Supporting Information for

Norbornene Homopolymerization and Copolymerization with ethylene by Phosphine-sulfonate Nickel Catalysts

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Table S1. NB homopolymerization with **1a-1c** and their $B(C_6F_5)_3$ adduct.[a]

entry	cat	[cat] (μmol)	$B(C_6F_5)_3$ (equiv.)	T (^oC)	T (min)	Yield (%)	Act.[b]	M_w[c] (10^5)	PDI
1	**1a**	10	1	50	2	31	9.3	2.51	3.08
2	**1b**	10	1	50	2	42	12.6	4.73	2.76
3	**1c**	10	1	50	2	81	24.3	3.12	2.78
4	**1a**	10	1	r.t.	20	71	2.1	7.43	2.39
5	**1b**	10	1	r.t.	20	77	2.4	4.39	2.93
6	**1c**	10	1	r.t.	20	84	2.5	3.23	3.07
7	**1c**	10	1	r.t.	2	7	2.1	3.72	2.91
8	**1c**	10	2	r.t.	2	25	7.5	7.24	2.78
9	**1c**	10	4	r.t.	2	41	12.3	4.58	2.60

[a]Polymerization conditions: chlorobenzene = 10ml, NB = 1g (10.6 mmol). [b]Activity is in unit of 10^5 g mol^{-1} h^{-1}. [c]Determined by GPC using universal calibration.

Data for 2D spectrum of **1c**.

Key ^{1}H-^{1}H **COSY** correlations ($CDCl_3$, 25 ℃) δ/δ 8.18 (H^1-Ar)/7.51 ($H^{2,3,4}$-Ar); Cy δ/δ 2.13/1.21; 2.03/1.56; 2.03/1.52; 1.71/1.21; 1.21/1.12; 1.19/1.82; 1.19/2.25 1.19/0.82. Key **HSQC** correlations ($CDCl_3$, 25 ℃) δ/δ 128.3 (C^1-Ar)/7.51 (H^1-Ar); 132.4 (C^2-Ar)/7.51 (H^2-Ar); 130.8 (C^3-Ar)/7.51 (H^3-Ar); 130.0 (C^4-Ar)/7.51 (H^4-Ar); 112.5 (C, allyl)/5.55 (H, allyl); Cy, 29.5/2.16; 35.7/2.02; 26.7/1.69; 28.8/1.53; 25.9/1.21; 29.5/1.20

NMR spectrum

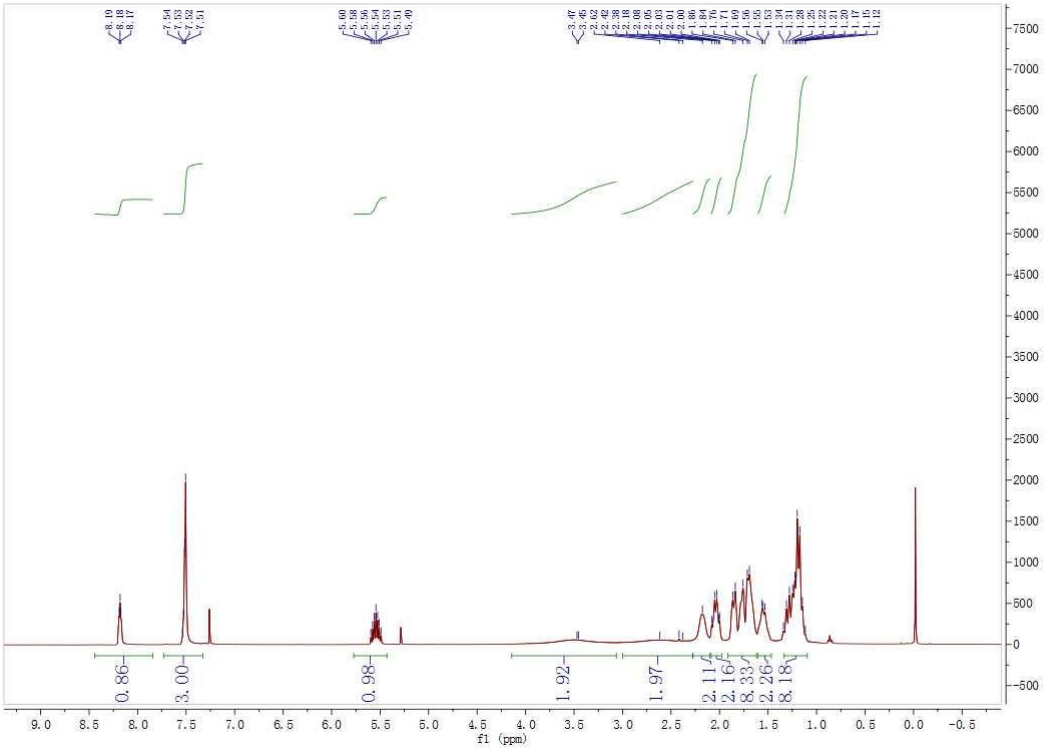

Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **1c**.

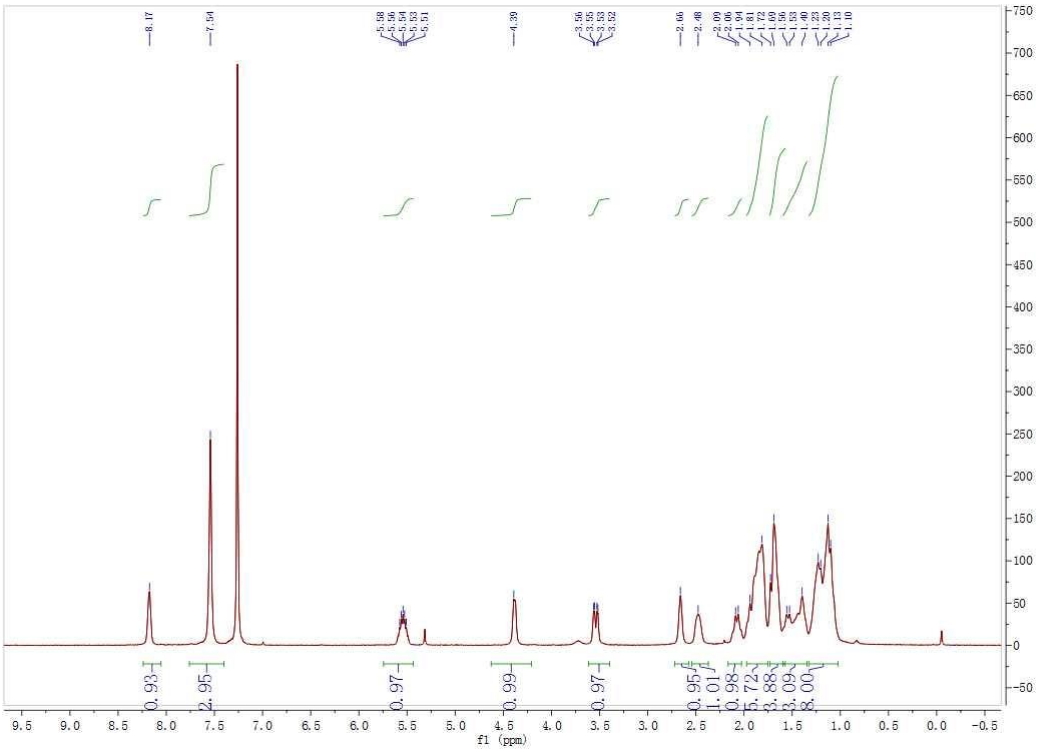

Figure S2. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, -50 ^{o}C) of **1c**.

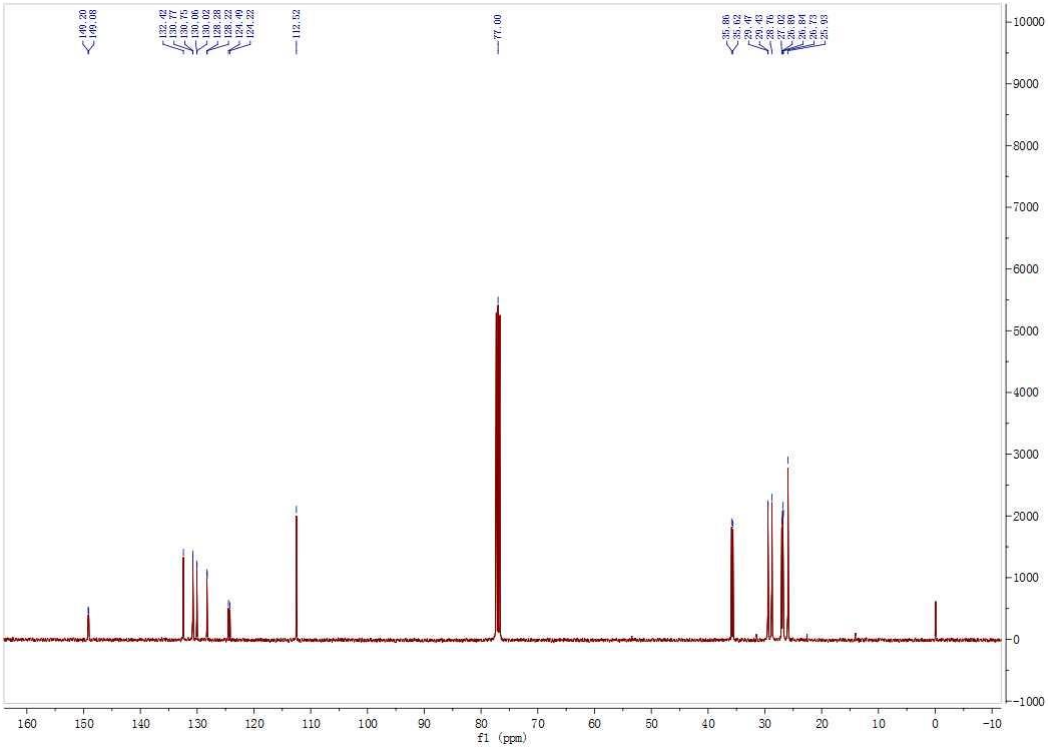

Figure S3. ^{13}C {^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **1c**.

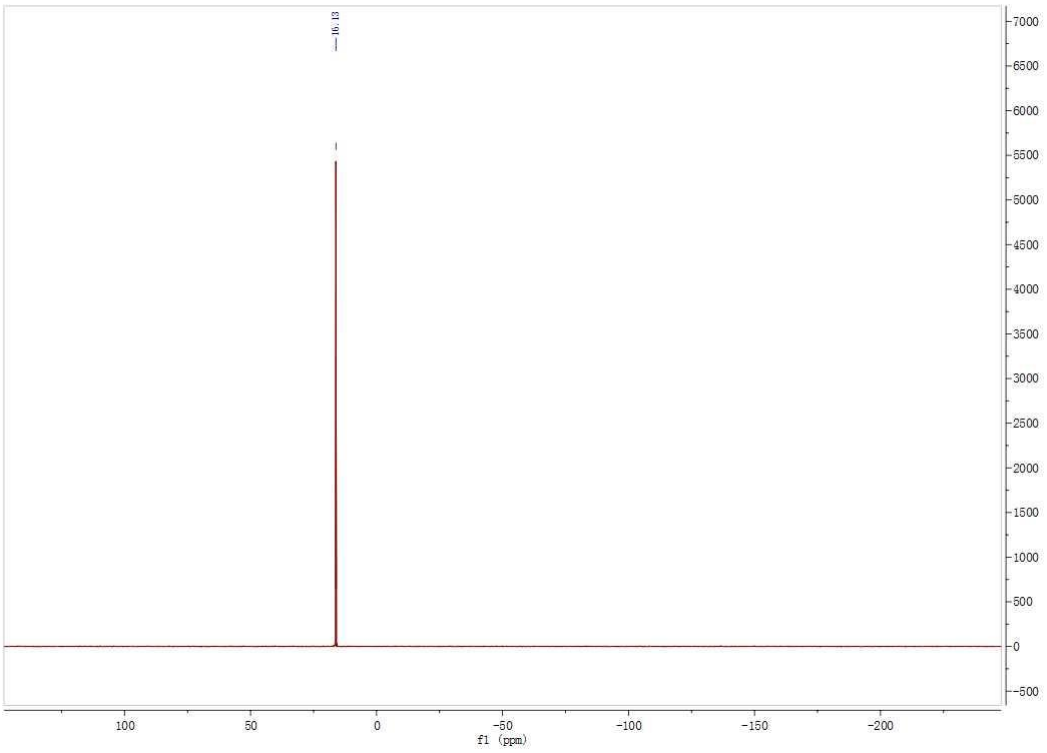

Figure S4. ^{31}P NMR spectrum ($CDCl_3$) of **1c**.

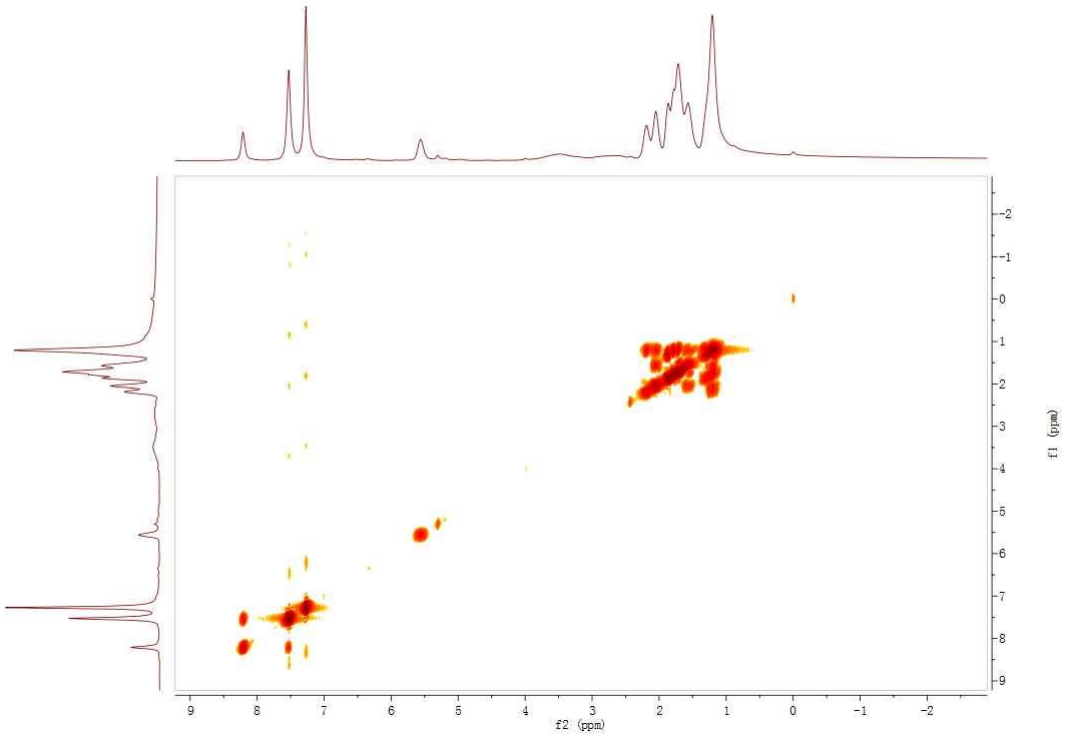

Figure S5.^{1}H-^{1}H COSY NMR($CDCl_3$, 25 ^{o}C) of **1c**.

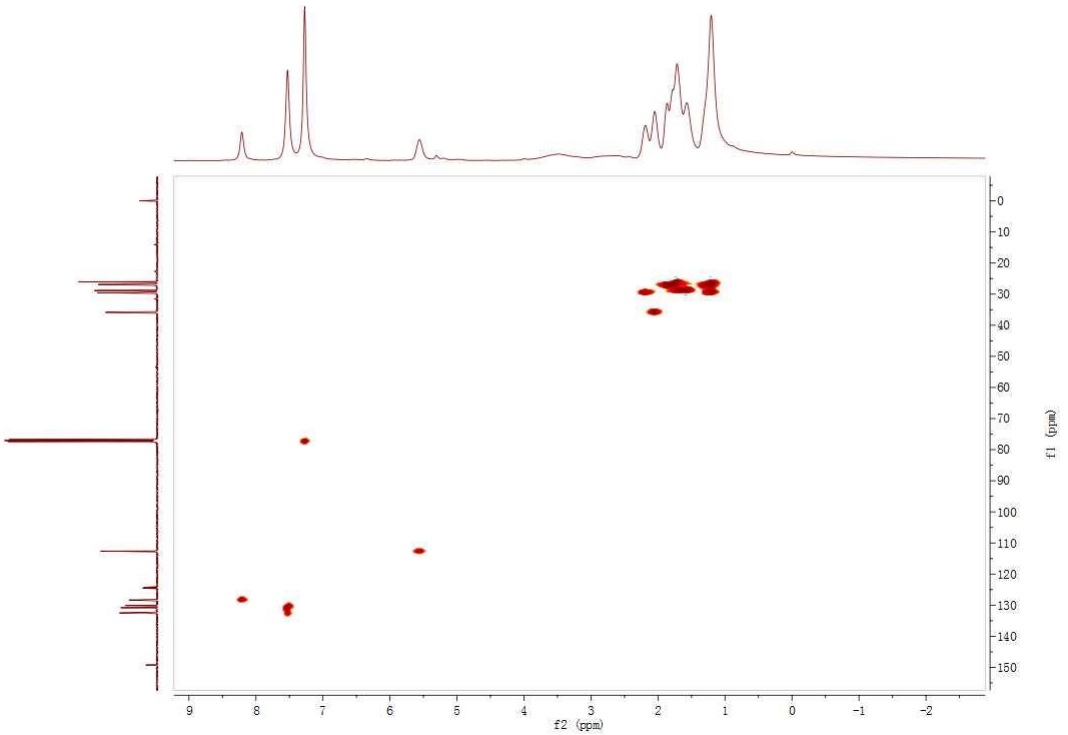

Figure S6. ^{1}H-^{13}C HSQC NMR ($CDCl_3$, 25 ^{o}C) of **1c**.

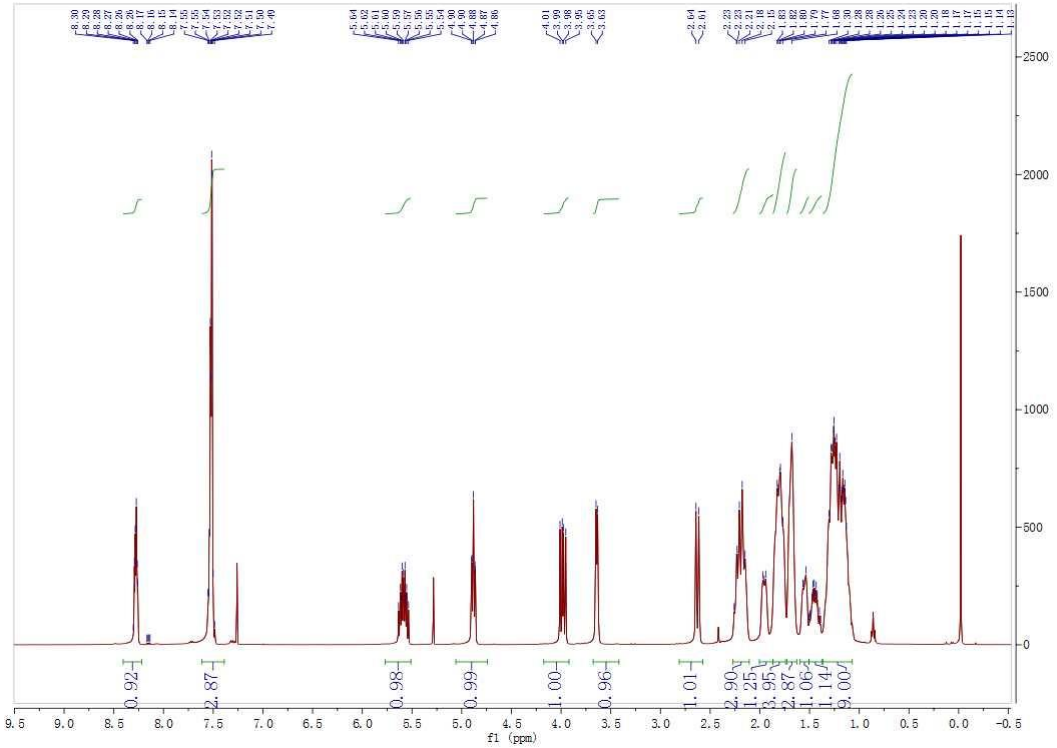

Figure S7. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **2**.

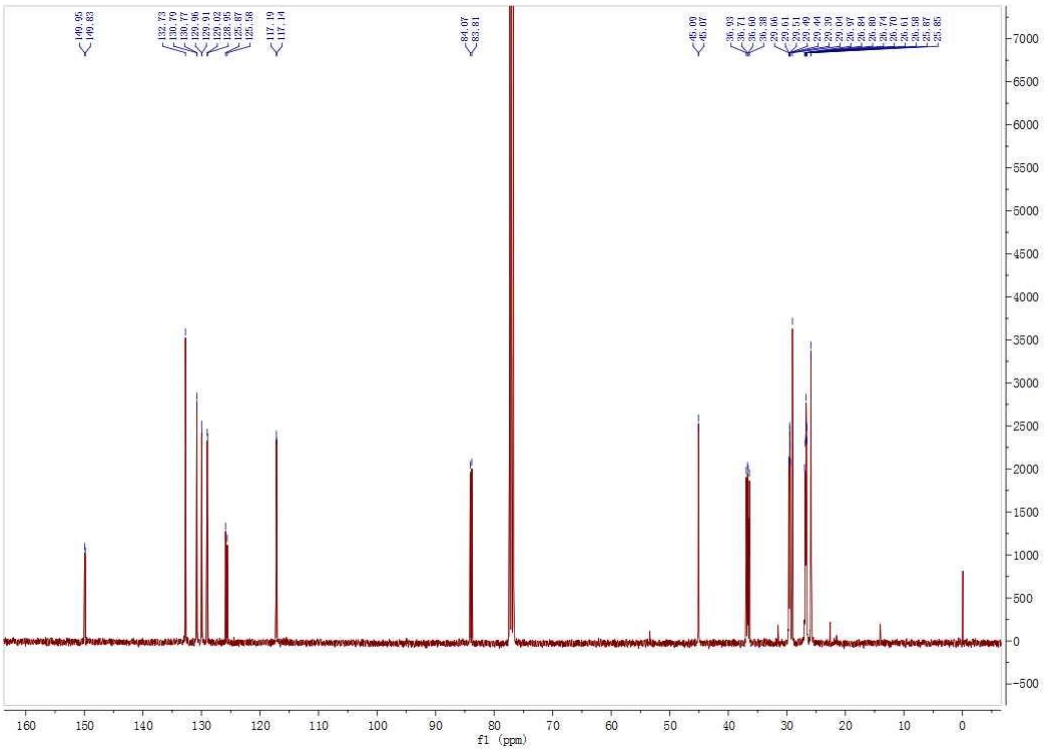

Figure S8. ^{13}C {^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **2**.

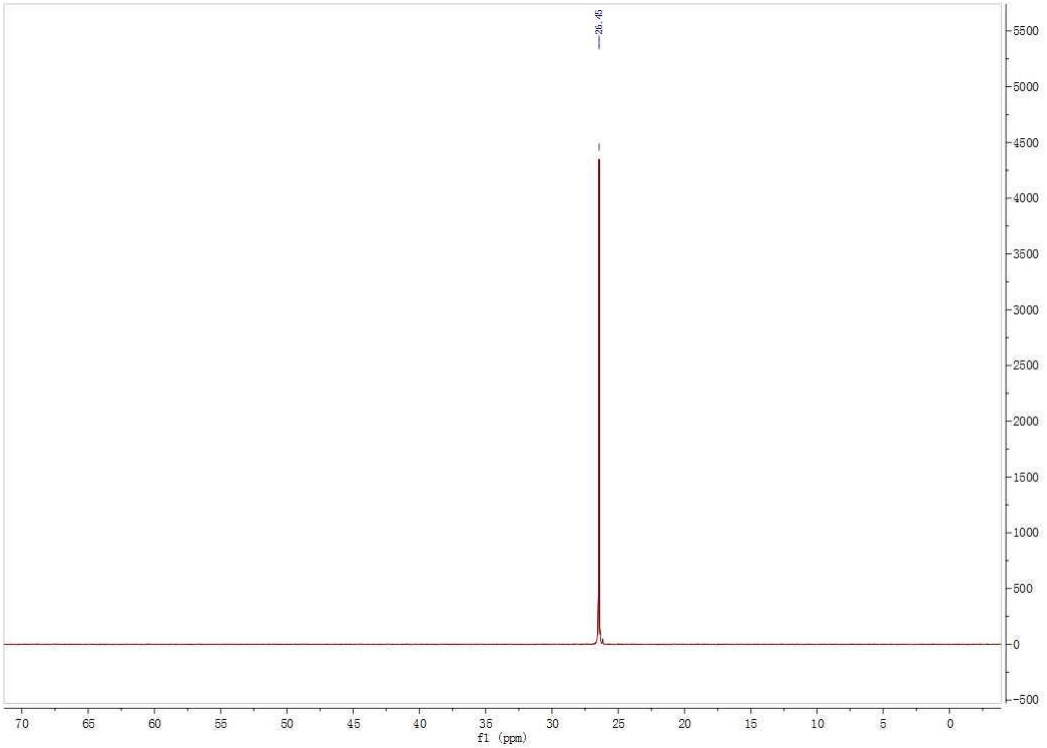

Figure S9. ^{31}P NMR spectrum ($CDCl_3$) of **2**.

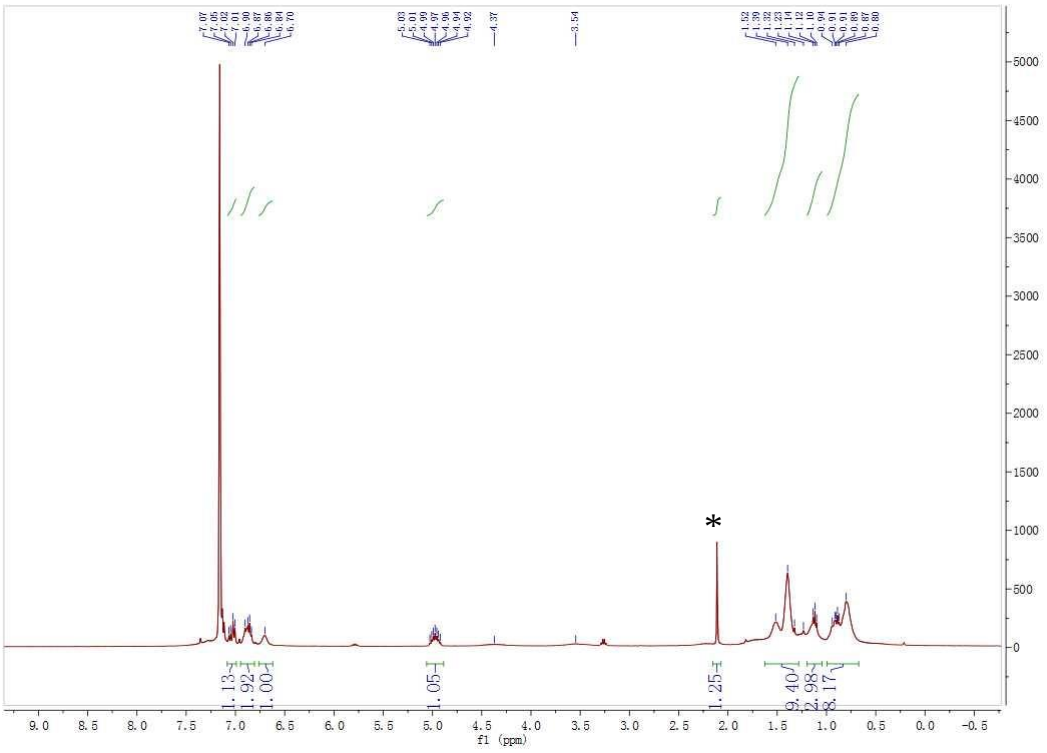

Figure S10. ^{1}H NMR spectrum (400 MHz, C_6D_6) of **3c** (* = toluene).

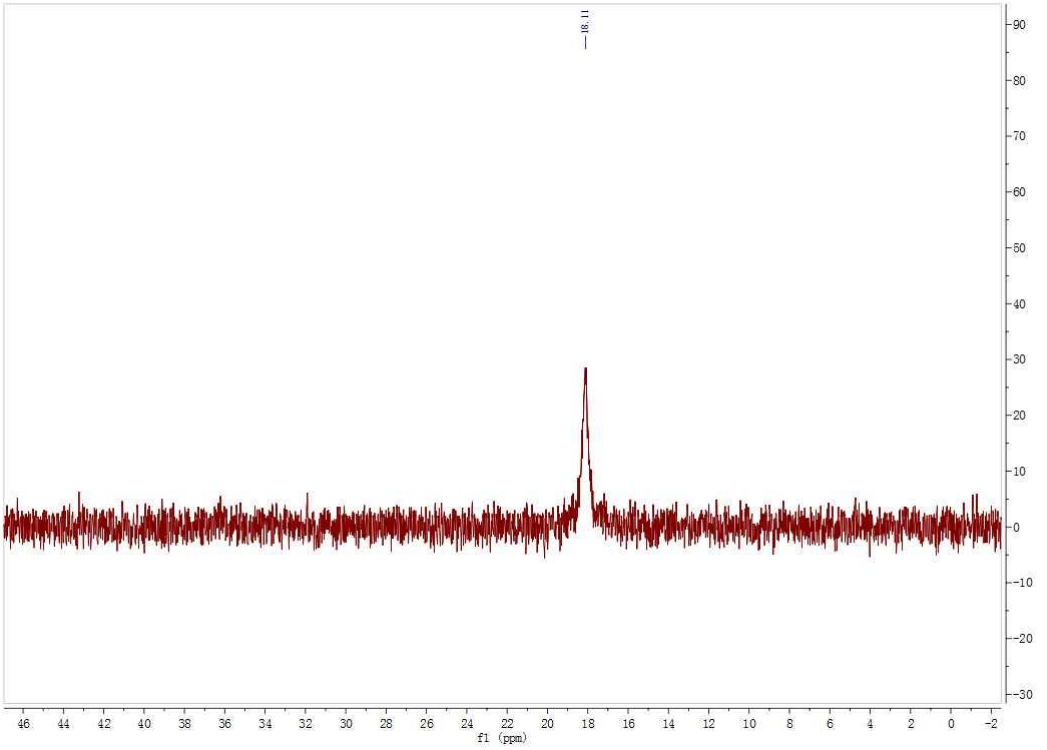

Figure S11. ^{31}P NMR spectrum (C_6D_6) of **3c**.

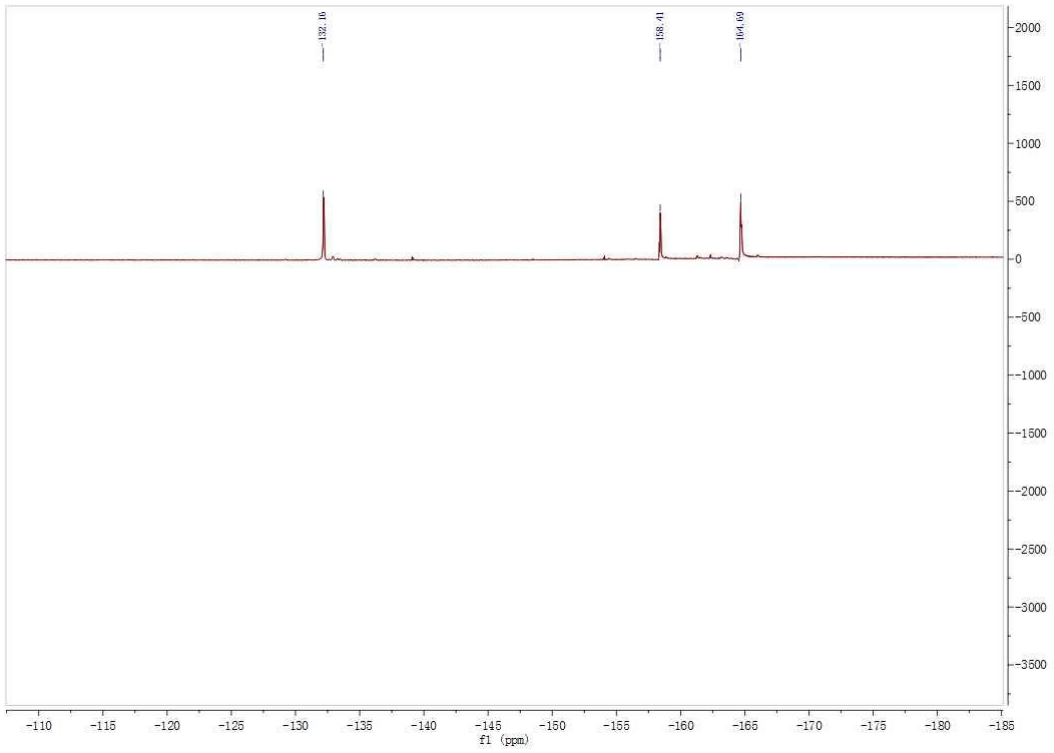

Figure S12. ^{19}F NMR spectrum (C_6D_6) of **3c**.

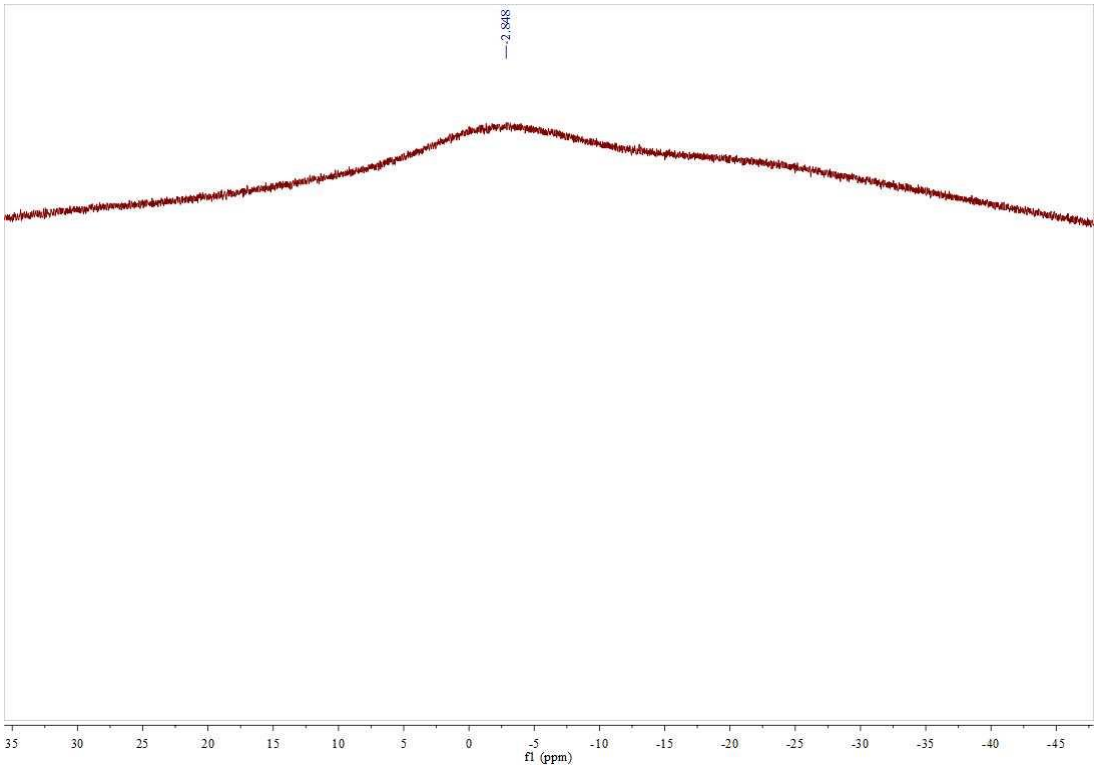

Figure S13. ^{11}B NMR spectrum (C_6D_6) of **3c**.

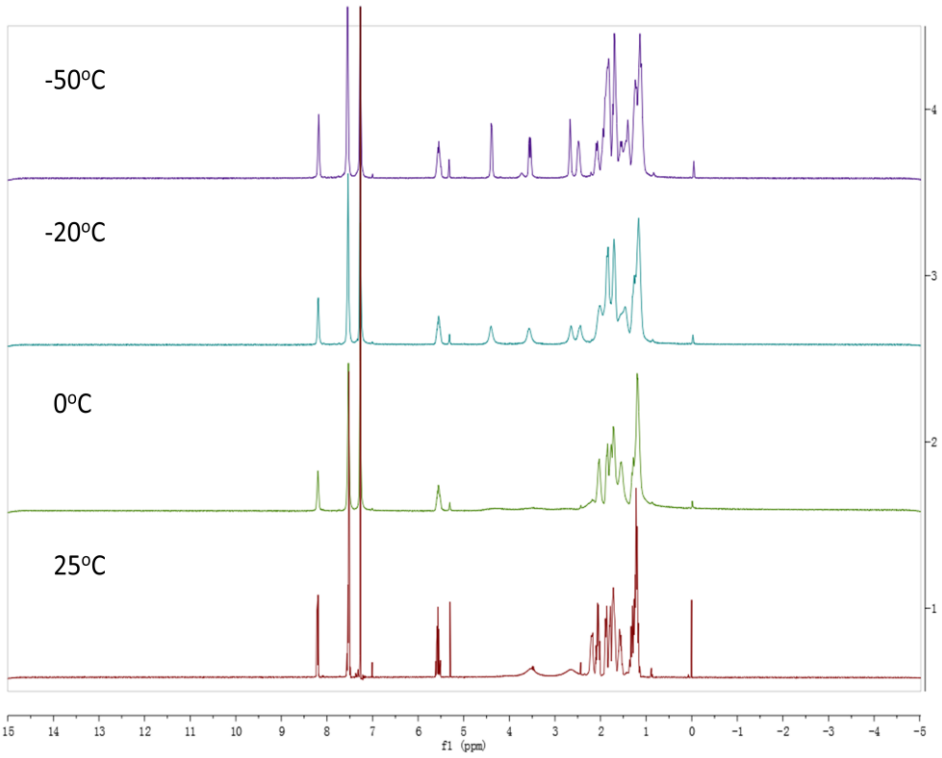

Figure S14. VT ^{1}H NMR (400 MHz, $CDCl_3$) of **1c** at 25°C, 0 °C, -20 °C, -50 °C.

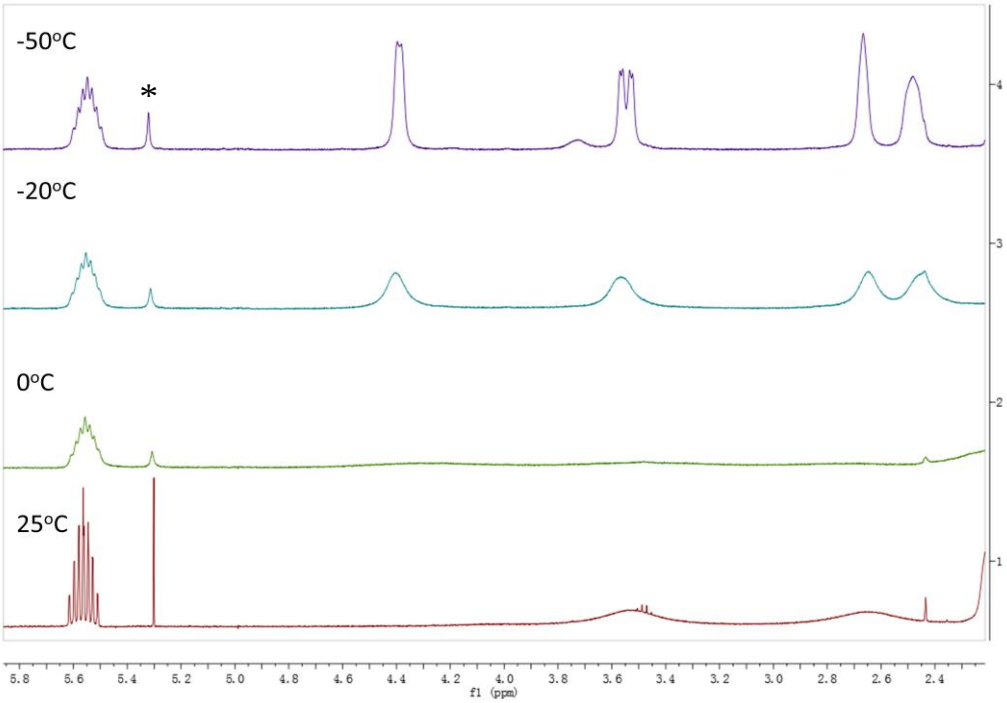

Figure **S15**. VT ^{1}H NMR of **1c** at 25°C, 0 °C, -20 °C, -50 °C: expansion of the δ 5.8-2.3 region (* = CH_2Cl_2).

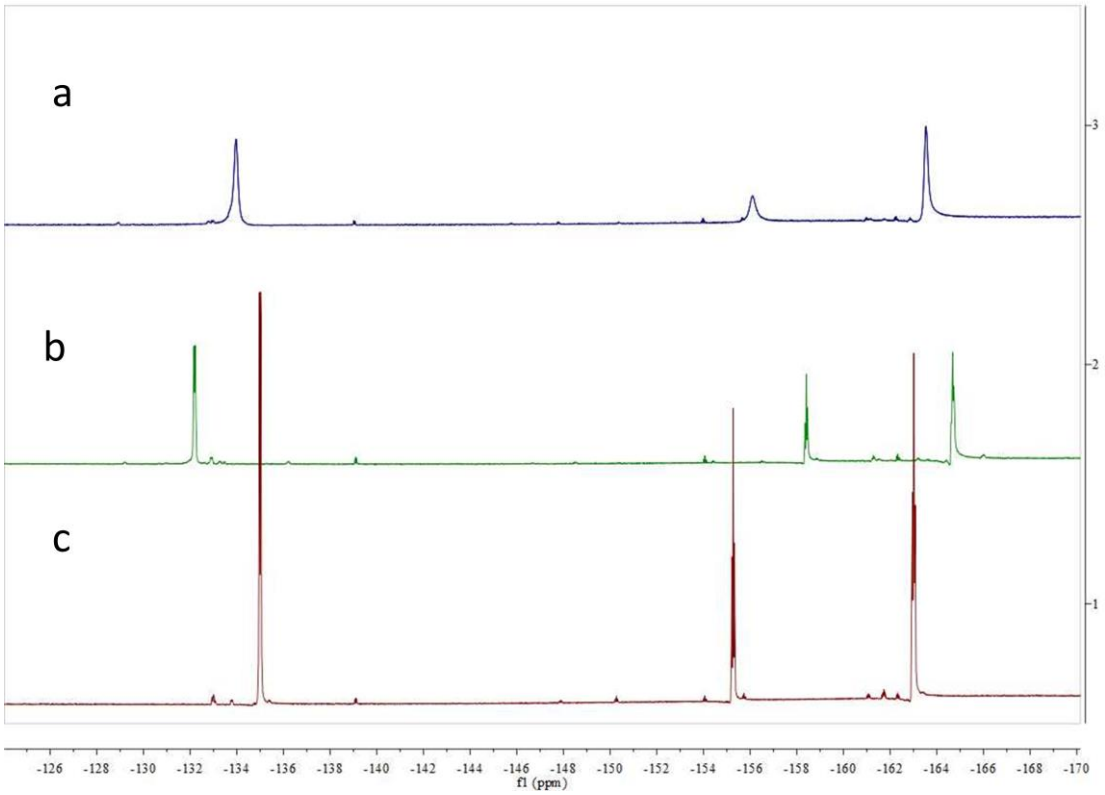

Figure **S16**. Exchange of **3c** and free $B(C_6F_5)_3$ in C_6D_6 at 25 °C. a) ^{19}F NMR of **3c** in the presence of 1 equiv. of $B(C_6F_5)_3$ at 25°C in C_6D_6; b) ^{19}F NMR of **3c** at 25°C in C_6D_6; c) ^{19}F NMR of free $B(C_6F_5)_3$ at 25°C in C_6D_6.

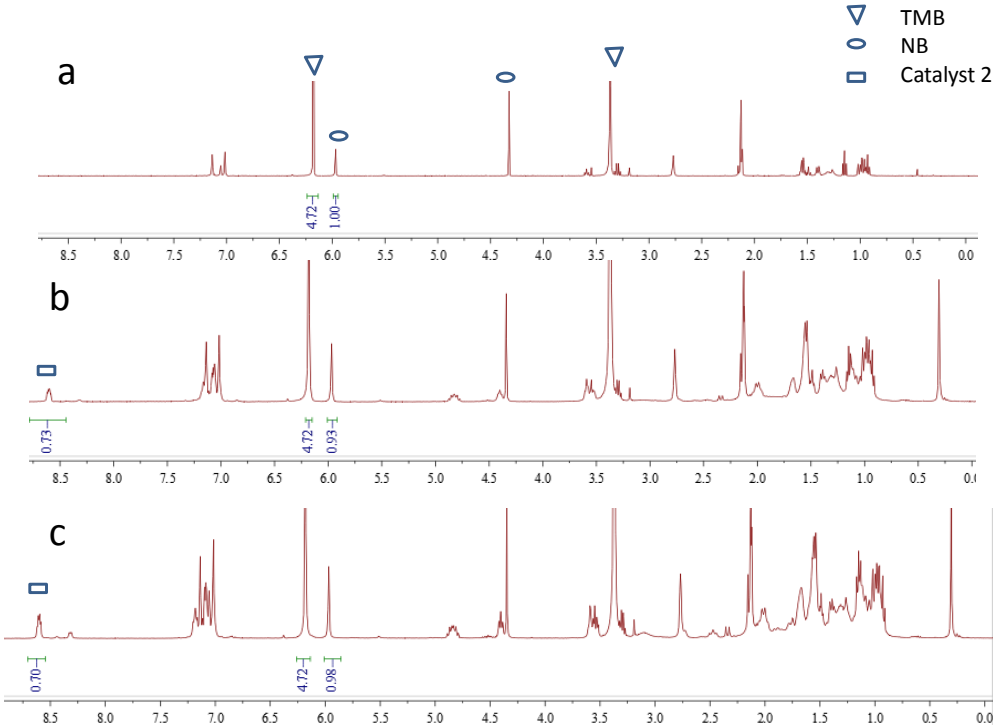

Figure **S17**. ^{1}H NMR spectra complex **2** with NB. a) NB and internal standard TMB in

toluene-d8 (Blank test); b) NB, internal standard TMB and 1.4 eq. of complex **2** in toluene-d8 at 25 ^{o}C for 0.5h; c) NB , internal standard TMB and 1.4 eq. of complex **2** in toluene-d8 at 90 ^{o}C for 6h.

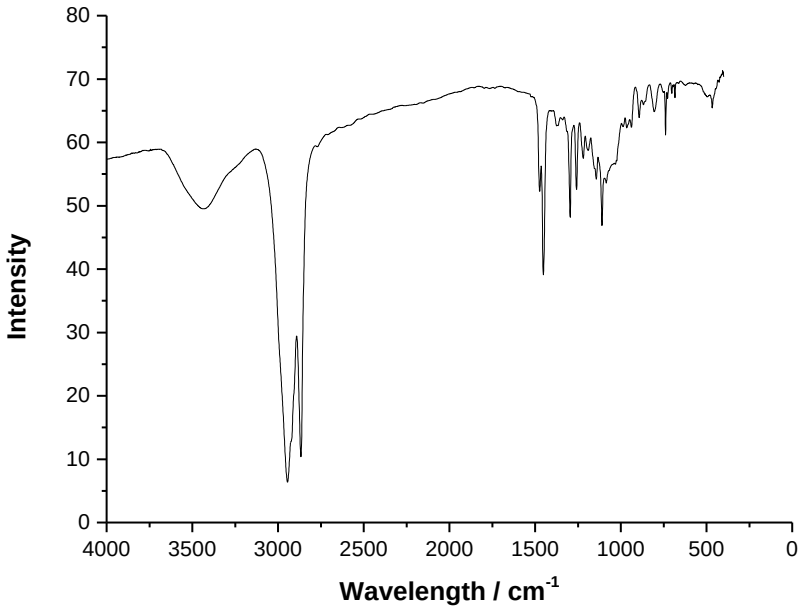

Figure S18. FTIR spectrum of PNB prepared by catalyst **1c** (table 1, entry 6).

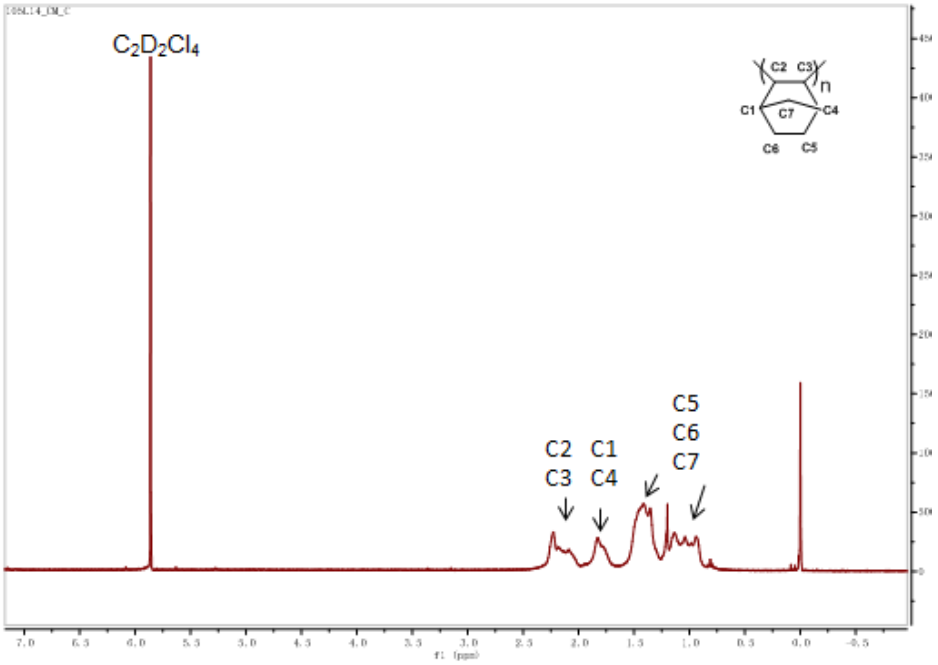

Figure S19. ^{1}H NMR spectrum of PNB in $C_2D_2Cl_4$ at 120 ^{o}C prepared by catalyst **1c** (table 1, entry 6).

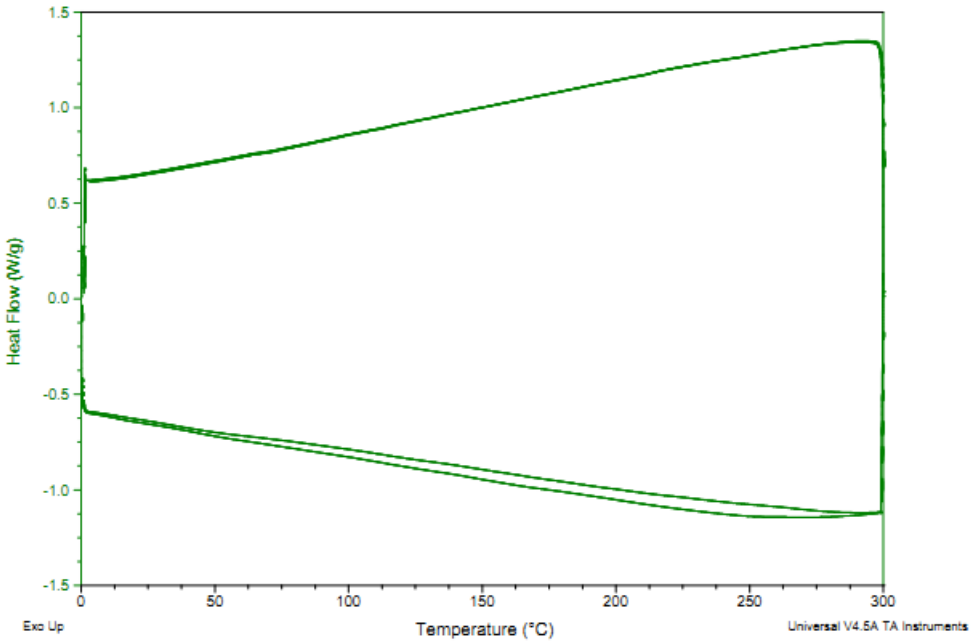

Figure S20. DSC of PNB prepared by catalyst **1c** (table 1, entry 6).

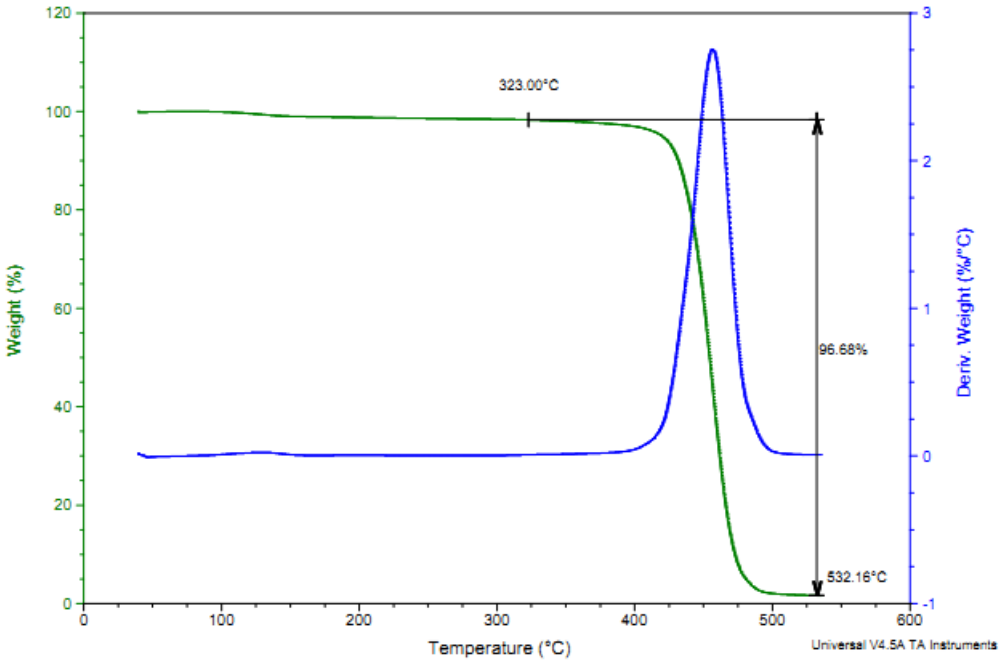

Figure S21. TGA of PNB prepared by catalyst **1c** (table 1, entry 6).

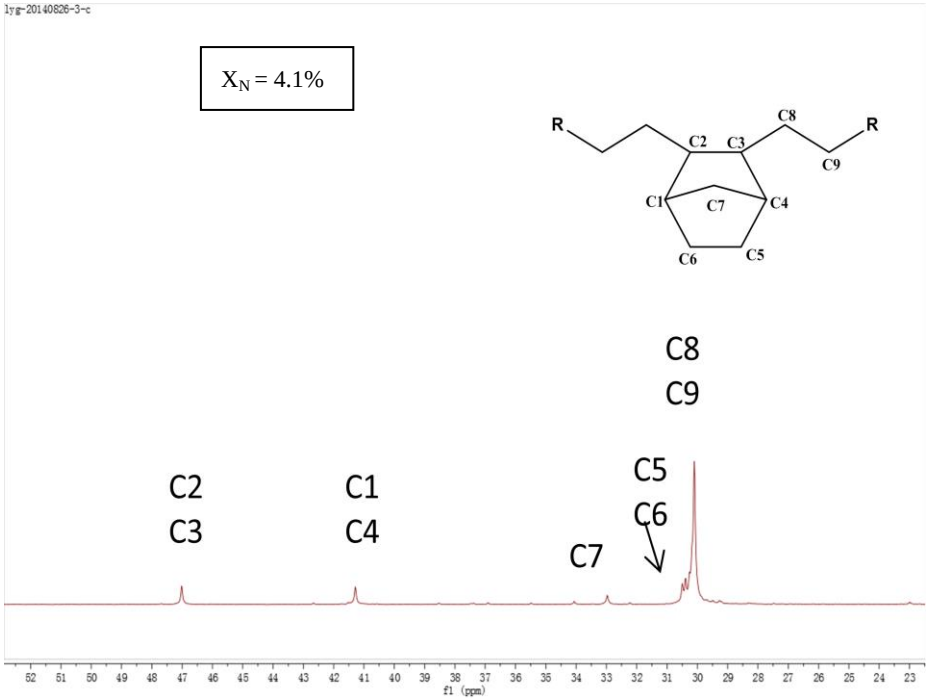

Figure S22. ^{13}C NMR of P(E-NB) prepared by catalyst **1c** (Table 3 ,entry 4) in $C_2D_2Cl_4$ at 120 ^oC.

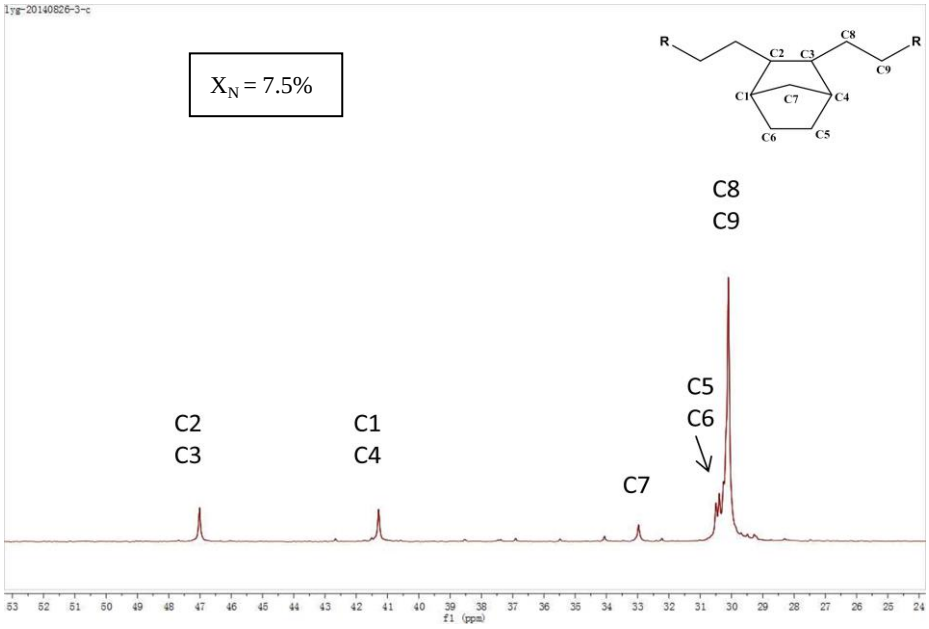

Figure S23. ^{13}C NMR of P(E-NB) prepared by catalyst **1c** (Table 3 ,entry 5) in $C_2D_2Cl_4$ at 120 ^oC.

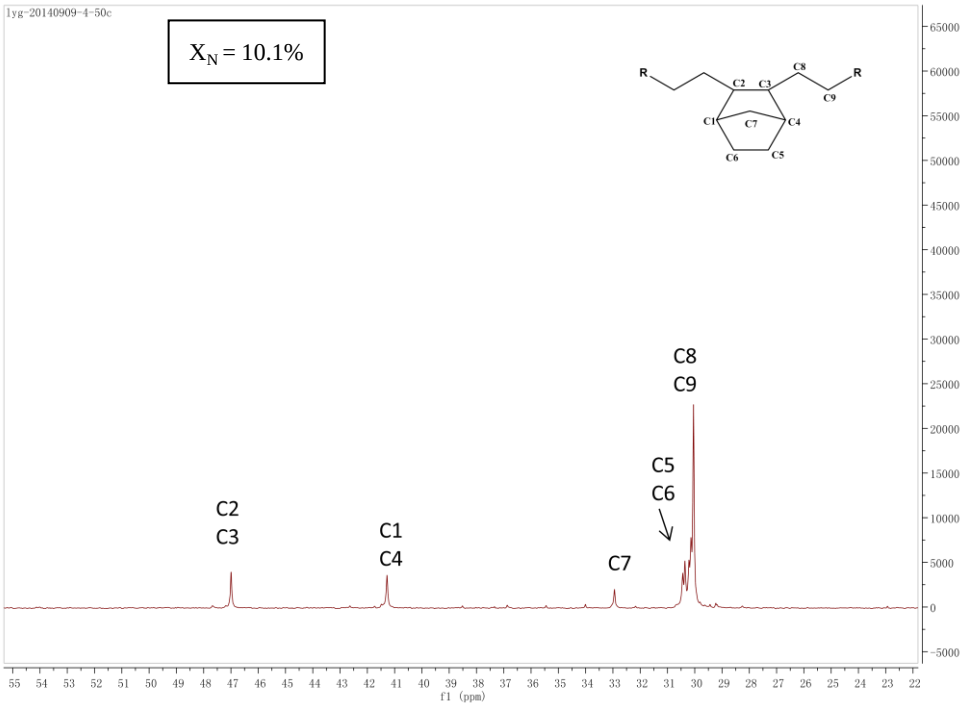

Figure S24. ^{13}C NMR of P(E-NB) prepared by catalyst **1c** (Table 3, entry 6) in $C_2D_2Cl_4$ at 120 ^oC.

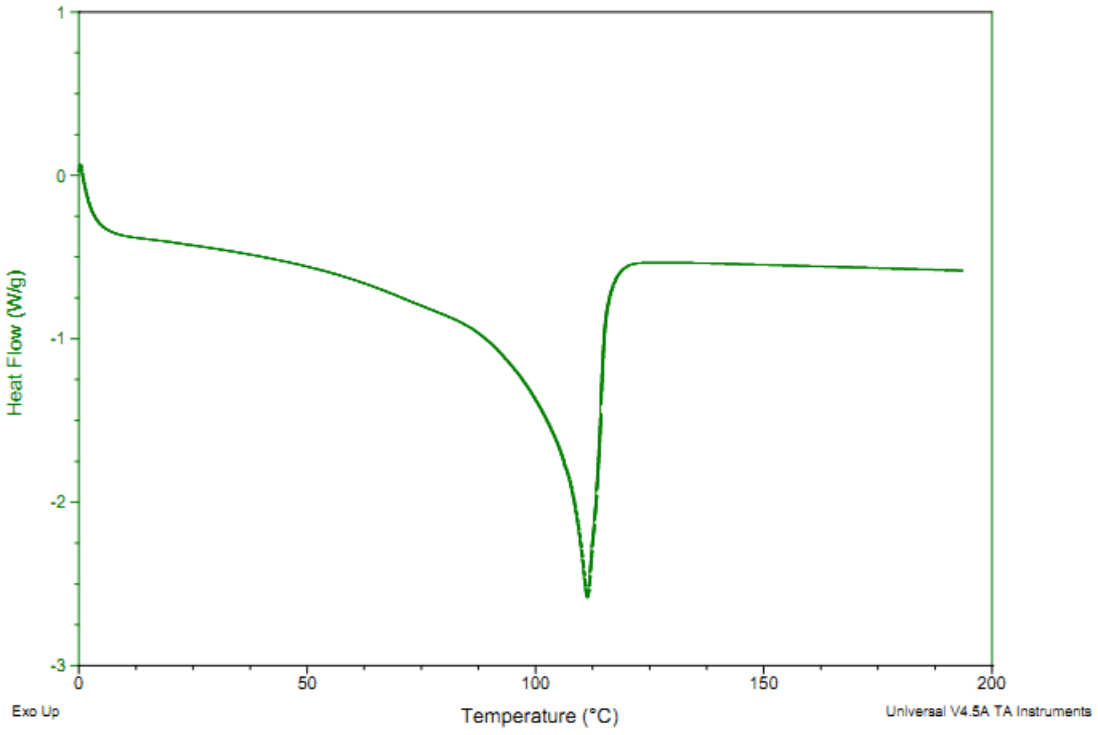

Figure S25. DSC of P(E-NB) prepared by catalyst **1c** (Table 3, entry 4).

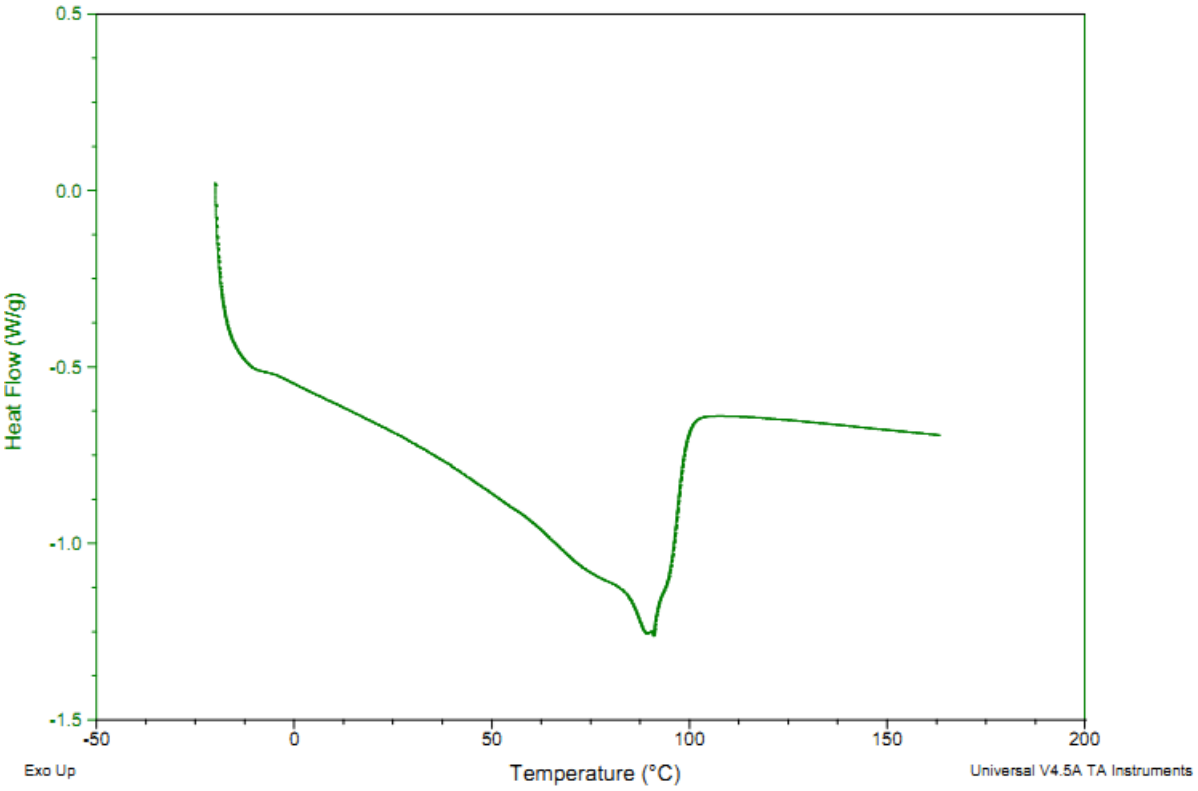

Figure S26. DSC of P(E-NB) prepared by catalyst **1c** (Table 3, entry 5).

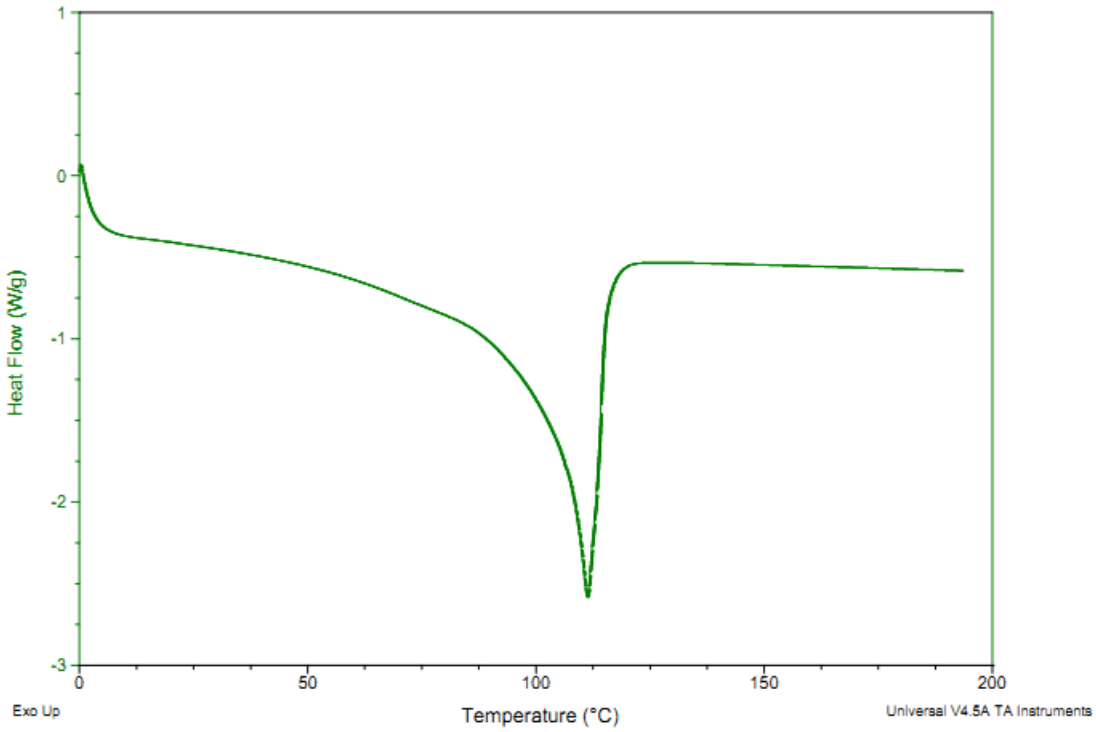

Figure S27. DSC of P(E-NB) prepared by catalyst **1c** (Table 3, entry 7).

X-ray crystallography data

Table S2. Crystal data and structure refinement for **1c**.

data	**1c**
Empirical formula	$C_{21}H_{31}NiO_3PS$
Formula Wt	453.20
Temp. (K)	290(2)
Cryst syst	Monoclinic
Space group	$P2_1/n$
a (Å)	9.56849(3)
b (Å)	16.3520(5)
c (Å)	13.9609(4)
α (deg)	90
β (deg)	95.255(3)
γ (deg)	90
V ($Å^3$)	2175.18(11)
Z	4
D_t (Mg/m^3)	1.384

abs coeff (mm^{-1})	1.080
F(000)	960.0
Crystal size (mm)	0.36×0.32×0.29
θ range (deg)	6.368 to 52.744
Index ranges	-11 <= h <= 11,
	-20 <= k <= 19,
	-17 <= l <= 17
No. of reflns collected	13781
No. of indep reflns	4436 [R(int) = 0.0224]
No. of data / restraints / params	4436 / 1 / 244
Goodness-of-fit on F^2	1.032
Final R indices [I > 2σ(I)]	R1 = 0.0332,
	wR2 = 0.0814
R indices (all data)	R1 = 0.0418,
	wR2 = 0.0859
Largest diff peak & hole (e·Å^{-3})	0.47 and -0.32

Table S3. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **1c**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ni1	6356.6(3)	2427.4(2)	6925.5(2)	37.02(10)
P1	8339.6(5)	1871.9(3)	6567.6(4)	29.80(12)
S1	8025.2(7)	3908.4(3)	6911.5(4)	49.26(16)
O1	6727.5(17)	3509.2(9)	6480.4(12)	50.1(4)
O3	7996(2)	4766.3(10)	6693.6(16)	76.8(6)
O2	8322(2)	3694.5(12)	7906.6(12)	67.0(5)
C15	7302(3)	1032.6(15)	3771.2(16)	50.8(6)
C2	9593(2)	2648.0(12)	6167.7(14)	34.1(4)
C3	10720(2)	2381.8(14)	5686.8(17)	44.3(5)
C7	9275(2)	1292.6(12)	7559.6(14)	34.2(4)
C14	7416(2)	1603.1(13)	4639.7(15)	42.8(5)
C18	7331(3)	392.9(13)	5734.6(16)	48.1(6)
C16	6552(3)	245.1(17)	3977.9(18)	57.7(7)
C13	8133(2)	1172.4(11)	5523.7(13)	32.0(4)
C10	11454(3)	867.3(18)	9106.1(19)	64.4(7)
C1	9407(2)	3479.9(13)	6290.6(15)	42.3(5)
C17	7222(3)	-173.4(15)	4861.4(18)	57.5(7)
C5	11444(3)	3758.4(18)	5449(2)	69.2(8)
C6	10339(3)	4031.2(16)	5925(2)	61.2(7)
C4	11638(3)	2934.4(18)	5330.2(19)	58.2(7)
C8	10603(3)	834.8(16)	7343.1(17)	52.9(6)
C9	11173(3)	331.1(18)	8218.4(18)	63.1(7)
C12	9567(3)	1835.5(15)	8445.5(16)	50.4(6)
C11	10139(3)	1329.0(18)	9307.4(17)	64.2(7)
C21	4478(3)	2755(2)	7410(3)	75.5(9)
C19	5619(3)	1458.8(17)	7574(2)	57.5(6)
C20	4525(3)	1942.7(19)	7201(3)	70.9(8)

Table S4. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **1c**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni1	35.18(16)	36.73(17)	39.12(16)	-6.09(11)	3.32(12)	6.13(11)
P1	32.5(3)	25.9(3)	31.3(3)	-2.05(19)	4.6(2)	1.11(19)
S1	63.3(4)	30.0(3)	53.2(3)	-11.7(2)	-1.6(3)	4.4(3)
O1	51.9(9)	36.2(8)	60.5(10)	-1.7(7)	-3.8(8)	8.9(7)
O3	95.3(15)	27.9(9)	106.4(16)	-12.6(10)	4.8(13)	3.9(9)
O2	83.5(13)	69.3(13)	46.7(10)	-20.6(9)	-2.0(9)	11.8(10)
C15	59.5(15)	55.5(15)	36.6(12)	-7.1(10)	1.1(11)	-10.1(12)
C2	33.8(10)	37.8(11)	30(1)	-4.7(8)	-0.3(8)	-3.3(8)
C3	44.4(12)	42.6(13)	46.4(13)	-0.5(10)	7.5(10)	-6.1(10)
C7	36.3(10)	32.6(10)	33.7(10)	2.1(8)	3.2(8)	2.8(8)

C14	50.2(12)	37.6(12)	39.4(11)	-1.6(9)	-1.2(10)	-0.1(10)
C18	66.6(15)	34.2(12)	45.7(12)	-5(1)	16.2(12)	-12.8(11)
C16	58.7(15)	63.8(16)	52.0(14)	-22.0(13)	12.3(12)	-24.2(13)
C13	35.5(10)	28.1(10)	33.2(10)	-4.6(8)	6.5(8)	-1.2(8)
C10	66.3(17)	70.0(18)	53.2(15)	6.8(13)	-14.4(13)	16.5(14)
C1	49.2(12)	35.7(11)	40.8(12)	-2.4(9)	-3.4(10)	-8.2(10)
C17	77.9(18)	37.4(13)	60.5(15)	-15.8(12)	25.0(14)	-20.0(12)
C5	74.1(19)	63.6(18)	71.8(18)	5.8(15)	16.5(16)	-33.3(15)
C6	75.9(18)	38.4(13)	68.4(17)	0.5(12)	2.0(15)	-20.7(13)
C4	52.3(15)	67.6(18)	57.0(15)	1.1(13)	17.3(12)	-15.7(13)
C8	53.2(14)	63.1(16)	42.4(12)	1.3(11)	4.8(11)	24.3(12)
C9	71.0(18)	63.9(17)	52.8(14)	3.5(13)	-3.8(13)	34.3(14)
C12	59.0(15)	50.0(14)	40.4(12)	-6.4(10)	-5.1(11)	14.6(11)
C11	83(2)	71.8(18)	35.9(12)	-3.1(12)	-4.7(13)	20.9(15)
C21	54.0(16)	80(2)	97(2)	-12.6(18)	30.1(17)	19.0(15)
C19	53.9(14)	58.8(16)	62.8(16)	5.6(13)	21.8(13)	1.1(12)
C20	44.3(14)	74(2)	98(2)	1.4(17)	23.3(15)	1.3(13)

Table S5. Bond Lengths for **1c**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ni1	P1	2.2020(6)	C3	C4	1.384(3)
Ni1	O1	1.9189(16)	C7	C8	1.529(3)
Ni1	C21	2.049(3)	C7	C12	1.527(3)
Ni1	C19	1.986(3)	C14	C13	1.528(3)
Ni1	C20	1.992(3)	C18	C13	1.531(3)
P1	C2	1.866(2)	C18	C17	1.527(3)
P1	C7	1.841(2)	C16	C17	1.502(4)
P1	C13	1.8489(19)	C10	C9	1.522(4)
S1	O1	1.4809(17)	C10	C11	1.516(4)
S1	O3	1.4352(19)	C1	C6	1.397(3)
S1	O2	1.4356(19)	C5	C6	1.374(4)
S1	C1	1.789(2)	C5	C4	1.372(4)
C15	C14	1.526(3)	C8	C9	1.532(3)
C15	C16	1.515(3)	C12	C11	1.521(3)
C2	C3	1.392(3)	C21	C20	1.362(4)
C2	C1	1.385(3)	C19	C20	1.375(4)

Table S6. Bond Angles for **1c**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°

O1	Ni1	P1	96.78(5)	C4	C3	C2	121.0(2)
O1	Ni1	C21	93.42(11)	C8	C7	P1	117.31(14)
O1	Ni1	C19	165.24(9)	C12	C7	P1	110.51(14)
O1	Ni1	C20	128.41(10)	C12	C7	C8	110.56(18)
C21	Ni1	P1	169.43(10)	C15	C14	C13	110.75(18)
C19	Ni1	P1	97.13(8)	C17	C18	C13	110.49(18)
C19	Ni1	C21	72.48(12)	C17	C16	C15	111.7(2)
C19	Ni1	C20	40.46(11)	C14	C13	P1	111.05(13)
C20	Ni1	P1	132.15(9)	C14	C13	C18	110.06(18)
C20	Ni1	C21	39.35(12)	C18	C13	P1	112.51(14)
C2	P1	Ni1	112.20(7)	C11	C10	C9	110.5(2)
C7	P1	Ni1	114.28(7)	C2	C1	S1	123.60(17)
C7	P1	C2	107.08(9)	C2	C1	C6	119.7(2)
C7	P1	C13	106.51(9)	C6	C1	S1	116.68(19)
C13	P1	Ni1	113.70(7)	C16	C17	C18	111.8(2)
C13	P1	C2	102.12(9)	C4	C5	C6	119.7(2)
O1	S1	C1	105.07(10)	C5	C6	C1	120.8(2)
O3	S1	O1	110.20(11)	C5	C4	C3	120.0(3)
O3	S1	O2	116.20(12)	C7	C8	C9	110.31(19)
O3	S1	C1	106.32(12)	C10	C9	C8	111.3(2)
O2	S1	O1	111.74(12)	C11	C12	C7	110.49(19)
O2	S1	C1	106.48(11)	C10	C11	C12	111.7(2)
S1	O1	Ni1	116.60(9)	C20	C21	Ni1	68.09(15)
C16	C15	C14	111.66(19)	C20	C19	Ni1	70.04(16)
C3	C2	P1	118.63(16)	C21	C20	Ni1	72.55(17)
C1	C2	P1	122.56(16)	C21	C20	C19	121.3(3)
C1	C2	C3	118.7(2)	C19	C20	Ni1	69.51(16)

Table S7. Torsion Angles for **1c**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ni1	P1	C2	C3	-163.61(15)	C2	P1	C13	C18	170.55(16)
Ni1	P1	C2	C1	13.3(2)	C2	C3	C4	C5	0.0(4)
Ni1	P1	C7	C8	175.45(15)	C2	C1	C6	C5	-0.4(4)
Ni1	P1	C7	C12	-56.58(17)	C3	C2	C1	S1	-178.87(17)
Ni1	P1	C13	C14	55.51(15)	C3	C2	C1	C6	0.6(3)
Ni1	P1	C13	C18	-68.36(16)	C7	P1	C2	C3	70.24(18)
Ni1	C21	C20	C19	51.7(3)	C7	P1	C2	C1	-112.87(18)
Ni1	C19	C20	C21	-53.0(3)	C7	P1	C13	C14	-177.72(14)
P1	C2	C3	C4	176.57(19)	C7	P1	C13	C18	58.40(17)
P1	C2	C1	S1	4.2(3)	C7	C8	C9	C10	-56.6(3)
P1	C2	C1	C6	-176.28(18)	C7	C12	C11	C10	56.9(3)

P1	C7	C8	C9	-175.25(19)	C14	C15	C16	C17	-54.2(3)
P1	C7	C12	C11	171.50(18)	C16	C15	C14	C13	55.6(3)
S1	C1	C6	C5	179.2(2)	C13	P1	C2	C3	-41.48(19)
O1	S1	C1	C2	-50.2(2)	C13	P1	C2	C1	135.41(18)
O1	S1	C1	C6	130.35(19)	C13	P1	C7	C8	49.04(19)
O3	S1	O1	Ni1	-166.10(12)	C13	P1	C7	C12	177.00(15)
O3	S1	C1	C2	-167.00(19)	C13	C18	C17	C16	-56.2(3)
O3	S1	C1	C6	13.5(2)	C1	S1	O1	Ni1	79.75(12)
O2	S1	O1	Ni1	-35.31(14)	C1	C2	C3	C4	-0.4(3)
O2	S1	C1	C2	68.5(2)	C17	C18	C13	P1	-178.49(17)
O2	S1	C1	C6	-111.0(2)	C17	C18	C13	C14	57.1(3)
C15	C14	C13	P1	177.75(16)	C6	C5	C4	C3	0.2(4)
C15	C14	C13	C18	-57.0(2)	C4	C5	C6	C1	-0.1(4)
C15	C16	C17	C18	54.6(3)	C8	C7	C12	C11	-56.9(3)
C2	P1	C7	C8	-59.64(19)	C9	C10	C11	C12	-56.2(3)
C2	P1	C7	C12	68.32(17)	C12	C7	C8	C9	56.8(3)
C2	P1	C13	C14	-65.58(16)	C11	C10	C9	C8	56.0(3)

Table S8. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **1c**.

Atom	*x*	*y*	*z*	U(eq)
H15A	6794	1307	3230	61
H15B	8235	906	3595	61
H3	10859	1824	5604	53
H7	8616	873	7740	41
H14A	6485	1779	4773	51
H14B	7951	2085	4497	51
H18A	7812	113	6282	58
H18B	6397	535	5896	58
H16A	5579	364	4066	69
H16B	6569	-119	3431	69
H13	9074	1010	5372	38
H10A	11763	529	9656	77
H10B	12197	1253	9006	77
H17A	8154	-357	4741	69
H17B	6673	-651	4998	69
H5	12058	4131	5207	83
H6	10210	4590	6005	73
H4	12386	2747	5010	70
H8A	11309	1223	7180	63
H8B	10392	475	6796	63
H9A	10498	-89	8344	76
H9B	12036	63	8080	76

H12A	10242	2254	8316	60
H12B	8707	2104	8589	60
H11A	10350	1687	9856	77
H11B	9428	943	9470	77
H21A	4491	2902	8084	91
H21B	3859	3091	6985	91
H19A	5725	934	7266	69
H19B	5788	1440	8269	69
H20	3900	1732	6662	85

Table S9. Crystal data and structure refinement for **3c**.

data	**3c**
Empirical formula	$C_{39}H_{31}BF_{15}NiO_3PS \cdot C_7H_8$
Formula Wt	1057.32
Temp. (K)	291(2)
Cryst syst	Orthorhombic
Space group	$Pna2_1$
a (Å)	24.5629(3)
b (Å)	15.6599(2)
c (Å)	11.5597(10)
α (deg)	90
β (deg)	90
γ (deg)	90
V ($Å^3$)	4446.47(9)
Z	4
D_t (Mg/m^3)	1.579
abs coeff (mm^{-1})	2.356
F(000)	2152.0
Crystal size (mm)	0.36×0.32×0.27
θ range (deg)	6.694 to 139.148
Index ranges	-29 <= h <= 25,
	-18 <= k <= 17,
	-8<= l <= 13
No. of reflns collected	11103
No. of indep reflns	5783 [R(int) = 0.0226]
No. of data / restraints / params	5783 / 1 /614
Goodness-of-fit on F^2	1.048
Final R indices [I > 2σ(I)]	R1 = 0.0332,
	wR2 = 0.0906
R indices (all data)	R1 = 0.0355,
	wR2 = 0.0937
Largest diff peak & hole ($e \cdot Å^{-3}$)	0.28 and -0.26

Table S10. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3c**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Ni1	6480.6(2)	5298.3(4)	9061.4(6)	50.79(18)
S1	5594.5(3)	5603.5(5)	7343.2(8)	41.70(19)
P1	6969.1(3)	5205.7(6)	7460.3(9)	46.5(2)
F1	5043.1(9)	6429.5(16)	9384(2)	63.1(6)
03	5758.4(8)	6522.4(14)	7561(2)	43.3(5)
F11	6026.8(11)	7597.7(17)	9324(2)	67.1(7)
F10	6189.4(8)	7187.5(16)	5244(2)	59.9(6)
F5	4754.6(11)	8782.7(16)	6901(3)	73.8(7)
F7	4081.4(11)	6758(2)	4028(4)	89.9(10)
F6	4315.4(9)	7069.4(18)	6186(3)	72.2(7)
F15	5834.9(12)	8817.1(16)	5603(3)	71.4(7)
F14	6583.7(14)	9957.4(19)	6130(4)	95.3(10)
F8	4885.9(16)	6641(2)	2400(3)	95.1(10)
F3	3555.7(10)	8233(2)	9955(3)	92(1)
F9	5937.6(13)	6866(2)	3044(3)	83.5(8
O2	5782.3(10)	5105.3(16)	8340(2)	49.3(6)
F12	6755.8(14)	8792(2)	9840(3)	96.5(10)
F13	7060.2(13)	9968(2)	8250(4)	104.1(12)
C1	5976.5(13)	5277(2)	6121(3)	41.5(7)
C32	6057.5(16)	8755(2)	6658(4)	56.3(10)
C19	5267.5(14)	7207(2)	5833(4)	47.5(8)
C6	6545.9(14)	5146(2)	6143(4)	45.9(8)
C3	5933.6(17)	4921(3)	4102(4)	58.1(9)
C24	4738.4(15)	7065(3)	5449(4)	56.3(10)
C30	4763.5(14)	7112(2)	9002(4)	52.1(9)
C4	6497.9(17)	4805(3)	4095(5)	62.7(10)
C25	4934.3(14)	7570(2)	8045(4)	49.6(8)
C28	4004.5(16)	8027(3)	9346(5)	64.5(12)
C29	4303.2(17)	7322(3)	9645(4)	61.2(11)
C7	7460.3(13)	6090(3)	7253(4)	53.9(9)
C2	5679.8(14)	5151(2)	5116(4)	48.9(8)
C20	5655.6(15)	7127(2)	4962(4)	50.2(9)
C23	4607.8(17)	6884(3)	4312(5)	66.2(13)
C21	5538.2(19)	6949(3)	3829(4)	59.1(10)
C31	5901.7(13)	8112(2)	7424(4)	48.1(8)
C22	5006(2)	6825(3)	3496(4)	67.9(12)
C33	6444.0(18)	9371(3)	6923(5)	67.3(12)
C36	6145.8(15)	8169(2)	8491(4)	52.9(9)
C8	7718.6(19)	6174(3)	6061(5)	70.7(12)

C14	7005.7(16)	3436(3)	7319(7)	80.6(16)
C26	4621.6(15)	8296(3)	7819(4)	56.5(9)
C13	7372.9(13)	4209(2)	7323(4)	52.5(9)
B1	5446.1(14)	7358(2)	7180(4)	44.4(9)
C5	6788.9(15)	4906(3)	5106(4)	56.4(10)
C35	6522.8(18)	8788(3)	8786(5)	67.4(13)
C16	7778(2)	2526(3)	8045(6)	87.5(17)
C34	6673.0(18)	9382(3)	7986(5)	71.2(14)
C37	7078(2)	5456(5)	10176(5)	96.2(19)
C18	7810(2)	4128(3)	8257(6)	81.6(15)
C17	8137(2)	3305(3)	8065(7)	91.0(19)
C10	7910(2)	7729(3)	6426(7)	92.2(19)
C40	4982(4)	8914(5)	2327(8)	109(2)
C15	7337(2)	2610(3)	7141(7)	90.8(19)
C45	5168(4)	9281(5)	3334(8)	111(2)
C9	8139(2)	6899(4)	6033(6)	85.7(16)
C12	7213.4(16)	6941(3)	7615(6)	71.8(13)
C43	4287(4)	9246(6)	4184(10)	126(3)
C44	4817(4)	9427(6)	4220(10)	129(3)
C11	7651(2)	7641(3)	7615(7)	88.6(19)
C39	6143(3)	5333(5)	10706(5)	89.4(18)
C41	4429(5)	8707(5)	2273(10)	136(3)
C38	6616(3)	5704(7)	10654(6)	120(3)
C42	4096(4)	8863(5)	3225(12)	133(3)
O1	5029.5(8)	5508.5(17)	7091(3)	52.3(7)
F4	3874.2(11)	9216.3(19)	8146(4)	89.2(10)
F2	4154.5(12)	6852(2)	10560(3)	79.3(8)
C27	4165.9(17)	8525(3)	8435(5)	66.5(13)
C46	5396(6)	8764(8)	1340(10)	214(7)
O2	5782.3(10)	5105.3(16)	8340(2)	49.3(6)
F12	6755.8(14)	8792(2)	9840(3)	96.5(10)
F13	7060.2(13)	9968(2)	8250(4)	104.1(12)
C1	5976.5(13)	5277(2)	6121(3)	41.5(7)
C32	6057.5(16)	8755(2)	6658(4)	56.3(10)
C19	5267.5(14)	7207(2)	5833(4)	47.5(8)
C6	6545.9(14)	5146(2)	6143(4)	45.9(8)
C3	5933.6(17)	4921(3)	4102(4)	58.1(9)
C24	4738.4(15)	7065(3)	5449(4)	56.3(10)
C30	4763.5(14)	7112(2)	9002(4)	52.1(9)
C4	6497.9(17)	4805(3)	4095(5)	62.7(10)
C25	4934.3(14)	7570(2)	8045(4)	49.6(8)
C28	4004.5(16)	8027(3)	9346(5)	64.5(12)
C29	4303.2(17)	7322(3)	9645(4)	61.2(11)
C7	7460.3(13)	6090(3)	7253(4)	53.9(9)

C2	5679.8(14)	5151(2)	5116(4)	48.9(8)
C20	5655.6(15)	7127(2)	4962(4)	50.2(9)
C23	4607.8(17)	6884(3)	4312(5)	66.2(13)
C21	5538.2(19)	6949(3)	3829(4)	59.1(10)
C31	5901.7(13)	8112(2)	7424(4)	48.1(8)
C22	5006(2)	6825(3)	3496(4)	67.9(12)
C33	6444.0(18)	9371(3)	6923(5)	67.3(12)
C36	6145.8(15)	8169(2)	8491(4)	52.9(9)
C8	7718.6(19)	6174(3)	6061(5)	70.7(12)
C14	7005.7(16)	3436(3)	7319(7)	80.6(16)
C26	4621.6(15)	8296(3)	7819(4)	56.5(9)
C13	7372.9(13)	4209(2)	7323(4)	52.5(9)
B1	5446.1(14)	7358(2)	7180(4)	44.4(9)
C5	6788.9(15)	4906(3)	5106(4)	56.4(10)
C35	6522.8(18)	8788(3)	8786(5)	67.4(13)
C16	7778(2)	2526(3)	8045(6)	87.5(17)
C34	6673.0(18)	9382(3)	7986(5)	71.2(14)
C37	7078(2)	5456(5)	10176(5)	96.2(19)
C18	7810(2)	4128(3)	8257(6)	81.6(15)
C17	8137(2)	3305(3)	8065(7)	91.0(19)
C10	7910(2)	7729(3)	6426(7)	92.2(19)
C40	4982(4)	8914(5)	2327(8)	109(2)
C15	7337(2)	2610(3)	7141(7)	90.8(19)
C45	5168(4)	9281(5)	3334(8)	111(2)
C9	8139(2)	6899(4)	6033(6)	85.7(16)
C12	7213.4(16)	6941(3)	7615(6)	71.8(13)

Table S11. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **3c**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
Ni1	45.6(3)	59.1(4)	47.7(4)	1.2(3)	-1.1(3)	3.7(3)
S1	30.7(3)	40.5(4)	54.0(5)	1.4(4)	0.5(4)	-1.4(3)
P1	33.0(3)	57.5(5)	49.1(5)	1.1(5)	-2.2(4)	3.7(3)
F1	59.1(12)	60.9(13)	69.4(16)	5.8(12)	8.7(12)	7.8(10)
O3	34.5(9)	41.0(11)	54.5(15)	-2.0(12)	-5.7(11)	0.3(8)
F11	77.3(15)	65.4(15)	58.7(16)	2.9(12)	-10.9(13)	-5.9(12)
F10	45.5(10)	69.9(14)	64.5(14)	1.5(12)	3.9(11)	-11.6(10)
F5	80.9(16)	57.3(13)	83.2(19)	6.1(14)	-0.3(15)	18.0(12)
F7	66.1(14)	84.8(18)	119(3)	-21(2)	-47.4(18)	7.2(13)
F6	36.9(10)	84.7(17)	95(2)	-21.4(16)	-8.0(12)	3.3(11)
F15	88.1(17)	56.6(13)	69.5(16)	15.4(12)	-13.6(15)	-15.0(12)
F14	105(2)	63.0(15)	118(3)	17.3(19)	7(2)	-32.4(15)

F8	132(3)	90(2)	62.6(17)	-6.6(17)	-38.7(19)	-8.2(18)
F3	54.5(13)	109(2)	112(3)	-39(2)	17.6(16)	12.5(14)
F9	104(2)	90(2)	56.1(15)	-1.7(15)	14.2(16)	-19.9(16)
O2	44.5(11)	49.1(13)	54.3(15)	8.1(12)	1.8(12)	0.1(10)
F12	100(2)	100(2)	90(2)	-12.0(19)	-43(2)	-21.4(18)
F13	83.6(18)	79.7(18)	149(3)	-11(2)	-29(2)	-37.8(15)
C1	34.9(15)	38.6(15)	51(2)	2.4(16)	-2.3(15)	0.3(12)
C32	52.8(19)	46.1(19)	70(3)	0.0(19)	-7(2)	-0.9(16)
C19	40.9(16)	40.1(16)	61(2)	2.2(17)	-8.6(17)	-0.1(13)
C6	34.5(16)	51.1(19)	52(2)	-0.7(17)	0.1(15)	1.3(13)
C3	59(2)	64(2)	52(2)	0(2)	-14(2)	-2.6(17)
C24	43.9(18)	48.1(19)	77(3)	-4(2)	-11(2)	3.2(15)
C30	43.1(16)	51.7(19)	61(2)	-9(2)	-0.8(19)	0.2(15)
C4	57(2)	81(3)	50(2)	-8(3)	4(2)	5.1(19)
C25	41.1(16)	48.0(18)	60(2)	-9.1(19)	-3.9(17)	2.1(14)
C28	45.7(18)	73(3)	74(3)	-24(2)	6(2)	3.2(18)
C29	47.4(19)	70(3)	66(3)	-12(2)	5.6(19)	-7.5(18)
C7	36.1(14)	61(2)	64(3)	5(2)	-5.9(18)	0.2(13)
C2	40.6(16)	45.6(18)	61(2)	-0.8(18)	-8.0(18)	-0.9(14)
C20	48.7(19)	43.5(18)	58(2)	7.6(18)	-1.8(18)	-4.6(15)
C23	57(2)	54(2)	88(4)	-6(2)	-29(3)	5.0(18)
C21	72(2)	52(2)	53(2)	5.4(19)	-3(2)	-6.5(18)
C31	40.5(14)	41.4(16)	62(2)	-4.2(19)	-2.0(18)	-0.7(12)
C22	93(3)	53(2)	58(3)	2(2)	-23(3)	-3(2)
C33	59(2)	47(2)	95(4)	5(2)	6(3)	-12.7(17)
C36	49.4(17)	45.7(19)	64(2)	-3.3(19)	-6.5(19)	1.9(15)
C8	60(2)	78(3)	74(3)	6(3)	6(2)	-8(2)
C14	48.5(18)	62(2)	131(5)	4(3)	-2(3)	0.2(17)
C26	48.1(18)	53(2)	69(3)	-7(2)	-5.2(19)	3.8(15)
C13	36.7(14)	63(2)	58(2)	5(2)	1.7(17)	6.5(14)
B1	36.3(15)	41.3(17)	56(2)	0.7(18)	-1.8(17)	0.4(14)
C5	38.5(16)	77(3)	54(2)	-2(2)	-3.4(18)	6.7(16)
C35	58(2)	61(2)	83(4)	-13(2)	-20(2)	-3.6(18)
C16	89(3)	66(3)	108(4)	17(3)	6(4)	22(2)
C34	52(2)	58(2)	103(4)	-9(3)	-12(3)	-15.1(18)
C37	75(3)	154(6)	60(3)	-14(4)	-15(3)	7(4)
C18	74(3)	74(3)	97(4)	0(3)	-32(3)	15(2)
C17	67(3)	84(3)	123(5)	12(4)	-27(3)	26(2)
C10	69(3)	71(3)	136(6)	25(4)	-2(4)	-10(2)
C40	138(6)	85(4)	105(5)	16(4)	-18(5)	23(4)
C15	76(3)	62(3)	135(6)	3(3)	-10(4)	4(2)
C45	132(6)	90(4)	112(6)	13(5)	-23(5)	-6(4)
C9	62(3)	93(4)	102(5)	14(4)	7(3)	-15(3)
C12	49.3(19)	65(2)	101(4)	-7(3)	-1(3)	4.3(17)

C43	130(7)	104(5)	144(8)	14(6)	-25(7)	20(5)
C44	143(7)	118(6)	127(8)	0(6)	-31(7)	6(5)
C11	64(2)	64(3)	137(6)	-3(3)	6(3)	-3(2)
C39	82(3)	140(6)	46(3)	0(3)	8(3)	1(3)
C41	170(8)	102(5)	138(8)	-29(6)	-71(7)	27(6)
C38	96(4)	208(9)	57(3)	-25(5)	-5(3)	-18(5)
C42	111(6)	92(5)	195(11)	5(6)	-28(7)	9(4)
O1	30.6(10)	55.9(13)	70.4(18)	-0.9(14)	0.7(11)	-4.1(9)
F4	67.5(15)	75.7(16)	124(3)	-20.3(19)	-12.1(17)	31.0(13)
F2	72.2(16)	91(2)	74.5(18)	-6.9(16)	24.0(15)	-9.2(14)
C27	50.3(19)	57(2)	92(3)	-22(3)	-11(2)	16.5(18)
C46	286(16)	226(14)	130(9)	44(9)	55(11)	114(12)

Table S12. Bond Length for **3c**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ni1	P1	2.2105(12)	C30	C29	1.392(6)
Ni1	O2	1.931(3)	C4	C5	1.379(7)
Ni1	C37	1.968(6)	C25	C26	1.396(5)
Ni1	C39	2.075(5)	C25	B1	1.640(5)
Ni1	C38	1.976(7)	C28	C29	1.370(7)
S1	O3	1.515(2)	C28	C27	1.368(8)
S1	O2	1.466(3)	C29	F2	1.339(6)
S1	C1	1.771(4)	C7	C8	1.522(7)
S1	O1	1.426(2)	C7	C12	1.521(6)
P1	C6	1.846(4)	C20	C21	1.370(6)
P1	C7	1.853(4)	C23	C22	1.361(8)
P1	C13	1.856(4)	C21	C22	1.377(7)
F1	C30	1.344(5)	C31	C36	1.375(6)
O3	B1	1.580(4)	C31	B1	1.652(5)
F11	C36	1.346(5)	C33	C34	1.351(8)
F10	C20	1.354(4)	C36	C35	1.383(6)
F5	C26	1.347(6)	C8	C9	1.537(7)
F7	C23	1.349(5)	C14	C13	1.510(6)
F6	C24	1.344(5)	C14	C15	1.541(6)
F15	C32	1.340(5)	C26	C27	1.375(6)
F14	C33	1.343(6)	C13	C18	1.527(6)
F8	C22	1.333(6)	C35	C34	1.363(7)
F3	C28	1.347(5)	C16	C17	1.507(8)
F9	C21	1.343(5)	C16	C15	1.512(9)
F12	C35	1.347(6)	C37	C38	1.321(9)
F13	C34	1.356(5)	C18	C17	1.535(7)
C1	C6	1.414(5)	C10	C9	1.488(8)

C1	C2	1.386(6)	C10	C11	1.520(10)
C32	C31	1.394(6)	C40	C45	1.376(12)
C32	C33	1.387(6)	C40	C41	1.397(13)
C19	C24	1.391(5)	C40	C46	1.546(14)
C19	C20	1.391(6)	C45	C44	1.357(13)
C19	B1	1.635(6)	C12	C11	1.535(6)
C6	C5	1.391(6)	C43	C44	1.333(12)
C3	C4	1.398(6)	C43	C42	1.345(13)
C3	C2	1.376(7)	C39	C38	1.301(10)
C24	C23	1.382(7)	C41	C42	1.392(15)
C30	C25	1.384(6)	F4	C27	1.340(5)

Table S13. Bond Angles for **3c**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Ni1	P1	96.32(9)	C22	C23	C24	120.4(4)
O2	Ni1	C37	164.7(2)	F9	C21	C20	120.8(4)
O2	Ni1	C39	92.56(19)	F9	C21	C22	119.4(4)
O2	Ni1	C38	127.0(2)	C20	C21	C22	119.7(5)
C37	Ni1	P1	98.71(19)	C32	C31	B1	126.4(4)
C37	Ni1	C39	72.3(3)	C36	C31	C32	113.8(3)
C37	Ni1	C38	39.1(3)	C36	C31	B1	119.7(4)
C39	Ni1	P1	170.37(19)	F8	C22	C23	121.0(5)
C38	Ni1	P1	135.2(2)	F8	C22	C21	120.4(5)
C38	Ni1	C39	37.4(3)	C23	C22	C21	118.6(4)
O3	S1	C1	105.41(15)	F14	C33	C32	119.9(5)
O2	S1	O3	106.93(16)	F14	C33	C34	120.4(4)
O2	S1	C1	107.86(15)	C34	C33	C32	119.7(5)
O1	S1	O3	113.05(14)	F11	C36	C31	120.3(3)
O1	S1	O2	114.29(16)	F11	C36	C35	115.8(4)
O1	S1	C1	108.82(17)	C31	C36	C35	123.9(4)
C6	P1	Ni1	112.85(12)	C7	C8	C9	111.3(5)
C6	P1	C7	107.34(18)	C13	C14	C15	111.0(4)
C6	P1	C13	100.83(18)	F5	C26	C25	118.3(4)
C7	P1	Ni1	114.38(15)	F5	C26	C27	117.2(4)
C7	P1	C13	105.65(16)	C27	C26	C25	124.3(5)
C13	P1	Ni1	114.62(14)	C14	C13	P1	110.8(2)
S1	O3	B1	127.7(2)	C14	C13	C18	110.8(4)
S1	O2	Ni1	122.39(16)	C18	C13	P1	112.6(3)
C6	C1	S1	123.5(3)	O3	B1	C19	106.0(3)
C2	C1	S1	115.6(3)	O3	B1	C25	111.7(3)
C2	C1	C6	121.0(4)	O3	B1	C31	102.5(2)

F15	C32	C31	121.2(4)	C19	B1	C25	113.9(3)
F15	C32	C33	115.5(4)	C19	B1	C31	116.6(3)
C33	C32	C31	123.3(4)	C25	B1	C31	105.7(3)
C24	C19	C20	113.3(4)	C4	C5	C6	122.6(3)
C24	C19	B1	125.3(4)	F12	C35	C36	120.7(5)
C20	C19	B1	121.2(3)	F12	C35	C34	119.7(4)
C1	C6	P1	124.4(3)	C34	C35	C36	119.5(5)
C5	C6	P1	118.9(3)	C17	C16	C15	111.0(5)
C5	C6	C1	116.6(4)	F13	C34	C35	119.9(5)
C2	C3	C4	119.2(4)	C33	C34	F13	120.4(5)
F6	C24	C19	121.2(4)	C33	C34	C35	119.7(4)
F6	C24	C23	115.1(4)	C38	C37	Ni1	70.7(4)
C23	C24	C19	123.6(4)	C13	C18	C17	109.6(5)
F1	C30	C25	121.3(3)	C16	C17	C18	112.0(4)
F1	C30	C29	115.3(4)	C9	C10	C11	110.8(5)
C25	C30	C29	123.4(4)	C45	C40	C41	117.2(9)
C5	C4	C3	119.6(5)	C45	C40	C46	118.0(10)
C30	C25	C26	113.9(4)	C41	C40	C46	124.8(10)
C30	C25	B1	127.9(3)	C16	C15	C14	111.1(5)
C26	C25	B1	118.2(4)	C44	C45	C40	119.9(9)
F3	C28	C29	120.0(5)	C10	C9	C8	112.6(4)
F3	C28	C27	120.2(4)	C7	C12	C11	110.2(3)
C27	C28	C29	119.9(4)	C44	C43	C42	117.4(11)
C28	C29	C30	119.4(5)	C43	C44	C45	124.1(10)
F2	C29	C30	120.9(4)	C10	C11	C12	111.0(5)
F2	C29	C28	119.7(4)	C38	C39	Ni1	67.2(4)
C8	C7	P1	116.9(3)	C42	C41	C40	119.7(9)
C12	C7	P1	111.0(3)	C37	C38	Ni1	70.1(4)
C12	C7	C8	109.9(4)	C39	C38	Ni1	75.4(4)
C3	C2	C1	120.9(3)	C39	C38	C37	130.9(9)
F10	C20	C19	118.9(4)	C43	C42	C41	121.6(9)
F10	C20	C21	116.6(4)	C28	C27	C26	119.0(4)
C21	C20	C19	124.4(4)	F4	C27	C28	119.8(4)
F7	C23	C24	119.0(5)	F4	C27	C26	121.1(5)
F7	C23	C22	120.6(5)				

Table S14. Torsion Angles for **3c**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ni1	P1	C6	C1	9.3(3)	C30	C25	C26	C27	-3.5(6)
Ni1	P1	C6	C5	-166.5(3)	C30	C25	B1	O3	-0.4(5)
Ni1	P1	C7	C8	-167.0(3)	C30	C25	B1	C19	119.6(4)
Ni1	P1	C7	C12	-39.9(4)	C30	C25	B1	C31	-111.1(4)
Ni1	P1	C13	C14	60.6(4)	C4	C3	C2	C1	0.7(6)
Ni1	P1	C13	C18	-64.2(4)	C25	C30	C29	C28	-1.5(7)
Ni1	C37	C38	C39	48.1(9)	C25	C30	C29	F2	179.5(4)
Ni1	C39	C38	C37	-46.3(8)	C25	C26	C27	C28	1.1(7)
S1	O3	B1	C19	-45.2(4)	C25	C26	C27	F4	-177.7(4)
S1	O3	B1	C25	79.4(4)	C29	C30	C25	C26	3.7(6)
S1	O3	B1	C31	-167.9(3)	C29	C30	C25	B1	-176.3(4)
S1	C1	C6	P1	5.2(5)	C29	C28	C27	C26	1.4(7)
S1	C1	C6	C5	-178.8(3)	C29	C28	C27	F4	-179.8(4)
S1	C1	C2	C3	178.1(3)	C7	P1	C6	C1	-117.6(3)
P1	C6	C5	C4	176.8(4)	C7	P1	C6	C5	66.5(4)
P1	C7	C8	C9	-176.8(3)	C7	P1	C13	C14	-172.5(4)
P1	C7	C12	C11	171.3(4)	C7	P1	C13	C18	62.7(4)
P1	C13	C18	C17	-178.2(4)	C7	C8	C9	C10	-54.5(7)
F1	C30	C25	C26	-175.4(4)	C7	C12	C11	C10	58.4(6)
F1	C30	C25	B1	4.6(6)	C2	C1	C6	P1	-174.5(3)
F1	C30	C29	C28	177.6(4)	C2	C1	C6	C5	1.5(5)
F1	C30	C29	F2	-1.4(6)	C2	C3	C4	C5	1.3(7)
O3	S1	O2	Ni1	-40.7(2)	C20	C19	C24	F6	176.3(3)
O3	S1	C1	C6	70.1(3)	C20	C19	C24	C23	-1.6(6)
O3	S1	C1	C2	-110.2(3)	C20	C19	B1	O3	-65.0(4)
F11	C36	C35	F12	1.1(6)	C20	C19	B1	C25	171.8(3)
F11	C36	C35	C34	178.9(4)	C20	C19	B1	C31	48.3(5)
F10	C20	C21	F9	-1.9(6)	C20	C21	C22	F8	-179.2(4)
F10	C20	C21	C22	175.9(4)	C20	C21	C22	C23	0.0(7)
F5	C26	C27	C28	177.4(4)	C31	C32	C33	F14	178.2(4)
F5	C26	C27	F4	-1.4(6)	C31	C32	C33	C34	-2.5(7)
F7	C23	C22	F8	-0.1(7)	C31	C36	C35	F12	-178.4(4)
F7	C23	C22	C21	-179.2(4)	C31	C36	C35	C34	-0.6(7)
F6	C24	C23	F7	2.1(6)	C33	C32	C31	C36	3.2(6)
F6	C24	C23	C22	-177.2(4)	C33	C32	C31	B1	179.9(4)
F15	C32	C31	C36	-176.5(4)	C36	C31	B1	O3	-52.5(4)
F15	C32	C31	B1	0.3(6)	C36	C31	B1	C19	-167.8(3)
F15	C32	C33	F14	-2.1(7)	C36	C31	B1	C25	64.5(4)
F15	C32	C33	C34	177.1(4)	C36	C35	C34	F13	-177.1(4)
F14	C33	C34	F13	-2.2(7)	C36	C35	C34	C33	1.4(7)
F14	C33	C34	C35	179.3(5)	C8	C7	C12	C11	-57.8(6)

F3	C28	C29	C30	179.5(4)	C14	C13	C18	C17	57.0(6)
F3	C28	C29	F2	-1.6(7)	C26	C25	B1	O3	179.6(3)
F3	C28	C27	C26	-179.2(4)	C26	C25	B1	C19	-60.4(4)
F3	C28	C27	F4	-0.4(7)	C26	C25	B1	C31	68.9(4)
F9	C21	C22	F8	-1.3(7)	C13	P1	C6	C1	132.1(3)
F9	C21	C22	C23	177.8(4)	C13	P1	C6	C5	-43.8(4)
O2	S1	O3	B1	-147.0(3)	C13	P1	C7	C8	66.0(4)
O2	S1	C1	C6	-43.9(3)	C13	P1	C7	C12	-166.9(3)
O2	S1	C1	C2	135.8(3)	C13	C14	C15	C16	55.8(8)
F12	C35	C34	F13	0.7(7)	C13	C18	C17	C16	-56.6(7)
F12	C35	C34	C33	179.2(5)	B1	C19	C24	F6	2.3(6)
C1	S1	O3	B1	98.4(3)	B1	C19	C24	C23	-175.6(4)
C1	S1	O2	Ni1	72.2(2)	B1	C19	C20	F10	-0.8(5)
C1	C6	C5	C4	0.6(6)	B1	C19	C20	C21	175.9(4)
C32	C31	C36	F11	178.9(3)	B1	C25	C26	F5	0.2(5)
C32	C31	C36	C35	-1.6(6)	B1	C25	C26	C27	176.5(4)
C32	C31	B1	O3	130.9(4)	B1	C31	C36	F11	2.0(5)
C32	C31	B1	C19	15.6(5)	B1	C31	C36	C35	-178.6(4)
C32	C31	B1	C25	-112.0(4)	C17	C16	C15	C14	-54.8(7)
C32	C33	C34	F13	178.5(4)	C40	C45	C44	C43	-0.9(13)
C32	C33	C34	C35	0.1(7)	C40	C41	C42	C43	3.2(13)
C19	C24	C23	F7	-179.9(4)	C15	C14	C13	P1	177.0(5)
C19	C24	C23	C22	0.9(7)	C15	C14	C13	C18	-57.1(7)
C19	C20	C21	F9	-178.7(4)	C15	C16	C17	C18	55.9(8)
C19	C20	C21	C22	-0.9(6)	C45	C40	C41	C42	-1.1(11)
C6	P1	C7	C8	-41.0(3)	C9	C10	C11	C12	-56.3(6)
C6	P1	C7	C12	86.1(4)	C12	C7	C8	C9	55.5(5)
C6	P1	C13	C14	-60.9(4)	C44	C43	C42	C41	-4.0(13)
C6	P1	C13	C18	174.3(4)	C11	C10	C9	C8	54.3(7)
C6	C1	C2	C3	-2.2(6)	C41	C40	C45	C44	0.0(11)
C3	C4	C5	C6	-2.0(7)	C42	C43	C44	C45	2.9(14)
C24	C19	C20	F10	-175.1(3)	O1	S1	O3	B1	-20.4(3)
C24	C19	C20	C21	1.6(6)	O1	S1	O2	Ni1	-166.61(18)
C24	C19	B1	O3	108.6(4)	O1	S1	C1	C6	-168.4(3)
C24	C19	B1	C25	-14.6(5)	O1	S1	C1	C2	11.3(3)
C24	C19	B1	C31	-138.1(4)	C27	C28	C29	C30	-1.2(7)
C24	C23	C22	F8	179.1(4)	C27	C28	C29	F2	177.8(4)
C24	C23	C22	C21	0.0(7)	C46	C40	C45	C44	179.7(8)
C30	C25	C26	F5	-179.7(3)	C46	C40	C41	C42	179.2(8)

Table S15. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3c**.

Atom	x	y	z	U(eq)
H3	5732	4844	3429	70
H4	6676	4661	3412	75
H7	7760	5982	7792	65
H2	5304	5222	5128	59
H8A	7437	6285	5493	85
H8B	7895	5640	5858	85
H14A	6740	3492	6703	97
H14B	6811	3404	8047	97
H13	7559	4228	6574	63
H5	7162	4809	5094	68
H16A	7613	2448	8800	105
H16B	7998	2025	7880	105
H37A	7242	4941	10486	115
H37B	7340	5901	9999	115
H18A	7640	4114	9014	98
H18B	8051	4618	8227	98
H17A	8332	3346	7337	109
H17B	8404	3246	8678	109
H10A	7638	7923	5876	111
H10B	8197	8154	6457	111
H15A	7095	2121	7186	109
H15B	7501	2616	6377	109
H45	5533	9428	3407	134
H9A	8444	6748	6525	103
H9B	8275	6963	5250	103
H12A	7058	6889	8382	86
H12B	6924	7094	7083	86
H43	4058	9379	4799	151
H44	4955	9668	4894	155
H11A	7488	8180	7837	106
H11B	7930	7501	8178	106
H39A	5828	5698	10815	107
H39B	6124	4797	11124	107
H41	4284	8467	1605	164
H38	6590	6327	10721	144
H42	3733	8698	3197	159
H46A	5213	8511	690	321
H46B	5678	8388	1604	321
H46C	5552	9300	1113	321