Electronic Supporting Information for:

C–H Activation of Ethers by Pyridine Tethered $PC_{sp3}P$ type Iridium Complexes

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1 X-ray Data for Compounds 6, 9, 10 and 11

X−Ray crystal structure of [(PC^{Py}P)Ir(COD)] (6). Single crystals were obtained as pale orange blocks by diffusion of *n*-pentane into a concentrated THF solution at room temperature in the glovebox. Crystal and refinement data for **6**: $C_{50}H_{44}IrNP_2$; M_r = 913.00; Monoclinic; space group $P2_1/n$; a = 9.9433(4) Å; b = 24.0410(9) Å; c = 15.8819(6) Å; α = 90°; β = 91.8887(14)°; γ = 90°; V = 3794.5(3) Å^3; Z = 4; T = 120(2) K; λ = 0.71073 Å; μ = 3.641 mm^{-1}; d_{calc} = 1.598 g·cm^{-3}; 53230 reflections collected; 6681 unique (R_{int} = 0.0281); giving R_1 = 0.0149, wR_2 = 0.0326 for 6197 data with [I>2σ(I)] and R_1 = 0.0175, wR_2 = 0.0332 for all 6681 data. Residual electron density (e$^-$·Å^{-3}) max/min: 0.346/−0.393.

X−Ray crystal structure of [(PC^{Py}P)IrH(C$_4$H$_7$O)] (9). Single crystals were obtained in the glovebox as pale-yellow blocks by diffusion of *n*-pentane into a concentrated THF solution at room temperature in the presence of small amount of NBE. Crystal and refinement data for **9**: $C_{46}H_{40}IrNOP_2$; M_r = 876.93; Monoclinic; space group $C2/c$; a = 42.2630(17) Å; b = 9.1164(4) Å; c = 18.8750(7) Å; α = 90°; β = 92.105(3)°; γ = 90°; V = 7267.4(5) Å^3; Z = 8; T = 120(2) K; λ = 0.71073 Å; μ = 3.801 mm^{-1}; d_{calc} = 1.603 g·cm^{-3}; 55245 reflections collected; 6399 unique (R_{int} = 0.0551); giving R_1 = 0.0296, wR_2 = 0.0608 for 5483 data with [I>2σ(I)] and R_1 = 0.0393, wR_2 = 0.0635 for all 6399 data. Residual electron density (e$^-$·Å^{-3}) max/min: 1.100/−0.612. The deprotonated THF molecule substituent on the iridium atom is disordered over two positions and this disorder was modeled (occupancy is 44% for one and 56% for the other position)

X−Ray crystal structure of [(PC^{Py}P)IrH(CH$_2$O^{t}Bu] (10). Single crystals were obtained as pale-yellow blocks by diffusion of *n*-pentane into a concentrated THF solution at −35 °C in the glovebox. Crystal and refinement data for **10**: $C_{47}H_{44}IrNOP_2$; M_r = 892.97; Monoclinic; space group $P2_1/c$; a = 17.280(3) Å; b = 14.146(2) Å; c = 18.792(3) Å; α = 90°; β = 104.829(2)°; γ = 90°; V = 4440.5(11) Å^3; Z = 4; T = 120(2) K; λ = 0.71073 Å; μ = 3.111 mm^{-1}; d_{calc} = 1.336 g·cm^{-3}; 66672 reflections collected; 7823 unique (R_{int} = 0.0705); giving R_1 = 0.0315, wR_2 = 0.0676 for 6216 data with [I>2σ(I)] and R_1 = 0.0493, wR_2 = 0.0723 for all 7823 data. Residual electron density (e$^-$·Å^{-3}) max/min: 0.997/−0.515. A highly disordered molecule of *n*-pentane was removed using the SQUEEZE function in PLATON.

X−Ray crystal structure of [(PC^{Py}P)IrH(C$_4$H$_7$O)(CCHPh)] (11). Single crystals were obtained as red needles by diffusion of *n*-pentane into a concentrated THF solution at room temperature in the glovebox. Crystal and refinement data for **11**: $C_{54}H_{46}IrNOP_2$; M_r = 979.06; Triclinic; space group $P\bar{1}$; a = 10.4635(10) Å; b = 13.3359(12) Å; c = 15.8836(15) Å; α = 77.710(2)°; β = 80.875(3)°; γ = 85.402(2)°; V = 2135.7(3) Å^3; Z = 2; T = 120(2) K; λ = 0.71073 Å; μ = 3.242 mm^{-1}; d_{calc} = 1.522 g·cm^{-3}; 18693 reflections collected; 7517 unique (R_{int} = 0.0626); giving R_1 = 0.0436, wR_2 = 0.0868 for 6065 data with [I>2σ(I)] and R_1 = 0.0635, wR_2 = 0.0919 for all 7517 data. Residual electron density (e$^-$·Å^{-3}) max/min: 3.649/−3.069. The deprotonated THF molecule substituent on the iridium atom is disordered over two positions and this disorder was modeled (occupancy is 80% for one and 20% for the other position).

Table S1. Crystal data and structure refinement for **6**, **9**, **10** and **11**.

Compound:	**6**	**9**	**10**	**11**
Identification code:	pc7	pc25	pc13	pc8b
Empirical formula:	$C_{50}H_{44}IrNP_2$	$C_{46}H_{40}IrNOP_2$	$C_{47}H_{44}IrNOP_2$	$C_{54}H_{46}IrNOP_2$
Formula weight:	913.00	876.93	892.97	979.06
Temperature:	120(2) K	120(2) K	120(2) K	120(2) K
Wavelength:	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system:	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group:	$P2_1/n$	$C2/c$	$P2_1/c$	$P\bar{1}$
Unit cell dimensions:	a = 9.9433(4) Å	a = 42.2630(17)	a = 17.280(3) Å	a = 10.4635(10) Å
	b = 24.0410(9) Å	b = 9.1164(4) Å	b = 14.146(2) Å	b = 13.3359(12) Å
	c = 15.8819(6) Å	c = 18.8750(7) Å	c = 18.792(3) Å	c = 15.8836(15) Å
	α = 90°	α = 90°	α = 90°	α = 77.710(2)°
	β = 91.8887(14)°	β = 92.105(3)°	β = 104.829(2)°	β = 80.875(3)°
	γ = 90°	γ = 90°	γ = 90°	γ = 85.402(2)°
Volume:	3794.5(3) Å^3	7267.4(5) Å^3	4440.5(11) Å^3	2135.7(3) Å^3
Z:	4	8	4	2
Density (calculated):	1.598 g·cm^{-3}	1.603 g·cm^{-3}	1.336 g·cm^{-3}	1.522 g·cm^{-3}
Absorption coefficient (μ):	3.641 mm^{-1}	3.801 mm^{-1}	3.111 mm^{-1}	3.242 mm^{-1}
F(000):	1832	3504	1792	984
Crystal size:	0.04 × 0.03 × 0.03 mm^3	0.11 × 0.09 × 0.08 mm^3	0.09 × 0.08 × 0.08 mm^3	0.09 × 0.08 × 0.07 mm^3
θ range for data collection:	1.54 to 25.00°	0.96 to 25.00°	1.22 to 25.00°	1.56 to 25.00°
Index ranges:	$-7 \le h \le 11$	$-50 \le h \le 50$	$-20 \le h \le 20$	$-12 \le h \le 11$
	$-28 \le k \le 28$	$-7 \le k \le 10$	$-16 \le k \le 16$	$-15 \le k \le 14$
	$-18 \le l \le 18$	$-22 \le l \le 22$	$-22 \le l \le 22$	$-18 \le l \le 16$
Reflections collected:	53230	55245	66672	18693
Independent reflections:	6681 [R_{int} = 0.0281]	6399 [R_{int} = 0.0551]	7823 [R_{int} = 0.0705]	7517 [R_{int} = 0.0626]
Completeness to θ = 25.00°:	100.0 %	100.0 %	100.0 %	100.0 %
Absorption correction:	Semi-empirical	Semi-empirical	Semi-empirical	Semi-empirical
Max. and min. transmission:	0.7073 and 0.5743	0.7457 and 0.6140	0.7455 and 0.6604	0.7454 and 0.6201
Refinement method:	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters:	6681 / 0 / 487	6399 / 0 / 453	7823 / 0 / 476	7517 / 0 / 537
Goodness-of-fit on F^2:	1.049	1.052	1.047	0.981
Final R indices [I>2σ(I)]:	R_1 = 0.0149, wR_2 = 0.0326	R_1 = 0.0296, wR_2 = 0.0608	R_1 = 0.0315, wR_2 = 0.0676	R_1 = 0.0436, wR_2 = 0.0868
R indices (all data):	R_1 = 0.0175, wR_2 = 0.0332	R_1 = 0.0393, wR_2 = 0.0635	R_1 = 0.0493, wR_2 = 0.0723	R_1 = 0.0635, wR_2 = 0.0919
Largest diff. peak and hole:	0.346 and −0.393 e$^-$·Å^{-3}	1.100 and −0.612 e$^-$·Å^{-3}	0.997 and −0.515 e$^-$·Å^{-3}	3.649 and −3.069 e$^-$·Å^{-3}

2 NMR Spectra

2.1 NMR Spectra for PC^{Py}(OH)P (2)

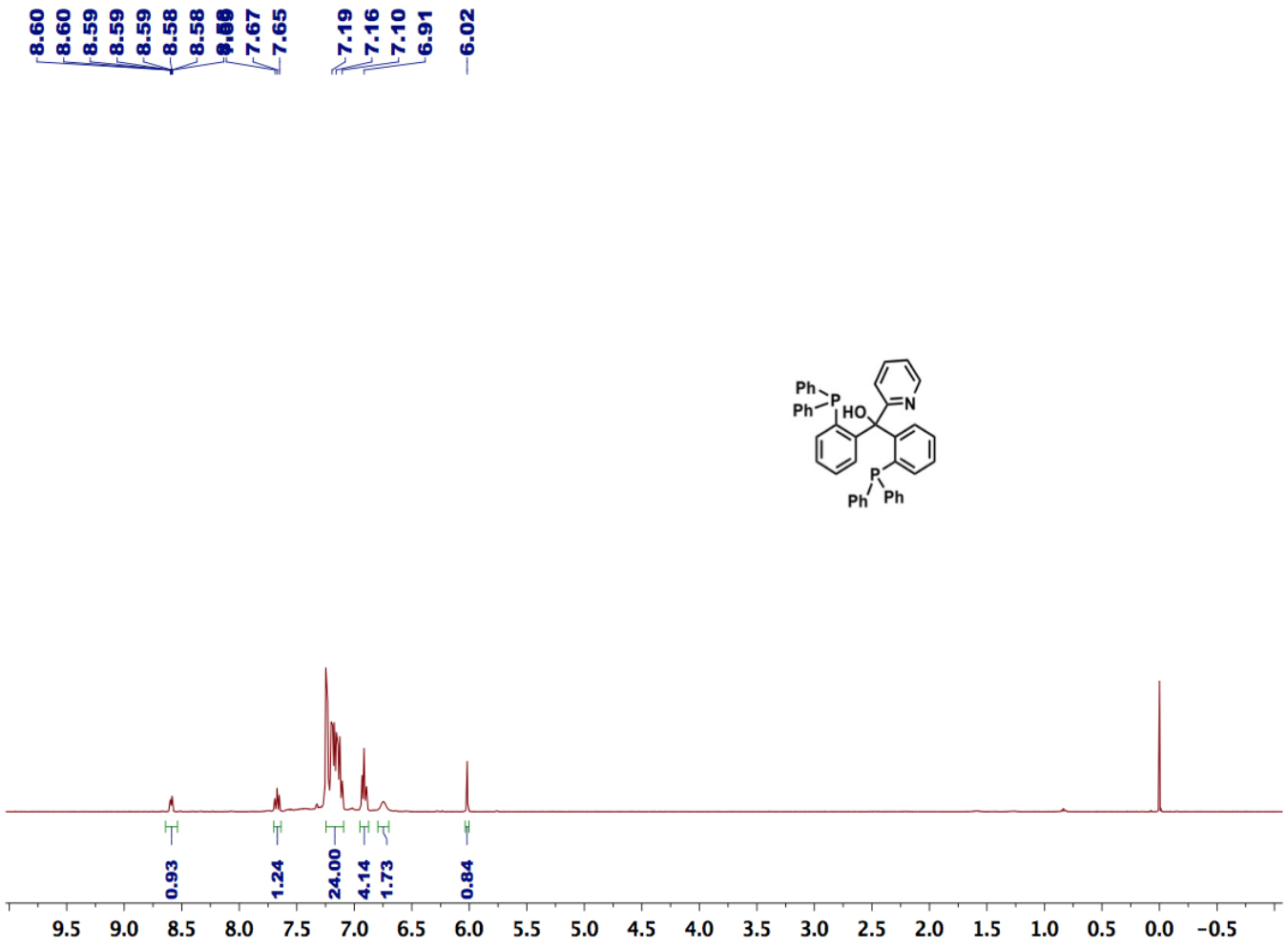

Figure S1. ^{1}H NMR spectrum for PC^{Py}(OH)P (**2**).

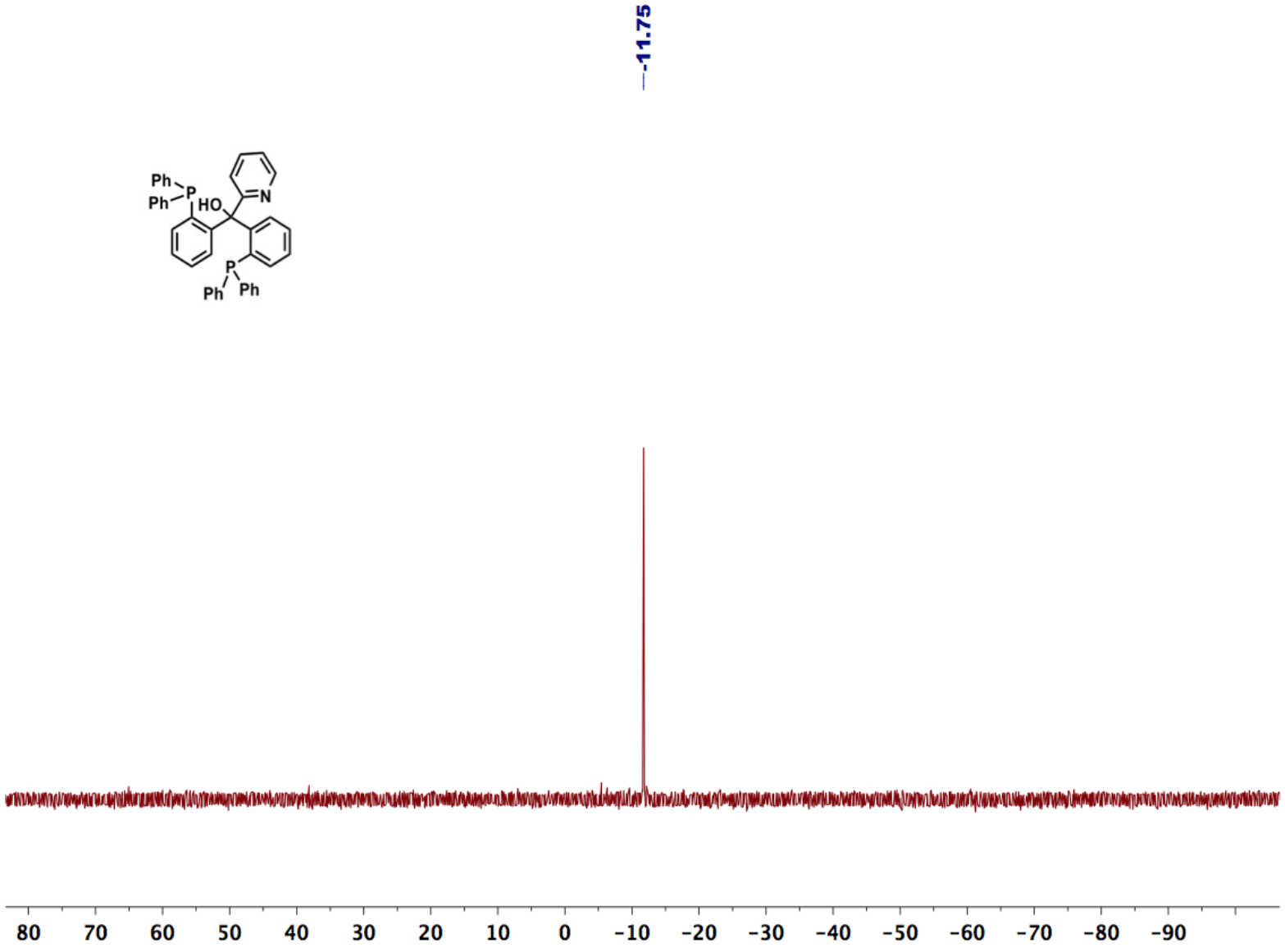

Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum for $PC^{Py}(OH)P$ (**2**).

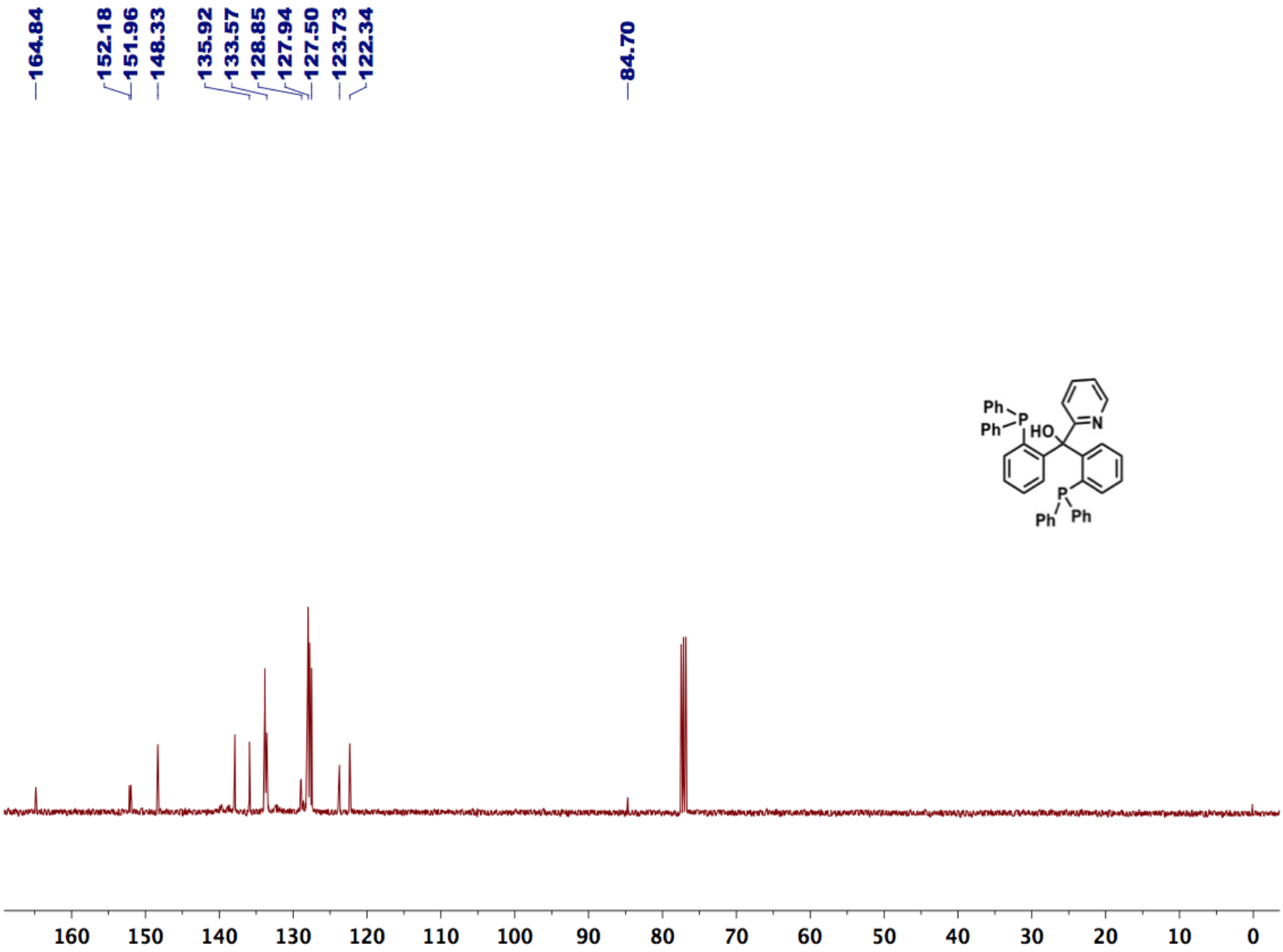

Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum for $PC^{Py}(OH)P$ (**2**).

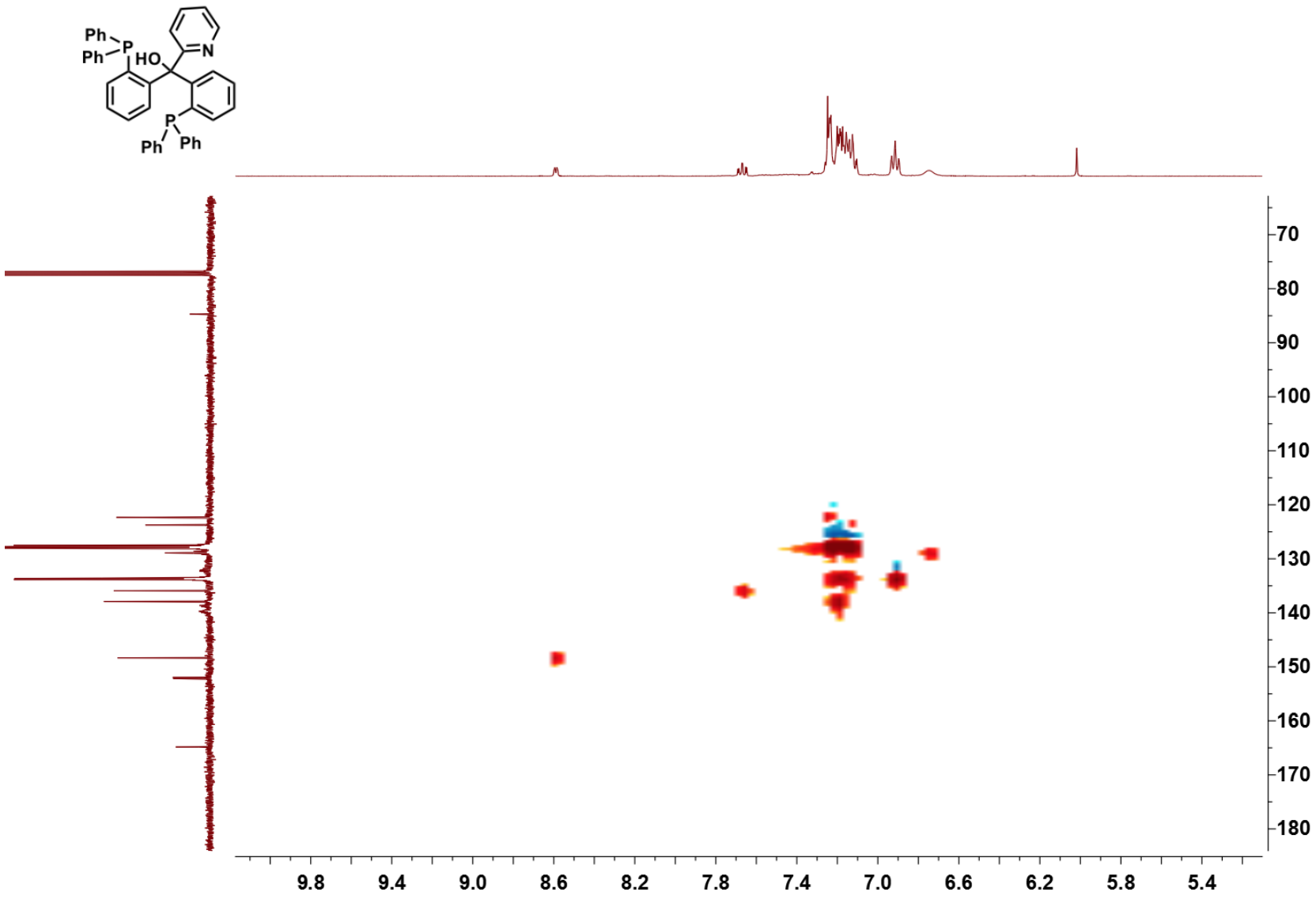

Figure S4. ^{1}H-^{13}C HSQC NMR spectrum for $PC^{Py}(OH)P$ (**2**).

2.2 NMR Spectra for P(O)C^{Py}(OH)P(O) (3)

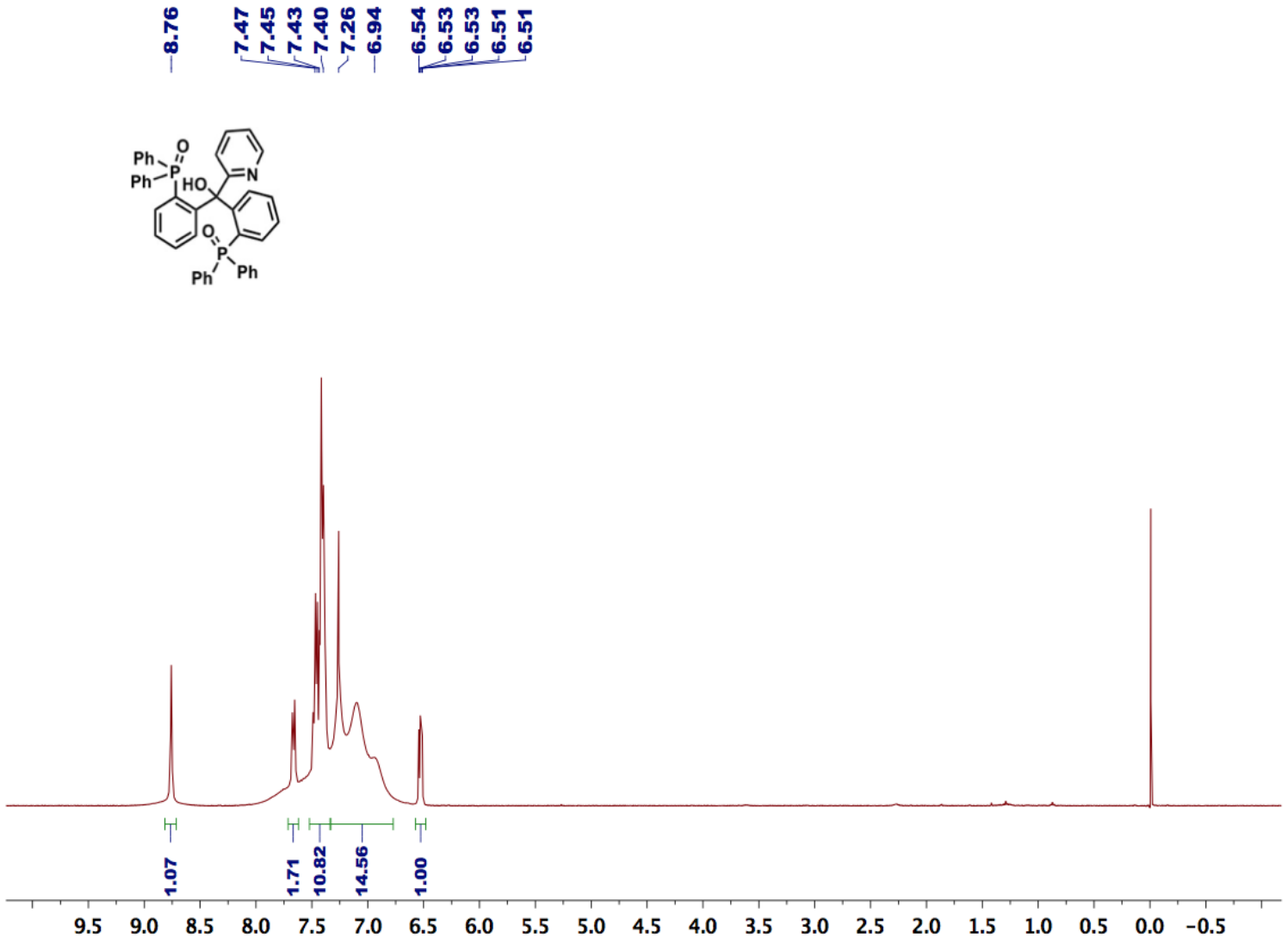

Figure S5. ^{1}H NMR spectrum for P(O)C^{Py}(OH)P(O) (**3**).

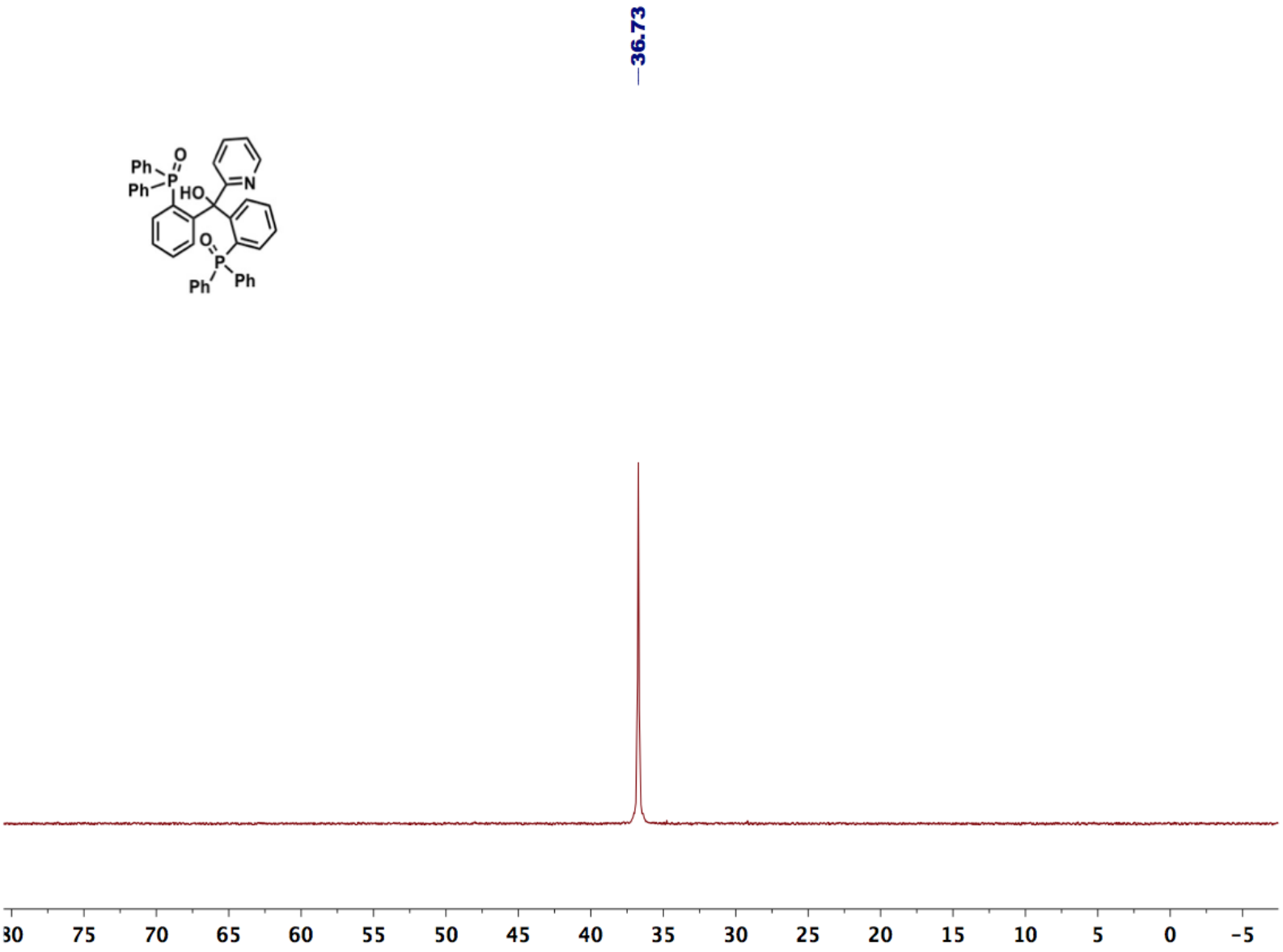

Figure S6. $^{31}P\{^{1}H\}$ NMR spectrum for $P(O)C^{Py}(OH)P(O)$ (**3**).

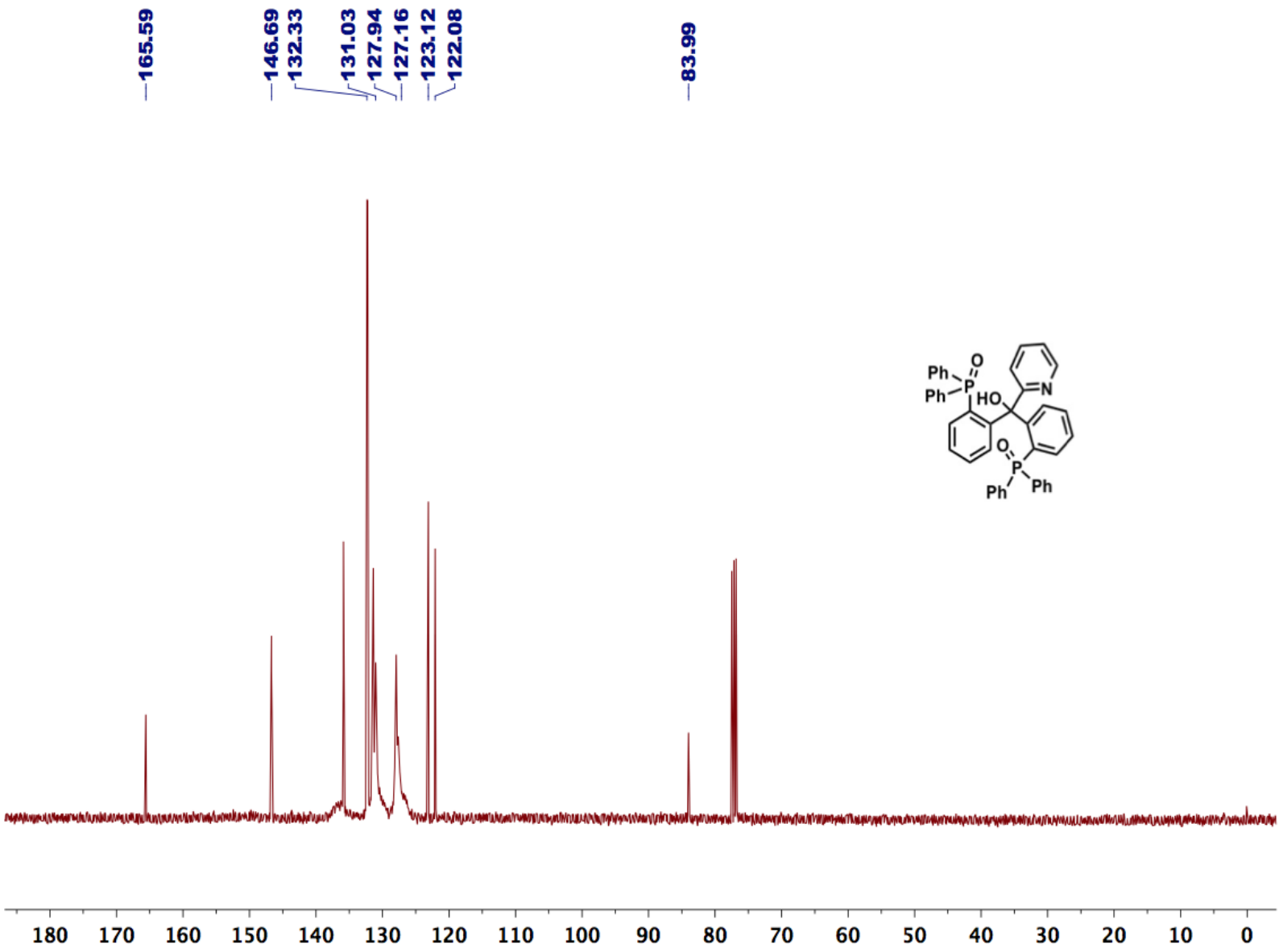

Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum for $P(O)C^{Py}(OH)P(O)$ (**3**).

2.3 NMR Spectra for P(O)C^{Py}HP(O) (4)

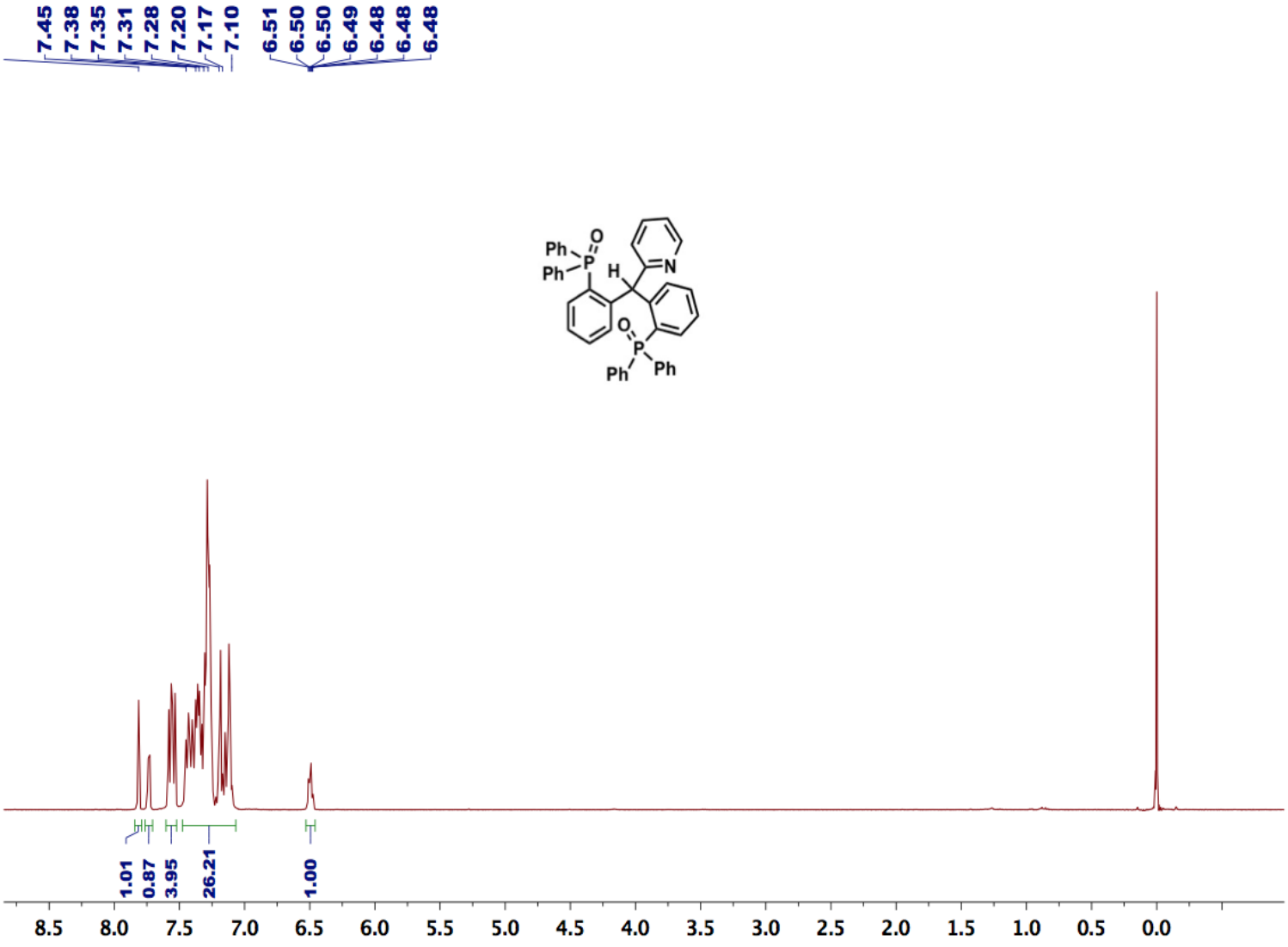

Figure S8. ^{1}H NMR spectrum for P(O)C^{Py}HP(O) (**4**).

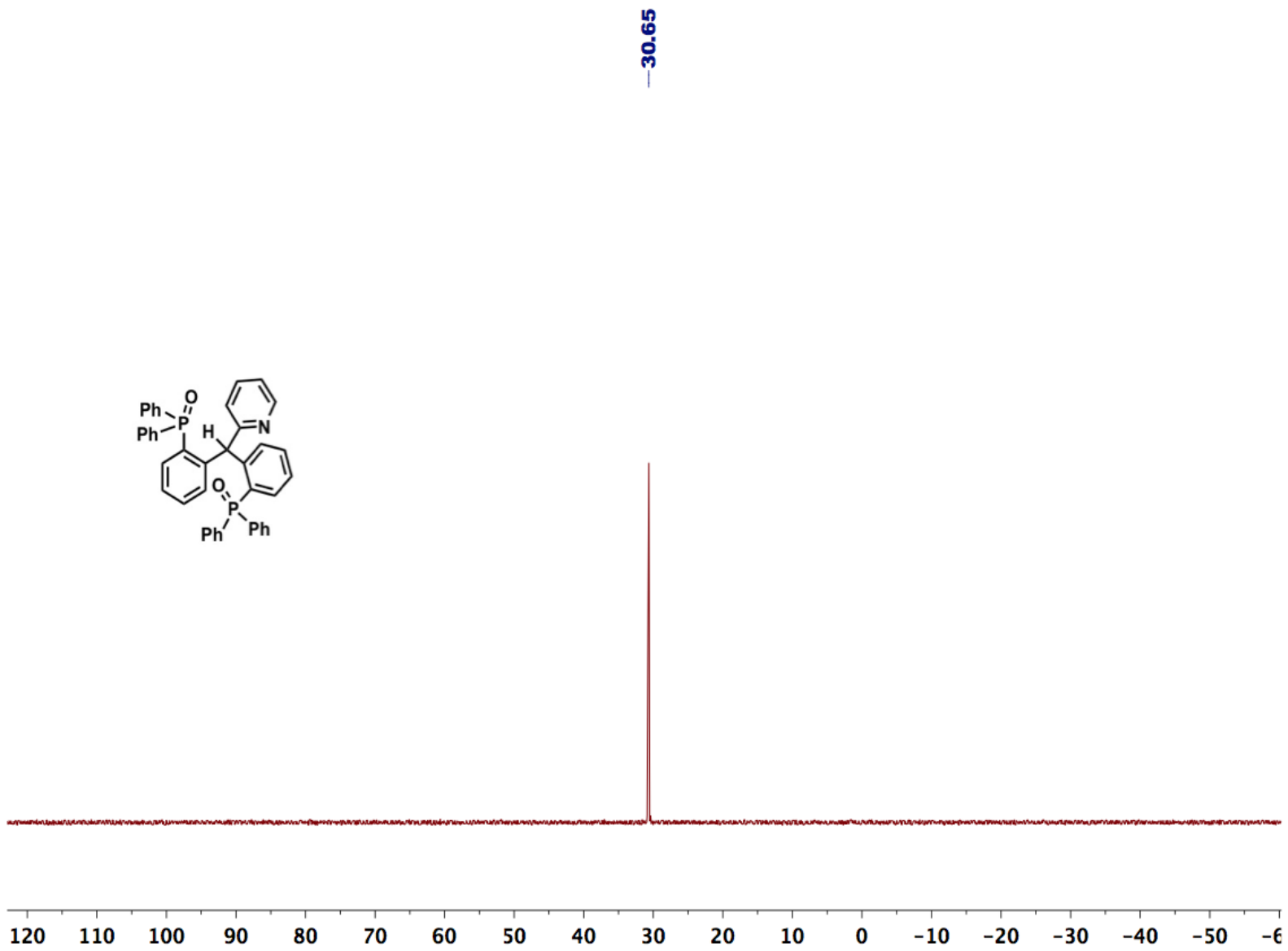

Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum for $P(O)C^{Py}HP(O)$ (**4**).

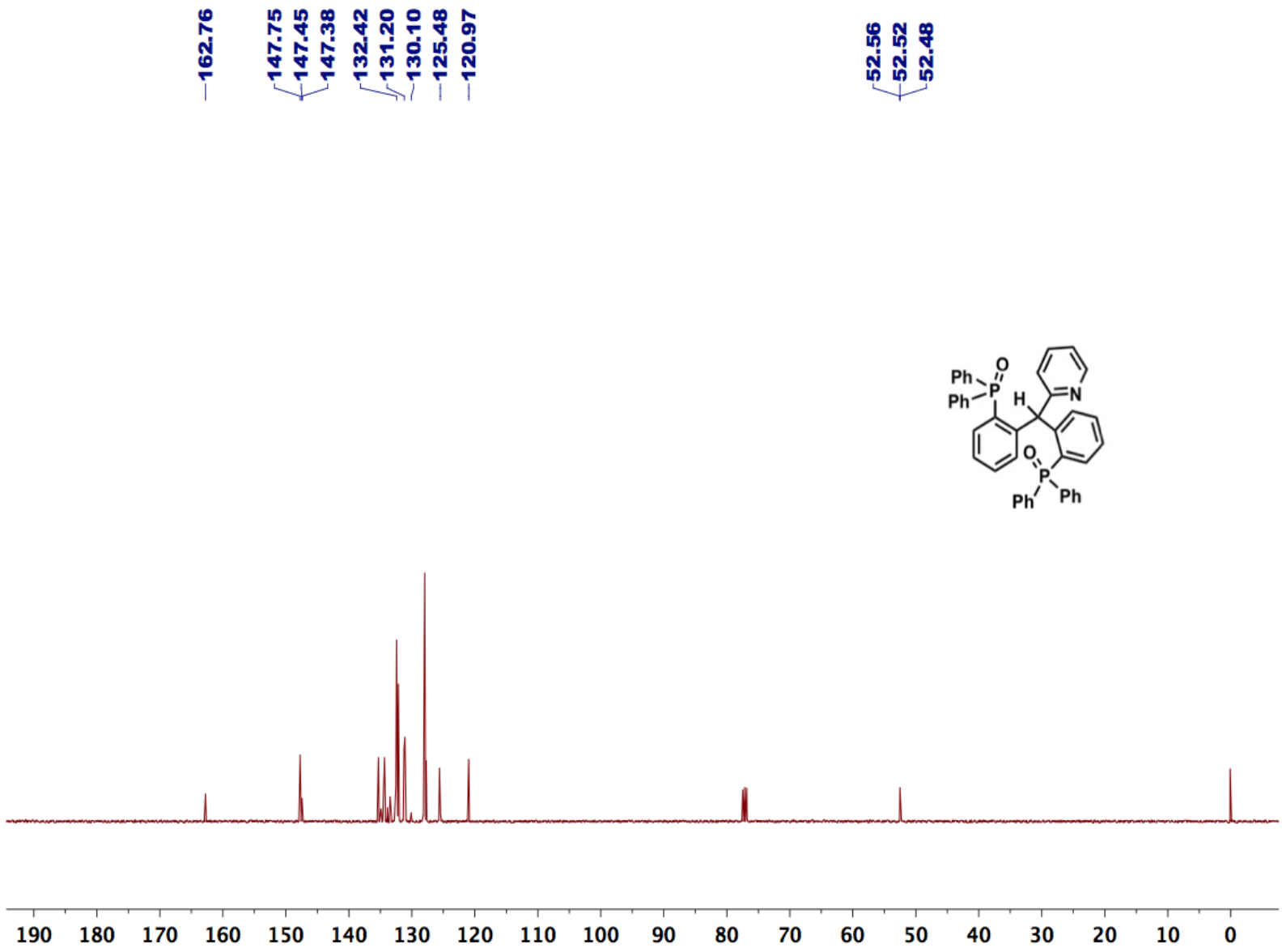

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum for $P(O)C^{Py}HP(O)$ (**4**).

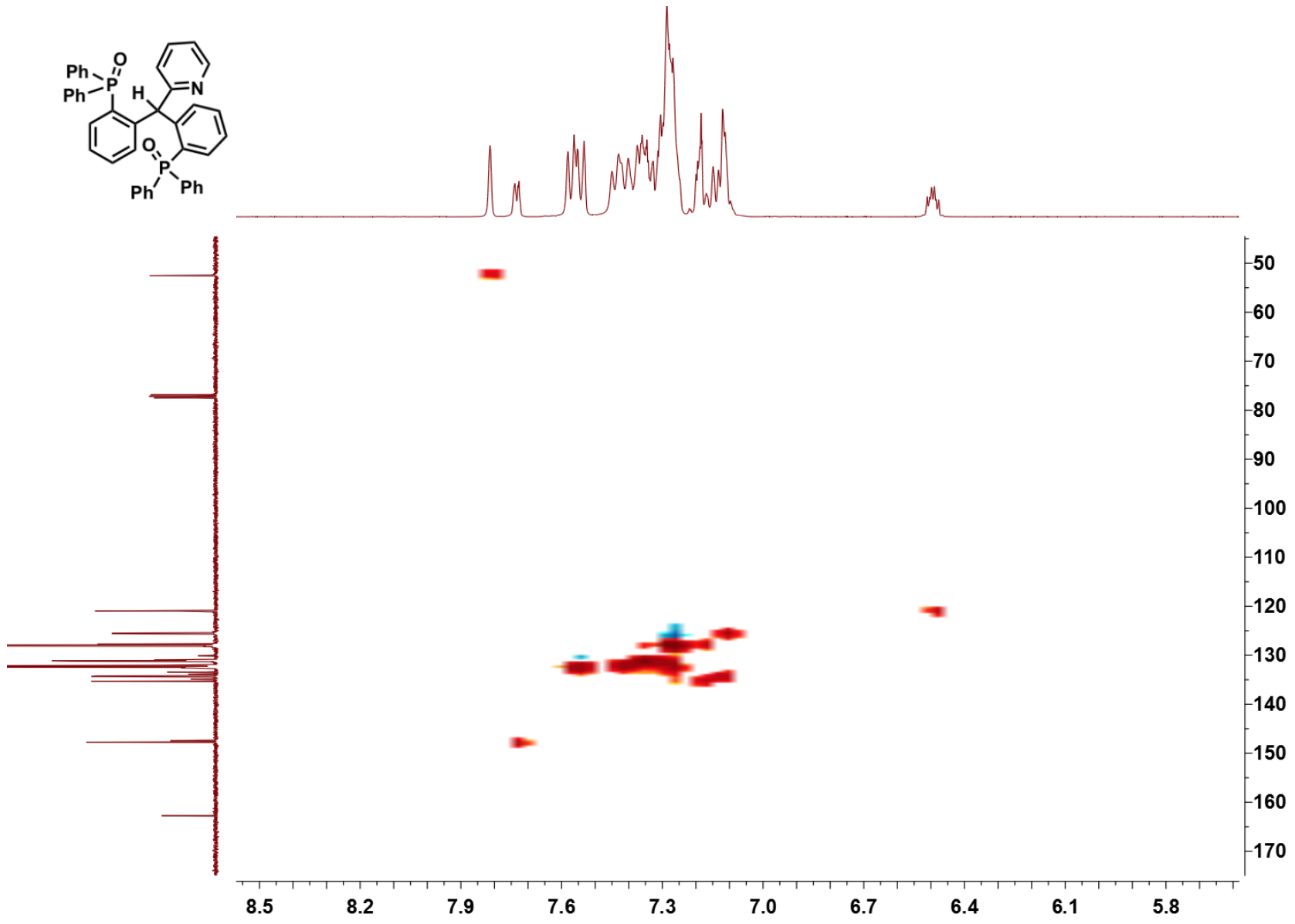

Figure S11. ^{1}H-^{13}C HSQC NMR spectrum for P(O)C^{Py}HP(O) (**4**).

2.4 NMR Spectra for PC^{Py}HP (5)

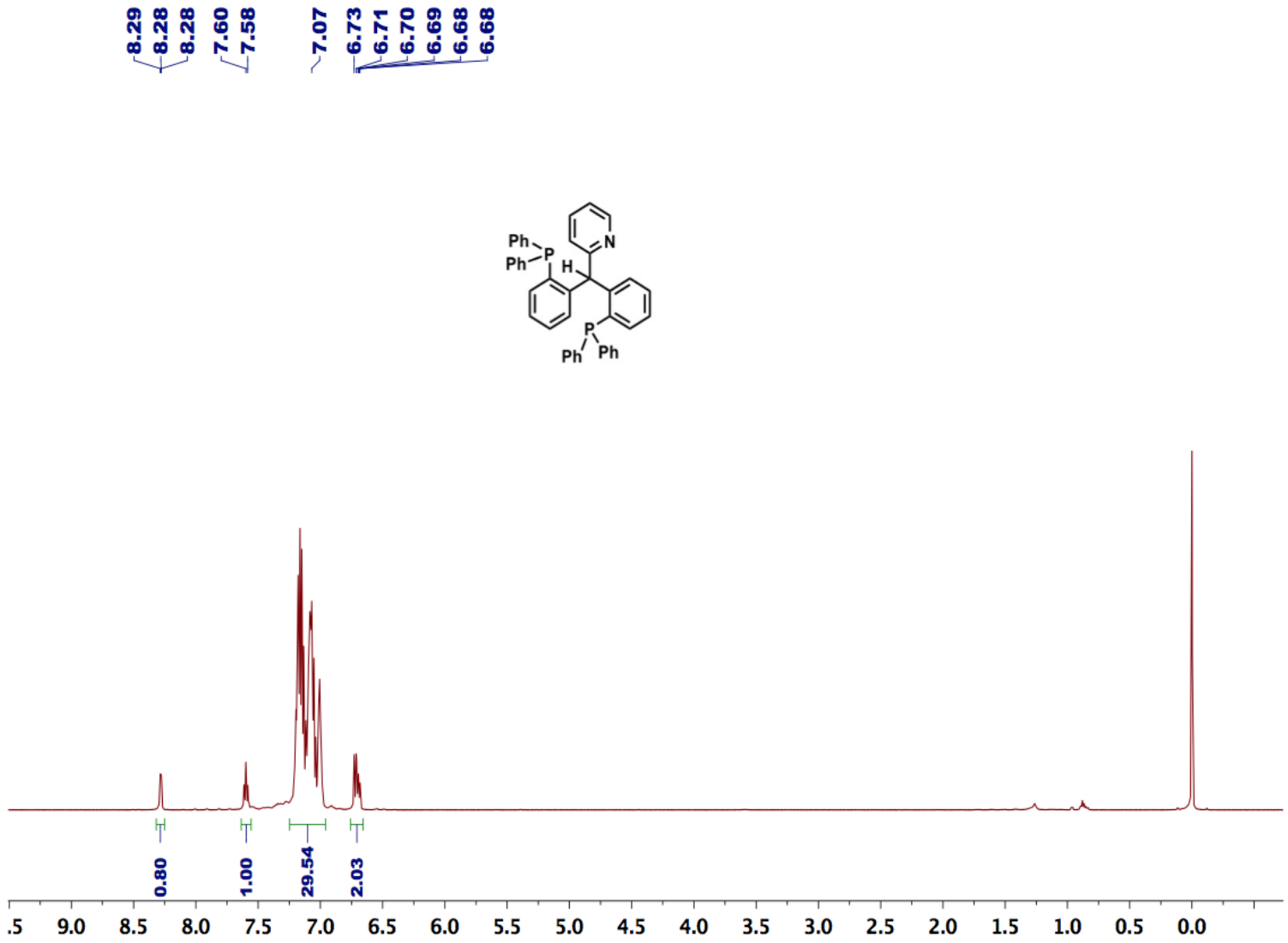

Figure S12. ^{1}H NMR spectrum for PC^{Py}HP (**5**).

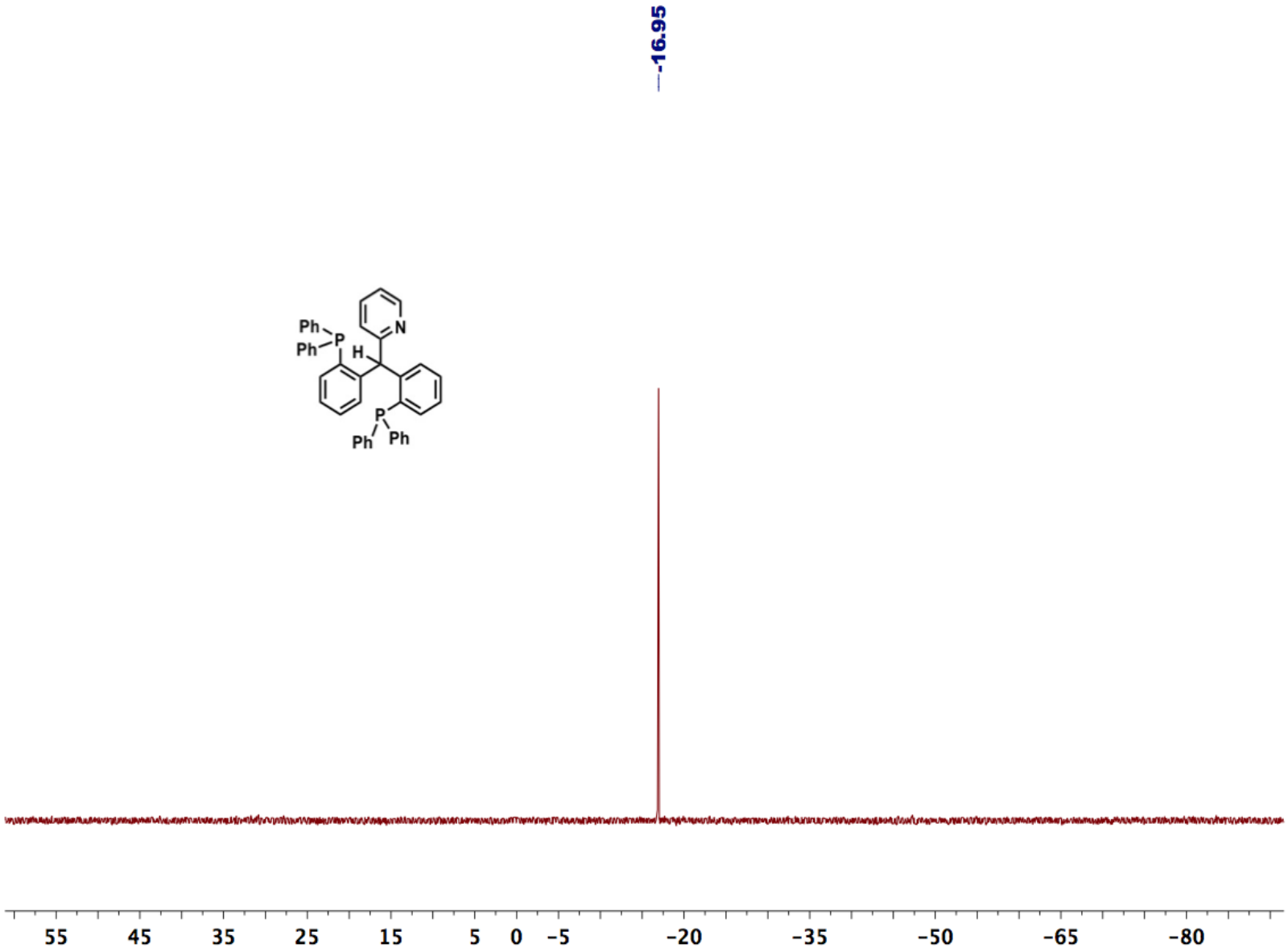

Figure S13. $^{31}P\{^{1}H\}$ NMR spectrum for $PC^{Py}HP$ (**5**).

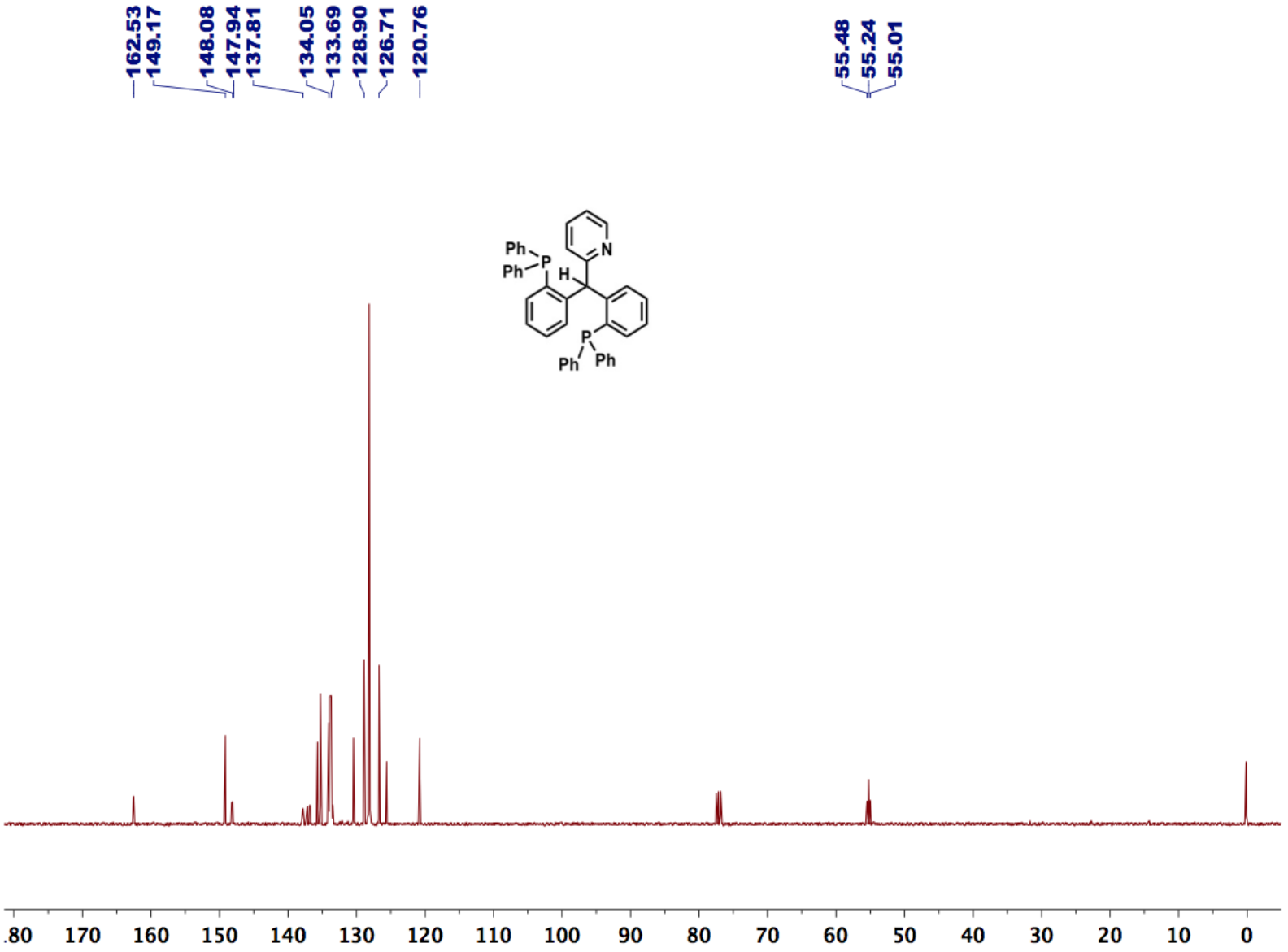

Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum for $PC^{Py}HP$ (**5**).

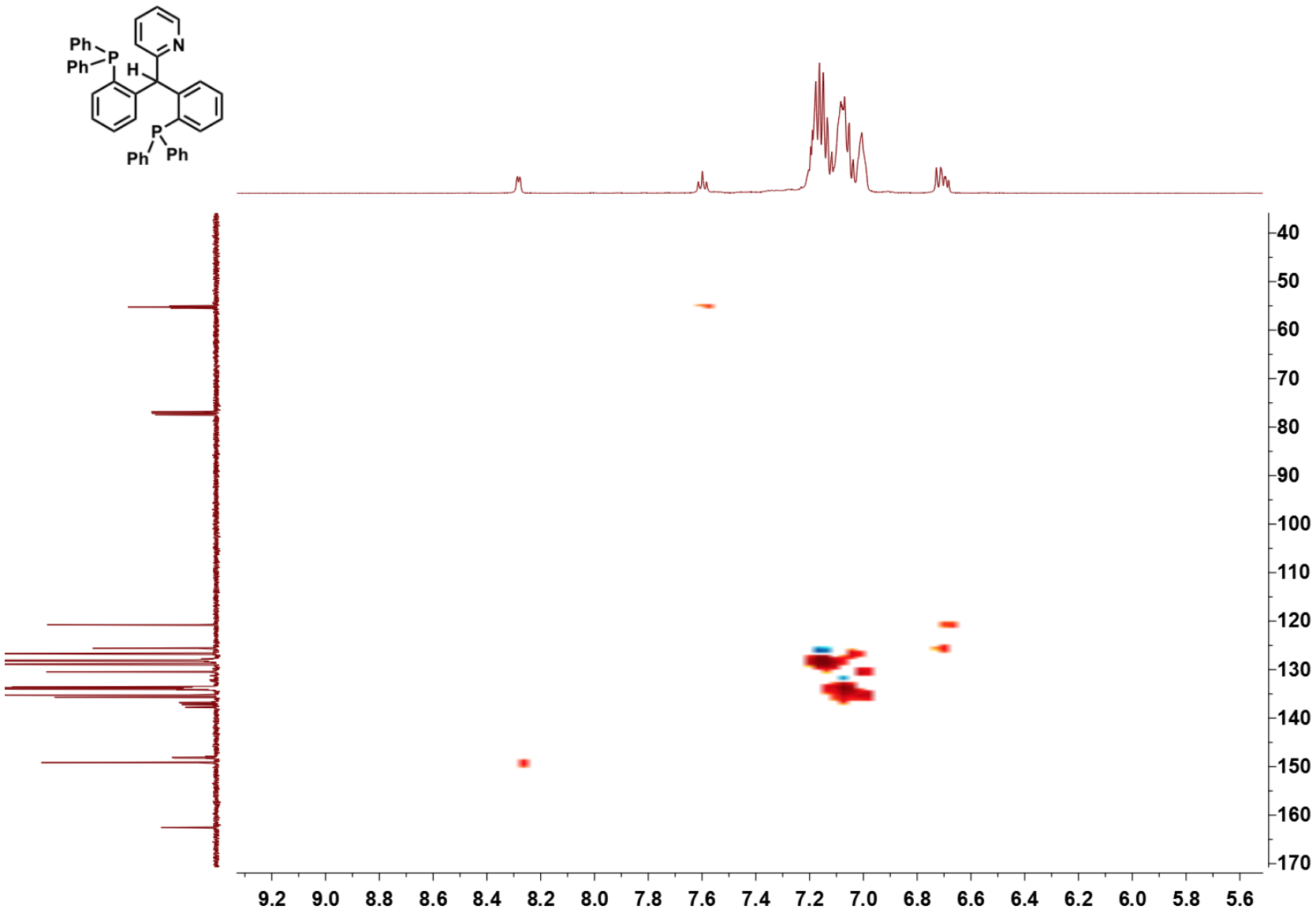

Figure S15. ^{1}H-^{13}C HSQC NMR spectrum for $PC^{Py}HP$ (**5**).

2.5 NMR Spectra for [(PC^{Py}P)Ir(COD)] (6)

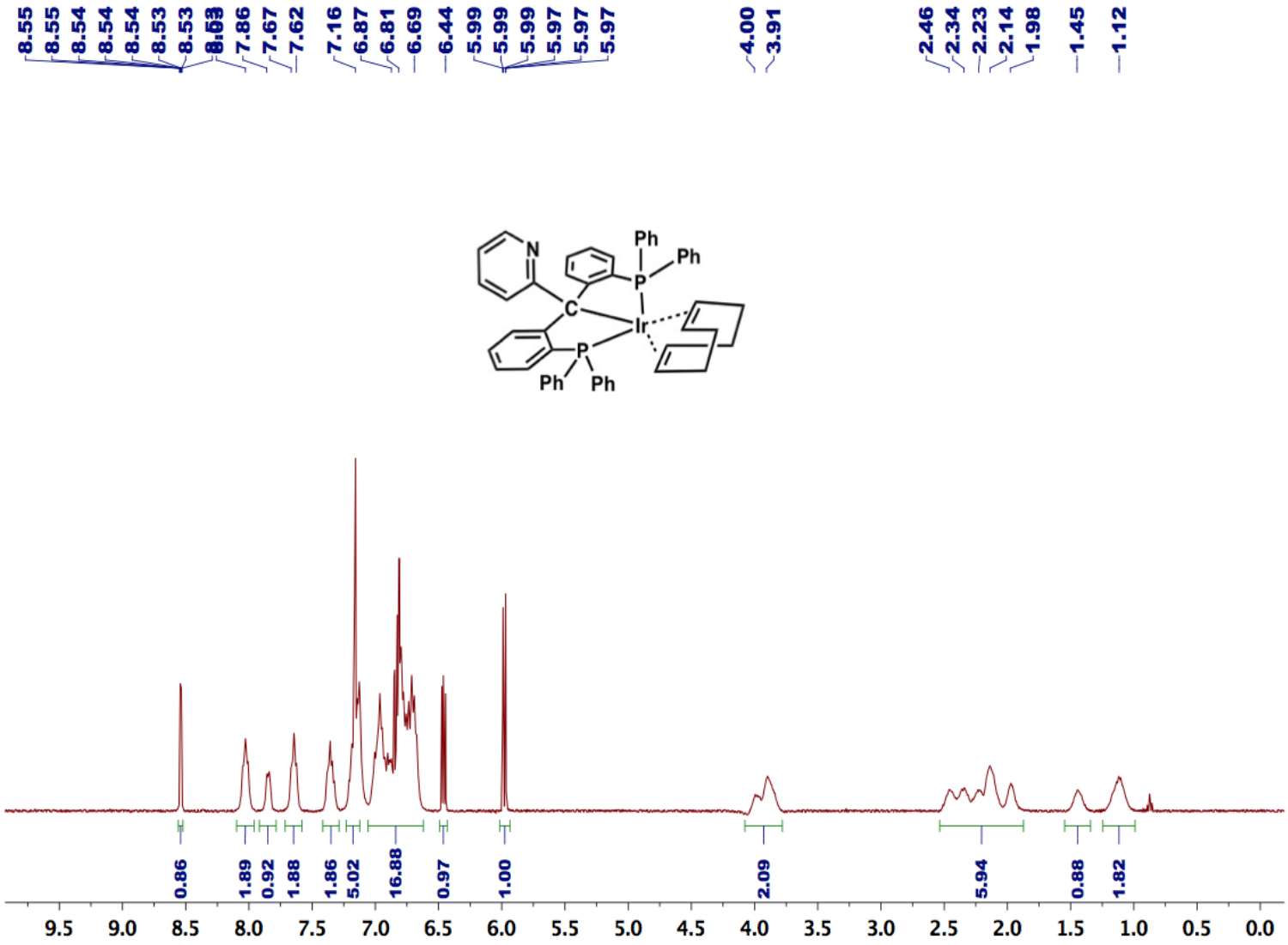

Figure S16. ^{1}H NMR spectrum for [(PC^{Py}P)Ir(COD)] (**6**).

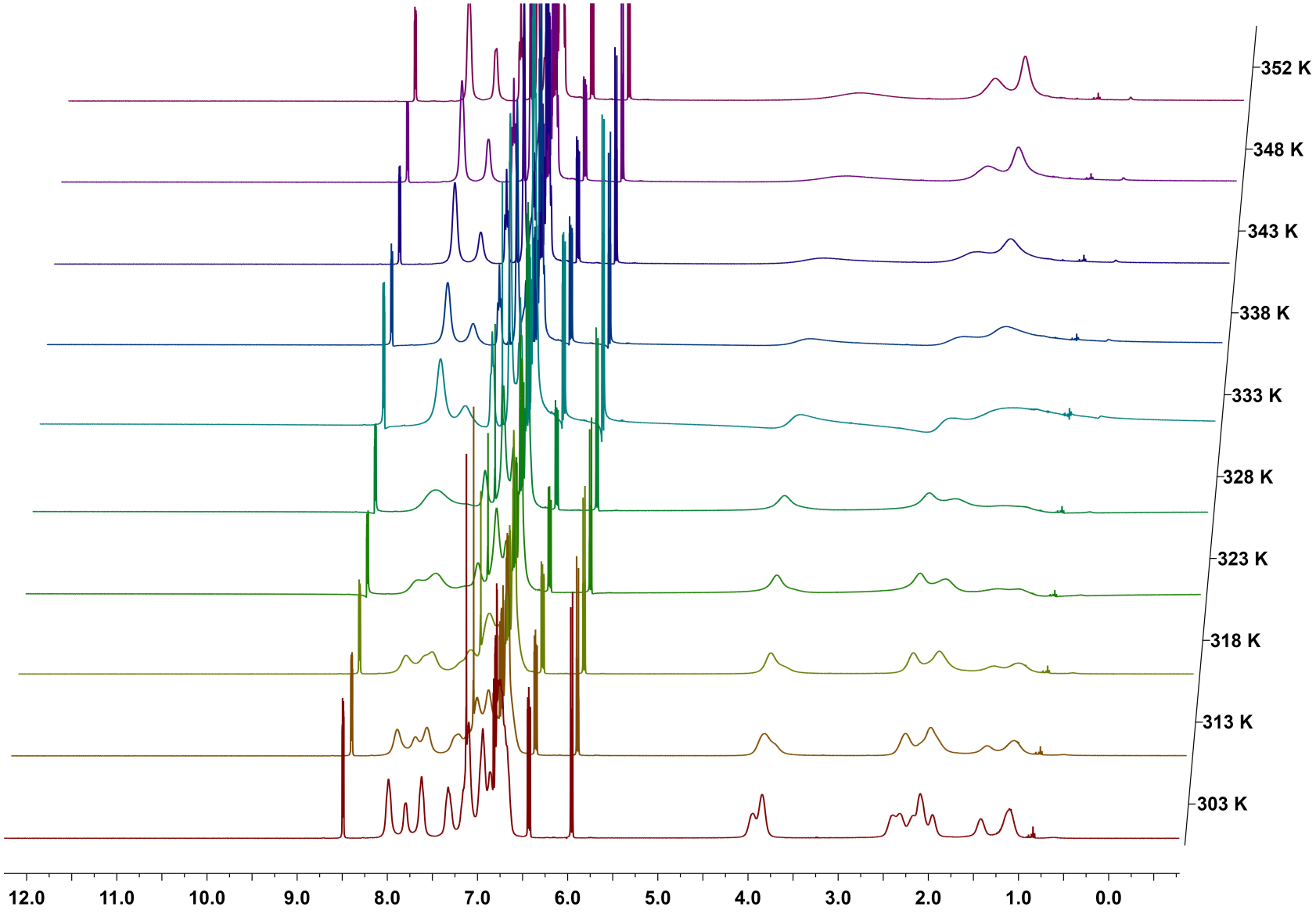

Figure S17. Variable temperature ^{1}H NMR spectrum for [(PC^{Py}P)Ir(COD)] (**6**).

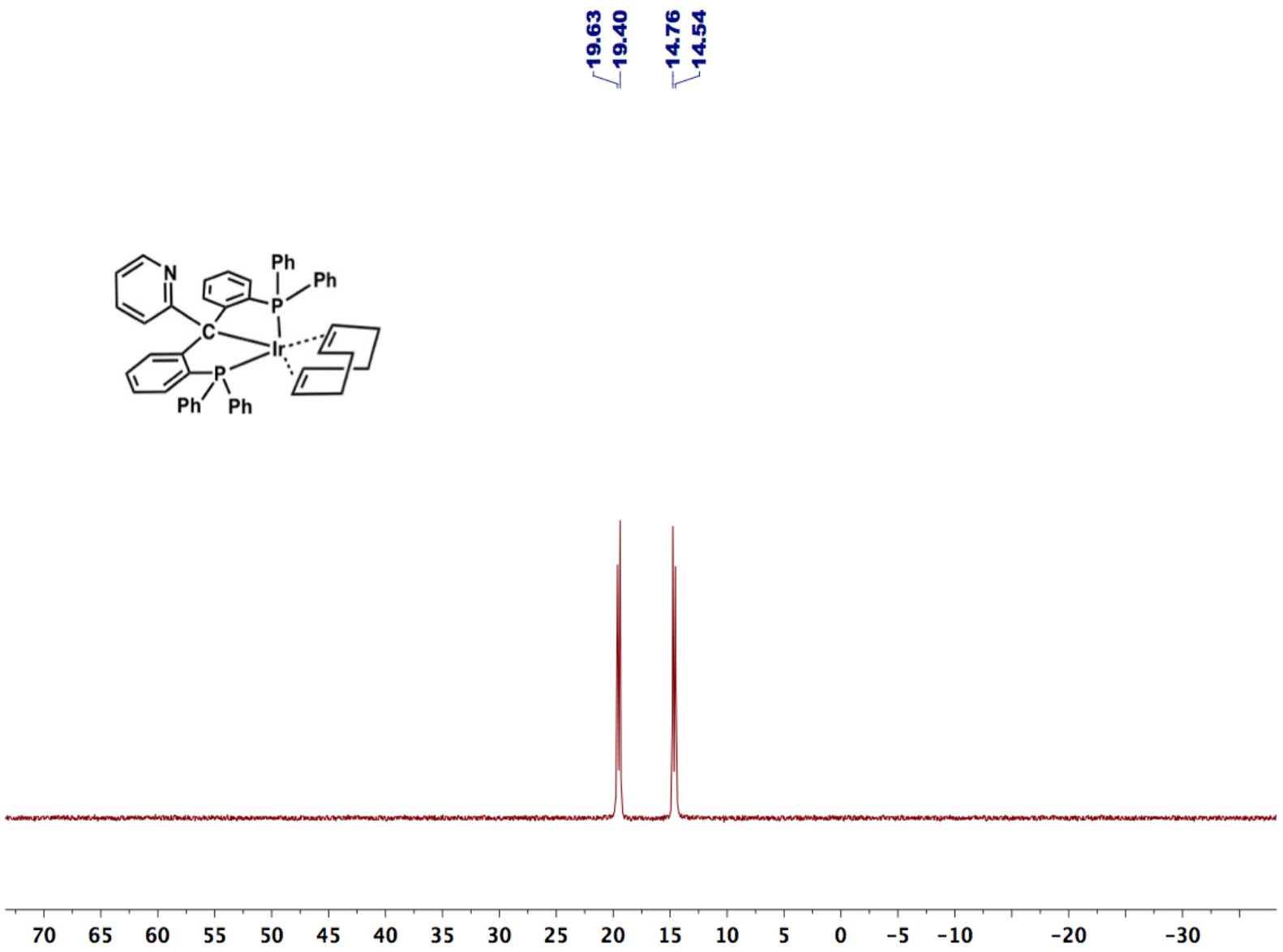

Figure S18. $^{31}P\{^{1}H\}$ NMR spectrum for [($PC^{Py}P$)Ir(COD)] (**6**).

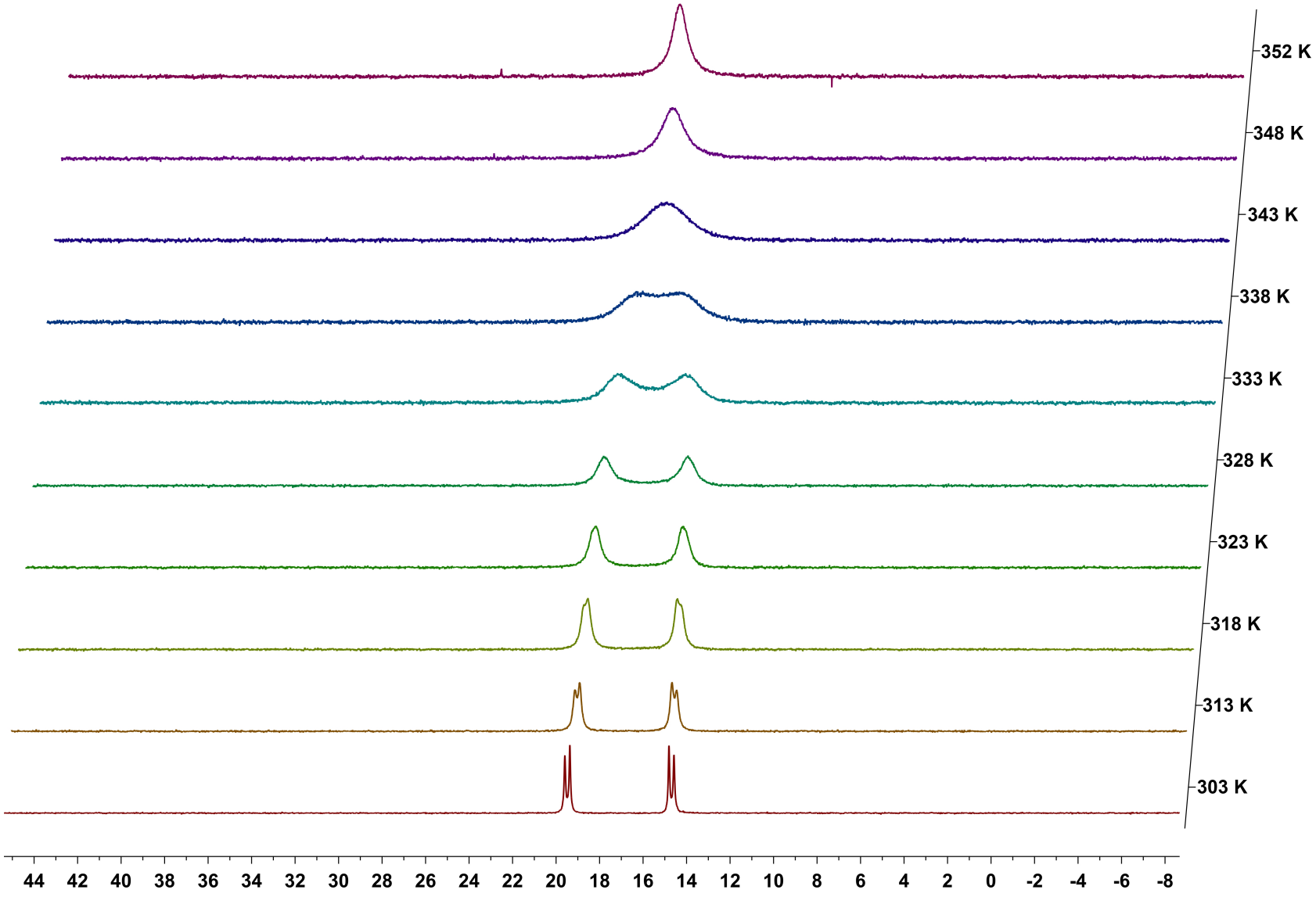

Figure S19. Variable temperature $^{31}P\{^{1}H\}$ NMR spectrum for [($PC^{Py}P$)Ir(COD)] (**6**).

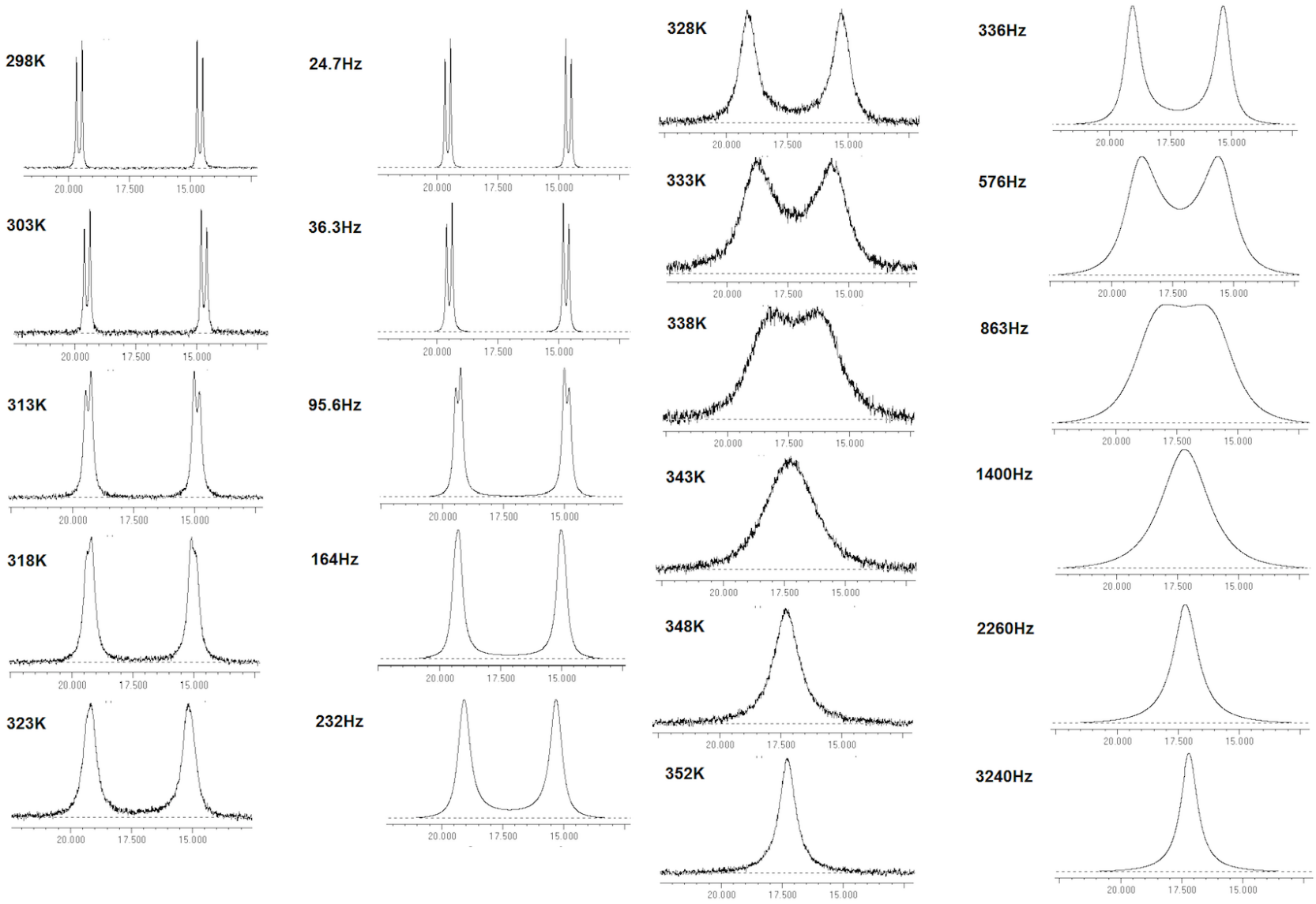

Figure S20. Experimental and simulated $^{31}P\{^{1}H\}$ NMR spectra for **6**.

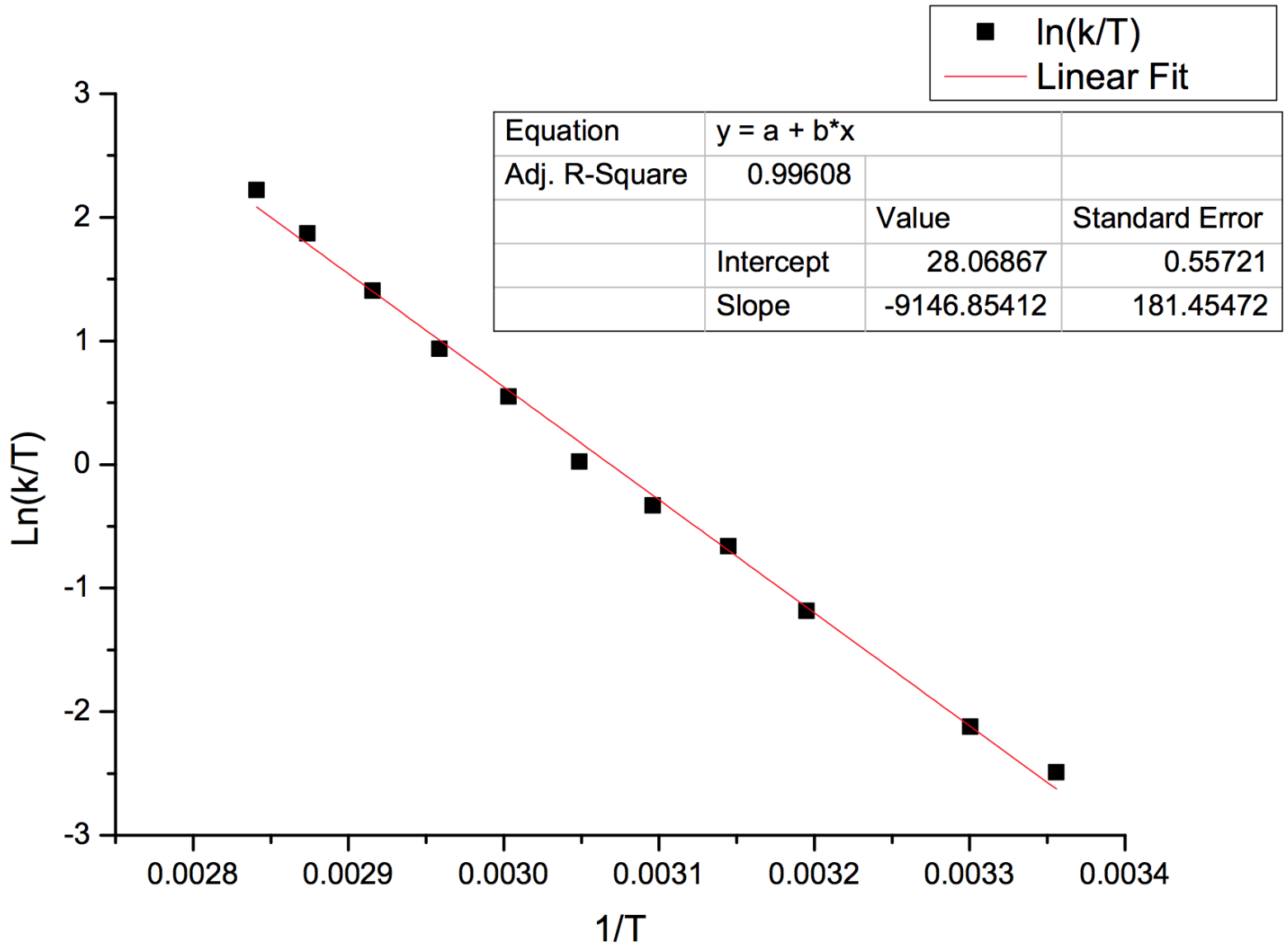

Figure S21. Eyring plot and analysis for [(PC^{Py}P)Ir(COD)] (**6**).

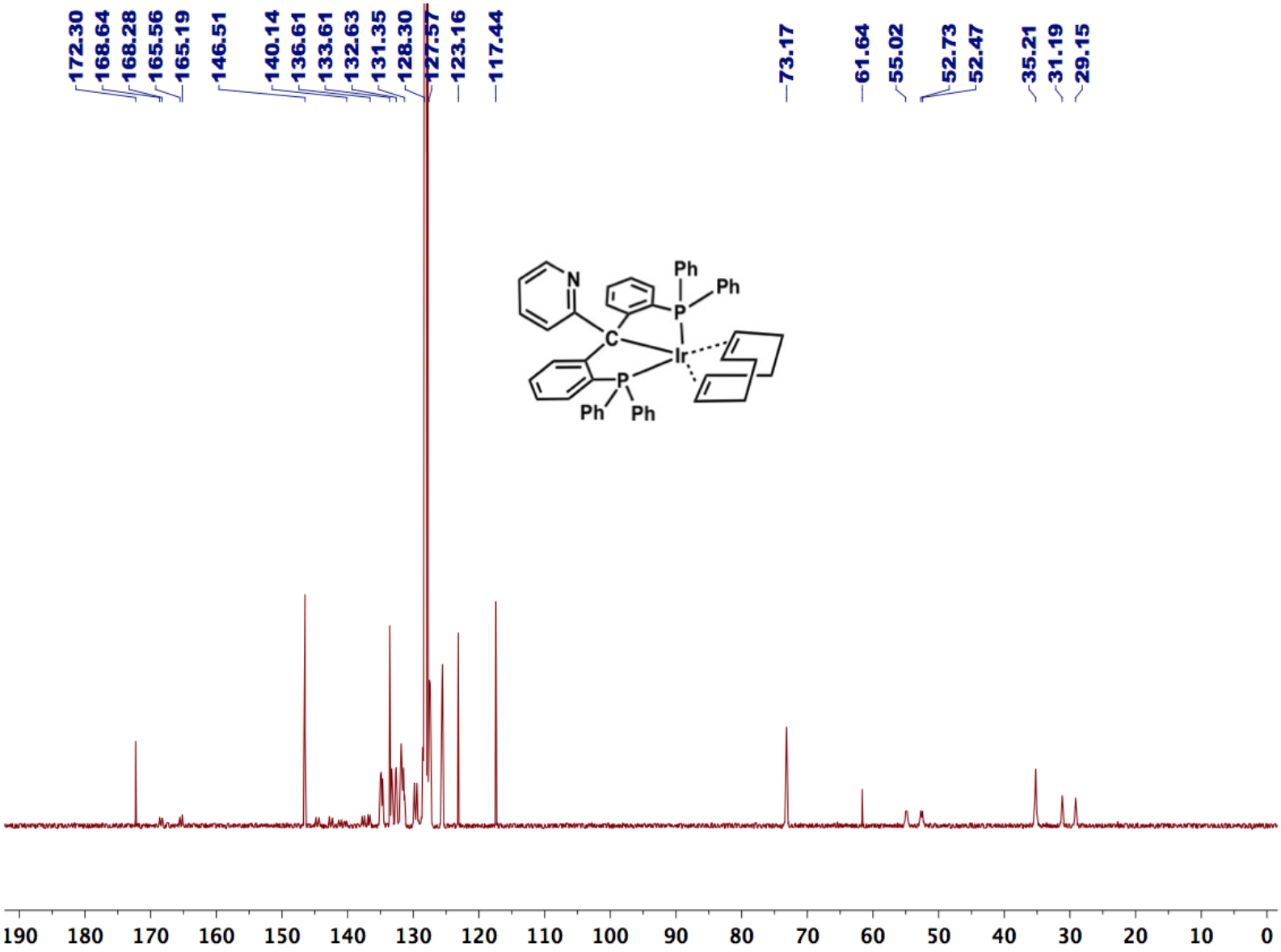

Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum for [($PC^{Py}P$)Ir(COD)] (**6**).

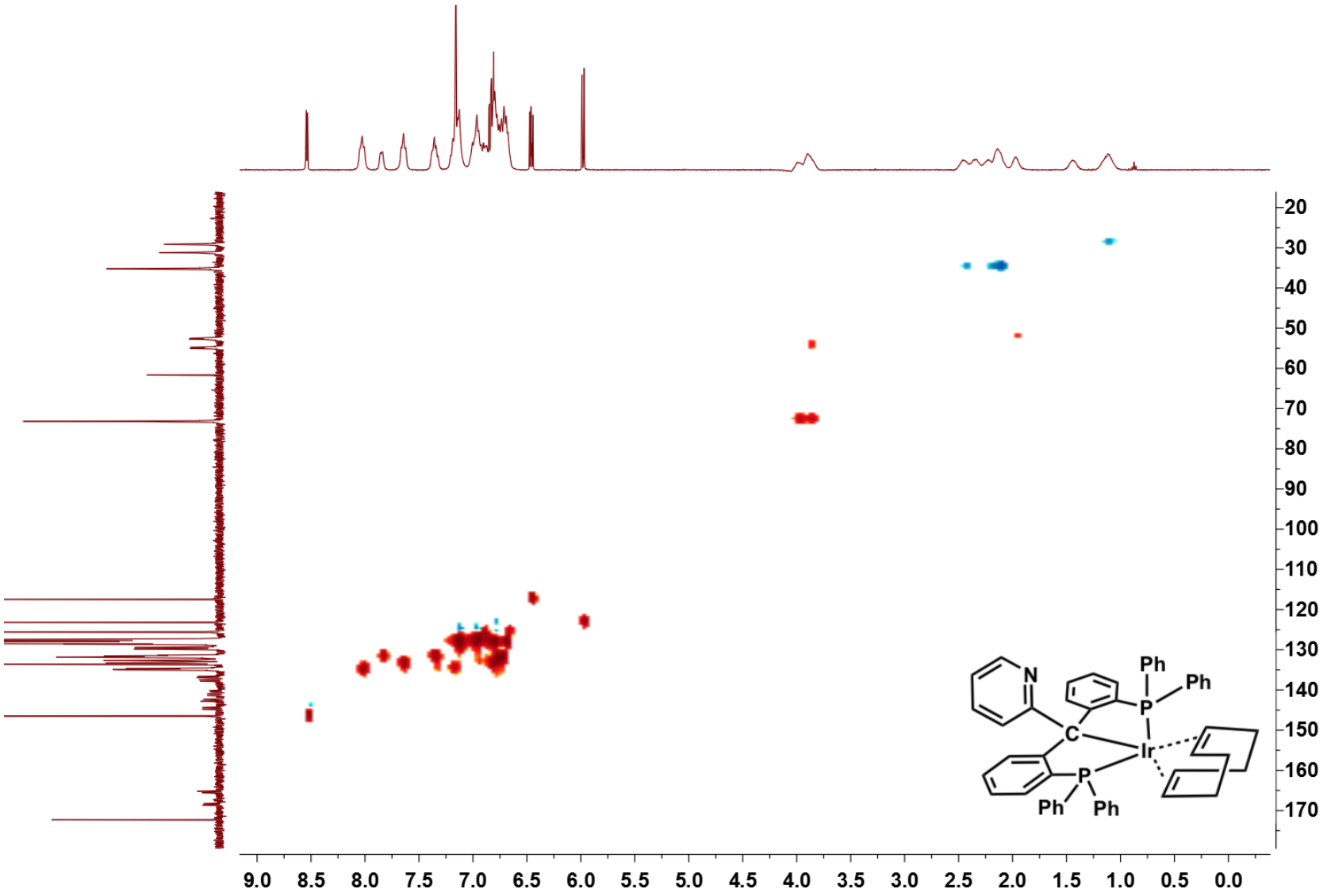

Figure S23. ^{1}H-^{13}C HSQC NMR spectrum for [(PC^{Py}P)Ir(COD)] (**6**).

2.6 NMR Spectra for [(PC^{Py}P)Ir(COE)] (7)

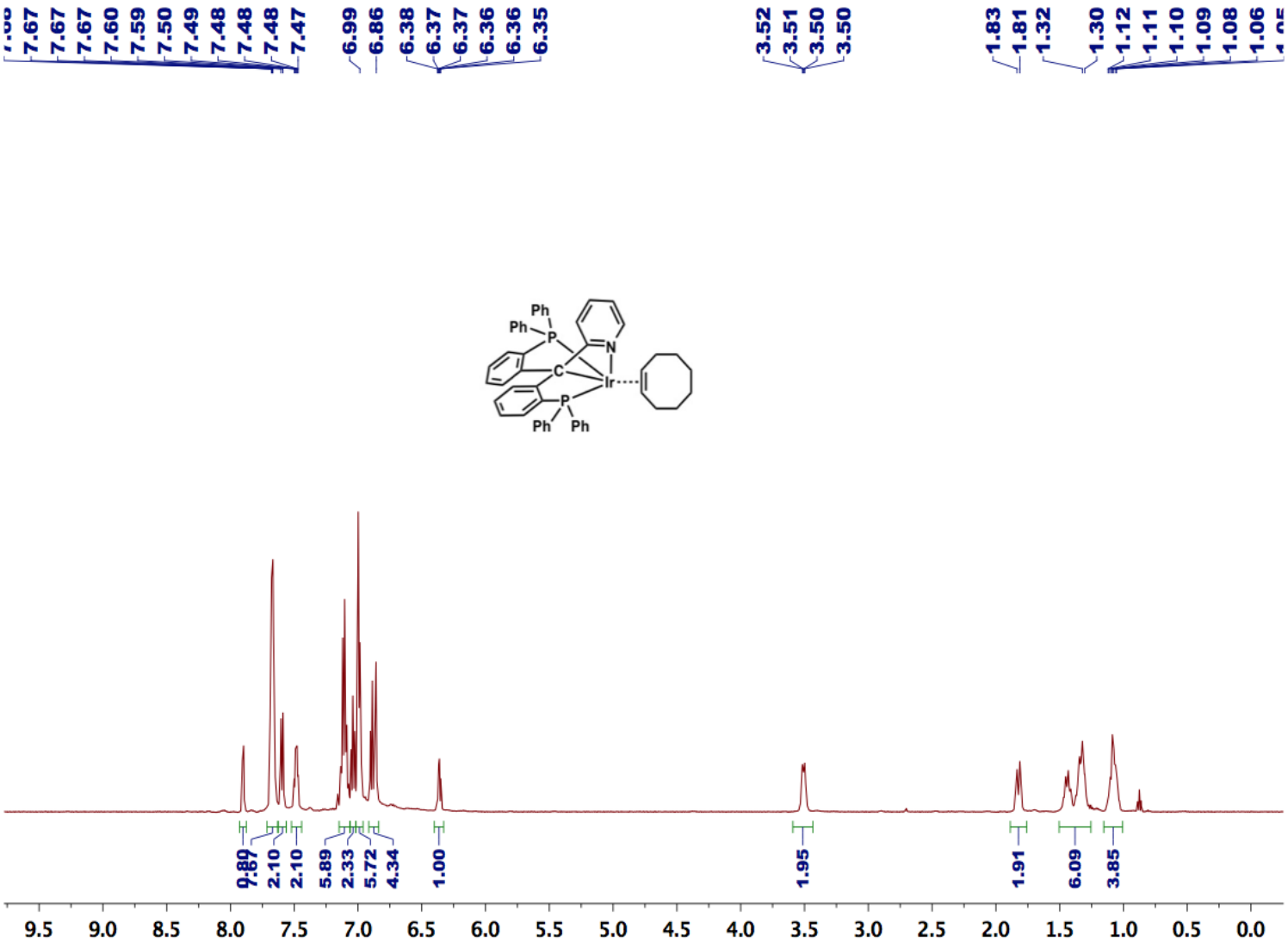

Figure S24. ^{1}H NMR spectrum for [(PC^{Py}P)Ir(COE)] (**7**).

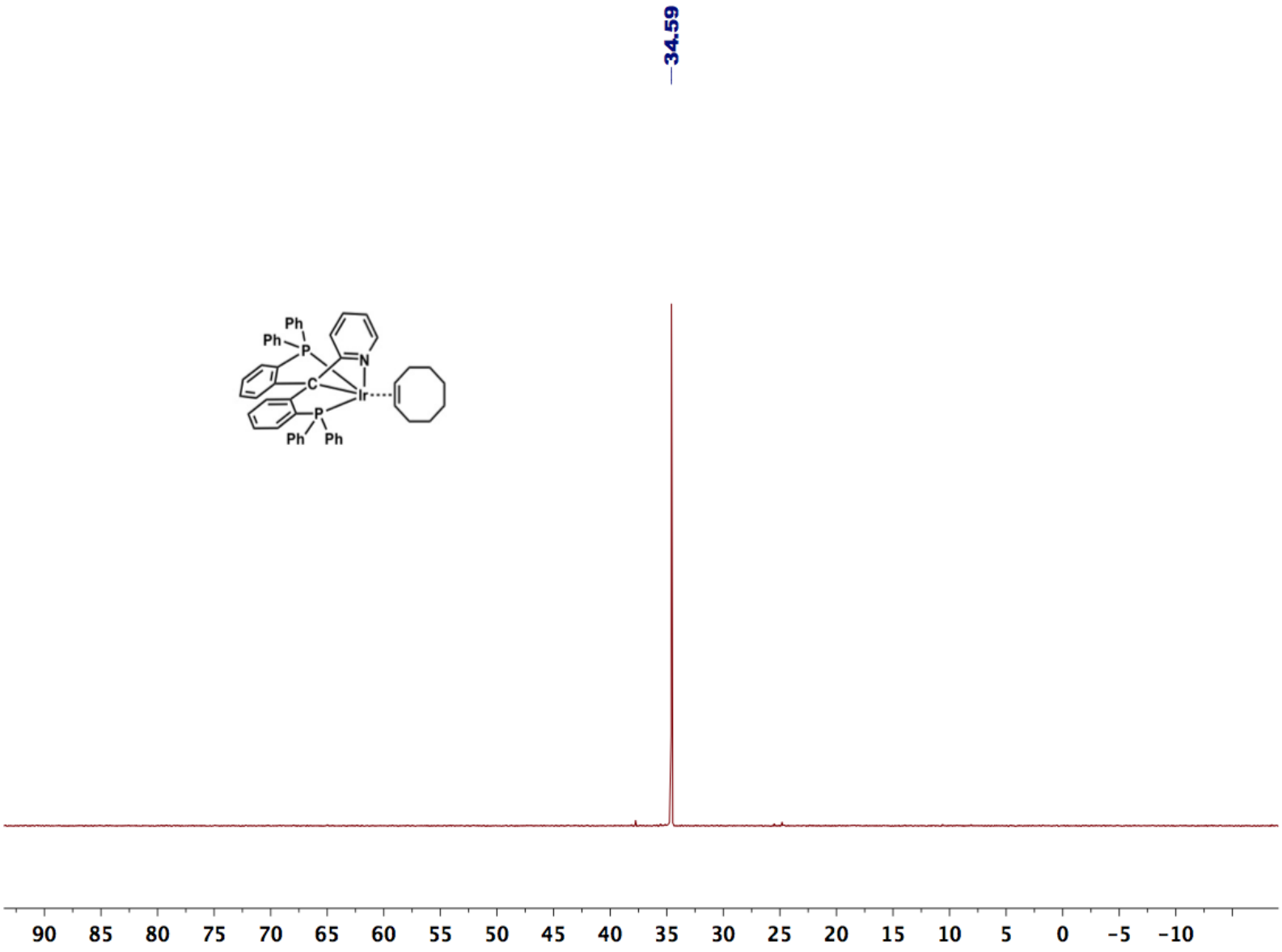

Figure S25. $^{31}P\{^{1}H\}$ NMR spectrum for [($PC^{Py}P$)Ir(COE)] (**7**).

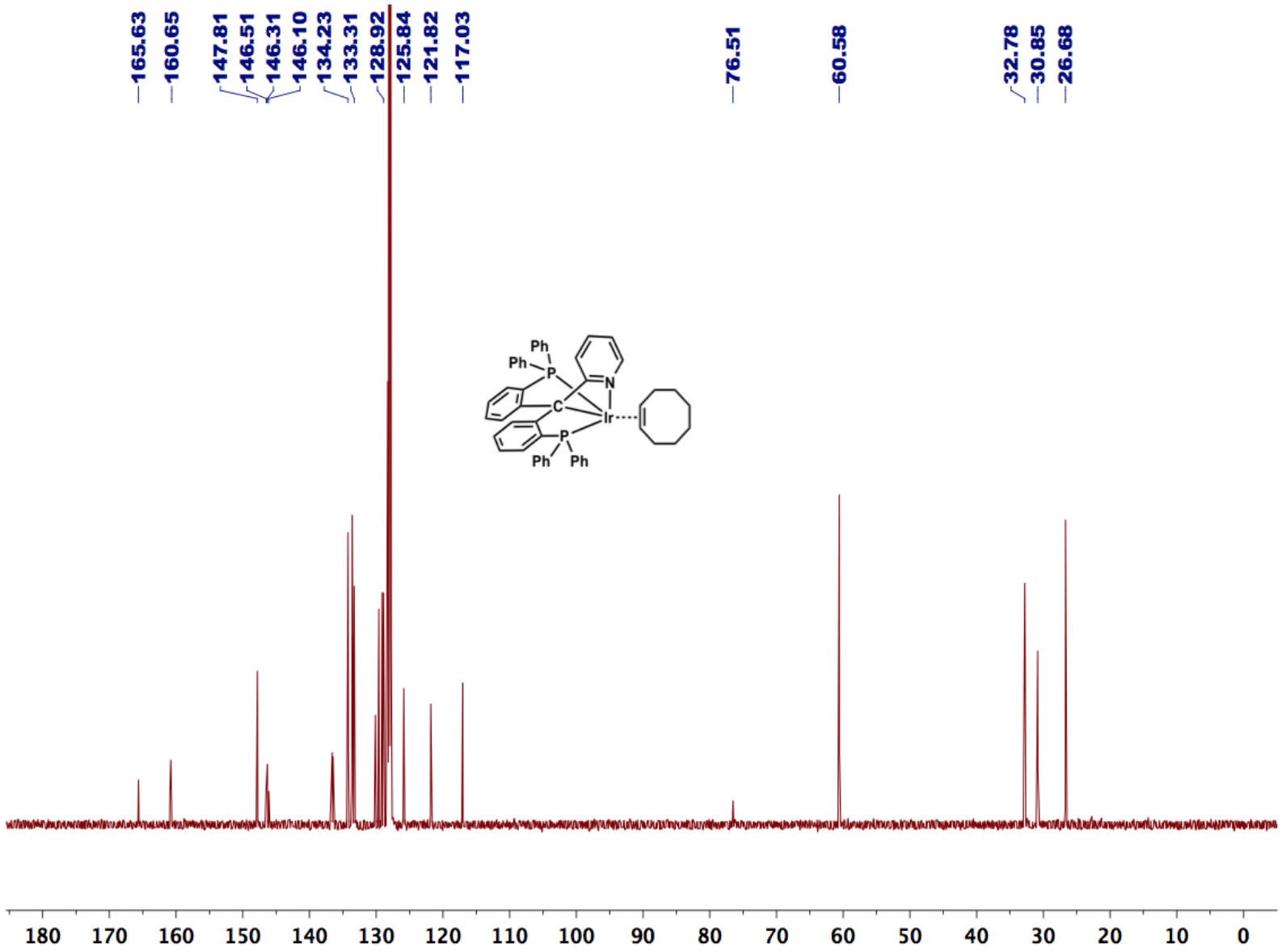

Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum for [($PC^{Py}P$)Ir(COE)] (**7**).

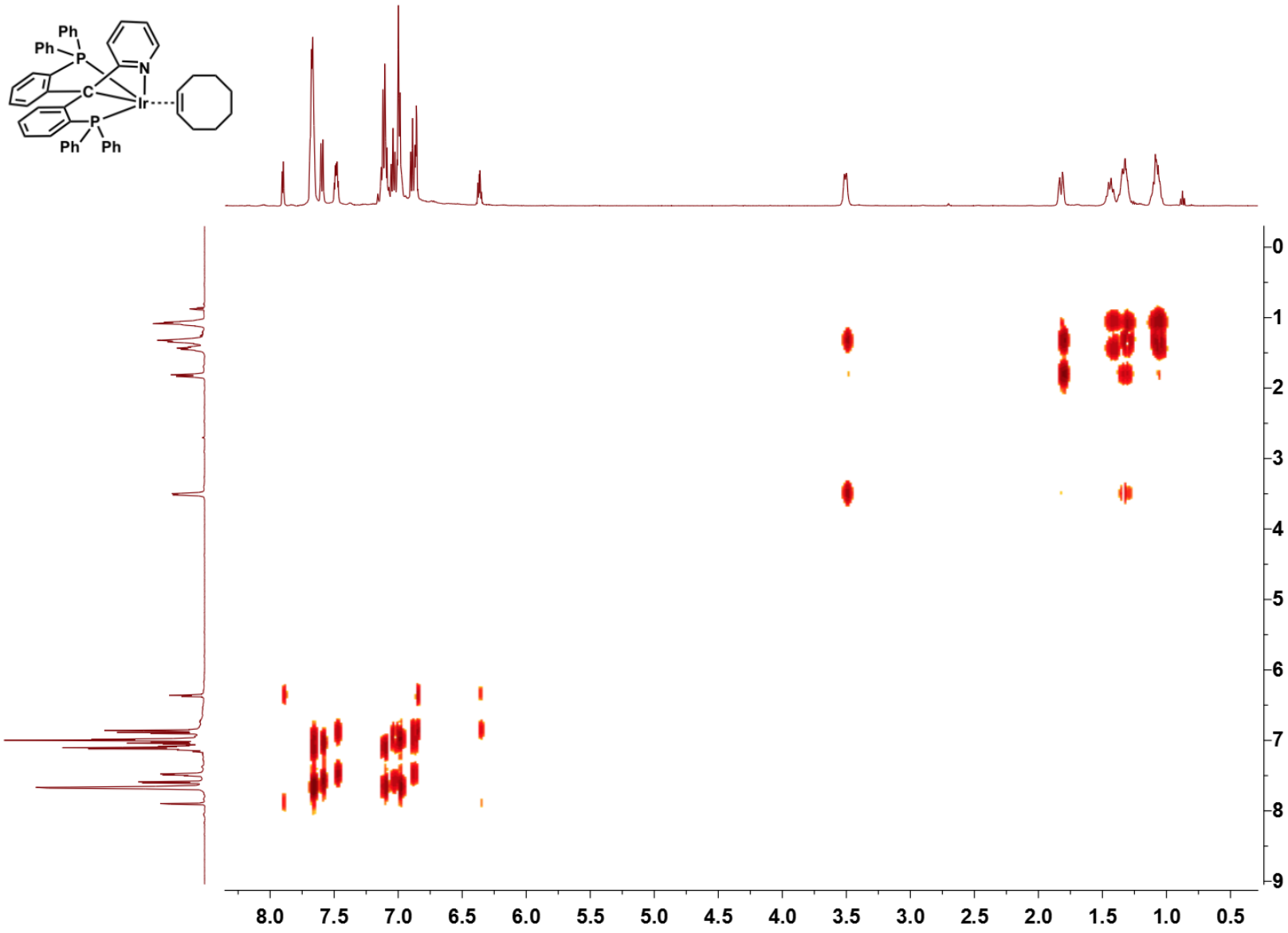

Figure S27. ^{1}H-^{1}H COSY NMR spectrum for [(PC^{Py}P)Ir(COE)] (**7**).

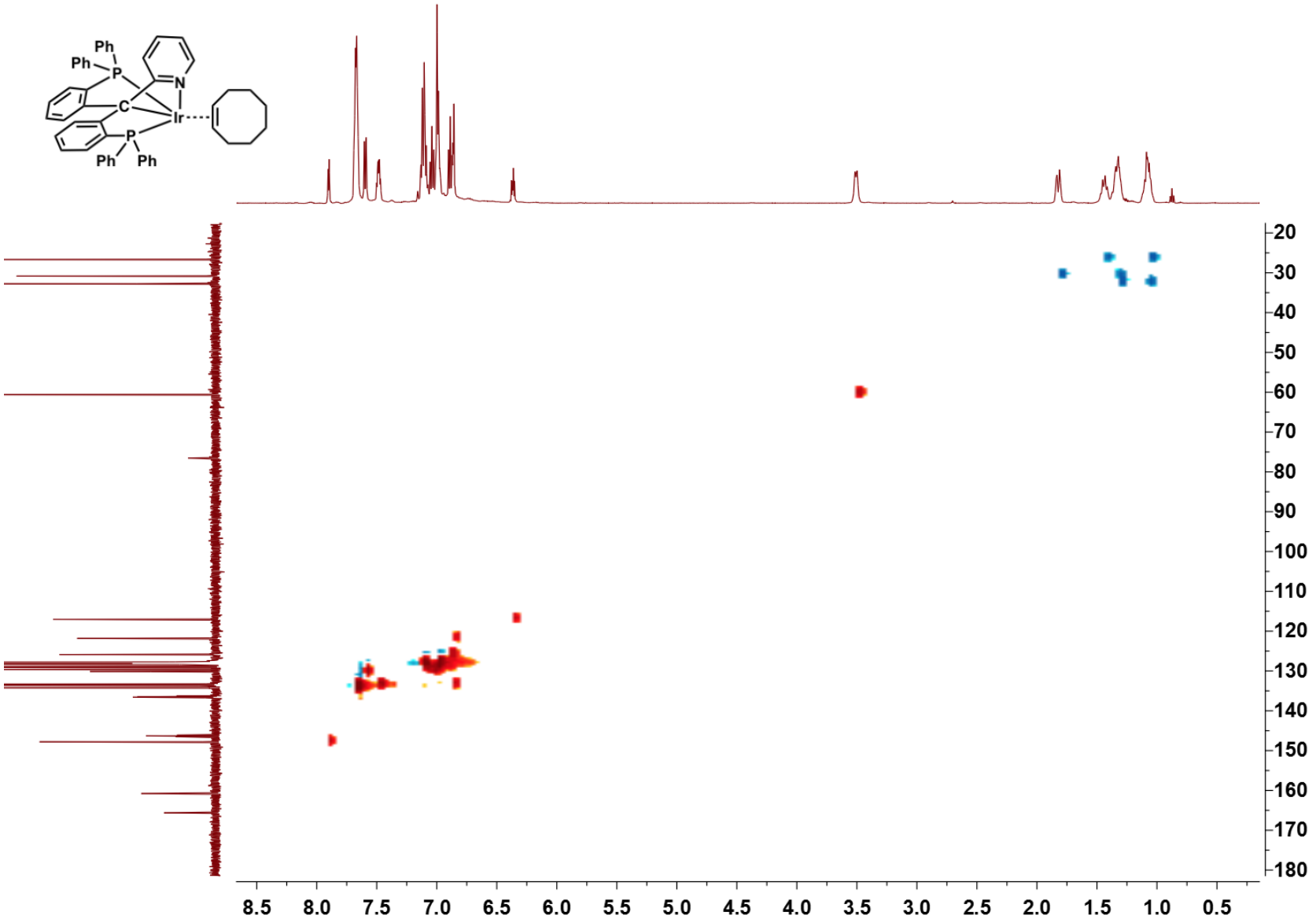

Figure S28. ^{1}H-^{13}C HSQC NMR spectrum for [(PC^{Py}P)Ir(COE)] (**7**).

2.7 NMR Spectra for [(PC^{Py}P)Ir(H)$_2$] (8)

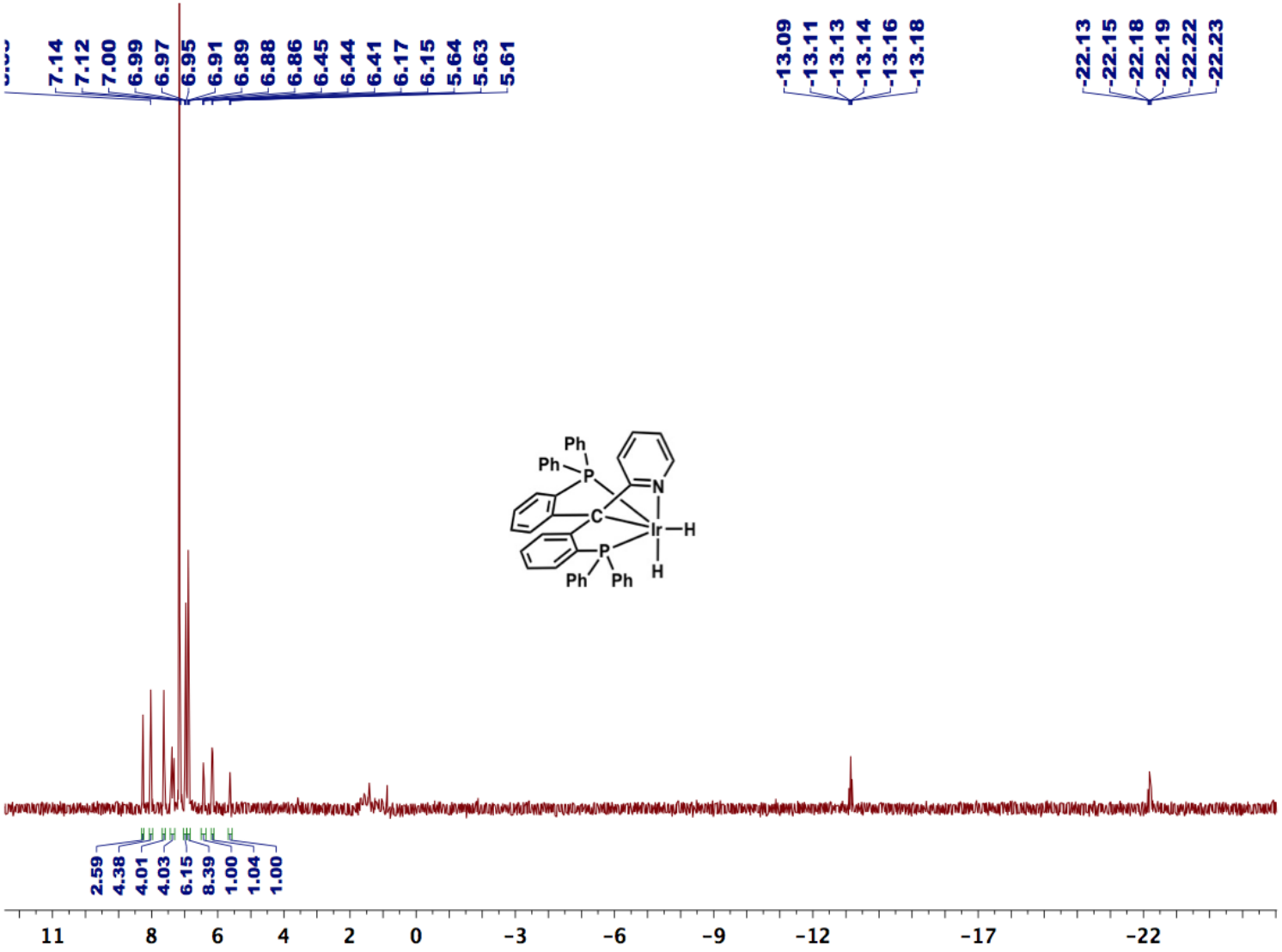

Figure S29. ^{1}H NMR spectrum for [(PC^{Py}P)Ir(H)$_2$] (**8**).

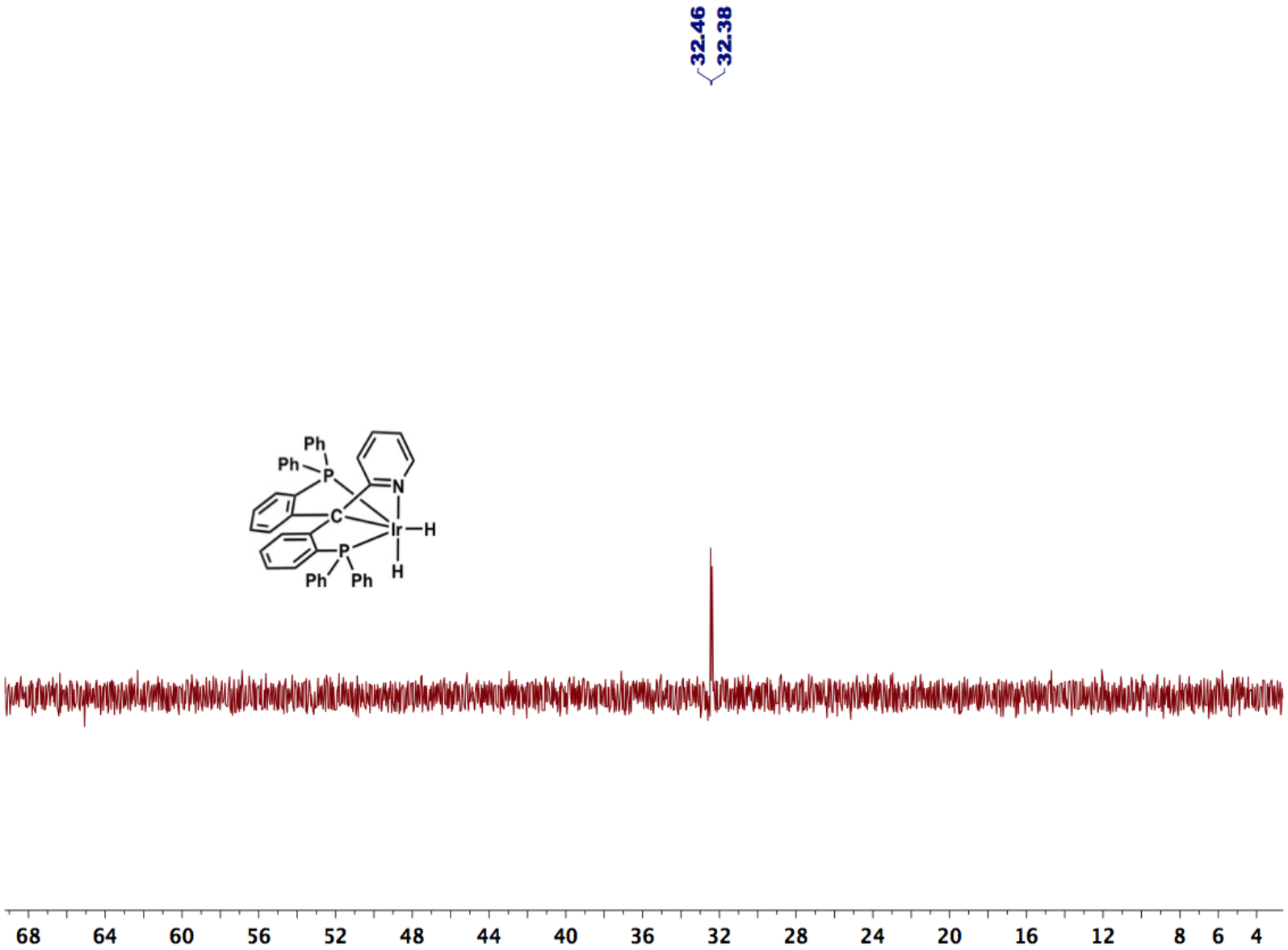

Figure S30. ^{31}P spectrum for [($PC^{Py}P$)Ir($H)_2$] (**8**).

2.8 NMR Spectra for [(PC^{Py}P)IrH(C$_4$H$_7$O)] (**9**)

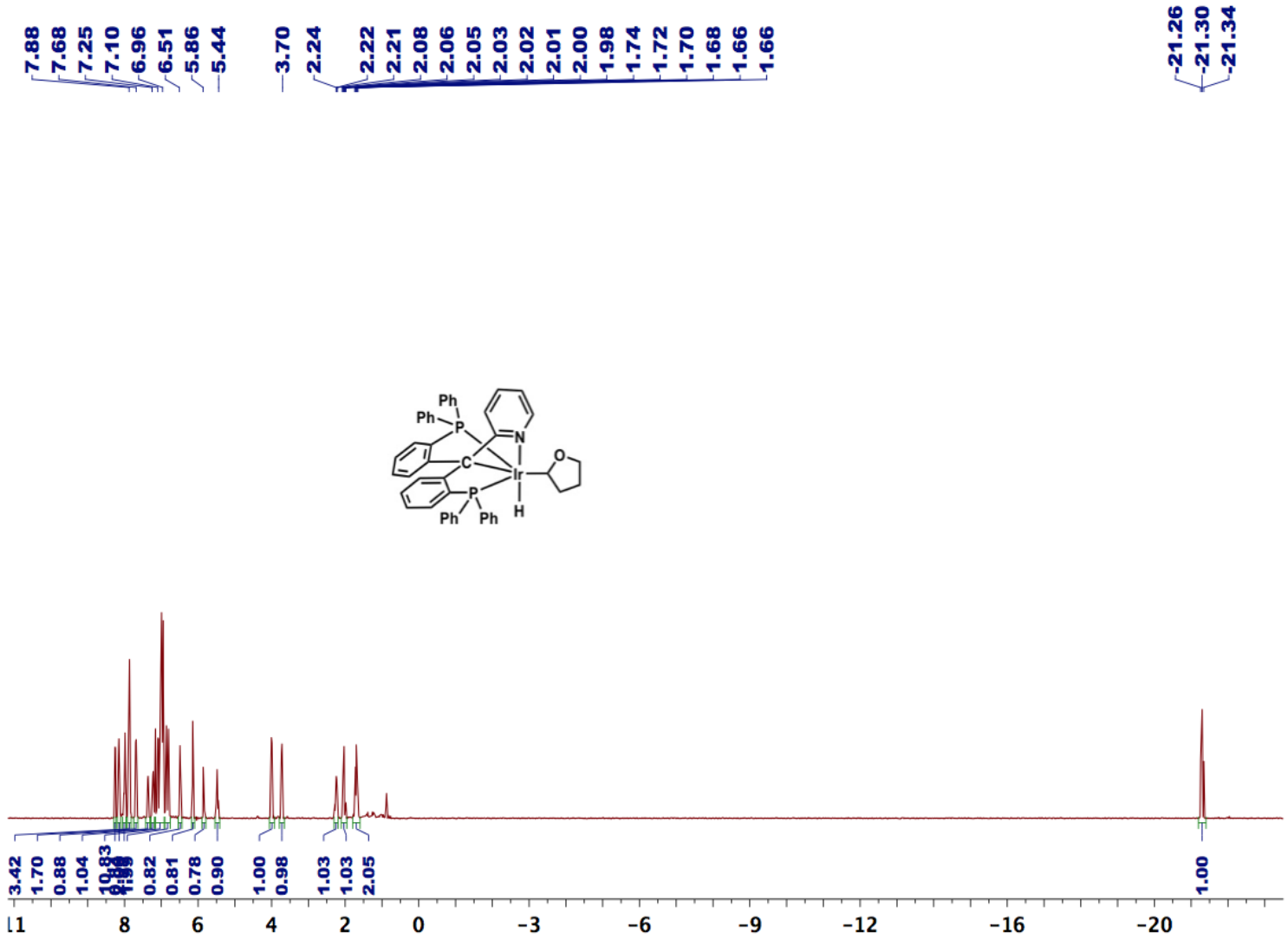

Figure S31. ^{1}H NMR spectrum for [(PC^{Py}P)IrH(C$_4$H$_7$O)] (**9**).

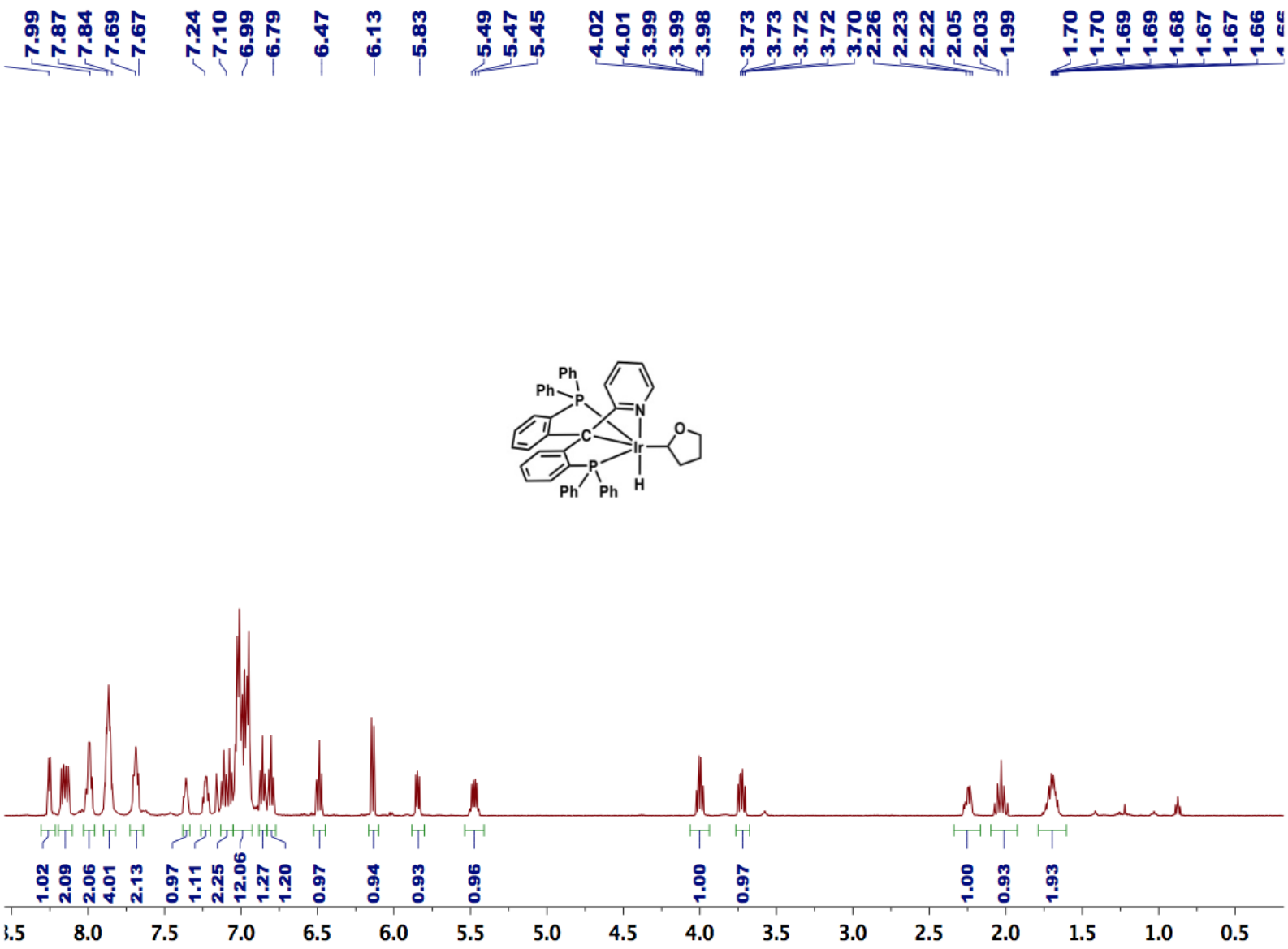

Figure S32. ^{1}H NMR spectrum for [(PC^{Py}P)IrH(C$_4$H$_7$O)] (**9**).

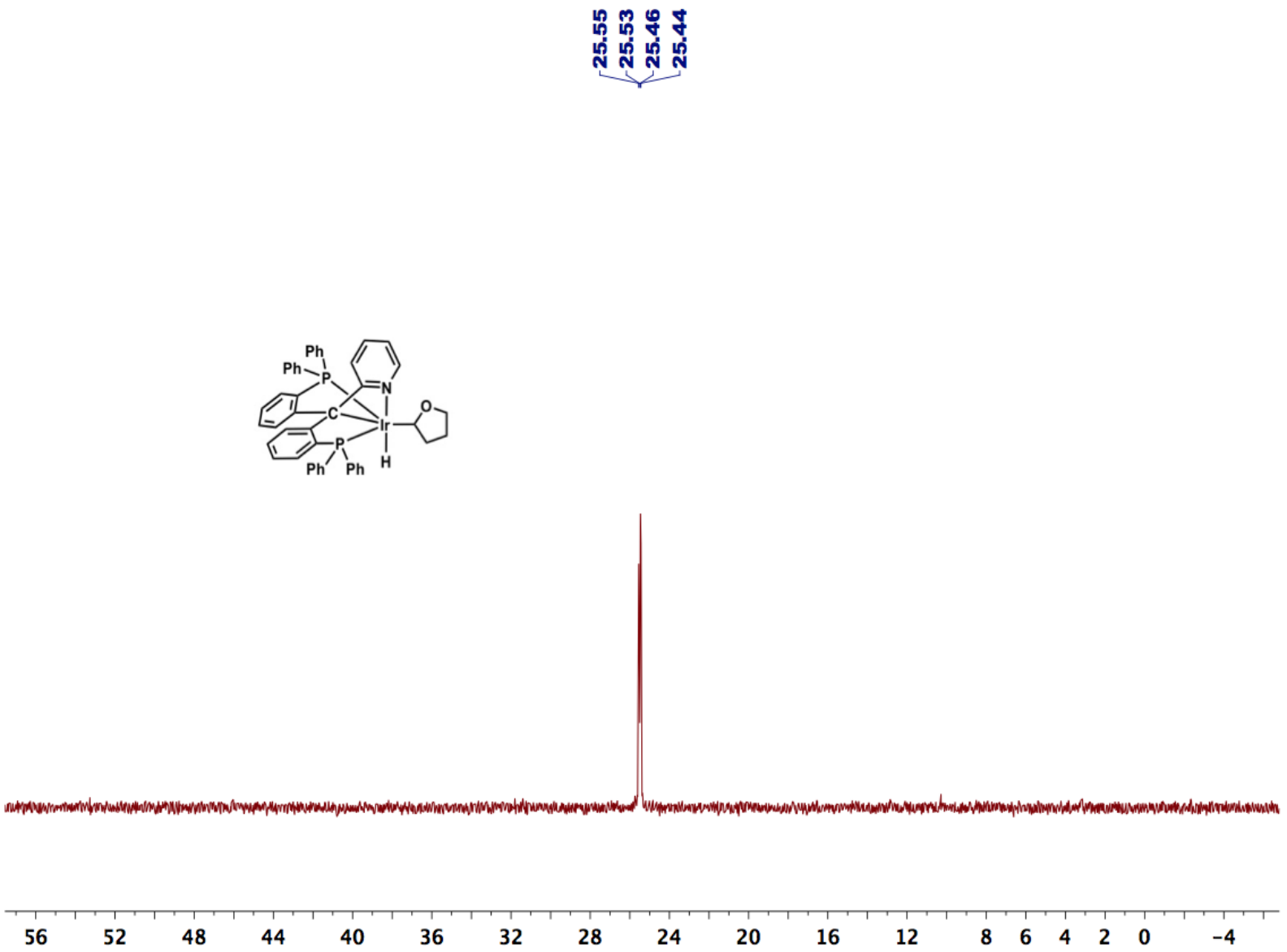

Figure S33. $^{31}P\{^{1}H\}$ NMR spectrum for [($PC^{Py}P$)IrH(C_4H_7O)] (**9**).

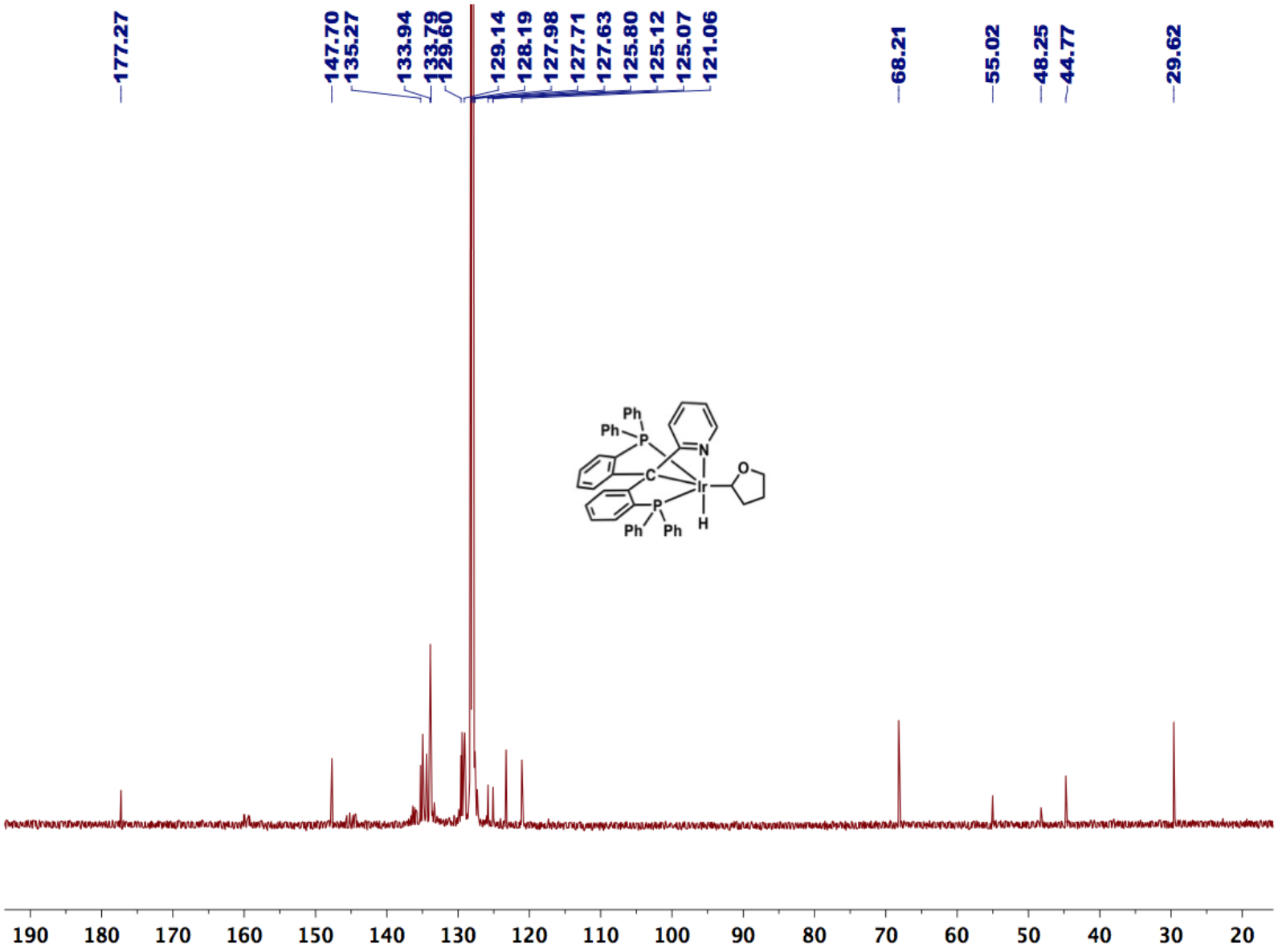

Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum for [($PC^{Py}P$)IrH(C_4H_7O)] (**9**).

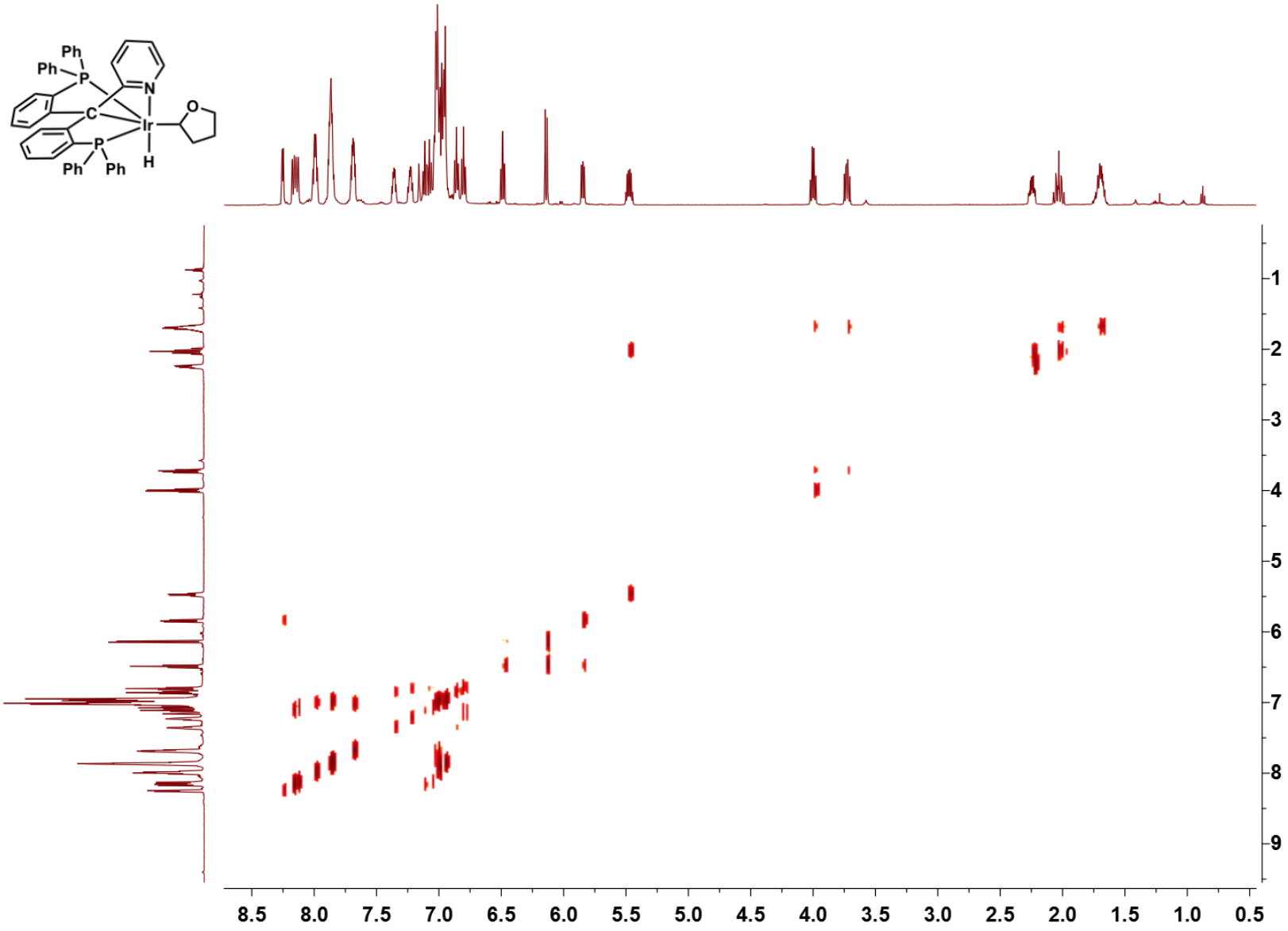

Figure S35. ^{1}H-^{1}H COSY NMR spectrum for [(PC^{Py}P)IrH(C$_4$H$_7$O)] (**9**).

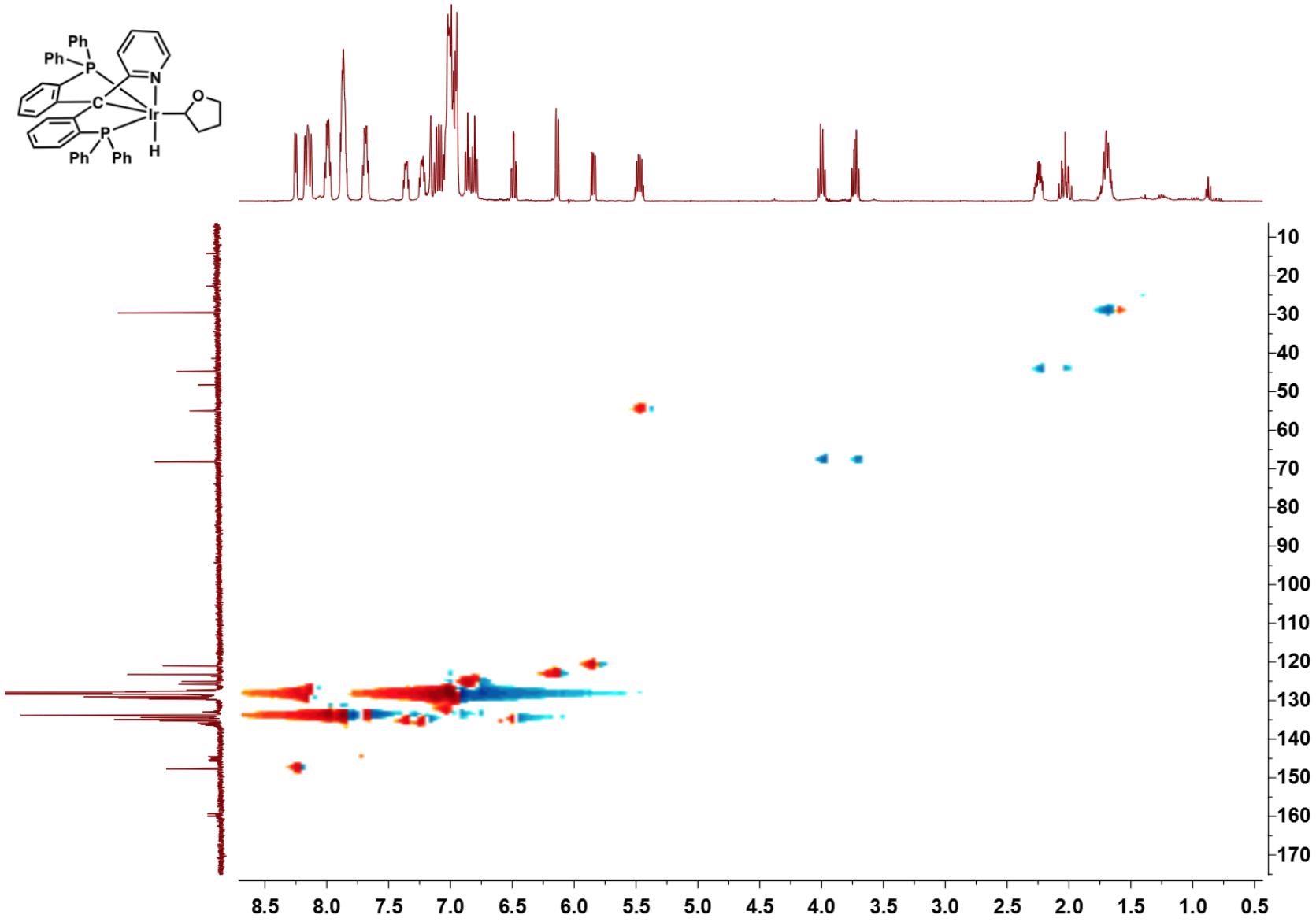

Figure S36. ^{1}H-^{13}C HSQC NMR spectrum for [($PC^{Py}P$)IrH(C_4H_7O)] (**9**).

2.9 NMR Spectra for [(PC^{Py}P)IrH(CH$_2$O^{t}Bu)] (10)

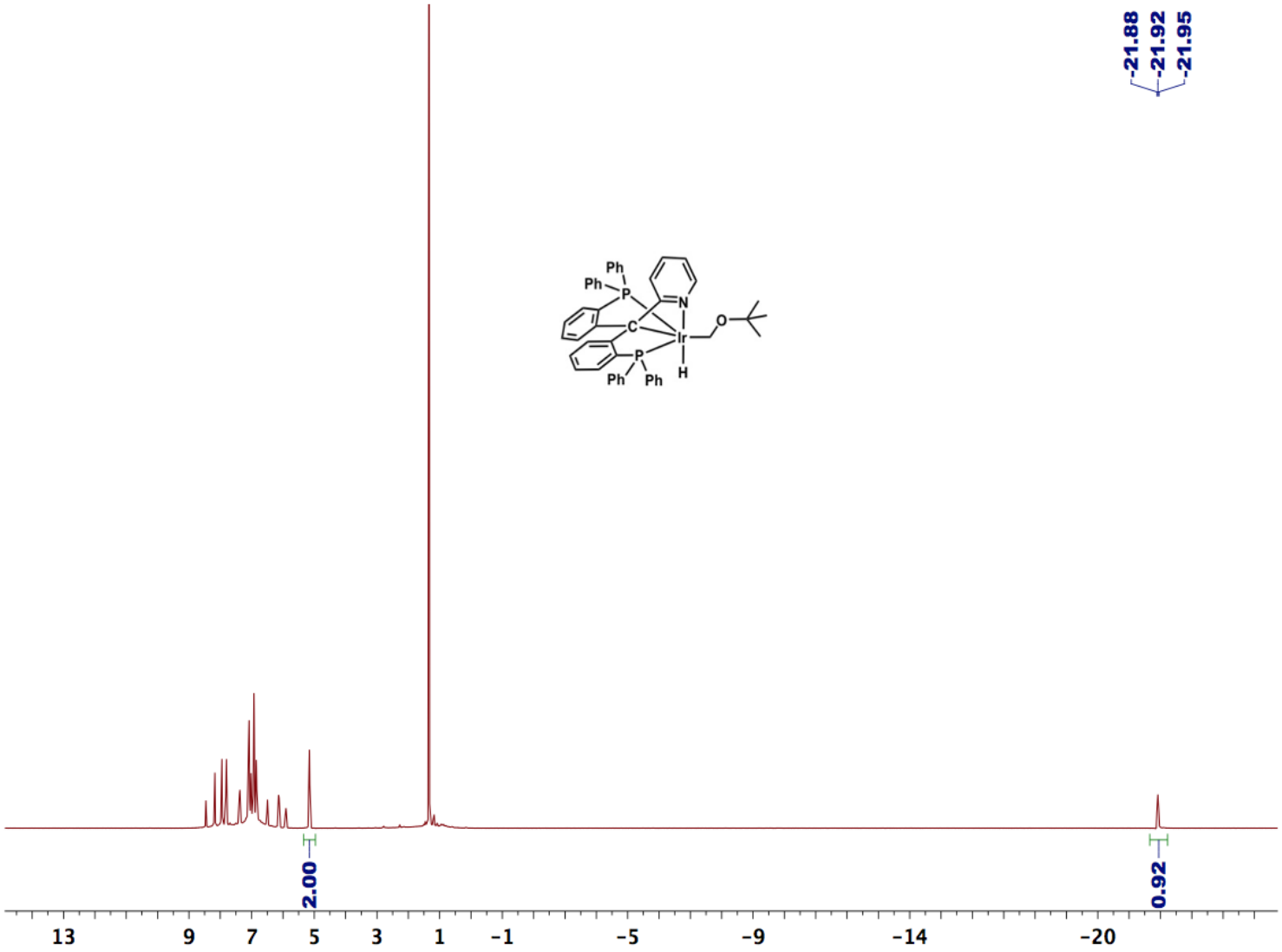

Figure S37. ^{1}H NMR spectrum for [(PC^{Py}P)IrH(CH$_2$O^{t}Bu)] (**10**).

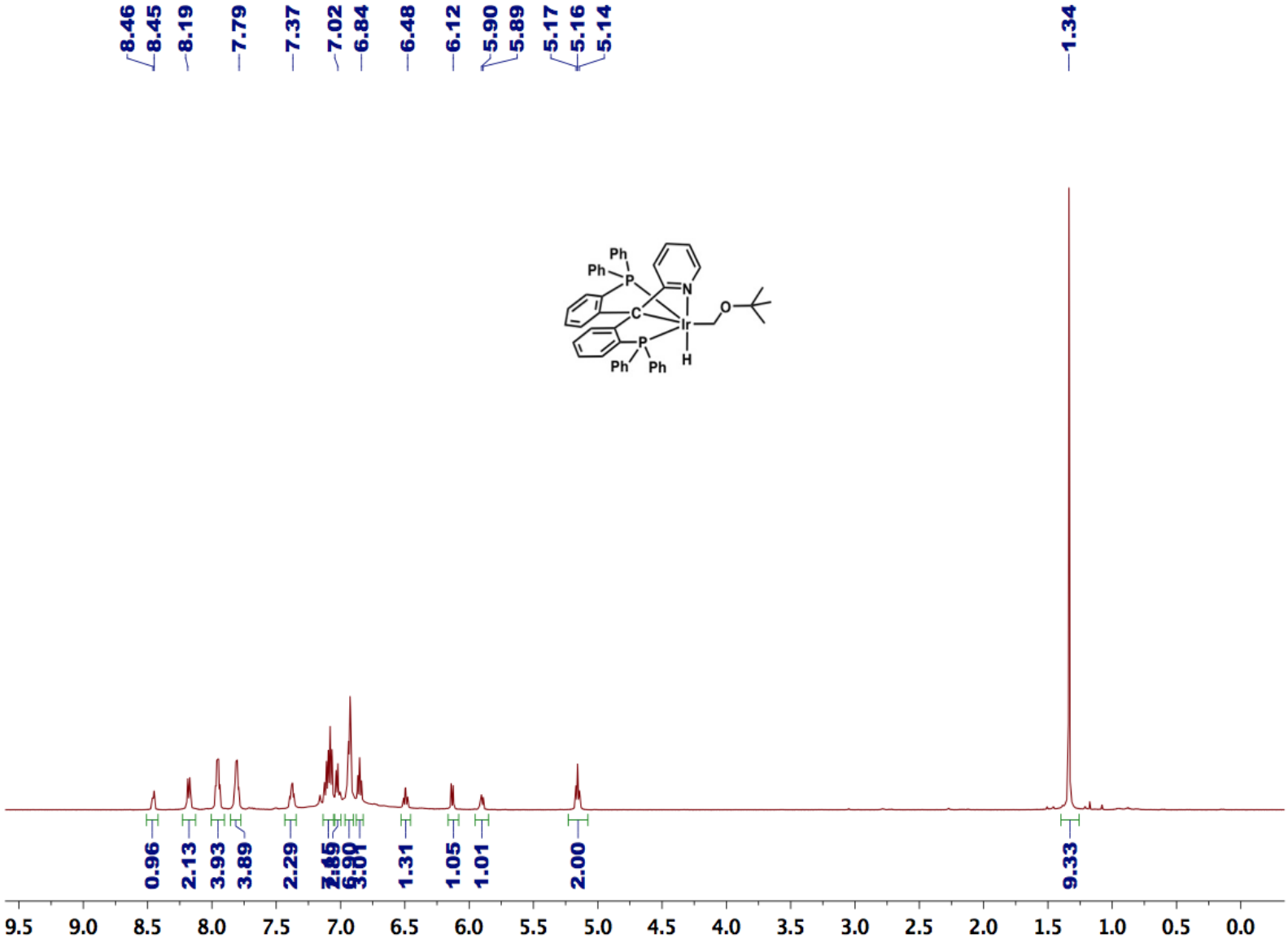

Figure S38. ^{1}H NMR spectrum for [(PC^{Py}P)IrH(CH$_2$O^{t}Bu)] (**10**).

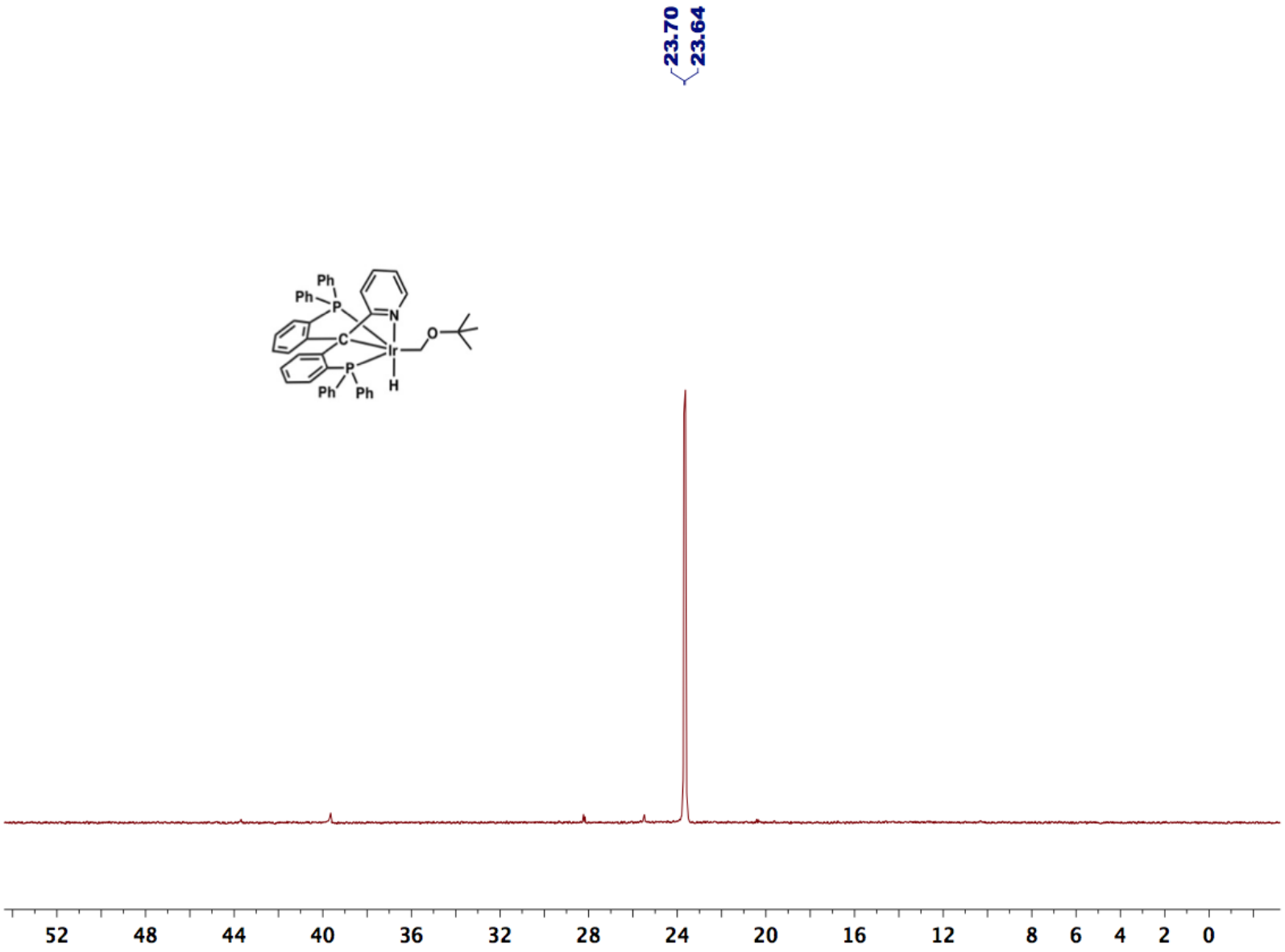

Figure S39. ^{31}P spectrum for [(PC^{Py}P)IrH(CH$_2$O^{t}Bu)] (**10**).

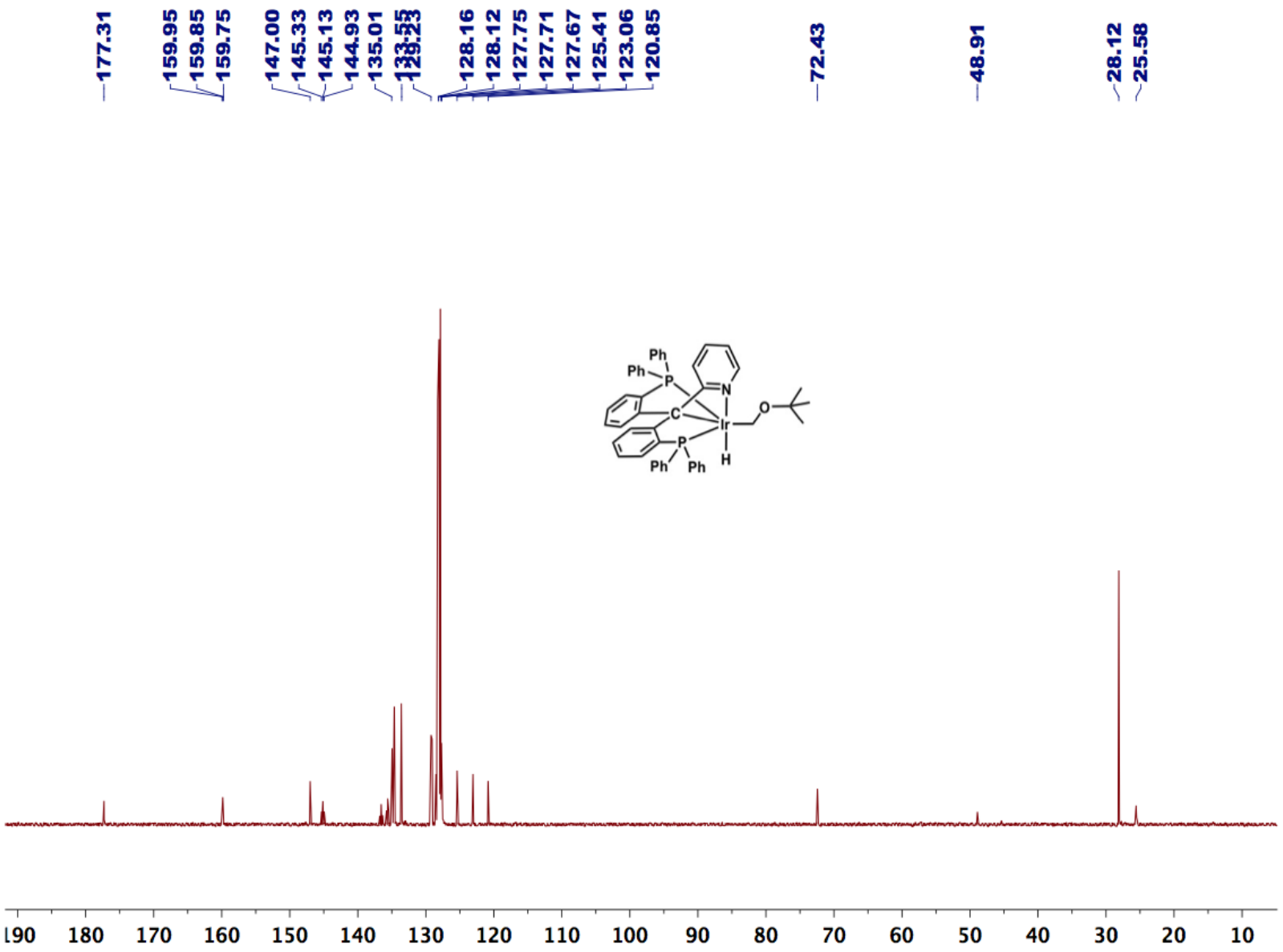

Figure S40. $^{13}C\{^{1}H\}$ NMR spectrum for [($PC^{Py}P$)IrH($CH_2O'Bu$)] (**10**).

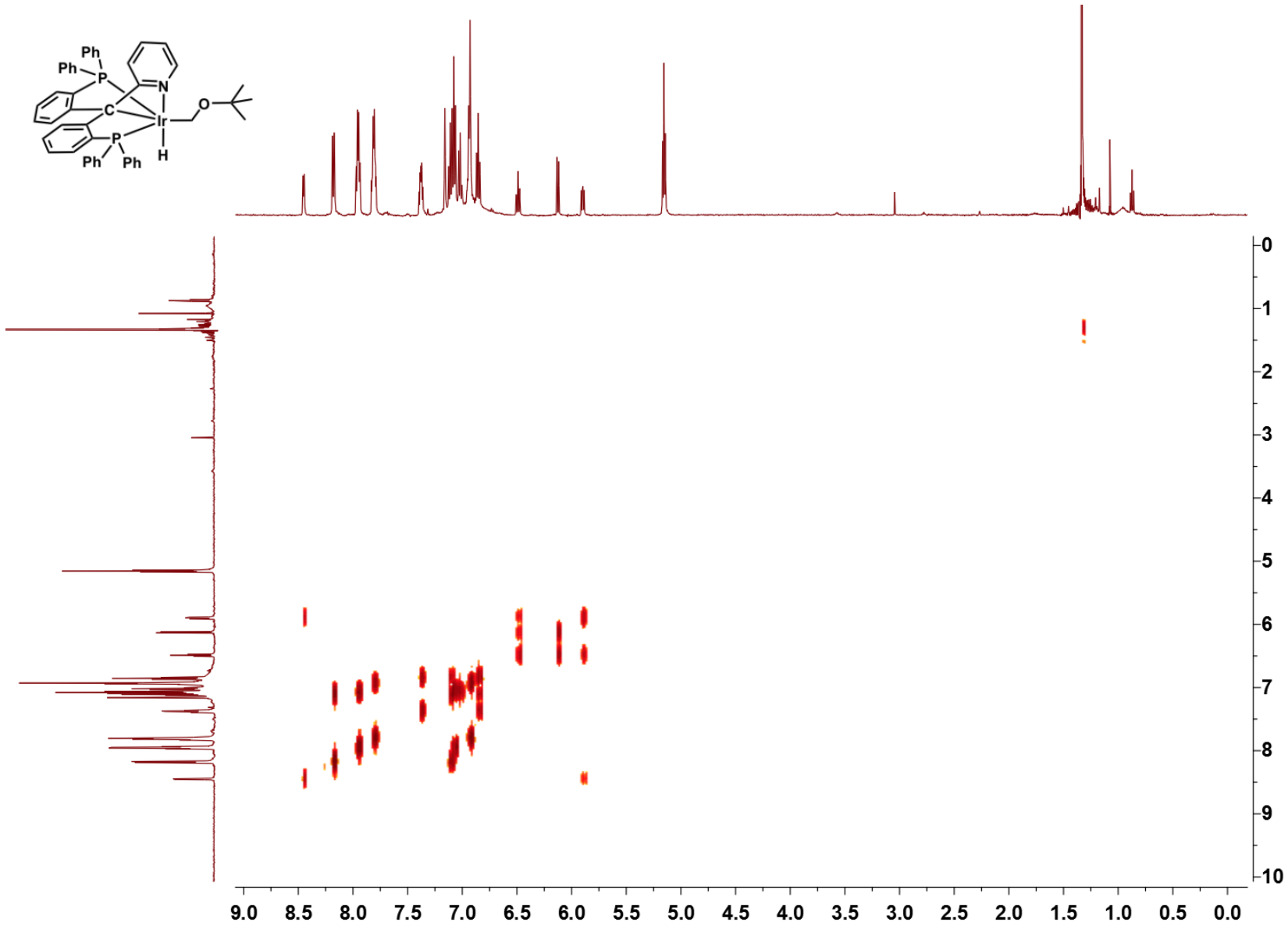

Figure S41. ^{1}H-^{1}H COSY NMR spectrum for [(PC^{Py}P)IrH(CH$_2$O^{t}Bu)] (**10**).

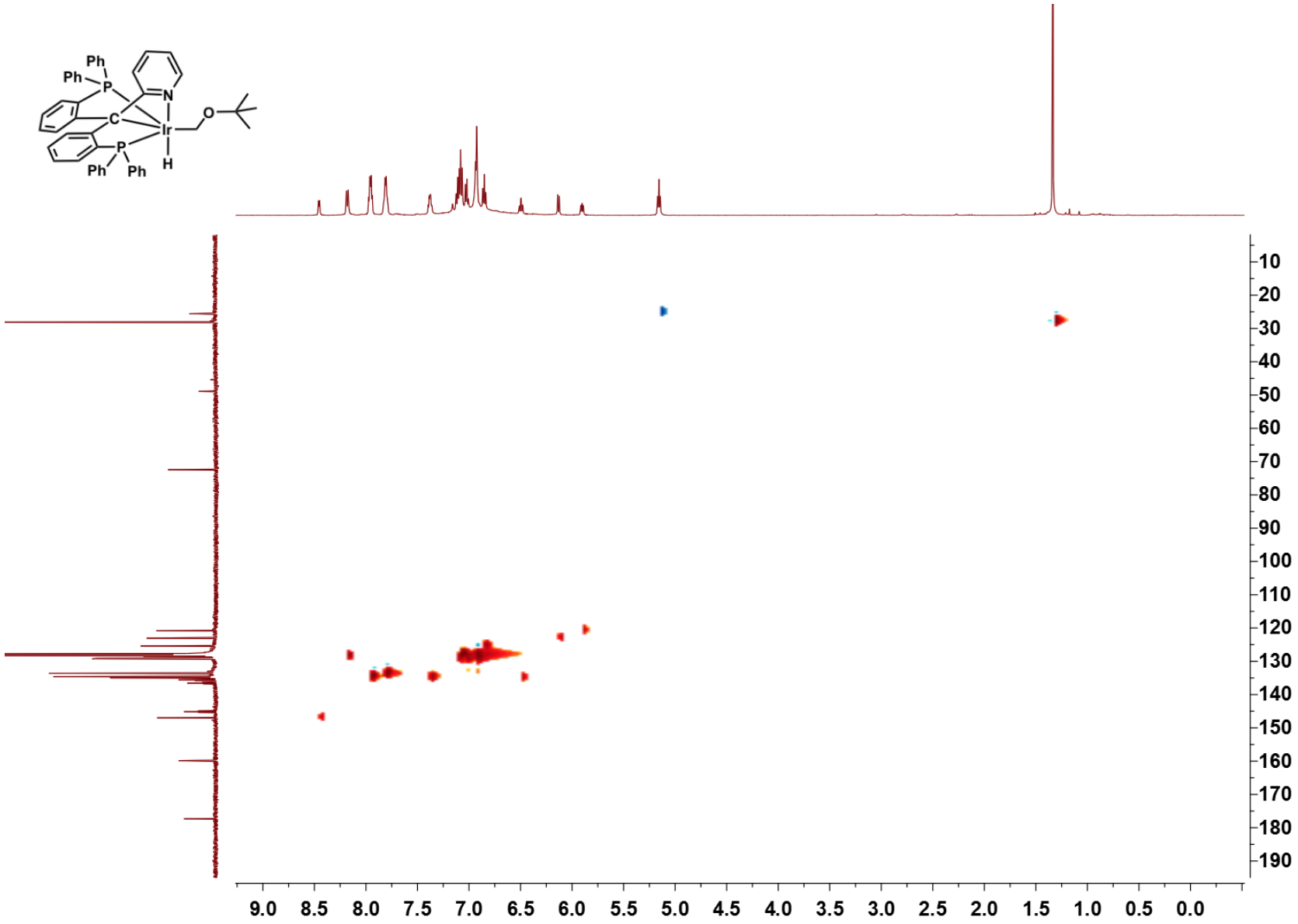

Figure S42. ^{1}H-^{13}C HSQC NMR spectrum for [($PC^{Py}P$)IrH(CH_2O^tBu)] (**10**).

2.10 NMR Spectra for [(PC^{Py}P)IrH(C$_4$H$_7$O)(CCHPh)] (11)

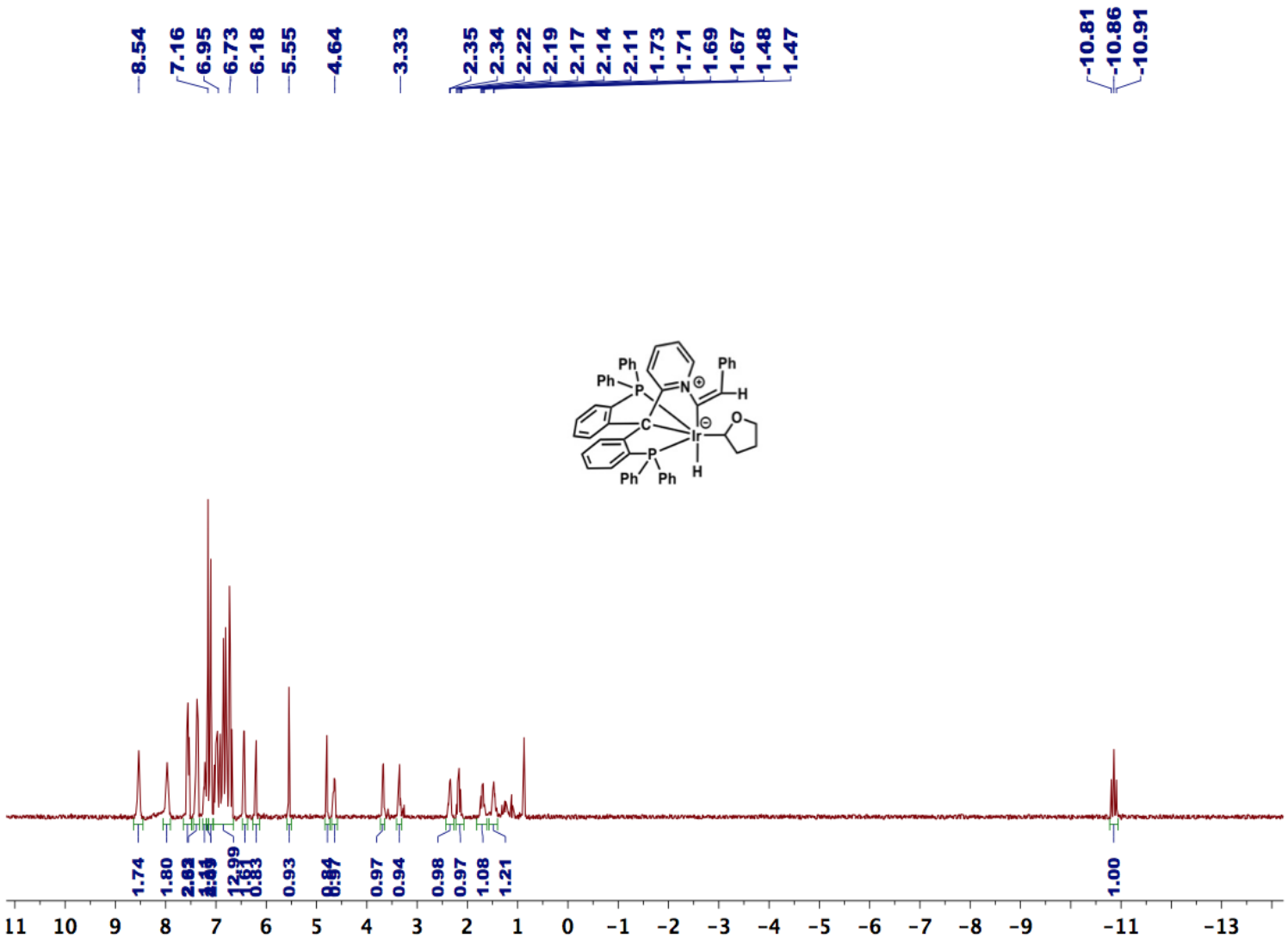

Figure S43. ^{1}H NMR spectrum for [(PC^{Py}P)IrH(C$_4$H$_7$O)(CCHPh)] (**11**).

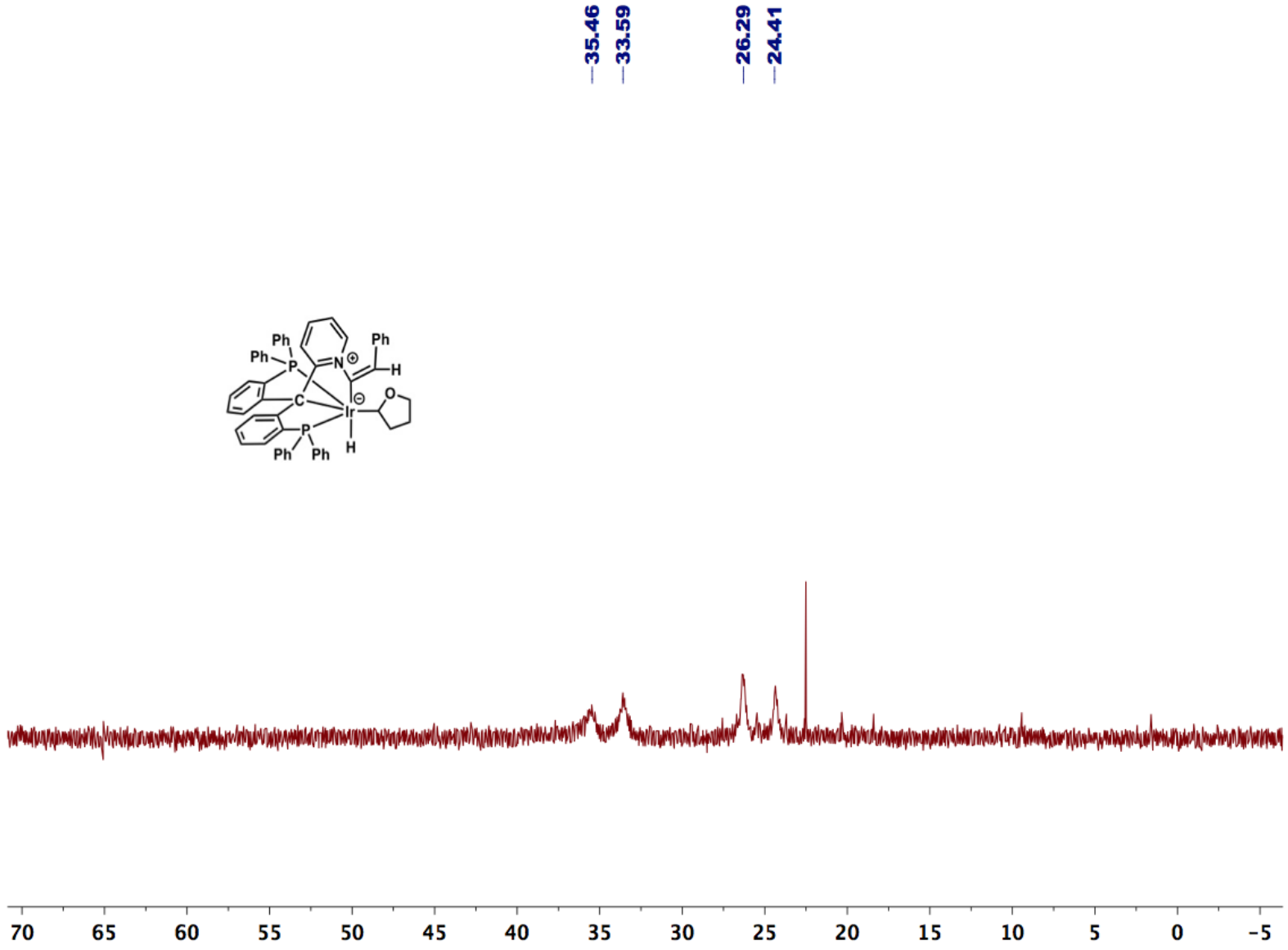

Figure S44. $^{31}P\{^{1}H\}$ NMR spectrum for [($PC^{Py}P$)IrH(C_4H_7O)(CCHPh)] (**11**).

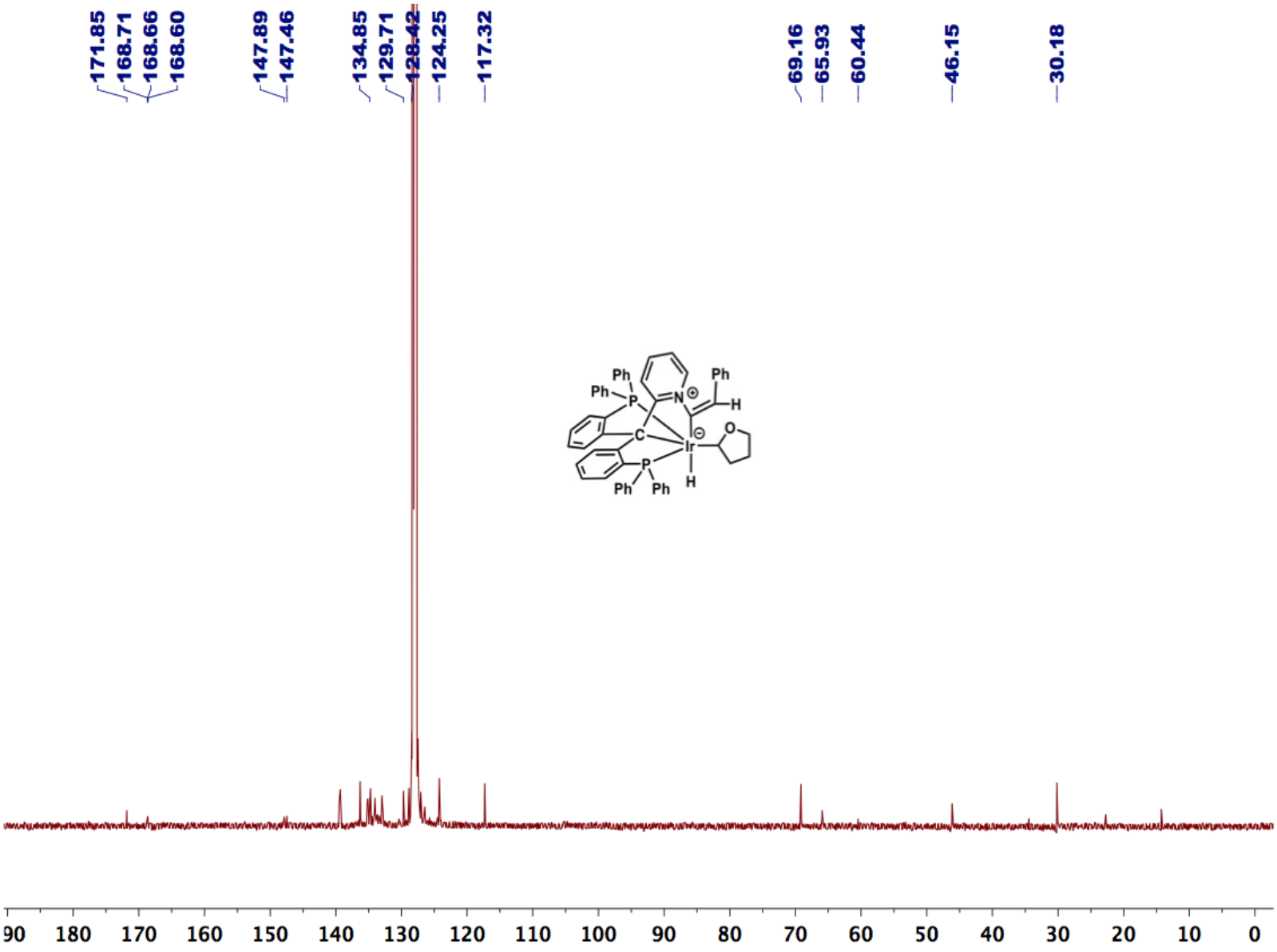

Figure S45. $^{13}C\{^{1}H\}$ NMR spectrum for [($PC^{Py}P$)IrH(C_4H_7O)(CCHPh)] (**11**).

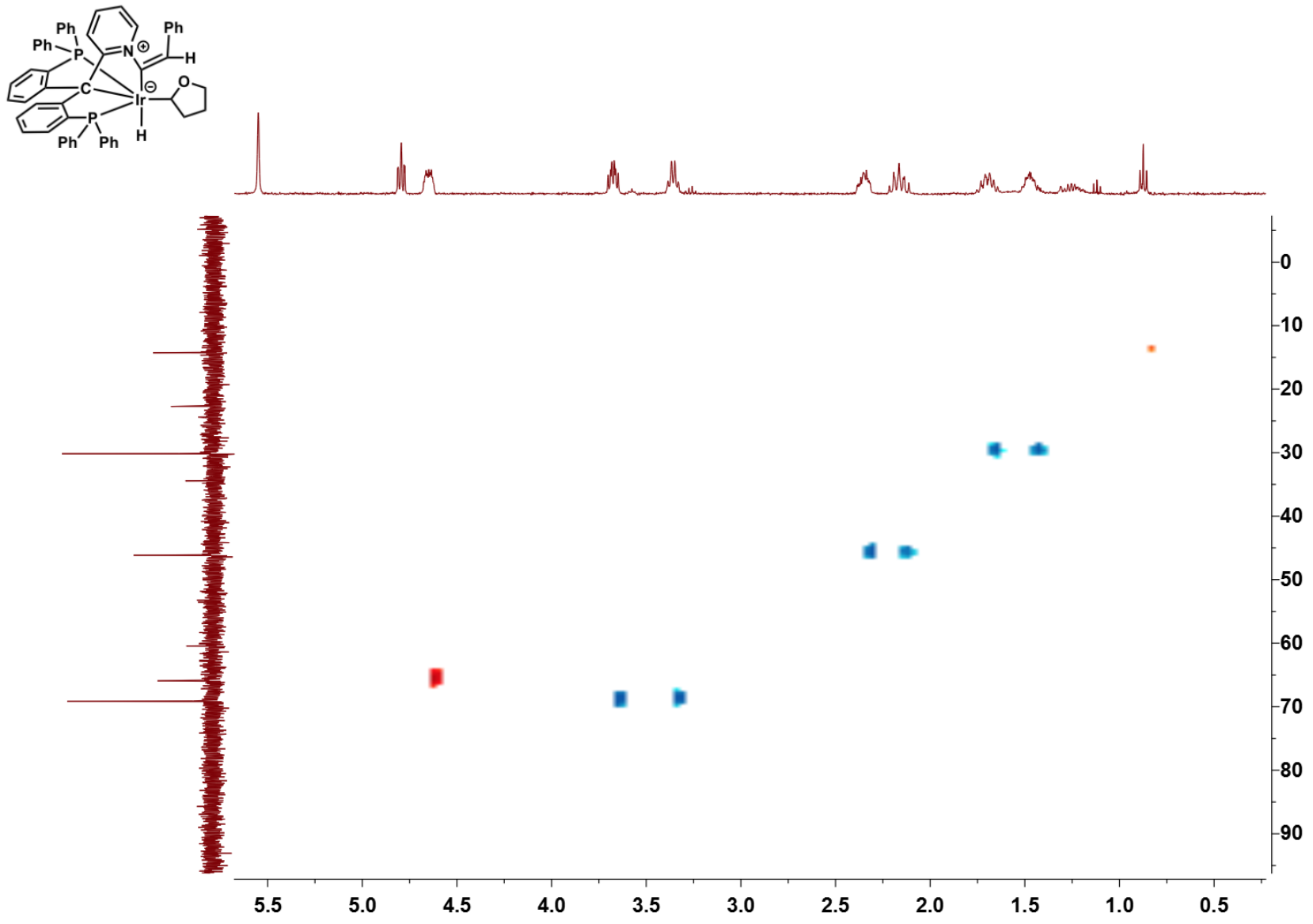

Figure S46. ^{1}H-^{13}C HSQC NMR spectrum for [($PC^{Py}P$)IrH(C_4H_7O)(CCHPh)] (**11**).

2.11 NMR Spectra for [(PC^{Py}P)IrD(C$_6$D$_5$)]

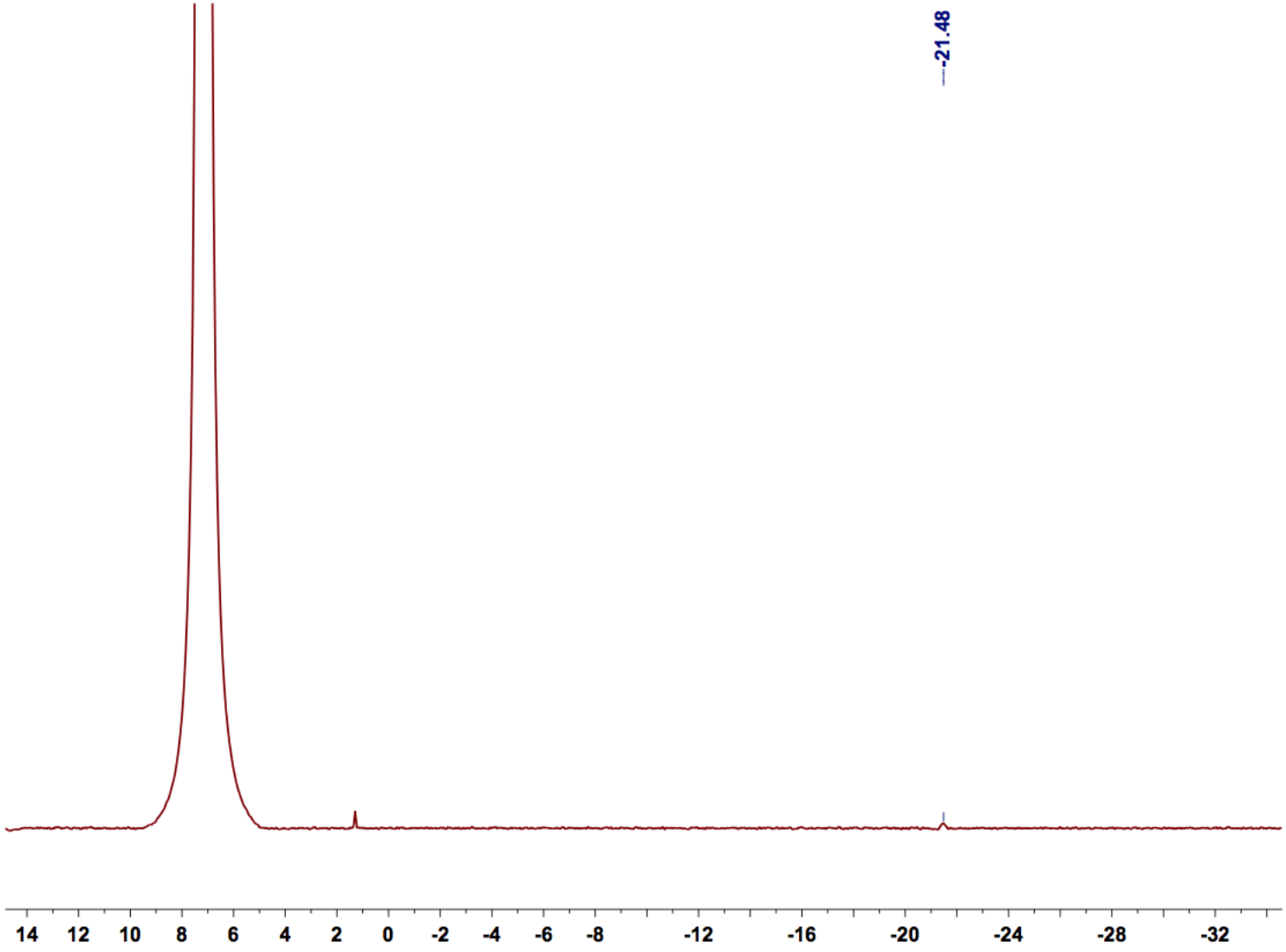

Figure S47. ^{2}H NMR spectrum for [(PC^{Py}P)IrD(C$_6$D$_5$)].

3 Crystallographic tables

3.1 Crystal data for [(PC^{Py}P)Ir(COD)] (6)

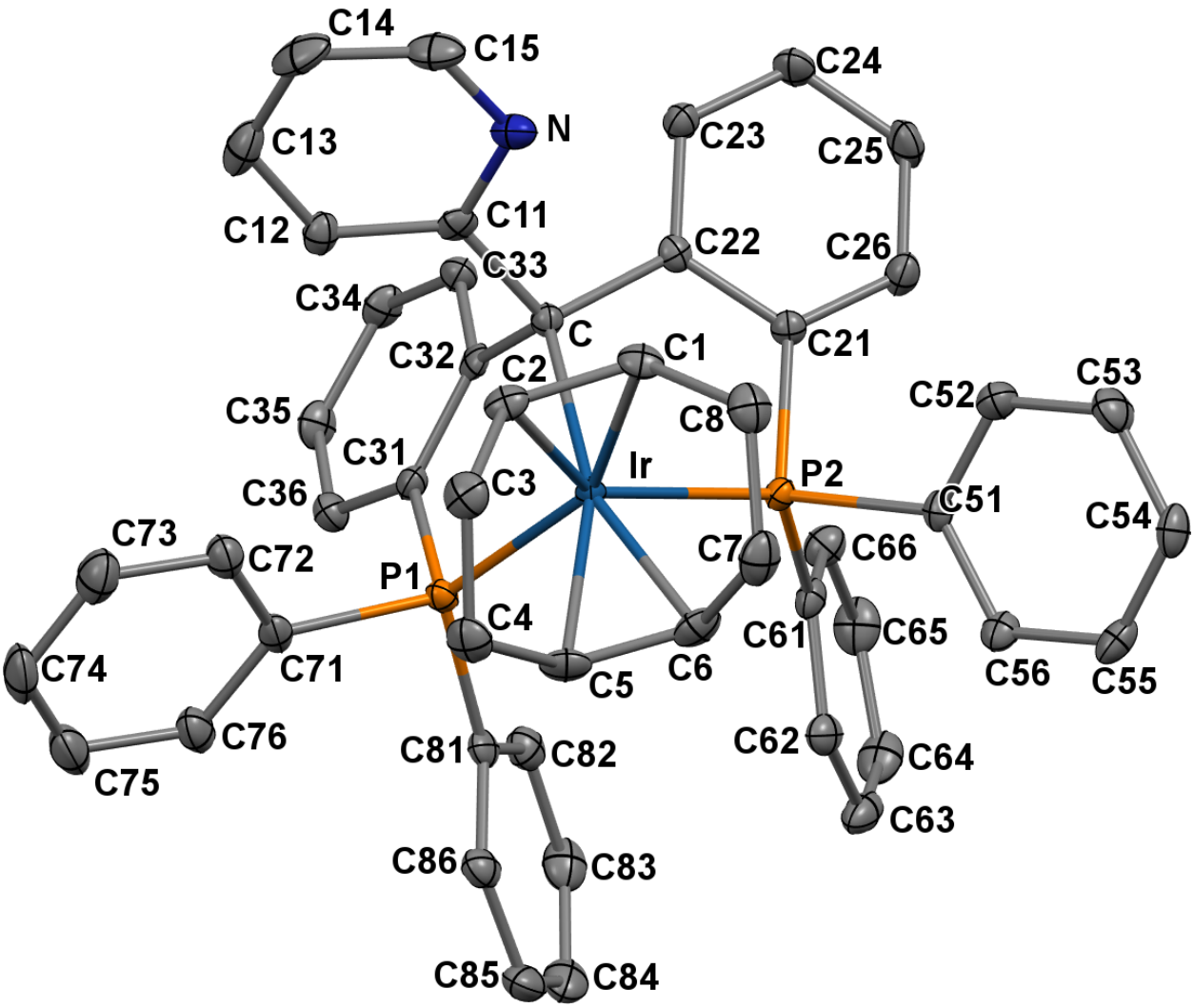

Figure S48. Thermal-ellipsoid representation of [(PC^{Py}P)Ir(COD)] (**6**) at 50% probability. Hydrogen atoms were omitted for clarity.

Table S2. Crystal data and structure refinement for [($PC^{Py}P$)Ir(COD)] (**6**).

Identification code:	pc7	
Empirical formula:	$C_{50}H_{44}IrNP_2$	
Formula weight:	913.00	
Temperature:	120(2) K	
Wavelength:	0.71073 Å	
Crystal system:	Monoclinic	
Space group:	$P2_1/n$	
Unit cell dimensions:	a = 9.9433(4) Å	$\alpha = 90°$
	b = 24.0410(9) Å	$\beta = 91.8887(14)°$
	c = 15.8819(6) Å	$\gamma = 90°$
Volume:	3794.5(3) $Å^3$	
Z:	4	
Density (calculated):	1.598 $g \cdot cm^{-3}$	
Absorption coefficient (μ):	3.641 mm^{-1}	
F(000):	1832	
Crystal size:	$0.04 \times 0.03 \times 0.03$ mm^3	
θ range for data collection:	1.54 to 25.00°	
Index ranges:	$-7 \leq h \leq 11$, $-28 \leq k \leq 28$, $-18 \leq l \leq 18$	
Reflections collected:	53230	
Independent reflections:	6681 [R_{int} = 0.0281]	
Completeness to θ = 25.00°:	100.0 %	
Absorption correction:	Semi-empirical from equivalents	
Max. and min. transmission:	0.7073 and 0.5743	
Refinement method:	Full-matrix least-squares on F^2	
Data / restraints / parameters:	6681 / 0 / 487	
Goodness-of-fit on F^2:	1.049	
Final R indices [I>2σ(I)]:	R_1 = 0.0149, wR_2 = 0.0326	
R indices (all data):	R_1 = 0.0175, wR_2 = 0.0332	
Largest diff. peak and hole:	0.346 and −0.393 $e^- \cdot Å^{-3}$	

Table S3. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for [(PC^{Py}P)Ir(COD)] (**6**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	x	y	z	U(eq)
Ir	0.47012(1)	0.11211(1)	0.75326(1)	0.010(1)
C(1)	0.4557(2)	0.02436(8)	0.73296(13)	0.016(1)
P(2)	0.49360(5)	0.14602(2)	0.61840(3)	0.011(1)
C(2)	0.4525(2)	0.03536(8)	0.82204(13)	0.016(1)
C(5)	0.2637(2)	0.11912(9)	0.80258(14)	0.019(1)
C(4)	0.2409(2)	0.08027(9)	0.87535(14)	0.021(1)
C(3)	0.3245(2)	0.02716(9)	0.87056(14)	0.020(1)
C(6)	0.2528(2)	0.10324(9)	0.71816(14)	0.019(1)
C(7)	0.2136(2)	0.04490(10)	0.68996(14)	0.023(1)
C(8)	0.3332(2)	0.00539(9)	0.68239(14)	0.022(1)
C(21)	0.6567(2)	0.11993(8)	0.58971(12)	0.012(1)
C(15)	0.7925(2)	−0.03252(9)	0.82304(15)	0.025(1)
C(14)	0.8304(2)	−0.02604(10)	0.90616(15)	0.029(1)
C(13)	0.8273(2)	0.02711(10)	0.93893(14)	0.025(1)
C(12)	0.7857(2)	0.07096(9)	0.88838(13)	0.017(1)
C(11)	0.7477(2)	0.06096(8)	0.80434(13)	0.014(1)
C(22)	0.7358(2)	0.09819(8)	0.65566(12)	0.012(1)
C(83)	0.4551(3)	0.34693(9)	0.74406(14)	0.024(1)
C(23)	0.8576(2)	0.07328(9)	0.63503(13)	0.016(1)
C(84)	0.3239(3)	0.35732(9)	0.76314(14)	0.027(1)
C(24)	0.8986(2)	0.07074(9)	0.55300(13)	0.020(1)
C(85)	0.2528(2)	0.31825(9)	0.80719(14)	0.024(1)
C(25)	0.8200(2)	0.09385(10)	0.48809(13)	0.022(1)
C(86)	0.3138(2)	0.26883(9)	0.83239(13)	0.018(1)
C(26)	0.6995(2)	0.11845(9)	0.50682(13)	0.018(1)
C(31)	0.6962(2)	0.19999(8)	0.82571(12)	0.014(1)
C(32)	0.7635(2)	0.16142(8)	0.77751(12)	0.013(1)
C(33)	0.9003(2)	0.17098(9)	0.76514(13)	0.016(1)
C(34)	0.9655(2)	0.21658(9)	0.79965(13)	0.018(1)
C(35)	0.8985(2)	0.25338(9)	0.85016(13)	0.019(1)
C(36)	0.7642(2)	0.24470(9)	0.86338(13)	0.018(1)
C(54)	0.2091(2)	0.07023(9)	0.41030(13)	0.021(1)
C(55)	0.1758(2)	0.11976(9)	0.44756(13)	0.019(1)
C(56)	0.2604(2)	0.14319(9)	0.50887(13)	0.016(1)
C(61)	0.4965(2)	0.21983(8)	0.58814(12)	0.015(1)
C(62)	0.3806(2)	0.25226(9)	0.59375(13)	0.017(1)
C(63)	0.3766(2)	0.30588(9)	0.56230(14)	0.023(1)
C(64)	0.4905(3)	0.32924(9)	0.52893(14)	0.026(1)
C(65)	0.6086(3)	0.29936(9)	0.52911(14)	0.025(1)
C(66)	0.6114(2)	0.24465(9)	0.55723(13)	0.019(1)

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Table S3. – continued from previous page

atom	x	y	x	U(eq)
C(71)	0.5000(2)	0.18514(9)	0.95051(13)	0.016(1)
C(72)	0.5087(2)	0.13349(10)	0.98965(13)	0.020(1)
C(73)	0.5009(2)	0.12865(11)	1.07642(14)	0.028(1)
C(74)	0.4847(2)	0.17590(11)	1.12482(14)	0.031(1)
C(75)	0.4772(2)	0.22739(11)	1.08710(14)	0.029(1)
C(76)	0.4849(2)	0.23236(10)	1.00059(13)	0.022(1)
N	0.75361(18)	0.00924(7)	0.77184(11)	0.019(1)
C(82)	0.5160(2)	0.29682(9)	0.76638(13)	0.019(1)
C(81)	0.4463(2)	0.25692(8)	0.81096(13)	0.015(1)
C	0.6944(2)	0.10700(8)	0.74700(12)	0.012(1)
C(53)	0.3273(2)	0.04400(9)	0.43496(14)	0.023(1)
C(52)	0.4119(2)	0.06743(9)	0.49605(13)	0.019(1)
C(51)	0.3808(2)	0.11785(8)	0.53408(12)	0.013(1)
P(1)	0.51838(5)	0.18831(2)	0.83562(3)	0.012(1)
H(1)	0.5415	0.0069	0.7150	0.020
H(2)	0.5365	0.0243	0.8541	0.019
H(5)	0.2347	0.1583	0.8130	0.023
H(4A)	0.1443	0.0703	0.8758	0.026
H(4B)	0.2640	0.0998	0.9288	0.026
H(3A)	0.3488	0.0145	0.9284	0.025
H(3B)	0.2695	−0.0023	0.8429	0.025
H(6)	0.2174	0.1332	0.6798	0.023
H(7A)	0.1651	0.0472	0.6346	0.028
H(7B)	0.1508	0.0291	0.7307	0.028
H(8A)	0.3069	−0.0321	0.7018	0.027
H(8B)	0.3563	0.0024	0.6224	0.027
H(15)	0.7938	−0.0690	0.8002	0.030
H(14)	0.8578	−0.0569	0.9399	0.035
H(13)	0.8537	0.0335	0.9961	0.031
H(12)	0.7829	0.1076	0.9106	0.020
H(83)	0.5048	0.3743	0.7153	0.029
H(23)	0.9135	0.0577	0.6786	0.019
H(84)	0.2822	0.3912	0.7461	0.033
H(24)	0.9811	0.0531	0.5408	0.024
H(85)	0.1618	0.3252	0.8203	0.029
H(25)	0.8489	0.0927	0.4317	0.026
H(86)	0.2653	0.2428	0.8645	0.022
H(26)	0.6450	0.1345	0.4630	0.022
H(33)	0.9493	0.1455	0.7322	0.019
H(34)	1.0576	0.2228	0.7886	0.021
H(35)	0.9443	0.2841	0.8753	0.023
H(36)	0.7172	0.2694	0.8986	0.021

Continued on next page

Table S3. – continued from previous page

atom	x	y	x	U(eq)
H(54)	0.1513	0.0543	0.3681	0.025
H(55)	0.0943	0.1380	0.4312	0.023
H(56)	0.2356	0.1773	0.5342	0.019
H(62)	0.3037	0.2373	0.6195	0.021
H(63)	0.2955	0.3267	0.5636	0.028
H(64)	0.4871	0.3657	0.5060	0.031
H(65)	0.6884	0.3162	0.5099	0.030
H(66)	0.6926	0.2239	0.5554	0.023
H(72)	0.5202	0.1010	0.9565	0.024
H(73)	0.5067	0.0931	1.1024	0.034
H(74)	0.4788	0.1728	1.1842	0.037
H(75)	0.4667	0.2597	1.1207	0.035
H(76)	0.4798	0.2681	0.9751	0.026
H(82)	0.6059	0.2898	0.7511	0.022
H(53)	0.3507	0.0096	0.4098	0.027
H(52)	0.4929	0.0488	0.5124	0.023

Table S4. Anisotropic displacement parameters (Å^2) for [(PC^{Py}P)Ir(COD)] (**6**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ...+ 2hka^*b^*U_{12}]$.

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir	0.0086(1)	0.0111(1)	0.0097(1)	−0.0001(1)	0.0006(1)	−0.0004(1)
C(1)	0.0176(12)	0.0094(10)	0.0224(11)	−0.0008(8)	0.0027(9)	−0.0007(9)
P(2)	0.0099(3)	0.0123(3)	0.0110(2)	0.0008(2)	−0.0006(2)	0.0000(2)
C(2)	0.0142(11)	0.0118(10)	0.0210(11)	0.0038(9)	0.0010(9)	−0.0008(9)
C(5)	0.0096(11)	0.0191(11)	0.0285(12)	0.0000(9)	0.0048(9)	0.0016(9)
C(4)	0.0164(12)	0.0276(13)	0.0206(12)	−0.0006(10)	0.0061(9)	−0.0026(10)
C(3)	0.0203(12)	0.0206(12)	0.0206(11)	0.0047(9)	0.0039(10)	−0.0031(10)
C(6)	0.0093(11)	0.0230(12)	0.0254(12)	0.0051(9)	−0.0010(9)	−0.0002(9)
C(7)	0.0168(12)	0.0321(13)	0.0211(12)	0.0012(10)	−0.0034(10)	−0.0080(10)
C(8)	0.0251(13)	0.0192(12)	0.0220(12)	−0.0010(9)	0.0002(10)	−0.0051(10)
C(21)	0.0107(10)	0.0139(10)	0.0128(10)	0.0002(8)	0.0011(8)	−0.0019(8)
C(15)	0.0252(13)	0.0162(11)	0.0348(14)	0.0047(10)	0.0063(11)	0.0062(10)
C(14)	0.0243(13)	0.0293(14)	0.0340(14)	0.0187(11)	0.0024(11)	0.0090(11)
C(13)	0.0186(12)	0.0408(15)	0.0168(11)	0.0104(10)	−0.0024(10)	−0.0032(11)
C(12)	0.0131(11)	0.0223(11)	0.0143(10)	0.0011(9)	−0.0003(9)	−0.0026(9)
C(11)	0.0069(10)	0.0180(11)	0.0170(10)	0.0025(9)	0.0026(8)	0.0002(9)
C(22)	0.0119(11)	0.0114(10)	0.0129(10)	−0.0013(8)	0.0005(8)	−0.0033(8)
C(83)	0.0347(15)	0.0157(11)	0.0222(12)	−0.0013(9)	−0.0030(11)	−0.0047(10)
C(23)	0.0132(11)	0.0203(11)	0.0143(10)	−0.0002(9)	−0.0010(9)	0.0008(9)
C(84)	0.0397(16)	0.0173(12)	0.0244(12)	−0.0059(10)	−0.0057(11)	0.0084(11)
C(24)	0.0132(11)	0.0284(12)	0.0183(11)	−0.0038(9)	0.0030(9)	0.0027(10)
C(85)	0.0228(13)	0.0256(13)	0.0249(12)	−0.0104(10)	−0.0018(10)	0.0085(10)
C(25)	0.0200(12)	0.0328(13)	0.0123(11)	−0.0017(9)	0.0043(9)	−0.0015(10)
C(86)	0.0180(12)	0.0185(11)	0.0185(11)	−0.0062(9)	−0.0002(9)	−0.0001(9)
C(26)	0.0146(11)	0.0259(12)	0.0135(10)	0.0029(9)	−0.0012(9)	−0.0007(10)
C(31)	0.0113(11)	0.0180(11)	0.0114(10)	0.0007(8)	−0.0019(8)	0.0014(9)
C(32)	0.0132(11)	0.0154(10)	0.0092(9)	0.0053(8)	−0.0006(8)	0.0006(9)
C(33)	0.0138(11)	0.0198(11)	0.0140(10)	0.0001(9)	0.0022(9)	0.0017(9)
C(34)	0.0107(11)	0.0227(12)	0.0196(11)	0.0026(9)	−0.0012(9)	−0.0041(9)
C(35)	0.0183(12)	0.0189(11)	0.0193(11)	−0.0021(9)	−0.0044(9)	−0.0061(9)
C(36)	0.0184(12)	0.0183(11)	0.0158(11)	−0.0041(9)	−0.0002(9)	0.0014(9)
C(54)	0.0225(13)	0.0239(12)	0.0154(11)	−0.0005(9)	−0.0057(9)	−0.0070(10)
C(55)	0.0161(12)	0.0192(12)	0.0216(11)	0.0055(9)	−0.0072(9)	−0.0016(9)
C(56)	0.0185(12)	0.0130(11)	0.0170(11)	0.0010(8)	−0.0026(9)	−0.0008(9)
C(61)	0.0159(11)	0.0155(11)	0.0121(10)	−0.0001(8)	−0.0043(9)	−0.0017(9)
C(62)	0.0156(12)	0.0173(11)	0.0184(11)	−0.0050(9)	−0.0042(9)	−0.0016(9)
C(63)	0.0260(13)	0.0175(11)	0.0254(12)	−0.0050(10)	−0.0124(10)	0.0047(10)
C(64)	0.0370(15)	0.0141(11)	0.0252(12)	0.0030(9)	−0.0076(11)	−0.0021(11)
C(65)	0.0291(14)	0.0223(12)	0.0227(12)	0.0042(10)	0.0003(10)	−0.0093(11)
C(66)	0.0172(12)	0.0194(11)	0.0208(11)	0.0019(9)	−0.0011(9)	−0.0015(9)

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Table S4. – continued from previous page

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(71)	0.0098(11)	0.0263(12)	0.0131(10)	−0.0039(9)	0.0006(9)	−0.0010(9)
C(72)	0.0179(12)	0.0260(12)	0.0155(11)	−0.0022(9)	0.0011(9)	−0.0012(10)
C(73)	0.0257(14)	0.0390(15)	0.0193(12)	0.0056(11)	−0.0007(10)	−0.0006(11)
C(74)	0.0279(14)	0.0536(17)	0.0115(11)	−0.0033(11)	0.0002(10)	−0.0014(12)
C(75)	0.0255(14)	0.0424(15)	0.0194(12)	−0.0117(11)	0.0013(10)	0.0014(12)
C(76)	0.0189(12)	0.0290(13)	0.0178(11)	−0.0078(10)	−0.0012(10)	−0.0006(10)
N	0.0168(10)	0.0167(9)	0.0222(10)	0.0012(8)	0.0040(8)	0.0037(8)
C(82)	0.0193(12)	0.0187(11)	0.0178(11)	−0.0041(9)	−0.0008(9)	−0.0025(9)
C(81)	0.0160(11)	0.0161(11)	0.0131(10)	−0.0063(8)	−0.0029(9)	−0.0002(9)
C	0.0116(10)	0.0139(10)	0.0106(10)	0.0001(8)	0.0003(8)	−0.0003(9)
C(53)	0.0255(13)	0.0209(12)	0.0211(12)	−0.0082(9)	−0.0003(10)	−0.0006(10)
C(52)	0.0158(12)	0.0214(11)	0.0197(11)	−0.0013(9)	−0.0004(9)	0.0026(9)
C(51)	0.0136(11)	0.0145(10)	0.0099(10)	0.0023(8)	0.0008(8)	−0.0034(9)
P(1)	0.0105(3)	0.0143(3)	0.0120(3)	−0.0021(2)	0.0010(2)	−0.0001(2)

Table S5. Distances [Å] for [(PC^{Py}P)Ir(COD)] (**6**).

atom – atom	distance	atom – atom	distance
Ir – C(1)	2.138(2)	Ir – C(2)	2.154(2)
Ir – C(6)	2.224(2)	Ir – C(5)	2.227(2)
Ir – C	2.239(2)	Ir – P(1)	2.2925(5)
Ir – P(2)	2.3106(5)	C(1) – C(2)	1.441(3)
C(1) – C(8)	1.507(3)	C(1) – H(1)	1.0000
P(2) – C(21)	1.811(2)	P(2) – C(61)	1.839(2)
P(2) – C(51)	1.847(2)	C(2) – C(3)	1.522(3)
C(2) – H(2)	1.0000	C(5) – C(6)	1.395(3)
C(5) – C(4)	1.509(3)	C(5) – H(5)	1.0000
C(4) – C(3)	1.527(3)	C(4) – H(4A)	0.9900
C(4) – H(4B)	0.9900	C(3) – H(3A)	0.9900
C(3) – H(3B)	0.9900	C(6) – C(7)	1.519(3)
C(6) – H(6)	1.0000	C(7) – C(8)	1.530(3)
C(7) – H(7A)	0.9900	C(7) – H(7B)	0.9900
C(8) – H(8A)	0.9900	C(8) – H(8B)	0.9900
C(21) – C(22)	1.391(3)	C(21) – C(26)	1.397(3)
C(15) – N	1.341(3)	C(15) – C(14)	1.370(3)
C(15) – H(15)	0.9500	C(14) – C(13)	1.380(3)
C(14) – H(14)	0.9500	C(13) – C(12)	1.380(3)
C(13) – H(13)	0.9500	C(12) – C(11)	1.396(3)
C(12) – H(12)	0.9500	C(11) – N	1.348(3)
C(11) – C	1.518(3)	C(22) – C(23)	1.400(3)
C(22) – C	1.536(3)	C(83) – C(84)	1.372(3)
C(83) – C(82)	1.389(3)	C(83) – H(83)	0.9500
C(23) – C(24)	1.379(3)	C(23) – H(23)	0.9500
C(84) – C(85)	1.380(3)	C(84) – H(84)	0.9500
C(24) – C(25)	1.389(3)	C(24) – H(24)	0.9500
C(85) – C(86)	1.387(3)	C(85) – H(85)	0.9500
C(25) – C(26)	1.377(3)	C(25) – H(25)	0.9500
C(86) – C(81)	1.401(3)	C(86) – H(86)	0.9500
C(26) – H(26)	0.9500	C(31) – C(32)	1.388(3)
C(31) – C(36)	1.394(3)	C(31) – P(1)	1.803(2)
C(32) – C(33)	1.400(3)	C(32) – C	1.548(3)
C(33) – C(34)	1.378(3)	C(33) – H(33)	0.9500
C(34) – C(35)	1.381(3)	C(34) – H(34)	0.9500
C(35) – C(36)	1.374(3)	C(35) – H(35)	0.9500
C(36) – H(36)	0.9500	C(54) – C(55)	1.375(3)
C(54) – C(53)	1.379(3)	C(54) – H(54)	0.9500
C(55) – C(56)	1.385(3)	C(55) – H(55)	0.9500
C(56) – C(51)	1.390(3)	C(56) – H(56)	0.9500
C(61) – C(66)	1.393(3)	C(61) – C(62)	1.396(3)

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Table S5. – continued from previous page

atom – atom	distance	atom – atom	distance
C(62) – C(63)	1.383(3)	C(62) – H(62)	0.9500
C(63) – C(64)	1.385(3)	C(63) – H(63)	0.9500
C(64) – C(65)	1.376(3)	C(64) – H(64)	0.9500
C(65) – C(66)	1.389(3)	C(65) – H(65)	0.9500
C(66) – H(66)	0.9500	C(71) – C(72)	1.390(3)
C(71) – C(76)	1.397(3)	C(71) – P(1)	1.841(2)
C(72) – C(73)	1.388(3)	C(72) – H(72)	0.9500
C(73) – C(74)	1.384(3)	C(73) – H(73)	0.9500
C(74) – C(75)	1.376(4)	C(74) – H(74)	0.9500
C(75) – C(76)	1.384(3)	C(75) – H(75)	0.9500
C(76) – H(76)	0.9500	C(82) – C(81)	1.391(3)
C(82) – H(82)	0.9500	C(81) – P(1)	1.836(2)
C(53) – C(52)	1.383(3)	C(53) – H(53)	0.9500
C(52) – C(51)	1.394(3)	C(52) – H(52)	0.9500

Table S6. Angles [°] for [(PC^{Py}P)Ir(COD)] (**6**).

atom – atom – atom	angle	atom – atom – atom	angle
C(1) – Ir – C(2)	39.22(8)	C(1) – Ir – C(6)	78.92(8)
C(2) – Ir – C(6)	87.16(8)	C(1) – Ir – C(5)	94.00(8)
C(2) – Ir – C(5)	78.19(8)	C(6) – Ir – C(5)	36.53(8)
C(1) – Ir – C	90.06(8)	C(2) – Ir – C	94.20(8)
C(6) – Ir – C	160.83(8)	C(5) – Ir – C	161.90(8)
C(1) – Ir – P(1)	152.39(6)	C(2) – Ir – P(1)	114.46(6)
C(6) – Ir – P(1)	113.77(6)	C(5) – Ir – P(1)	85.23(6)
C – Ir – P(1)	83.06(5)	C(1) – Ir – P(2)	102.51(6)
C(2) – Ir – P(2)	141.68(6)	C(6) – Ir – P(2)	85.90(6)
C(5) – Ir – P(2)	114.95(6)	C – Ir – P(2)	81.20(5)
P(1) – Ir – P(2)	102.789(19)	C(2) – C(1) – C(8)	122.35(19)
C(2) – C(1) – Ir	71.00(11)	C(8) – C(1) – Ir	115.33(14)
C(2) – C(1) – H(1)	113.8	C(8) – C(1) – H(1)	113.8
Ir – C(1) – H(1)	113.8	C(21) – P(2) – C(61)	104.27(10)
C(21) – P(2) – C(51)	102.59(9)	C(61) – P(2) – C(51)	100.29(9)
C(21) – P(2) – Ir	103.28(7)	C(61) – P(2) – Ir	125.84(7)
C(51) – P(2) – Ir	117.73(6)	C(1) – C(2) – C(3)	121.28(19)
C(1) – C(2) – Ir	69.78(11)	C(3) – C(2) – Ir	116.80(14)
C(1) – C(2) – H(2)	114.0	C(3) – C(2) – H(2)	114.0
Ir – C(2) – H(2)	114.0	C(6) – C(5) – C(4)	123.9(2)
C(6) – C(5) – Ir	71.61(12)	C(4) – C(5) – Ir	112.73(14)
C(6) – C(5) – H(5)	113.8	C(4) – C(5) – H(5)	113.8
Ir – C(5) – H(5)	113.8	C(5) – C(4) – C(3)	112.53(18)
C(5) – C(4) – H(4A)	109.1	C(3) – C(4) – H(4A)	109.1
C(5) – C(4) – H(4B)	109.1	C(3) – C(4) – H(4B)	109.1
H(4A) – C(4) – H(4B)	107.8	C(2) – C(3) – C(4)	112.51(18)
C(2) – C(3) – H(3A)	109.1	C(4) – C(3) – H(3A)	109.1
C(2) – C(3) – H(3B)	109.1	C(4) – C(3) – H(3B)	109.1
H(3A) – C(3) – H(3B)	107.8	C(5) – C(6) – C(7)	123.2(2)
C(5) – C(6) – Ir	71.86(12)	C(7) – C(6) – Ir	113.60(15)
C(5) – C(6) – H(6)	113.8	C(7) – C(6) – H(6)	113.8
Ir – C(6) – H(6)	113.8	C(6) – C(7) – C(8)	113.80(18)
C(6) – C(7) – H(7A)	108.8	C(8) – C(7) – H(7A)	108.8
C(6) – C(7) – H(7B)	108.8	C(8) – C(7) – H(7B)	108.8
H(7A) – C(7) – H(7B)	107.7	C(1) – C(8) – C(7)	112.76(18)
C(1) – C(8) – H(8A)	109.0	C(7) – C(8) – H(8A)	109.0
C(1) – C(8) – H(8B)	109.0	C(7) – C(8) – H(8B)	109.0
H(8A) – C(8) – H(8B)	107.8	C(22) – C(21) – C(26)	121.17(19)
C(22) – C(21) – P(2)	115.45(15)	C(26) – C(21) – P(2)	123.30(16)
N – C(15) – C(14)	124.3(2)	N – C(15) – H(15)	117.8
C(14) – C(15) – H(15)	117.8	C(15) – C(14) – C(13)	117.4(2)

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Table S6. – continued from previous page

atom – atom – atom	angle	atom – atom – atom	angle
C(15) – C(14) – H(14)	121.3	C(13) – C(14) – H(14)	121.3
C(14) – C(13) – C(12)	119.9(2)	C(14) – C(13) – H(13)	120.1
C(12) – C(13) – H(13)	120.1	C(13) – C(12) – C(11)	119.4(2)
C(13) – C(12) – H(12)	120.3	C(11) – C(12) – H(12)	120.3
N – C(11) – C(12)	120.74(19)	N – C(11) – C	117.49(18)
C(12) – C(11) – C	121.74(18)	C(21) – C(22) – C(23)	117.19(18)
C(21) – C(22) – C	119.79(18)	C(23) – C(22) – C	122.76(18)
C(84) – C(83) – C(82)	120.7(2)	C(84) – C(83) – H(83)	119.6
C(82) – C(83) – H(83)	119.6	C(24) – C(23) – C(22)	121.6(2)
C(24) – C(23) – H(23)	119.2	C(22) – C(23) – H(23)	119.2
C(83) – C(84) – C(85)	119.7(2)	C(83) – C(84) – H(84)	120.2
C(85) – C(84) – H(84)	120.2	C(23) – C(24) – C(25)	120.5(2)
C(23) – C(24) – H(24)	119.8	C(25) – C(24) – H(24)	119.8
C(84) – C(85) – C(86)	120.2(2)	C(84) – C(85) – H(85)	119.9
C(86) – C(85) – H(85)	119.9	C(26) – C(25) – C(24)	118.9(2)
C(26) – C(25) – H(25)	120.5	C(24) – C(25) – H(25)	120.5
C(85) – C(86) – C(81)	120.7(2)	C(85) – C(86) – H(86)	119.6
C(81) – C(86) – H(86)	119.6	C(25) – C(26) – C(21)	120.6(2)
C(25) – C(26) – H(26)	119.7	C(21) – C(26) – H(26)	119.7
C(32) – C(31) – C(36)	121.09(19)	C(32) – C(31) – P(1)	115.83(15)
C(36) – C(31) – P(1)	123.08(16)	C(31) – C(32) – C(33)	117.09(19)
C(31) – C(32) – C	121.39(18)	C(33) – C(32) – C	121.19(18)
C(34) – C(33) – C(32)	121.4(2)	C(34) – C(33) – H(33)	119.3
C(32) – C(33) – H(33)	119.3	C(33) – C(34) – C(35)	120.7(2)
C(33) – C(34) – H(34)	119.6	C(35) – C(34) – H(34)	119.6
C(36) – C(35) – C(34)	118.8(2)	C(36) – C(35) – H(35)	120.6
C(34) – C(35) – H(35)	120.6	C(35) – C(36) – C(31)	120.7(2)
C(35) – C(36) – H(36)	119.6	C(31) – C(36) – H(36)	119.6
C(55) – C(54) – C(53)	119.3(2)	C(55) – C(54) – H(54)	120.4
C(53) – C(54) – H(54)	120.4	C(54) – C(55) – C(56)	120.4(2)
C(54) – C(55) – H(55)	119.8	C(56) – C(55) – H(55)	119.8
C(55) – C(56) – C(51)	121.4(2)	C(55) – C(56) – H(56)	119.3
C(51) – C(56) – H(56)	119.3	C(66) – C(61) – C(62)	118.1(2)
C(66) – C(61) – P(2)	121.72(17)	C(62) – C(61) – P(2)	120.14(16)
C(63) – C(62) – C(61)	120.8(2)	C(63) – C(62) – H(62)	119.6
C(61) – C(62) – H(62)	119.6	C(62) – C(63) – C(64)	120.1(2)
C(62) – C(63) – H(63)	119.9	C(64) – C(63) – H(63)	119.9
C(65) – C(64) – C(63)	119.7(2)	C(65) – C(64) – H(64)	120.1
C(63) – C(64) – H(64)	120.1	C(64) – C(65) – C(66)	120.2(2)
C(64) – C(65) – H(65)	119.9	C(66) – C(65) – H(65)	119.9
C(65) – C(66) – C(61)	120.7(2)	C(65) – C(66) – H(66)	119.6
C(61) – C(66) – H(66)	119.6	C(72) – C(71) – C(76)	118.5(2)

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Table S6. – continued from previous page

atom – atom – atom	angle	atom – atom – atom	angle
C(72) – C(71) – P(1)	118.25(16)	C(76) – C(71) – P(1)	123.13(17)
C(73) – C(72) – C(71)	120.9(2)	C(73) – C(72) – H(72)	119.5
C(71) – C(72) – H(72)	119.5	C(74) – C(73) – C(72)	119.6(2)
C(74) – C(73) – H(73)	120.2	C(72) – C(73) – H(73)	120.2
C(75) – C(74) – C(73)	120.1(2)	C(75) – C(74) – H(74)	119.9
C(73) – C(74) – H(74)	119.9	C(74) – C(75) – C(76)	120.4(2)
C(74) – C(75) – H(75)	119.8	C(76) – C(75) – H(75)	119.8
C(75) – C(76) – C(71)	120.4(2)	C(75) – C(76) – H(76)	119.8
C(71) – C(76) – H(76)	119.8	C(15) – N – C(11)	118.27(19)
C(83) – C(82) – C(81)	120.5(2)	C(83) – C(82) – H(82)	119.7
C(81) – C(82) – H(82)	119.7	C(82) – C(81) – C(86)	118.1(2)
C(82) – C(81) – P(1)	122.07(17)	C(86) – C(81) – P(1)	119.70(16)
C(11) – C – C(22)	111.53(16)	C(11) – C – C(32)	106.62(16)
C(22) – C – C(32)	106.42(16)	C(11) – C – Ir	110.00(13)
C(22) – C – Ir	110.36(13)	C(32) – C – Ir	111.82(13)
C(54) – C(53) – C(52)	120.4(2)	C(54) – C(53) – H(53)	119.8
C(52) – C(53) – H(53)	119.8	C(53) – C(52) – C(51)	121.3(2)
C(53) – C(52) – H(52)	119.3	C(51) – C(52) – H(52)	119.3
C(56) – C(51) – C(52)	117.23(19)	C(56) – C(51) – P(2)	123.00(15)
C(52) – C(51) – P(2)	119.67(16)	C(31) – P(1) – C(81)	102.63(10)
C(31) – P(1) – C(71)	102.86(9)	C(81) – P(1) – C(71)	101.40(9)
C(31) – P(1) – Ir	105.20(7)	C(81) – P(1) – Ir	121.56(7)
C(71) – P(1) – Ir	120.44(7)		

3.2 Crystal data for [(PC^{Py}P)IrH(C$_4$H$_7$O)] (9)

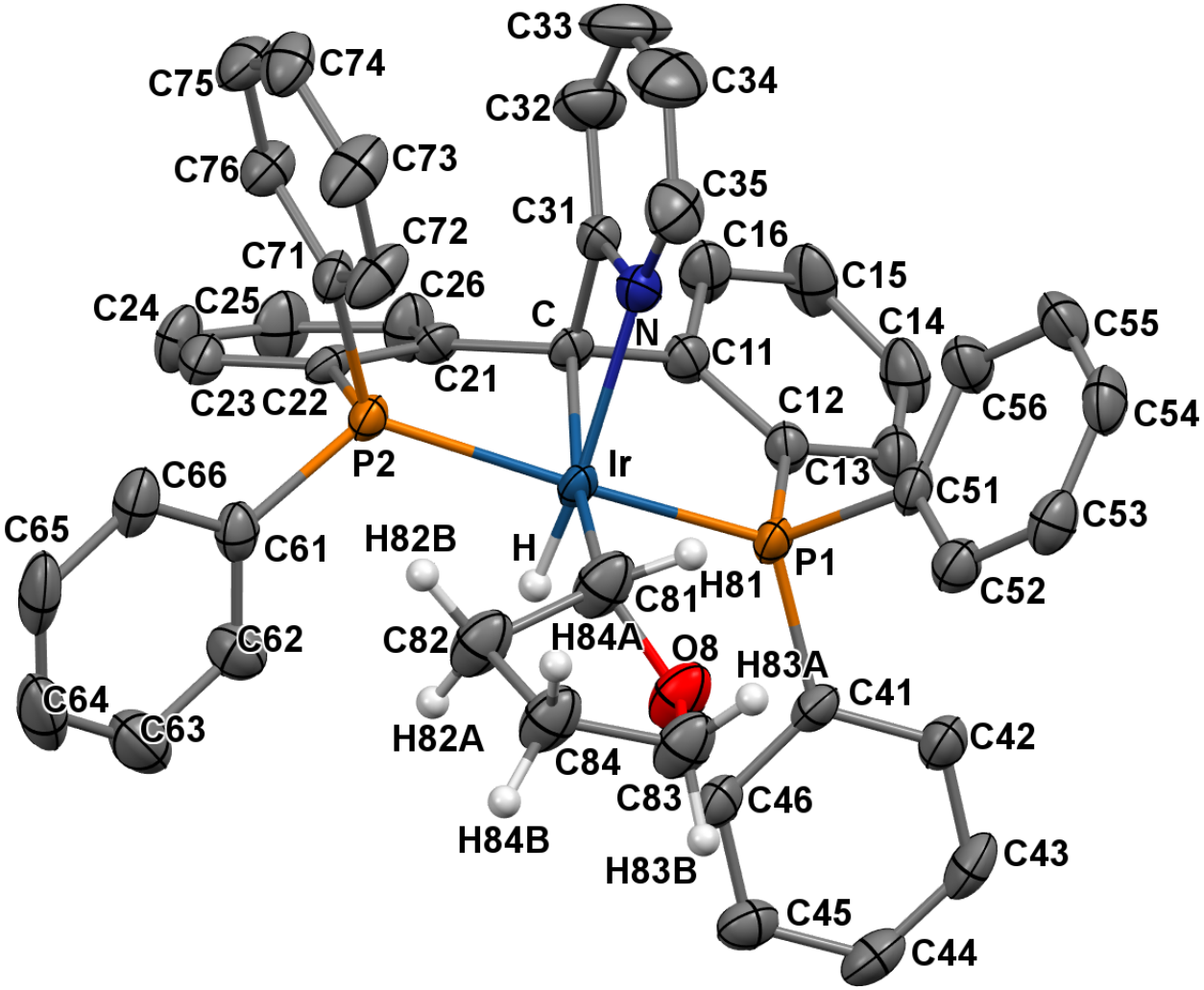

Figure S49. Thermal-ellipsoid representation of [(PC^{Py}P)IrH(C$_4$H$_7$O)] (**9**) at 50% probability. Most hydrogen atoms were omitted for clarity.

Table S7. Crystal data and structure refinement for [($PC^{Py}P$)IrH(C_4H_7O)] (**9**).

Identification code:	pc25	
Empirical formula:	$C_{46}H_{40}IrNOP_2$	
Formula weight:	876.93	
Temperature:	120(2) K	
Wavelength:	0.71073 Å	
Crystal system:	Monoclinic	
Space group:	$C2/c$	
Unit cell dimensions:	a = 42.2630(17) Å	$\alpha = 90°$
	b = 9.1164(4) Å	$\beta = 92.105(3)°$
	c = 18.8750(7) Å	$\gamma = 90°$
Volume:	7267.4(5) Å^3	
Z:	8	
Density (calculated):	1.603 g·cm^{-3}	
Absorption coefficient (μ):	3.801 mm^{-1}	
F(000):	3504	
Crystal size:	0.11 × 0.09 × 0.08 mm^3	
θ range for data collection:	0.96 to 25.00°	
Index ranges:	$-50 \le h \le 50$, $-7 \le k \le 10$, $-22 \le l \le 22$	
Reflections collected:	55245	
Independent reflections:	6399 [R_{int} = 0.0551]	
Completeness to θ = 25.00°:	100.0 %	
Absorption correction:	Semi-empirical from equivalents	
Max. and min. transmission:	0.7457 and 0.6140	
Refinement method:	Full-matrix least-squares on F^2	
Data / restraints / parameters:	6399 / 0 / 453	
Goodness-of-fit on F^2:	1.052	
Final R indices [I>2σ(I)]:	R_1 = 0.0296, wR_2 = 0.0608	
R indices (all data):	R_1 = 0.0393, wR_2 = 0.0635	
Largest diff. peak and hole:	1.100 and −0.612 e$^-$·Å^{-3}	

Table S8. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for [($PC^{Py}P$)IrH(C_4H_7O)] (**9**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	x	y	z	U(eq)
Ir	0.37122(1)	0.68136(2)	0.94636(1)	0.022(1)
P(1)	0.33075(2)	0.80016(13)	0.89185(6)	0.025(1)
P(2)	0.42025(2)	0.60135(13)	0.98088(6)	0.023(1)
C	0.39490(9)	0.7132(5)	0.8462(2)	0.024(1)
C(11)	0.37608(10)	0.8015(5)	0.7916(2)	0.029(1)
O(8)	0.32064(19)	0.7021(10)	1.0526(4)	0.044(1)
C(83)	0.3060(3)	0.6315(15)	1.1113(7)	0.044(1)
C(84)	0.3329(3)	0.5588(18)	1.1530(7)	0.044(1)
C(82)	0.3619(3)	0.5895(16)	1.1074(6)	0.044(1)
O(9)	0.35668(13)	0.4943(8)	1.0748(3)	0.044(1)
C(92)	0.3367(2)	0.4794(12)	1.1342(5)	0.044(1)
C(93)	0.3181(3)	0.6184(12)	1.1409(6)	0.044(1)
C(94)	0.3319(2)	0.7125(12)	1.0836(5)	0.044(1)
C(12)	0.34601(10)	0.8548(5)	0.8065(2)	0.027(1)
C(13)	0.32836(10)	0.9350(5)	0.7561(2)	0.035(1)
C(14)	0.33976(12)	0.9624(6)	0.6903(3)	0.044(1)
C(15)	0.36869(11)	0.9016(7)	0.6731(2)	0.046(1)
C(16)	0.38607(11)	0.8221(6)	0.7224(2)	0.039(1)
C(21)	0.42974(9)	0.7524(5)	0.8582(2)	0.026(1)
C(26)	0.44713(10)	0.8477(6)	0.8171(2)	0.038(1)
C(25)	0.47882(11)	0.8789(6)	0.8342(3)	0.042(1)
C(24)	0.49406(10)	0.8141(6)	0.8905(3)	0.038(1)
C(23)	0.47738(10)	0.7229(5)	0.9336(3)	0.031(1)
C(22)	0.44537(9)	0.6949(5)	0.9187(2)	0.024(1)
C(31)	0.38925(9)	0.5525(5)	0.8285(2)	0.029(1)
C(32)	0.40159(12)	0.4626(7)	0.7780(3)	0.049(1)
C(33)	0.39121(16)	0.3196(7)	0.7732(4)	0.070(2)
C(34)	0.36965(15)	0.2682(7)	0.8175(3)	0.062(2)
C(35)	0.35798(12)	0.3608(6)	0.8674(3)	0.043(1)
C(41)	0.31342(9)	0.9668(5)	0.9277(2)	0.027(1)
C(42)	0.28533(10)	1.0246(6)	0.8989(2)	0.036(1)
C(43)	0.27420(11)	1.1563(6)	0.9227(3)	0.041(1)
C(44)	0.29027(11)	1.2318(6)	0.9758(3)	0.041(1)
C(45)	0.31743(11)	1.1725(5)	1.0062(3)	0.037(1)
C(46)	0.32882(10)	1.0412(5)	0.9826(2)	0.031(1)
N	0.36801(8)	0.4988(4)	0.87330(19)	0.028(1)
C(51)	0.29615(9)	0.6882(5)	0.8685(2)	0.029(1)
C(52)	0.27337(10)	0.6652(5)	0.9181(2)	0.033(1)
C(53)	0.24873(10)	0.5686(6)	0.9048(3)	0.039(1)

Continued on next page

Table S8. – continued from previous page

atom	x	y	x	U(eq)
C(54)	0.24693(11)	0.4911(6)	0.8427(3)	0.042(1)
C(55)	0.26934(11)	0.5112(6)	0.7926(3)	0.047(1)
C(56)	0.29389(11)	0.6088(6)	0.8053(3)	0.041(1)
C(61)	0.43820(10)	0.6498(5)	1.0669(2)	0.030(1)
C(62)	0.43475(12)	0.7914(6)	1.0910(3)	0.040(1)
C(63)	0.44795(13)	0.8356(7)	1.1554(3)	0.056(2)
C(64)	0.46467(12)	0.7366(9)	1.1965(3)	0.058(2)
C(65)	0.46874(11)	0.5961(8)	1.1731(3)	0.053(2)
C(66)	0.45577(10)	0.5522(6)	1.1085(2)	0.039(1)
C(71)	0.42967(9)	0.4068(5)	0.9713(2)	0.028(1)
C(72)	0.41017(11)	0.3034(5)	1.0010(3)	0.042(1)
C(73)	0.41620(12)	0.1557(5)	0.9940(3)	0.047(1)
C(74)	0.44171(11)	0.1089(6)	0.9572(3)	0.039(1)
C(75)	0.46117(11)	0.2106(5)	0.9276(3)	0.039(1)
C(76)	0.45507(10)	0.3582(5)	0.9340(3)	0.033(1)
C(81)	0.34439(12)	0.6066(6)	1.0343(3)	0.044(1)
H	0.3774(11)	0.795(6)	0.978(3)	0.051(15)
H(83A)	0.2903	0.5577	1.0942	0.053
H(83B)	0.2952	0.7044	1.1409	0.053
H(84A)	0.3291	0.4521	1.1579	0.053
H(84B)	0.3357	0.6027	1.2008	0.053
H(82A)	0.3731	0.6804	1.1222	0.053
H(82B)	0.3769	0.5062	1.1081	0.053
H(92A)	0.3498	0.4620	1.1780	0.053
H(92B)	0.3222	0.3950	1.1269	0.053
H(93A)	0.3215	0.6631	1.1884	0.053
H(93B)	0.2952	0.6012	1.1318	0.053
H(94A)	0.3154	0.7744	1.0601	0.053
H(94B)	0.3490	0.7765	1.1035	0.053
H(13)	0.3081	0.9712	0.7675	0.042
H(14)	0.3281	1.0216	0.6571	0.053
H(15)	0.3764	0.9152	0.6270	0.055
H(16)	0.4055	0.7796	0.7092	0.047
H(26)	0.4372	0.8924	0.7766	0.045
H(25)	0.4899	0.9466	0.8060	0.050
H(24)	0.5160	0.8315	0.9001	0.046
H(23)	0.4877	0.6786	0.9737	0.037
H(32)	0.4170	0.4984	0.7470	0.059
H(33)	0.3994	0.2567	0.7382	0.084
H(34)	0.3626	0.1694	0.8143	0.074
H(35)	0.3424	0.3259	0.8983	0.052
H(42)	0.2738	0.9728	0.8627	0.043

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Table S8. – continued from previous page

atom	x	y	x	U(eq)
H(43)	0.2552	1.1958	0.9023	0.050
H(44)	0.2827	1.3241	0.9913	0.049
H(45)	0.3284	1.2227	1.0437	0.044
H(46)	0.3475	1.0009	1.0042	0.038
H(52)	0.2747	0.7165	0.9619	0.040
H(53)	0.2330	0.5558	0.9389	0.047
H(54)	0.2301	0.4233	0.8341	0.050
H(55)	0.2679	0.4580	0.7493	0.056
H(56)	0.3094	0.6220	0.7706	0.049
H(62)	0.4230	0.8600	1.0627	0.049
H(63)	0.4455	0.9338	1.1711	0.067
H(64)	0.4734	0.7655	1.2415	0.070
H(65)	0.4806	0.5283	1.2016	0.063
H(66)	0.4589	0.4547	1.0925	0.047
H(72)	0.3924	0.3346	1.0265	0.050
H(73)	0.4026	0.0860	1.0148	0.057
H(74)	0.4459	0.0071	0.9523	0.047
H(75)	0.4790	0.1789	0.9024	0.047
H(76)	0.4685	0.4273	0.9124	0.040
H(81)	0.3250	0.5628	1.0111	0.053

Table S9. Anisotropic displacement parameters (Å^2) for [(PC^{Py}P)IrH(C$_4$H$_7$O)] (**9**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ...+ 2hka^*b^*U_{12}]$.

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir	0.0147(1)	0.0310(1)	0.0206(1)	−0.0004(1)	0.0036(1)	0.0042(1)
P(1)	0.0154(5)	0.0358(7)	0.0233(6)	−0.0012(5)	0.0012(4)	0.0053(5)
P(2)	0.0160(5)	0.0279(7)	0.0264(6)	0.0003(5)	0.0012(4)	0.0038(5)
C	0.017(2)	0.035(3)	0.021(2)	−0.0019(19)	0.0062(17)	0.0006(18)
C(11)	0.022(2)	0.041(3)	0.024(2)	−0.003(2)	0.0024(18)	−0.001(2)
O(8)	0.0363(17)	0.057(2)	0.0393(19)	0.0124(15)	0.0124(13)	0.0112(14)
C(83)	0.0363(17)	0.057(2)	0.0393(19)	0.0124(15)	0.0124(13)	0.0112(14)
C(84)	0.0363(17)	0.057(2)	0.0393(19)	0.0124(15)	0.0124(13)	0.0112(14)
C(82)	0.0363(17)	0.057(2)	0.0393(19)	0.0124(15)	0.0124(13)	0.0112(14)
O(9)	0.0363(17)	0.057(2)	0.0393(19)	0.0124(15)	0.0124(13)	0.0112(14)
C(92)	0.0363(17)	0.057(2)	0.0393(19)	0.0124(15)	0.0124(13)	0.0112(14)
C(93)	0.0363(17)	0.057(2)	0.0393(19)	0.0124(15)	0.0124(13)	0.0112(14)
C(94)	0.0363(17)	0.057(2)	0.0393(19)	0.0124(15)	0.0124(13)	0.0112(14)
C(12)	0.021(2)	0.038(3)	0.023(2)	0.000(2)	−0.0010(18)	−0.0007(19)
C(13)	0.026(2)	0.046(3)	0.031(3)	0.002(2)	−0.005(2)	0.003(2)
C(14)	0.040(3)	0.060(4)	0.030(3)	0.011(3)	−0.011(2)	−0.003(3)
C(15)	0.035(3)	0.082(4)	0.020(2)	0.007(3)	0.001(2)	−0.007(3)
C(16)	0.027(2)	0.064(4)	0.027(2)	0.002(3)	0.0039(19)	0.001(2)
C(21)	0.018(2)	0.035(3)	0.025(2)	−0.006(2)	0.0068(18)	0.0017(19)
C(26)	0.026(2)	0.056(4)	0.031(3)	0.011(2)	0.004(2)	−0.003(2)
C(25)	0.026(2)	0.056(3)	0.043(3)	0.011(3)	0.011(2)	−0.009(2)
C(24)	0.018(2)	0.048(3)	0.048(3)	0.006(3)	0.005(2)	−0.001(2)
C(23)	0.023(2)	0.032(3)	0.038(3)	−0.003(2)	−0.001(2)	0.003(2)
C(22)	0.019(2)	0.024(2)	0.029(2)	−0.003(2)	0.0080(17)	0.0045(18)
C(31)	0.020(2)	0.040(3)	0.027(2)	−0.008(2)	0.0008(18)	0.002(2)
C(32)	0.046(3)	0.058(4)	0.046(3)	−0.016(3)	0.017(3)	−0.002(3)
C(33)	0.083(5)	0.059(4)	0.069(4)	−0.040(4)	0.021(4)	0.002(4)
C(34)	0.067(4)	0.041(4)	0.078(5)	−0.023(3)	0.003(4)	−0.007(3)
C(35)	0.036(3)	0.039(3)	0.055(3)	−0.002(3)	0.001(2)	−0.009(2)
C(41)	0.023(2)	0.031(3)	0.029(2)	0.002(2)	0.0058(18)	0.009(2)
C(42)	0.026(2)	0.048(3)	0.034(3)	−0.002(2)	0.001(2)	0.009(2)
C(43)	0.026(2)	0.047(3)	0.051(3)	0.011(3)	0.003(2)	0.015(2)
C(44)	0.034(3)	0.036(3)	0.053(3)	0.001(3)	0.012(2)	0.012(2)
C(45)	0.034(3)	0.038(3)	0.039(3)	−0.004(2)	0.011(2)	0.003(2)
C(46)	0.019(2)	0.039(3)	0.036(3)	−0.001(2)	0.0032(19)	0.003(2)
N	0.0225(19)	0.034(2)	0.028(2)	−0.0049(17)	0.0013(15)	−0.0008(17)
C(51)	0.016(2)	0.038(3)	0.032(2)	0.001(2)	−0.0015(18)	0.005(2)
C(52)	0.026(2)	0.042(3)	0.032(3)	0.001(2)	0.0026(19)	0.005(2)
C(53)	0.022(2)	0.048(3)	0.048(3)	0.002(3)	0.005(2)	0.001(2)
C(54)	0.024(2)	0.049(3)	0.051(3)	0.000(3)	−0.009(2)	−0.004(2)

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Table S9. – continued from previous page

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(55)	0.036(3)	0.067(4)	0.036(3)	−0.017(3)	−0.008(2)	−0.006(3)
C(56)	0.028(3)	0.063(4)	0.033(3)	−0.012(3)	0.001(2)	−0.005(2)
C(61)	0.019(2)	0.042(3)	0.030(2)	0.004(2)	0.0007(18)	−0.003(2)
C(62)	0.043(3)	0.048(3)	0.031(3)	−0.003(2)	−0.001(2)	0.001(2)
C(63)	0.046(3)	0.078(5)	0.044(3)	−0.019(3)	0.000(3)	−0.009(3)
C(64)	0.034(3)	0.111(6)	0.030(3)	−0.007(3)	−0.006(2)	−0.006(3)
C(65)	0.024(3)	0.096(5)	0.037(3)	0.016(3)	−0.007(2)	0.007(3)
C(66)	0.023(2)	0.057(3)	0.038(3)	0.012(3)	0.000(2)	0.005(2)
C(71)	0.018(2)	0.031(3)	0.035(3)	0.001(2)	−0.0024(18)	0.0043(19)
C(72)	0.026(2)	0.033(3)	0.069(4)	0.008(3)	0.015(2)	0.003(2)
C(73)	0.034(3)	0.029(3)	0.079(4)	0.012(3)	0.012(3)	0.000(2)
C(74)	0.033(3)	0.031(3)	0.054(3)	0.006(3)	−0.002(2)	0.006(2)
C(75)	0.031(3)	0.036(3)	0.051(3)	−0.002(2)	0.005(2)	0.011(2)
C(76)	0.028(2)	0.030(3)	0.042(3)	0.002(2)	0.005(2)	0.003(2)
C(81)	0.0363(17)	0.057(2)	0.0393(19)	0.0124(15)	0.0124(13)	0.0112(14)

Table S10. Distances [Å] for [($PC^{Py}P$)IrH(C_4H_7O)] (**9**).

atom – atom	distance	atom – atom	distance
Ir – C(81)	2.155(5)	Ir – N	2.163(4)
Ir – C	2.191(4)	Ir – P(1)	2.2421(11)
Ir – P(2)	2.2696(10)	Ir – H	1.22(5)
P(1) – C(51)	1.824(4)	P(1) – C(12)	1.826(4)
P(1) – C(41)	1.827(4)	P(2) – C(61)	1.821(5)
P(2) – C(22)	1.823(4)	P(2) – C(71)	1.828(5)
C – C(11)	1.511(6)	C – C(31)	1.520(6)
C – C(21)	1.524(6)	C(11) – C(12)	1.399(6)
C(11) – C(16)	1.400(6)	O(8) – C(81)	1.382(9)
O(8) – C(83)	1.442(14)	C(83) – C(84)	1.511(17)
C(83) – H(83A)	0.9900	C(83) – H(83B)	0.9900
C(84) – C(82)	1.549(15)	C(84) – H(84A)	0.9900
C(84) – H(84B)	0.9900	C(82) – C(81)	1.547(13)
C(82) – H(82A)	0.9900	C(82) – H(82B)	0.9900
O(9) – C(81)	1.368(7)	O(9) – C(92)	1.433(10)
C(92) – C(93)	1.500(14)	C(92) – H(92A)	0.9900
C(92) – H(92B)	0.9900	C(93) – C(94)	1.515(13)
C(93) – H(93A)	0.9900	C(93) – H(93B)	0.9900
C(94) – C(81)	1.453(11)	C(94) – H(94A)	0.9900
C(94) – H(94B)	0.9900	C(12) – C(13)	1.394(6)
C(13) – C(14)	1.372(6)	C(13) – H(13)	0.9500
C(14) – C(15)	1.392(7)	C(14) – H(14)	0.9500
C(15) – C(16)	1.371(7)	C(15) – H(15)	0.9500
C(16) – H(16)	0.9500	C(21) – C(26)	1.392(6)
C(21) – C(22)	1.400(6)	C(26) – C(25)	1.396(6)
C(26) – H(26)	0.9500	C(25) – C(24)	1.357(7)
C(25) – H(25)	0.9500	C(24) – C(23)	1.375(6)
C(24) – H(24)	0.9500	C(23) – C(22)	1.395(6)
C(23) – H(23)	0.9500	C(31) – N	1.348(5)
C(31) – C(32)	1.373(6)	C(32) – C(33)	1.378(8)
C(32) – H(32)	0.9500	C(33) – C(34)	1.343(9)
C(33) – H(33)	0.9500	C(34) – C(35)	1.370(8)
C(34) – H(34)	0.9500	C(35) – N	1.330(6)
C(35) – H(35)	0.9500	C(41) – C(46)	1.380(6)
C(41) – C(42)	1.391(6)	C(42) – C(43)	1.371(7)
C(42) – H(42)	0.9500	C(43) – C(44)	1.374(7)
C(43) – H(43)	0.9500	C(44) – C(45)	1.376(7)
C(44) – H(44)	0.9500	C(45) – C(46)	1.370(6)
C(45) – H(45)	0.9500	C(46) – H(46)	0.9500
C(51) – C(52)	1.384(6)	C(51) – C(56)	1.396(6)
C(52) – C(53)	1.380(6)	C(52) – H(52)	0.9500

Continued on next page

Table S10. – continued from previous page

atom – atom	distance	atom – atom	distance
C(53) – C(54)	1.368(7)	C(53) – H(53)	0.9500
C(54) – C(55)	1.375(7)	C(54) – H(54)	0.9500
C(55) – C(56)	1.381(7)	C(55) – H(55)	0.9500
C(56) – H(56)	0.9500	C(61) – C(62)	1.379(7)
C(61) – C(66)	1.385(6)	C(62) – C(63)	1.378(7)
C(62) – H(62)	0.9500	C(63) – C(64)	1.370(9)
C(63) – H(63)	0.9500	C(64) – C(65)	1.368(9)
C(64) – H(64)	0.9500	C(65) – C(66)	1.377(7)
C(65) – H(65)	0.9500	C(66) – H(66)	0.9500
C(71) – C(76)	1.379(6)	C(71) – C(72)	1.384(6)
C(72) – C(73)	1.377(7)	C(72) – H(72)	0.9500
C(73) – C(74)	1.372(7)	C(73) – H(73)	0.9500
C(74) – C(75)	1.373(7)	C(74) – H(74)	0.9500
C(75) – C(76)	1.376(7)	C(75) – H(75)	0.9500
C(76) – H(76)	0.9500	C(81) – H(81)	1.0000

Table S11. Angles [°] for [($PC^{Py}P$)IrH(C_4H_7O)] (**9**).

atom – atom – atom	angle	atom – atom – atom	angle
C(81) – Ir – N	103.03(19)	C(81) – Ir – C	167.6(2)
N – Ir – C	64.64(15)	C(81) – Ir – P(1)	95.29(14)
N – Ir – P(1)	92.88(10)	C – Ir – P(1)	84.54(11)
C(81) – Ir – P(2)	100.24(14)	N – Ir – P(2)	88.33(10)
C – Ir – P(2)	81.32(11)	P(1) – Ir – P(2)	163.73(4)
C(81) – Ir – H	90(2)	N – Ir – H	167(2)
C – Ir – H	103(2)	P(1) – Ir – H	88(2)
P(2) – Ir – H	87(2)	C(51) – P(1) – C(12)	104.2(2)
C(51) – P(1) – C(41)	103.1(2)	C(12) – P(1) – C(41)	105.0(2)
C(51) – P(1) – Ir	115.60(15)	C(12) – P(1) – Ir	104.38(14)
C(41) – P(1) – Ir	122.75(14)	C(61) – P(2) – C(22)	103.1(2)
C(61) – P(2) – C(71)	103.8(2)	C(22) – P(2) – C(71)	104.84(19)
C(61) – P(2) – Ir	121.61(15)	C(22) – P(2) – Ir	102.24(14)
C(71) – P(2) – Ir	118.91(14)	C(11) – C – C(31)	106.8(3)
C(11) – C – C(21)	117.3(4)	C(31) – C – C(21)	113.7(3)
C(11) – C – Ir	114.4(3)	C(31) – C – Ir	89.4(2)
C(21) – C – Ir	111.9(3)	C(12) – C(11) – C(16)	116.7(4)
C(12) – C(11) – C	120.5(4)	C(16) – C(11) – C	122.6(4)
C(81) – O(8) – C(83)	104.3(8)	O(8) – C(83) – C(84)	105.0(9)
O(8) – C(83) – H(83A)	110.7	C(84) – C(83) – H(83A)	110.7
O(8) – C(83) – H(83B)	110.7	C(84) – C(83) – H(83B)	110.7
H(83A) – C(83) – H(83B)	108.8	C(83) – C(84) – C(82)	103.1(9)
C(83) – C(84) – H(84A)	111.1	C(82) – C(84) – H(84A)	111.1
C(83) – C(84) – H(84B)	111.1	C(82) – C(84) – H(84B)	111.1
H(84A) – C(84) – H(84B)	109.1	C(81) – C(82) – C(84)	98.8(8)
C(81) – C(82) – H(82A)	112.0	C(84) – C(82) – H(82A)	112.0
C(81) – C(82) – H(82B)	112.0	C(84) – C(82) – H(82B)	112.0
H(82A) – C(82) – H(82B)	109.7	C(81) – O(9) – C(92)	106.6(6)
O(9) – C(92) – C(93)	108.2(7)	O(9) – C(92) – H(92A)	110.1
C(93) – C(92) – H(92A)	110.1	O(9) – C(92) – H(92B)	110.1
C(93) – C(92) – H(92B)	110.1	H(92A) – C(92) – H(92B)	108.4
C(92) – C(93) – C(94)	101.6(7)	C(92) – C(93) – H(93A)	111.5
C(94) – C(93) – H(93A)	111.5	C(92) – C(93) – H(93B)	111.5
C(94) – C(93) – H(93B)	111.5	H(93A) – C(93) – H(93B)	109.3
C(81) – C(94) – C(93)	103.8(8)	C(81) – C(94) – H(94A)	111.0
C(93) – C(94) – H(94A)	111.0	C(81) – C(94) – H(94B)	111.0
C(93) – C(94) – H(94B)	111.0	H(94A) – C(94) – H(94B)	109.0
C(13) – C(12) – C(11)	120.8(4)	C(13) – C(12) – P(1)	123.2(3)
C(11) – C(12) – P(1)	115.9(3)	C(14) – C(13) – C(12)	121.1(4)
C(14) – C(13) – H(13)	119.4	C(12) – C(13) – H(13)	119.4
C(13) – C(14) – C(15)	118.7(5)	C(13) – C(14) – H(14)	120.7

Continued on next page

Table S11. – continued from previous page

atom – atom – atom	angle	atom – atom – atom	angle
C(15) – C(14) – H(14)	120.7	C(16) – C(15) – C(14)	120.4(4)
C(16) – C(15) – H(15)	119.8	C(14) – C(15) – H(15)	119.8
C(15) – C(16) – C(11)	122.1(4)	C(15) – C(16) – H(16)	118.9
C(11) – C(16) – H(16)	118.9	C(26) – C(21) – C(22)	116.4(4)
C(26) – C(21) – C	126.2(4)	C(22) – C(21) – C	117.3(4)
C(21) – C(26) – C(25)	121.3(4)	C(21) – C(26) – H(26)	119.3
C(25) – C(26) – H(26)	119.3	C(24) – C(25) – C(26)	121.1(5)
C(24) – C(25) – H(25)	119.5	C(26) – C(25) – H(25)	119.5
C(25) – C(24) – C(23)	119.1(4)	C(25) – C(24) – H(24)	120.4
C(23) – C(24) – H(24)	120.4	C(24) – C(23) – C(22)	120.4(4)
C(24) – C(23) – H(23)	119.8	C(22) – C(23) – H(23)	119.8
C(23) – C(22) – C(21)	121.4(4)	C(23) – C(22) – P(2)	122.7(3)
C(21) – C(22) – P(2)	115.6(3)	N – C(31) – C(32)	119.8(5)
N – C(31) – C	108.4(4)	C(32) – C(31) – C	131.8(4)
C(31) – C(32) – C(33)	118.8(5)	C(31) – C(32) – H(32)	120.6
C(33) – C(32) – H(32)	120.6	C(34) – C(33) – C(32)	120.7(6)
C(34) – C(33) – H(33)	119.6	C(32) – C(33) – H(33)	119.6
C(33) – C(34) – C(35)	118.8(6)	C(33) – C(34) – H(34)	120.6
C(35) – C(34) – H(34)	120.6	N – C(35) – C(34)	121.2(5)
N – C(35) – H(35)	119.4	C(34) – C(35) – H(35)	119.4
C(46) – C(41) – C(42)	118.6(4)	C(46) – C(41) – P(1)	120.1(3)
C(42) – C(41) – P(1)	121.2(4)	C(43) – C(42) – C(41)	120.1(5)
C(43) – C(42) – H(42)	119.9	C(41) – C(42) – H(42)	119.9
C(42) – C(43) – C(44)	120.7(5)	C(42) – C(43) – H(43)	119.6
C(44) – C(43) – H(43)	119.6	C(43) – C(44) – C(45)	119.3(5)
C(43) – C(44) – H(44)	120.4	C(45) – C(44) – H(44)	120.4
C(46) – C(45) – C(44)	120.4(5)	C(46) – C(45) – H(45)	119.8
C(44) – C(45) – H(45)	119.8	C(45) – C(46) – C(41)	120.8(4)
C(45) – C(46) – H(46)	119.6	C(41) – C(46) – H(46)	119.6
C(35) – N – C(31)	120.6(4)	C(35) – N – Ir	142.5(3)
C(31) – N – Ir	95.3(3)	C(52) – C(51) – C(56)	118.2(4)
C(52) – C(51) – P(1)	119.5(4)	C(56) – C(51) – P(1)	121.7(3)
C(53) – C(52) – C(51)	120.8(5)	C(53) – C(52) – H(52)	119.6
C(51) – C(52) – H(52)	119.6	C(54) – C(53) – C(52)	120.2(4)
C(54) – C(53) – H(53)	119.9	C(52) – C(53) – H(53)	119.9
C(53) – C(54) – C(55)	120.2(5)	C(53) – C(54) – H(54)	119.9
C(55) – C(54) – H(54)	119.9	C(54) – C(55) – C(56)	119.9(5)
C(54) – C(55) – H(55)	120.0	C(56) – C(55) – H(55)	120.0
C(55) – C(56) – C(51)	120.6(4)	C(55) – C(56) – H(56)	119.7
C(51) – C(56) – H(56)	119.7	C(62) – C(61) – C(66)	118.4(5)
C(62) – C(61) – P(2)	118.4(4)	C(66) – C(61) – P(2)	123.2(4)
C(63) – C(62) – C(61)	121.3(5)	C(63) – C(62) – H(62)	119.3

Continued on next page

Table S11. – continued from previous page

atom – atom – atom	angle	atom – atom – atom	angle
C(61) – C(62) – H(62)	119.3	C(64) – C(63) – C(62)	119.4(6)
C(64) – C(63) – H(63)	120.3	C(62) – C(63) – H(63)	120.3
C(65) – C(64) – C(63)	120.1(5)	C(65) – C(64) – H(64)	119.9
C(63) – C(64) – H(64)	119.9	C(64) – C(65) – C(66)	120.5(5)
C(64) – C(65) – H(65)	119.7	C(66) – C(65) – H(65)	119.7
C(65) – C(66) – C(61)	120.2(5)	C(65) – C(66) – H(66)	119.9
C(61) – C(66) – H(66)	119.9	C(76) – C(71) – C(72)	118.3(4)
C(76) – C(71) – P(2)	122.6(4)	C(72) – C(71) – P(2)	119.1(3)
C(73) – C(72) – C(71)	120.8(4)	C(73) – C(72) – H(72)	119.6
C(71) – C(72) – H(72)	119.6	C(74) – C(73) – C(72)	120.3(5)
C(74) – C(73) – H(73)	119.9	C(72) – C(73) – H(73)	119.9
C(73) – C(74) – C(75)	119.4(5)	C(73) – C(74) – H(74)	120.3
C(75) – C(74) – H(74)	120.3	C(74) – C(75) – C(76)	120.5(5)
C(74) – C(75) – H(75)	119.7	C(76) – C(75) – H(75)	119.7
C(75) – C(76) – C(71)	120.7(5)	C(75) – C(76) – H(76)	119.6
C(71) – C(76) – H(76)	119.6	O(9) – C(81) – O(8)	126.6(5)
O(9) – C(81) – C(94)	106.2(6)	O(8) – C(81) – C(82)	99.7(6)
C(94) – C(81) – C(82)	70.7(7)	O(9) – C(81) – Ir	117.8(4)
O(8) – C(81) – Ir	113.6(5)	C(94) – C(81) – Ir	119.8(5)
C(82) – C(81) – Ir	118.1(5)	O(9) – C(81) – H(81)	103.6
O(8) – C(81) – H(81)	76.6	C(94) – C(81) – H(81)	103.6
C(82) – C(81) – H(81)	135.1	Ir – C(81) – H(81)	103.6

3.3 Crystal data for [(PC^{Py}P)IrH(CH$_2$O^{t}Bu] (10)

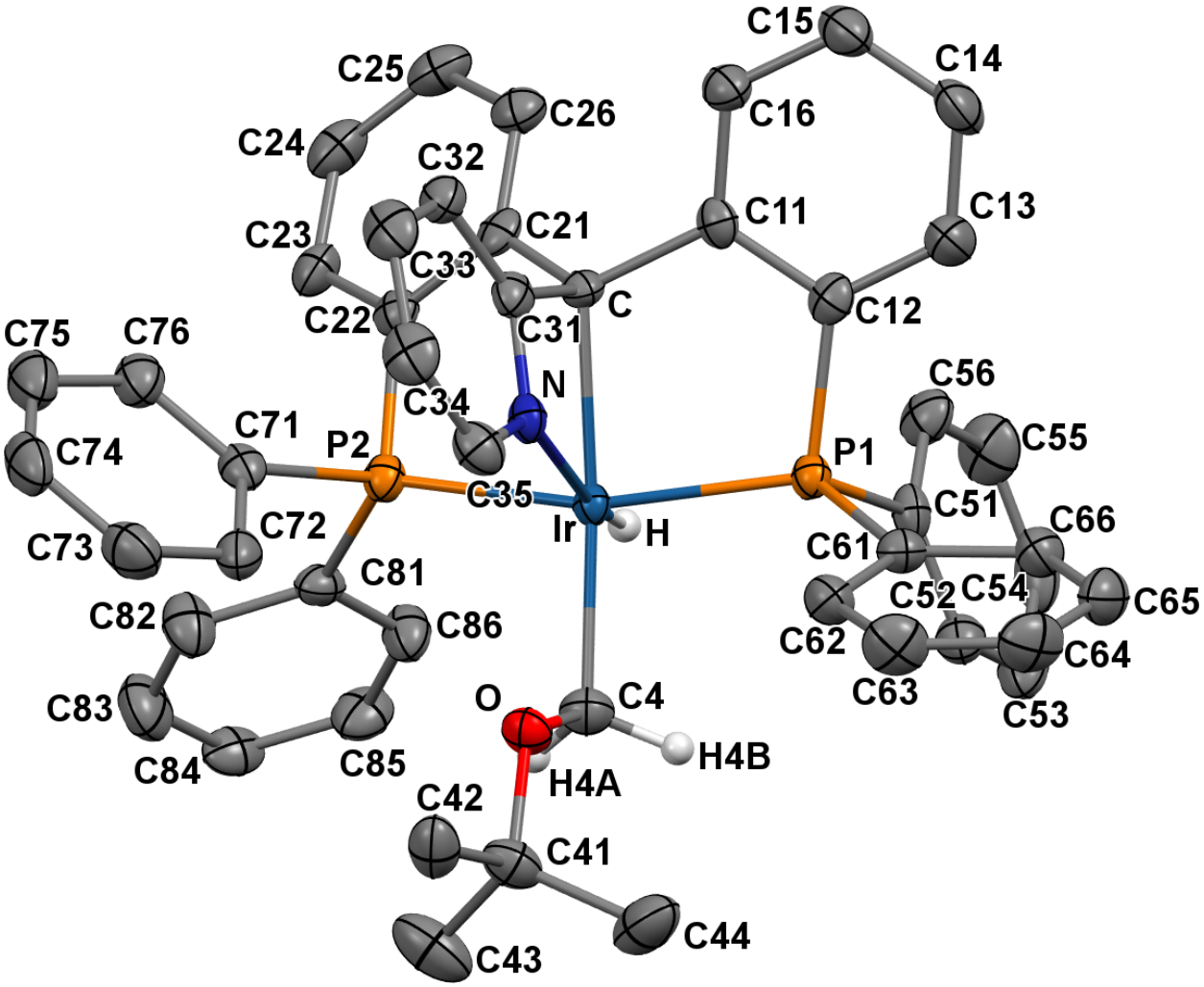

Figure S50. Thermal-ellipsoid representation of [(PC^{Py}P)IrH(CH$_2$O^{t}Bu] (**10**) at 50% probability. Most hydrogen atoms were omitted for clarity.

Table S12. Crystal data and structure refinement for [($PC^{Py}P$)IrH(CH_2O^tBu] (**10**).

Identification code:	pc13	
Empirical formula:	$C_{47}H_{44}IrNOP_2$	
Formula weight:	892.97	
Temperature:	120(2) K	
Wavelength:	0.71073 Å	
Crystal system:	Monoclinic	
Space group:	$P2_1/c$	
Unit cell dimensions:	a = 17.280(3) Å	α = 90°
	b = 14.146(2) Å	β = 104.829(2)°
	c = 18.792(3) Å	γ = 90°
Volume:	4440.5(11) $Å^3$	
Z:	4	
Density (calculated):	1.336 $g{\cdot}cm^{-3}$	
Absorption coefficient (μ):	3.111 mm^{-1}	
F(000):	1792	
Crystal size:	0.09 × 0.08 × 0.08 mm^3	
θ range for data collection:	1.22 to 25.00°	
Index ranges:	$-20 \le h \le 20$, $-16 \le k \le 16$, $-22 \le l \le 22$	
Reflections collected:	66672	
Independent reflections:	7823 [R_{int} = 0.0705]	
Completeness to θ = 25.00°:	100.0 %	
Absorption correction:	Semi-empirical from equivalents	
Max. and min. transmission:	0.7455 and 0.6604	
Refinement method:	Full-matrix least-squares on F^2	
Data / restraints / parameters:	7823 / 0 / 476	
Goodness-of-fit on F^2:	1.047	
Final R indices [I>2σ(I)]:	R_1 = 0.0315, wR_2 = 0.0676	
R indices (all data):	R_1 = 0.0493, wR_2 = 0.0723	
Largest diff. peak and hole:	0.997 and −0.515 $e^{-}{\cdot}Å^{-3}$	

Table S13. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for [($PC^{Py}P$)IrH(CH_2O^tBu] (**10**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	x	y	z	U(eq)
Ir	0.69522(1)	−0.00712(1)	0.85598(1)	0.017(1)
P(2)	0.75925(7)	−0.14313(8)	0.90053(7)	0.023(1)
O	0.68995(18)	−0.0466(2)	0.70329(15)	0.025(1)
C(4)	0.6344(3)	−0.0552(3)	0.7493(2)	0.028(1)
N	0.8084(2)	0.0503(2)	0.84134(19)	0.020(1)
C	0.7768(3)	0.0498(3)	0.9555(2)	0.020(1)
C(11)	0.7569(3)	0.1525(3)	0.9727(2)	0.022(1)
C(12)	0.6910(3)	0.1990(3)	0.9288(2)	0.024(1)
C(13)	0.6768(3)	0.2935(3)	0.9409(3)	0.033(1)
C(14)	0.7284(3)	0.3445(3)	0.9953(3)	0.036(1)
C(15)	0.7956(3)	0.2999(3)	1.0379(3)	0.035(1)
C(16)	0.8100(3)	0.2059(3)	1.0268(3)	0.028(1)
P(1)	0.62861(7)	0.12964(8)	0.85371(6)	0.020(1)
C(21)	0.7952(2)	−0.0204(3)	1.0179(2)	0.023(1)
C(22)	0.7913(3)	−0.1167(3)	0.9993(2)	0.023(1)
C(23)	0.8054(3)	−0.1864(3)	1.0534(3)	0.029(1)
C(24)	0.8219(3)	−0.1625(4)	1.1271(3)	0.036(1)
C(25)	0.8242(3)	−0.0682(4)	1.1464(3)	0.034(1)
C(26)	0.8115(3)	0.0018(3)	1.0931(2)	0.029(1)
C(31)	0.8424(3)	0.0589(3)	0.9143(2)	0.024(1)
C(32)	0.9238(3)	0.0715(3)	0.9413(3)	0.027(1)
C(33)	0.9705(3)	0.0790(3)	0.8916(3)	0.034(1)
C(34)	0.9352(3)	0.0751(3)	0.8172(3)	0.032(1)
C(35)	0.8531(3)	0.0589(3)	0.7930(3)	0.030(1)
C(41)	0.6634(3)	−0.0740(3)	0.6273(2)	0.032(1)
C(42)	0.7381(3)	−0.0661(3)	0.6000(3)	0.035(1)
C(43)	0.6354(4)	−0.1758(4)	0.6197(3)	0.051(2)
C(44)	0.6000(3)	−0.0061(4)	0.5847(3)	0.048(2)
C(51)	0.5328(3)	0.1220(3)	0.8771(2)	0.024(1)
C(52)	0.4627(3)	0.1059(3)	0.8228(3)	0.028(1)
C(53)	0.3917(3)	0.0886(3)	0.8425(3)	0.036(1)
C(54)	0.3898(3)	0.0873(3)	0.9151(3)	0.038(1)
C(55)	0.4592(3)	0.1041(4)	0.9690(3)	0.043(1)
C(56)	0.5308(3)	0.1216(3)	0.9503(3)	0.032(1)
C(61)	0.6098(3)	0.2091(3)	0.7739(2)	0.024(1)
C(62)	0.6527(3)	0.1940(3)	0.7216(2)	0.030(1)
C(63)	0.6460(3)	0.2590(4)	0.6643(3)	0.038(1)
C(64)	0.5966(3)	0.3355(4)	0.6589(3)	0.040(1)
C(65)	0.5525(3)	0.3499(3)	0.7095(3)	0.034(1)

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Table S13. – continued from previous page

atom	x	y	x	U(eq)
C(66)	0.5583(3)	0.2866(3)	0.7664(3)	0.029(1)
C(71)	0.8524(3)	−0.1768(3)	0.8767(2)	0.024(1)
C(72)	0.8551(3)	−0.1646(3)	0.8040(3)	0.032(1)
C(73)	0.9250(3)	−0.1899(4)	0.7828(3)	0.040(1)
C(74)	0.9883(3)	−0.2303(4)	0.8338(3)	0.040(1)
C(75)	0.9835(3)	−0.2436(4)	0.9046(3)	0.041(1)
C(76)	0.9169(3)	−0.2162(3)	0.9266(3)	0.033(1)
C(81)	0.7058(3)	−0.2563(3)	0.8929(2)	0.025(1)
C(82)	0.7399(3)	−0.3417(3)	0.8811(3)	0.037(1)
C(83)	0.6966(3)	−0.4250(4)	0.8746(3)	0.045(2)
C(84)	0.6188(3)	−0.4232(3)	0.8793(3)	0.032(1)
C(85)	0.5842(3)	−0.3398(3)	0.8905(3)	0.036(1)
C(86)	0.6268(3)	−0.2563(3)	0.8957(3)	0.033(1)
H(4A)	0.6177	−0.1219	0.7514	0.033
H(4B)	0.5862	−0.0163	0.7292	0.033
H(13)	0.6307	0.3235	0.9110	0.039
H(14)	0.7180	0.4091	1.0034	0.043
H(15)	0.8323	0.3343	1.0753	0.042
H(16)	0.8568	0.1767	1.0564	0.033
H	0.635(3)	−0.043(4)	0.885(3)	0.059(16)
H(23)	0.8037	−0.2511	1.0396	0.034
H(24)	0.8314	−0.2103	1.1639	0.043
H(25)	0.8346	−0.0512	1.1969	0.041
H(26)	0.8139	0.0662	1.1078	0.034
H(32)	0.9474	0.0749	0.9928	0.033
H(33)	1.0268	0.0869	0.9088	0.041
H(34)	0.9664	0.0834	0.7827	0.039
H(35)	0.8286	0.0539	0.7418	0.036
H(42A)	0.7256	−0.0832	0.5478	0.053
H(42B)	0.7792	−0.1091	0.6282	0.053
H(42C)	0.7581	−0.0010	0.6063	0.053
H(43A)	0.5815	−0.1799	0.6275	0.077
H(43B)	0.6723	−0.2148	0.6564	0.077
H(43C)	0.6343	−0.1988	0.5702	0.077
H(44A)	0.5902	−0.0186	0.5319	0.072
H(44B)	0.6187	0.0591	0.5951	0.072
H(44C)	0.5502	−0.0151	0.5998	0.072
H(52)	0.4633	0.1066	0.7724	0.034
H(53)	0.3438	0.0776	0.8052	0.043
H(54)	0.3411	0.0749	0.9280	0.045
H(55)	0.4582	0.1037	1.0193	0.051
H(56)	0.5783	0.1333	0.9878	0.038

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Table S13. – continued from previous page

atom	x	y	x	U(eq)
H(62)	0.6862	0.1401	0.7247	0.036
H(63)	0.6761	0.2500	0.6290	0.046
H(64)	0.5926	0.3792	0.6197	0.048
H(65)	0.5182	0.4032	0.7051	0.041
H(66)	0.5272	0.2959	0.8008	0.035
H(72)	0.8103	−0.1394	0.7689	0.038
H(73)	0.9284	−0.1792	0.7338	0.048
H(74)	1.0351	−0.2488	0.8197	0.048
H(75)	1.0270	−0.2723	0.9392	0.049
H(76)	0.9154	−0.2244	0.9764	0.040
H(82)	0.7938	−0.3431	0.8775	0.044
H(83)	0.7207	−0.4832	0.8668	0.054
H(84)	0.5889	−0.4802	0.8749	0.039
H(85)	0.5305	−0.3390	0.8947	0.043
H(86)	0.6015	−0.1982	0.9013	0.040

Table S14. Anisotropic displacement parameters (Å^2) for [(PC^{Py}P)IrH(CH$_2$O^{t}Bu] (**10**). The anisotropic displacement factor exponent takes the form: $-2\pi^2$[h^{2}a*^{2}U$_{11}$ + ...+ 2hka*b*U$_{12}$].

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir	0.0154(1)	0.0164(1)	0.0193(1)	0.0000(1)	0.0057(1)	0.0000(1)
P(2)	0.0192(6)	0.0204(6)	0.0279(6)	0.0012(5)	0.0055(5)	0.0002(5)
O	0.0292(19)	0.0282(17)	0.0200(16)	−0.0013(13)	0.0090(14)	0.0015(14)
C(4)	0.029(3)	0.030(3)	0.024(2)	−0.001(2)	0.006(2)	−0.002(2)
N	0.017(2)	0.0181(19)	0.027(2)	0.0003(16)	0.0096(17)	0.0010(15)
C	0.016(2)	0.022(2)	0.020(2)	−0.0033(18)	0.0016(19)	−0.0017(18)
C(11)	0.022(3)	0.023(2)	0.025(2)	−0.0006(19)	0.012(2)	0.0021(19)
C(12)	0.018(3)	0.029(3)	0.026(2)	0.002(2)	0.010(2)	0.0005(19)
C(13)	0.036(3)	0.030(3)	0.030(3)	−0.003(2)	0.004(2)	0.004(2)
C(14)	0.047(3)	0.024(3)	0.037(3)	−0.008(2)	0.012(3)	0.004(2)
C(15)	0.031(3)	0.035(3)	0.039(3)	−0.013(2)	0.010(3)	−0.002(2)
C(16)	0.022(3)	0.030(3)	0.030(3)	−0.005(2)	0.005(2)	−0.001(2)
P(1)	0.0163(6)	0.0207(6)	0.0239(6)	0.0000(5)	0.0061(5)	0.0016(5)
C(21)	0.011(2)	0.029(3)	0.030(2)	0.003(2)	0.0029(19)	−0.0007(18)
C(22)	0.015(2)	0.028(3)	0.025(2)	0.000(2)	0.006(2)	0.0003(19)
C(23)	0.022(3)	0.028(3)	0.033(3)	0.007(2)	0.002(2)	0.003(2)
C(24)	0.026(3)	0.041(3)	0.036(3)	0.012(2)	0.001(2)	0.000(2)
C(25)	0.026(3)	0.048(3)	0.025(3)	0.005(2)	0.001(2)	−0.003(2)
C(26)	0.022(2)	0.033(3)	0.029(2)	−0.001(2)	0.0032(19)	−0.003(2)
C(31)	0.023(3)	0.016(2)	0.031(3)	−0.0009(19)	0.005(2)	−0.0003(19)
C(32)	0.022(3)	0.027(2)	0.032(3)	−0.003(2)	0.004(2)	0.002(2)
C(33)	0.022(3)	0.038(3)	0.047(3)	−0.005(2)	0.017(2)	−0.005(2)
C(34)	0.025(3)	0.035(3)	0.043(3)	0.000(2)	0.020(2)	−0.006(2)
C(35)	0.034(3)	0.025(3)	0.033(3)	−0.002(2)	0.013(2)	−0.003(2)
C(41)	0.041(3)	0.031(3)	0.025(3)	−0.004(2)	0.012(2)	−0.005(2)
C(42)	0.044(3)	0.038(3)	0.027(3)	0.006(2)	0.015(2)	0.013(2)
C(43)	0.071(4)	0.043(3)	0.051(4)	−0.017(3)	0.035(3)	−0.017(3)
C(44)	0.034(3)	0.080(4)	0.029(3)	−0.001(3)	0.004(2)	0.012(3)
C(51)	0.022(3)	0.020(2)	0.034(3)	0.002(2)	0.013(2)	0.0043(19)
C(52)	0.023(3)	0.026(3)	0.034(3)	−0.002(2)	0.006(2)	−0.002(2)
C(53)	0.022(3)	0.030(3)	0.055(4)	−0.003(2)	0.008(3)	−0.001(2)
C(54)	0.028(3)	0.031(3)	0.062(4)	0.003(3)	0.027(3)	0.005(2)
C(55)	0.039(3)	0.057(4)	0.040(3)	0.004(3)	0.024(3)	0.005(3)
C(56)	0.021(3)	0.043(3)	0.034(3)	0.002(2)	0.009(2)	0.003(2)
C(61)	0.024(3)	0.025(2)	0.022(2)	−0.0012(19)	0.004(2)	−0.002(2)
C(62)	0.030(3)	0.031(3)	0.028(3)	−0.003(2)	0.007(2)	0.003(2)
C(63)	0.048(4)	0.042(3)	0.029(3)	0.007(2)	0.016(3)	−0.002(3)
C(64)	0.052(4)	0.037(3)	0.028(3)	0.011(2)	0.008(3)	−0.002(3)
C(65)	0.038(3)	0.026(3)	0.035(3)	0.004(2)	0.004(3)	0.004(2)
C(66)	0.032(3)	0.026(2)	0.029(3)	−0.002(2)	0.007(2)	0.002(2)

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Table S14. – continued from previous page

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(71)	0.019(3)	0.022(2)	0.033(3)	−0.005(2)	0.009(2)	−0.0046(19)
C(72)	0.026(3)	0.025(3)	0.040(3)	−0.005(2)	0.001(2)	0.003(2)
C(73)	0.042(4)	0.042(3)	0.039(3)	−0.011(2)	0.016(3)	0.000(3)
C(74)	0.025(3)	0.038(3)	0.060(4)	−0.015(3)	0.015(3)	0.004(2)
C(75)	0.027(3)	0.038(3)	0.057(4)	−0.010(3)	0.008(3)	0.004(2)
C(76)	0.026(3)	0.030(3)	0.042(3)	−0.004(2)	0.007(2)	0.000(2)
C(81)	0.027(3)	0.021(2)	0.023(2)	−0.0005(19)	0.000(2)	−0.004(2)
C(82)	0.032(3)	0.025(3)	0.056(3)	−0.002(2)	0.016(3)	−0.004(2)
C(83)	0.049(4)	0.024(3)	0.062(4)	−0.005(2)	0.013(3)	0.002(3)
C(84)	0.037(3)	0.023(3)	0.033(3)	0.004(2)	0.002(2)	−0.012(2)
C(85)	0.028(3)	0.031(3)	0.044(3)	0.003(2)	0.002(2)	−0.010(2)
C(86)	0.022(3)	0.027(3)	0.050(3)	−0.004(2)	0.009(2)	−0.001(2)

Table S15. Distances [Å] for [($PC^{Py}P$)IrH(CH_2O^tBu] (**10**).

atom – atom	distance	atom – atom	distance
Ir – C(4)	2.123(4)	Ir – C	2.187(4)
Ir – N	2.199(3)	Ir – P(1)	2.2459(11)
Ir – P(2)	2.2699(12)	Ir – H	1.39(5)
P(2) – C(22)	1.835(4)	P(2) – C(81)	1.836(4)
P(2) – C(71)	1.840(5)	O – C(41)	1.437(5)
O – C(4)	1.451(5)	C(4) – H(4A)	0.9900
C(4) – H(4B)	0.9900	N – C(35)	1.341(6)
N – C(31)	1.352(5)	C – C(21)	1.507(6)
C – C(31)	1.532(6)	C – C(11)	1.546(6)
C(11) – C(12)	1.389(6)	C(11) – C(16)	1.404(6)
C(12) – C(13)	1.388(6)	C(12) – P(1)	1.826(5)
C(13) – C(14)	1.376(7)	C(13) – H(13)	0.9500
C(14) – C(15)	1.384(7)	C(14) – H(14)	0.9500
C(15) – C(16)	1.377(6)	C(15) – H(15)	0.9500
C(16) – H(16)	0.9500	P(1) – C(51)	1.821(5)
P(1) – C(61)	1.836(4)	C(21) – C(26)	1.404(6)
C(21) – C(22)	1.404(6)	C(22) – C(23)	1.392(6)
C(23) – C(24)	1.382(6)	C(23) – H(23)	0.9500
C(24) – C(25)	1.380(7)	C(24) – H(24)	0.9500
C(25) – C(26)	1.386(6)	C(25) – H(25)	0.9500
C(26) – H(26)	0.9500	C(31) – C(32)	1.380(6)
C(32) – C(33)	1.387(6)	C(32) – H(32)	0.9500
C(33) – C(34)	1.376(7)	C(33) – H(33)	0.9500
C(34) – C(35)	1.393(6)	C(34) – H(34)	0.9500
C(35) – H(35)	0.9500	C(41) – C(42)	1.511(7)
C(41) – C(43)	1.514(7)	C(41) – C(44)	1.521(7)
C(42) – H(42A)	0.9800	C(42) – H(42B)	0.9800
C(42) – H(42C)	0.9800	C(43) – H(43A)	0.9800
C(43) – H(43B)	0.9800	C(43) – H(43C)	0.9800
C(44) – H(44A)	0.9800	C(44) – H(44B)	0.9800
C(44) – H(44C)	0.9800	C(51) – C(56)	1.385(6)
C(51) – C(52)	1.389(6)	C(52) – C(53)	1.391(6)
C(52) – H(52)	0.9500	C(53) – C(54)	1.373(7)
C(53) – H(53)	0.9500	C(54) – C(55)	1.378(7)
C(54) – H(54)	0.9500	C(55) – C(56)	1.391(7)
C(55) – H(55)	0.9500	C(56) – H(56)	0.9500
C(61) – C(62)	1.392(6)	C(61) – C(66)	1.396(6)
C(62) – C(63)	1.397(6)	C(62) – H(62)	0.9500
C(63) – C(64)	1.365(7)	C(63) – H(63)	0.9500
C(64) – C(65)	1.377(7)	C(64) – H(64)	0.9500
C(65) – C(66)	1.379(6)	C(65) – H(65)	0.9500

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Table S15. – continued from previous page

atom – atom	distance	atom – atom	distance
C(66) – H(66)	0.9500	C(71) – C(76)	1.378(6)
C(71) – C(72)	1.389(6)	C(72) – C(73)	1.411(7)
C(72) – H(72)	0.9500	C(73) – C(74)	1.380(7)
C(73) – H(73)	0.9500	C(74) – C(75)	1.368(7)
C(74) – H(74)	0.9500	C(75) – C(76)	1.374(7)
C(75) – H(75)	0.9500	C(76) – H(76)	0.9500
C(81) – C(86)	1.379(6)	C(81) – C(82)	1.387(6)
C(82) – C(83)	1.384(7)	C(82) – H(82)	0.9500
C(83) – C(84)	1.371(7)	C(83) – H(83)	0.9500
C(84) – C(85)	1.363(7)	C(84) – H(84)	0.9500
C(85) – C(86)	1.383(6)	C(85) – H(85)	0.9500
C(86) – H(86)	0.9500		

Table S16. Angles [°] for [(PC^{Py}P)IrH(CH$_2$O^{t}Bu] (**10**).

atom – atom – atom	angle	atom – atom – atom	angle
C(4) – Ir – C	168.58(16)	C(4) – Ir – N	103.95(15)
C – Ir – N	64.64(15)	C(4) – Ir – P(1)	97.52(13)
C – Ir – P(1)	85.06(11)	N – Ir – P(1)	98.47(9)
C(4) – Ir – P(2)	98.82(13)	C – Ir – P(2)	81.39(12)
N – Ir – P(2)	89.66(9)	P(1) – Ir – P(2)	159.42(4)
C(4) – Ir – H	91(2)	C – Ir – H	101(2)
N – Ir – H	165(2)	P(1) – Ir – H	84(2)
P(2) – Ir – H	84(2)	C(22) – P(2) – C(81)	105.8(2)
C(22) – P(2) – C(71)	104.0(2)	C(81) – P(2) – C(71)	102.1(2)
C(22) – P(2) – Ir	101.13(15)	C(81) – P(2) – Ir	121.50(15)
C(71) – P(2) – Ir	120.26(15)	C(41) – O – C(4)	118.5(3)
O – C(4) – Ir	107.0(3)	O – C(4) – H(4A)	110.3
Ir – C(4) – H(4A)	110.3	O – C(4) – H(4B)	110.3
Ir – C(4) – H(4B)	110.3	H(4A) – C(4) – H(4B)	108.6
C(35) – N – C(31)	120.2(4)	C(35) – N – Ir	143.5(3)
C(31) – N – Ir	94.3(3)	C(21) – C – C(31)	114.3(4)
C(21) – C – C(11)	118.1(4)	C(31) – C – C(11)	105.1(3)
C(21) – C – Ir	112.6(3)	C(31) – C – Ir	89.8(3)
C(11) – C – Ir	113.3(3)	C(12) – C(11) – C(16)	117.4(4)
C(12) – C(11) – C	120.9(4)	C(16) – C(11) – C	121.2(4)
C(13) – C(12) – C(11)	120.7(4)	C(13) – C(12) – P(1)	123.4(4)
C(11) – C(12) – P(1)	115.9(3)	C(14) – C(13) – C(12)	121.3(5)
C(14) – C(13) – H(13)	119.4	C(12) – C(13) – H(13)	119.4
C(13) – C(14) – C(15)	118.6(4)	C(13) – C(14) – H(14)	120.7
C(15) – C(14) – H(14)	120.7	C(16) – C(15) – C(14)	120.7(5)
C(16) – C(15) – H(15)	119.7	C(14) – C(15) – H(15)	119.7
C(15) – C(16) – C(11)	121.3(4)	C(15) – C(16) – H(16)	119.4
C(11) – C(16) – H(16)	119.4	C(51) – P(1) – C(12)	103.8(2)
C(51) – P(1) – C(61)	104.6(2)	C(12) – P(1) – C(61)	104.4(2)
C(51) – P(1) – Ir	115.92(14)	C(12) – P(1) – Ir	104.47(15)
C(61) – P(1) – Ir	121.73(15)	C(26) – C(21) – C(22)	116.9(4)
C(26) – C(21) – C	125.7(4)	C(22) – C(21) – C	117.3(4)
C(23) – C(22) – C(21)	121.2(4)	C(23) – C(22) – P(2)	123.1(3)
C(21) – C(22) – P(2)	115.6(3)	C(24) – C(23) – C(22)	120.7(4)
C(24) – C(23) – H(23)	119.6	C(22) – C(23) – H(23)	119.6
C(25) – C(24) – C(23)	119.0(5)	C(25) – C(24) – H(24)	120.5
C(23) – C(24) – H(24)	120.5	C(24) – C(25) – C(26)	120.8(5)
C(24) – C(25) – H(25)	119.6	C(26) – C(25) – H(25)	119.6
C(25) – C(26) – C(21)	121.4(4)	C(25) – C(26) – H(26)	119.3
C(21) – C(26) – H(26)	119.3	N – C(31) – C(32)	121.5(4)
N – C(31) – C	108.6(4)	C(32) – C(31) – C	129.9(4)

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Table S16. – continued from previous page

atom – atom – atom	angle	atom – atom – atom	angle
C(31) – C(32) – C(33)	118.5(5)	C(31) – C(32) – H(32)	120.8
C(33) – C(32) – H(32)	120.8	C(34) – C(33) – C(32)	119.9(5)
C(34) – C(33) – H(33)	120.0	C(32) – C(33) – H(33)	120.0
C(33) – C(34) – C(35)	119.2(5)	C(33) – C(34) – H(34)	120.4
C(35) – C(34) – H(34)	120.4	N – C(35) – C(34)	120.6(4)
N – C(35) – H(35)	119.7	C(34) – C(35) – H(35)	119.7
O – C(41) – C(42)	103.5(4)	O – C(41) – C(43)	111.3(4)
C(42) – C(41) – C(43)	108.5(4)	O – C(41) – C(44)	110.9(4)
C(42) – C(41) – C(44)	109.7(4)	C(43) – C(41) – C(44)	112.4(5)
C(41) – C(42) – H(42A)	109.5	C(41) – C(42) – H(42B)	109.5
H(42A) – C(42) – H(42B)	109.5	C(41) – C(42) – H(42C)	109.5
H(42A) – C(42) – H(42C)	109.5	H(42B) – C(42) – H(42C)	109.5
C(41) – C(43) – H(43A)	109.5	C(41) – C(43) – H(43B)	109.5
H(43A) – C(43) – H(43B)	109.5	C(41) – C(43) – H(43C)	109.5
H(43A) – C(43) – H(43C)	109.5	H(43B) – C(43) – H(43C)	109.5
C(41) – C(44) – H(44A)	109.5	C(41) – C(44) – H(44B)	109.5
H(44A) – C(44) – H(44B)	109.5	C(41) – C(44) – H(44C)	109.5
H(44A) – C(44) – H(44C)	109.5	H(44B) – C(44) – H(44C)	109.5
C(56) – C(51) – C(52)	119.4(4)	C(56) – C(51) – P(1)	119.7(4)
C(52) – C(51) – P(1)	120.5(3)	C(51) – C(52) – C(53)	119.7(5)
C(51) – C(52) – H(52)	120.1	C(53) – C(52) – H(52)	120.1
C(54) – C(53) – C(52)	120.9(5)	C(54) – C(53) – H(53)	119.6
C(52) – C(53) – H(53)	119.6	C(53) – C(54) – C(55)	119.4(5)
C(53) – C(54) – H(54)	120.3	C(55) – C(54) – H(54)	120.3
C(54) – C(55) – C(56)	120.4(5)	C(54) – C(55) – H(55)	119.8
C(56) – C(55) – H(55)	119.8	C(51) – C(56) – C(55)	120.2(5)
C(51) – C(56) – H(56)	119.9	C(55) – C(56) – H(56)	119.9
C(62) – C(61) – C(66)	119.4(4)	C(62) – C(61) – P(1)	117.9(3)
C(66) – C(61) – P(1)	122.5(4)	C(61) – C(62) – C(63)	119.2(4)
C(61) – C(62) – H(62)	120.4	C(63) – C(62) – H(62)	120.4
C(64) – C(63) – C(62)	120.4(5)	C(64) – C(63) – H(63)	119.8
C(62) – C(63) – H(63)	119.8	C(63) – C(64) – C(65)	120.7(5)
C(63) – C(64) – H(64)	119.6	C(65) – C(64) – H(64)	119.6
C(64) – C(65) – C(66)	119.8(5)	C(64) – C(65) – H(65)	120.1
C(66) – C(65) – H(65)	120.1	C(65) – C(66) – C(61)	120.3(5)
C(65) – C(66) – H(66)	119.8	C(61) – C(66) – H(66)	119.8
C(76) – C(71) – C(72)	119.6(4)	C(76) – C(71) – P(2)	123.0(4)
C(72) – C(71) – P(2)	117.3(4)	C(71) – C(72) – C(73)	119.6(5)
C(71) – C(72) – H(72)	120.2	C(73) – C(72) – H(72)	120.2
C(74) – C(73) – C(72)	119.5(5)	C(74) – C(73) – H(73)	120.3
C(72) – C(73) – H(73)	120.3	C(75) – C(74) – C(73)	119.8(5)
C(75) – C(74) – H(74)	120.1	C(73) – C(74) – H(74)	120.1

Continued on next page

Table S16. – continued from previous page

atom – atom – atom	angle	atom – atom – atom	angle
C(74) – C(75) – C(76)	121.2(5)	C(74) – C(75) – H(75)	119.4
C(76) – C(75) – H(75)	119.4	C(75) – C(76) – C(71)	120.2(5)
C(75) – C(76) – H(76)	119.9	C(71) – C(76) – H(76)	119.9
C(86) – C(81) – C(82)	118.2(4)	C(86) – C(81) – P(2)	118.7(3)
C(82) – C(81) – P(2)	123.1(4)	C(83) – C(82) – C(81)	120.9(5)
C(83) – C(82) – H(82)	119.6	C(81) – C(82) – H(82)	119.6
C(84) – C(83) – C(82)	119.7(5)	C(84) – C(83) – H(83)	120.2
C(82) – C(83) – H(83)	120.2	C(85) – C(84) – C(83)	120.2(5)
C(85) – C(84) – H(84)	119.9	C(83) – C(84) – H(84)	119.9
C(84) – C(85) – C(86)	120.2(5)	C(84) – C(85) – H(85)	119.9
C(86) – C(85) – H(85)	119.9	C(81) – C(86) – C(85)	120.8(5)
C(81) – C(86) – H(86)	119.6	C(85) – C(86) – H(86)	119.6

3.4 Crystal data for [(PC^{Py}P)IrH(C$_4$H$_7$O)(CCHPh)] (11)

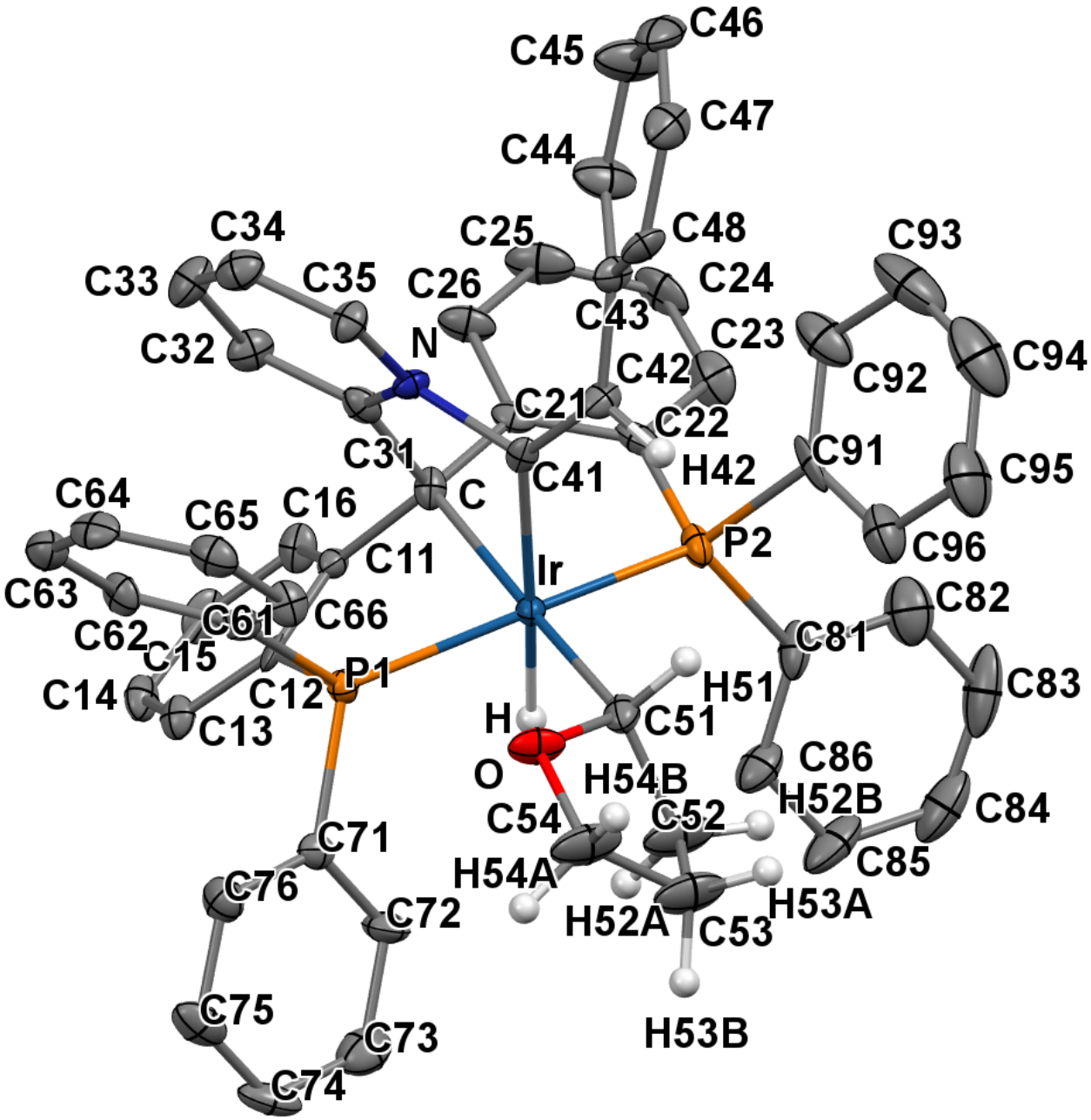

Figure S51. Thermal-ellipsoid representation of [(PC^{Py}P)IrH(C$_4$H$_7$O)(CCHPh)] (**11**) at 50% probability. Most hydrogen atoms were omitted for clarity.

Table S17. Crystal data and structure refinement for [($PC^{Py}P$)IrH(C_4H_7O)(CCHPh)] (**11**).

Identification code:	pc8b	
Empirical formula:	$C_{54}H_{46}IrNOP_2$	
Formula weight:	979.06	
Temperature:	120(2) K	
Wavelength:	0.71073 Å	
Crystal system:	Triclinic	
Space group:	$P\bar{1}$	
Unit cell dimensions:	a = 10.4635(10) Å	α = 77.710(2)°
	b = 13.3359(12) Å	β = 80.875(3)°
	c = 15.8836(15) Å	γ = 85.402(2)°
Volume:	2135.7(3) $Å^3$	
Z:	2	
Density (calculated):	1.522 $g{\cdot}cm^{-3}$	
Absorption coefficient (μ):	3.242 mm^{-1}	
F(000):	984	
Crystal size:	0.09 × 0.08 × 0.07 mm^3	
θ range for data collection:	1.56 to 25.00°	
Index ranges:	$-12 \le h \le 11$, $-15 \le k \le 14$, $-18 \le l \le 16$	
Reflections collected:	18693	
Independent reflections:	7517 [R_{int} = 0.0626]	
Completeness to θ = 25.00°:	100.0 %	
Absorption correction:	Semi-empirical from equivalents	
Max. and min. transmission:	0.7454 and 0.6201	
Refinement method:	Full-matrix least-squares on F^2	
Data / restraints / parameters:	7517 / 0 / 537	
Goodness-of-fit on F^2:	0.981	
Final R indices [I>2σ(I)]:	R_1 = 0.0436, wR_2 = 0.0868	
R indices (all data):	R_1 = 0.0635, wR_2 = 0.0919	
Largest diff. peak and hole:	3.649 and −3.069 $e^{-}{\cdot}Å^{-3}$	

Table S18. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for [($PC^{Py}P$)IrH(C_4H_7O)(CCHPh)] (**11**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	x	y	z	U(eq)
Ir	0.60637(2)	0.74861(2)	0.74056(2)	0.013(1)
P(2)	0.69118(17)	0.72679(12)	0.60604(10)	0.019(1)
N	0.8112(5)	0.6610(4)	0.8458(3)	0.014(1)
C	0.7879(6)	0.8220(4)	0.7394(4)	0.016(1)
C(11)	0.7525(6)	0.9297(4)	0.7589(4)	0.013(1)
C(12)	0.6432(6)	0.9402(4)	0.8217(4)	0.015(1)
C(13)	0.6110(6)	1.0321(4)	0.8479(4)	0.018(1)
C(14)	0.6834(6)	1.1178(5)	0.8107(4)	0.021(2)
C(15)	0.7855(7)	1.1107(5)	0.7464(4)	0.023(2)
C(16)	0.8218(6)	1.0179(5)	0.7200(4)	0.020(2)
P(1)	0.54113(15)	0.82871(12)	0.85293(10)	0.014(1)
C(21)	0.8829(6)	0.8195(4)	0.6565(4)	0.018(2)
C(22)	0.8489(6)	0.7833(5)	0.5870(4)	0.021(2)
C(23)	0.9341(7)	0.7896(5)	0.5085(4)	0.029(2)
C(24)	1.0570(7)	0.8268(5)	0.5012(4)	0.030(2)
C(25)	1.0953(7)	0.8560(5)	0.5720(5)	0.034(2)
C(26)	1.0105(6)	0.8521(5)	0.6485(5)	0.025(2)
C(31)	0.8429(6)	0.7613(5)	0.8184(4)	0.018(1)
C(32)	0.9201(6)	0.8001(5)	0.8674(4)	0.022(2)
C(33)	0.9591(7)	0.7418(5)	0.9414(4)	0.028(2)
C(34)	0.9170(6)	0.6418(5)	0.9705(4)	0.025(2)
C(35)	0.8439(6)	0.6041(5)	0.9217(4)	0.019(1)
C(41)	0.7156(6)	0.6235(4)	0.7998(4)	0.013(1)
C(42)	0.7293(6)	0.5237(4)	0.7946(4)	0.018(1)
C(43)	0.8350(6)	0.4467(4)	0.8104(4)	0.018(1)
C(44)	0.9651(7)	0.4702(5)	0.7770(5)	0.034(2)
C(45)	1.0635(7)	0.3948(5)	0.7832(6)	0.041(2)
C(46)	1.0374(7)	0.2942(5)	0.8232(5)	0.034(2)
C(47)	0.9110(7)	0.2704(5)	0.8578(5)	0.029(2)
C(48)	0.8109(6)	0.3472(5)	0.8504(4)	0.021(2)
C(51)	0.4389(6)	0.6635(5)	0.7529(4)	0.020(2)
C(61)	0.5665(6)	0.7681(5)	0.9640(4)	0.018(1)
C(54)	0.2482(9)	0.6190(8)	0.8455(7)	0.040(2)
C(53)	0.2186(10)	0.6454(8)	0.7545(7)	0.040(2)
O	0.3774(6)	0.6443(4)	0.8435(4)	0.025(2)
C(52)	0.3257(10)	0.7080(8)	0.7042(8)	0.040(2)
O(1)	0.372(2)	0.686(2)	0.6728(17)	0.025(2)
C(56)	0.206(5)	0.611(4)	0.783(3)	0.040(2)
C(55)	0.267(4)	0.612(3)	0.688(3)	0.040(2)

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Table S18. – continued from previous page

atom	x	y	x	U(eq)
C(57)	0.315(5)	0.659(4)	0.823(3)	0.040(2)
C(62)	0.6192(6)	0.8172(5)	1.0184(4)	0.020(2)
C(63)	0.6323(6)	0.7677(5)	1.1035(4)	0.024(2)
C(64)	0.5992(6)	0.6662(5)	1.1328(4)	0.024(2)
C(65)	0.5503(6)	0.6147(5)	1.0799(4)	0.024(2)
C(66)	0.5332(6)	0.6654(4)	0.9957(4)	0.020(2)
C(71)	0.3780(6)	0.8920(4)	0.8688(4)	0.017(1)
C(72)	0.3248(6)	0.9412(5)	0.7954(5)	0.024(2)
C(73)	0.2064(7)	0.9964(5)	0.8036(5)	0.033(2)
C(74)	0.1428(7)	1.0050(5)	0.8850(5)	0.031(2)
C(75)	0.1955(6)	0.9569(5)	0.9583(5)	0.029(2)
C(76)	0.3131(6)	0.8997(5)	0.9501(4)	0.024(2)
C(81)	0.6127(7)	0.7851(5)	0.5102(4)	0.027(2)
C(82)	0.6546(8)	0.7545(6)	0.4304(5)	0.042(2)
C(83)	0.5953(10)	0.7999(7)	0.3574(5)	0.052(3)
C(84)	0.4969(9)	0.8744(7)	0.3637(5)	0.047(2)
C(85)	0.4559(8)	0.9029(6)	0.4416(5)	0.043(2)
C(86)	0.5118(7)	0.8579(5)	0.5148(5)	0.030(2)
C(91)	0.7226(7)	0.5959(5)	0.5878(4)	0.025(2)
C(92)	0.8425(8)	0.5437(5)	0.5849(5)	0.037(2)
C(93)	0.8539(10)	0.4394(6)	0.5775(5)	0.055(3)
C(94)	0.7441(11)	0.3906(6)	0.5745(6)	0.058(3)
C(95)	0.6250(10)	0.4405(6)	0.5773(5)	0.049(2)
C(96)	0.6135(8)	0.5429(5)	0.5840(5)	0.034(2)
H(13)	0.5388	1.0371	0.8916	0.022
H(14)	0.6621	1.1807	0.8299	0.025
H(15)	0.8325	1.1700	0.7192	0.027
H(16)	0.8935	1.0143	0.6757	0.024
H(23)	0.9080	0.7686	0.4606	0.035
H(24)	1.1144	0.8322	0.4480	0.036
H(25)	1.1803	0.8788	0.5677	0.041
H(26)	1.0383	0.8717	0.6966	0.031
H(32)	0.9461	0.8689	0.8486	0.026
H(33)	1.0139	0.7688	0.9725	0.033
H(34)	0.9390	0.6008	1.0234	0.030
H(35)	0.8150	0.5362	0.9412	0.023
H(42)	0.6569	0.4987	0.7776	0.022
H(44)	0.9851	0.5389	0.7500	0.041
H(45)	1.1501	0.4121	0.7598	0.050
H(46)	1.1053	0.2424	0.8268	0.040
H(47)	0.8918	0.2020	0.8865	0.035
H(48)	0.7245	0.3295	0.8738	0.025

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Table S18. – continued from previous page

atom	x	y	x	U(eq)
H(51)	0.4675	0.5957	0.7372	0.024
H	0.537(5)	0.849(4)	0.694(4)	0.014(15)
H(54A)	0.1881	0.6582	0.8827	0.048
H(54B)	0.2381	0.5447	0.8695	0.048
H(53A)	0.2148	0.5824	0.7315	0.048
H(53B)	0.1345	0.6848	0.7517	0.048
H(52A)	0.3075	0.7818	0.7054	0.048
H(52B)	0.3426	0.6995	0.6430	0.048
H(56A)	0.1871	0.5407	0.8154	0.048
H(56B)	0.1240	0.6546	0.7853	0.048
H(55A)	0.3037	0.5425	0.6812	0.048
H(55B)	0.2032	0.6349	0.6474	0.048
H(57A)	0.2870	0.7289	0.8334	0.048
H(57B)	0.3328	0.6149	0.8791	0.048
H(62)	0.6466	0.8854	0.9973	0.024
H(63)	0.6637	0.8034	1.1412	0.029
H(64)	0.6106	0.6320	1.1902	0.029
H(65)	0.5283	0.5451	1.1004	0.029
H(66)	0.4985	0.6299	0.9593	0.024
H(72)	0.3695	0.9372	0.7392	0.029
H(73)	0.1693	1.0282	0.7530	0.039
H(74)	0.0630	1.0439	0.8904	0.037
H(75)	0.1519	0.9626	1.0144	0.034
H(76)	0.3486	0.8660	1.0008	0.029
H(82)	0.7225	0.7033	0.4260	0.050
H(83)	0.6230	0.7794	0.3034	0.063
H(84)	0.4577	0.9059	0.3140	0.057
H(85)	0.3881	0.9543	0.4457	0.051
H(86)	0.4804	0.8774	0.5688	0.036
H(92)	0.9173	0.5780	0.5878	0.044
H(93)	0.9362	0.4035	0.5748	0.065
H(94)	0.7516	0.3203	0.5702	0.069
H(95)	0.5506	0.4054	0.5748	0.059
H(96)	0.5306	0.5778	0.5861	0.041

Table S19. Anisotropic displacement parameters (Å^2) for [(PC^{Py}P)IrH(C$_4$H$_7$O)(CCHPh)] (**11**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ...+ 2hka^*b^*U_{12}]$.

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir	0.0137(1)	0.0124(1)	0.0121(1)	−0.0036(1)	−0.0031(1)	0.0007(1)
P(2)	0.0293(11)	0.0170(9)	0.0117(9)	−0.0050(7)	−0.0034(7)	0.0030(7)
N	0.011(3)	0.013(3)	0.017(3)	−0.001(2)	−0.004(2)	−0.002(2)
C	0.023(4)	0.012(3)	0.012(3)	−0.001(2)	−0.003(3)	−0.004(3)
C(11)	0.013(3)	0.012(3)	0.016(3)	−0.003(2)	−0.005(3)	0.000(2)
C(12)	0.019(4)	0.017(3)	0.013(3)	−0.004(3)	−0.011(3)	−0.003(3)
C(13)	0.026(4)	0.017(3)	0.011(3)	0.000(3)	−0.004(3)	−0.002(3)
C(14)	0.032(4)	0.012(3)	0.021(4)	−0.004(3)	−0.009(3)	−0.001(3)
C(15)	0.030(4)	0.016(3)	0.022(4)	0.004(3)	−0.005(3)	−0.018(3)
C(16)	0.027(4)	0.019(4)	0.011(3)	0.002(3)	0.000(3)	−0.009(3)
P(1)	0.0142(9)	0.0137(8)	0.0137(9)	−0.0036(6)	−0.0013(7)	−0.0021(7)
C(21)	0.018(4)	0.012(3)	0.022(4)	0.000(3)	−0.002(3)	0.004(3)
C(22)	0.022(4)	0.018(3)	0.019(4)	−0.001(3)	0.002(3)	0.009(3)
C(23)	0.040(5)	0.028(4)	0.013(4)	0.003(3)	0.005(3)	−0.005(3)
C(24)	0.034(5)	0.032(4)	0.016(4)	−0.001(3)	0.014(3)	0.005(3)
C(25)	0.020(4)	0.035(4)	0.036(5)	0.009(3)	0.009(3)	0.000(3)
C(26)	0.016(4)	0.023(4)	0.031(4)	0.002(3)	0.006(3)	−0.001(3)
C(31)	0.016(4)	0.018(3)	0.018(4)	−0.004(3)	0.004(3)	−0.002(3)
C(32)	0.020(4)	0.019(4)	0.026(4)	0.000(3)	−0.003(3)	−0.006(3)
C(33)	0.031(4)	0.031(4)	0.023(4)	−0.001(3)	−0.012(3)	−0.007(3)
C(34)	0.023(4)	0.028(4)	0.021(4)	0.001(3)	−0.005(3)	−0.001(3)
C(35)	0.023(4)	0.018(3)	0.016(4)	0.000(3)	−0.006(3)	−0.003(3)
C(41)	0.010(3)	0.019(3)	0.009(3)	−0.002(2)	0.003(2)	−0.007(3)
C(42)	0.020(4)	0.011(3)	0.023(4)	0.000(3)	−0.009(3)	−0.002(3)
C(43)	0.016(4)	0.011(3)	0.029(4)	−0.005(3)	−0.007(3)	−0.003(3)
C(44)	0.027(4)	0.016(4)	0.055(5)	−0.003(3)	−0.002(4)	0.001(3)
C(45)	0.020(4)	0.026(4)	0.076(6)	−0.008(4)	−0.005(4)	−0.004(3)
C(46)	0.029(5)	0.028(4)	0.051(5)	−0.014(4)	−0.024(4)	0.013(3)
C(47)	0.034(5)	0.017(4)	0.038(5)	−0.004(3)	−0.014(4)	−0.001(3)
C(48)	0.013(4)	0.025(4)	0.026(4)	−0.003(3)	−0.008(3)	−0.005(3)
C(51)	0.027(4)	0.018(3)	0.019(4)	−0.005(3)	−0.010(3)	0.005(3)
C(61)	0.011(3)	0.025(4)	0.016(4)	−0.004(3)	0.001(3)	−0.001(3)
C(54)	0.018(3)	0.036(4)	0.064(5)	0.002(3)	−0.012(3)	−0.008(3)
C(53)	0.018(3)	0.036(4)	0.064(5)	0.002(3)	−0.012(3)	−0.008(3)
O	0.012(3)	0.023(3)	0.036(4)	0.002(3)	0.000(3)	−0.006(3)
C(52)	0.018(3)	0.036(4)	0.064(5)	0.002(3)	−0.012(3)	−0.008(3)
O(1)	0.012(3)	0.023(3)	0.036(4)	0.002(3)	0.000(3)	−0.006(3)
C(56)	0.018(3)	0.036(4)	0.064(5)	0.002(3)	−0.012(3)	−0.008(3)
C(55)	0.018(3)	0.036(4)	0.064(5)	0.002(3)	−0.012(3)	−0.008(3)
C(57)	0.018(3)	0.036(4)	0.064(5)	0.002(3)	−0.012(3)	−0.008(3)

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Table S19. – continued from previous page

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(62)	0.023(4)	0.024(4)	0.011(3)	−0.003(3)	0.003(3)	−0.001(3)
C(63)	0.020(4)	0.030(4)	0.024(4)	−0.008(3)	−0.003(3)	0.000(3)
C(64)	0.024(4)	0.029(4)	0.014(4)	0.005(3)	−0.004(3)	0.007(3)
C(65)	0.024(4)	0.024(4)	0.020(4)	0.000(3)	0.003(3)	0.001(3)
C(66)	0.025(4)	0.013(3)	0.020(4)	0.000(3)	0.000(3)	−0.006(3)
C(71)	0.016(4)	0.012(3)	0.023(4)	−0.004(3)	−0.003(3)	−0.002(3)
C(72)	0.018(4)	0.025(4)	0.029(4)	−0.006(3)	−0.004(3)	0.009(3)
C(73)	0.036(5)	0.025(4)	0.037(5)	0.001(3)	−0.014(4)	0.000(3)
C(74)	0.018(4)	0.015(4)	0.053(5)	−0.003(3)	0.004(4)	0.004(3)
C(75)	0.020(4)	0.025(4)	0.038(5)	−0.008(3)	0.010(3)	−0.006(3)
C(76)	0.025(4)	0.028(4)	0.019(4)	−0.005(3)	0.000(3)	−0.002(3)
C(81)	0.045(5)	0.024(4)	0.013(4)	−0.003(3)	−0.008(3)	−0.008(3)
C(82)	0.058(6)	0.040(5)	0.027(5)	−0.006(4)	−0.001(4)	−0.009(4)
C(83)	0.096(8)	0.050(6)	0.015(4)	−0.001(4)	−0.010(4)	−0.038(5)
C(84)	0.059(6)	0.054(6)	0.032(5)	0.005(4)	−0.026(4)	−0.021(5)
C(85)	0.050(6)	0.034(5)	0.049(6)	0.005(4)	−0.036(4)	−0.006(4)
C(86)	0.036(5)	0.026(4)	0.028(4)	0.002(3)	−0.017(3)	−0.003(3)
C(91)	0.049(5)	0.015(3)	0.008(3)	−0.005(3)	0.005(3)	0.005(3)
C(92)	0.048(5)	0.025(4)	0.028(4)	−0.001(3)	0.008(4)	0.007(4)
C(93)	0.066(7)	0.035(5)	0.050(6)	−0.006(4)	0.015(5)	0.020(5)
C(94)	0.090(8)	0.026(5)	0.052(6)	−0.013(4)	0.011(5)	−0.002(5)
C(95)	0.074(7)	0.028(5)	0.050(6)	−0.019(4)	−0.007(5)	−0.007(4)
C(96)	0.050(5)	0.026(4)	0.028(4)	−0.010(3)	−0.003(4)	0.000(4)

Table S20. Distances [Å] for [($PC^{Py}P$)IrH(C_4H_7O)(CCHPh)] (**11**).

atom – atom	distance	atom – atom	distance
Ir – C(41)	2.084(6)	Ir – C(51)	2.124(7)
Ir – C	2.201(6)	Ir – P(2)	2.2493(17)
Ir – P(1)	2.2585(16)	Ir – H	1.57(5)
P(2) – C(22)	1.824(7)	P(2) – C(91)	1.825(6)
P(2) – C(81)	1.840(7)	N – C(35)	1.357(7)
N – C(31)	1.367(7)	N – C(41)	1.501(7)
C – C(31)	1.510(8)	C – C(21)	1.524(8)
C – C(11)	1.537(8)	C(11) – C(16)	1.406(8)
C(11) – C(12)	1.412(8)	C(12) – C(13)	1.377(8)
C(12) – P(1)	1.836(6)	C(13) – C(14)	1.392(9)
C(13) – H(13)	0.9500	C(14) – C(15)	1.369(9)
C(14) – H(14)	0.9500	C(15) – C(16)	1.395(9)
C(15) – H(15)	0.9500	C(16) – H(16)	0.9500
P(1) – C(61)	1.828(6)	P(1) – C(71)	1.847(6)
C(21) – C(22)	1.399(9)	C(21) – C(26)	1.416(9)
C(22) – C(23)	1.404(9)	C(23) – C(24)	1.394(10)
C(23) – H(23)	0.9500	C(24) – C(25)	1.389(10)
C(24) – H(24)	0.9500	C(25) – C(26)	1.381(9)
C(25) – H(25)	0.9500	C(26) – H(26)	0.9500
C(31) – C(32)	1.402(9)	C(32) – C(33)	1.365(9)
C(32) – H(32)	0.9500	C(33) – C(34)	1.398(9)
C(33) – H(33)	0.9500	C(34) – C(35)	1.362(9)
C(34) – H(34)	0.9500	C(35) – H(35)	0.9500
C(41) – C(42)	1.346(8)	C(42) – C(43)	1.462(8)
C(42) – H(42)	0.9500	C(43) – C(48)	1.369(8)
C(43) – C(44)	1.415(9)	C(44) – C(45)	1.380(9)
C(44) – H(44)	0.9500	C(45) – C(46)	1.385(10)
C(45) – H(45)	0.9500	C(46) – C(47)	1.384(10)
C(46) – H(46)	0.9500	C(47) – C(48)	1.405(9)
C(47) – H(47)	0.9500	C(48) – H(48)	0.9500
C(51) – O	1.457(8)	C(51) – O(1)	1.51(3)
C(51) – C(52)	1.528(11)	C(51) – C(57)	1.56(5)
C(51) – H(51)	1.0000	C(61) – C(62)	1.389(9)
C(61) – C(66)	1.406(8)	C(54) – O	1.415(11)
C(54) – C(53)	1.489(15)	C(54) – H(54A)	0.9900
C(54) – H(54B)	0.9900	C(53) – C(52)	1.475(14)
C(53) – H(53A)	0.9900	C(53) – H(53B)	0.9900
C(52) – H(52A)	0.9900	C(52) – H(52B)	0.9900
O(1) – C(55)	1.50(4)	C(56) – C(55)	1.55(7)
C(56) – C(57)	1.63(7)	C(56) – H(56A)	0.9900
C(56) – H(56B)	0.9900	C(55) – H(55A)	0.9900

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Table S20. – continued from previous page

atom – atom	distance	atom – atom	distance
C(55) – H(55B)	0.9900	C(57) – H(57A)	0.9900
C(57) – H(57B)	0.9900	C(62) – C(63)	1.395(9)
C(62) – H(62)	0.9500	C(63) – C(64)	1.388(9)
C(63) – H(63)	0.9500	C(64) – C(65)	1.370(9)
C(64) – H(64)	0.9500	C(65) – C(66)	1.397(9)
C(65) – H(65)	0.9500	C(66) – H(66)	0.9500
C(71) – C(76)	1.381(9)	C(71) – C(72)	1.386(9)
C(72) – C(73)	1.392(9)	C(72) – H(72)	0.9500
C(73) – C(74)	1.380(10)	C(73) – H(73)	0.9500
C(74) – C(75)	1.379(10)	C(74) – H(74)	0.9500
C(75) – C(76)	1.397(9)	C(75) – H(75)	0.9500
C(76) – H(76)	0.9500	C(81) – C(86)	1.380(10)
C(81) – C(82)	1.408(10)	C(82) – C(83)	1.401(11)
C(82) – H(82)	0.9500	C(83) – C(84)	1.380(12)
C(83) – H(83)	0.9500	C(84) – C(85)	1.366(11)
C(84) – H(84)	0.9500	C(85) – C(86)	1.383(9)
C(85) – H(85)	0.9500	C(86) – H(86)	0.9500
C(91) – C(92)	1.384(10)	C(91) – C(96)	1.406(10)
C(92) – C(93)	1.415(10)	C(92) – H(92)	0.9500
C(93) – C(94)	1.377(13)	C(93) – H(93)	0.9500
C(94) – C(95)	1.365(12)	C(94) – H(94)	0.9500
C(95) – C(96)	1.386(10)	C(95) – H(95)	0.9500
C(96) – H(96)	0.9500		

Table S21. Angles [°] for [(PC^{Py}P)IrH(C$_4$H$_7$O)(CCHPh)] (**11**).

atom – atom – atom	angle	atom – atom – atom	angle
C(41) – Ir – C(51)	94.1(2)	C(41) – Ir – C	79.5(2)
C(51) – Ir – C	173.3(2)	C(41) – Ir – P(2)	92.59(16)
C(51) – Ir – P(2)	96.73(18)	C – Ir – P(2)	85.65(16)
C(41) – Ir – P(1)	100.92(16)	C(51) – Ir – P(1)	97.86(18)
C – Ir – P(1)	81.53(16)	P(2) – Ir – P(1)	159.29(6)
C(41) – Ir – H	174(2)	C(51) – Ir – H	92(2)
C – Ir – H	95(2)	P(2) – Ir – H	86(2)
P(1) – Ir – H	79(2)	C(22) – P(2) – C(91)	106.1(3)
C(22) – P(2) – C(81)	105.7(3)	C(91) – P(2) – C(81)	99.8(3)
C(22) – P(2) – Ir	103.8(2)	C(91) – P(2) – Ir	118.3(2)
C(81) – P(2) – Ir	121.7(2)	C(35) – N – C(31)	121.0(5)
C(35) – N – C(41)	120.6(5)	C(31) – N – C(41)	117.1(5)
C(31) – C – C(21)	110.9(5)	C(31) – C – C(11)	105.3(5)
C(21) – C – C(11)	114.9(5)	C(31) – C – Ir	104.7(4)
C(21) – C – Ir	112.5(4)	C(11) – C – Ir	107.9(4)
C(16) – C(11) – C(12)	117.7(5)	C(16) – C(11) – C	125.0(6)
C(12) – C(11) – C	117.4(5)	C(13) – C(12) – C(11)	121.0(6)
C(13) – C(12) – P(1)	124.2(5)	C(11) – C(12) – P(1)	114.4(4)
C(12) – C(13) – C(14)	120.5(6)	C(12) – C(13) – H(13)	119.7
C(14) – C(13) – H(13)	119.7	C(15) – C(14) – C(13)	119.4(6)
C(15) – C(14) – H(14)	120.3	C(13) – C(14) – H(14)	120.3
C(14) – C(15) – C(16)	121.2(6)	C(14) – C(15) – H(15)	119.4
C(16) – C(15) – H(15)	119.4	C(15) – C(16) – C(11)	120.2(6)
C(15) – C(16) – H(16)	119.9	C(11) – C(16) – H(16)	119.9
C(61) – P(1) – C(12)	105.7(3)	C(61) – P(1) – C(71)	102.9(3)
C(12) – P(1) – C(71)	101.2(3)	C(61) – P(1) – Ir	121.3(2)
C(12) – P(1) – Ir	101.0(2)	C(71) – P(1) – Ir	121.7(2)
C(22) – C(21) – C(26)	117.9(6)	C(22) – C(21) – C	121.7(6)
C(26) – C(21) – C	120.4(6)	C(21) – C(22) – C(23)	120.7(7)
C(21) – C(22) – P(2)	116.1(5)	C(23) – C(22) – P(2)	123.2(6)
C(24) – C(23) – C(22)	119.8(7)	C(24) – C(23) – H(23)	120.1
C(22) – C(23) – H(23)	120.1	C(25) – C(24) – C(23)	119.9(6)
C(25) – C(24) – H(24)	120.0	C(23) – C(24) – H(24)	120.0
C(26) – C(25) – C(24)	120.3(7)	C(26) – C(25) – H(25)	119.8
C(24) – C(25) – H(25)	119.8	C(25) – C(26) – C(21)	121.1(7)
C(25) – C(26) – H(26)	119.5	C(21) – C(26) – H(26)	119.5
N – C(31) – C(32)	117.3(5)	N – C(31) – C	117.1(5)
C(32) – C(31) – C	125.6(5)	C(33) – C(32) – C(31)	121.9(6)
C(33) – C(32) – H(32)	119.1	C(31) – C(32) – H(32)	119.1
C(32) – C(33) – C(34)	118.9(6)	C(32) – C(33) – H(33)	120.5
C(34) – C(33) – H(33)	120.5	C(35) – C(34) – C(33)	118.7(6)

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Table S21. – continued from previous page

atom – atom – atom	angle	atom – atom – atom	angle
C(35) – C(34) – H(34)	120.6	C(33) – C(34) – H(34)	120.6
N – C(35) – C(34)	121.8(6)	N – C(35) – H(35)	119.1
C(34) – C(35) – H(35)	119.1	C(42) – C(41) – N	116.3(5)
C(42) – C(41) – Ir	133.6(5)	N – C(41) – Ir	109.3(4)
C(41) – C(42) – C(43)	131.9(6)	C(41) – C(42) – H(42)	114.1
C(43) – C(42) – H(42)	114.1	C(48) – C(43) – C(44)	117.6(6)
C(48) – C(43) – C(42)	121.3(6)	C(44) – C(43) – C(42)	120.9(5)
C(45) – C(44) – C(43)	121.0(6)	C(45) – C(44) – H(44)	119.5
C(43) – C(44) – H(44)	119.5	C(44) – C(45) – C(46)	120.7(7)
C(44) – C(45) – H(45)	119.6	C(46) – C(45) – H(45)	119.6
C(47) – C(46) – C(45)	119.0(6)	C(47) – C(46) – H(46)	120.5
C(45) – C(46) – H(46)	120.5	C(46) – C(47) – C(48)	120.1(6)
C(46) – C(47) – H(47)	120.0	C(48) – C(47) – H(47)	120.0
C(43) – C(48) – C(47)	121.6(6)	C(43) – C(48) – H(48)	119.2
C(47) – C(48) – H(48)	119.2	O – C(51) – O(1)	127.0(11)
O – C(51) – C(52)	102.4(6)	O(1) – C(51) – C(57)	98(2)
C(52) – C(51) – C(57)	73.6(18)	O – C(51) – Ir	109.2(4)
O(1) – C(51) – Ir	114.0(10)	C(52) – C(51) – Ir	120.8(5)
C(57) – C(51) – Ir	128.1(19)	O – C(51) – H(51)	107.9
O(1) – C(51) – H(51)	86.7	C(52) – C(51) – H(51)	107.9
C(57) – C(51) – H(51)	113.7	Ir – C(51) – H(51)	107.9
C(62) – C(61) – C(66)	118.0(6)	C(62) – C(61) – P(1)	123.6(5)
C(66) – C(61) – P(1)	118.3(5)	O – C(54) – C(53)	107.7(8)
O – C(54) – H(54A)	110.2	C(53) – C(54) – H(54A)	110.2
O – C(54) – H(54B)	110.2	C(53) – C(54) – H(54B)	110.2
H(54A) – C(54) – H(54B)	108.5	C(52) – C(53) – C(54)	105.2(9)
C(52) – C(53) – H(53A)	110.7	C(54) – C(53) – H(53A)	110.7
C(52) – C(53) – H(53B)	110.7	C(54) – C(53) – H(53B)	110.7
H(53A) – C(53) – H(53B)	108.8	C(54) – O – C(51)	107.8(7)
C(53) – C(52) – C(51)	101.9(8)	C(53) – C(52) – H(52A)	111.4
C(51) – C(52) – H(52A)	111.4	C(53) – C(52) – H(52B)	111.4
C(51) – C(52) – H(52B)	111.4	H(52A) – C(52) – H(52B)	109.2
C(55) – O(1) – C(51)	107(2)	C(55) – C(56) – C(57)	104(3)
C(55) – C(56) – H(56A)	111.0	C(57) – C(56) – H(56A)	111.0
C(55) – C(56) – H(56B)	111.0	C(57) – C(56) – H(56B)	111.0
H(56A) – C(56) – H(56B)	109.0	O(1) – C(55) – C(56)	103(3)
O(1) – C(55) – H(55A)	111.2	C(56) – C(55) – H(55A)	111.2
O(1) – C(55) – H(55B)	111.2	C(56) – C(55) – H(55B)	111.2
H(55A) – C(55) – H(55B)	109.1	C(51) – C(57) – C(56)	105(4)
C(51) – C(57) – H(57A)	110.7	C(56) – C(57) – H(57A)	110.7
C(51) – C(57) – H(57B)	110.7	C(56) – C(57) – H(57B)	110.7
H(57A) – C(57) – H(57B)	108.8	C(61) – C(62) – C(63)	120.8(6)

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Table S21. – continued from previous page

atom – atom – atom	angle	atom – atom – atom	angle
C(61) – C(62) – H(62)	119.6	C(63) – C(62) – H(62)	119.6
C(64) – C(63) – C(62)	119.8(6)	C(64) – C(63) – H(63)	120.1
C(62) – C(63) – H(63)	120.1	C(65) – C(64) – C(63)	120.8(6)
C(65) – C(64) – H(64)	119.6	C(63) – C(64) – H(64)	119.6
C(64) – C(65) – C(66)	119.4(6)	C(64) – C(65) – H(65)	120.3
C(66) – C(65) – H(65)	120.3	C(65) – C(66) – C(61)	121.1(6)
C(65) – C(66) – H(66)	119.4	C(61) – C(66) – H(66)	119.4
C(76) – C(71) – C(72)	119.2(6)	C(76) – C(71) – P(1)	122.6(5)
C(72) – C(71) – P(1)	118.0(5)	C(71) – C(72) – C(73)	120.4(6)
C(71) – C(72) – H(72)	119.8	C(73) – C(72) – H(72)	119.8
C(74) – C(73) – C(72)	120.1(7)	C(74) – C(73) – H(73)	120.0
C(72) – C(73) – H(73)	120.0	C(75) – C(74) – C(73)	119.9(6)
C(75) – C(74) – H(74)	120.1	C(73) – C(74) – H(74)	120.1
C(74) – C(75) – C(76)	120.0(7)	C(74) – C(75) – H(75)	120.0
C(76) – C(75) – H(75)	120.0	C(71) – C(76) – C(75)	120.5(6)
C(71) – C(76) – H(76)	119.8	C(75) – C(76) – H(76)	119.8
C(86) – C(81) – C(82)	118.7(7)	C(86) – C(81) – P(2)	121.5(5)
C(82) – C(81) – P(2)	119.8(6)	C(83) – C(82) – C(81)	119.6(8)
C(83) – C(82) – H(82)	120.2	C(81) – C(82) – H(82)	120.2
C(84) – C(83) – C(82)	120.2(8)	C(84) – C(83) – H(83)	119.9
C(82) – C(83) – H(83)	119.9	C(85) – C(84) – C(83)	119.9(7)
C(85) – C(84) – H(84)	120.1	C(83) – C(84) – H(84)	120.1
C(84) – C(85) – C(86)	120.8(8)	C(84) – C(85) – H(85)	119.6
C(86) – C(85) – H(85)	119.6	C(81) – C(86) – C(85)	120.8(7)
C(81) – C(86) – H(86)	119.6	C(85) – C(86) – H(86)	119.6
C(92) – C(91) – C(96)	118.6(6)	C(92) – C(91) – P(2)	125.0(6)
C(96) – C(91) – P(2)	116.2(5)	C(91) – C(92) – C(93)	120.2(8)
C(91) – C(92) – H(92)	119.9	C(93) – C(92) – H(92)	119.9
C(94) – C(93) – C(92)	119.1(8)	C(94) – C(93) – H(93)	120.5
C(92) – C(93) – H(93)	120.5	C(95) – C(94) – C(93)	121.7(8)
C(95) – C(94) – H(94)	119.1	C(93) – C(94) – H(94)	119.1
C(94) – C(95) – C(96)	119.4(9)	C(94) – C(95) – H(95)	120.3
C(96) – C(95) – H(95)	120.3	C(95) – C(96) – C(91)	121.0(8)
C(95) – C(96) – H(96)	119.5	C(91) – C(96) – H(96)	119.5