Supporting Information for:

Ethylene Polymerization by Salicylaldimine Nickel(II) Complexes Containing Dibenzhydryl Moiety

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Content

^{1}H NMR, ^{13}C NMR, ^{31}P NMR of the ligands.

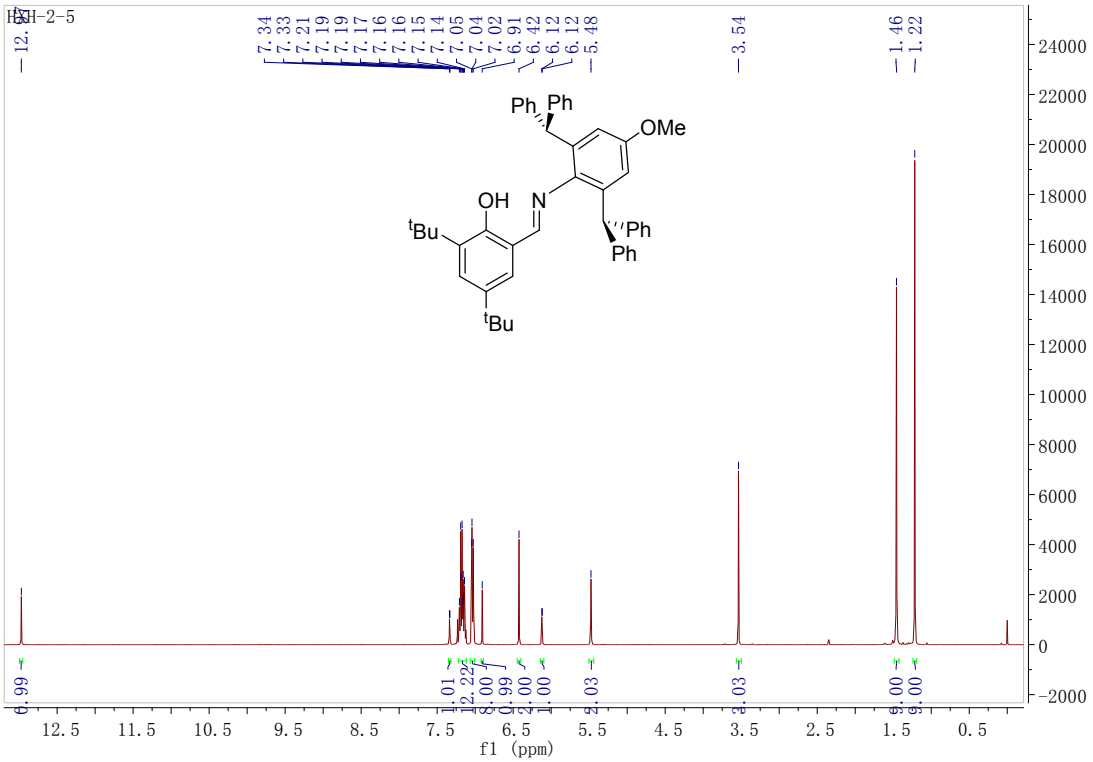

Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, ppm) of $\mathbf{L_1}$.

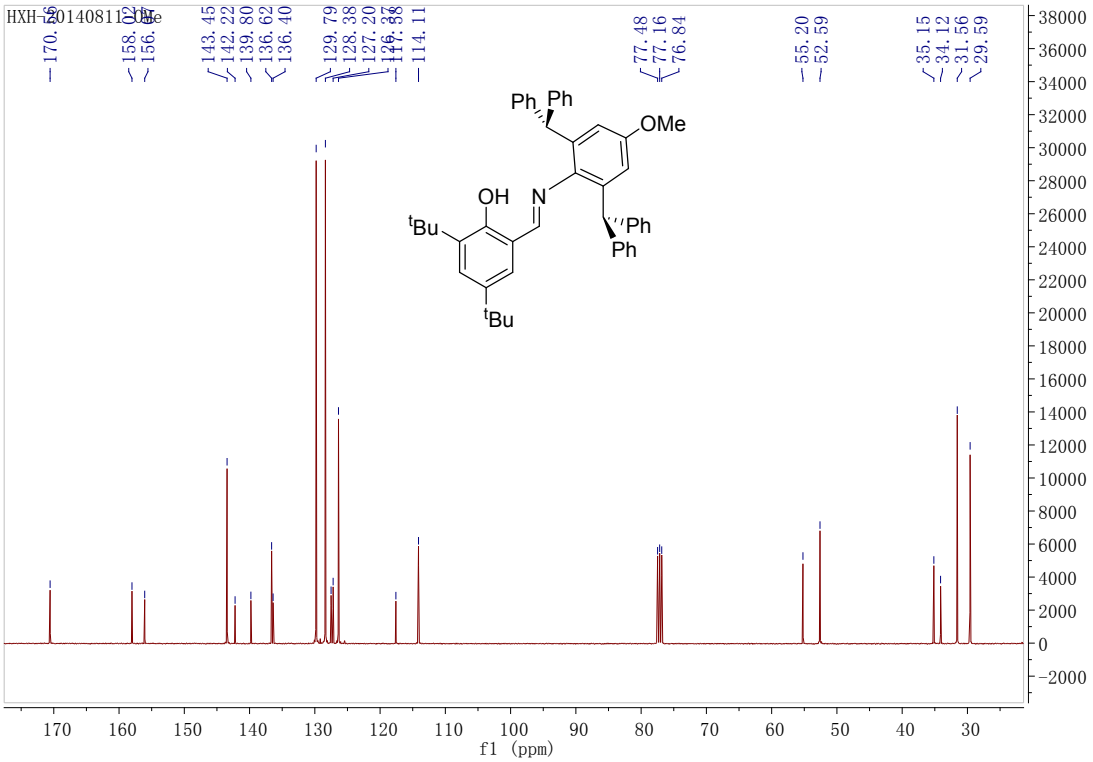

Figure S2. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, ppm) of $\mathbf{L_1}$.

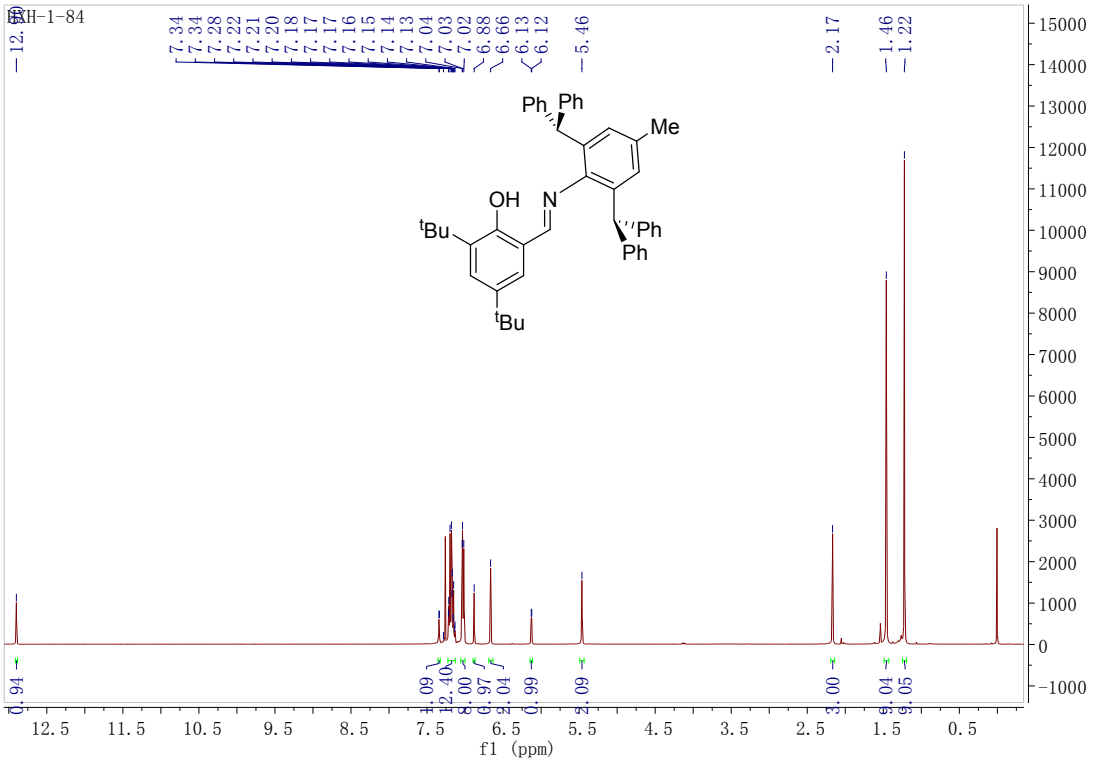

Figure S3. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, ppm) of $\mathbf{L_2}$.

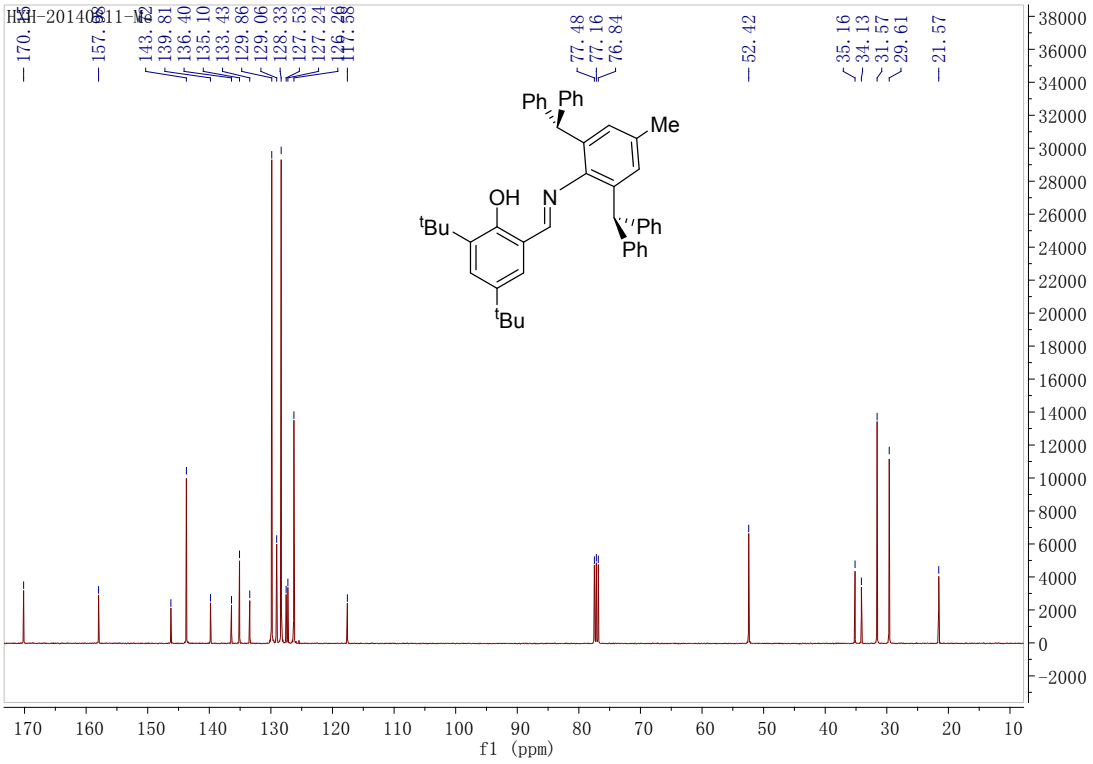

Figure S4. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, ppm) of $\mathbf{L_2}$.

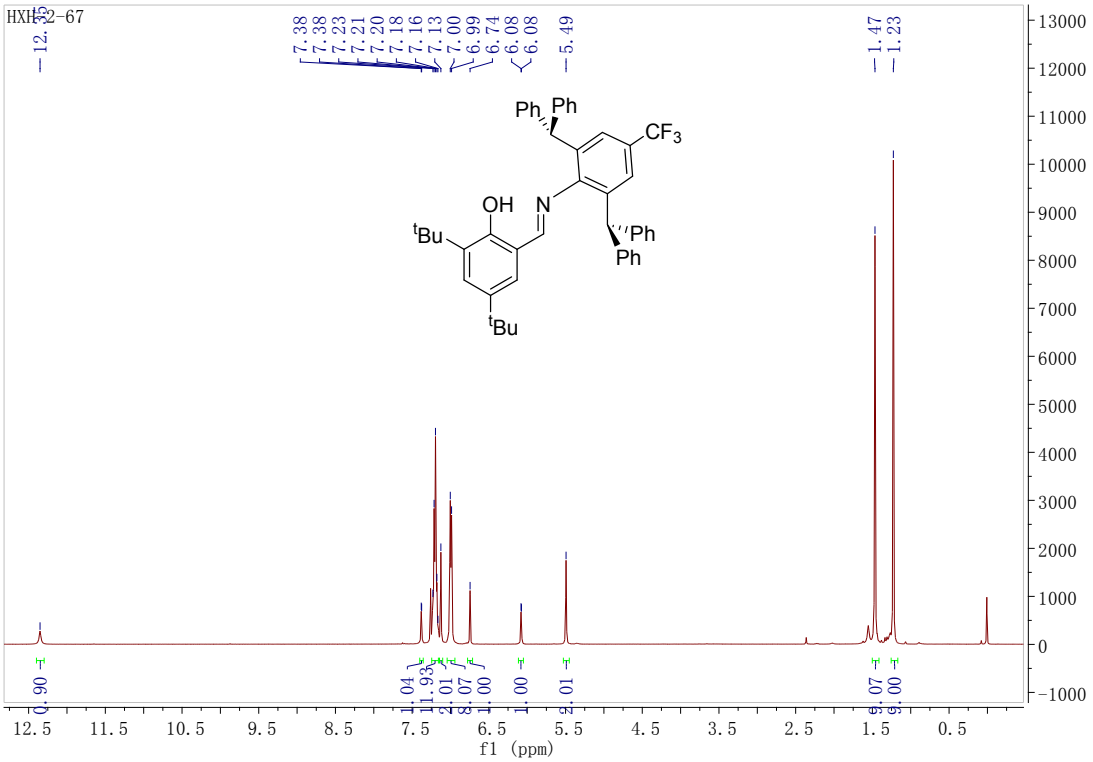

Figure S5. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, ppm) of $\mathbf{L_4}$.

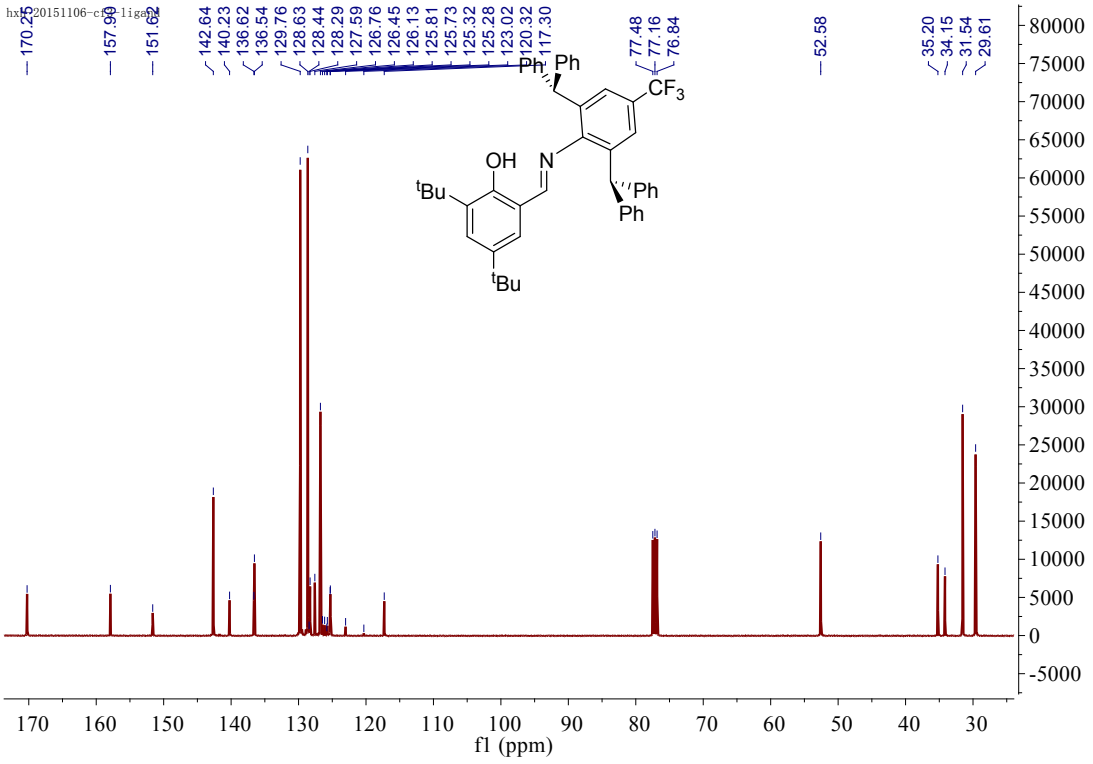

Figure S6. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, ppm) of $\mathbf{L_4}$.

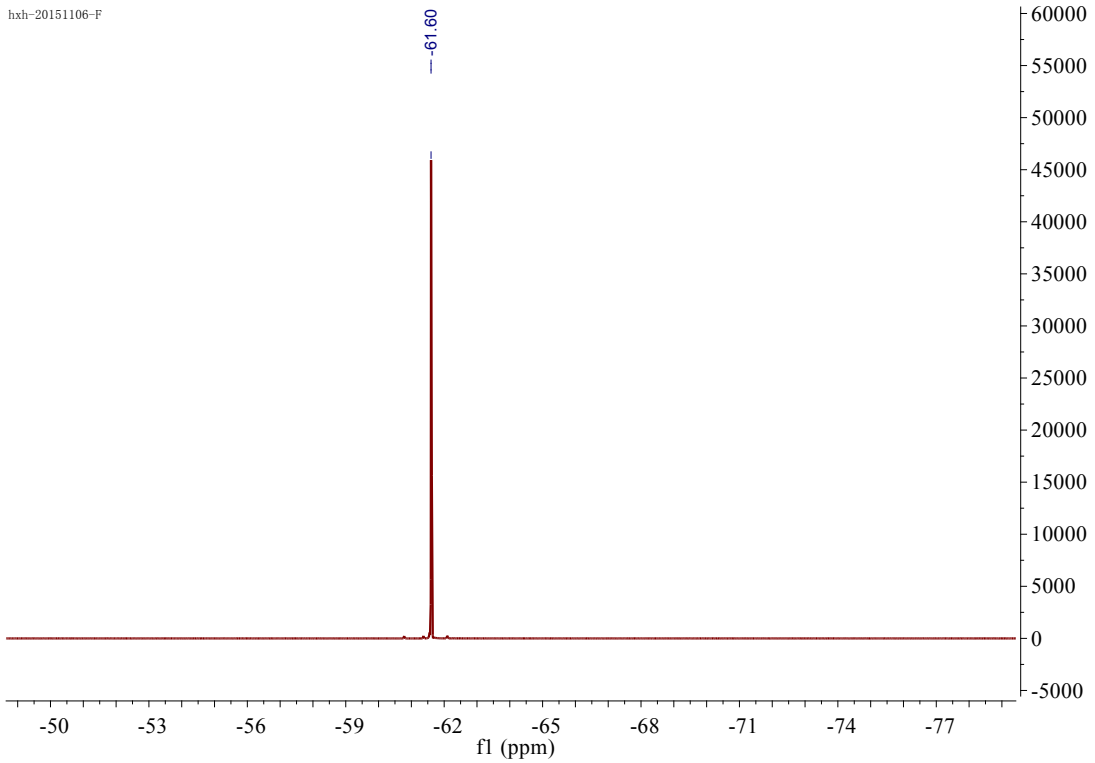

Figure S7. ^{19}F NMR spectrum (282 MHz, $CDCl_3$, ppm) of $\mathbf{L_4}$.

^{1}H NMR, ^{13}C NMR, ^{31}P NMR of the Nickel(II) Complexes.

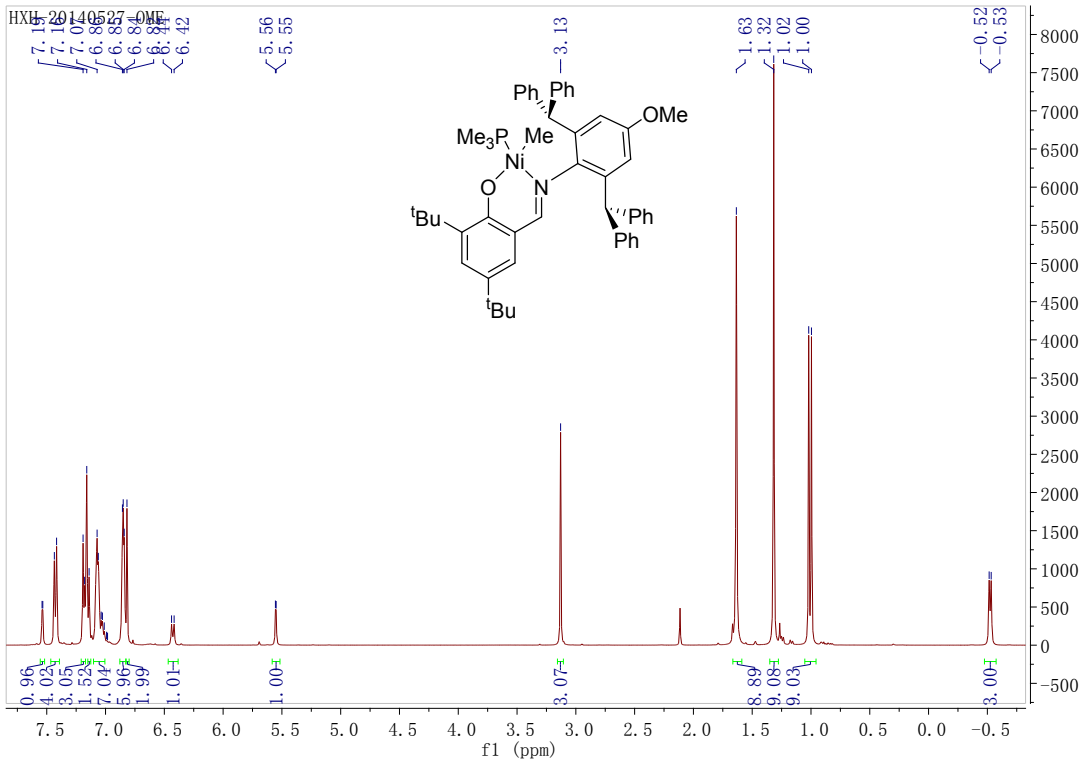

Figure S8. ^{1}H NMR spectrum（400 MHz, C_6D_6, ppm）of **1**.

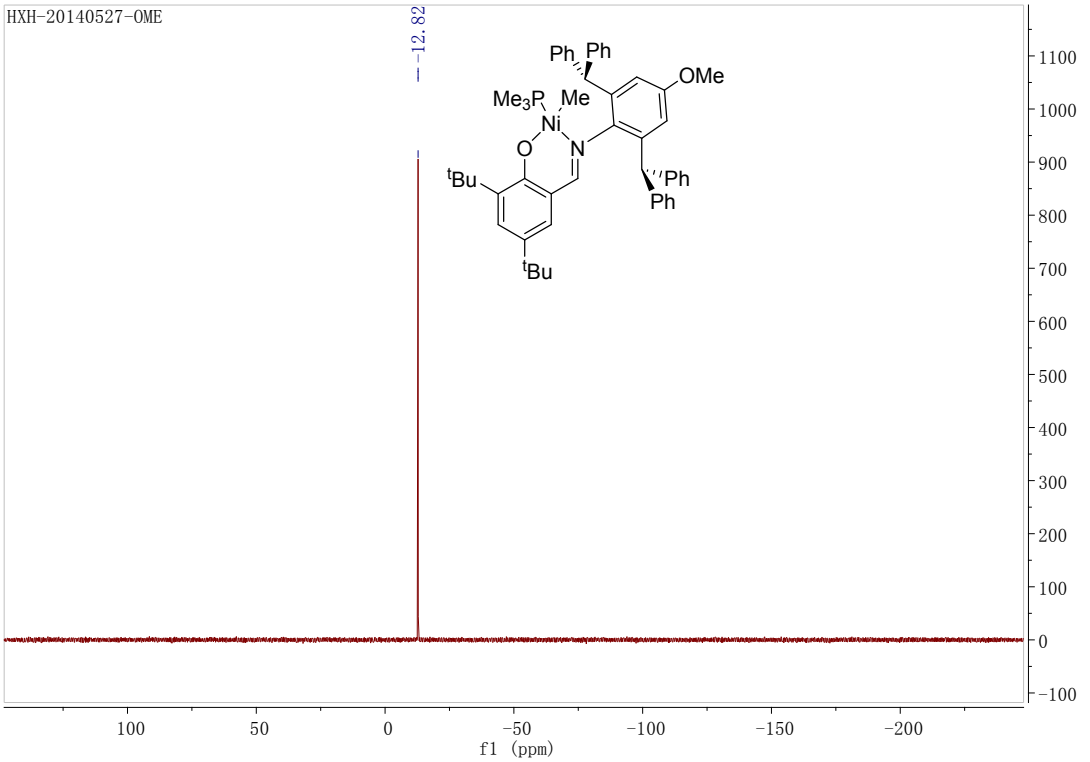

Figure S9. ^{31}P NMR spectrum（162 MHz, C_6D_6, ppm）of **1**.

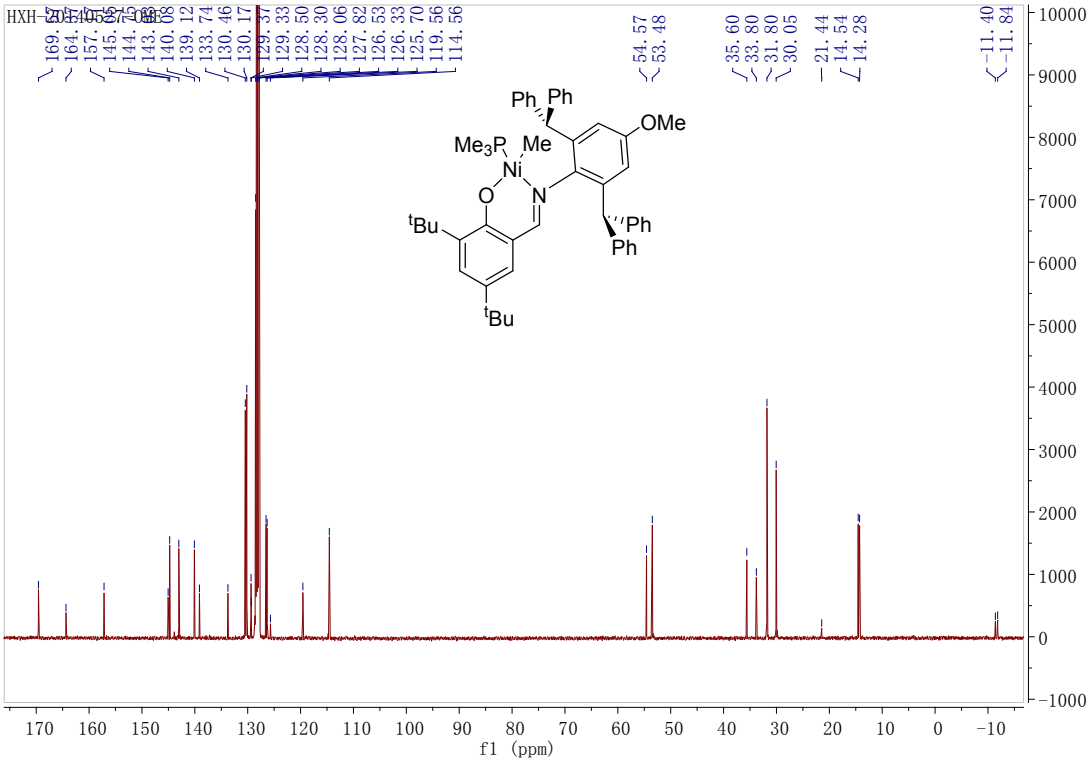

Figure S10. ^{13}C NMR spectrum (100 MHz, C_6D_6, ppm) of **1**.

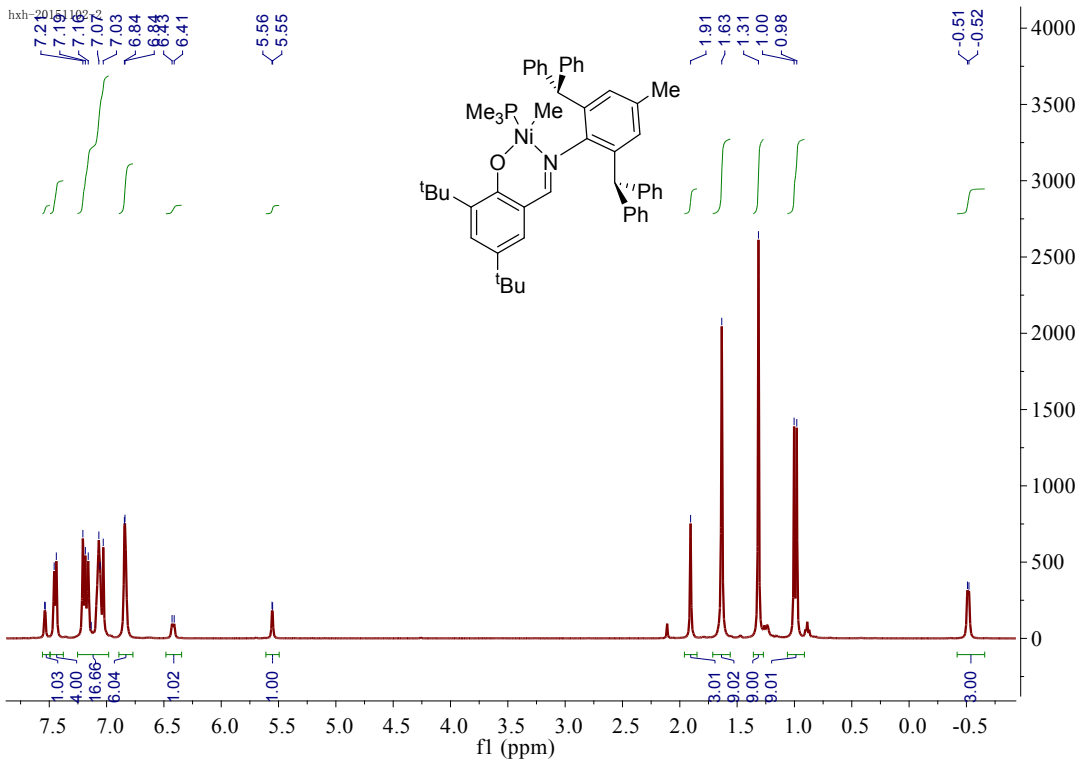

Figure S11. ^{1}H NMR spectrum（400 MHz, C_6D_6, ppm）of **2**.

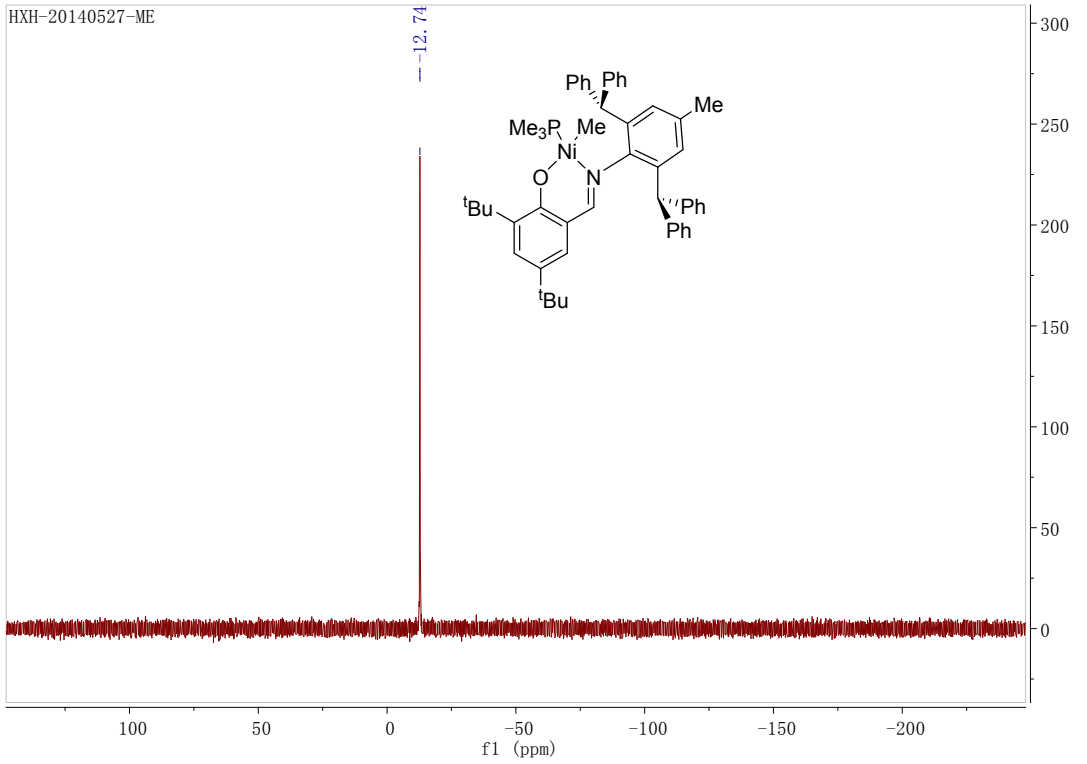

Figure S12. ^{31}P NMR spectrum (162 MHz, C_6D_6, ppm) of **2**.

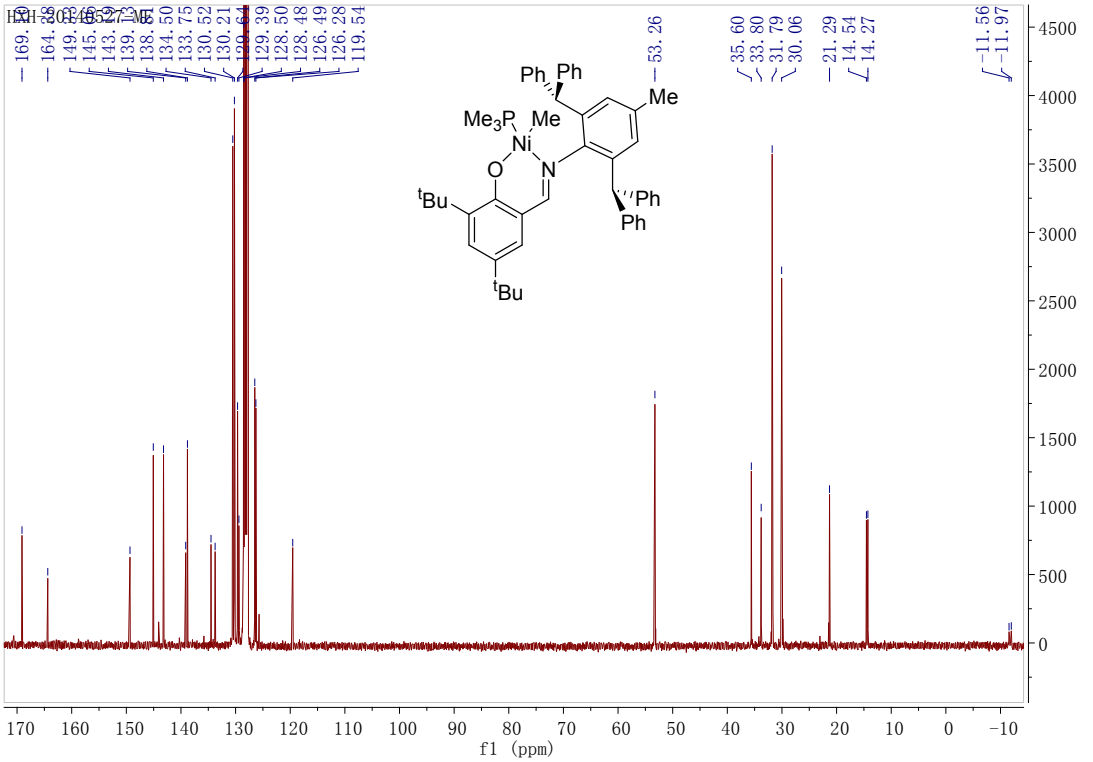

Figure S13. ^{13}C NMR spectrum (100 MHz, C_6D_6, ppm) of **2**.

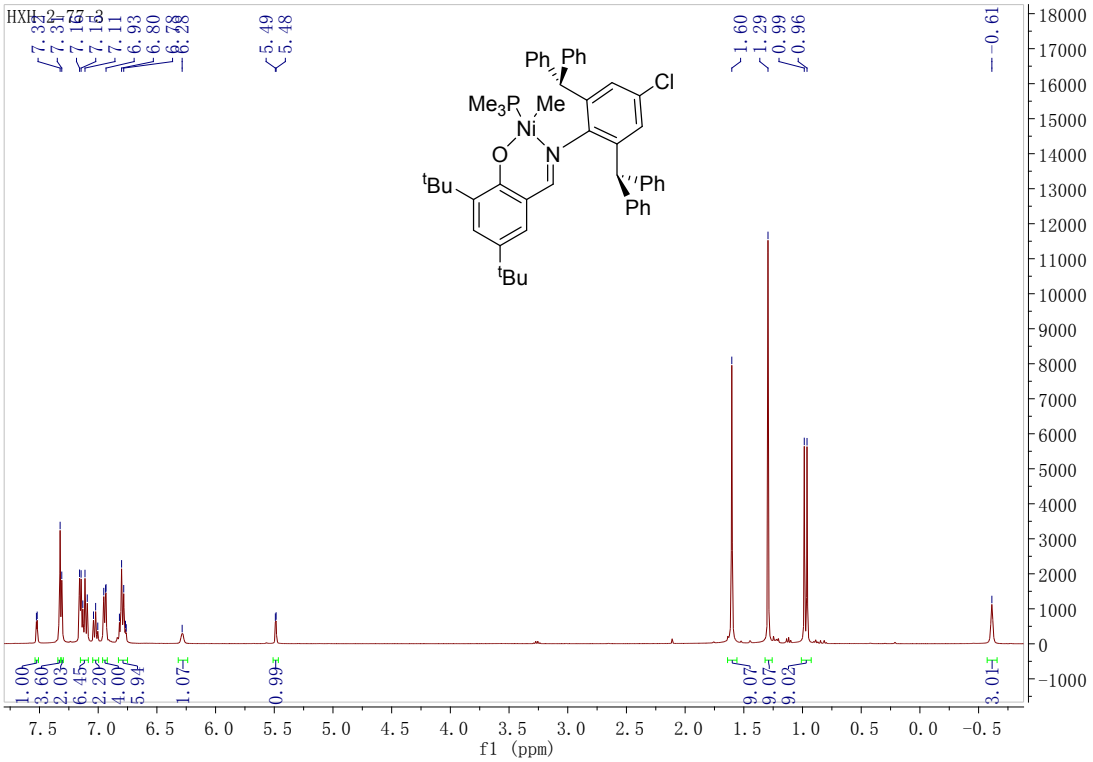

Figure S14. ^{1}H NMR spectrum (400 MHz, C_6D_6, ppm) of **3**.

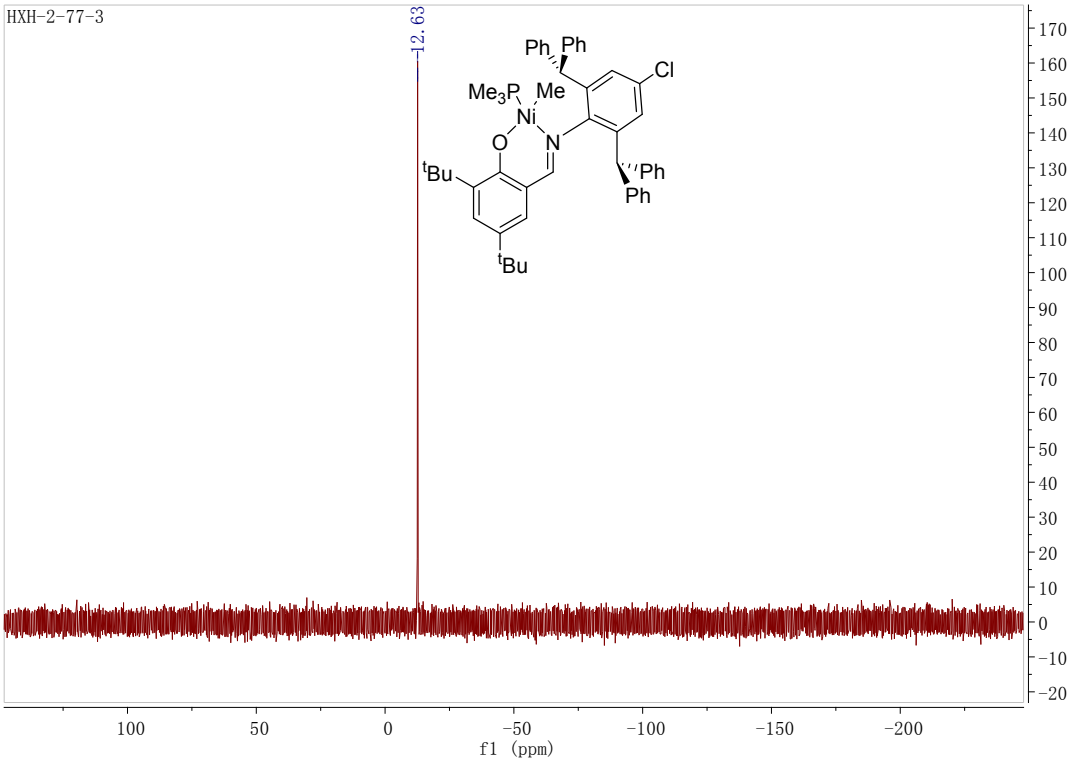

Figure S15. ^{31}P NMR spectrum (162 MHz, C_6D_6, ppm) of **3**.

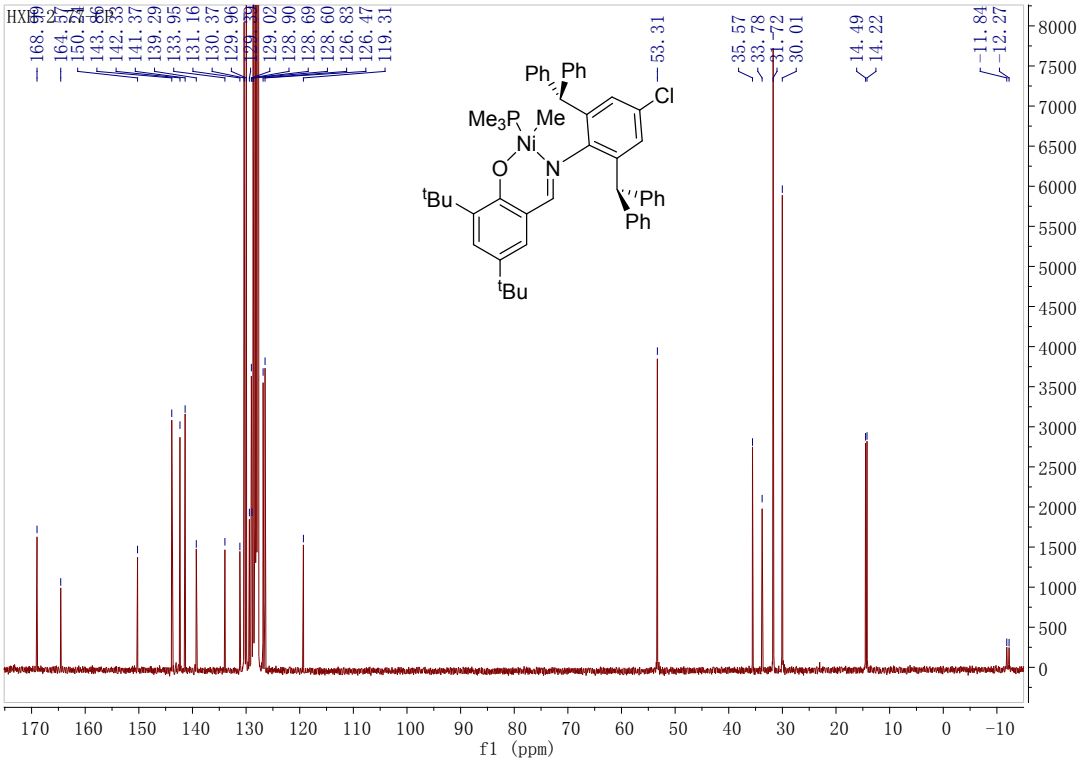

Figure S16. ^{13}C NMR spectrum (100 MHz, C_6D_6, ppm) of **3**.

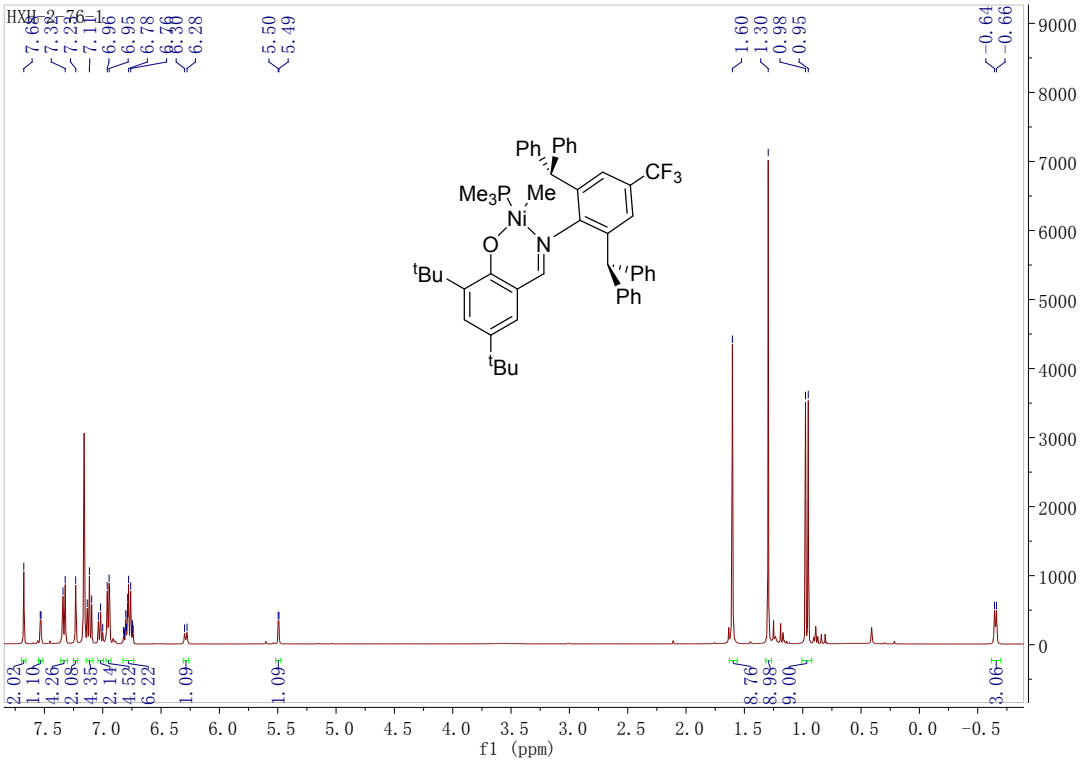

Figure S17. ^{1}H NMR spectrum (400 MHz, C_6D_6, ppm) of **4**.

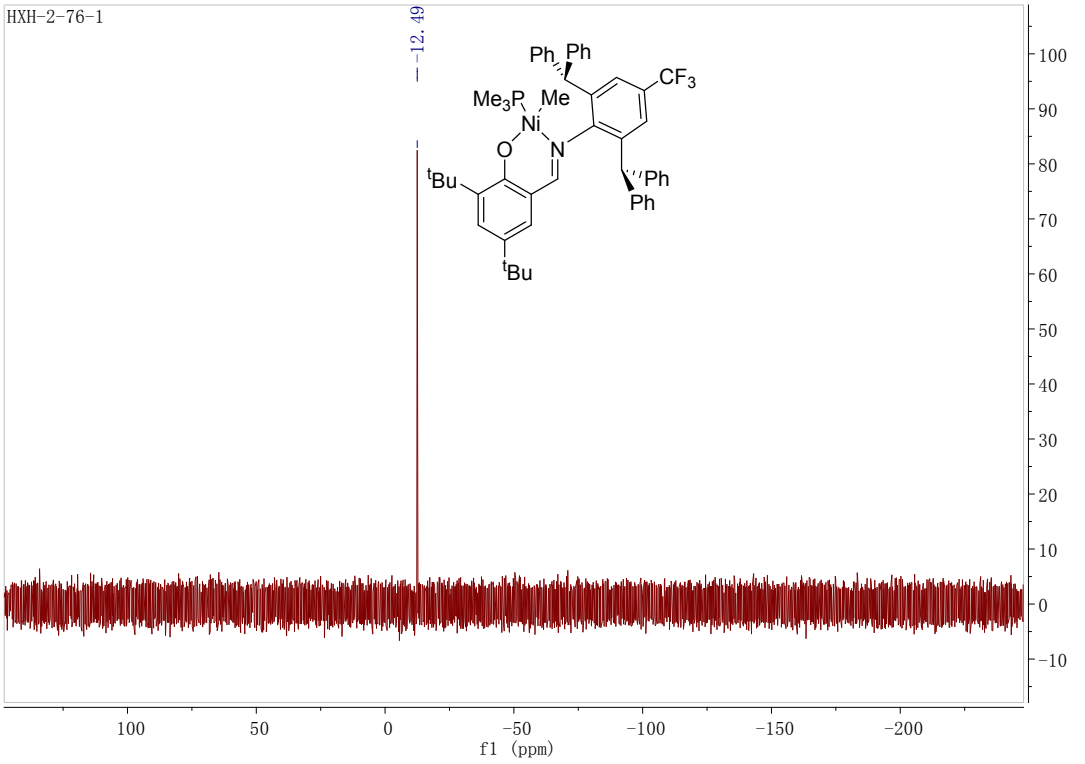

Figure S18. ^{31}P NMR spectrum (162 MHz, C_6D_6, ppm) of **4**.

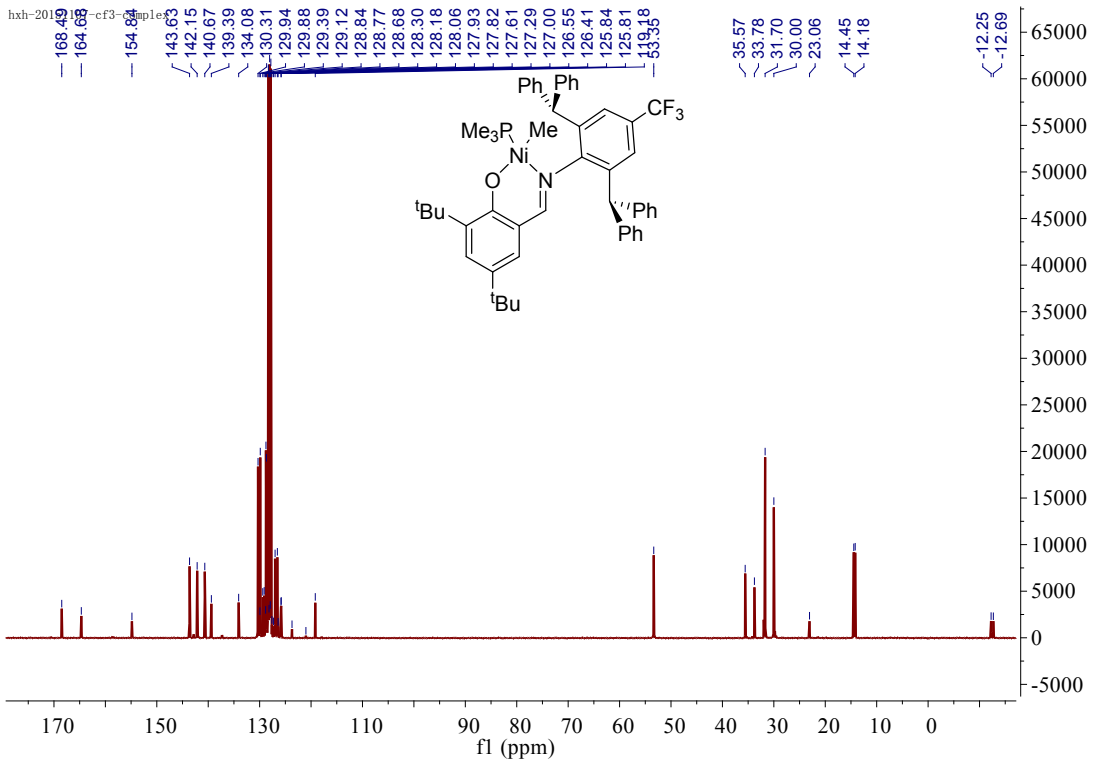

Figure S19. ^{13}C NMR spectrum (100 MHz, C_6D_6, ppm) of **4**.

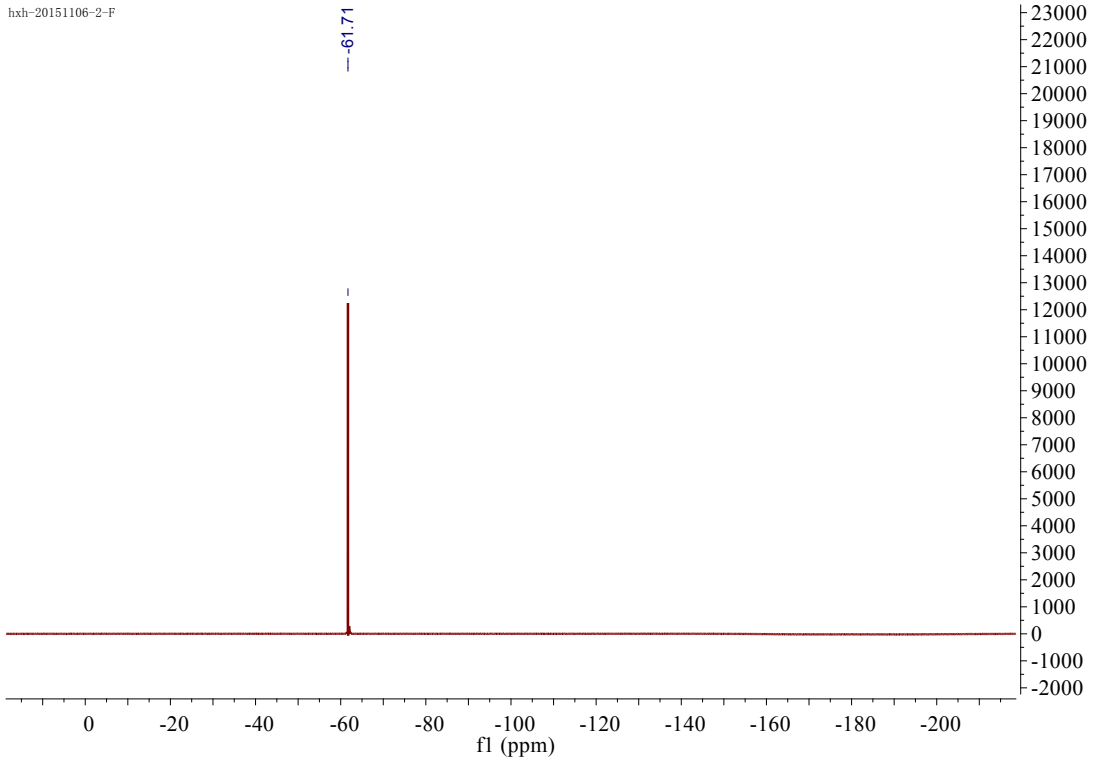

Figure S20. ^{19}F NMR spectrum (282 MHz, C_6D_6, ppm) of **4**.

^{1}H NMR, ^{13}C NMR of the Polyethylene.

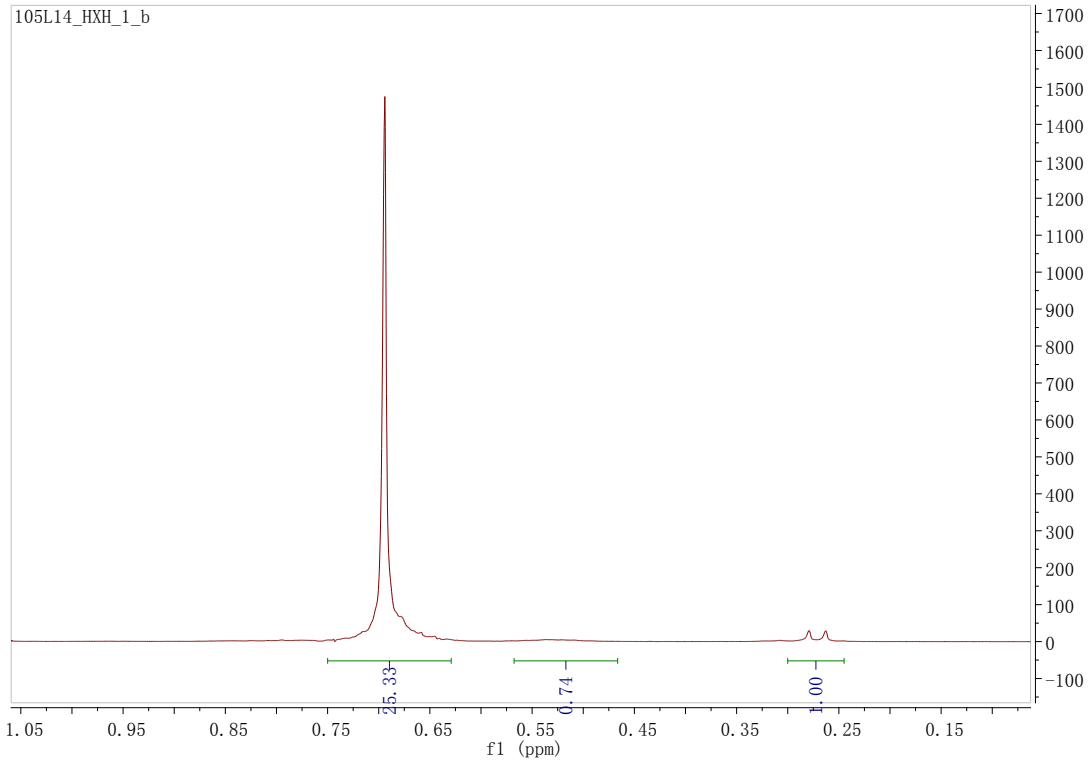

Figure S21. ^{1}H NMR spectrum (400 MHz, d^{2}-1,1,2,2-Tetrachloroethane, 100 °C, ppm) of polyethylene generated by complex **1** at 25°C.

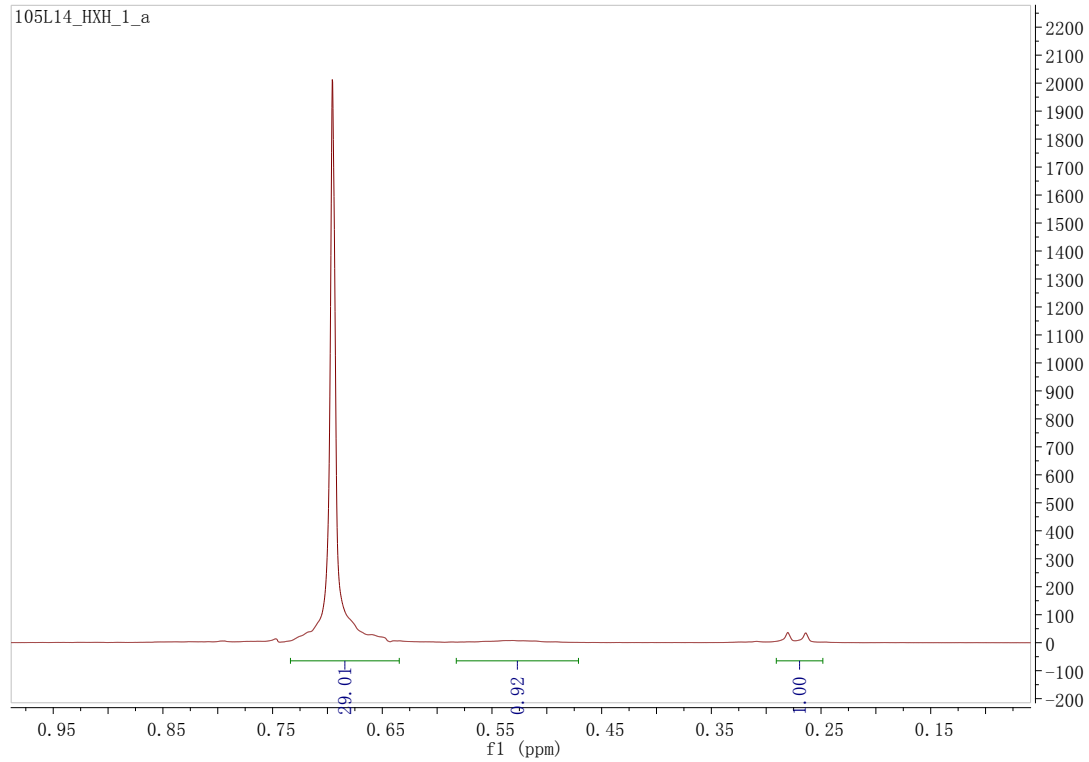

Figure S22. ^{1}H NMR spectrum (400 MHz, d^{2}-1,1,2,2-Tetrachloroethane, 100 °C, ppm) of polyethylene generated by complex **2** at 25 °C.

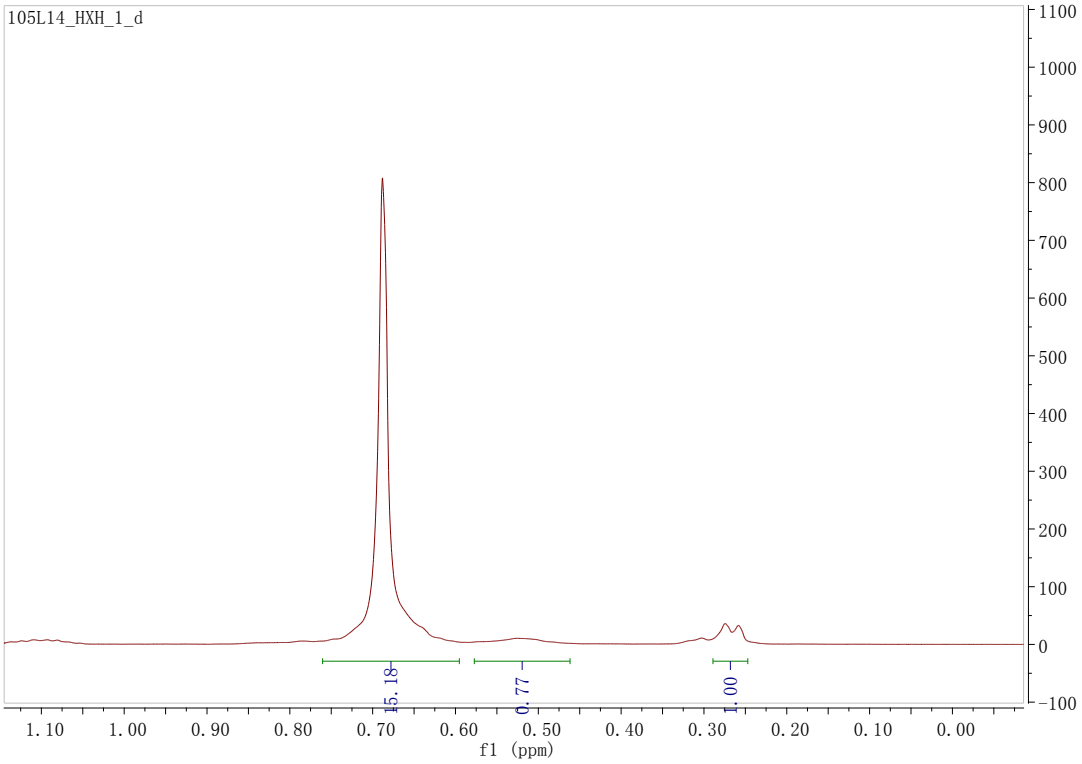

Figure S23. ^{1}H NMR spectrum (400 MHz, d^2-1,1,2,2-Tetrachloroethane, 100 °C, ppm) of polyethylene generated by complex **3** at 25 °C.

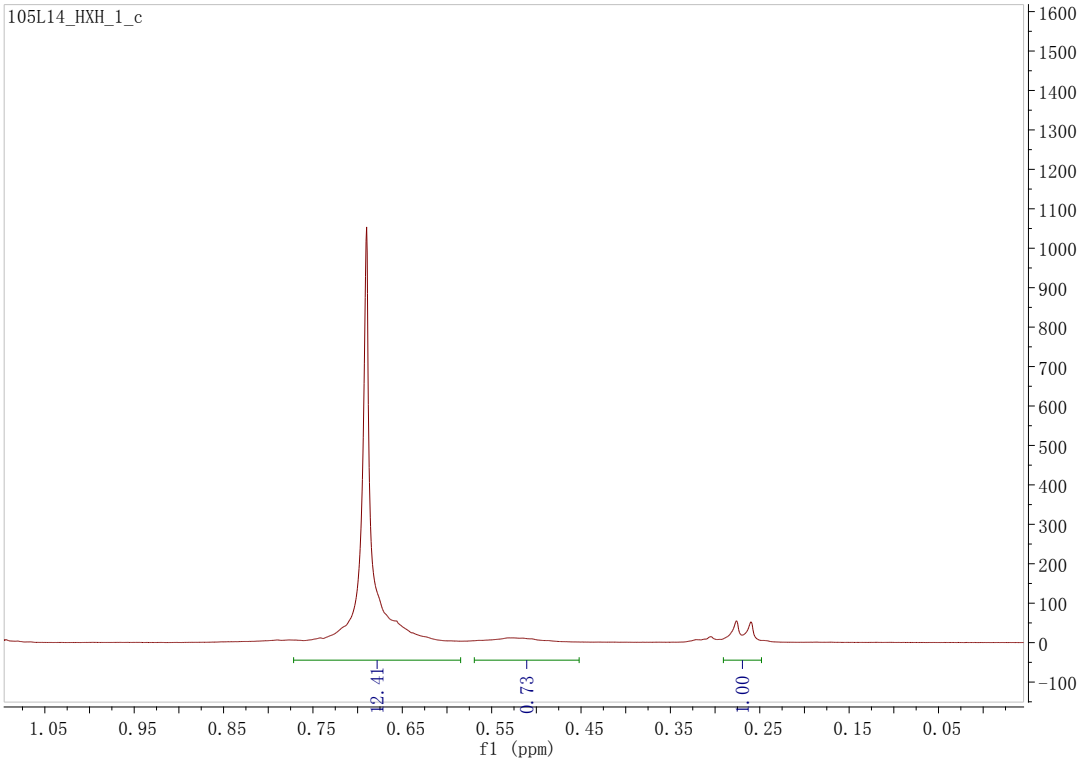

Figure S24. ^{1}H NMR spectrum (400 MHz, d^2-1,1,2,2-Tetrachloroethane, 100 °C, ppm) of polyethylene generated by complex **4** at 25 °C.

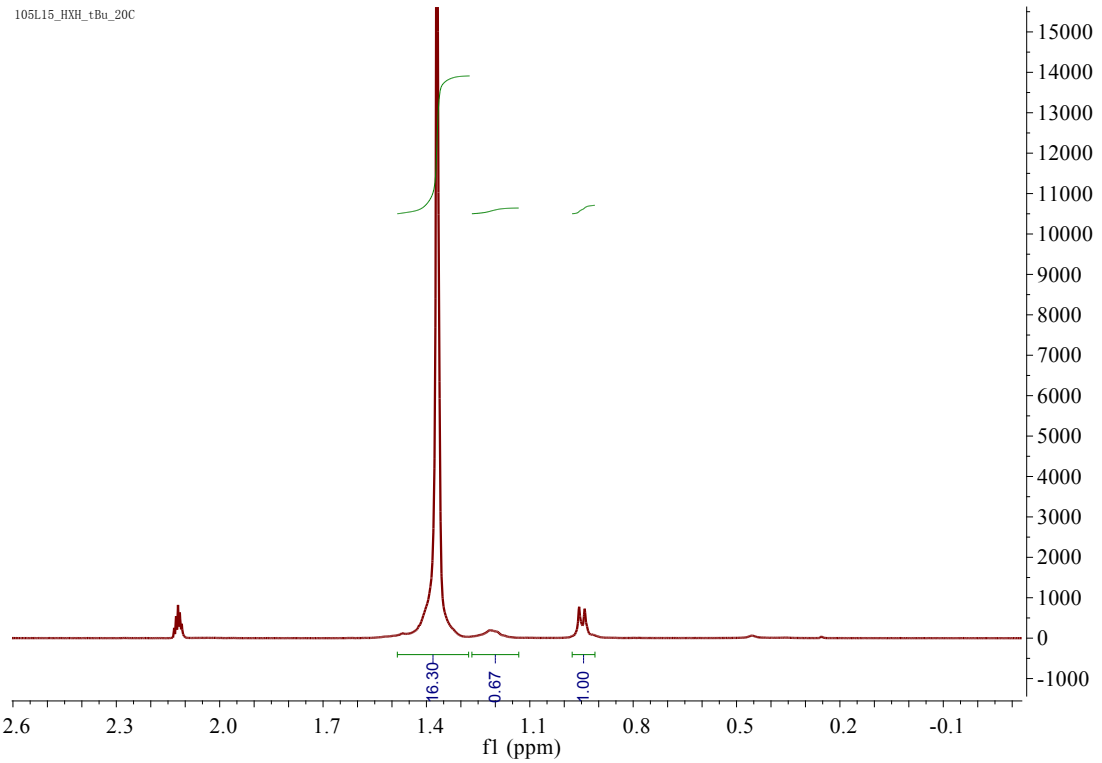

Figure S25. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 80 °C, ppm) of polyethylene generated by complex **5** at 25 °C.

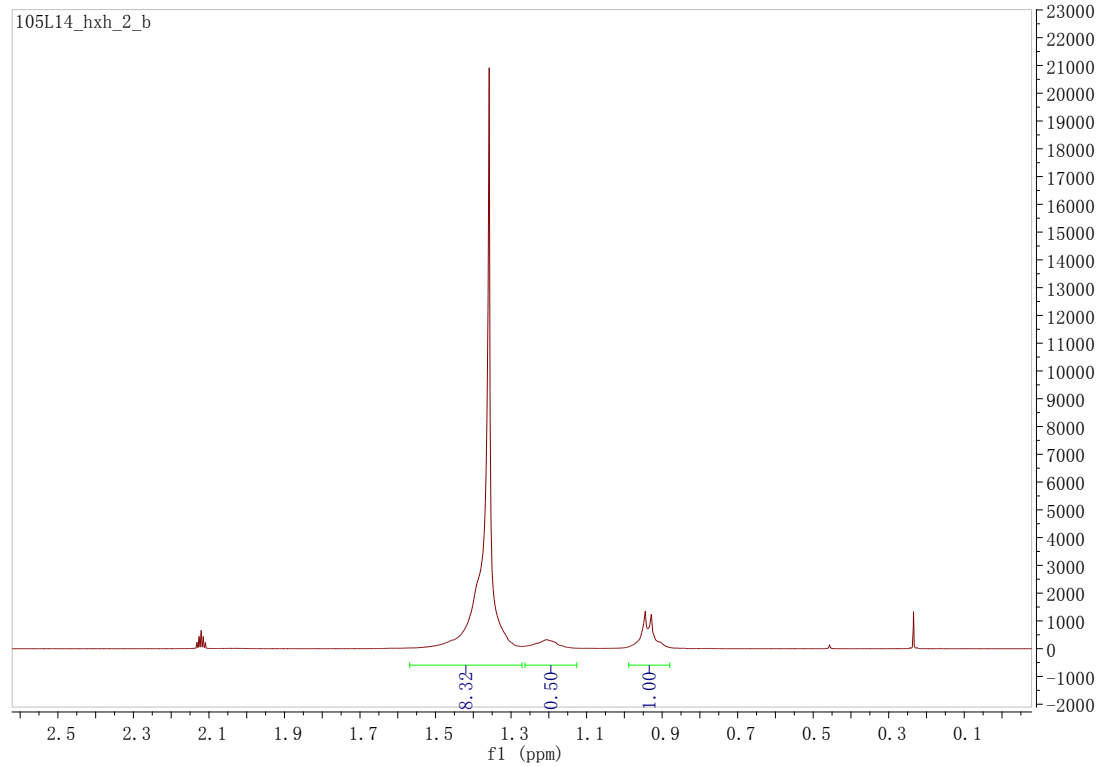

Figure S26. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 80 °C, ppm) of polyethylene generated by complex **1** at 50 °C.

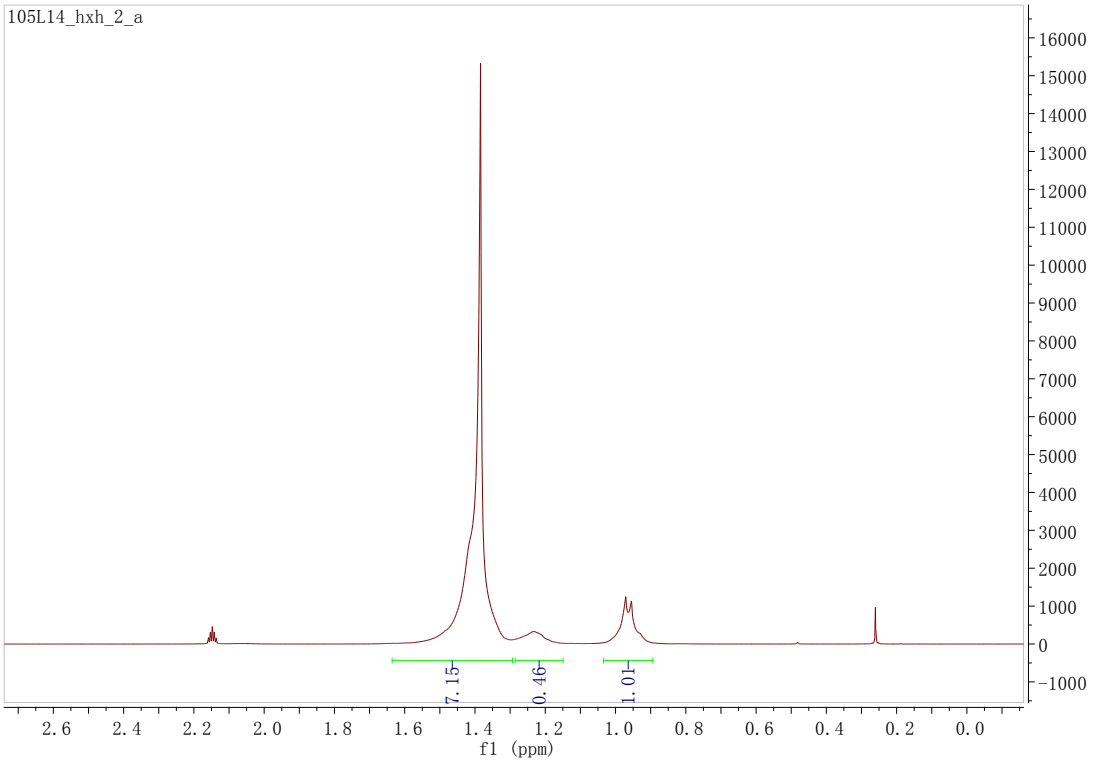

Figure S27. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 80 °C, ppm) of polyethylene generated by complex **2** at 50 °C.

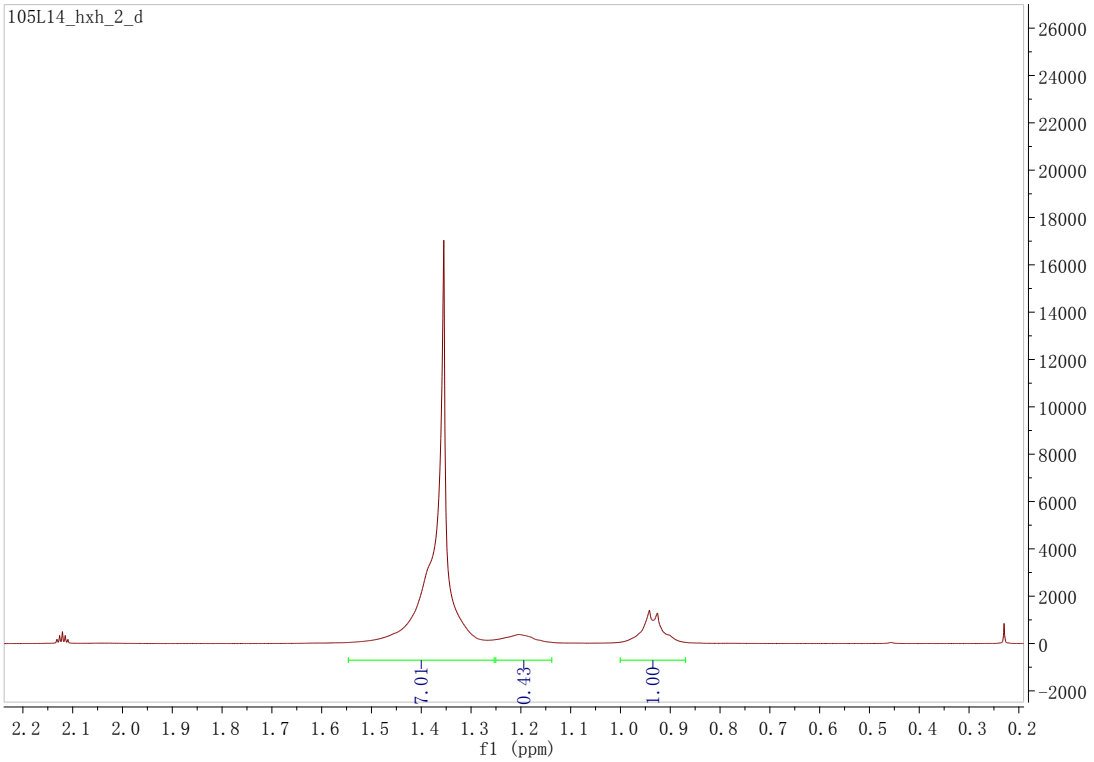

Figure S28. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 80 °C, ppm) of polyethylene generated by complex **3** at 50 °C.

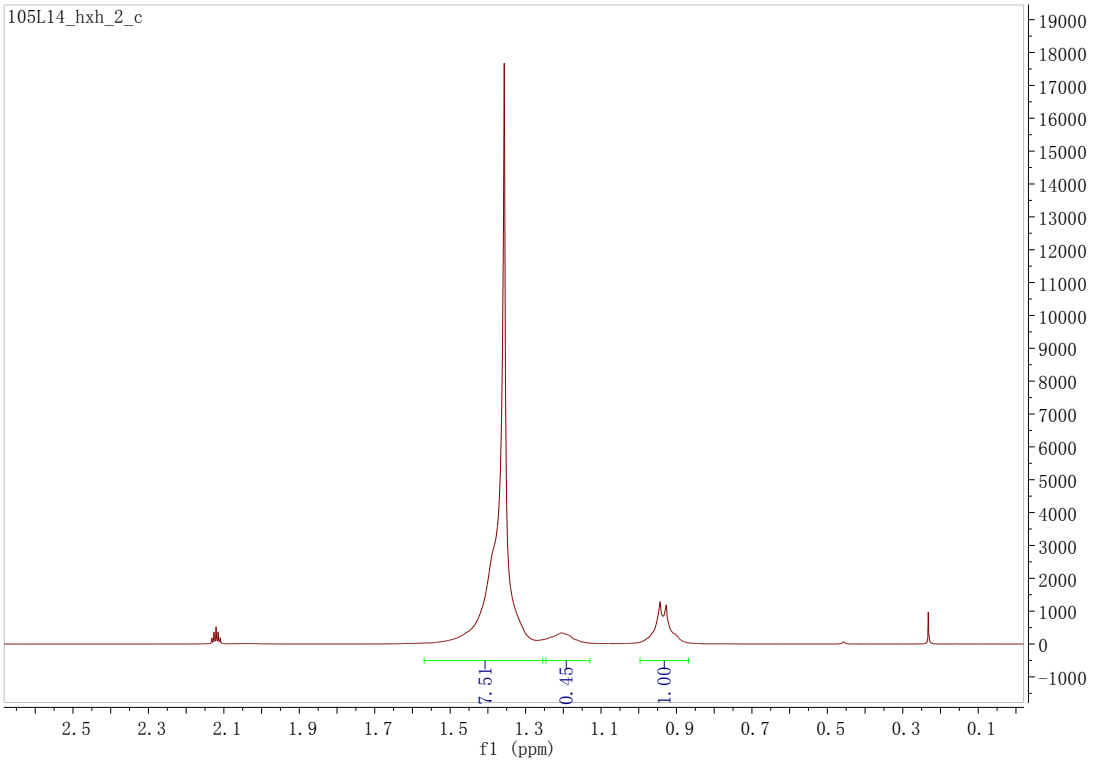

Figure S29. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 80 °C, ppm) of polyethylene generated by complex **4** at 50 °C.

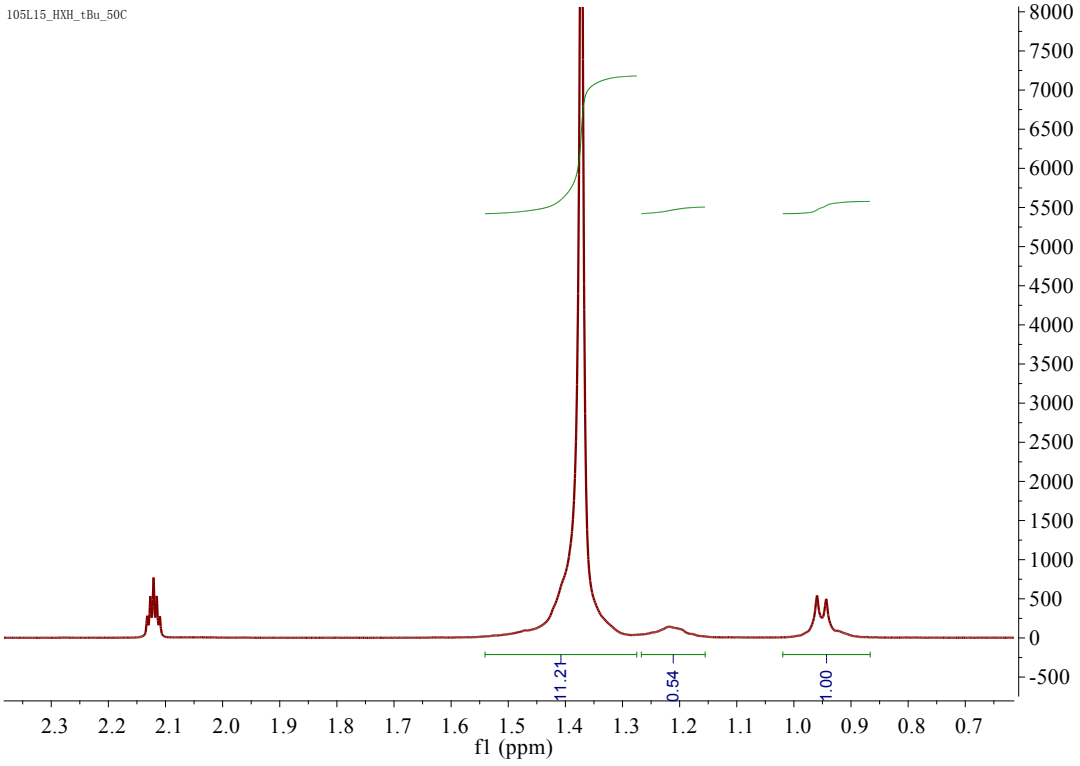

Figure S30. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 80 °C, ppm) of polyethylene generated by complex **5** at 50 °C.

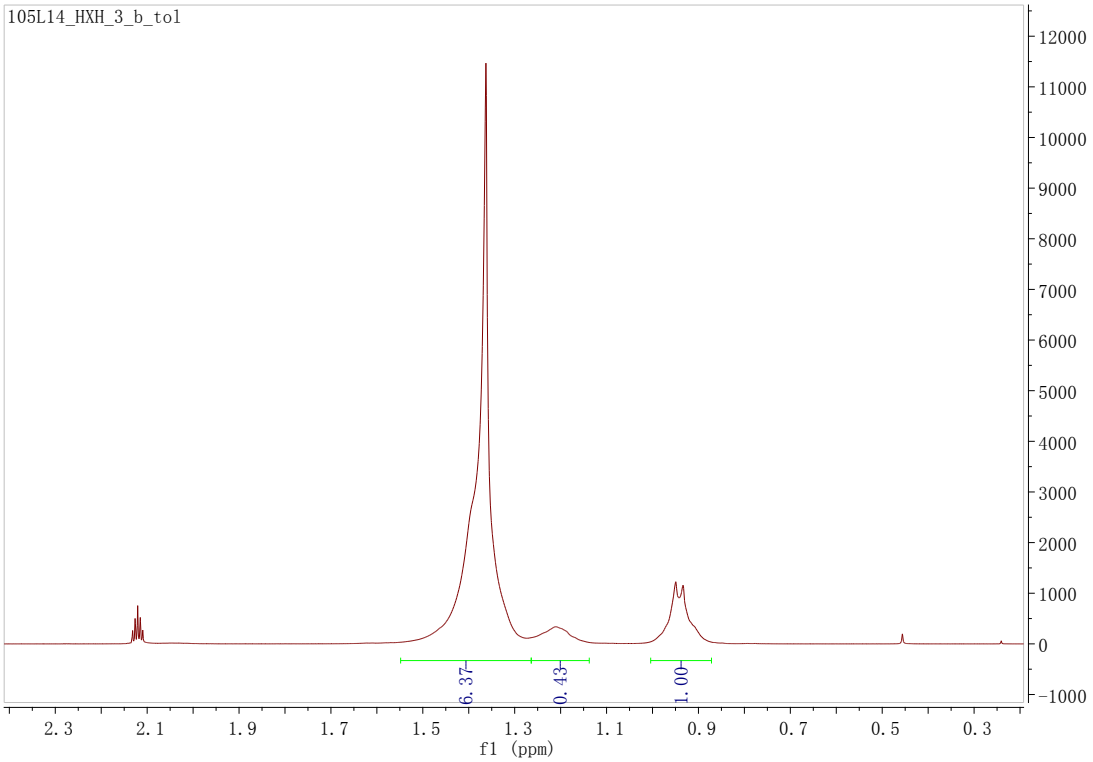

Figure S31. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 80 °C, ppm) of polyethylene generated by complex **1** at 80 °C.

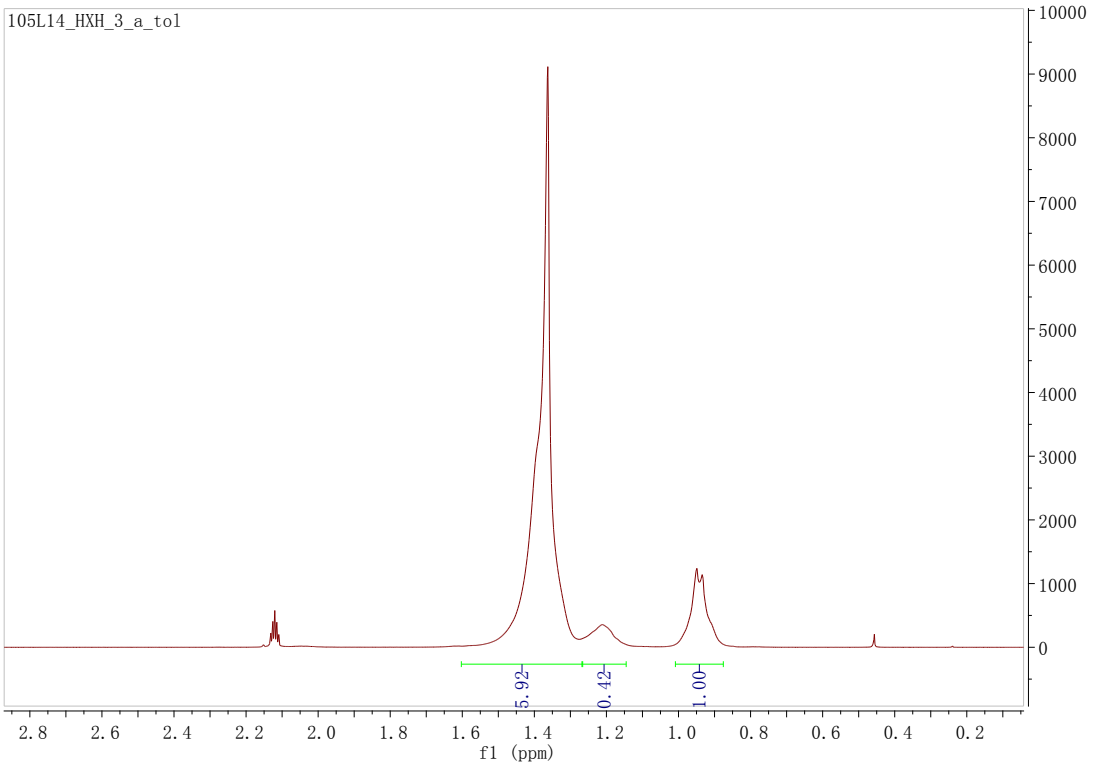

Figure S32. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 80 °C, ppm) of polyethylene generated by complex **2** at 80 °C.

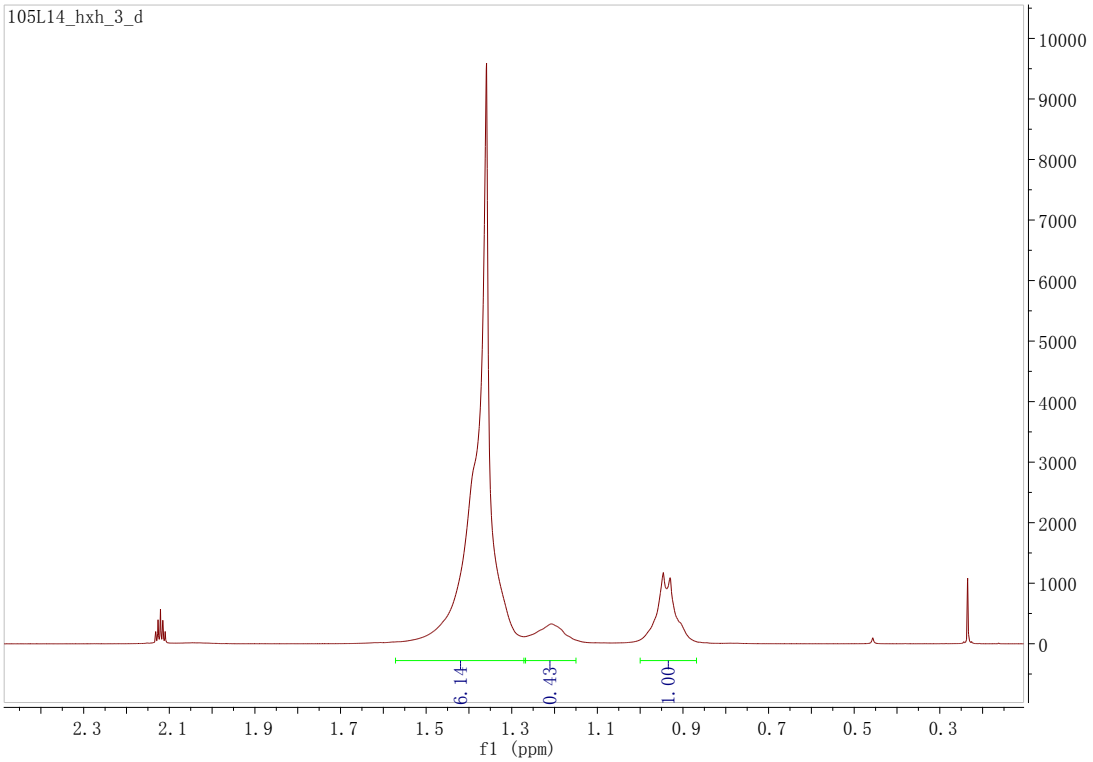

Figure S33. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 80 °C, ppm) of polyethylene generated by complex **3** at 80 °C.

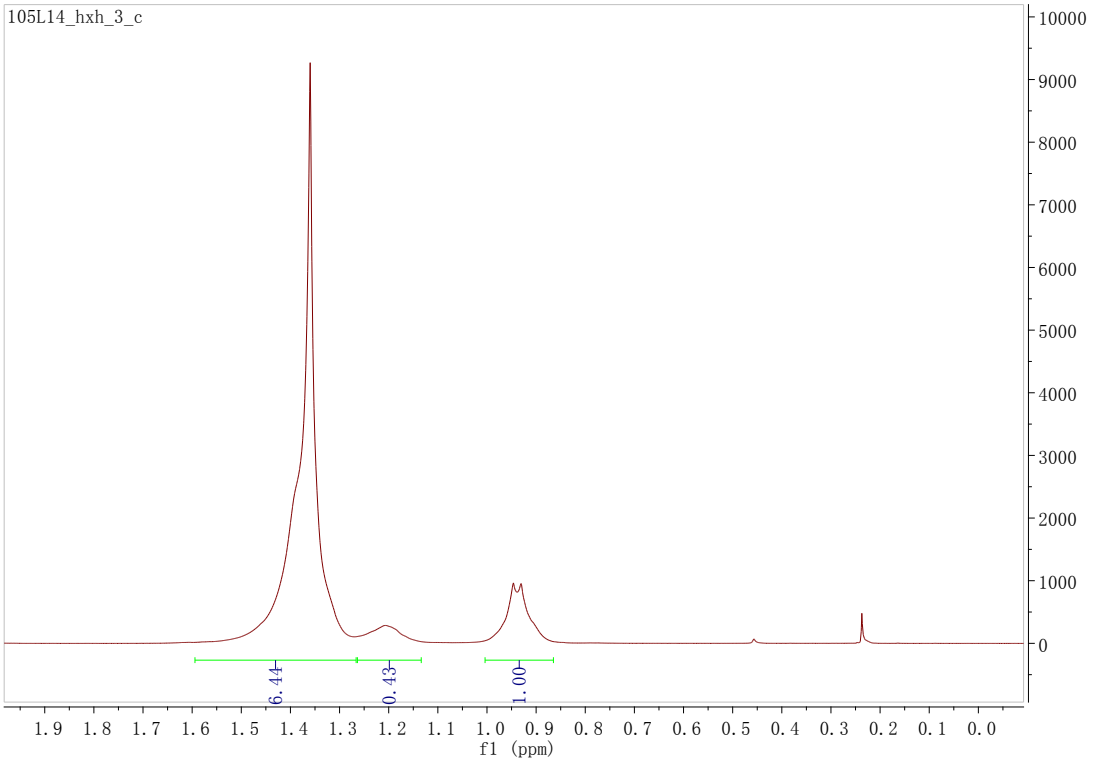

Figure S34. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 80 °C, ppm) of polyethylene generated by complex **4** at 80 °C.

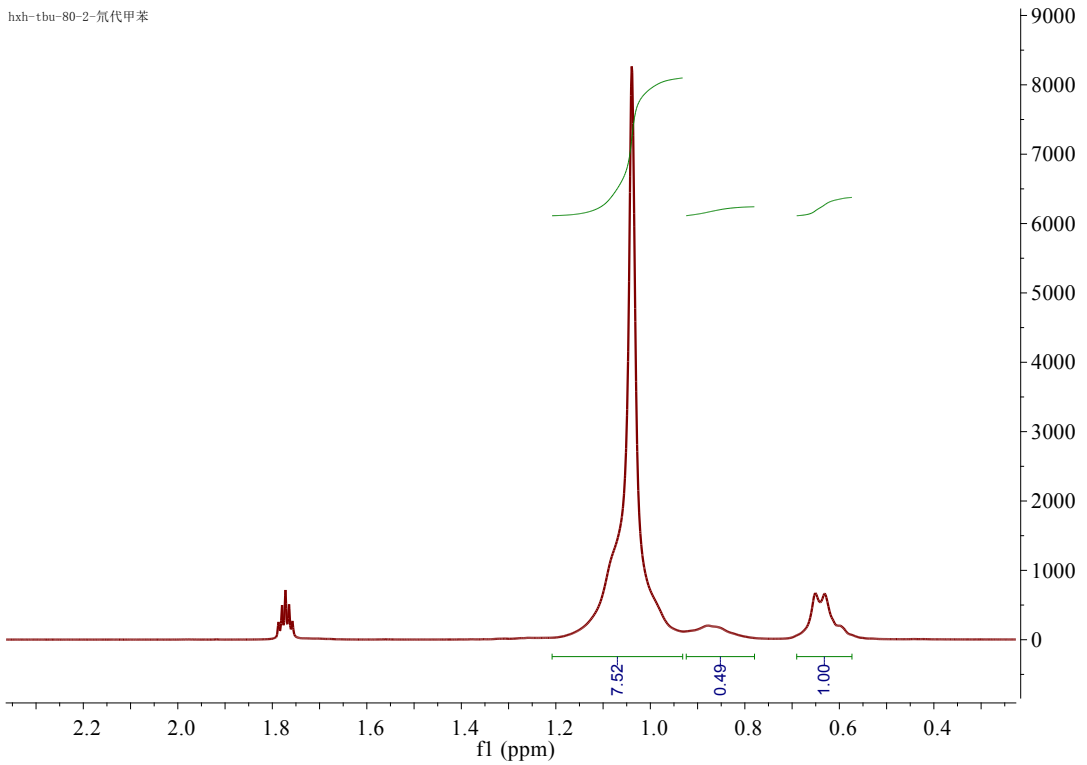

Figure S35. ^{1}H NMR spectrum (400 MHz, d^{6}-toluene, 25 °C, ppm) of polyeth ylene generated by complex **5** at 80 °C.

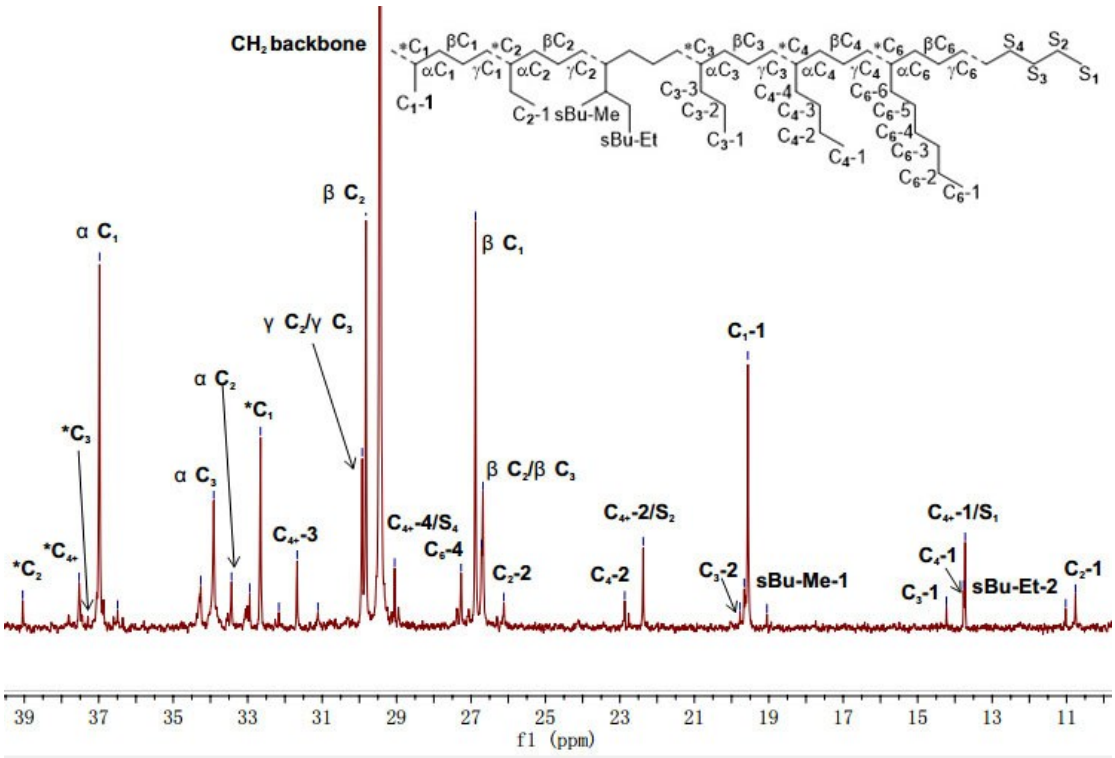

Figure S36. ^{13}C NMR spectrum (400 MHz, d^{2}-1,1,2,2-Tetrachloroethane, 80 °C,p pm) of polyethylene generated by complex **1** at 50 °C.

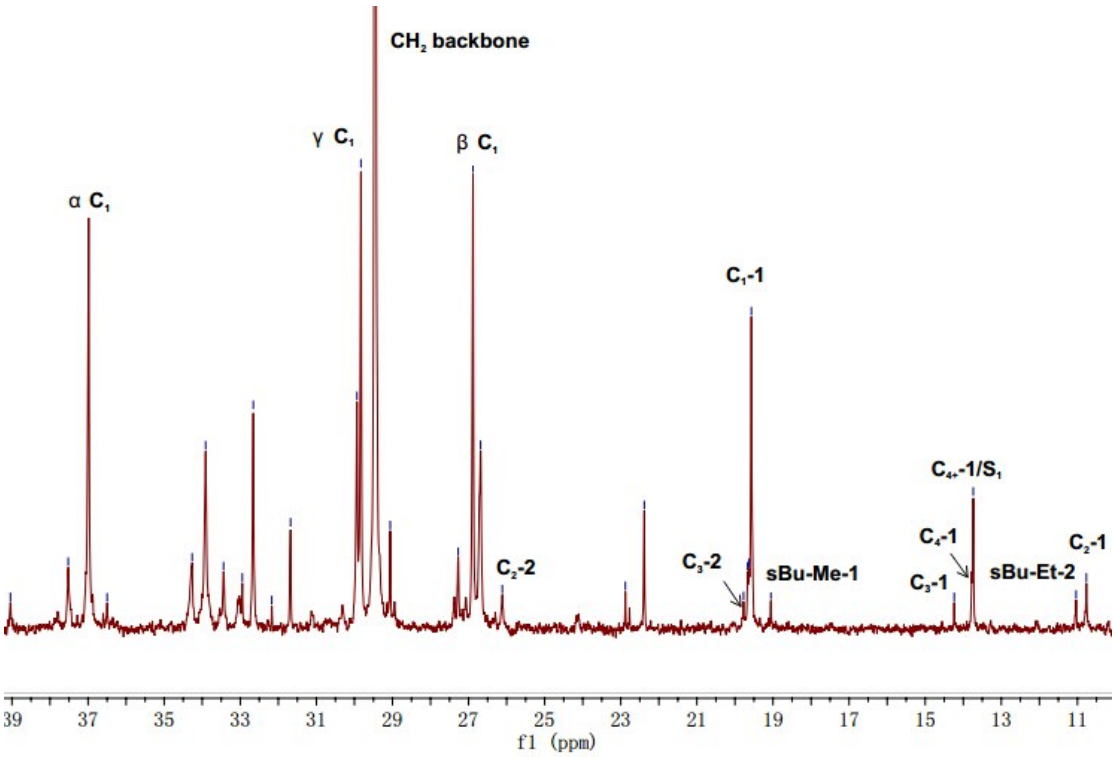

Figure S37. ^{13}C NMR spectrum (400 MHz, d^2-1,1,2,2-Tetrachloroethane, 80 °C,ppm) of polyethylene generated by complex **2** at 50 °C.

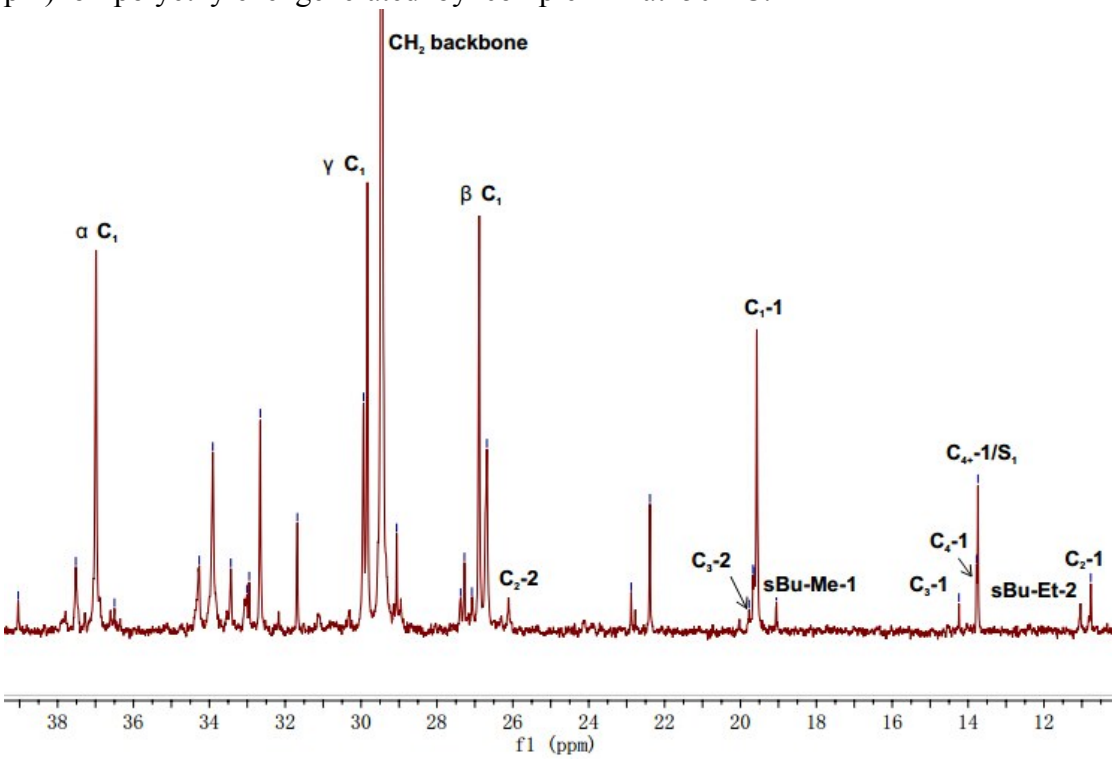

Figure S38. ^{13}C NMR spectrum (400 MHz, d^2-1,1,2,2-Tetrachloroethane, 80 °C,ppm) of polyethylene generated by complex **3** at 50 °C.

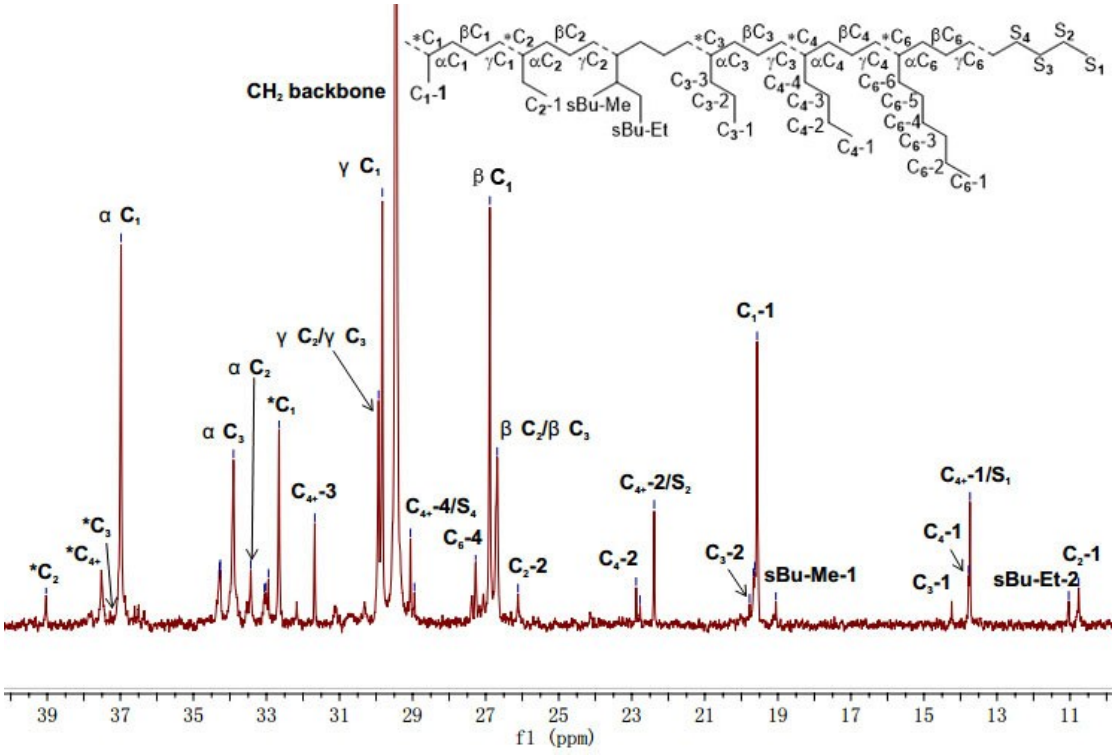

Figure S39. ^{13}C NMR spectrum (400 MHz, 1,1,2,2-Tetrachloroethane-d^2, 80 °C, ppm) of polyethylene generated by complex **4** at 50 °C.

DSC of Polyethylene generated by precatalyst 4.

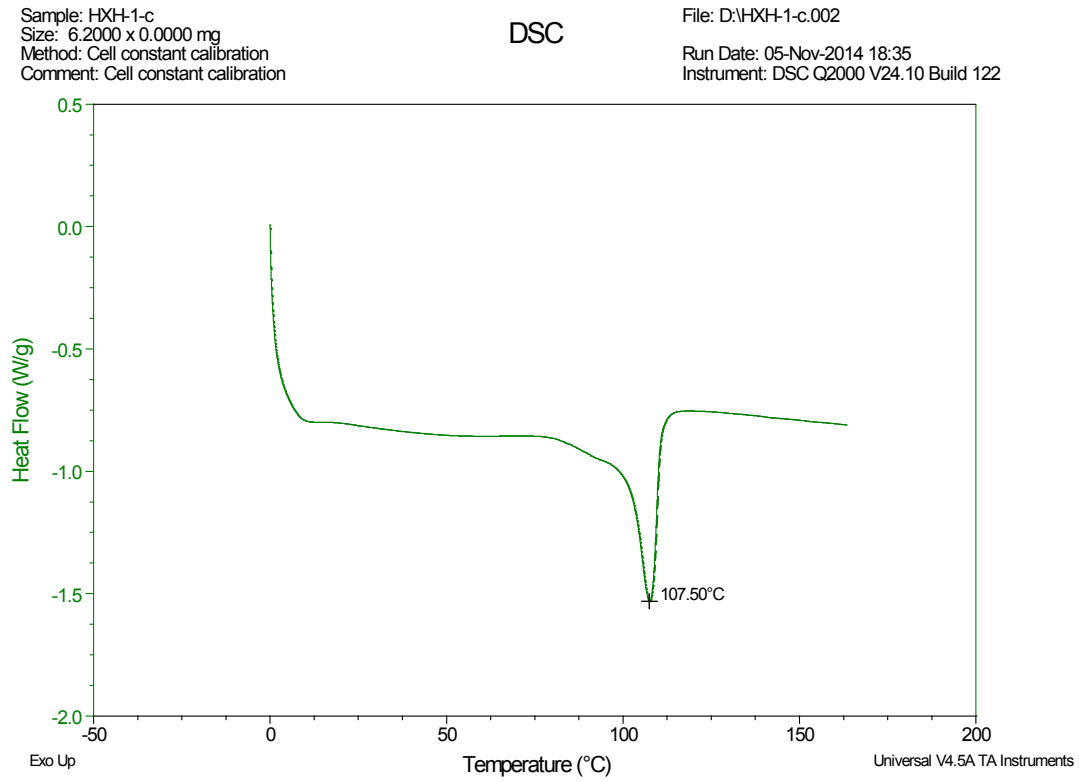

Figure S40. DSC of Polyethylene generated by precatalyst **4** (Table 1, entry 4).

X-Ray Crystallography of complex 1 and 2.

Table S1. Crystal data and structure refinement for **[2,4-di-tert-butyl-6-((2,6-di benzhydryl-4-methoxyphenylimino)methyl)-phenolato]-Ni(Ⅱ)-methyl(trimethyl phosphine)**

data	**1**
Identification code	HXH-1-163
Empirical formula	$C_{52}H_{60}NNiO_2P$
Formula weight	820.69
Temperature/K	290(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.8638(3)
b/Å	16.9433(4)
c/Å	25.4176(5)
α/°	90
β/°	98.390(2)
γ/°	90

Volume/Å^3	4628.51(19)
Z	4
ρ_{calc}g/cm^3	1.178
μ/mm^{-1}	1.222
F(000)	1752.0
Crystal size/mm^3	0.350 × 0.320 × 0.220
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.29 to 139.848
Index ranges	-12 ≤ h ≤ 13, -11 ≤ k ≤ 20, -30 ≤ l ≤ 29
Reflections collected	18287
Independent reflections	8386 [R_{int} = 0.0277, R_{sigma} = 0.0354]
Data/restraints/parameters	8386/47/551
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0554, wR_2 = 0.1495
Final R indexes [all data]	R_1 = 0.0757, wR_2 = 0.1665
Largest diff. peak/hole / e Å^{-3}	0.43/-0.39

Table S2. **Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.**

Atom	*x*	*y*	*z*	U(eq)
Ni1	1654.4(4)	1571.5(3)	5618.9(2)	53.97(16)
P1	2771.4(12)	541.5(7)	5763.3(5)	99.8(4)
O1	1489.0(18)	1371.6(12)	4869.1(7)	60.8(5)
O2	356(2)	4736.2(13)	7109.3(9)	74.7(6)
N1	595(2)	2486.9(13)	5522.1(8)	49.3(5)
C21	-473(3)	3014.7(16)	6235.4(10)	52.3(6)
C36	2525(2)	3635.2(17)	5719.6(11)	53.8(6)
C17	1423(2)	3644.5(16)	6037.1(10)	50.1(6)
C37	3661(3)	4069.4(19)	6005.5(12)	61.5(7)
C6	-164(2)	2259.6(16)	4576.7(10)	48.8(6)
C43	2156(2)	3883.1(17)	5144.2(11)	54.0(6)
C20	-541(3)	3578.5(16)	6631.4(11)	56.5(7)
C19	354(3)	4158.9(16)	6726.7(11)	56.1(7)
C22	-1435(3)	2356.7(16)	6131.3(11)	57.2(7)
C5	-1061(2)	2544.2(17)	4165.0(11)	55.6(6)
C7	-108(2)	2648.1(16)	5076.6(10)	49.4(6)
C16	498(2)	3061.5(15)	5934.7(10)	48.7(6)
C18	1332(3)	4192.2(17)	6433.2(11)	55.2(6)

C1	706(2)	1670.0(16)	4482.8(10)	52.4(6)
C48	2429(3)	3398.8(18)	4737.2(12)	60.5(7)
C29	-1956(3)	2114.5(18)	6640.0(12)	68.6(8)
C4	-1129(3)	2280.7(19)	3653.2(11)	61.1(7)
C23	-2458(3)	2546.8(18)	5673.2(11)	58.0(7)
C2	712(3)	1440.9(18)	3938.9(11)	62.0(7)
C8	1720(4)	883(2)	3784.0(14)	85.4(11)
C12	-2104(3)	2583(2)	3204.9(13)	78.3(9)
C46	1201(3)	4789(2)	4476.1(14)	76.9(9)
C44	1529(3)	4583(2)	5006.0(12)	65.7(8)
C35	-555(3)	4683(2)	7450.5(14)	85.6(11)
C3	-203(3)	1742(2)	3558.2(11)	66.4(8)
C28	-2971(3)	3291(2)	5598.4(14)	72.4(9)
C47	2086(3)	3604(2)	4211.2(13)	76.4(9)
C42	4322(3)	3738(3)	6450.1(13)	79.9(10)
C45	1462(3)	4299(2)	4080.0(14)	80.4(10)
C25	-3822(4)	2114(3)	4893.2(17)	95.0(12)
C41	5370(4)	4101(3)	6720.9(17)	100.9(14)
C52	1947(4)	1698(2)	6382.4(13)	96.6(13)
C38	4077(3)	4775(2)	5835.7(19)	94.5(12)
C27	-3900(3)	3438(3)	5171.1(17)	87.9(11)
C24	-2897(3)	1961(2)	5316.3(14)	76.1(9)
C26	-4314(3)	2851(3)	4819.0(17)	91.4(12)
C30	-3191(4)	2170(3)	6687.2(18)	104.0(14)
C34	-1162(5)	1821(3)	7064.9(17)	112.0(16)
C11	3012(4)	1246(3)	3958(2)	118.9(17)
C40	5762(4)	4802(3)	6548(2)	112.1(17)
C33	-1601(6)	1608(3)	7535.3(19)	135(2)
C10	1589(5)	74(3)	4034.7(18)	117.5(17)
C9	1587(5)	751(3)	3180.6(16)	131(2)
C39	5131(4)	5140(3)	6107(2)	126.2(19)
C32	-2820(7)	1673(3)	7574(2)	134(2)
C31	-3616(6)	1951(4)	7158(2)	139(2)
C13	-3385(7)	2481(7)	3370(3)	122(2)
C15	-2141(10)	2085(7)	2686(4)	123(3)
C14	-1834(11)	3408(6)	3066(5)	133(3)
C13'	-2947(10)	3270(9)	3396(5)	122(2)
C15'	-2828(13)	1934(9)	2916(5)	123(3)
C14'	-1380(14)	3024(9)	2801(6)	133(3)
C50	3537(11)	212(7)	6370(3)	188(4)

C49	3937(5)	424(4)	5303(3)	114(2)
C51	1788(7)	-349(3)	5544(3)	122(2)
C51'	2500(18)	-89(8)	6346(6)	122(2)
C49'	4400(11)	859(9)	6093(7)	114(2)
C50'	3217(19)	-194(10)	5349(5)	188(4)

Table S3. **Anisotropic Displacement Parameters ($Å^2×10^3$) for 1. 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	62.7(3)	52.6(3)	43.4(3)	-1.9(2)	-3.0(2)	8.9(2)
P1	119.4(8)	90.0(7)	83.1(7)	0.0(6)	-8.6(6)	53.0(6)
O1	66.0(11)	66.6(12)	46.3(10)	-9.6(9)	-3.8(9)	18.5(10)
O2	92.6(15)	71.4(13)	61.7(13)	-23.6(11)	17.0(11)	-3.7(12)
N1	57.8(12)	50.7(12)	38.2(11)	-2.0(9)	3.4(9)	4.4(10)
C21	65.2(16)	49.1(14)	42.2(13)	3.0(11)	6.8(12)	1.7(12)
C36	53.6(14)	56.9(15)	49.0(15)	-1.7(12)	0.9(12)	6.0(12)
C17	55.6(14)	53.2(15)	39.6(13)	2.6(11)	0.6(11)	6.5(12)
C37	54.1(15)	70.9(19)	58.1(17)	-9.8(15)	3.0(13)	6.6(14)
C6	50.3(13)	54.8(15)	40.4(13)	-0.9(11)	3.6(11)	2.2(11)
C43	47.7(14)	64.7(17)	49.2(15)	-0.1(13)	5.2(11)	-1.0(12)
C20	71.3(17)	55.9(16)	44.0(14)	-2.1(12)	14.1(13)	2.1(14)
C19	74.5(18)	52.0(15)	41.0(14)	-6.8(12)	5.6(13)	3.7(13)
C22	72.0(17)	48.5(15)	51.2(15)	-2.3(12)	9.5(13)	-2.2(13)
C5	53.4(14)	64.7(17)	47.1(14)	1.1(13)	2.1(11)	5.1(13)
C7	51.8(13)	52.3(14)	43.8(14)	0.7(12)	6.5(11)	4.9(12)
C16	61.1(15)	46.4(14)	37.0(12)	0.7(11)	1.4(11)	7.7(12)
C18	61.2(16)	54.3(15)	48.0(15)	-3.2(12)	1.7(12)	-0.8(13)
C1	56.8(15)	56.9(15)	42.4(14)	-3.5(12)	3.3(12)	1.3(12)
C48	62.1(16)	69.2(18)	51.9(16)	-0.7(14)	14.4(13)	-1.2(14)
C29	98(2)	56.4(17)	52.5(17)	0.6(14)	14.5(16)	-16.1(16)
C4	62.1(16)	75.2(19)	43.5(15)	5.0(14)	-0.2(12)	-1.3(15)
C23	59.9(15)	64.0(17)	52.6(15)	1.5(14)	16.7(13)	-2.8(13)
C2	70.8(18)	68.5(18)	45.9(15)	-6.6(13)	5.9(13)	8.8(15)
C8	108(3)	96(3)	52.6(18)	-11.7(18)	12.0(18)	36(2)
C12	80(2)	101(3)	47.5(16)	7.2(17)	-10.9(15)	9.8(19)
C46	70.8(19)	92(2)	68(2)	24.9(19)	8.0(16)	14.9(18)
C44	63.9(17)	76(2)	57.0(17)	4.6(15)	8.8(14)	13.0(15)
C35	96(2)	97(3)	66(2)	-30(2)	19.4(19)	9(2)
C3	83(2)	78(2)	37.2(14)	-4.6(14)	5.0(14)	0.3(17)

C28	74(2)	73(2)	72(2)	2.5(17)	16.2(17)	6.3(16)
C47	87(2)	95(3)	49.1(17)	-2.1(17)	18.6(16)	-5(2)
C42	73(2)	105(3)	57.1(19)	0.7(19)	-6.3(16)	-1.0(19)
C45	80(2)	107(3)	53.3(18)	15.8(19)	7.0(16)	0(2)
C25	83(2)	112(3)	84(3)	-14(2)	-6(2)	-7(2)
C41	78(2)	142(4)	73(2)	-19(3)	-21.6(19)	12(3)
C52	147(3)	89(2)	48.0(17)	4.1(17)	-6(2)	52(2)
C38	78(2)	80(2)	115(3)	9(2)	-22(2)	-10.2(19)
C27	75(2)	98(3)	90(3)	16(2)	13(2)	21(2)
C24	79(2)	76(2)	71(2)	-6.7(18)	2.7(17)	-4.6(17)
C26	66(2)	129(4)	77(2)	10(3)	4.7(18)	10(2)
C30	113(3)	118(3)	90(3)	31(3)	46(3)	8(3)
C34	119(3)	137(4)	74(3)	37(3)	-6(2)	-43(3)
C11	85(3)	158(4)	117(4)	-21(3)	26(3)	39(3)
C40	74(2)	111(4)	140(4)	-45(3)	-22(3)	-2(2)
C33	169(5)	153(5)	72(3)	42(3)	-17(3)	-72(4)
C10	176(5)	91(3)	86(3)	-14(2)	20(3)	50(3)
C9	172(5)	162(5)	61(2)	-19(3)	26(3)	72(4)
C39	93(3)	95(3)	173(5)	3(3)	-39(3)	-19(2)
C32	198(6)	136(4)	73(3)	12(3)	37(4)	-70(4)
C31	152(5)	174(5)	107(4)	40(4)	69(4)	0(4)
C13	88(4)	182(6)	86(4)	21(5)	-16(3)	40(5)
C15	123(6)	147(6)	82(5)	-4(5)	-40(4)	10(5)
C14	147(6)	120(6)	115(6)	43(5)	-30(5)	11(5)
C13'	88(4)	182(6)	86(4)	21(5)	-16(3)	40(5)
C15'	123(6)	147(6)	82(5)	-4(5)	-40(4)	10(5)
C14'	147(6)	120(6)	115(6)	43(5)	-30(5)	11(5)
C50	222(6)	186(6)	134(4)	40(5)	-45(5)	70(5)
C49	71(3)	113(4)	161(6)	22(4)	21(3)	32(3)
C51	137(5)	56(3)	178(7)	16(4)	40(5)	-1(3)
C51'	137(5)	56(3)	178(7)	16(4)	40(5)	-1(3)
C49'	71(3)	113(4)	161(6)	22(4)	21(3)	32(3)
C50'	222(6)	186(6)	134(4)	40(5)	-45(5)	70(5)

Table S4. **Bond Lengths for 1.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ni1	O1	1.9183(19)	C1	C2	1.437(4)
Ni1	N1	1.926(2)	C48	C47	1.379(4)
Ni1	C52	1.932(3)	C29	C30	1.367(5)

Ni1	P1	2.1268(10)	C29	C34	1.373(5)
P1	C50	1.733(6)	C4	C3	1.405(4)
P1	C50'	1.745(9)	C4	C12	1.526(4)
P1	C49	1.857(6)	C23	C28	1.380(4)
P1	C51'	1.885(14)	C23	C24	1.381(4)
P1	C51	1.885(7)	C2	C3	1.380(4)
P1	C49'	1.921(13)	C2	C8	1.541(4)
O1	C1	1.304(3)	C8	C10	1.528(6)
O2	C19	1.379(3)	C8	C9	1.536(5)
O2	C35	1.411(4)	C8	C11	1.536(6)
N1	C7	1.299(3)	C12	C15'	1.481(14)
N1	C16	1.446(3)	C12	C14	1.483(10)
C21	C16	1.392(4)	C12	C13	1.521(9)
C21	C20	1.397(4)	C12	C15	1.561(10)
C21	C22	1.525(4)	C12	C14'	1.571(15)
C36	C43	1.518(4)	C12	C13'	1.601(13)
C36	C37	1.527(4)	C46	C45	1.366(5)
C36	C17	1.538(4)	C46	C44	1.386(4)
C17	C18	1.384(4)	C28	C27	1.393(5)
C17	C16	1.406(4)	C47	C45	1.375(5)
C37	C42	1.367(4)	C42	C41	1.386(5)
C37	C38	1.370(5)	C25	C26	1.360(6)
C6	C5	1.407(4)	C25	C24	1.385(5)
C6	C1	1.419(4)	C41	C40	1.356(7)
C6	C7	1.424(4)	C38	C39	1.392(5)
C43	C48	1.386(4)	C27	C26	1.369(6)
C43	C44	1.388(4)	C30	C31	1.395(6)
C20	C19	1.380(4)	C34	C33	1.398(6)
C19	C18	1.385(4)	C40	C39	1.354(7)
C22	C23	1.522(4)	C33	C32	1.346(8)
C22	C29	1.541(4)	C32	C31	1.350(8)
C5	C4	1.367(4)			

Table S5. **Bond Angles for 1.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ni1	N1	92.73(8)	O1	C1	C6	121.6(2)
O1	Ni1	C52	174.50(12)	O1	C1	C2	121.7(2)
N1	Ni1	C52	92.68(12)	C6	C1	C2	116.7(2)
O1	Ni1	P1	89.71(7)	C47	C48	C43	121.1(3)

N1	Ni1	P1	176.70(8)	C30	C29	C34	117.9(4)
C52	Ni1	P1	84.93(11)	C30	C29	C22	122.7(3)
C50	P1	C49	104.1(5)	C34	C29	C22	119.4(3)
C50'	P1	C51'	99.2(6)	C5	C4	C3	115.8(3)
C50	P1	C51	100.5(5)	C5	C4	C12	122.5(3)
C49	P1	C51	97.9(3)	C3	C4	C12	121.7(3)
C50'	P1	C49'	98.3(6)	C28	C23	C24	118.2(3)
C51'	P1	C49'	93.1(8)	C28	C23	C22	122.2(3)
C50	P1	Ni1	127.3(4)	C24	C23	C22	119.6(3)
C50'	P1	Ni1	133.1(6)	C3	C2	C1	118.1(3)
C49	P1	Ni1	113.8(2)	C3	C2	C8	120.9(3)
C51'	P1	Ni1	116.8(5)	C1	C2	C8	121.0(3)
C51	P1	Ni1	108.7(2)	C10	C8	C9	106.5(4)
C49'	P1	Ni1	108.1(4)	C10	C8	C11	112.1(4)
C1	O1	Ni1	129.48(17)	C9	C8	C11	107.1(4)
C19	O2	C35	117.4(3)	C10	C8	C2	109.3(3)
C7	N1	C16	113.3(2)	C9	C8	C2	112.2(3)
C7	N1	Ni1	123.03(18)	C11	C8	C2	109.6(3)
C16	N1	Ni1	123.70(16)	C14	C12	C13	113.1(7)
C16	C21	C20	118.7(3)	C15'	C12	C4	112.4(6)
C16	C21	C22	120.1(2)	C14	C12	C4	110.8(5)
C20	C21	C22	121.2(2)	C13	C12	C4	108.6(4)
C43	C36	C37	114.0(2)	C14	C12	C15	106.8(7)
C43	C36	C17	112.7(2)	C13	C12	C15	105.1(6)
C37	C36	C17	112.5(2)	C4	C12	C15	112.3(5)
C18	C17	C16	118.7(2)	C15'	C12	C14'	108.1(8)
C18	C17	C36	122.2(2)	C4	C12	C14'	106.8(5)
C16	C17	C36	119.1(2)	C15'	C12	C13'	113.8(8)
C42	C37	C38	117.4(3)	C4	C12	C13'	112.5(4)
C42	C37	C36	119.1(3)	C14'	C12	C13'	102.4(8)
C38	C37	C36	123.5(3)	C45	C46	C44	120.7(3)
C5	C6	C1	121.5(2)	C46	C44	C43	120.5(3)
C5	C6	C7	116.1(2)	C2	C3	C4	125.5(3)
C1	C6	C7	122.2(2)	C23	C28	C27	120.2(3)
C48	C43	C44	117.9(3)	C45	C47	C48	120.3(3)
C48	C43	C36	120.0(3)	C37	C42	C41	121.5(4)
C44	C43	C36	122.1(3)	C46	C45	C47	119.3(3)
C19	C20	C21	120.2(3)	C26	C25	C24	120.4(4)
O2	C19	C20	123.9(3)	C40	C41	C42	120.1(4)
O2	C19	C18	115.4(3)	C37	C38	C39	121.2(4)

C20	C19	C18	120.7(2)	C26	C27	C28	120.7(4)
C23	C22	C21	112.6(2)	C23	C24	C25	121.1(4)
C23	C22	C29	112.5(3)	C25	C26	C27	119.4(4)
C21	C22	C29	112.0(2)	C29	C30	C31	120.6(5)
C4	C5	C6	122.1(3)	C29	C34	C33	120.8(5)
N1	C7	C6	128.6(2)	C39	C40	C41	119.7(4)
C21	C16	C17	121.1(2)	C32	C33	C34	120.3(5)
C21	C16	N1	120.1(2)	C40	C39	C38	120.1(5)
C17	C16	N1	118.8(2)	C33	C32	C31	119.7(5)
C17	C18	C19	120.5(3)	C32	C31	C30	120.7(5)

Table S6. **Torsion Angles for 1.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C43	C36	C17	C18	-110.5(3)	C29	C22	C23	C28	87.4(3)
C37	C36	C17	C18	20.1(4)	C21	C22	C23	C24	139.6(3)
C43	C36	C17	C16	71.7(3)	C29	C22	C23	C24	-92.7(3)
C37	C36	C17	C16	-157.7(2)	O1	C1	C2	C3	175.5(3)
C43	C36	C37	C42	-158.9(3)	C6	C1	C2	C3	-6.8(4)
C17	C36	C37	C42	71.2(4)	O1	C1	C2	C8	-5.2(5)
C43	C36	C37	C38	20.0(4)	C6	C1	C2	C8	172.4(3)
C17	C36	C37	C38	-110.0(4)	C3	C2	C8	C10	-115.9(4)
C37	C36	C43	C48	104.0(3)	C1	C2	C8	C10	64.9(4)
C17	C36	C43	C48	-126.2(3)	C3	C2	C8	C9	2.1(5)
C37	C36	C43	C44	-77.0(3)	C1	C2	C8	C9	-177.1(4)
C17	C36	C43	C44	52.8(4)	C3	C2	C8	C11	121.0(4)
C16	C21	C20	C19	-1.3(4)	C1	C2	C8	C11	-58.2(5)
C22	C21	C20	C19	178.6(3)	C5	C4	C12	C15'	-126.1(8)
C35	O2	C19	C20	5.6(4)	C3	C4	C12	C15'	57.3(8)
C35	O2	C19	C18	-174.3(3)	C5	C4	C12	C14	71.0(7)
C21	C20	C19	O2	-180.0(3)	C3	C4	C12	C14	-105.6(7)
C21	C20	C19	C18	0.0(4)	C5	C4	C12	C13	-53.8(6)
C16	C21	C22	C23	-83.0(3)	C3	C4	C12	C13	129.6(6)
C20	C21	C22	C23	97.1(3)	C5	C4	C12	C15	-169.7(6)
C16	C21	C22	C29	149.1(3)	C3	C4	C12	C15	13.7(7)
C20	C21	C22	C29	-30.8(4)	C5	C4	C12	C14'	115.5(7)
C1	C6	C5	C4	-1.2(4)	C3	C4	C12	C14'	-61.1(7)
C7	C6	C5	C4	173.1(3)	C5	C4	C12	C13'	4.0(8)
C16	N1	C7	C6	173.6(3)	C3	C4	C12	C13'	-172.6(7)
Ni1	N1	C7	C6	-6.5(4)	C45	C46	C44	C43	1.6(5)

C5	C6	C7	N1	177.3(3)	C48	C43	C44	C46	-0.6(4)
C1	C6	C7	N1	-8.4(4)	C36	C43	C44	C46	-179.7(3)
C20	C21	C16	C17	2.3(4)	C1	C2	C3	C4	2.2(5)
C22	C21	C16	C17	-177.5(2)	C8	C2	C3	C4	-177.0(3)
C20	C21	C16	N1	180.0(2)	C5	C4	C3	C2	3.1(5)
C22	C21	C16	N1	0.1(4)	C12	C4	C3	C2	179.9(3)
C18	C17	C16	C21	-2.1(4)	C24	C23	C28	C27	-0.3(5)
C36	C17	C16	C21	175.8(2)	C22	C23	C28	C27	179.6(3)
C18	C17	C16	N1	-179.8(2)	C43	C48	C47	C45	0.0(5)
C36	C17	C16	N1	-1.9(3)	C38	C37	C42	C41	0.2(5)
C7	N1	C16	C21	82.5(3)	C36	C37	C42	C41	179.1(3)
Ni1	N1	C16	C21	-97.4(3)	C44	C46	C45	C47	-1.7(5)
C7	N1	C16	C17	-99.8(3)	C48	C47	C45	C46	1.0(5)
Ni1	N1	C16	C17	80.3(3)	C37	C42	C41	C40	0.2(6)
C16	C17	C18	C19	0.8(4)	C42	C37	C38	C39	-0.1(6)
C36	C17	C18	C19	-177.0(2)	C36	C37	C38	C39	-179.0(4)
O2	C19	C18	C17	-179.8(3)	C23	C28	C27	C26	-0.3(6)
C20	C19	C18	C17	0.3(4)	C28	C23	C24	C25	0.2(5)
Ni1	O1	C1	C6	3.2(4)	C22	C23	C24	C25	-179.7(3)
Ni1	O1	C1	C2	-179.3(2)	C26	C25	C24	C23	0.4(6)
C5	C6	C1	O1	-175.9(3)	C24	C25	C26	C27	-1.0(6)
C7	C6	C1	O1	10.1(4)	C28	C27	C26	C25	1.0(6)
C5	C6	C1	C2	6.5(4)	C34	C29	C30	C31	1.4(7)
C7	C6	C1	C2	-167.5(3)	C22	C29	C30	C31	-179.3(4)
C44	C43	C48	C47	-0.2(4)	C30	C29	C34	C33	-1.8(7)
C36	C43	C48	C47	178.9(3)	C22	C29	C34	C33	178.9(4)
C23	C22	C29	C30	-8.1(5)	C42	C41	C40	C39	-0.6(7)
C21	C22	C29	C30	119.8(4)	C29	C34	C33	C32	1.4(8)
C23	C22	C29	C34	171.1(3)	C41	C40	C39	C38	0.7(8)
C21	C22	C29	C34	-60.9(4)	C37	C38	C39	C40	-0.3(8)
C6	C5	C4	C3	-3.6(4)	C34	C33	C32	C31	-0.6(9)
C6	C5	C4	C12	179.6(3)	C33	C32	C31	C30	0.2(10)
C21	C22	C23	C28	-40.3(4)	C29	C30	C31	C32	-0.6(9)

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 1.

Atom	*x*	*y*	*z*	U(eq)
H36	2776	3081	5707	65
H20	-1192	3562	6831	68

H22	-995	1895	6021	69
H5	-1625	2924	4244	67
H7	-645	3073	5085	59
H18	1930	4585	6503	66
H48	2851	2927	4820	73
H46	799	5267	4389	92
H44	1327	4917	5271	79
H35A	-1368	4698	7244	128
H35B	-464	5119	7694	128
H35C	-452	4197	7646	128
H3	-207	1575	3209	80
H28	-2695	3695	5834	87
H47	2278	3271	3944	92
H42	4062	3259	6573	96
H45	1220	4434	3725	96
H25	-4109	1711	4659	114
H41	5806	3864	7022	121
H52A	1658	1238	6548	145
H52B	1506	2154	6480	145
H52C	2822	1765	6499	145
H38	3648	5014	5534	113
H27	-4243	3941	5125	106
H24	-2565	1455	5361	91
H26	-4926	2955	4532	110
H30	-3752	2356	6403	125
H34	-321	1763	7039	134
H11A	3071	1740	3779	178
H11B	3640	892	3869	178
H11C	3131	1332	4335	178
H40	6460	5049	6732	134
H33	-1049	1422	7823	162
H10A	1662	128	4414	176
H10B	2232	-270	3948	176
H10C	790	-146	3900	176
H9A	811	492	3061	196
H9B	2261	428	3100	196
H9C	1606	1251	3004	196
H39	5402	5618	5984	151
H32	-3111	1527	7886	161
H31	-4457	1997	7186	167

H13A	-3517	1935	3446	182
H13B	-4009	2653	3087	182
H13C	-3438	2791	3682	182
H15A	-1392	2174	2535	184
H15B	-2847	2241	2435	184
H15C	-2207	1535	2768	184
H14A	-1802	3735	3376	199
H14B	-2478	3595	2795	199
H14C	-1048	3429	2936	199
H13D	-3476	3055	3631	182
H13E	-3449	3499	3092	182
H13F	-2422	3669	3579	182
H15D	-2268	1537	2823	184
H15E	-3310	2139	2599	184
H15F	-3374	1707	3140	184
H14D	-1014	3497	2963	199
H14E	-1946	3158	2488	199
H14F	-737	2688	2706	199
H50A	4130	602	6517	282
H50B	3962	-273	6319	282
H50C	2943	124	6609	282
H49A	3518	318	4950	172
H49B	4483	-7	5419	172
H49C	4414	900	5299	172
H51A	1125	-391	5754	183
H51B	2293	-815	5590	183
H51C	1444	-294	5176	183
H51D	2557	233	6660	183
H51E	3118	-497	6400	183
H51F	1688	-323	6277	183
H49D	4736	1235	5870	172
H49E	4934	405	6143	172
H49F	4343	1095	6432	172
H50D	2846	-686	5427	282
H50E	4107	-245	5407	282
H50F	2943	-55	4984	282

Table S8. **Atomic Occupancy for 1.**

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***

C13	0.565(5)	H13A	0.565(5)	H13B	0.565(5)
H13C	0.565(5)	C15	0.565(5)	H15A	0.565(5)
H15B	0.565(5)	H15C	0.565(5)	C14	0.565(5)
H14A	0.565(5)	H14B	0.565(5)	H14C	0.565(5)
C13'	0.435(5)	H13D	0.435(5)	H13E	0.435(5)
H13F	0.435(5)	C15'	0.435(5)	H15D	0.435(5)
H15E	0.435(5)	H15F	0.435(5)	C14'	0.435(5)
H14D	0.435(5)	H14E	0.435(5)	H14F	0.435(5)
C50	0.698(4)	H50A	0.698(4)	H50B	0.698(4)
H50C	0.698(4)	C49	0.698(4)	H49A	0.698(4)
H49B	0.698(4)	H49C	0.698(4)	C51	0.698(4)
H51A	0.698(4)	H51B	0.698(4)	H51C	0.698(4)
C51'	0.302(4)	H51D	0.302(4)	H51E	0.302(4)
H51F	0.302(4)	C49'	0.302(4)	H49D	0.302(4)
H49E	0.302(4)	H49F	0.302(4)	C50'	0.302(4)
H50D	0.302(4)	H50E	0.302(4)	H50F	0.302(4)

Table S9. Crystal data and structure refinement for **[2,4-di-tert-butyl-6-((2,6-di benzhydryl-4-methoxyphenylimino)methyl)-phenolato]-Ni(Ⅱ)-methyl(trimethyl phosphine)**

data	**2**
Identification code	HXH-2-19
Empirical formula	C52H60NNiOP
Formula weight	804.69
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P21/n
a/Å	10.7570(5)
b/Å	16.9845(6)
c/Å	25.3737(10)
α/°	90
β/°	97.853(4)
γ/°	90
Volume/Å3	4592.4(3)
Z	4
ρcalcg/cm3	1.164
μ/mm-1	0.494
F(000)	1720.0
Crystal size/mm3	0.36 × 0.32 × 0.22

Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.79 to 58.312
Index ranges	-14 ≤ h ≤ 12, -21 ≤ k ≤ 20, -30 ≤ l ≤ 31
Reflections collected	25593
Independent reflections	10561 [Rint = 0.0372, Rsigma = 0.0602]
Data/restraints/parameters	10561/18/522
Goodness-of-fit on F2	1.018
Final R indexes [I>=2σ (I)]	R1 = 0.0570, wR2 = 0.1247
Final R indexes [all data]	R1 = 0.1041, wR2 = 0.1468
Largest diff. peak/hole / e Å-3	0.36/-0.32

Table S10. Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103) for 2. Ueq is defined as 1/3 of of the t race of the orthogonalised UIJ tensor.

Atom	x	y	z	U(eq)
Ni1	6644.8(3)	1571.1(2)	5639.8(2)	40.98(12)
P1	7700.1(9)	504.6(5)	5763.9(4)	65.2(3)
O1	6554.7(18)	1395.2(10)	4884.8(7)	47.0(5)
N1	5575(2)	2486.5(12)	5539.9(8)	37.8(5)
C22	4453(3)	2992.7(15)	6253(1)	41.8(6)
C24	7503(3)	3632.0(15)	5752.3(11)	42.1(6)
C20	5261(3)	4134.3(15)	6765.7(11)	45.9(7)
C21	4375(3)	3550.7(15)	6652.5(11)	46.5(7)
C2	4863(2)	2259.2(14)	4589.8(10)	37.3(6)
C26	7449(3)	3442.4(18)	4767.1(12)	51.3(7)
C4	5822(3)	1473.4(16)	3950.6(11)	46.6(7)
C19	6251(3)	4168.2(15)	6468.0(11)	44.5(7)
C25	7164(2)	3910.3(16)	5179.8(11)	44.1(6)
C44	2480(3)	2524.1(17)	5680.4(12)	47.7(7)
C1	4883(2)	2641.2(15)	5092.6(10)	38.4(6)
C6	3911(3)	2264.8(16)	3664.6(11)	46.3(7)
C30	6572(3)	4625.7(18)	5053.6(13)	56.6(8)
C18	6372(2)	3631.4(14)	6064.2(10)	38.4(6)
C7	3953(3)	2525.1(16)	4178.5(11)	44.5(6)
C3	5769(2)	1690.7(15)	4495.4(10)	39.4(6)
C38	2960(3)	2064.8(17)	6643.9(12)	55.7(8)
C5	4881(3)	1754.3(17)	3569.3(11)	50.5(7)
C37	3490(3)	2332.4(16)	6142.9(11)	47.1(7)
C32	8647(3)	4034.5(18)	6054.5(12)	50.3(7)
C17	5449(2)	3051.2(14)	5956.3(10)	37.7(6)

C12	2901(3)	2542.1(19)	3217.2(12)	57.9(8)
C23	5170(3)	4704.1(19)	7220.7(13)	64.0(9)
C45	1956(3)	3268.9(19)	5609.4(13)	60.6(8)
C27	7148(3)	3674(2)	4242.3(13)	68.4(9)
C28	6577(3)	4386(2)	4125.6(14)	76.1(11)
C49	2055(3)	1947(2)	5314.9(13)	60.4(8)
C29	6289(3)	4862(2)	4525.2(15)	69.2(10)
C8	6887(3)	955(2)	3794.1(12)	65.1(9)
C33	9310(3)	3656(2)	6481.6(13)	67.7(9)
C48	1156(3)	2107(3)	4889.8(15)	78.0(11)
C31	9090(3)	4762(2)	5921.4(17)	80.5(11)
C47	659(3)	2843(3)	4818.1(15)	76.8(11)
C34	10367(4)	3981(3)	6772.0(16)	87.7(12)
C46	1050(3)	3423(2)	5177.2(16)	73.3(10)
C9	8152(4)	1349(3)	3986.1(16)	87.6(12)
C43	1695(4)	2030(2)	6674.6(16)	87.3(12)
C39	3764(4)	1827(3)	7084.1(16)	91.6(13)
C10	6809(4)	134(2)	4035.9(16)	95.4(14)
C40	3305(6)	1585(3)	7548.6(18)	116.9(19)
C11	6808(4)	848(3)	3187.9(14)	104.4(16)
C16	6893(4)	1676(2)	6407.3(13)	85.8(13)
C42	1258(5)	1774(3)	7138(2)	113.8(17)
C35	10776(4)	4701(3)	6636(2)	100.8(15)
C41	2076(6)	1563(3)	7572.4(19)	117.4(19)
C51	8967(4)	409(3)	5362(2)	113.6(17)
C36	10144(4)	5084(3)	6214(2)	109.3(17)
C50	6706(5)	-338(2)	5540(2)	122.3(19)
C52	8424(8)	168(4)	6396(2)	212(4)
C13	1600(5)	2443(5)	3393(2)	102(2)
C14	2862(7)	2043(4)	2707(3)	97(2)
C15	3128(8)	3383(4)	3086(3)	114(3)
C13'	2062(12)	3247(11)	3411(5)	102(2)
C15'	3644(16)	2952(9)	2789(7)	114(3)
C14'	2169(15)	1877(9)	2970(6)	97(2)

Table S11. **Anisotropic Displacement Parameters (Å2×103) for 2. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].**

Atom	U11	U22	U33	U23	U13	U12
Ni1	50.6(2)	38.87(19)	30.96(19)	-1.13(15)	-3.34(14)	6.66(15)

P1	83.4(7)	57.6(5)	52.1(5)	7.8(4)	0.6(4)	27.6(4)
O1	56.6(12)	49.5(11)	32.1(10)	-4.8(8)	-3.8(8)	15.4(9)
N1	46.2(13)	35.8(11)	30.3(12)	-2.1(9)	1.2(9)	1.5(9)
C22	54.1(17)	36.8(14)	34.4(15)	0.1(11)	5.7(12)	0.7(12)
C24	46.7(16)	39.5(14)	38.8(15)	-2.4(11)	1.2(12)	0.6(11)
C20	65.7(19)	40.6(15)	30.8(15)	-4.5(12)	4.3(13)	4.9(13)
C21	56.4(18)	46.5(16)	38.3(16)	-2.4(12)	12.7(13)	1.0(13)
C2	41.2(15)	38.9(14)	30.0(13)	-1.7(11)	-1.4(11)	1.2(11)
C26	51.3(18)	58.5(18)	45.8(17)	1.4(14)	12.4(13)	1.8(14)
C4	54.8(18)	51.7(16)	32.0(15)	-6.0(12)	1.5(12)	6.2(13)
C19	53.6(17)	37.8(14)	39.8(16)	-4.0(12)	-2.0(13)	-2.4(12)
C25	39.2(15)	51.5(16)	41.1(16)	2.0(13)	3.7(12)	-1.0(12)
C44	48.5(17)	50.2(16)	46.1(17)	0.8(13)	13.2(13)	-4.0(13)
C1	39.6(15)	36.8(13)	37.7(15)	-0.8(11)	1.9(11)	2.8(11)
C6	49.8(17)	50.7(16)	35.1(15)	3.4(13)	-5.6(12)	-2.4(13)
C30	58.2(19)	59.8(19)	51.8(19)	5.4(15)	7.7(15)	8.5(15)
C18	45.7(16)	37.0(14)	31.6(14)	1.1(11)	2.1(11)	3.5(11)
C7	42.6(16)	46.3(15)	43.2(16)	0.4(13)	0.2(12)	2.5(12)
C3	43.7(15)	40.2(14)	32.2(14)	-1.7(11)	-2.6(11)	0.5(11)
C38	74(2)	46.6(17)	47.1(18)	2.7(14)	8.7(15)	-14.1(15)
C5	61.2(19)	58.7(18)	29.8(15)	-6.8(13)	-0.5(13)	0.5(14)
C37	57.0(18)	41.2(15)	43.4(17)	-0.8(13)	7.9(13)	-3.4(13)
C32	43.2(16)	59.4(18)	47.7(18)	-9.2(14)	4.5(13)	1.2(14)
C17	47.9(16)	35.1(13)	28.3(13)	-0.7(11)	-1.3(11)	7.1(11)
C12	63(2)	68(2)	37.0(17)	5.4(15)	-10.3(14)	7.2(16)
C23	85(2)	62(2)	46.0(19)	-18.1(16)	12.7(16)	-2.6(17)
C45	64(2)	61(2)	57(2)	-2.5(16)	10.7(16)	6.0(16)
C27	80(2)	84(2)	43.4(19)	2.3(18)	19.4(17)	0(2)
C28	79(3)	105(3)	44(2)	23(2)	8.0(17)	8(2)
C49	62(2)	59.5(19)	58(2)	-5.8(16)	2.1(16)	-5.4(16)
C29	68(2)	76(2)	64(2)	27.3(19)	9.8(18)	15.5(18)
C8	80(2)	76(2)	38.4(18)	-10.3(16)	5.6(16)	26.2(19)
C33	62(2)	88(2)	50(2)	-0.6(18)	-3.5(16)	-6.6(18)
C48	66(2)	95(3)	69(3)	-14(2)	-4.7(19)	-8(2)
C31	68(2)	69(2)	99(3)	4(2)	-9(2)	-12.2(19)
C47	51(2)	115(3)	62(2)	2(2)	1.0(17)	6(2)
C34	67(3)	127(4)	62(3)	-19(2)	-15.5(19)	-1(3)
C46	66(2)	83(3)	72(3)	12(2)	11.1(19)	21.6(19)
C9	67(3)	121(3)	76(3)	-7(2)	16(2)	26(2)
C43	83(3)	113(3)	69(3)	21(2)	23(2)	-7(2)

C39	93(3)	110(3)	68(3)	37(2)	-3(2)	-30(2)
C10	131(4)	71(2)	81(3)	-17(2)	3(3)	39(2)
C40	135(5)	136(4)	71(3)	50(3)	-16(3)	-57(4)
C11	125(4)	143(4)	45(2)	-22(2)	8(2)	62(3)
C16	140(4)	77(2)	35.2(18)	-1.8(17)	-10(2)	53(2)
C42	108(4)	159(5)	82(3)	26(3)	42(3)	-22(3)
C35	63(3)	122(4)	111(4)	-49(3)	-11(2)	-16(3)
C41	161(5)	127(4)	66(3)	23(3)	22(3)	-62(4)
C51	84(3)	119(4)	143(5)	22(3)	32(3)	40(3)
C36	87(3)	82(3)	149(5)	-7(3)	-18(3)	-32(2)
C50	145(5)	60(3)	170(6)	2(3)	49(4)	-3(3)
C52	363(11)	175(6)	80(4)	14(4)	-35(5)	182(7)
C13	60(3)	172(6)	69(3)	28(4)	-14(3)	23(4)
C14	100(5)	122(4)	58(4)	-10(3)	-31(3)	21(4)
C15	138(6)	90(5)	98(5)	41(4)	-39(4)	8(4)
C13'	60(3)	172(6)	69(3)	28(4)	-14(3)	23(4)
C15'	138(6)	90(5)	98(5)	41(4)	-39(4)	8(4)
C14'	100(5)	122(4)	58(4)	-10(3)	-31(3)	21(4)

Table S12. Bond Lengths for 2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ni1	P1	2.1381(9)	C6	C5	1.403(4)
Ni1	O1	1.9284(18)	C6	C12	1.534(4)
Ni1	N1	1.930(2)	C30	C29	1.393(4)
Ni1	C16	1.937(3)	C18	C17	1.399(4)
P1	C51	1.817(4)	C38	C37	1.531(4)
P1	C50	1.830(5)	C38	C43	1.375(5)
P1	C52	1.780(5)	C38	C39	1.376(5)
O1	C3	1.309(3)	C32	C33	1.373(4)
N1	C1	1.296(3)	C32	C31	1.382(5)
N1	C17	1.447(3)	C12	C13	1.535(7)
C22	C21	1.399(4)	C12	C14	1.543(7)
C22	C37	1.526(4)	C12	C15	1.495(7)
C22	C17	1.394(4)	C12	C13'	1.616(15)
C24	C25	1.524(4)	C12	C15'	1.594(17)
C24	C18	1.539(4)	C12	C14'	1.467(15)
C24	C32	1.521(4)	C45	C46	1.389(5)
C20	C21	1.378(4)	C27	C28	1.369(5)
C20	C19	1.388(4)	C28	C29	1.366(5)
C20	C23	1.520(4)	C49	C48	1.374(5)

C2	C1	1.429(3)	C8	C9	1.535(5)
C2	C7	1.405(4)	C8	C10	1.531(5)
C2	C3	1.415(4)	C8	C11	1.540(4)
C26	C25	1.382(4)	C33	C34	1.382(5)
C26	C27	1.384(4)	C48	C47	1.362(5)
C4	C3	1.439(4)	C31	C36	1.380(5)
C4	C5	1.386(4)	C47	C46	1.369(5)
C4	C8	1.540(4)	C34	C35	1.360(6)
C19	C18	1.391(4)	C43	C42	1.394(5)
C25	C30	1.389(4)	C39	C40	1.400(6)
C44	C37	1.522(4)	C40	C41	1.333(7)
C44	C45	1.387(4)	C42	C41	1.361(7)
C44	C49	1.383(4)	C35	C36	1.354(6)
C6	C7	1.372(4)			

Table S13. Bond Angles for 2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ni1	P1	88.20(6)	C2	C3	C4	117.1(2)
O1	Ni1	N1	92.64(8)	C43	C38	C37	122.9(3)
O1	Ni1	C16	173.85(12)	C43	C38	C39	117.3(3)
N1	Ni1	P1	175.37(7)	C39	C38	C37	119.8(3)
N1	Ni1	C16	93.21(11)	C4	C5	C6	125.6(3)
C16	Ni1	P1	86.11(10)	C22	C37	C38	112.7(2)
C51	P1	Ni1	114.66(15)	C44	C37	C22	112.3(2)
C51	P1	C50	101.9(2)	C44	C37	C38	113.3(2)
C50	P1	Ni1	109.95(16)	C33	C32	C24	119.0(3)
C52	P1	Ni1	124.27(18)	C33	C32	C31	116.9(3)
C52	P1	C51	102.0(3)	C31	C32	C24	124.1(3)
C52	P1	C50	101.2(3)	C22	C17	N1	120.2(2)
C3	O1	Ni1	129.06(17)	C22	C17	C18	121.4(2)
C1	N1	Ni1	122.61(18)	C18	C17	N1	118.3(2)
C1	N1	C17	113.9(2)	C6	C12	C13	109.4(3)
C17	N1	Ni1	123.48(16)	C6	C12	C14	112.8(3)
C21	C22	C37	121.6(2)	C6	C12	C13'	111.8(5)
C17	C22	C21	118.0(2)	C6	C12	C15'	105.6(6)
C17	C22	C37	120.4(2)	C13	C12	C14	105.2(4)
C25	C24	C18	112.8(2)	C15	C12	C6	109.7(4)
C32	C24	C25	114.4(2)	C15	C12	C13	110.7(5)
C32	C24	C18	112.5(2)	C15	C12	C14	108.9(5)
C21	C20	C19	118.5(2)	C15'	C12	C13'	103.6(9)

C21	C20	C23	120.1(3)	C14'	C12	C6	111.3(6)
C19	C20	C23	121.4(3)	C14'	C12	C13'	114.3(9)
C20	C21	C22	122.0(3)	C14'	C12	C15'	109.6(9)
C7	C2	C1	116.2(2)	C44	C45	C46	120.2(3)
C7	C2	C3	121.3(2)	C28	C27	C26	119.9(3)
C3	C2	C1	122.3(2)	C29	C28	C27	120.2(3)
C25	C26	C27	121.2(3)	C48	C49	C44	121.3(3)
C3	C4	C8	121.5(2)	C28	C29	C30	120.1(3)
C5	C4	C3	117.5(2)	C4	C8	C11	112.6(3)
C5	C4	C8	121.0(3)	C9	C8	C4	109.2(3)
C20	C19	C18	122.0(3)	C9	C8	C11	107.1(3)
C26	C25	C24	119.7(2)	C10	C8	C4	109.5(3)
C26	C25	C30	118.1(3)	C10	C8	C9	111.4(3)
C30	C25	C24	122.2(3)	C10	C8	C11	107.1(3)
C45	C44	C37	122.0(3)	C32	C33	C34	122.3(4)
C49	C44	C37	120.1(3)	C47	C48	C49	120.5(4)
C49	C44	C45	117.9(3)	C36	C31	C32	120.6(4)
N1	C1	C2	128.8(2)	C48	C47	C46	119.5(4)
C7	C6	C5	115.7(2)	C35	C34	C33	119.6(4)
C7	C6	C12	122.2(3)	C47	C46	C45	120.6(3)
C5	C6	C12	122.0(3)	C38	C43	C42	120.8(4)
C25	C30	C29	120.5(3)	C38	C39	C40	121.0(4)
C19	C18	C24	122.6(2)	C41	C40	C39	120.8(4)
C19	C18	C17	118.1(2)	C41	C42	C43	120.6(5)
C17	C18	C24	119.3(2)	C36	C35	C34	119.2(4)
C6	C7	C2	122.1(3)	C40	C41	C42	119.4(4)
O1	C3	C2	121.5(2)	C35	C36	C31	121.4(4)
O1	C3	C4	121.4(2)				

Table S14. **Torsion Angles for 2.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ni1	O1	C3	C2	4.2(4)	C5	C4	C3	C2	-8.4(4)
Ni1	O1	C3	C4	-178.24(19)	C5	C4	C8	C9	122.4(3)
Ni1	N1	C1	C2	-8.0(4)	C5	C4	C8	C10	-115.4(3)
Ni1	N1	C17	C22	-96.6(3)	C5	C4	C8	C11	3.6(5)
Ni1	N1	C17	C18	81.0(3)	C5	C6	C7	C2	-3.9(4)
C24	C25	C30	C29	179.4(3)	C5	C6	C12	C13	132.0(4)
C24	C18	C17	N1	-2.0(3)	C5	C6	C12	C14	15.2(5)
C24	C18	C17	C22	175.5(2)	C5	C6	C12	C15	-106.4(5)
C24	C32	C33	C34	179.3(3)	C5	C6	C12	C13'	-169.1(7)

C24	C32	C31	C36	-179.4(4)	C5	C6	C12	C15'	-57.1(8)
C20	C19	C18	C24	-176.4(2)	C5	C6	C12	C14'	61.7(8)
C20	C19	C18	C17	0.9(4)	C37	C22	C21	C20	178.0(3)
C21	C22	C37	C44	97.9(3)	C37	C22	C17	N1	0.2(4)
C21	C22	C37	C38	-31.6(4)	C37	C22	C17	C18	-177.3(2)
C21	C22	C17	N1	179.8(2)	C37	C44	C45	C46	179.0(3)
C21	C22	C17	C18	2.3(4)	C37	C44	C49	C48	-179.1(3)
C21	C20	C19	C18	-0.3(4)	C37	C38	C43	C42	179.3(4)
C26	C25	C30	C29	-0.6(4)	C37	C38	C39	C40	179.5(4)
C26	C27	C28	C29	-0.9(6)	C32	C24	C25	C26	103.7(3)
C19	C20	C21	C22	0.7(4)	C32	C24	C25	C30	-76.2(3)
C19	C18	C17	N1	-179.4(2)	C32	C24	C18	C19	22.0(4)
C19	C18	C17	C22	-1.9(4)	C32	C24	C18	C17	-155.3(2)
C25	C24	C18	C19	-109.3(3)	C32	C33	C34	C35	0.0(6)
C25	C24	C18	C17	73.5(3)	C32	C31	C36	C35	0.2(7)
C25	C24	C32	C33	-156.1(3)	C17	N1	C1	C2	173.3(3)
C25	C24	C32	C31	22.6(4)	C17	C22	C21	C20	-1.6(4)
C25	C26	C27	C28	1.2(5)	C17	C22	C37	C44	-82.6(3)
C25	C30	C29	C28	0.9(5)	C17	C22	C37	C38	148.0(3)
C44	C45	C46	C47	0.3(5)	C12	C6	C7	C2	178.7(3)
C44	C49	C48	C47	-0.1(6)	C12	C6	C5	C4	-179.6(3)
C1	N1	C17	C22	82.2(3)	C23	C20	C21	C22	-177.1(3)
C1	N1	C17	C18	-100.3(3)	C23	C20	C19	C18	177.4(3)
C1	C2	C7	C6	173.4(3)	C45	C44	C37	C22	-40.8(4)
C1	C2	C3	O1	10.8(4)	C45	C44	C37	C38	88.4(3)
C1	C2	C3	C4	-166.9(2)	C45	C44	C49	C48	1.0(5)
C18	C24	C25	C26	-125.9(3)	C27	C26	C25	C24	179.6(3)
C18	C24	C25	C30	54.1(3)	C27	C26	C25	C30	-0.5(4)
C18	C24	C32	C33	73.5(3)	C27	C28	C29	C30	-0.2(6)
C18	C24	C32	C31	-107.9(3)	C49	C44	C37	C22	139.3(3)
C7	C2	C1	N1	176.2(3)	C49	C44	C37	C38	-91.5(3)
C7	C2	C3	O1	-174.5(2)	C49	C44	C45	C46	-1.1(5)
C7	C2	C3	C4	7.9(4)	C49	C48	C47	C46	-0.8(6)
C7	C6	C5	C4	3.0(4)	C8	C4	C3	O1	-6.7(4)
C7	C6	C12	C13	-50.8(5)	C8	C4	C3	C2	171.0(3)
C7	C6	C12	C14	-167.5(4)	C8	C4	C5	C6	-176.2(3)
C7	C6	C12	C15	70.8(5)	C33	C32	C31	C36	-0.7(6)
C7	C6	C12	C13'	8.1(8)	C33	C34	C35	C36	-0.5(7)
C7	C6	C12	C15'	120.1(8)	C48	C47	C46	C45	0.6(6)
C7	C6	C12	C14'	-121.0(8)	C31	C32	C33	C34	0.6(5)

C3	C2	C1	N1	-8.8(4)	C34	C35	C36	C31	0.4(8)
C3	C2	C7	C6	-1.6(4)	C43	C38	C37	C22	126.8(3)
C3	C4	C5	C6	3.2(4)	C43	C38	C37	C44	-2.2(4)
C3	C4	C8	C9	-57.0(4)	C43	C38	C39	C40	-2.1(6)
C3	C4	C8	C10	65.2(4)	C43	C42	C41	C40	-1.6(9)
C3	C4	C8	C11	-175.8(3)	C39	C38	C37	C22	-54.9(4)
C38	C43	C42	C41	0.9(8)	C39	C38	C37	C44	176.2(3)
C38	C39	C40	C41	1.5(8)	C39	C38	C43	C42	0.9(6)
C5	C4	C3	O1	173.9(3)	C39	C40	C41	C42	0.4(8)

Table S15. Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for 2.

Atom	x	y	z	U(eq)
H24	7740	3078	5727	50
H21	3704	3527	6848	56
H26	7851	2963	4843	62
H19	6851	4562	6541	53
H1	4324	3057	5100	46
H30	6363	4949	5324	68
H7	3360	2890	4257	53
H5	4894	1590	3220	61
H37	3950	1880	6028	57
H23A	5855	5071	7245	96
H23B	5208	4416	7548	96
H23C	4390	4985	7156	96
H45	2212	3667	5852	73
H27	7333	3348	3969	82
H28	6385	4545	3773	91
H49	2384	1442	5358	72
H29	5903	5345	4444	83
H33	9039	3163	6579	81
H48	886	1710	4649	94
H31	8674	5036	5633	97
H47	57	2950	4527	92
H34	10795	3709	7059	105
H46	705	3925	5131	88
H9A	8219	1830	3793	131
H9B	8822	1001	3926	131
H9C	8208	1462	4359	131
H43	1125	2179	6383	105

H39	4624	1827	7073	110
H10A	6882	176	4416	143
H10B	7478	-188	3941	143
H10C	6018	-102	3902	143
H40	3866	1439	7844	140
H11A	6047	574	3056	157
H11B	7516	548	3109	157
H11C	6810	1355	3020	157
H16A	6548	1225	6563	129
H16B	6480	2143	6506	129
H16C	7775	1711	6533	129
H42	399	1746	7150	137
H35	11482	4927	6830	121
H41	1779	1404	7883	141
H51A	8648	502	4995	170
H51B	9311	-113	5401	170
H51C	9610	786	5478	170
H36	10426	5575	6119	131
H50A	6147	-446	5796	183
H50B	7223	-791	5506	183
H50C	6226	-220	5202	183
H52A	8999	561	6555	318
H52B	8872	-311	6353	318
H52C	7793	73	6622	318
H13A	1469	1899	3473	154
H13B	967	2611	3112	154
H13C	1552	2755	3705	154
H14A	2707	1503	2787	146
H14B	3652	2085	2572	146
H14C	2203	2232	2444	146
H15A	2494	3555	2806	171
H15B	3939	3433	2972	171
H15C	3096	3703	3396	171
H13D	2604	3652	3577	154
H13E	1549	3046	3662	154
H13F	1535	3463	3110	154
H15D	4084	3405	2946	171
H15E	3061	3113	2488	171
H15F	4234	2586	2676	171
H14D	1545	2068	2693	146

H14E	1766	1610	3234	146
H14F	2718	1518	2823	146

Table S16. Atomic Occupancy for 2.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
C13	0.681(4)	H13A	0.681(4)	H13B	0.681(4)
H13C	0.681(4)	C14	0.681(4)	H14A	0.681(4)
H14B	0.681(4)	H14C	0.681(4)	C15	0.681(4)
H15A	0.681(4)	H15B	0.681(4)	H15C	0.681(4)
C13'	0.319(4)	H13D	0.319(4)	H13E	0.319(4)
H13F	0.319(4)	C15'	0.319(4)	H15D	0.319(4)
H15E	0.319(4)	H15F	0.319(4)	C14'	0.319(4)
H14D	0.319(4)	H14E	0.319(4)	H14F	0.319(4)