500
C(22)-C(27)	1.391(5)
C(22)-C(23)	1.392(5)
C(22)-P(1)	1.834(3)
C(23)-C(24)	1.391(5)
C(23)-H(26)	0.9500
C(24)-C(25)	1.372(6)
C(24)-H(23)	0.9500
C(25)-C(26)	1.384(6)
C(25)-H(34)	0.9500
C(26)-C(27)	1.391(5)
C(26)-H(39)	0.9500
C(27)-H(25)	0.9500
C(28)-C(29)	1.534(4)
C(28)-P(1)	1.846(3)
C(28)-H(18A)	0.9900
C(28)-H(18B)	0.9900
C(29)-P(2)	1.843(3)
C(29)-H(16A)	0.9900
C(29)-H(16B)	0.9900
C(30)-C(35)	1.384(5)
C(30)-C(31)	1.385(5)
C(30)-P(2)	1.831(3)
C(31)-C(32)	1.389(5)
C(31)-H(10)	0.9500
C(32)-C(33)	1.370(6)
C(32)-H(33)	0.9500

C(33)-C(34)	1.373(6)
C(33)-H(30)	0.9500
C(34)-C(35)	1.397(5)
C(34)-H(38)	0.9500
C(35)-H(28)	0.9500
C(36)-C(37)	1.388(5)
C(36)-C(41)	1.398(4)
C(36)-P(2)	1.835(3)
C(37)-C(38)	1.393(5)
C(37)-H(15)	0.9500
C(38)-C(39)	1.373(6)
C(38)-H(29)	0.9500
C(39)-C(40)	1.375(6)
C(39)-H(27)	0.9500
C(40)-C(41)	1.390(5)
C(40)-H(36)	0.9500
C(41)-H(31)	0.9500
N(1)-Si(1)	1.713(3)
N(1)-Ni(1)	1.875(2)
P(1)-Ni(1)	2.1978(8)
P(2)-Ni(1)	2.1922(8)

C(6)-C(1)-N(1)	121.2(3)
C(6)-C(1)-C(2)	117.7(3)
N(1)-C(1)-C(2)	121.0(3)
C(3)-C(2)-C(1)	120.3(3)
C(3)-C(2)-C(10)	118.7(3)
C(1)-C(2)-C(10)	121.0(3)
C(4)-C(3)-C(2)	121.2(4)
C(4)-C(3)-H(20)	119.4
C(2)-C(3)-H(20)	119.4
C(5)-C(4)-C(3)	118.9(4)
C(5)-C(4)-H(37)	120.6
C(3)-C(4)-H(37)	120.6
C(4)-C(5)-C(6)	122.2(3)
C(4)-C(5)-H(32)	118.9

C(6)-C(5)-H(32)	118.9
C(5)-C(6)-C(1)	119.6(4)
C(5)-C(6)-C(7)	119.8(3)
C(1)-C(6)-C(7)	120.6(3)
C(6)-C(7)-C(8)	111.6(3)
C(6)-C(7)-C(9)	111.2(5)
C(8)-C(7)-C(9)	112.0(4)
C(6)-C(7)-H(40)	107.3
C(8)-C(7)-H(40)	107.3
C(9)-C(7)-H(40)	107.3
C(7)-C(8)-H(17A)	109.5
C(7)-C(8)-H(17B)	109.5
H(17A)-C(8)-H(17B)	109.5
C(7)-C(8)-H(17C)	109.5
H(17A)-C(8)-H(17C)	109.5
H(17B)-C(8)-H(17C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(12)-C(10)-C(11)	105.9(5)
C(12)-C(10)-C(2)	116.1(3)
C(11)-C(10)-C(2)	112.7(4)
C(12)-C(10)-H(10A)	107.2
C(11)-C(10)-H(10A)	107.2
C(2)-C(10)-H(10A)	107.2
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5

H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(1)-C(13)-H(48A)	109.5
Si(1)-C(13)-H(48B)	109.5
H(48A)-C(13)-H(48B)	109.5
Si(1)-C(13)-H(48C)	109.5
H(48A)-C(13)-H(48C)	109.5
H(48B)-C(13)-H(48C)	109.5
Si(1)-C(14)-H(41A)	109.5
Si(1)-C(14)-H(41B)	109.5
H(41A)-C(14)-H(41B)	109.5
Si(1)-C(14)-H(41C)	109.5
H(41A)-C(14)-H(41C)	109.5
H(41B)-C(14)-H(41C)	109.5
Si(1)-C(15)-H(46A)	109.5
Si(1)-C(15)-H(46B)	109.5
H(46A)-C(15)-H(46B)	109.5
Si(1)-C(15)-H(46C)	109.5
H(46A)-C(15)-H(46C)	109.5
H(46B)-C(15)-H(46C)	109.5
C(21)-C(16)-C(17)	118.8(4)
C(21)-C(16)-P(1)	123.6(3)
C(17)-C(16)-P(1)	117.5(3)
C(16)-C(17)-C(18)	120.1(5)
C(16)-C(17)-H(35)	120.0
C(18)-C(17)-H(35)	120.0
C(19)-C(18)-C(17)	120.7(5)
C(19)-C(18)-H(7)	119.6
C(17)-C(18)-H(7)	119.6
C(18)-C(19)-C(20)	119.9(4)
C(18)-C(19)-H(19)	120.0
C(20)-C(19)-H(19)	120.0
C(19)-C(20)-C(21)	120.7(5)
C(19)-C(20)-H(45)	119.6

C(21)-C(20)-H(45)	119.6
C(16)-C(21)-C(20)	119.8(5)
C(16)-C(21)-H(42)	120.1
C(20)-C(21)-H(42)	120.1
C(27)-C(22)-C(23)	119.2(3)
C(27)-C(22)-P(1)	122.0(3)
C(23)-C(22)-P(1)	118.7(2)
C(24)-C(23)-C(22)	120.5(3)
C(24)-C(23)-H(26)	119.8
C(22)-C(23)-H(26)	119.8
C(25)-C(24)-C(23)	119.6(3)
C(25)-C(24)-H(23)	120.2
C(23)-C(24)-H(23)	120.2
C(24)-C(25)-C(26)	120.8(3)
C(24)-C(25)-H(34)	119.6
C(26)-C(25)-H(34)	119.6
C(25)-C(26)-C(27)	119.8(4)
C(25)-C(26)-H(39)	120.1
C(27)-C(26)-H(39)	120.1
C(26)-C(27)-C(22)	120.1(3)
C(26)-C(27)-H(25)	120.0
C(22)-C(27)-H(25)	120.0
C(29)-C(28)-P(1)	107.0(2)
C(29)-C(28)-H(18A)	110.3
P(1)-C(28)-H(18A)	110.3
C(29)-C(28)-H(18B)	110.3
P(1)-C(28)-H(18B)	110.3
H(18A)-C(28)-H(18B)	108.6
C(28)-C(29)-P(2)	108.0(2)
C(28)-C(29)-H(16A)	110.1
P(2)-C(29)-H(16A)	110.1
C(28)-C(29)-H(16B)	110.1
P(2)-C(29)-H(16B)	110.1
H(16A)-C(29)-H(16B)	108.4
C(35)-C(30)-C(31)	118.8(3)
C(35)-C(30)-P(2)	123.2(3)

C(31)-C(30)-P(2)	117.9(2)
C(30)-C(31)-C(32)	120.6(3)
C(30)-C(31)-H(10)	119.7
C(32)-C(31)-H(10)	119.7
C(33)-C(32)-C(31)	120.2(4)
C(33)-C(32)-H(33)	119.9
C(31)-C(32)-H(33)	119.9
C(32)-C(33)-C(34)	119.9(3)
C(32)-C(33)-H(30)	120.0
C(34)-C(33)-H(30)	120.0
C(33)-C(34)-C(35)	120.2(4)
C(33)-C(34)-H(38)	119.9
C(35)-C(34)-H(38)	119.9
C(30)-C(35)-C(34)	120.2(4)
C(30)-C(35)-H(28)	119.9
C(34)-C(35)-H(28)	119.9
C(37)-C(36)-C(41)	118.6(3)
C(37)-C(36)-P(2)	117.7(2)
C(41)-C(36)-P(2)	123.7(2)
C(36)-C(37)-C(38)	120.3(3)
C(36)-C(37)-H(15)	119.9
C(38)-C(37)-H(15)	119.9
C(39)-C(38)-C(37)	120.6(4)
C(39)-C(38)-H(29)	119.7
C(37)-C(38)-H(29)	119.7
C(38)-C(39)-C(40)	119.7(3)
C(38)-C(39)-H(27)	120.1
C(40)-C(39)-H(27)	120.1
C(39)-C(40)-C(41)	120.4(3)
C(39)-C(40)-H(36)	119.8
C(41)-C(40)-H(36)	119.8
C(40)-C(41)-C(36)	120.3(3)
C(40)-C(41)-H(31)	119.8
C(36)-C(41)-H(31)	119.8
C(1)-N(1)-Si(1)	125.0(2)
C(1)-N(1)-Ni(1)	114.09(19)

Si(1)-N(1)-Ni(1)	120.29(15)
N(1)-Si(1)-C(14)	113.09(16)
N(1)-Si(1)-C(15)	110.6(2)
C(14)-Si(1)-C(15)	108.2(2)
N(1)-Si(1)-C(13)	110.86(16)
C(14)-Si(1)-C(13)	105.2(2)
C(15)-Si(1)-C(13)	108.7(2)
C(16)-P(1)-C(22)	102.85(14)
C(16)-P(1)-C(28)	105.89(17)
C(22)-P(1)-C(28)	100.79(15)
C(16)-P(1)-Ni(1)	124.08(12)
C(22)-P(1)-Ni(1)	113.47(11)
C(28)-P(1)-Ni(1)	107.19(10)
C(30)-P(2)-C(36)	104.01(13)
C(30)-P(2)-C(29)	104.07(14)
C(36)-P(2)-C(29)	104.27(14)
C(30)-P(2)-Ni(1)	120.46(11)
C(36)-P(2)-Ni(1)	114.63(10)
C(29)-P(2)-Ni(1)	107.83(10)
N(1)-Ni(1)-P(2)	135.50(9)
N(1)-Ni(1)-P(1)	136.81(9)
P(2)-Ni(1)-P(1)	87.68(3)

Table S12. Bond lengths [Å] and angles [°] for Compound 7.

C(1)-O(1)	1.321(3)
C(1)-C(2)	1.423(4)
C(1)-C(6)	1.423(3)
C(2)-C(3)	1.399(3)
C(2)-C(11)	1.541(4)
C(3)-C(4)	1.380(3)
C(3)-H(033)	0.9500
C(4)-C(5)	1.393(4)
C(4)-C(15)	1.508(3)
C(5)-C(6)	1.390(3)
C(5)-H(022)	0.9500

C(6)-C(7)	1.539(4)
C(7)-C(9)	1.532(4)
C(7)-C(8)	1.534(4)
C(7)-C(10)	1.538(4)
C(8)-H(10D)	0.9800
C(8)-H(10E)	0.9800
C(8)-H(10F)	0.9800
C(9)-H(08M)	0.9800
C(9)-H(08N)	0.9800
C(9)-H(08O)	0.9800
C(10)-H(06A)	0.9800
C(10)-H(06B)	0.9800
C(10)-H(06C)	0.9800
C(11)-C(13)	1.529(4)
C(11)-C(12)	1.534(4)
C(11)-C(14)	1.540(4)
C(12)-H(09J)	0.9800
C(12)-H(09K)	0.9800
C(12)-H(09L)	0.9800
C(13)-H(08J)	0.9800
C(13)-H(08K)	0.9800
C(13)-H(08L)	0.9800
C(14)-H(11A)	0.9800
C(14)-H(11B)	0.9800
C(14)-H(11C)	0.9800
C(15)-H(08G)	0.9800
C(15)-H(08H)	0.9800
C(15)-H(08I)	0.9800
C(16)-N(1)	1.361(3)
C(16)-N(2)	1.362(3)
C(16)-Ni(1)	1.880(2)
C(17)-C(18)	1.326(4)
C(17)-N(2)	1.399(3)
C(17)-H(087)	0.9500
C(18)-N(1)	1.396(3)
C(18)-H(023)	0.9500

C(19)-C(20)	1.396(4)
C(19)-C(24)	1.404(4)
C(19)-N(1)	1.435(3)
C(20)-C(21)	1.398(4)
C(20)-C(28)	1.510(4)
C(21)-C(22)	1.370(5)
C(21)-H(093)	0.9500
C(22)-C(23)	1.392(5)
C(22)-H(119)	0.9500
C(23)-C(24)	1.381(4)
C(23)-H(109)	0.9500
C(24)-C(25)	1.521(4)
C(25)-C(26)	1.468(5)
C(25)-C(27)	1.498(4)
C(25)-H(102)	1.0000
C(26)-H(13S)	0.9800
C(26)-H(13T)	0.9800
C(26)-H(13U)	0.9800
C(27)-H(12P)	0.9800
C(27)-H(12Q)	0.9800
C(27)-H(12R)	0.9800
C(28)-C(29)	1.533(4)
C(28)-C(30)	1.534(4)
C(28)-H(042)	1.0000
C(29)-H(09A)	0.9800
C(29)-H(09B)	0.9800
C(29)-H(09C)	0.9800
C(30)-H(12J)	0.9800
C(30)-H(12K)	0.9800
C(30)-H(12L)	0.9800
C(31)-C(32)	1.381(4)
C(31)-C(36)	1.410(4)
C(31)-N(2)	1.439(3)
C(32)-C(33)	1.401(4)
C(32)-C(40)	1.516(4)
C(33)-C(34)	1.376(5)

C(33)-H(110)	0.9500
C(34)-C(35)	1.350(5)
C(34)-H(123)	0.9500
C(35)-C(36)	1.390(5)
C(35)-H(128)	0.9500
C(36)-C(37)	1.510(5)
C(37)-C(38)	1.495(5)
C(37)-C(39)	1.519(4)
C(37)-H(107)	1.0000
C(38)-H(13\$)	0.9800
C(38)-H(13V)	0.9800
C(38)-H(13W)	0.9800
C(39)-H(131)	0.9800
C(39)-H(13)	0.9800
C(39)-H(13M)	0.9800
C(40)-C(41)	1.518(4)
C(40)-C(42)	1.534(4)
C(40)-H(081)	1.0000
C(41)-H(11S)	0.9800
C(41)-H(11T)	0.9800
C(41)-H(11U)	0.9800
C(42)-H(10J)	0.9800
C(42)-H(10K)	0.9800
C(42)-H(10L)	0.9800
C(43)-O(2)	1.337(3)
C(43)-C(48)	1.423(4)
C(43)-C(44)	1.425(4)
C(44)-C(45)	1.381(4)
C(44)-C(53)	1.532(4)
C(45)-C(46)	1.382(4)
C(45)-H(047)	0.9500
C(46)-C(47)	1.389(4)
C(46)-C(57)	1.508(4)
C(47)-C(48)	1.392(4)
C(47)-H(061)	0.9500
C(48)-C(49)	1.546(4)

C(49)-C(51)	1.524(4)
C(49)-C(52)	1.536(4)
C(49)-C(50)	1.550(4)
C(50)-H(10M)	0.9800
C(50)-H(10N)	0.9800
C(50)-H(10O)	0.9800
C(51)-H(11J)	0.9800
C(51)-H(11K)	0.9800
C(51)-H(11L)	0.9800
C(52)-H(12M)	0.9800
C(52)-H(12N)	0.9800
C(52)-H(12O)	0.9800
C(53)-C(54)	1.534(4)
C(53)-C(56)	1.542(4)
C(53)-C(55)	1.556(4)
C(54)-H(12G)	0.9800
C(54)-H(12H)	0.9800
C(54)-H(12I)	0.9800
C(55)-H(12A)	0.9800
C(55)-H(12B)	0.9800
C(55)-H(12C)	0.9800
C(56)-H(09P)	0.9800
C(56)-H(09Q)	0.9800
C(56)-H(09R)	0.9800
C(57)-H(11M)	0.9800
C(57)-H(11N)	0.9800
C(57)-H(11O)	0.9800
C(58)-N(3)	1.360(3)
C(58)-N(4)	1.365(3)
C(58)-Ni(2)	1.863(3)
C(59)-C(60)	1.334(4)
C(59)-N(4)	1.386(3)
C(59)-H(039)	0.9500
C(60)-N(3)	1.391(3)
C(60)-H(054)	0.9500
C(61)-C(62)	1.389(4)

C(61)-C(66)	1.404(4)
C(61)-N(3)	1.443(3)
C(62)-C(63)	1.396(4)
C(62)-C(70)	1.514(4)
C(63)-C(64)	1.387(4)
C(63)-H(065)	0.9500
C(64)-C(65)	1.365(4)
C(64)-H(089)	0.9500
C(65)-C(66)	1.399(4)
C(65)-H(071)	0.9500
C(66)-C(67)	1.512(4)
C(67)-C(69)	1.510(5)
C(67)-C(68)	1.530(5)
C(67)-H(105)	1.0000
C(68)-H(132)	0.9800
C(68)-H(13N)	0.9800
C(68)-H(13O)	0.9800
C(69)-H(13P)	0.9800
C(69)-H(13Q)	0.9800
C(69)-H(13R)	0.9800
C(70)-C(72)	1.497(4)
C(70)-C(71)	1.531(4)
C(70)-H(073)	1.0000
C(71)-H(12D)	0.9800
C(71)-H(12E)	0.9800
C(71)-H(12F)	0.9800
C(72)-H(13A)	0.9800
C(72)-H(13B)	0.9800
C(72)-H(13C)	0.9800
C(73)-C(78)	1.394(4)
C(73)-C(74)	1.395(3)
C(73)-N(4)	1.438(3)
C(74)-C(75)	1.394(4)
C(74)-C(82)	1.513(4)
C(75)-C(76)	1.380(4)
C(75)-H(031)	0.9500

C(76)-C(77)	1.374(4)
C(76)-H(067)	0.9500
C(77)-C(78)	1.387(4)
C(77)-H(058)	0.9500
C(78)-C(79)	1.518(4)
C(79)-C(80)	1.479(4)
C(79)-C(81)	1.494(4)
C(79)-H(046)	1.0000
C(80)-H(13D)	0.9800
C(80)-H(13E)	0.9800
C(80)-H(13F)	0.9800
C(81)-H(12\$)	0.9800
C(81)-H(12V)	0.9800
C(81)-H(12W)	0.9800
C(82)-C(84)	1.524(4)
C(82)-C(83)	1.530(4)
C(82)-H(059)	1.0000
C(83)-H(11G)	0.9800
C(83)-H(11H)	0.9800
C(83)-H(11I)	0.9800
C(84)-H(10A)	0.9800
C(84)-H(10B)	0.9800
C(84)-H(10C)	0.9800
C(85)-O(3)	1.328(3)
C(85)-C(90)	1.423(3)
C(85)-C(86)	1.424(4)
C(86)-C(87)	1.382(4)
C(86)-C(95)	1.548(4)
C(87)-C(88)	1.384(4)
C(87)-H(048)	0.9500
C(88)-C(89)	1.392(4)
C(88)-C(99)	1.516(4)
C(89)-C(90)	1.389(4)
C(89)-H(041)	0.9500
C(90)-C(91)	1.535(4)
C(91)-C(93)	1.529(4)

C(91)-C(94)	1.542(4)
C(91)-C(92)	1.556(4)
C(92)-H(09D)	0.9800
C(92)-H(09E)	0.9800
C(92)-H(09F)	0.9800
C(93)-H(10G)	0.9800
C(93)-H(10H)	0.9800
C(93)-H(10I)	0.9800
C(94)-H(08A)	0.9800
C(94)-H(08B)	0.9800
C(94)-H(08C)	0.9800
C(95)-C(96)	1.525(4)
C(95)-C(98)	1.537(4)
C(95)-C(97)	1.540(4)
C(96)-H(07A)	0.9800
C(96)-H(07B)	0.9800
C(96)-H(07C)	0.9800
C(97)-H(07D)	0.9800
C(97)-H(07E)	0.9800
C(97)-H(07F)	0.9800
C(98)-H(09G)	0.9800
C(98)-H(09H)	0.9800
C(98)-H(09I)	0.9800
C(99)-H(11P)	0.9800
C(99)-H(11Q)	0.9800
C(99)-H(11R)	0.9800
C(100)-N(6)	1.357(3)
C(100)-N(5)	1.369(3)
C(100)-Ni(3)	1.875(3)
C(101)-C(102)	1.341(3)
C(101)-N(6)	1.392(3)
C(101)-H(034)	0.9500
C(102)-N(5)	1.383(3)
C(102)-H(027)	0.9500
C(103)-C(104)	1.396(3)
C(103)-C(108)	1.396(3)

C(103)-N(5)	1.442(3)
C(104)-C(105)	1.392(3)
C(104)-C(109)	1.523(3)
C(105)-C(106)	1.383(4)
C(105)-H(036)	0.9500
C(106)-C(107)	1.370(4)
C(106)-H(091)	0.9500
C(107)-C(108)	1.398(4)
C(107)-H(029)	0.9500
C(108)-C(112)	1.519(4)
C(109)-C(110)	1.517(4)
C(109)-C(111)	1.523(4)
C(109)-H(076)	1.0000
C(110)-H(11D)	0.9800
C(110)-H(11E)	0.9800
C(110)-H(11F)	0.9800
C(111)-H(08D)	0.9800
C(111)-H(08E)	0.9800
C(111)-H(08F)	0.9800
C(112)-C(113)	1.529(4)
C(112)-C(114)	1.532(4)
C(112)-H(052)	1.0000
C(113)-H(09M)	0.9800
C(113)-H(09N)	0.9800
C(113)-H(09O)	0.9800
C(114)-H(05A)	0.9800
C(114)-H(05B)	0.9800
C(114)-H(05C)	0.9800
C(115)-C(120)	1.394(3)
C(115)-C(116)	1.399(4)
C(115)-N(6)	1.448(3)
C(116)-C(117)	1.395(4)
C(116)-C(124)	1.522(3)
C(117)-C(118)	1.373(4)
C(117)-H(069)	0.9500
C(118)-C(119)	1.371(4)

C(118)-H(074)	0.9500
C(119)-C(120)	1.387(4)
C(119)-H(103)	0.9500
C(120)-C(121)	1.514(4)
C(121)-C(122)	1.525(4)
C(121)-C(123)	1.530(4)
C(121)-H(095)	1.0000
C(122)-H(13G)	0.9800
C(122)-H(13H)	0.9800
C(122)-H(13I)	0.9800
C(123)-H(11\$)	0.9800
C(123)-H(11V)	0.9800
C(123)-H(11W)	0.9800
C(124)-C(126)	1.494(4)
C(124)-C(125)	1.512(5)
C(124)-H(057)	1.0000
C(125)-H(13J)	0.9800
C(125)-H(13K)	0.9800
C(125)-H(13L)	0.9800
C(126)-H(12S)	0.9800
C(126)-H(12T)	0.9800
C(126)-H(12U)	0.9800
O(1)-Ni(1)	1.7612(19)
O(2)-Ni(2)	1.778(2)
O(3)-Ni(3)	1.8374(17)

O(1)-C(1)-C(2)	120.9(2)
O(1)-C(1)-C(6)	119.3(2)
C(2)-C(1)-C(6)	119.7(2)
C(3)-C(2)-C(1)	118.3(2)
C(3)-C(2)-C(11)	120.2(2)
C(1)-C(2)-C(11)	121.6(2)
C(4)-C(3)-C(2)	122.9(2)
C(4)-C(3)-H(033)	118.5
C(2)-C(3)-H(033)	118.5
C(3)-C(4)-C(5)	117.8(2)

C(3)-C(4)-C(15)	121.6(2)
C(5)-C(4)-C(15)	120.7(2)
C(6)-C(5)-C(4)	122.8(2)
C(6)-C(5)-H(022)	118.6
C(4)-C(5)-H(022)	118.6
C(5)-C(6)-C(1)	118.4(2)
C(5)-C(6)-C(7)	120.4(2)
C(1)-C(6)-C(7)	121.1(2)
C(9)-C(7)-C(8)	106.4(2)
C(9)-C(7)-C(10)	110.4(2)
C(8)-C(7)-C(10)	106.9(2)
C(9)-C(7)-C(6)	110.3(2)
C(8)-C(7)-C(6)	112.1(2)
C(10)-C(7)-C(6)	110.7(2)
C(7)-C(8)-H(10D)	109.5
C(7)-C(8)-H(10E)	109.5
H(10D)-C(8)-H(10E)	109.5
C(7)-C(8)-H(10F)	109.5
H(10D)-C(8)-H(10F)	109.5
H(10E)-C(8)-H(10F)	109.5
C(7)-C(9)-H(08M)	109.5
C(7)-C(9)-H(08N)	109.5
H(08M)-C(9)-H(08N)	109.5
C(7)-C(9)-H(08O)	109.5
H(08M)-C(9)-H(08O)	109.5
H(08N)-C(9)-H(08O)	109.5
C(7)-C(10)-H(06A)	109.5
C(7)-C(10)-H(06B)	109.5
H(06A)-C(10)-H(06B)	109.5
C(7)-C(10)-H(06C)	109.5
H(06A)-C(10)-H(06C)	109.5
H(06B)-C(10)-H(06C)	109.5
C(13)-C(11)-C(12)	107.1(2)
C(13)-C(11)-C(14)	111.2(3)
C(12)-C(11)-C(14)	106.2(3)
C(13)-C(11)-C(2)	109.4(2)

C(12)-C(11)-C(2)	112.1(2)
C(14)-C(11)-C(2)	110.8(2)
C(11)-C(12)-H(09J)	109.5
C(11)-C(12)-H(09K)	109.5
H(09J)-C(12)-H(09K)	109.5
C(11)-C(12)-H(09L)	109.5
H(09J)-C(12)-H(09L)	109.5
H(09K)-C(12)-H(09L)	109.5
C(11)-C(13)-H(08J)	109.5
C(11)-C(13)-H(08K)	109.5
H(08J)-C(13)-H(08K)	109.5
C(11)-C(13)-H(08L)	109.5
H(08J)-C(13)-H(08L)	109.5
H(08K)-C(13)-H(08L)	109.5
C(11)-C(14)-H(11A)	109.5
C(11)-C(14)-H(11B)	109.5
H(11A)-C(14)-H(11B)	109.5
C(11)-C(14)-H(11C)	109.5
H(11A)-C(14)-H(11C)	109.5
H(11B)-C(14)-H(11C)	109.5
C(4)-C(15)-H(08G)	109.5
C(4)-C(15)-H(08H)	109.5
H(08G)-C(15)-H(08H)	109.5
C(4)-C(15)-H(08I)	109.5
H(08G)-C(15)-H(08I)	109.5
H(08H)-C(15)-H(08I)	109.5
N(1)-C(16)-N(2)	103.7(2)
N(1)-C(16)-Ni(1)	127.60(19)
N(2)-C(16)-Ni(1)	128.7(2)
C(18)-C(17)-N(2)	107.1(2)
C(18)-C(17)-H(087)	126.4
N(2)-C(17)-H(087)	126.4
C(17)-C(18)-N(1)	106.8(2)
C(17)-C(18)-H(023)	126.6
N(1)-C(18)-H(023)	126.6
C(20)-C(19)-C(24)	123.3(3)

C(20)-C(19)-N(1)	118.8(2)
C(24)-C(19)-N(1)	118.0(2)
C(19)-C(20)-C(21)	116.9(3)
C(19)-C(20)-C(28)	122.4(2)
C(21)-C(20)-C(28)	120.7(3)
C(22)-C(21)-C(20)	121.3(3)
C(22)-C(21)-H(093)	119.4
C(20)-C(21)-H(093)	119.4
C(21)-C(22)-C(23)	120.4(3)
C(21)-C(22)-H(119)	119.8
C(23)-C(22)-H(119)	119.8
C(24)-C(23)-C(22)	121.1(3)
C(24)-C(23)-H(109)	119.4
C(22)-C(23)-H(109)	119.4
C(23)-C(24)-C(19)	117.1(3)
C(23)-C(24)-C(25)	121.0(3)
C(19)-C(24)-C(25)	121.9(3)
C(26)-C(25)-C(27)	111.9(4)
C(26)-C(25)-C(24)	113.3(3)
C(27)-C(25)-C(24)	109.9(3)
C(26)-C(25)-H(102)	107.1
C(27)-C(25)-H(102)	107.1
C(24)-C(25)-H(102)	107.1
C(25)-C(26)-H(13S)	109.5
C(25)-C(26)-H(13T)	109.5
H(13S)-C(26)-H(13T)	109.5
C(25)-C(26)-H(13U)	109.5
H(13S)-C(26)-H(13U)	109.5
H(13T)-C(26)-H(13U)	109.5
C(25)-C(27)-H(12P)	109.5
C(25)-C(27)-H(12Q)	109.5
H(12P)-C(27)-H(12Q)	109.5
C(25)-C(27)-H(12R)	109.5
H(12P)-C(27)-H(12R)	109.5
H(12Q)-C(27)-H(12R)	109.5
C(20)-C(28)-C(29)	109.2(2)

C(20)-C(28)-C(30)	113.9(2)
C(29)-C(28)-C(30)	110.3(2)
C(20)-C(28)-H(042)	107.7
C(29)-C(28)-H(042)	107.7
C(30)-C(28)-H(042)	107.7
C(28)-C(29)-H(09A)	109.5
C(28)-C(29)-H(09B)	109.5
H(09A)-C(29)-H(09B)	109.5
C(28)-C(29)-H(09C)	109.5
H(09A)-C(29)-H(09C)	109.5
H(09B)-C(29)-H(09C)	109.5
C(28)-C(30)-H(12J)	109.5
C(28)-C(30)-H(12K)	109.5
H(12J)-C(30)-H(12K)	109.5
C(28)-C(30)-H(12L)	109.5
H(12J)-C(30)-H(12L)	109.5
H(12K)-C(30)-H(12L)	109.5
C(32)-C(31)-C(36)	123.5(3)
C(32)-C(31)-N(2)	119.5(2)
C(36)-C(31)-N(2)	117.0(3)
C(31)-C(32)-C(33)	116.8(3)
C(31)-C(32)-C(40)	122.7(3)
C(33)-C(32)-C(40)	120.5(3)
C(34)-C(33)-C(32)	120.7(4)
C(34)-C(33)-H(110)	119.6
C(32)-C(33)-H(110)	119.6
C(35)-C(34)-C(33)	121.0(3)
C(35)-C(34)-H(123)	119.5
C(33)-C(34)-H(123)	119.5
C(34)-C(35)-C(36)	121.8(3)
C(34)-C(35)-H(128)	119.1
C(36)-C(35)-H(128)	119.1
C(35)-C(36)-C(31)	116.2(3)
C(35)-C(36)-C(37)	121.3(3)
C(31)-C(36)-C(37)	122.5(3)
C(38)-C(37)-C(36)	111.1(3)

C(38)-C(37)-C(39)	112.0(4)
C(36)-C(37)-C(39)	112.1(3)
C(38)-C(37)-H(107)	107.1
C(36)-C(37)-H(107)	107.1
C(39)-C(37)-H(107)	107.1
C(37)-C(38)-H(13\$)	109.5
C(37)-C(38)-H(13V)	109.5
H(13\$)-C(38)-H(13V)	109.5
C(37)-C(38)-H(13W)	109.5
H(13\$)-C(38)-H(13W)	109.5
H(13V)-C(38)-H(13W)	109.5
C(37)-C(39)-H(131)	109.5
C(37)-C(39)-H(13)	109.5
H(131)-C(39)-H(13)	109.5
C(37)-C(39)-H(13M)	109.5
H(131)-C(39)-H(13M)	109.5
H(13)-C(39)-H(13M)	109.5
C(32)-C(40)-C(41)	112.0(2)
C(32)-C(40)-C(42)	109.7(2)
C(41)-C(40)-C(42)	110.9(2)
C(32)-C(40)-H(081)	108.0
C(41)-C(40)-H(081)	108.0
C(42)-C(40)-H(081)	108.0
C(40)-C(41)-H(11S)	109.5
C(40)-C(41)-H(11T)	109.5
H(11S)-C(41)-H(11T)	109.5
C(40)-C(41)-H(11U)	109.5
H(11S)-C(41)-H(11U)	109.5
H(11T)-C(41)-H(11U)	109.5
C(40)-C(42)-H(10J)	109.5
C(40)-C(42)-H(10K)	109.5
H(10J)-C(42)-H(10K)	109.5
C(40)-C(42)-H(10L)	109.5
H(10J)-C(42)-H(10L)	109.5
H(10K)-C(42)-H(10L)	109.5
O(2)-C(43)-C(48)	121.0(3)

O(2)-C(43)-C(44)	118.8(3)
C(48)-C(43)-C(44)	119.9(2)
C(45)-C(44)-C(43)	118.1(3)
C(45)-C(44)-C(53)	121.3(2)
C(43)-C(44)-C(53)	120.6(2)
C(44)-C(45)-C(46)	123.3(2)
C(44)-C(45)-H(047)	118.3
C(46)-C(45)-H(047)	118.3
C(45)-C(46)-C(47)	117.6(2)
C(45)-C(46)-C(57)	121.1(2)
C(47)-C(46)-C(57)	121.4(3)
C(46)-C(47)-C(48)	123.0(3)
C(46)-C(47)-H(061)	118.5
C(48)-C(47)-H(061)	118.5
C(47)-C(48)-C(43)	117.8(2)
C(47)-C(48)-C(49)	120.4(3)
C(43)-C(48)-C(49)	121.8(2)
C(51)-C(49)-C(52)	107.4(3)
C(51)-C(49)-C(48)	112.7(2)
C(52)-C(49)-C(48)	109.9(2)
C(51)-C(49)-C(50)	106.4(2)
C(52)-C(49)-C(50)	110.3(3)
C(48)-C(49)-C(50)	110.1(2)
C(49)-C(50)-H(10M)	109.5
C(49)-C(50)-H(10N)	109.5
H(10M)-C(50)-H(10N)	109.5
C(49)-C(50)-H(10O)	109.5
H(10M)-C(50)-H(10O)	109.5
H(10N)-C(50)-H(10O)	109.5
C(49)-C(51)-H(11J)	109.5
C(49)-C(51)-H(11K)	109.5
H(11J)-C(51)-H(11K)	109.5
C(49)-C(51)-H(11L)	109.5
H(11J)-C(51)-H(11L)	109.5
H(11K)-C(51)-H(11L)	109.5
C(49)-C(52)-H(12M)	109.5

C(49)-C(52)-H(12N)	109.5
H(12M)-C(52)-H(12N)	109.5
C(49)-C(52)-H(12O)	109.5
H(12M)-C(52)-H(12O)	109.5
H(12N)-C(52)-H(12O)	109.5
C(44)-C(53)-C(54)	111.4(2)
C(44)-C(53)-C(56)	112.1(3)
C(54)-C(53)-C(56)	106.9(2)
C(44)-C(53)-C(55)	109.3(2)
C(54)-C(53)-C(55)	110.1(3)
C(56)-C(53)-C(55)	106.9(3)
C(53)-C(54)-H(12G)	109.5
C(53)-C(54)-H(12H)	109.5
H(12G)-C(54)-H(12H)	109.5
C(53)-C(54)-H(12I)	109.5
H(12G)-C(54)-H(12I)	109.5
H(12H)-C(54)-H(12I)	109.5
C(53)-C(55)-H(12A)	109.5
C(53)-C(55)-H(12B)	109.5
H(12A)-C(55)-H(12B)	109.5
C(53)-C(55)-H(12C)	109.5
H(12A)-C(55)-H(12C)	109.5
H(12B)-C(55)-H(12C)	109.5
C(53)-C(56)-H(09P)	109.5
C(53)-C(56)-H(09Q)	109.5
H(09P)-C(56)-H(09Q)	109.5
C(53)-C(56)-H(09R)	109.5
H(09P)-C(56)-H(09R)	109.5
H(09Q)-C(56)-H(09R)	109.5
C(46)-C(57)-H(11M)	109.5
C(46)-C(57)-H(11N)	109.5
H(11M)-C(57)-H(11N)	109.5
C(46)-C(57)-H(11O)	109.5
H(11M)-C(57)-H(11O)	109.5
H(11N)-C(57)-H(11O)	109.5
N(3)-C(58)-N(4)	103.4(2)

N(3)-C(58)-Ni(2)	127.50(17)
N(4)-C(58)-Ni(2)	129.05(19)
C(60)-C(59)-N(4)	107.1(2)
C(60)-C(59)-H(039)	126.4
N(4)-C(59)-H(039)	126.4
C(59)-C(60)-N(3)	106.6(2)
C(59)-C(60)-H(054)	126.7
N(3)-C(60)-H(054)	126.7
C(62)-C(61)-C(66)	123.5(2)
C(62)-C(61)-N(3)	118.2(2)
C(66)-C(61)-N(3)	118.3(2)
C(61)-C(62)-C(63)	117.1(2)
C(61)-C(62)-C(70)	122.3(2)
C(63)-C(62)-C(70)	120.6(2)
C(64)-C(63)-C(62)	121.0(3)
C(64)-C(63)-H(065)	119.5
C(62)-C(63)-H(065)	119.5
C(65)-C(64)-C(63)	120.4(3)
C(65)-C(64)-H(089)	119.8
C(63)-C(64)-H(089)	119.8
C(64)-C(65)-C(66)	121.6(3)
C(64)-C(65)-H(071)	119.2
C(66)-C(65)-H(071)	119.2
C(65)-C(66)-C(61)	116.5(3)
C(65)-C(66)-C(67)	121.4(2)
C(61)-C(66)-C(67)	122.1(2)
C(69)-C(67)-C(66)	113.3(3)
C(69)-C(67)-C(68)	110.7(3)
C(66)-C(67)-C(68)	109.9(3)
C(69)-C(67)-H(105)	107.6
C(66)-C(67)-H(105)	107.6
C(68)-C(67)-H(105)	107.6
C(67)-C(68)-H(132)	109.5
C(67)-C(68)-H(13N)	109.5
H(132)-C(68)-H(13N)	109.5
C(67)-C(68)-H(13O)	109.5

H(132)-C(68)-H(13O)	109.5
H(13N)-C(68)-H(13O)	109.5
C(67)-C(69)-H(13P)	109.5
C(67)-C(69)-H(13Q)	109.5
H(13P)-C(69)-H(13Q)	109.5
C(67)-C(69)-H(13R)	109.5
H(13P)-C(69)-H(13R)	109.5
H(13Q)-C(69)-H(13R)	109.5
C(72)-C(70)-C(62)	112.0(2)
C(72)-C(70)-C(71)	111.8(3)
C(62)-C(70)-C(71)	110.2(2)
C(72)-C(70)-H(073)	107.6
C(62)-C(70)-H(073)	107.6
C(71)-C(70)-H(073)	107.6
C(70)-C(71)-H(12D)	109.5
C(70)-C(71)-H(12E)	109.5
H(12D)-C(71)-H(12E)	109.5
C(70)-C(71)-H(12F)	109.5
H(12D)-C(71)-H(12F)	109.5
H(12E)-C(71)-H(12F)	109.5
C(70)-C(72)-H(13A)	109.5
C(70)-C(72)-H(13B)	109.5
H(13A)-C(72)-H(13B)	109.5
C(70)-C(72)-H(13C)	109.5
H(13A)-C(72)-H(13C)	109.5
H(13B)-C(72)-H(13C)	109.5
C(78)-C(73)-C(74)	123.7(2)
C(78)-C(73)-N(4)	117.7(2)
C(74)-C(73)-N(4)	118.5(2)
C(75)-C(74)-C(73)	116.9(2)
C(75)-C(74)-C(82)	120.9(2)
C(73)-C(74)-C(82)	122.1(2)
C(76)-C(75)-C(74)	120.6(3)
C(76)-C(75)-H(031)	119.7
C(74)-C(75)-H(031)	119.7
C(77)-C(76)-C(75)	120.6(3)

C(77)-C(76)-H(067)	119.7
C(75)-C(76)-H(067)	119.7
C(76)-C(77)-C(78)	121.5(3)
C(76)-C(77)-H(058)	119.2
C(78)-C(77)-H(058)	119.2
C(77)-C(78)-C(73)	116.6(2)
C(77)-C(78)-C(79)	121.1(2)
C(73)-C(78)-C(79)	122.3(2)
C(80)-C(79)-C(81)	110.5(3)
C(80)-C(79)-C(78)	114.5(3)
C(81)-C(79)-C(78)	111.9(2)
C(80)-C(79)-H(046)	106.5
C(81)-C(79)-H(046)	106.5
C(78)-C(79)-H(046)	106.5
C(79)-C(80)-H(13D)	109.5
C(79)-C(80)-H(13E)	109.5
H(13D)-C(80)-H(13E)	109.5
C(79)-C(80)-H(13F)	109.5
H(13D)-C(80)-H(13F)	109.5
H(13E)-C(80)-H(13F)	109.5
C(79)-C(81)-H(12\$)	109.5
C(79)-C(81)-H(12V)	109.5
H(12\$)-C(81)-H(12V)	109.5
C(79)-C(81)-H(12W)	109.5
H(12\$)-C(81)-H(12W)	109.5
H(12V)-C(81)-H(12W)	109.5
C(74)-C(82)-C(84)	110.6(2)
C(74)-C(82)-C(83)	112.5(2)
C(84)-C(82)-C(83)	110.6(2)
C(74)-C(82)-H(059)	107.7
C(84)-C(82)-H(059)	107.7
C(83)-C(82)-H(059)	107.7
C(82)-C(83)-H(11G)	109.5
C(82)-C(83)-H(11H)	109.5
H(11G)-C(83)-H(11H)	109.5
C(82)-C(83)-H(11I)	109.5

H(11G)-C(83)-H(11I)	109.5
H(11H)-C(83)-H(11I)	109.5
C(82)-C(84)-H(10A)	109.5
C(82)-C(84)-H(10B)	109.5
H(10A)-C(84)-H(10B)	109.5
C(82)-C(84)-H(10C)	109.5
H(10A)-C(84)-H(10C)	109.5
H(10B)-C(84)-H(10C)	109.5
O(3)-C(85)-C(90)	120.7(2)
O(3)-C(85)-C(86)	119.6(2)
C(90)-C(85)-C(86)	119.5(2)
C(87)-C(86)-C(85)	118.7(2)
C(87)-C(86)-C(95)	121.2(2)
C(85)-C(86)-C(95)	120.1(2)
C(86)-C(87)-C(88)	123.0(3)
C(86)-C(87)-H(048)	118.5
C(88)-C(87)-H(048)	118.5
C(87)-C(88)-C(89)	117.5(3)
C(87)-C(88)-C(99)	121.2(3)
C(89)-C(88)-C(99)	121.2(3)
C(90)-C(89)-C(88)	123.1(3)
C(90)-C(89)-H(041)	118.5
C(88)-C(89)-H(041)	118.5
C(89)-C(90)-C(85)	118.1(2)
C(89)-C(90)-C(91)	121.5(2)
C(85)-C(90)-C(91)	120.3(2)
C(93)-C(91)-C(90)	112.2(2)
C(93)-C(91)-C(94)	106.8(2)
C(90)-C(91)-C(94)	109.5(2)
C(93)-C(91)-C(92)	108.0(2)
C(90)-C(91)-C(92)	111.5(2)
C(94)-C(91)-C(92)	108.8(2)
C(91)-C(92)-H(09D)	109.5
C(91)-C(92)-H(09E)	109.5
H(09D)-C(92)-H(09E)	109.5
C(91)-C(92)-H(09F)	109.5

H(09D)-C(92)-H(09F)	109.5
H(09E)-C(92)-H(09F)	109.5
C(91)-C(93)-H(10G)	109.5
C(91)-C(93)-H(10H)	109.5
H(10G)-C(93)-H(10H)	109.5
C(91)-C(93)-H(10I)	109.5
H(10G)-C(93)-H(10I)	109.5
H(10H)-C(93)-H(10I)	109.5
C(91)-C(94)-H(08A)	109.5
C(91)-C(94)-H(08B)	109.5
H(08A)-C(94)-H(08B)	109.5
C(91)-C(94)-H(08C)	109.5
H(08A)-C(94)-H(08C)	109.5
H(08B)-C(94)-H(08C)	109.5
C(96)-C(95)-C(98)	110.1(2)
C(96)-C(95)-C(97)	106.8(2)
C(98)-C(95)-C(97)	107.5(2)
C(96)-C(95)-C(86)	110.3(2)
C(98)-C(95)-C(86)	110.2(2)
C(97)-C(95)-C(86)	111.9(2)
C(95)-C(96)-H(07A)	109.5
C(95)-C(96)-H(07B)	109.5
H(07A)-C(96)-H(07B)	109.5
C(95)-C(96)-H(07C)	109.5
H(07A)-C(96)-H(07C)	109.5
H(07B)-C(96)-H(07C)	109.5
C(95)-C(97)-H(07D)	109.5
C(95)-C(97)-H(07E)	109.5
H(07D)-C(97)-H(07E)	109.5
C(95)-C(97)-H(07F)	109.5
H(07D)-C(97)-H(07F)	109.5
H(07E)-C(97)-H(07F)	109.5
C(95)-C(98)-H(09G)	109.5
C(95)-C(98)-H(09H)	109.5
H(09G)-C(98)-H(09H)	109.5
C(95)-C(98)-H(09I)	109.5

H(09G)-C(98)-H(09I)	109.5
H(09H)-C(98)-H(09I)	109.5
C(88)-C(99)-H(11P)	109.5
C(88)-C(99)-H(11Q)	109.5
H(11P)-C(99)-H(11Q)	109.5
C(88)-C(99)-H(11R)	109.5
H(11P)-C(99)-H(11R)	109.5
H(11Q)-C(99)-H(11R)	109.5
N(6)-C(100)-N(5)	103.3(2)
N(6)-C(100)-Ni(3)	133.04(18)
N(5)-C(100)-Ni(3)	123.38(17)
C(102)-C(101)-N(6)	107.0(2)
C(102)-C(101)-H(034)	126.5
N(6)-C(101)-H(034)	126.5
C(101)-C(102)-N(5)	106.4(2)
C(101)-C(102)-H(027)	126.8
N(5)-C(102)-H(027)	126.8
C(104)-C(103)-C(108)	123.1(2)
C(104)-C(103)-N(5)	118.7(2)
C(108)-C(103)-N(5)	118.2(2)
C(105)-C(104)-C(103)	117.2(2)
C(105)-C(104)-C(109)	121.3(2)
C(103)-C(104)-C(109)	121.4(2)
C(106)-C(105)-C(104)	120.7(2)
C(106)-C(105)-H(036)	119.6
C(104)-C(105)-H(036)	119.6
C(107)-C(106)-C(105)	120.9(2)
C(107)-C(106)-H(091)	119.6
C(105)-C(106)-H(091)	119.6
C(106)-C(107)-C(108)	120.9(2)
C(106)-C(107)-H(029)	119.6
C(108)-C(107)-H(029)	119.6
C(103)-C(108)-C(107)	117.1(2)
C(103)-C(108)-C(112)	122.7(2)
C(107)-C(108)-C(112)	120.1(2)
C(110)-C(109)-C(111)	110.6(2)

C(110)-C(109)-C(104)	111.0(2)
C(111)-C(109)-C(104)	113.4(2)
C(110)-C(109)-H(076)	107.2
C(111)-C(109)-H(076)	107.2
C(104)-C(109)-H(076)	107.2
C(109)-C(110)-H(11D)	109.5
C(109)-C(110)-H(11E)	109.5
H(11D)-C(110)-H(11E)	109.5
C(109)-C(110)-H(11F)	109.5
H(11D)-C(110)-H(11F)	109.5
H(11E)-C(110)-H(11F)	109.5
C(109)-C(111)-H(08D)	109.5
C(109)-C(111)-H(08E)	109.5
H(08D)-C(111)-H(08E)	109.5
C(109)-C(111)-H(08F)	109.5
H(08D)-C(111)-H(08F)	109.5
H(08E)-C(111)-H(08F)	109.5
C(108)-C(112)-C(113)	109.8(2)
C(108)-C(112)-C(114)	112.3(2)
C(113)-C(112)-C(114)	111.2(2)
C(108)-C(112)-H(052)	107.8
C(113)-C(112)-H(052)	107.8
C(114)-C(112)-H(052)	107.8
C(112)-C(113)-H(09M)	109.5
C(112)-C(113)-H(09N)	109.5
H(09M)-C(113)-H(09N)	109.5
C(112)-C(113)-H(09O)	109.5
H(09M)-C(113)-H(09O)	109.5
H(09N)-C(113)-H(09O)	109.5
C(112)-C(114)-H(05A)	109.5
C(112)-C(114)-H(05B)	109.5
H(05A)-C(114)-H(05B)	109.5
C(112)-C(114)-H(05C)	109.5
H(05A)-C(114)-H(05C)	109.5
H(05B)-C(114)-H(05C)	109.5
C(120)-C(115)-C(116)	123.7(2)

C(120)-C(115)-N(6)	117.6(2)
C(116)-C(115)-N(6)	118.6(2)
C(117)-C(116)-C(115)	116.7(2)
C(117)-C(116)-C(124)	120.6(2)
C(115)-C(116)-C(124)	122.7(2)
C(118)-C(117)-C(116)	120.7(3)
C(118)-C(117)-H(069)	119.7
C(116)-C(117)-H(069)	119.7
C(119)-C(118)-C(117)	120.9(3)
C(119)-C(118)-H(074)	119.5
C(117)-C(118)-H(074)	119.5
C(118)-C(119)-C(120)	121.5(3)
C(118)-C(119)-H(103)	119.2
C(120)-C(119)-H(103)	119.2
C(119)-C(120)-C(115)	116.4(3)
C(119)-C(120)-C(121)	120.8(2)
C(115)-C(120)-C(121)	122.8(2)
C(120)-C(121)-C(122)	112.3(3)
C(120)-C(121)-C(123)	111.6(2)
C(122)-C(121)-C(123)	109.9(3)
C(120)-C(121)-H(095)	107.6
C(122)-C(121)-H(095)	107.6
C(123)-C(121)-H(095)	107.6
C(121)-C(122)-H(13G)	109.5
C(121)-C(122)-H(13H)	109.5
H(13G)-C(122)-H(13H)	109.5
C(121)-C(122)-H(13I)	109.5
H(13G)-C(122)-H(13I)	109.5
H(13H)-C(122)-H(13I)	109.5
C(121)-C(123)-H(11\$)	109.5
C(121)-C(123)-H(11V)	109.5
H(11\$)-C(123)-H(11V)	109.5
C(121)-C(123)-H(11W)	109.5
H(11\$)-C(123)-H(11W)	109.5
H(11V)-C(123)-H(11W)	109.5
C(126)-C(124)-C(125)	109.5(3)

C(126)-C(124)-C(116)	111.8(2)
C(125)-C(124)-C(116)	112.7(3)
C(126)-C(124)-H(057)	107.5
C(125)-C(124)-H(057)	107.5
C(116)-C(124)-H(057)	107.5
C(124)-C(125)-H(13J)	109.5
C(124)-C(125)-H(13K)	109.5
H(13J)-C(125)-H(13K)	109.5
C(124)-C(125)-H(13L)	109.5
H(13J)-C(125)-H(13L)	109.5
H(13K)-C(125)-H(13L)	109.5
C(124)-C(126)-H(12S)	109.5
C(124)-C(126)-H(12T)	109.5
H(12S)-C(126)-H(12T)	109.5
C(124)-C(126)-H(12U)	109.5
H(12S)-C(126)-H(12U)	109.5
H(12T)-C(126)-H(12U)	109.5
C(16)-N(1)-C(18)	111.4(2)
C(16)-N(1)-C(19)	124.2(2)
C(18)-N(1)-C(19)	124.0(2)
C(16)-N(2)-C(17)	111.0(2)
C(16)-N(2)-C(31)	124.6(2)
C(17)-N(2)-C(31)	124.1(2)
C(58)-N(3)-C(60)	111.6(2)
C(58)-N(3)-C(61)	121.7(2)
C(60)-N(3)-C(61)	126.7(2)
C(58)-N(4)-C(59)	111.3(2)
C(58)-N(4)-C(73)	122.8(2)
C(59)-N(4)-C(73)	125.7(2)
C(100)-N(5)-C(102)	111.9(2)
C(100)-N(5)-C(103)	121.6(2)
C(102)-N(5)-C(103)	126.5(2)
C(100)-N(6)-C(101)	111.4(2)
C(100)-N(6)-C(115)	124.1(2)
C(101)-N(6)-C(115)	124.2(2)
C(1)-O(1)-Ni(1)	168.2(2)

C(43)-O(2)-Ni(2)	151.0(2)
C(85)-O(3)-Ni(3)	131.82(15)
O(1)-Ni(1)-C(16)	173.30(10)
O(2)-Ni(2)-C(58)	168.99(11)
O(3)-Ni(3)-C(100)	162.19(9)

Table S13. Bond lengths [Å] and angles [°] for Compound 8.

C(1)-O(1)	1.2570(17)
C(1)-C(2)	1.4707(19)
C(1)-C(6)	1.4721(19)
C(1)-Ni(1)	2.4648(14)
C(2)-C(3)	1.4076(19)
C(2)-C(11)	1.5385(19)
C(2)-Ni(1)	2.2362(13)
C(3)-C(4)	1.409(2)
C(3)-Ni(1)	2.1701(14)
C(3)-H(3)	0.9500
C(4)-C(5)	1.410(2)
C(4)-C(15)	1.5067(19)
C(4)-Ni(1)	2.1949(14)
C(5)-C(6)	1.4037(19)
C(5)-Ni(1)	2.1803(13)
C(5)-H(5)	0.9500
C(6)-C(7)	1.5372(19)
C(6)-Ni(1)	2.2534(13)
C(7)-C(10)	1.5329(19)
C(7)-C(9)	1.534(2)
C(7)-C(8)	1.5375(19)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800

C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.5347(19)
C(11)-C(14)	1.5381(19)
C(11)-C(13)	1.5408(19)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(18)	1.5381(19)
C(16)-C(19)	1.542(2)
C(16)-C(17)	1.543(2)
C(16)-P(1)	1.9115(14)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(23)	1.531(2)
C(20)-C(21)	1.539(2)
C(20)-C(22)	1.5446(19)
C(20)-P(1)	1.9090(14)
C(21)-H(21A)	0.9800

C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(26)	1.538(2)
C(24)-C(27)	1.5401(19)
C(24)-C(25)	1.540(2)
C(24)-P(1)	1.9079(14)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
P(1)-Ni(1)	2.2333(4)

O(1)-C(1)-C(2)	122.29(12)
O(1)-C(1)-C(6)	122.18(12)
C(2)-C(1)-C(6)	115.42(12)
O(1)-C(1)-Ni(1)	142.50(10)
C(2)-C(1)-Ni(1)	63.47(7)
C(6)-C(1)-Ni(1)	64.15(7)
C(3)-C(2)-C(1)	119.06(12)
C(3)-C(2)-C(11)	120.79(12)
C(1)-C(2)-C(11)	119.29(12)
C(3)-C(2)-Ni(1)	68.84(8)
C(1)-C(2)-Ni(1)	80.48(8)
C(11)-C(2)-Ni(1)	130.46(9)
C(2)-C(3)-C(4)	122.71(13)

C(2)-C(3)-Ni(1)	73.94(8)
C(4)-C(3)-Ni(1)	72.13(8)
C(2)-C(3)-H(3)	118.6
C(4)-C(3)-H(3)	118.6
Ni(1)-C(3)-H(3)	127.5
C(3)-C(4)-C(5)	117.61(12)
C(3)-C(4)-C(15)	121.75(13)
C(5)-C(4)-C(15)	120.62(13)
C(3)-C(4)-Ni(1)	70.22(8)
C(5)-C(4)-Ni(1)	70.64(8)
C(15)-C(4)-Ni(1)	131.49(10)
C(6)-C(5)-C(4)	122.75(13)
C(6)-C(5)-Ni(1)	74.40(8)
C(4)-C(5)-Ni(1)	71.76(8)
C(6)-C(5)-H(5)	118.6
C(4)-C(5)-H(5)	118.6
Ni(1)-C(5)-H(5)	127.4
C(5)-C(6)-C(1)	119.18(12)
C(5)-C(6)-C(7)	120.90(12)
C(1)-C(6)-C(7)	119.27(11)
C(5)-C(6)-Ni(1)	68.73(8)
C(1)-C(6)-Ni(1)	79.85(8)
C(7)-C(6)-Ni(1)	130.16(9)
C(10)-C(7)-C(9)	107.52(12)
C(10)-C(7)-C(6)	112.04(11)
C(9)-C(7)-C(6)	110.68(11)
C(10)-C(7)-C(8)	107.91(12)
C(9)-C(7)-C(8)	109.51(11)
C(6)-C(7)-C(8)	109.11(11)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5

C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(14)	107.49(11)
C(12)-C(11)-C(2)	112.03(11)
C(14)-C(11)-C(2)	111.44(11)
C(12)-C(11)-C(13)	107.78(12)
C(14)-C(11)-C(13)	109.49(11)
C(2)-C(11)-C(13)	108.53(11)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(4)-C(15)-H(15A)	109.5

C(4)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(4)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(18)-C(16)-C(19)	108.67(12)
C(18)-C(16)-C(17)	108.65(11)
C(19)-C(16)-C(17)	105.51(12)
C(18)-C(16)-P(1)	116.21(10)
C(19)-C(16)-P(1)	108.79(9)
C(17)-C(16)-P(1)	108.48(10)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(23)-C(20)-C(21)	108.13(12)
C(23)-C(20)-C(22)	109.17(12)
C(21)-C(20)-C(22)	105.44(11)
C(23)-C(20)-P(1)	116.51(10)
C(21)-C(20)-P(1)	109.85(10)
C(22)-C(20)-P(1)	107.19(9)
C(20)-C(21)-H(21A)	109.5

C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(26)-C(24)-C(27)	108.07(11)
C(26)-C(24)-C(25)	105.92(12)
C(27)-C(24)-C(25)	109.13(12)
C(26)-C(24)-P(1)	109.05(10)
C(27)-C(24)-P(1)	115.68(10)
C(25)-C(24)-P(1)	108.56(9)
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(24)-C(27)-H(27A)	109.5

C(24)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(24)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(24)-P(1)-C(20)	108.74(6)
C(24)-P(1)-C(16)	108.28(6)
C(20)-P(1)-C(16)	108.26(6)
C(24)-P(1)-Ni(1)	114.42(5)
C(20)-P(1)-Ni(1)	104.22(4)
C(16)-P(1)-Ni(1)	112.65(4)
C(3)-Ni(1)-C(5)	67.32(5)
C(3)-Ni(1)-C(4)	37.65(5)
C(5)-Ni(1)-C(4)	37.60(5)
C(3)-Ni(1)-P(1)	131.74(4)
C(5)-Ni(1)-P(1)	131.35(4)
C(4)-Ni(1)-P(1)	124.92(4)
C(3)-Ni(1)-C(2)	37.22(5)
C(5)-Ni(1)-C(2)	79.48(5)
C(4)-Ni(1)-C(2)	67.79(5)
P(1)-Ni(1)-C(2)	145.82(4)
C(3)-Ni(1)-C(6)	79.32(5)
C(5)-Ni(1)-C(6)	36.87(5)
C(4)-Ni(1)-C(6)	67.44(5)
P(1)-Ni(1)-C(6)	145.34(4)
C(2)-Ni(1)-C(6)	67.30(5)
C(3)-Ni(1)-C(1)	64.36(5)
C(5)-Ni(1)-C(1)	64.21(5)
C(4)-Ni(1)-C(1)	76.49(5)
P(1)-Ni(1)-C(1)	158.59(3)
C(2)-Ni(1)-C(1)	36.05(5)
C(6)-Ni(1)-C(1)	36.01(5)