

SUPPORTING INFORMATION

Carbon-Carbon vs. Carbon-Oxygen bond activation in 2- and 3-Furonitriles with Nickel.

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INDEX OF FIGURES

Figure S1. $^{31}\text{P}\{^1\text{H}\}$ -NMR following up of stoichiometric reaction between complex (1) and 2-FN at room temperature in THF- d_8 . _____ S4

Figure S2. ^1H -NMR following up of stoichiometric reaction between complex (1) and 2-FN at room temperature in THF- d_8 . _____ S4

Figure S3. $^{31}\text{P}\{^1\text{H}\}$ -NMR following up of reaction between complex (1) and an excess of 2-FN at room temperature in THF- d_8 . * Impurity from complex (1). ___ S6

Figure S4. ^1H -NMR following up of reaction between complex (1) and an excess of 2-FN at room temperature in THF- d_8 . _____ S6

Figure S5. $^{31}\text{P}\{^1\text{H}\}$ -NMR following up of thermolysis of complex (7) at 100 °C in THF- d_8 . _____ S8

Figure S6. ^1H -NMR following up of thermolysis of complex (7) at 100 °C in THF- d_8 . _____ S9

Figure S7. $^{31}\text{P}\{^1\text{H}\}$ -NMR following up of reaction between complex (1) and 3-FN by 6 days at room temperature in THF- d_8 . _____ S12

Figure S8. ^1H -NMR following up of reaction between complex (1) and 3-FN by 6 days at room temperature in THF- d_8 . _____ S12

Figure S9. Comparison between ^1H -NMR spectrum of 3-FN and reaction solution after 6 days of reaction at room temperature by in THF- d_8 . _____ S13

INDEX OF SPECTRUMS

Spectrum S1. $^{31}\text{P}\{^1\text{H}\}$ -NMR spectrum of initial reaction between complex (1) and an excess of 2-FN in THF- d_8 at room temperature. Signals assigned to complex (2). _____ S5

Spectrum S2. ^1H -NMR spectrum of initial reaction between complex (1) and an excess of 2-FN in THF- d_8 at room temperature. Signals assigned to complex (2) and 2-FN. _____ S5

Spectrum S3. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of complex (7) in THF- d_8 at room temperature. Signals assigned to heteroaromatic carbons and nitrile carbon. __ S7

Spectrum S4. Mass spectrum of 2,2'-bifuryl, resulted from reaction of complex (7) at room temperature by 6 days in THF- d_8 . _____ S8

Spectrum S5. $^{31}\text{P}\{^1\text{H}\}$ -NMR spectrum of pure complex (9). _____ S9

Spectrum S6. ^1H -NMR spectrum of pure complex (9). _____ S10

Spectrum S7. Mass spectrum corresponding to 2-FN, obtained from thermolysis of complex (7) after 4 hours at 100 °C _____ S11

Spectrum S8. Mass spectrum corresponding to (5), obtained from thermolysis of complex (7) after 4 hours at 100 °C. _____ S11

Spectrum S9. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of complex (11) in THF- d_8 at room temperature. Signals assigned to heteroaromatic carbons and nitrile carbon. _ S13

Spectrum S10. Mass spectrum corresponding to (13), obtained from thermolysis of complex (11) after 4 hours at 100 °C. _____ S14

Spectrum S11. Mass spectrum corresponding to 3-FN, obtained from thermolysis of complex (11) after 4 hours at 100 °C. _____ S15

INDEX OF CRYSTALLOGRAPHIC TABLES

- Table S1.** *Crystal data and structure refinement for complex (7).* _____ S15
- Table S2.** *Atomic coordinates and equivalent isotropic displacement parameters for complex (7).* _____ S16
- Table S3.** *Bond lengths and angles for complex (7).* _____ S17
- Table S4.** *Anisotropic displacement parameters for complex (7).* _____ S22
- Table S5.** Torsion angles [°] for (7). _____ S22
- Table S6.** *Hydrogen bonds for complex (7).* _____ S24
- Table S7.** *Crystal data and structure refinement for complex (11).* _____ S24
- Table S8.** *Atomic coordinates and equivalent isotropic displacement parameters for complex (11).* _____ S25
- Table S9.** *Bond lengths and angles for complex (11).* _____ S26
- Table S10.** *Anisotropic displacement parameters for complex (11).* _____ S36
- Table S11.** Torsion angles [°] for (11). _____ S37
- Table S12.** *Hydrogen bonds for complex (11).* _____ S40

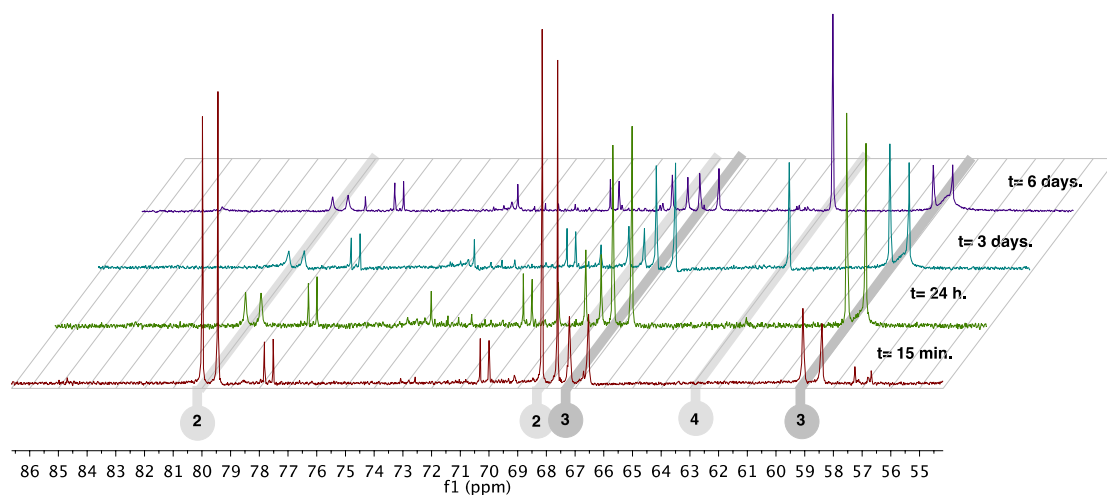


Figure S1. $^{31}\text{P}\{^1\text{H}\}$ -NMR following up of stoichiometric reaction between complex (1) and 2-FN at room temperature in THF-d_8 .

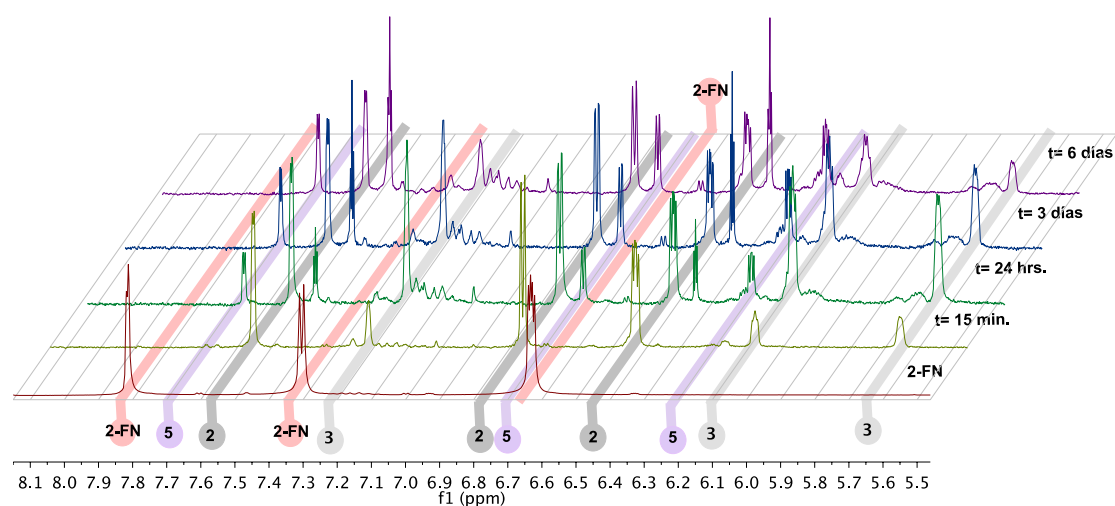
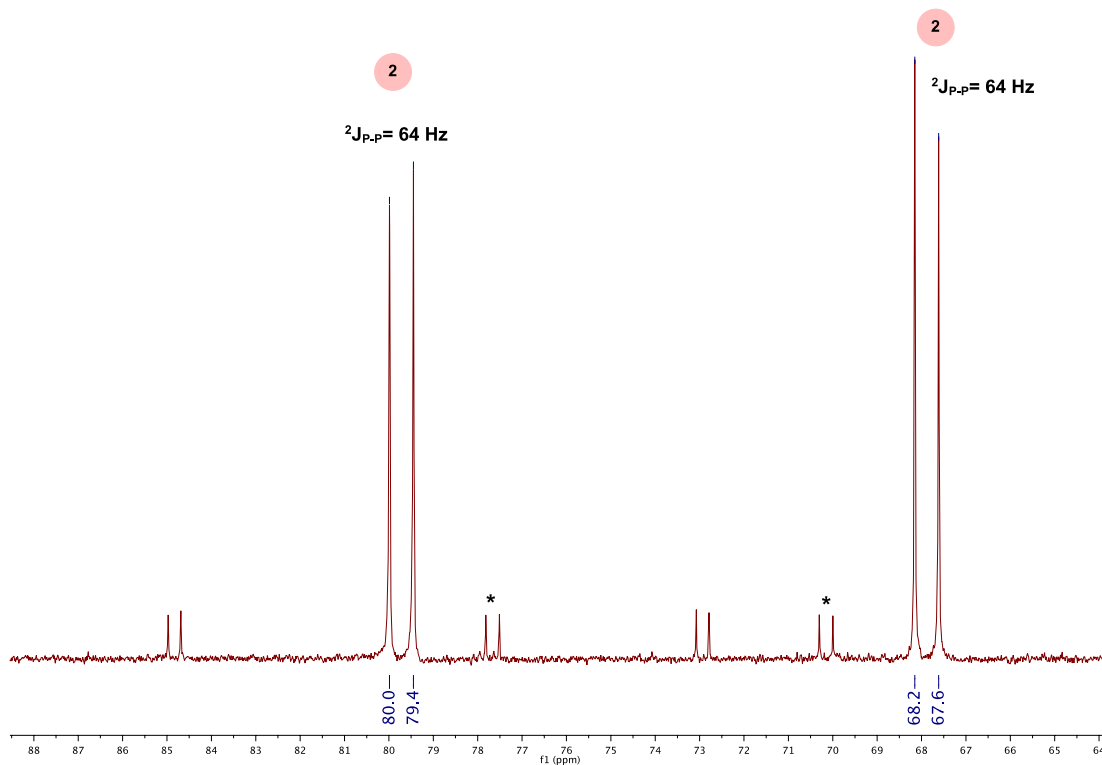
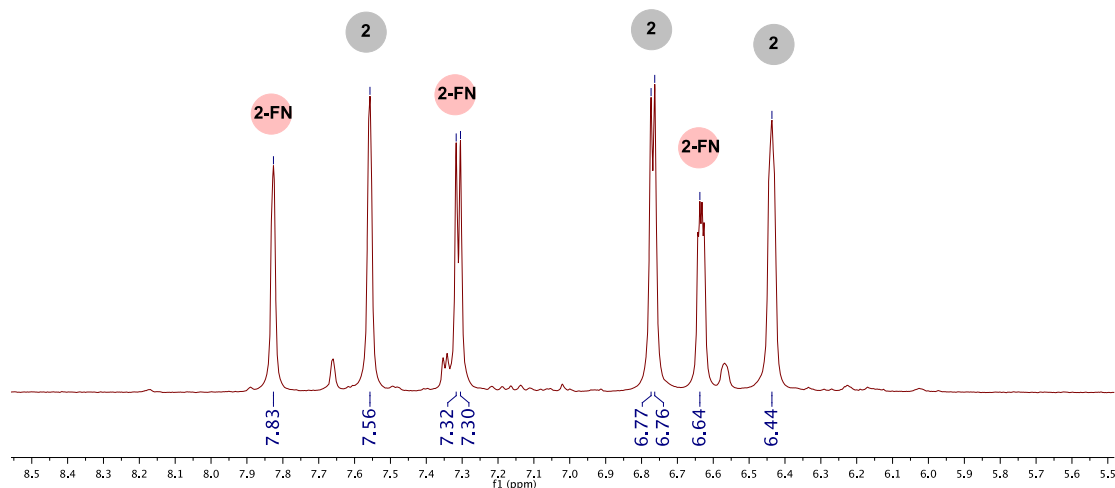


Figure S2. ^1H -NMR following up of stoichiometric reaction between complex (1) and 2-FN at room temperature in THF-d_8 .



Spectrum S1. $^{31}\text{P}\{^1\text{H}\}$ -NMR spectrum of initial reaction between complex (1) and an excess of 2-FN in THF- d_8 at room temperature. Signals assigned to complex (2). * Impurity from complex (1).



Spectrum S2. ^1H -NMR spectrum of initial reaction between complex (1) and an excess of 2-FN in THF- d_8 at room temperature. Signals assigned to complex (2) and 2-FN.

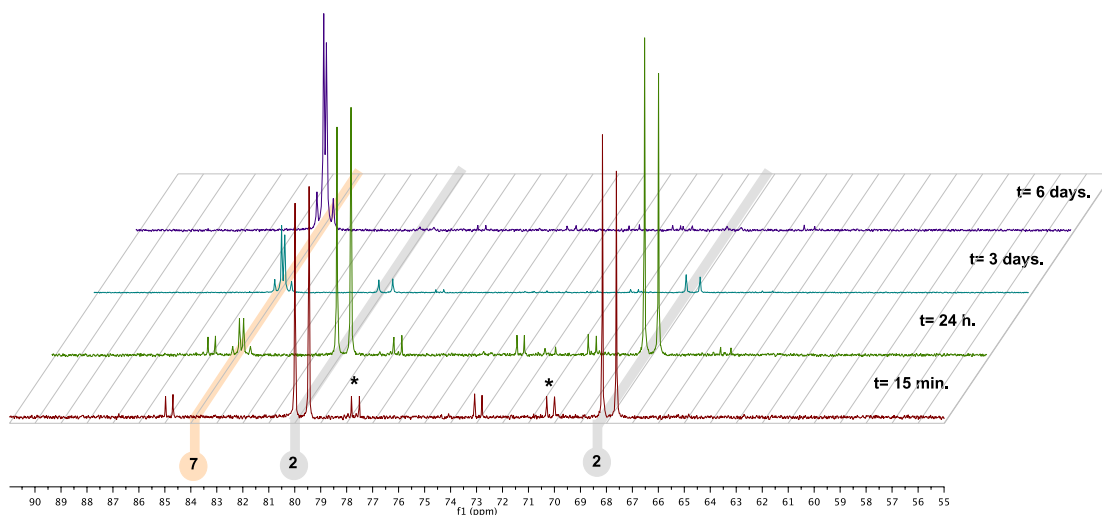


Figure S3. $^{31}\text{P}\{^1\text{H}\}$ -NMR following up of reaction between complex (1) and an excess of 2-FN at room temperature in THF-d_8 . * Impurity from complex (1).

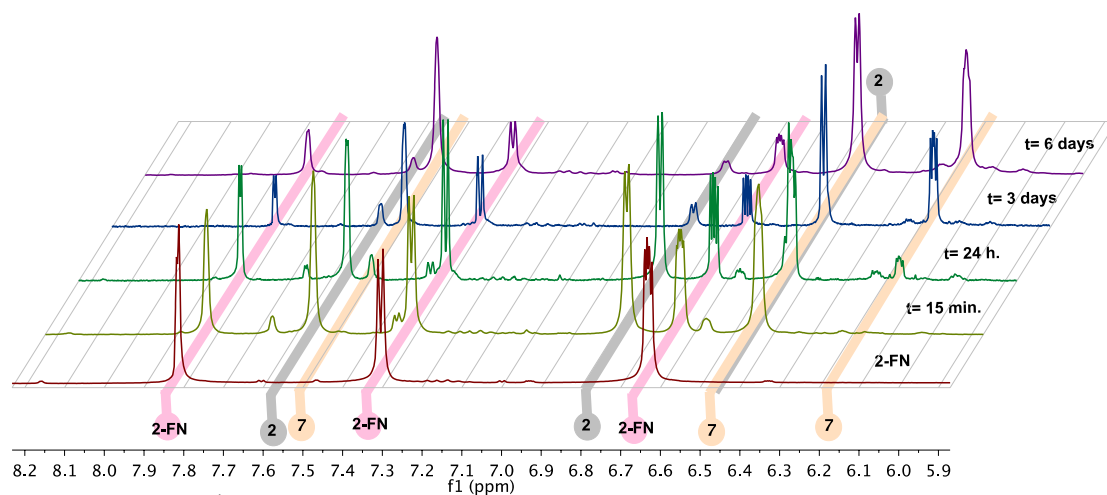
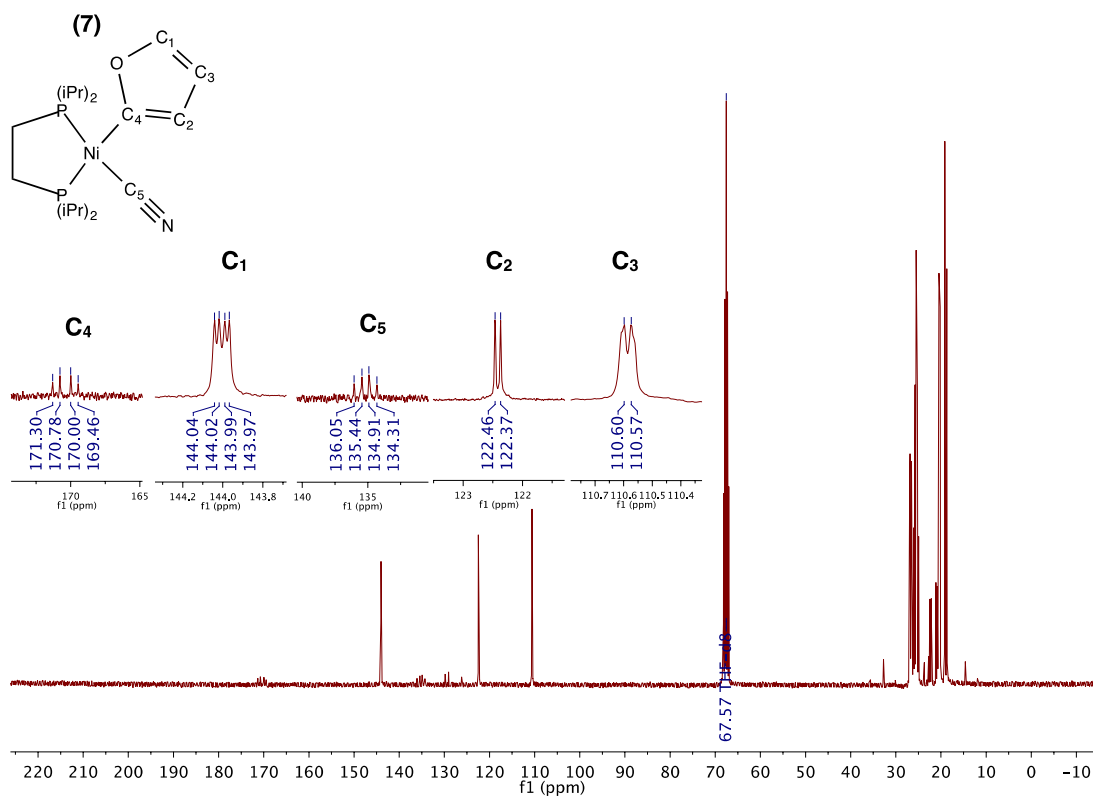
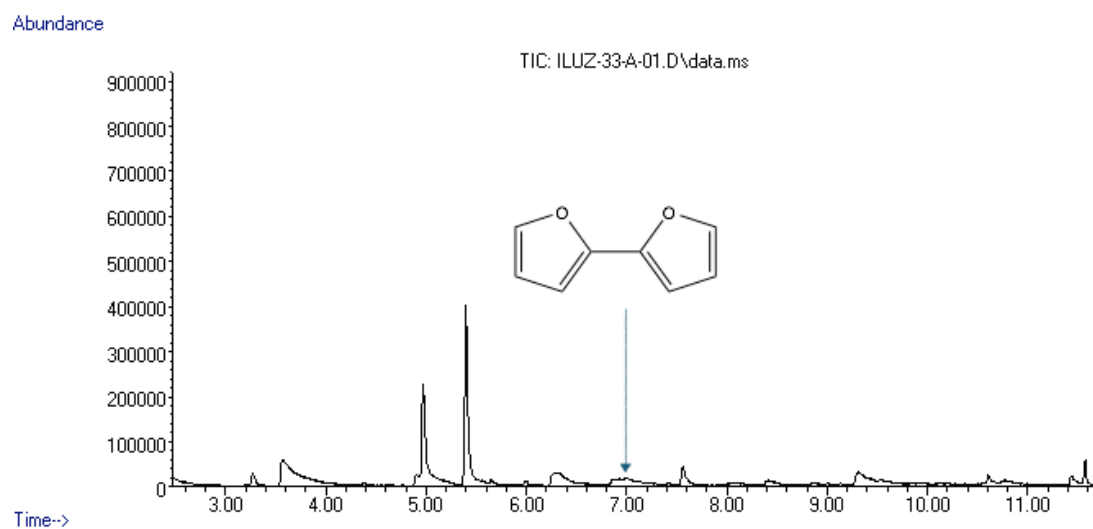


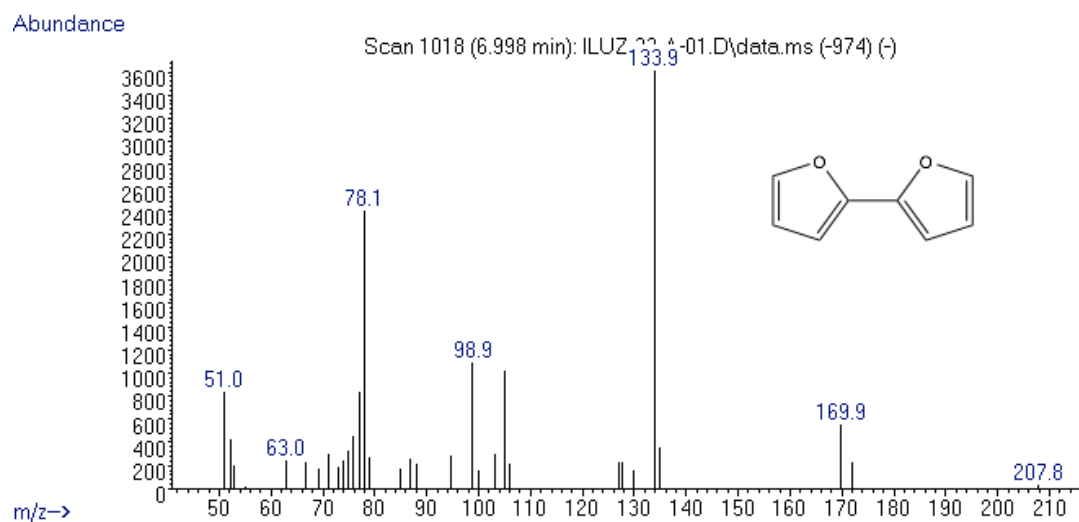
Figure S4. ^1H -NMR following up of reaction between complex (1) and an excess of 2-FN at room temperature in THF-d_8 .



Spectrum S3. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of complex **(7)** in THF- d_8 at room temperature. Signals assigned to heteroaromatic carbons and nitrile carbon.



Chromatogram S1. Chromatogram of reaction of complex **(7)** after 6 days at room temperature in TFH- d_8 . Peak assigned to compound 2,2'-bifuryl.



Spectrum S4. Mass spectrum of **2,2'-bifuryl**, resulted from reaction of complex **(7)** at room temperature by 6 days in THF- d_8 .

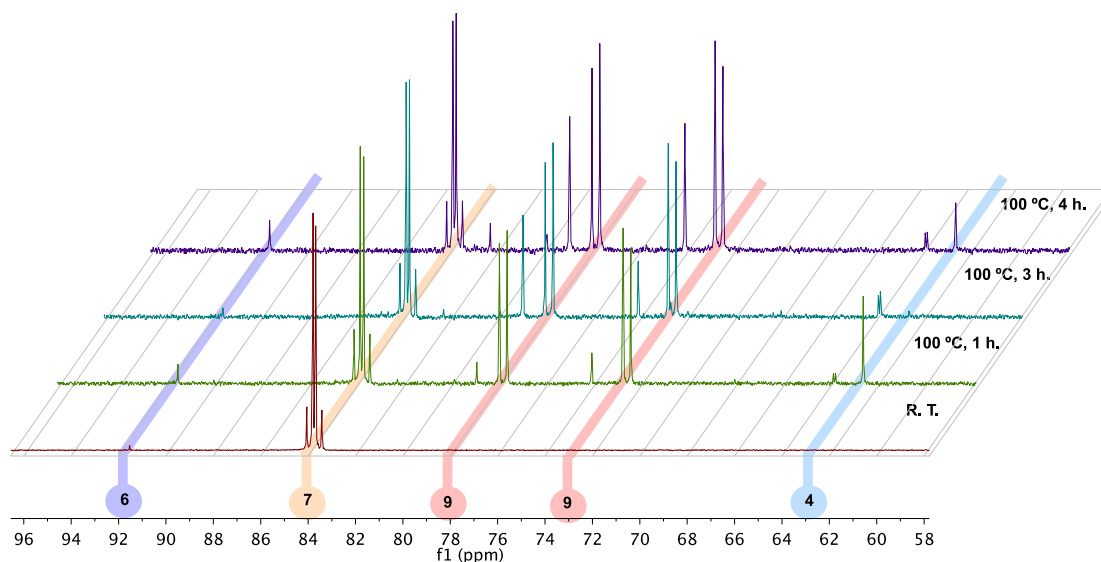


Figure S5. $^{31}\text{P}\{^1\text{H}\}$ -NMR following up of thermolysis of complex **(7)** at 100 °C in THF- d_8 .

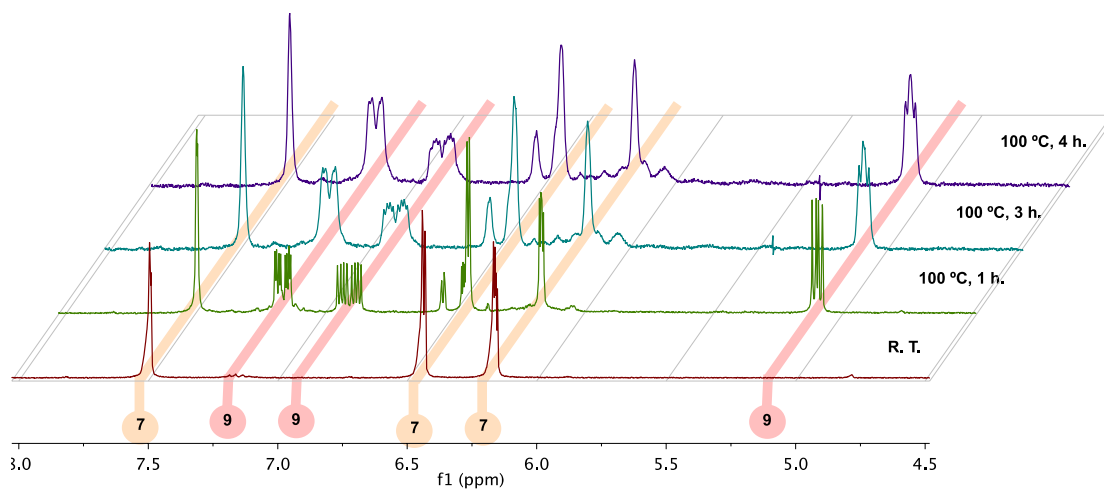
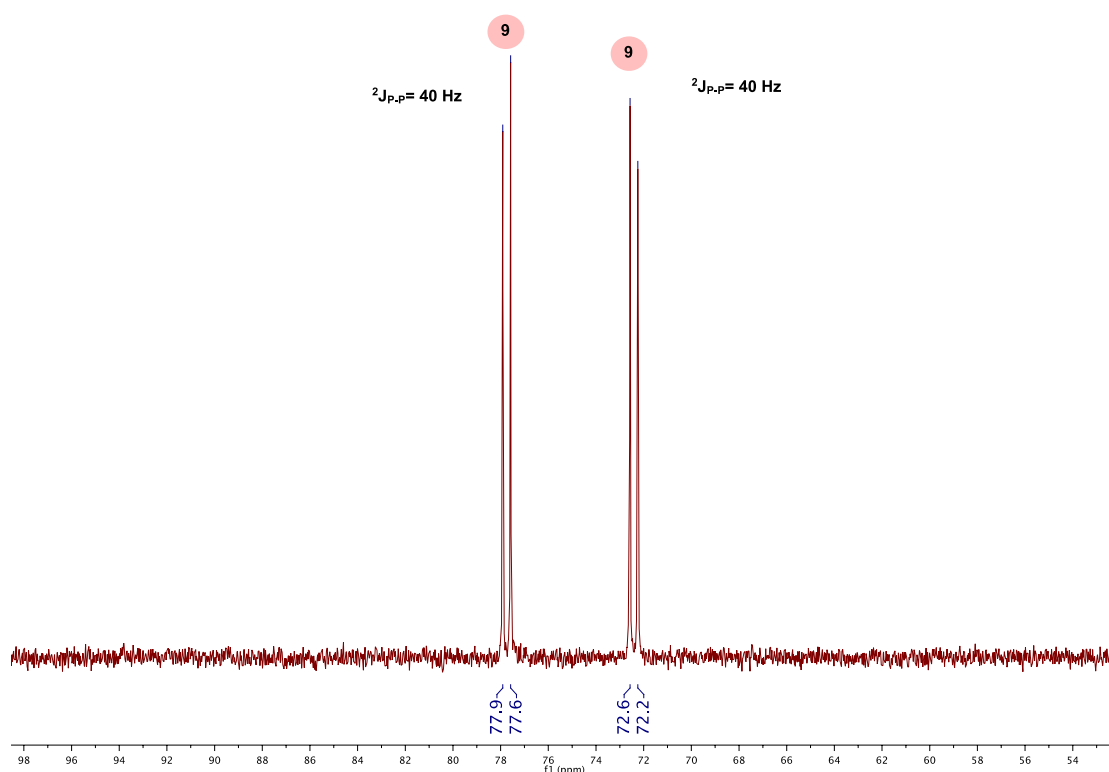
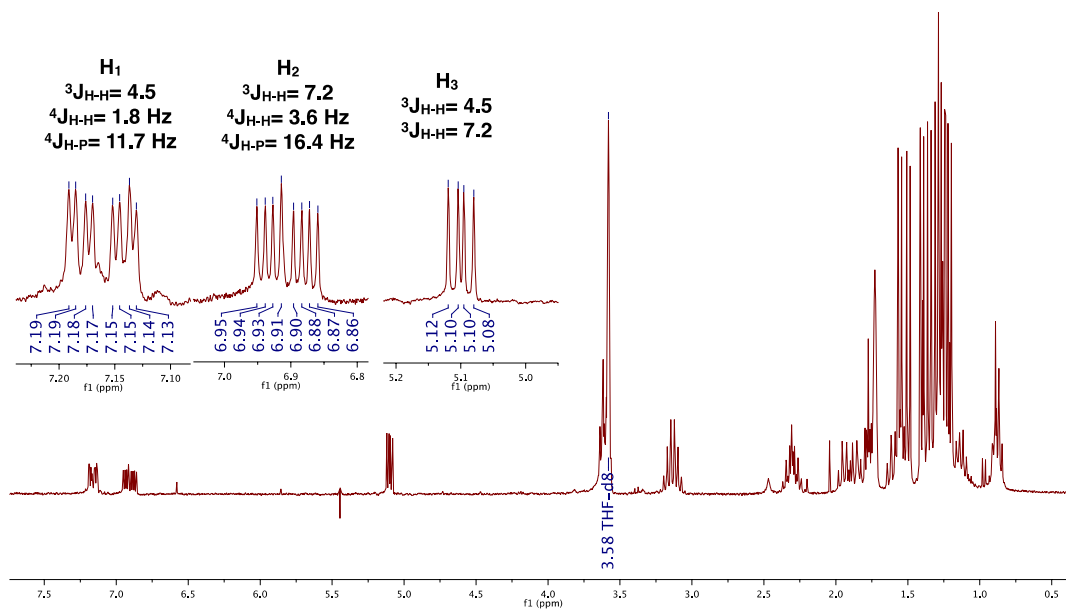
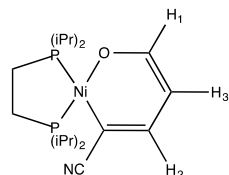


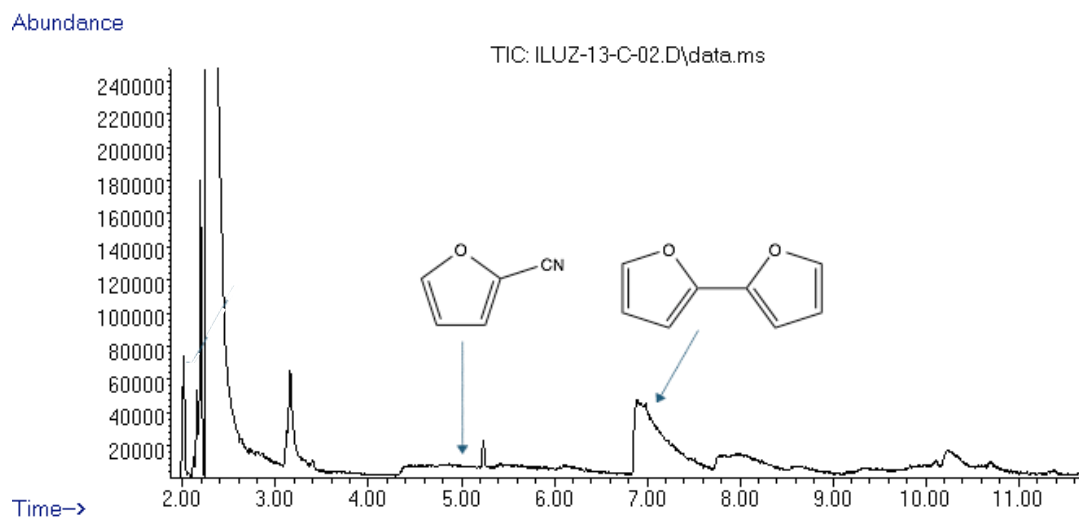
Figure S6. ^1H -NMR following up of thermolysis of complex (7) at 100 °C in THF- d_8 .



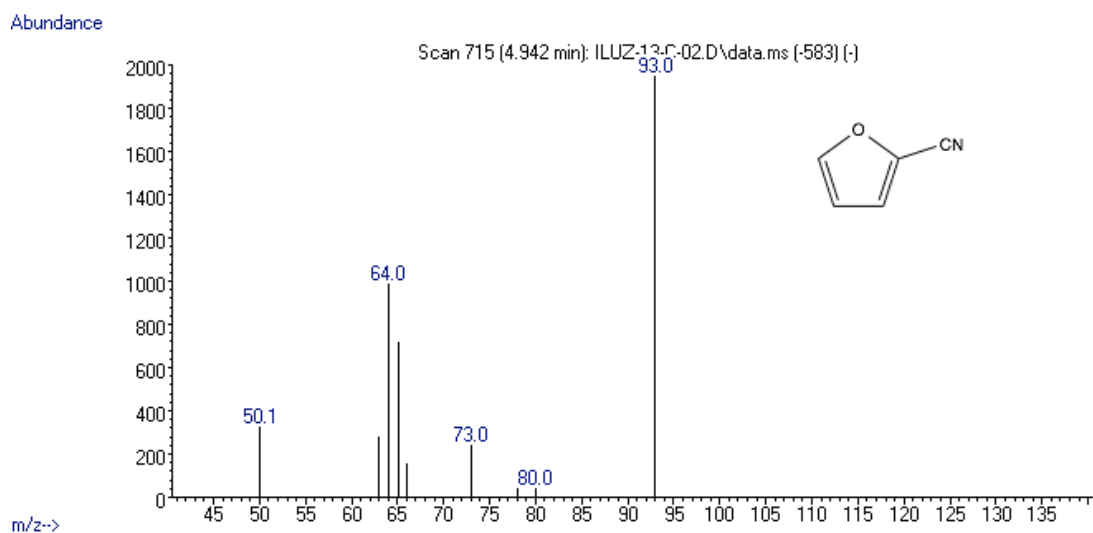
Spectrum S5. $^{31}\text{P}\{^1\text{H}\}$ -NMR spectrum of pure complex (9).



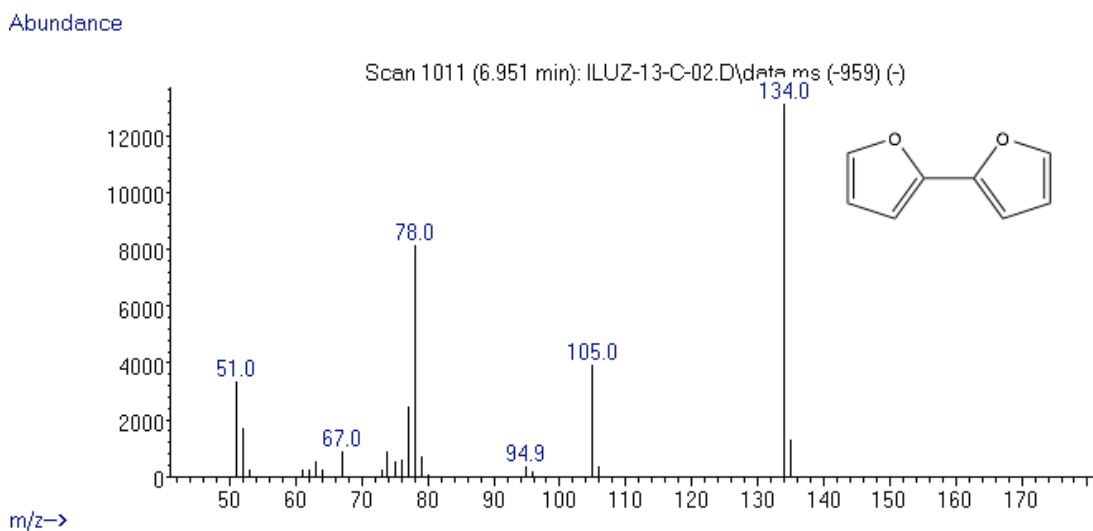
Spectrum S6. ¹H-NMR spectrum of pure complex (9).



Chromatogram S2. Chromatogram of thermolysis of complex (7) after 4 hours at 100 °C.



Spectrum S7. Mass spectrum corresponding to **2-FN**, obtained from thermolysis of complex **(7)** after 4 hours at 100 °C



Spectrum S8. Mass spectrum corresponding to **(5)**, obtained from thermolysis of complex **(7)** after 4 hours at 100 °C.

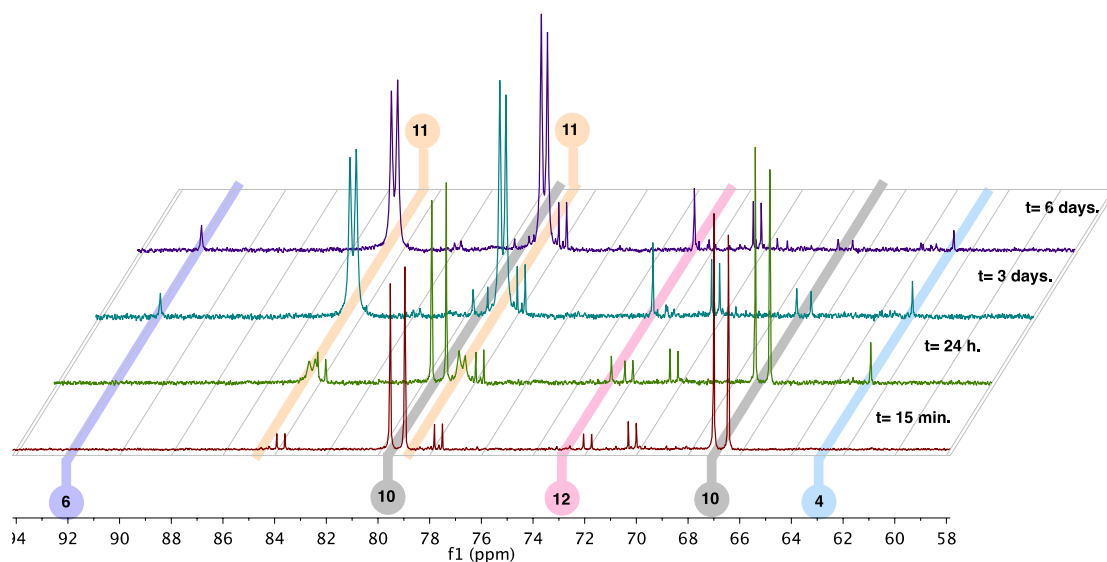


Figure S7. $^{31}\text{P}\{^1\text{H}\}$ -NMR following up of reaction between complex (1) and 3-FN by 6 days at room temperature in THF-d_8 .

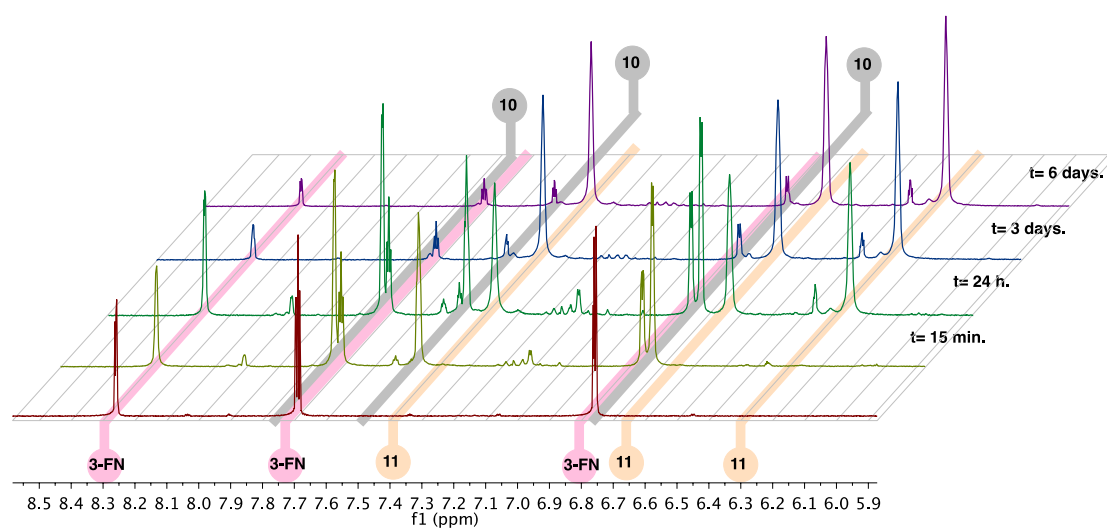


Figure S8. ^1H -NMR following up of reaction between complex (1) and 3-FN by 6 days at room temperature in THF-d_8 .

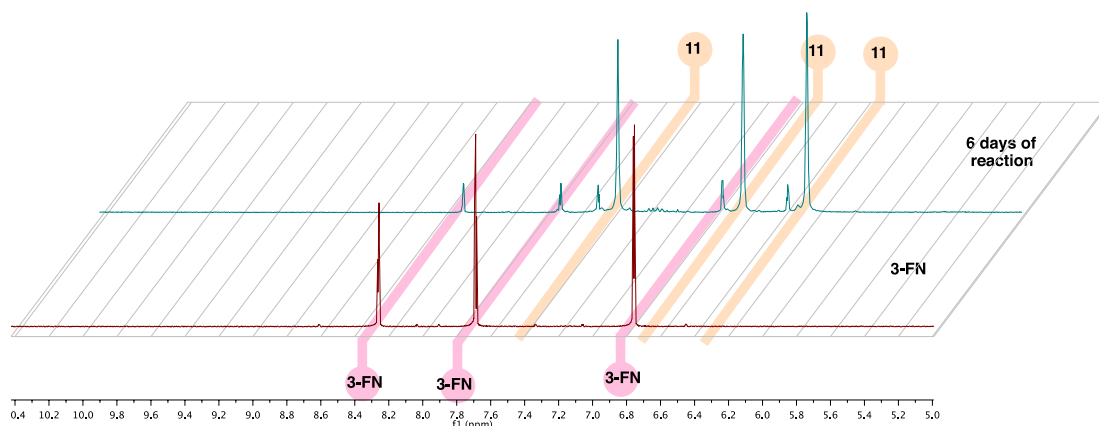
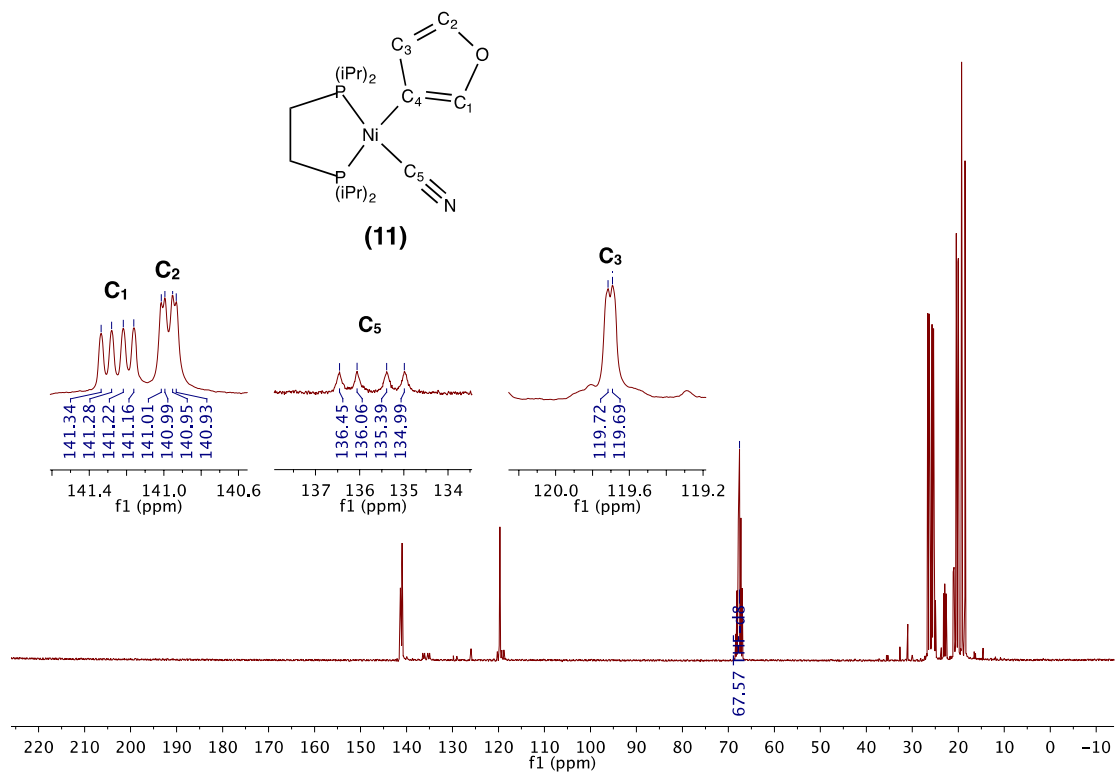
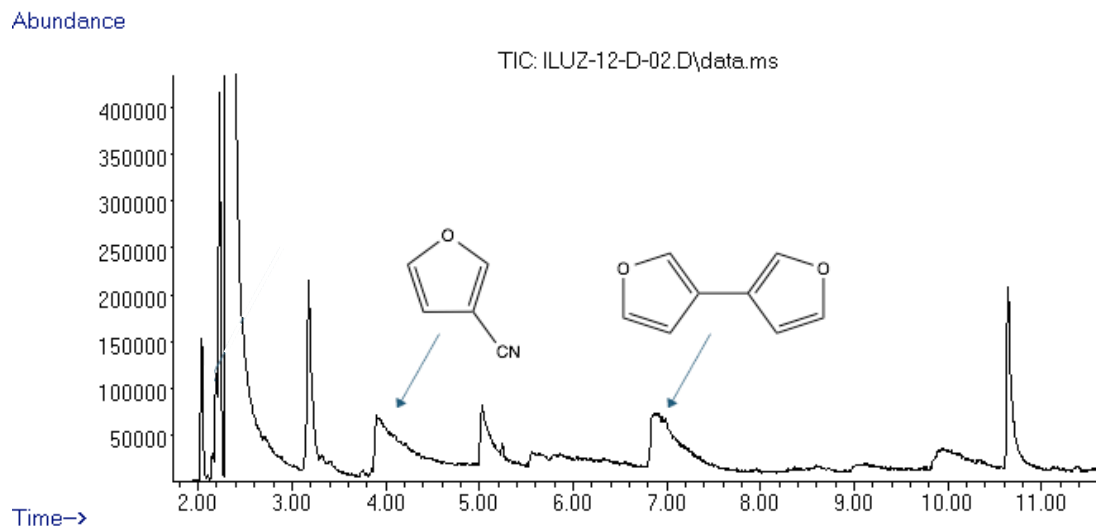


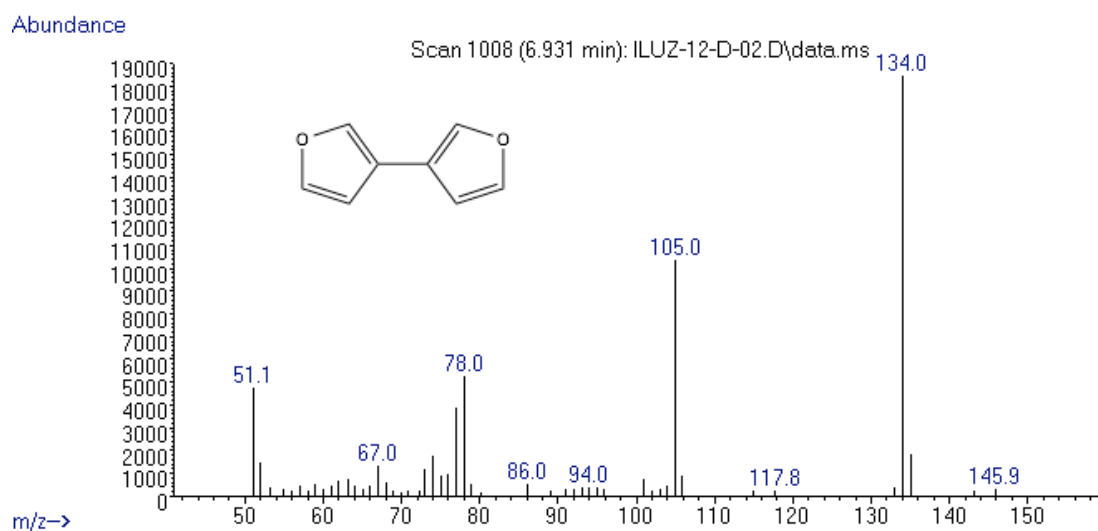
Figure S9. Comparison between ^1H -NMR spectrum of **3-FN** and reaction solution after 6 days of reaction at room temperature by in THF-d_8 .



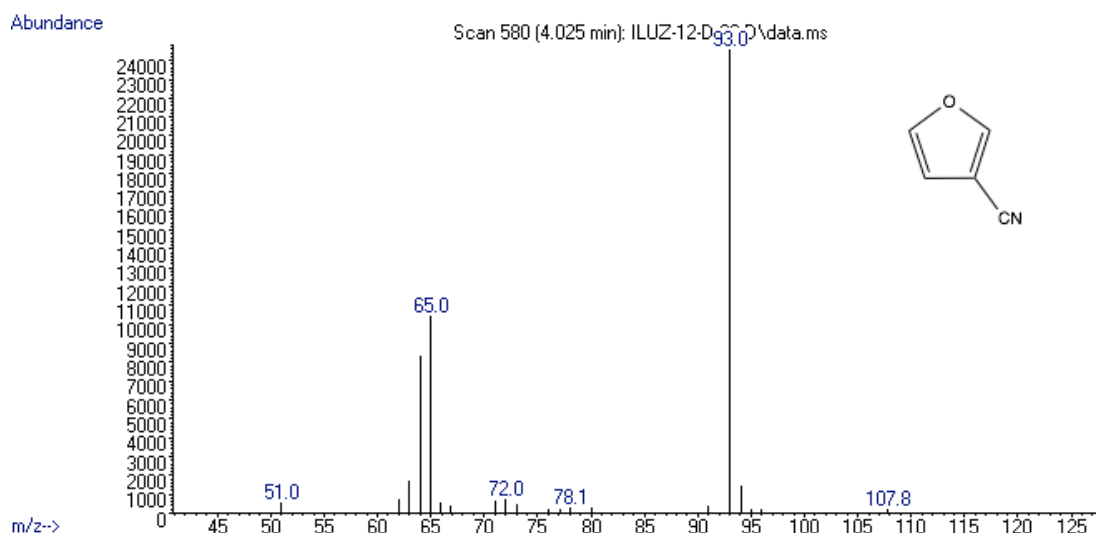
Spectrum S9. $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of complex **(11)** in THF-d_8 at room temperature. Signals assigned to heteroaromatic carbons and nitrile carbon.



Chromatogram S3. Chromatogram of thermolysis of complex **(11)** after 4 hours at 100 °C.



Spectrum S10. Mass spectrum corresponding to **(13)**, obtained from thermolysis of complex **(11)** after 4 hours at 100 °C.



Spectrum S11. Mass spectrum corresponding to **3-FN**, obtained from thermolysis of complex (**11**) after 4 hours at 100 °C.

Cristallographic data for complex (7).

Table S1. Crystal data and structure refinement for complex (7).

Identification code	7	
Empirical formula	C ₁₉ H ₃₅ N Ni O P ₂	
Formula weight	414.13	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /n	
Unit cell dimensions	a = 10.9347(15) Å	α = 90°.
	b = 14.4261(14) Å	β = 107.794(13)°.
	c = 13.9266(16) Å	γ = 90°.
Volume	2091.8(4) Å ³	
Z	4	
Density (calculated)	1.315 Mg/m ³	
Absorption coefficient	1.087 mm ⁻¹	
F(000)	888	
Crystal size	0.490 x 0.400 x 0.330 mm ³	
Theta range for data collection	3.436 to 29.582°.	
Index ranges	-10 ≤ h ≤ 13, -18 ≤ k ≤ 19, -18 ≤ l ≤ 19	

Reflections collected	10578	
Independent reflections	4940 [R(int) = 0.0366]	
Completeness to theta = 25.242°	99.4 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4940 / 0 / 225	
Goodness-of-fit on F²	1.078	
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.0800	
R indices (all data)	R1 = 0.0765, wR2 = 0.0939	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.645 and -0.463 e.Å ⁻³	

Table S2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	Z	U(eq)
C(1)	873(3)	8191(2)	6028(2)	26(1)
C(2)	2056(3)	8366(2)	5672(2)	26(1)
C(3)	2815(3)	6659(2)	4925(2)	29(1)
C(4)	1445(3)	6293(2)	4706(2)	36(1)
C(5)	3745(4)	5857(2)	5004(3)	46(1)
C(6)	4752(3)	7987(2)	6010(2)	27(1)
C(7)	5392(3)	8495(2)	6995(2)	38(1)
C(8)	4584(3)	8628(2)	5102(2)	36(1)
C(9)	1583(3)	8542(2)	8185(2)	25(1)
C(10)	2782(3)	9095(2)	8223(2)	35(1)
C(11)	1652(4)	8188(2)	9229(2)	42(1)
C(12)	-116(3)	6992(2)	7306(2)	26(1)
C(13)	-366(3)	6143(2)	6611(3)	37(1)
C(14)	-1290(3)	7622(2)	7093(3)	38(1)
C(15)	4648(3)	6100(2)	7748(2)	26(1)
C(16)	5223(3)	5526(2)	8525(2)	26(1)
C(17)	6413(3)	5211(2)	8436(2)	30(1)
C(18)	6521(3)	5599(2)	7607(3)	44(1)
C(19)	2698(3)	6188(2)	8508(2)	30(1)

O(1)	5483(2)	6144(2)	7158(2)	50(1)
Ni(1)	3078(1)	6778(1)	7425(1)	21(1)
P(1)	3243(1)	7427(1)	6044(1)	21(1)
P(2)	1341(1)	7603(1)	7248(1)	21(1)
N(1)	2399(3)	5816(2)	9127(2)	45(1)

Table S3. Bond lengths [Å] and angles [°] for **7**.

C(1)-C(2)	1.541(4)
C(1)-P(2)	1.827(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-P(1)	1.837(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(5)	1.522(4)
C(3)-C(4)	1.528(4)
C(3)-P(1)	1.852(3)
C(3)-H(3)	1.0000
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-C(7)	1.525(4)
C(6)-C(8)	1.531(4)
C(6)-P(1)	1.850(3)
C(6)-H(6)	1.0000
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(11)	1.521(4)

C(9)-C(10)	1.522(4)
C(9)-P(2)	1.842(3)
C(9)-H(9)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(14)	1.527(4)
C(12)-C(13)	1.533(4)
C(12)-P(2)	1.844(3)
C(12)-H(12)	1.0000
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)-C(16)	1.355(4)
C(15)-O(1)	1.404(3)
C(15)-Ni(1)	1.906(3)
C(16)-C(17)	1.419(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.321(4)
C(17)-H(17)	0.9500
C(18)-O(1)	1.365(4)
C(18)-H(18)	0.9500
C(19)-N(1)	1.145(4)
C(19)-Ni(1)	1.885(3)
Ni(1)-P(2)	2.1910(8)
Ni(1)-P(1)	2.1964(8)
C(2)-C(1)-P(2)	110.59(19)
C(2)-C(1)-H(1A)	109.5
P(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
P(2)-C(1)-H(1B)	109.5

H(1A)-C(1)-H(1B)	108.1
C(1)-C(2)-P(1)	112.23(19)
C(1)-C(2)-H(2A)	109.2
P(1)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2B)	109.2
P(1)-C(2)-H(2B)	109.2
H(2A)-C(2)-H(2B)	107.9
C(5)-C(3)-C(4)	110.1(3)
C(5)-C(3)-P(1)	113.7(2)
C(4)-C(3)-P(1)	110.8(2)
C(5)-C(3)-H(3)	107.3
C(4)-C(3)-H(3)	107.3
P(1)-C(3)-H(3)	107.3
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(7)-C(6)-C(8)	111.0(3)
C(7)-C(6)-P(1)	110.7(2)
C(8)-C(6)-P(1)	113.7(2)
C(7)-C(6)-H(6)	107.0
C(8)-C(6)-H(6)	107.0
P(1)-C(6)-H(6)	107.0
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5

C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(11)-C(9)-C(10)	110.6(3)
C(11)-C(9)-P(2)	112.7(2)
C(10)-C(9)-P(2)	110.2(2)
C(11)-C(9)-H(9)	107.7
C(10)-C(9)-H(9)	107.7
P(2)-C(9)-H(9)	107.7
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(14)-C(12)-C(13)	112.1(3)
C(14)-C(12)-P(2)	113.1(2)
C(13)-C(12)-P(2)	110.2(2)
C(14)-C(12)-H(12)	107.0
C(13)-C(12)-H(12)	107.0
P(2)-C(12)-H(12)	107.0
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5

C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(16)-C(15)-O(1)	105.6(3)
C(16)-C(15)-Ni(1)	131.8(2)
O(1)-C(15)-Ni(1)	122.6(2)
C(15)-C(16)-C(17)	109.9(3)
C(15)-C(16)-H(16)	125.0
C(17)-C(16)-H(16)	125.0
C(18)-C(17)-C(16)	105.6(3)
C(18)-C(17)-H(17)	127.2
C(16)-C(17)-H(17)	127.2
C(17)-C(18)-O(1)	111.1(3)
C(17)-C(18)-H(18)	124.4
O(1)-C(18)-H(18)	124.4
N(1)-C(19)-Ni(1)	176.0(3)
C(18)-O(1)-C(15)	107.8(2)
C(19)-Ni(1)-C(15)	88.98(13)
C(19)-Ni(1)-P(2)	86.57(9)
C(15)-Ni(1)-P(2)	173.04(9)
C(19)-Ni(1)-P(1)	172.07(10)
C(15)-Ni(1)-P(1)	96.68(9)
P(2)-Ni(1)-P(1)	88.28(3)
C(2)-P(1)-C(6)	103.28(14)
C(2)-P(1)-C(3)	103.23(14)
C(6)-P(1)-C(3)	103.74(13)
C(2)-P(1)-Ni(1)	108.75(9)
C(6)-P(1)-Ni(1)	121.40(10)
C(3)-P(1)-Ni(1)	114.49(10)
C(1)-P(2)-C(9)	104.86(14)
C(1)-P(2)-C(12)	105.25(14)
C(9)-P(2)-C(12)	105.06(13)
C(1)-P(2)-Ni(1)	110.09(10)
C(9)-P(2)-Ni(1)	112.80(10)
C(12)-P(2)-Ni(1)	117.75(10)

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^* 2U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	25(2)	24(2)	29(2)	6(1)	7(1)	8(1)
C(2)	32(2)	23(2)	25(1)	4(1)	12(1)	5(1)
C(3)	41(2)	25(2)	27(2)	-5(1)	19(1)	-4(1)
C(4)	39(2)	36(2)	33(2)	-8(2)	10(1)	-5(2)
C(5)	48(2)	36(2)	65(2)	-18(2)	32(2)	-6(2)
C(6)	27(2)	27(2)	31(2)	-1(1)	16(1)	-2(1)
C(7)	32(2)	47(2)	39(2)	-13(2)	16(2)	-12(2)
C(8)	44(2)	31(2)	43(2)	9(2)	27(2)	-1(2)
C(9)	27(2)	23(1)	27(2)	-2(1)	13(1)	0(1)
C(10)	34(2)	34(2)	41(2)	-10(2)	17(2)	-9(2)
C(11)	63(2)	35(2)	34(2)	-5(2)	25(2)	-4(2)
C(12)	23(2)	25(2)	35(2)	-1(1)	15(1)	-1(1)
C(13)	31(2)	28(2)	57(2)	-11(2)	23(2)	-9(1)
C(14)	25(2)	33(2)	60(2)	-13(2)	20(2)	-2(1)
C(15)	27(2)	24(2)	30(2)	2(1)	14(1)	2(1)
C(16)	26(2)	25(2)	25(2)	-1(1)	5(1)	1(1)
C(17)	26(2)	25(2)	36(2)	0(1)	4(1)	4(1)
C(18)	34(2)	48(2)	58(2)	14(2)	27(2)	18(2)
C(19)	32(2)	29(2)	31(2)	7(1)	15(1)	7(1)
O(1)	46(2)	62(2)	57(2)	30(1)	37(1)	28(1)
Ni(1)	23(1)	21(1)	22(1)	4(1)	11(1)	4(1)
P(1)	25(1)	20(1)	22(1)	2(1)	11(1)	2(1)
P(2)	21(1)	19(1)	24(1)	1(1)	10(1)	1(1)
N(1)	54(2)	44(2)	49(2)	19(2)	33(2)	20(2)

Table S5. Torsion angles [$^\circ$] for **7**.

P(2)-C(1)-C(2)-P(1)	34.9(3)
O(1)-C(15)-C(16)-C(17)	0.3(3)
Ni(1)-C(15)-C(16)-C(17)	-178.4(2)
C(15)-C(16)-C(17)-C(18)	-0.3(4)

C(16)-C(17)-C(18)-O(1)	0.1(4)
C(17)-C(18)-O(1)-C(15)	0.1(4)
C(16)-C(15)-O(1)-C(18)	-0.3(4)
Ni(1)-C(15)-O(1)-C(18)	178.6(2)
C(1)-C(2)-P(1)-C(6)	-158.0(2)
C(1)-C(2)-P(1)-C(3)	94.1(2)
C(1)-C(2)-P(1)-Ni(1)	-27.8(2)
C(7)-C(6)-P(1)-C(2)	84.2(2)
C(8)-C(6)-P(1)-C(2)	-41.6(2)
C(7)-C(6)-P(1)-C(3)	-168.4(2)
C(8)-C(6)-P(1)-C(3)	65.8(2)
C(7)-C(6)-P(1)-Ni(1)	-37.9(3)
C(8)-C(6)-P(1)-Ni(1)	-163.70(17)
C(5)-C(3)-P(1)-C(2)	174.8(2)
C(4)-C(3)-P(1)-C(2)	-60.6(2)
C(5)-C(3)-P(1)-C(6)	67.3(2)
C(4)-C(3)-P(1)-C(6)	-168.1(2)
C(5)-C(3)-P(1)-Ni(1)	-67.2(2)
C(4)-C(3)-P(1)-Ni(1)	57.5(2)
C(2)-C(1)-P(2)-C(9)	94.1(2)
C(2)-C(1)-P(2)-C(12)	-155.4(2)
C(2)-C(1)-P(2)-Ni(1)	-27.5(2)
C(11)-C(9)-P(2)-C(1)	165.7(2)
C(10)-C(9)-P(2)-C(1)	-70.2(2)
C(11)-C(9)-P(2)-C(12)	55.0(3)
C(10)-C(9)-P(2)-C(12)	179.1(2)
C(11)-C(9)-P(2)-Ni(1)	-74.5(2)
C(10)-C(9)-P(2)-Ni(1)	49.6(2)
C(14)-C(12)-P(2)-C(1)	-52.5(2)
C(13)-C(12)-P(2)-C(1)	73.9(2)
C(14)-C(12)-P(2)-C(9)	57.9(2)
C(13)-C(12)-P(2)-C(9)	-175.7(2)
C(14)-C(12)-P(2)-Ni(1)	-175.56(18)
C(13)-C(12)-P(2)-Ni(1)	-49.2(2)

Table S6. Hydrogen bonds for **7** [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
C(6)-H(6)...O(1)	1.00	2.53	3.080(4)	114.3
C(2)-H(2A)...N(1)#1	0.99	2.69	3.580(4)	149.8
C(2)-H(2A)...N(1)#1	0.99	2.69	3.580(4)	149.8
C(6)-H(6)...O(1)	1.00	2.53	3.080(4)	114.3

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1/2, y+1/2, -z+3/2$

Cristalographic data for complex (11).

Table S7. Crystal data and structure refinement for complex (11).

Identification code	11	
Empirical formula	C ₁₉ H ₃₅ N Ni O P ₂	
Formula weight	414.13	
Temperature	130(2) K	
Wavelength	0.71073 \AA	
Crystal system	Monoclinic	
Space group	P 2 ₁ /n	
Unit cell dimensions	a = 15.6451(9) \AA	$\alpha = 90^\circ$.
	b = 14.6989(13) \AA	$\beta = 103.432(6)^\circ$.
	c = 19.3297(15) \AA	$\gamma = 90^\circ$.
Volume	4323.6(6) \AA^3	
Z	8	
Density (calculated)	1.272 Mg/m ³	
Absorption coefficient	1.051 mm ⁻¹	
F(000)	1776	
Crystal size	0.450 x 0.280 x 0.100 mm ³	
Theta range for data collection	3.519 to 29.434 $^\circ$.	
Index ranges	-19 \leq h \leq 17, -14 \leq k \leq 19, -17 \leq l \leq 26	
Reflections collected	18841	
Independent reflections	9914 [R(int) = 0.0401]	
Completeness to theta = 25.242 $^\circ$	99.7 %	

Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9914 / 0 / 449	
Goodness-of-fit on F²	1.089	
Final R indices [I>2sigma(I)]	R1 = 0.0591, wR2 = 0.1437	
R indices (all data)	R1 = 0.1064, wR2 = 0.1738	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.053 and -0.788 e.Å ⁻³	

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **11**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	8825(3)	4758(3)	3182(2)	27(1)
C(2)	8742(3)	4734(3)	2375(2)	24(1)
C(3)	6915(3)	4818(3)	1573(2)	27(1)
C(4)	6581(3)	5220(4)	2189(3)	42(1)
C(5)	6154(3)	4417(4)	1011(3)	38(1)
C(6)	8175(3)	3640(3)	1112(2)	25(1)
C(7)	8846(3)	2872(3)	1289(3)	34(1)
C(8)	8526(3)	4428(4)	740(2)	36(1)
C(9)	8108(3)	3954(3)	4313(2)	29(1)
C(10)	7209(3)	4430(4)	4099(3)	41(1)
C(11)	8778(3)	4512(4)	4851(2)	38(1)
C(12)	9540(3)	3041(3)	3852(2)	26(1)
C(13)	9922(3)	2721(4)	3238(2)	34(1)
C(14)	9428(3)	2242(3)	4332(2)	34(1)
C(15)	6639(3)	2417(3)	1910(2)	26(1)
C(16)	5735(3)	2323(3)	1964(3)	32(1)
C(17)	5272(3)	1941(4)	1364(3)	36(1)
C(18)	6628(3)	2063(3)	1271(2)	32(1)
C(19)	7226(3)	2209(3)	3326(2)	28(1)
N(1)	7007(3)	1776(3)	3756(2)	37(1)
Ni(1)	7536(1)	2990(1)	2652(1)	22(1)
P(2)	8495(1)	3663(1)	3508(1)	23(1)

P(1)	7818(1)	4004(1)	1914(1)	21(1)
O(1)	5799(2)	1756(2)	910(2)	37(1)
C(20)	6331(3)	6402(3)	7748(2)	26(1)
C(21)	6295(3)	6457(3)	6938(2)	31(1)
C(22)	7128(3)	5694(3)	5855(2)	29(1)
C(23)	7986(3)	6227(4)	6093(3)	38(1)
C(24)	6482(4)	6186(4)	5258(3)	41(1)
C(25)	5645(3)	4759(3)	6218(2)	32(1)
C(26)	5835(3)	3933(4)	5785(3)	38(1)
C(27)	5175(3)	4466(4)	6786(3)	47(1)
C(28)	8141(3)	6513(3)	8582(2)	28(1)
C(29)	8538(3)	6875(4)	7980(3)	42(1)
C(30)	8855(3)	6128(4)	9198(3)	39(1)
C(31)	6899(3)	5276(3)	9002(2)	27(1)
C(32)	6569(3)	6038(4)	9415(2)	37(1)
C(33)	6216(3)	4516(3)	8793(3)	36(1)
C(34)	8454(3)	4095(3)	8226(2)	26(1)
C(35)	9366(3)	3994(3)	8198(3)	33(1)
C(36)	9786(3)	3546(4)	8786(3)	38(1)
C(37)	8410(3)	3672(3)	8826(2)	31(1)
C(38)	7923(3)	3937(3)	6809(2)	28(1)
N(2)	8134(3)	3498(3)	6373(2)	36(1)
Ni(2)	7586(1)	4698(1)	7481(1)	22(1)
P(3)	6667(1)	5387(1)	6620(1)	24(1)
P(4)	7259(1)	5688(1)	8218(1)	22(1)
O(2)	9216(2)	3319(2)	9195(2)	39(1)

Table S9. Bond lengths [\AA] and angles [$^\circ$] for **11**.

C(1)-C(2)	1.534(6)
C(1)-P(2)	1.846(5)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-P(1)	1.854(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900

C(3)-C(4)	1.526(6)
C(3)-C(5)	1.531(6)
C(3)-P(1)	1.852(4)
C(3)-H(3)	1.0000
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-C(7)	1.525(6)
C(6)-C(8)	1.532(6)
C(6)-P(1)	1.844(4)
C(6)-H(6)	1.0000
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(11)	1.532(6)
C(9)-C(10)	1.539(6)
C(9)-P(2)	1.846(4)
C(9)-H(9)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.522(6)
C(12)-C(14)	1.533(6)
C(12)-P(2)	1.856(4)
C(12)-H(12)	1.0000
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)-C(18)	1.335(6)
C(15)-C(16)	1.449(6)
C(15)-Ni(1)	1.951(4)
C(16)-C(17)	1.341(7)
C(16)-H(16)	0.9500
C(17)-O(1)	1.363(6)
C(17)-H(17)	0.9500
C(18)-O(1)	1.397(5)
C(18)-H(18)	0.9500
C(19)-N(1)	1.160(6)
C(19)-Ni(1)	1.883(5)
Ni(1)-P(1)	2.1788(12)
Ni(1)-P(2)	2.1930(12)
C(20)-C(21)	1.558(6)
C(20)-P(4)	1.849(4)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-P(3)	1.831(5)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(24)	1.529(6)
C(22)-C(23)	1.530(7)
C(22)-P(3)	1.844(5)
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)	1.519(7)
C(25)-C(26)	1.541(7)
C(25)-P(3)	1.854(4)
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(29)	1.535(6)
C(28)-C(30)	1.538(6)
C(28)-P(4)	1.850(4)
C(28)-H(28)	1.0000
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(33)	1.533(6)
C(31)-C(32)	1.533(6)
C(31)-P(4)	1.837(4)
C(31)-H(31)	1.0000
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(37)	1.331(6)
C(34)-C(35)	1.446(6)
C(34)-Ni(2)	1.948(4)
C(35)-C(36)	1.345(7)
C(35)-H(35)	0.9500
C(36)-O(2)	1.363(6)
C(36)-H(36)	0.9500
C(37)-O(2)	1.397(5)
C(37)-H(37)	0.9500
C(38)-N(2)	1.169(6)
C(38)-Ni(2)	1.880(5)

Ni(2)-P(4)	2.1793(12)
Ni(2)-P(3)	2.1801(12)
C(2)-C(1)-P(2)	111.3(3)
C(2)-C(1)-H(1A)	109.4
P(2)-C(1)-H(1A)	109.4
C(2)-C(1)-H(1B)	109.4
P(2)-C(1)-H(1B)	109.4
H(1A)-C(1)-H(1B)	108.0
C(1)-C(2)-P(1)	112.0(3)
C(1)-C(2)-H(2A)	109.2
P(1)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2B)	109.2
P(1)-C(2)-H(2B)	109.2
H(2A)-C(2)-H(2B)	107.9
C(4)-C(3)-C(5)	110.6(4)
C(4)-C(3)-P(1)	110.1(3)
C(5)-C(3)-P(1)	114.0(3)
C(4)-C(3)-H(3)	107.3
C(5)-C(3)-H(3)	107.3
P(1)-C(3)-H(3)	107.3
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(7)-C(6)-C(8)	111.2(4)
C(7)-C(6)-P(1)	110.7(3)
C(8)-C(6)-P(1)	112.8(3)
C(7)-C(6)-H(6)	107.3

C(8)-C(6)-H(6)	107.3
P(1)-C(6)-H(6)	107.3
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(11)-C(9)-C(10)	112.2(4)
C(11)-C(9)-P(2)	112.9(3)
C(10)-C(9)-P(2)	109.8(3)
C(11)-C(9)-H(9)	107.2
C(10)-C(9)-H(9)	107.2
P(2)-C(9)-H(9)	107.2
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(13)-C(12)-C(14)	110.8(4)
C(13)-C(12)-P(2)	110.2(3)
C(14)-C(12)-P(2)	112.3(3)
C(13)-C(12)-H(12)	107.8
C(14)-C(12)-H(12)	107.8

P(2)-C(12)-H(12)	107.8
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(18)-C(15)-C(16)	103.1(4)
C(18)-C(15)-Ni(1)	134.5(3)
C(16)-C(15)-Ni(1)	122.3(3)
C(17)-C(16)-C(15)	108.5(4)
C(17)-C(16)-H(16)	125.8
C(15)-C(16)-H(16)	125.8
C(16)-C(17)-O(1)	110.7(4)
C(16)-C(17)-H(17)	124.6
O(1)-C(17)-H(17)	124.6
C(15)-C(18)-O(1)	113.5(4)
C(15)-C(18)-H(18)	123.2
O(1)-C(18)-H(18)	123.2
N(1)-C(19)-Ni(1)	175.5(4)
C(19)-Ni(1)-C(15)	89.32(18)
C(19)-Ni(1)-P(1)	174.00(14)
C(15)-Ni(1)-P(1)	91.95(13)
C(19)-Ni(1)-P(2)	89.68(13)
C(15)-Ni(1)-P(2)	177.25(14)
P(1)-Ni(1)-P(2)	88.79(4)
C(9)-P(2)-C(1)	104.9(2)
C(9)-P(2)-C(12)	104.3(2)
C(1)-P(2)-C(12)	105.0(2)
C(9)-P(2)-Ni(1)	116.07(15)
C(1)-P(2)-Ni(1)	109.41(14)

C(12)-P(2)-Ni(1)	116.07(15)
C(6)-P(1)-C(3)	104.11(19)
C(6)-P(1)-C(2)	102.59(19)
C(3)-P(1)-C(2)	104.0(2)
C(6)-P(1)-Ni(1)	119.92(15)
C(3)-P(1)-Ni(1)	114.94(15)
C(2)-P(1)-Ni(1)	109.52(14)
C(17)-O(1)-C(18)	104.2(4)
C(21)-C(20)-P(4)	111.3(3)
C(21)-C(20)-H(20A)	109.4
P(4)-C(20)-H(20A)	109.4
C(21)-C(20)-H(20B)	109.4
P(4)-C(20)-H(20B)	109.4
H(20A)-C(20)-H(20B)	108.0
C(20)-C(21)-P(3)	110.7(3)
C(20)-C(21)-H(21A)	109.5
P(3)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
P(3)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	108.1
C(24)-C(22)-C(23)	111.4(4)
C(24)-C(22)-P(3)	114.1(3)
C(23)-C(22)-P(3)	111.3(3)
C(24)-C(22)-H(22)	106.5
C(23)-C(22)-H(22)	106.5
P(3)-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(27)-C(25)-C(26)	110.9(4)
C(27)-C(25)-P(3)	110.7(3)
C(26)-C(25)-P(3)	111.3(3)
C(27)-C(25)-H(25)	107.9
C(26)-C(25)-H(25)	107.9
P(3)-C(25)-H(25)	107.9
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(29)-C(28)-C(30)	111.4(4)
C(29)-C(28)-P(4)	109.7(3)
C(30)-C(28)-P(4)	113.3(3)
C(29)-C(28)-H(28)	107.4
C(30)-C(28)-H(28)	107.4
P(4)-C(28)-H(28)	107.4
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5

C(33)-C(31)-C(32)	111.8(4)
C(33)-C(31)-P(4)	110.6(3)
C(32)-C(31)-P(4)	113.1(3)
C(33)-C(31)-H(31)	107.0
C(32)-C(31)-H(31)	107.0
P(4)-C(31)-H(31)	107.0
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(37)-C(34)-C(35)	103.6(4)
C(37)-C(34)-Ni(2)	133.4(3)
C(35)-C(34)-Ni(2)	122.9(3)
C(36)-C(35)-C(34)	108.1(4)
C(36)-C(35)-H(35)	125.9
C(34)-C(35)-H(35)	125.9
C(35)-C(36)-O(2)	110.7(4)
C(35)-C(36)-H(36)	124.7
O(2)-C(36)-H(36)	124.7
C(34)-C(37)-O(2)	113.3(4)
C(34)-C(37)-H(37)	123.3
O(2)-C(37)-H(37)	123.3
N(2)-C(38)-Ni(2)	176.9(4)
C(38)-Ni(2)-C(34)	88.85(18)
C(38)-Ni(2)-P(4)	174.41(15)
C(34)-Ni(2)-P(4)	92.90(13)
C(38)-Ni(2)-P(3)	89.42(13)
C(34)-Ni(2)-P(3)	177.08(14)
P(4)-Ni(2)-P(3)	88.60(5)

C(21)-P(3)-C(22)	105.8(2)
C(21)-P(3)-C(25)	104.9(2)
C(22)-P(3)-C(25)	104.2(2)
C(21)-P(3)-Ni(2)	110.31(15)
C(22)-P(3)-Ni(2)	114.49(15)
C(25)-P(3)-Ni(2)	116.12(16)
C(31)-P(4)-C(20)	103.7(2)
C(31)-P(4)-C(28)	104.3(2)
C(20)-P(4)-C(28)	104.3(2)
C(31)-P(4)-Ni(2)	118.82(16)
C(20)-P(4)-Ni(2)	109.56(14)
C(28)-P(4)-Ni(2)	114.73(15)
C(36)-O(2)-C(37)	104.2(4)

Table S10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	28(2)	24(2)	28(2)	-4(2)	4(2)	-2(2)
C(2)	22(2)	21(2)	29(2)	2(2)	5(2)	-5(2)
C(3)	24(2)	31(3)	28(2)	6(2)	9(2)	6(2)
C(4)	39(3)	48(3)	42(3)	6(3)	16(2)	22(3)
C(5)	25(2)	40(3)	44(3)	12(2)	1(2)	4(2)
C(6)	21(2)	30(2)	25(2)	-6(2)	6(2)	-2(2)
C(7)	29(2)	40(3)	35(2)	-12(2)	10(2)	5(2)
C(8)	36(3)	49(3)	25(2)	-1(2)	12(2)	0(2)
C(9)	31(2)	33(3)	25(2)	-2(2)	12(2)	1(2)
C(10)	38(3)	54(3)	35(3)	-5(2)	16(2)	8(3)
C(11)	47(3)	40(3)	28(2)	-4(2)	10(2)	0(2)
C(12)	23(2)	27(2)	26(2)	2(2)	5(2)	0(2)
C(13)	26(2)	40(3)	37(3)	8(2)	11(2)	7(2)
C(14)	35(2)	33(3)	33(2)	4(2)	7(2)	8(2)
C(15)	21(2)	25(2)	30(2)	0(2)	2(2)	-5(2)
C(16)	28(2)	30(3)	36(2)	3(2)	4(2)	-3(2)
C(17)	25(2)	38(3)	44(3)	6(2)	3(2)	-3(2)

C(18)	26(2)	35(3)	32(2)	1(2)	4(2)	-3(2)
C(19)	18(2)	35(3)	28(2)	-9(2)	3(2)	-5(2)
N(1)	37(2)	39(2)	36(2)	6(2)	9(2)	-5(2)
Ni(1)	20(1)	24(1)	24(1)	0(1)	6(1)	0(1)
P(2)	23(1)	25(1)	21(1)	-1(1)	7(1)	0(1)
P(1)	19(1)	24(1)	21(1)	0(1)	6(1)	2(1)
O(1)	37(2)	34(2)	34(2)	-1(2)	-3(1)	-8(2)
C(20)	19(2)	25(2)	31(2)	-1(2)	3(2)	5(2)
C(21)	28(2)	35(3)	29(2)	3(2)	5(2)	4(2)
C(22)	36(2)	27(2)	25(2)	2(2)	7(2)	8(2)
C(23)	42(3)	44(3)	32(2)	-2(2)	17(2)	-4(2)
C(24)	51(3)	41(3)	31(2)	8(2)	8(2)	10(3)
C(25)	24(2)	36(3)	32(2)	-3(2)	-2(2)	-2(2)
C(26)	34(3)	38(3)	39(3)	-7(2)	2(2)	-2(2)
C(27)	30(3)	61(4)	52(3)	-20(3)	15(2)	-22(3)
C(28)	22(2)	31(3)	30(2)	-6(2)	5(2)	-8(2)
C(29)	34(3)	53(3)	41(3)	-5(3)	18(2)	-20(2)
C(30)	32(2)	35(3)	41(3)	-5(2)	-5(2)	-4(2)
C(31)	25(2)	32(2)	25(2)	2(2)	9(2)	-3(2)
C(32)	42(3)	43(3)	30(2)	-2(2)	16(2)	0(2)
C(33)	37(3)	38(3)	36(3)	0(2)	15(2)	-12(2)
C(34)	19(2)	29(2)	28(2)	-5(2)	3(2)	2(2)
C(35)	25(2)	35(3)	39(3)	0(2)	8(2)	-1(2)
C(36)	29(2)	39(3)	42(3)	-6(2)	-2(2)	2(2)
C(37)	33(2)	31(3)	28(2)	-3(2)	5(2)	7(2)
C(38)	20(2)	38(3)	26(2)	6(2)	2(2)	2(2)
N(2)	39(2)	37(2)	34(2)	-1(2)	14(2)	5(2)
Ni(2)	21(1)	25(1)	22(1)	0(1)	5(1)	1(1)
P(3)	23(1)	28(1)	22(1)	0(1)	5(1)	1(1)
P(4)	18(1)	24(1)	22(1)	-1(1)	5(1)	-2(1)
O(2)	41(2)	43(2)	30(2)	-1(2)	1(1)	8(2)

Table S11 Torsion angles [°] for **11**.

P(2)-C(1)-C(2)-P(1)	32.9(4)
C(18)-C(15)-C(16)-C(17)	-0.7(5)

Ni(1)-C(15)-C(16)-C(17)	177.4(3)
C(15)-C(16)-C(17)-O(1)	0.8(6)
C(16)-C(15)-C(18)-O(1)	0.4(5)
Ni(1)-C(15)-C(18)-O(1)	-177.4(3)
C(11)-C(9)-P(2)-C(1)	-52.9(4)
C(10)-C(9)-P(2)-C(1)	73.1(4)
C(11)-C(9)-P(2)-C(12)	57.2(4)
C(10)-C(9)-P(2)-C(12)	-176.8(3)
C(11)-C(9)-P(2)-Ni(1)	-173.8(3)
C(10)-C(9)-P(2)-Ni(1)	-47.8(4)
C(2)-C(1)-P(2)-C(9)	-152.8(3)
C(2)-C(1)-P(2)-C(12)	97.6(3)
C(2)-C(1)-P(2)-Ni(1)	-27.6(3)
C(13)-C(12)-P(2)-C(9)	177.7(3)
C(14)-C(12)-P(2)-C(9)	53.6(4)
C(13)-C(12)-P(2)-C(1)	-72.2(4)
C(14)-C(12)-P(2)-C(1)	163.7(3)
C(13)-C(12)-P(2)-Ni(1)	48.7(4)
C(14)-C(12)-P(2)-Ni(1)	-75.4(3)
C(7)-C(6)-P(1)-C(3)	-172.9(3)
C(8)-C(6)-P(1)-C(3)	61.8(3)
C(7)-C(6)-P(1)-C(2)	78.9(3)
C(8)-C(6)-P(1)-C(2)	-46.4(3)
C(7)-C(6)-P(1)-Ni(1)	-42.6(3)
C(8)-C(6)-P(1)-Ni(1)	-168.0(3)
C(4)-C(3)-P(1)-C(6)	-177.0(3)
C(5)-C(3)-P(1)-C(6)	58.0(4)
C(4)-C(3)-P(1)-C(2)	-69.9(4)
C(5)-C(3)-P(1)-C(2)	165.1(3)
C(4)-C(3)-P(1)-Ni(1)	49.8(4)
C(5)-C(3)-P(1)-Ni(1)	-75.1(3)
C(1)-C(2)-P(1)-C(6)	-153.2(3)
C(1)-C(2)-P(1)-C(3)	98.5(3)
C(1)-C(2)-P(1)-Ni(1)	-24.8(3)
C(16)-C(17)-O(1)-C(18)	-0.6(5)
C(15)-C(18)-O(1)-C(17)	0.1(5)
P(4)-C(20)-C(21)-P(3)	33.7(4)

C(37)-C(34)-C(35)-C(36)	-1.5(5)
Ni(2)-C(34)-C(35)-C(36)	-179.6(3)
C(34)-C(35)-C(36)-O(2)	1.5(6)
C(35)-C(34)-C(37)-O(2)	0.9(5)
Ni(2)-C(34)-C(37)-O(2)	178.8(3)
C(20)-C(21)-P(3)-C(22)	-151.8(3)
C(20)-C(21)-P(3)-C(25)	98.3(3)
C(20)-C(21)-P(3)-Ni(2)	-27.5(3)
C(24)-C(22)-P(3)-C(21)	-57.6(4)
C(23)-C(22)-P(3)-C(21)	69.5(4)
C(24)-C(22)-P(3)-C(25)	52.7(4)
C(23)-C(22)-P(3)-C(25)	179.8(3)
C(24)-C(22)-P(3)-Ni(2)	-179.4(3)
C(23)-C(22)-P(3)-Ni(2)	-52.3(4)
C(27)-C(25)-P(3)-C(21)	-68.2(4)
C(26)-C(25)-P(3)-C(21)	168.0(3)
C(27)-C(25)-P(3)-C(22)	-179.2(4)
C(26)-C(25)-P(3)-C(22)	57.0(4)
C(27)-C(25)-P(3)-Ni(2)	53.9(4)
C(26)-C(25)-P(3)-Ni(2)	-69.9(4)
C(33)-C(31)-P(4)-C(20)	76.0(4)
C(32)-C(31)-P(4)-C(20)	-50.2(4)
C(33)-C(31)-P(4)-C(28)	-175.1(3)
C(32)-C(31)-P(4)-C(28)	58.7(4)
C(33)-C(31)-P(4)-Ni(2)	-45.8(4)
C(32)-C(31)-P(4)-Ni(2)	-172.0(3)
C(21)-C(20)-P(4)-C(31)	-154.2(3)
C(21)-C(20)-P(4)-C(28)	96.9(3)
C(21)-C(20)-P(4)-Ni(2)	-26.4(3)
C(29)-C(28)-P(4)-C(31)	176.9(3)
C(30)-C(28)-P(4)-C(31)	51.7(4)
C(29)-C(28)-P(4)-C(20)	-74.6(4)
C(30)-C(28)-P(4)-C(20)	160.1(3)
C(29)-C(28)-P(4)-Ni(2)	45.2(4)
C(30)-C(28)-P(4)-Ni(2)	-80.0(3)
C(35)-C(36)-O(2)-C(37)	-0.9(5)
C(34)-C(37)-O(2)-C(36)	-0.1(5)

Table S12. Hydrogen bonds for **11** [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(3)-H(3)...N(1)#1	1.00	2.52	3.467(6)	158.6
C(17)-H(17)...N(2)#2	0.95	2.48	3.410(6)	164.5
C(20)-H(20B)...N(2)#3	0.99	2.55	3.525(6)	168.1
C(24)-H(24B)...O(2)#3	0.98	2.58	3.561(7)	175.5
C(28)-H(28)...N(2)#3	1.00	2.63	3.547(6)	152.9
C(36)-H(36)...N(1)#4	0.95	2.61	3.522(6)	159.8

Symmetry transformations used to generate equivalent atoms:

#1 $-x+3/2, y+1/2, -z+1/2$ #2 $x-1/2, -y+1/2, z-1/2$

#3 $-x+3/2, y+1/2, -z+3/2$ #4 $x+1/2, -y+1/2, z+1/2$