Supporting Information

Preparation, Structure and Norbornene Polymerization Study of Pyrrole-imine [N$^-$NP] Nickel(II) and Palladium(II) Complexes

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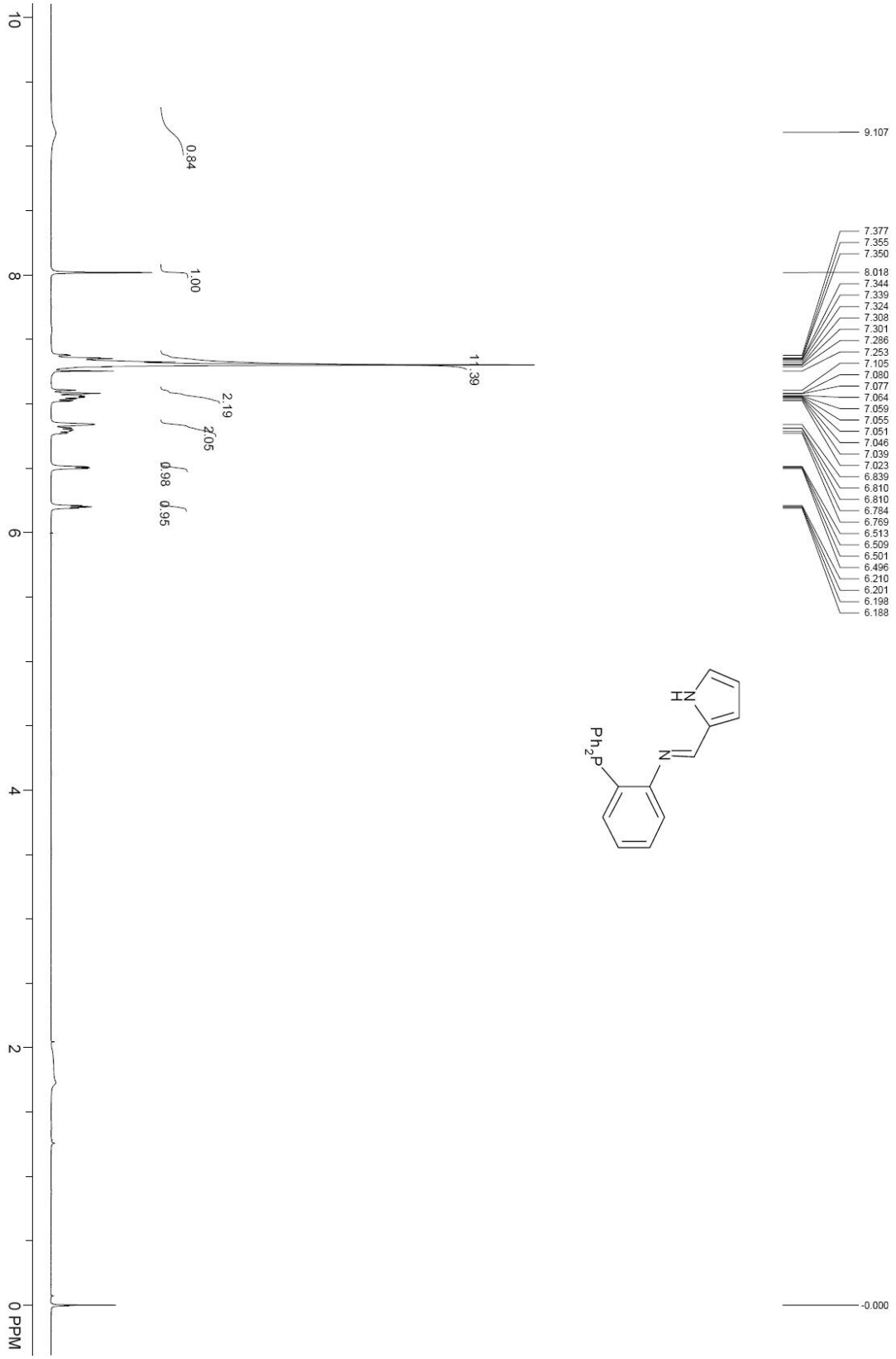
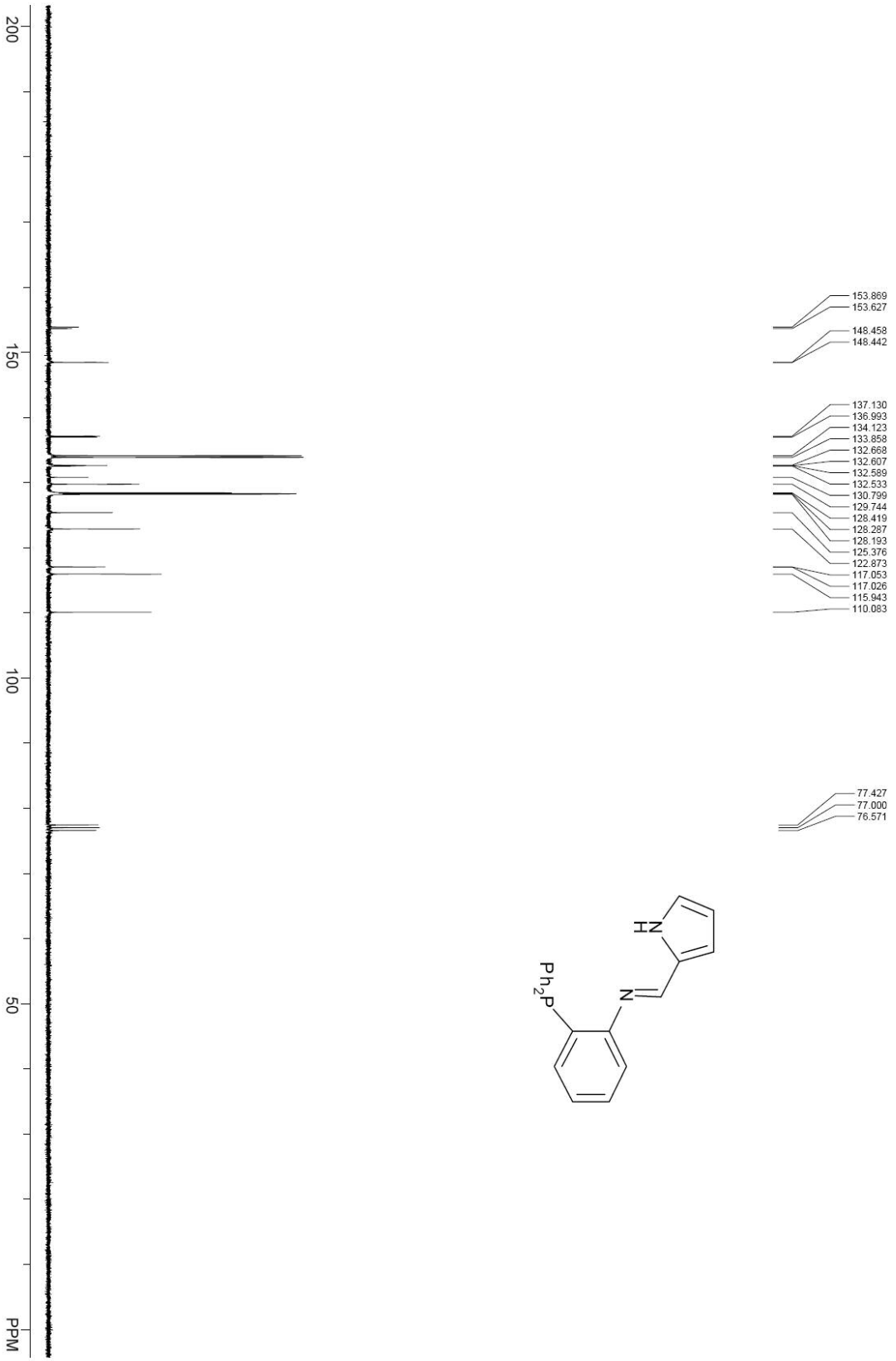
Content

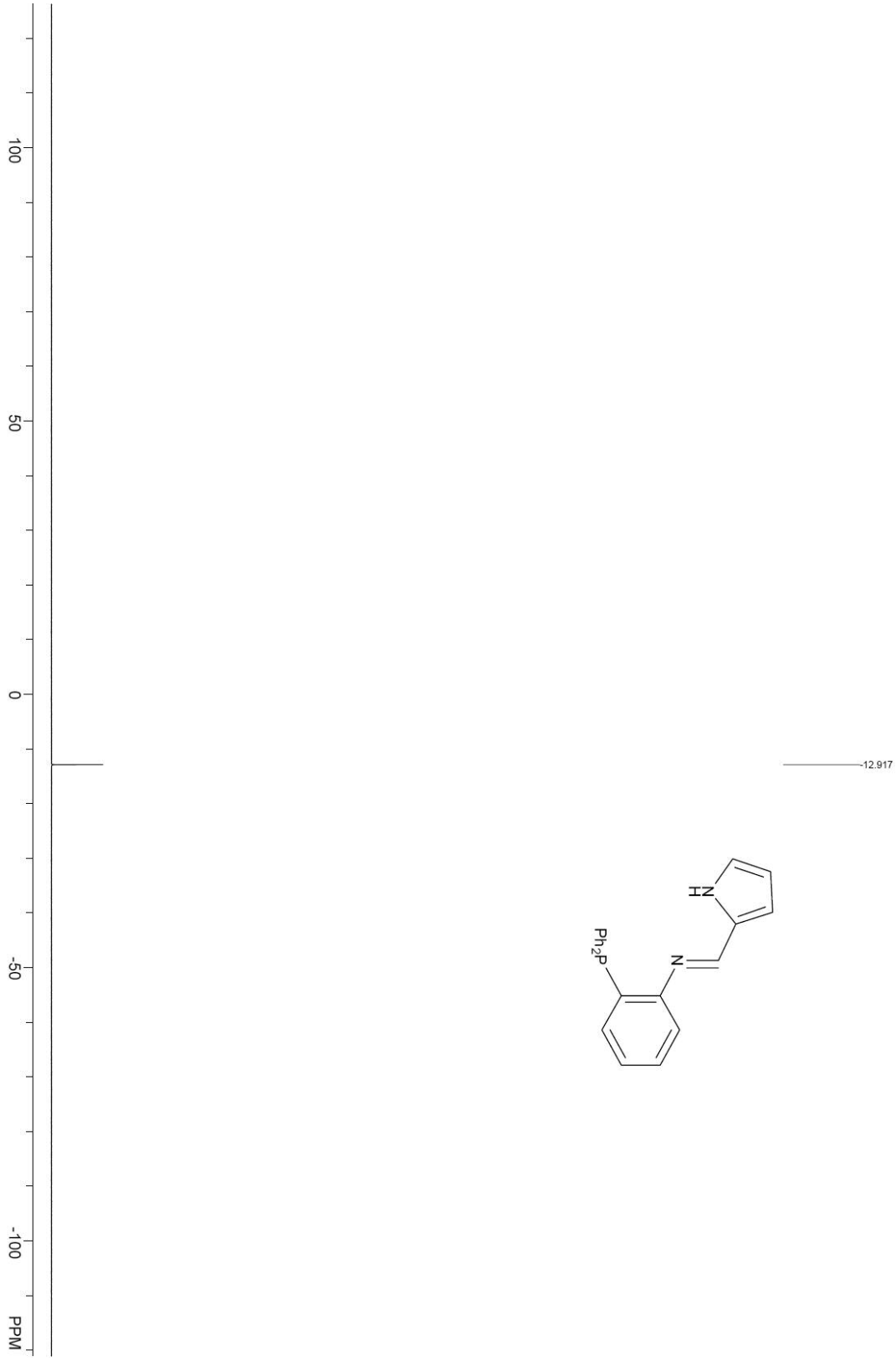
^{1}H NMR of the ligand L1 (300 MHz, $CDCl_3$)



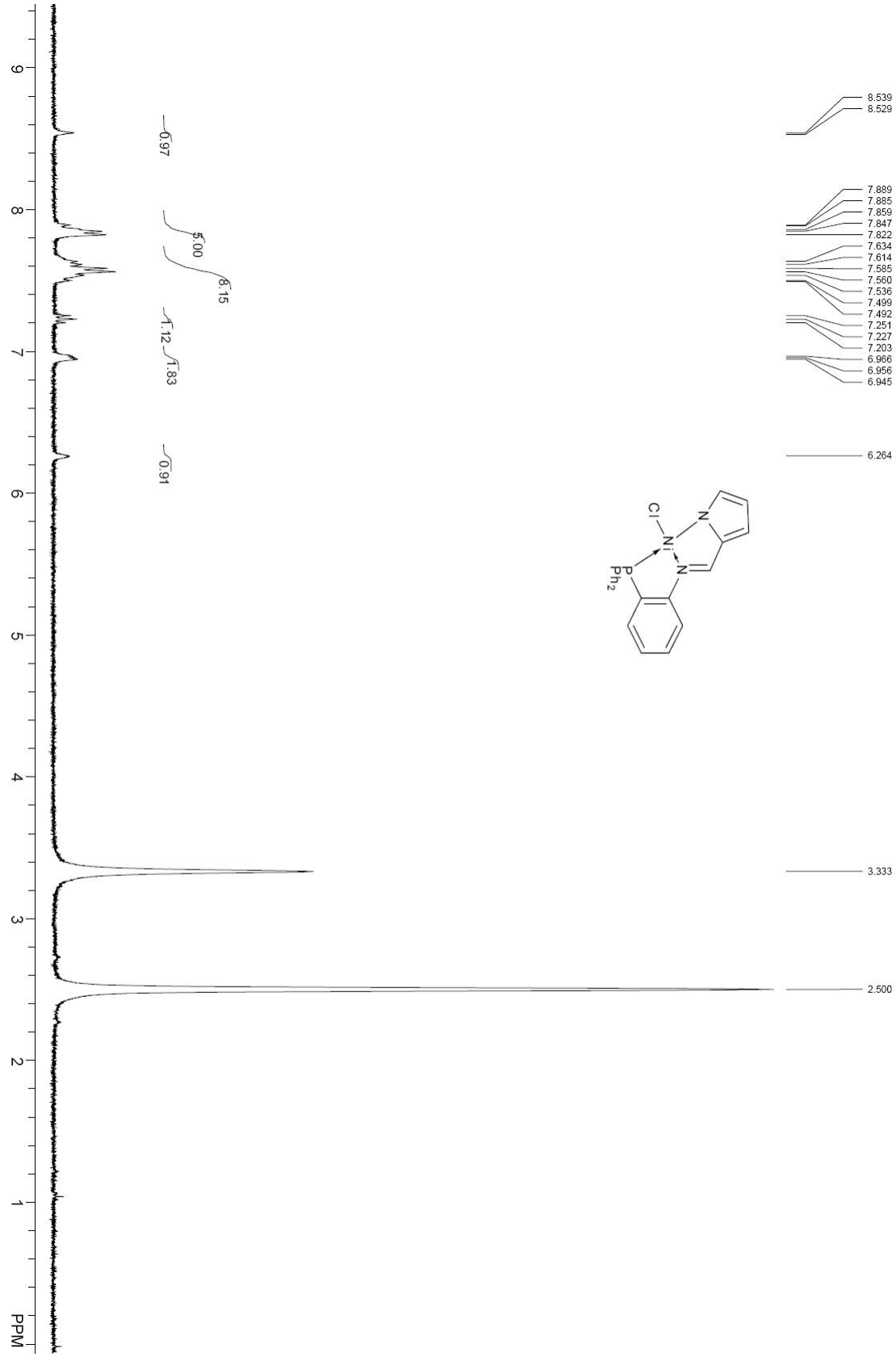
^{13}C NMR of the ligand L1 (75 MHz, $CDCl_3$)



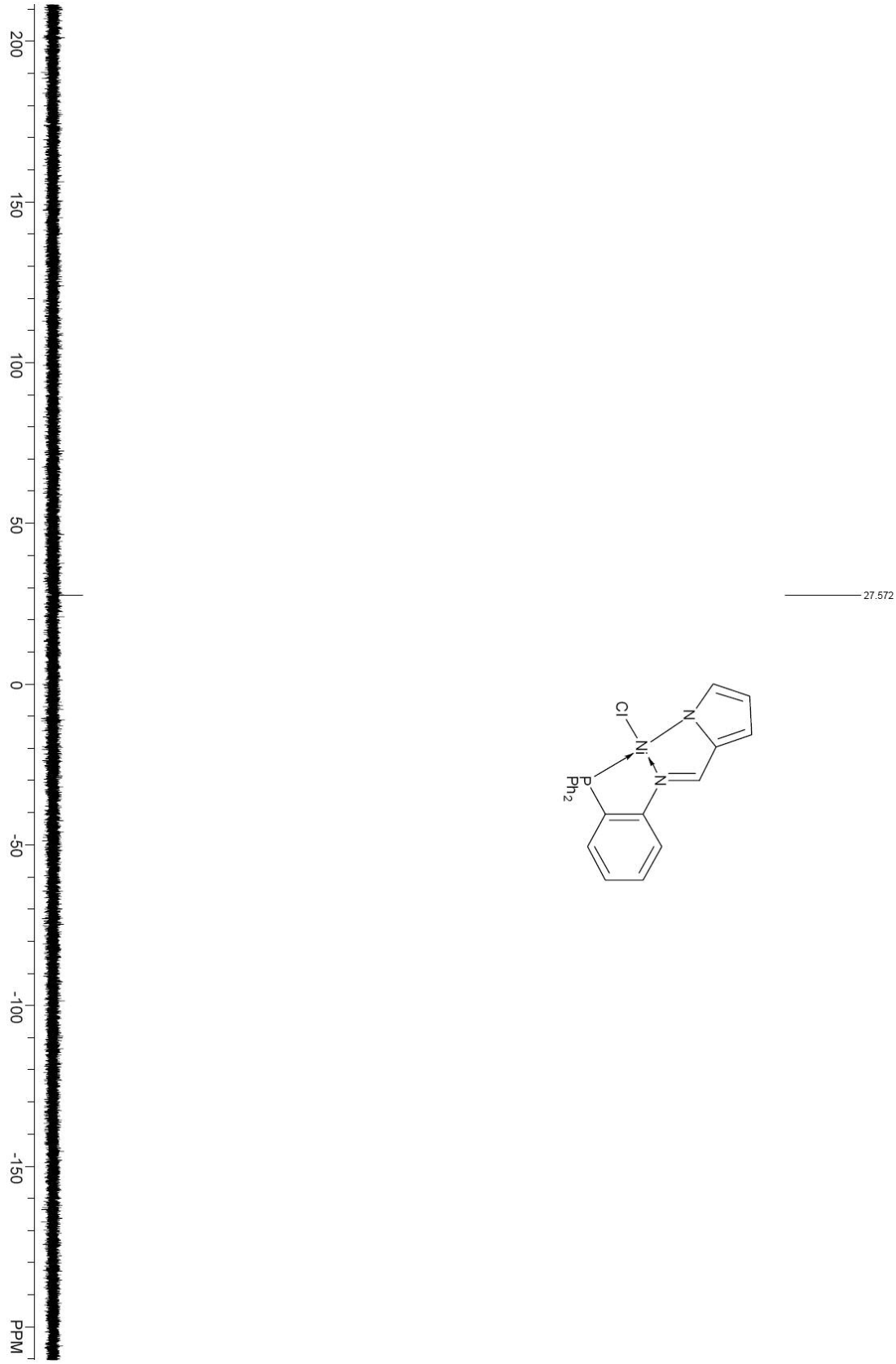
^{31}P NMR of the ligand L1 (121 MHz, $CDCl_3$)



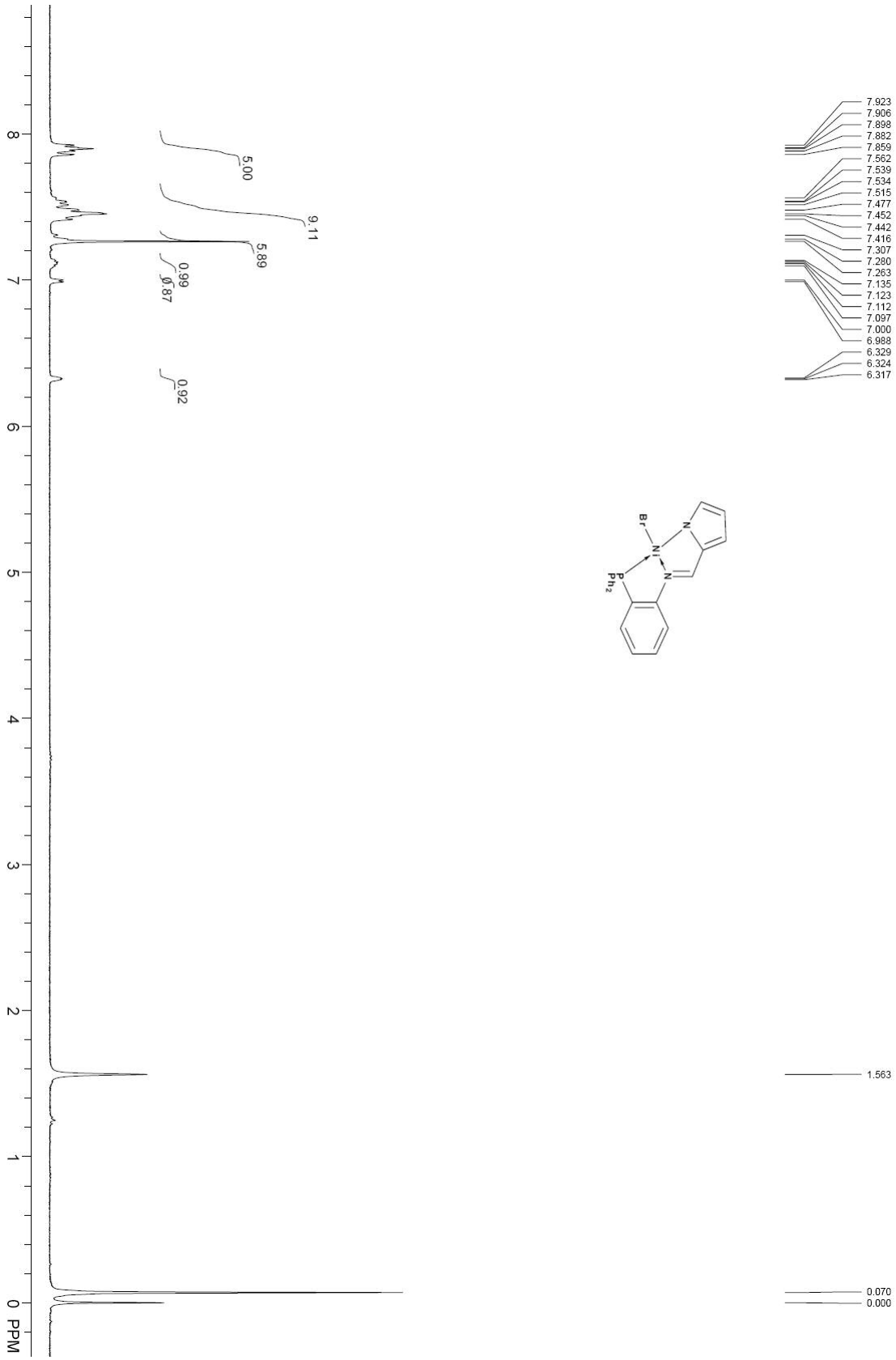
^{1}H NMR of the complex 1 (300 MHz, DMSO-d_6)



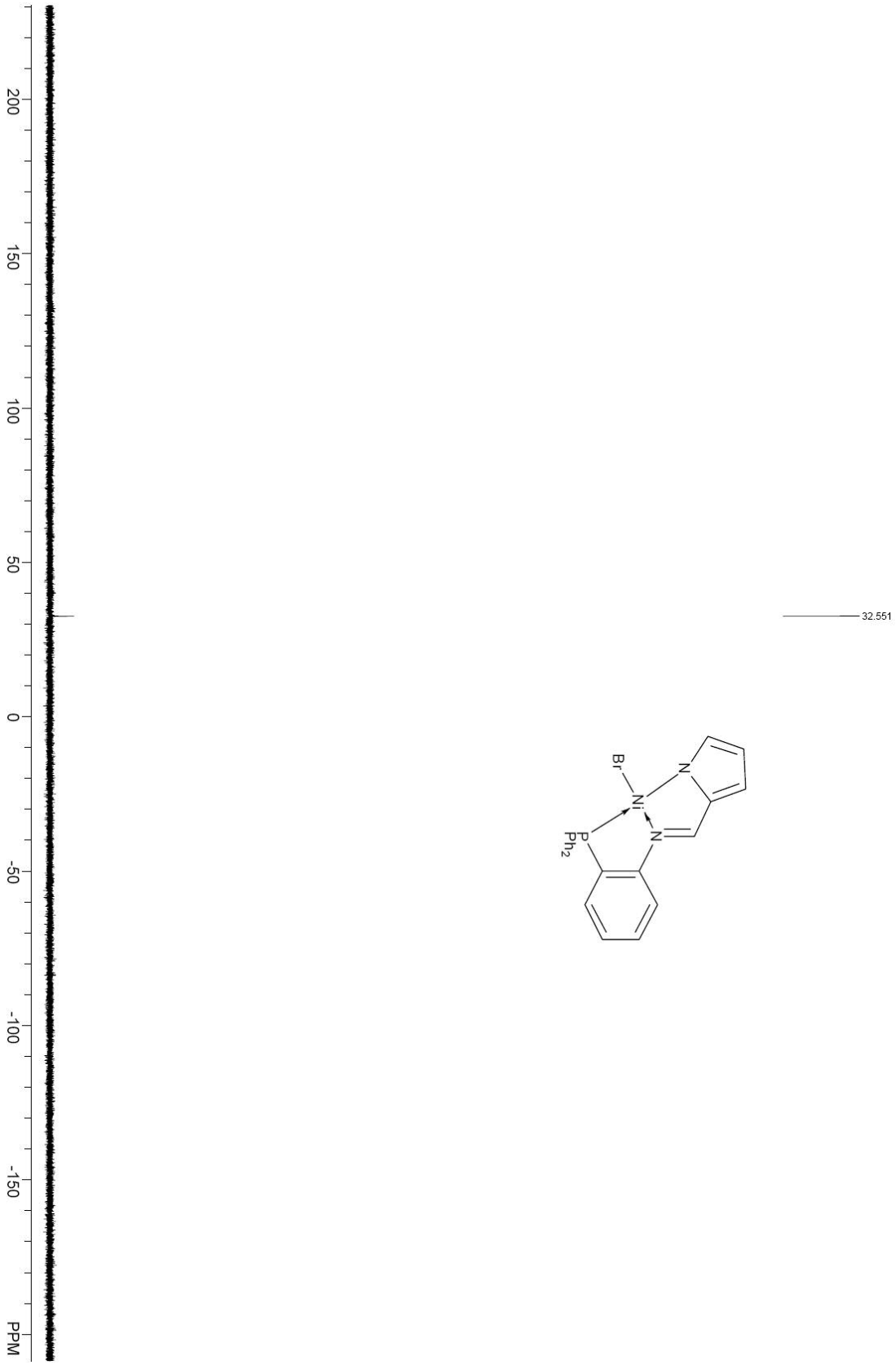
^{31}P NMR of the complex 1 (121 M, $CDCl_3$)



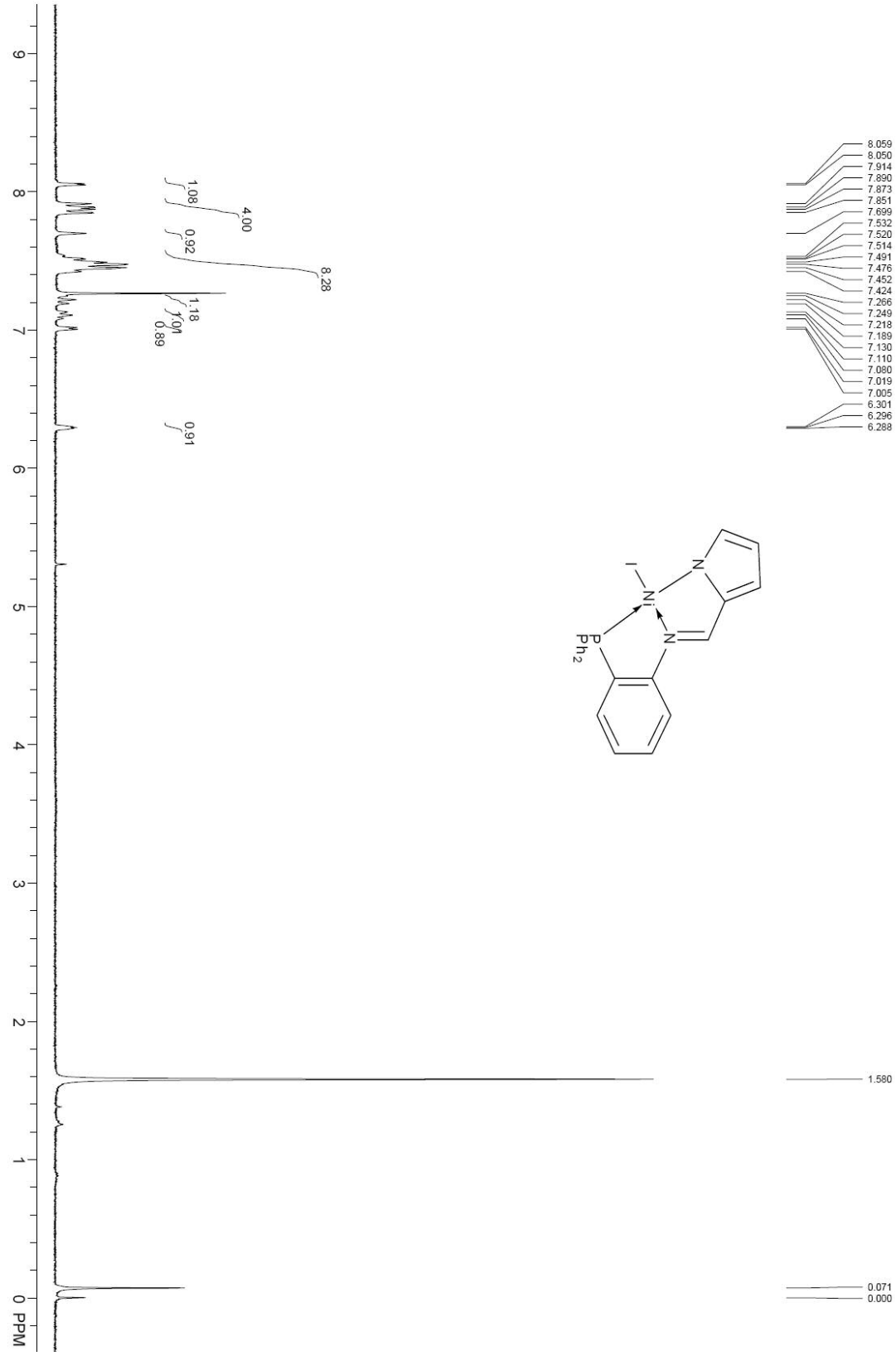
^{1}H NMR of the complex 2 (300 MHz, $CDCl_3$)



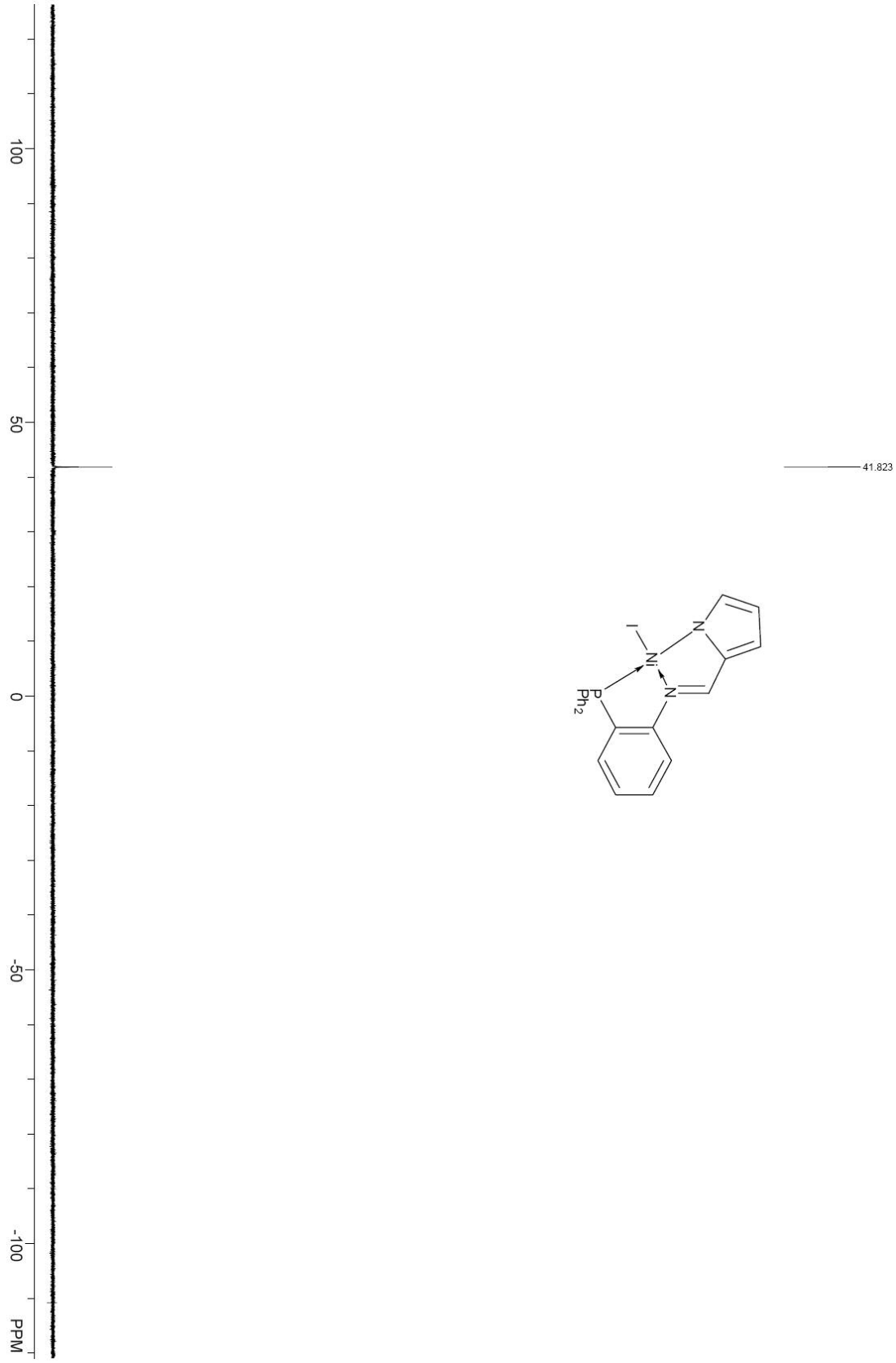
^{31}P NMR of the complex 2 (121 MHz, $CDCl_3$)



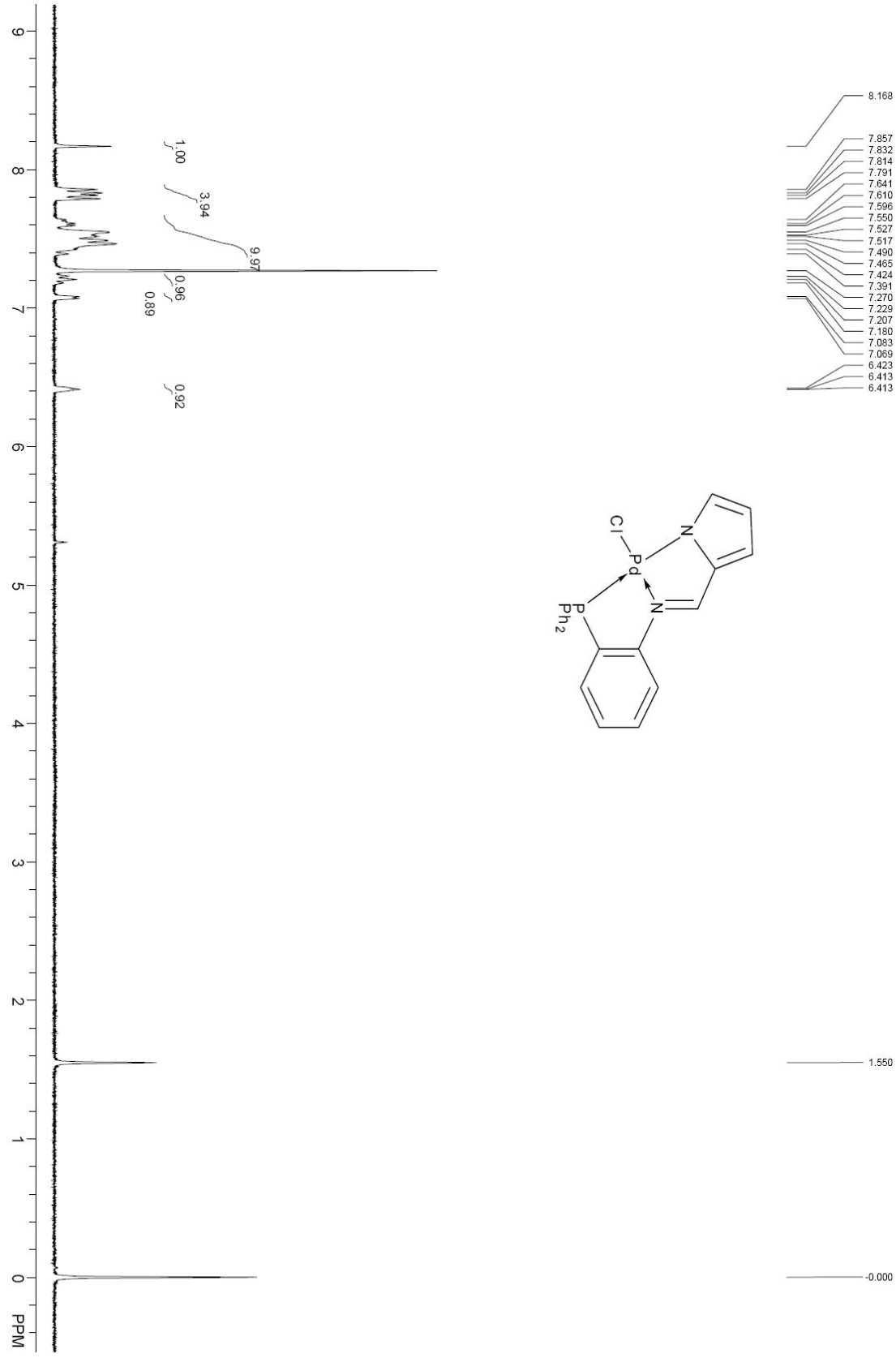
^{1}H NMR of the complex 3 (300 MHz, $CDCl_3$)



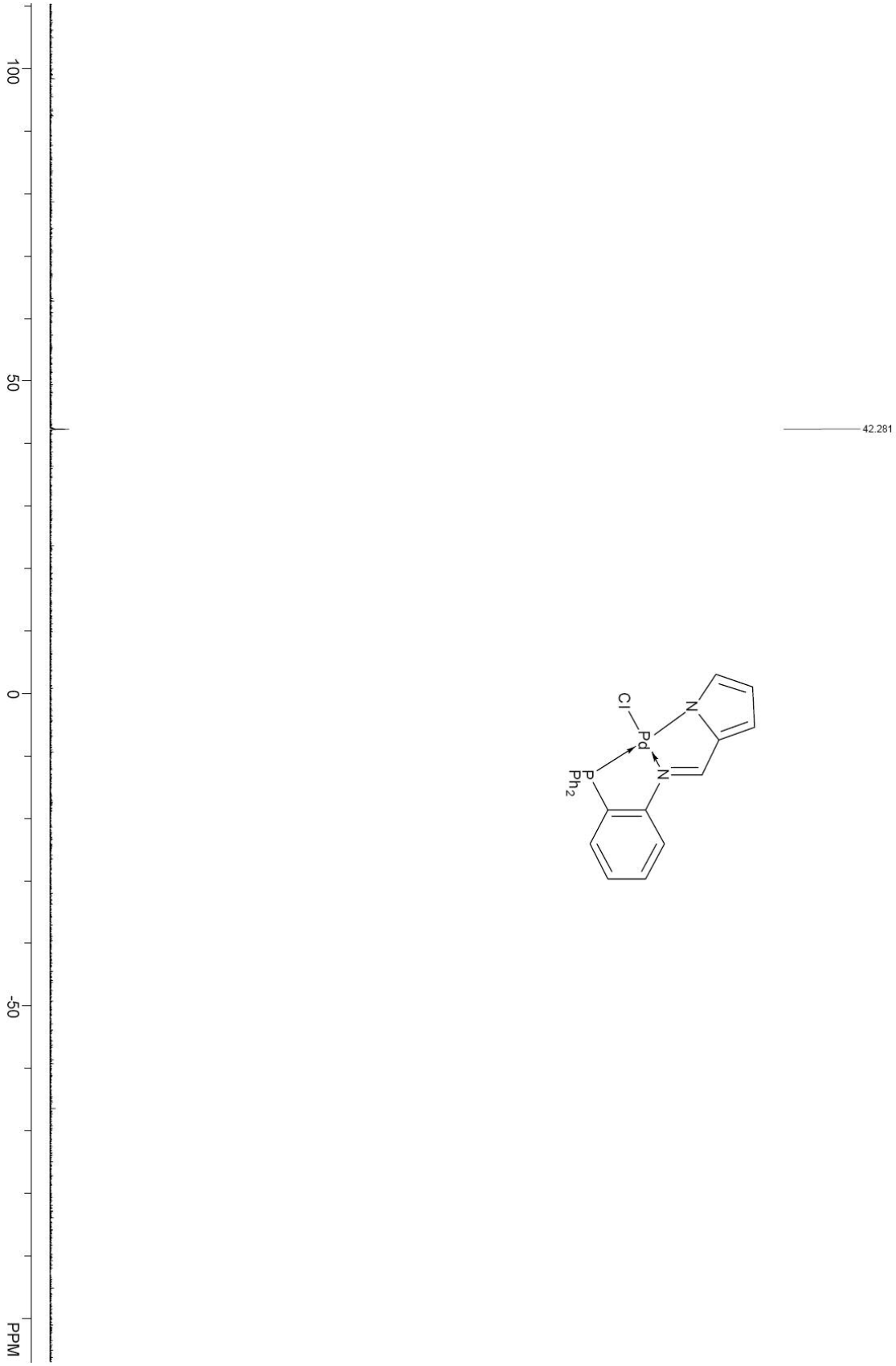
^{31}P NMR of the complex 3 (121 MHz, $CDCl_3$)



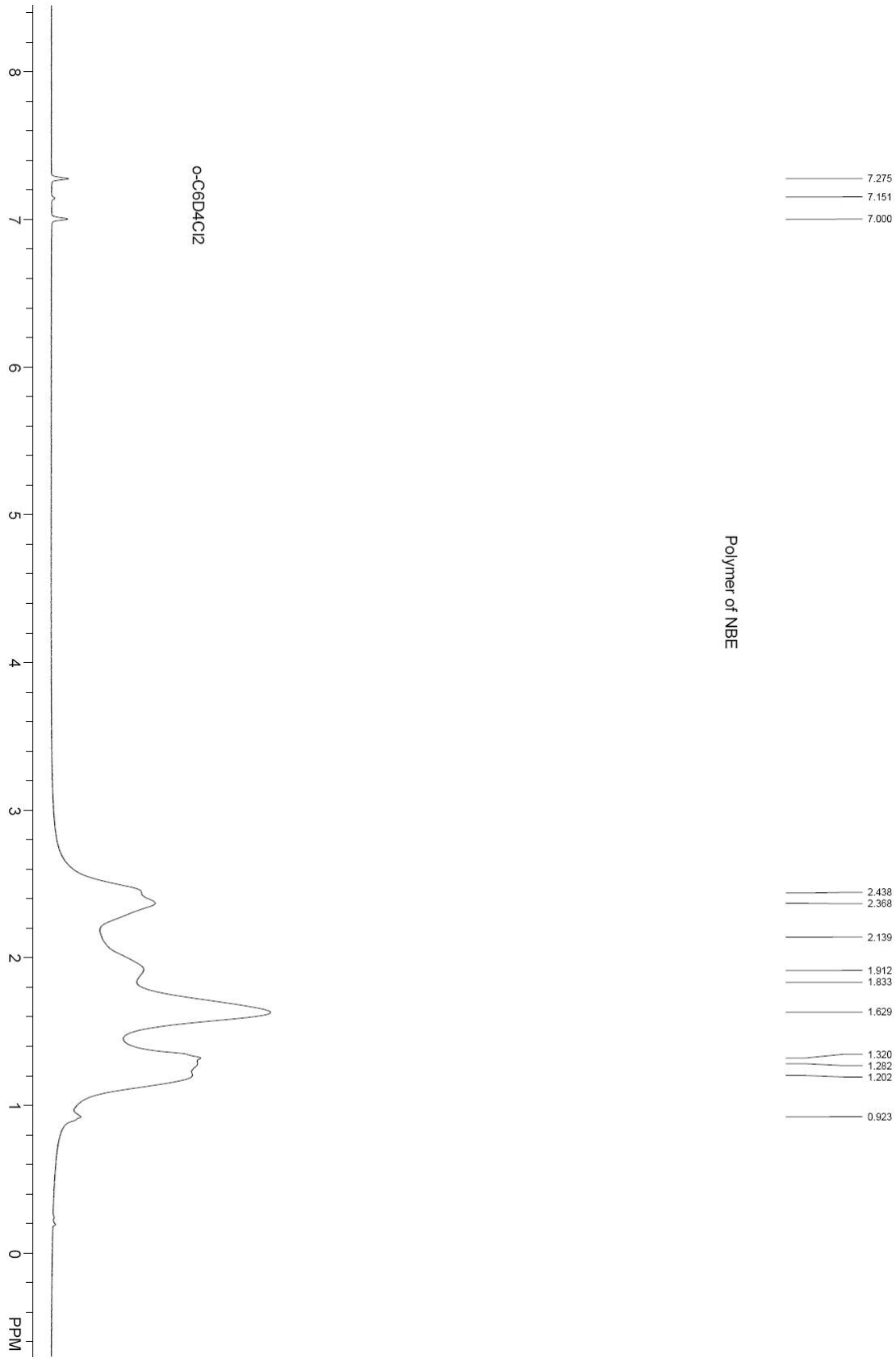
^{1}H NMR of the complex 4 (300 MHz, $CDCl_3$)



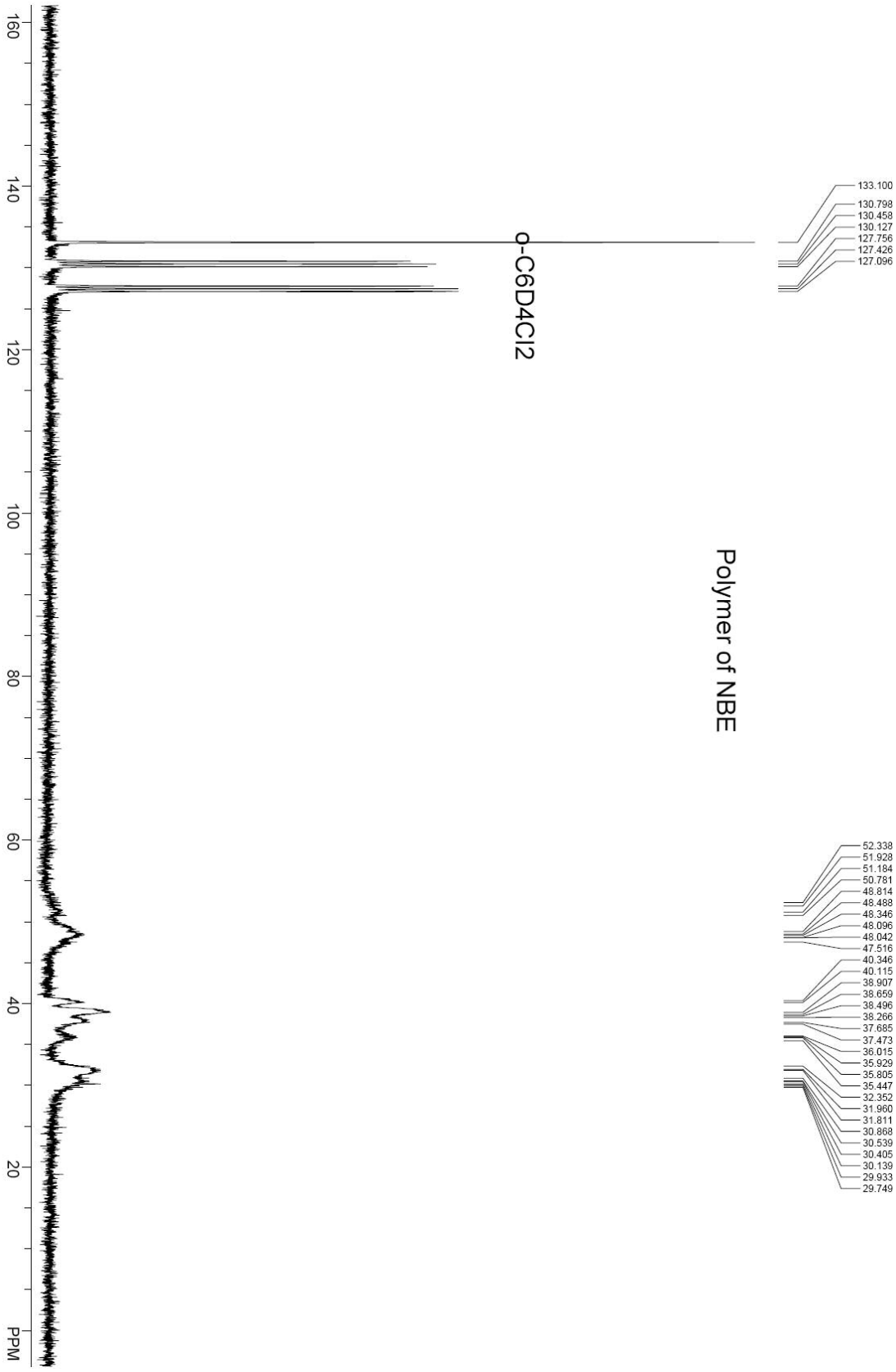
^{31}P NMR of the complex 4 (121 MHz, $CDCl_3$)



^{1}H NMR of the polymer (300 MHz, *o*-$C_6D_4Cl_2$, 110 ˚C)



^{13}C NMR of the polymer (75 MHz , *o*-$C_6D_4Cl_2$, 110 ˚C)



X-Ray of the complex 1 (cat. 1):

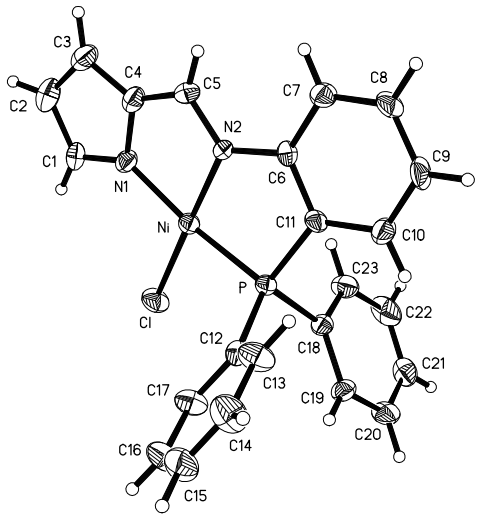


Table 1. Crystal data and structure refinement for cd22294.

Identification code	cd22294
Empirical formula	C23 H18 N2 Cl P Ni
Formula weight	447.52
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pna2(1)
Unit cell dimensions	a = 18.7870(18) A alpha = 90 deg. b = 8.8927(9) A beta = 90 deg. c = 11.8928(12) A gamma = 90 deg.
Volume	1986.9(3) A^3
Z, Calculated density	4, 1.496 Mg/m^3
Absorption coefficient	1.202 mm^-1
F(000)	920
Crystal size	0.358 x 0.229 x 0.035 mm
Theta range for data collection	2.17 to 28.26 deg.
Limiting indices	-24<=h<=24, -9<=k<=11, -14<=l<=15
Reflections collected / unique	11598 / 4420 [R(int) = 0.0931]
Completeness to theta = 25.49	99.9 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.69291
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4420 / 1 / 253
Goodness-of-fit on F^2	0.899
Final R indices [I>2sigma(I)]	R1 = 0.0507, wR2 = 0.0740
R indices (all data)	R1 = 0.1100, wR2 = 0.0826
Absolute structure parameter	0.02(2)
Largest diff. peak and hole	0.371 and -0.292 e.A^-3

X-Ray of the complex 2 (cat. 2):

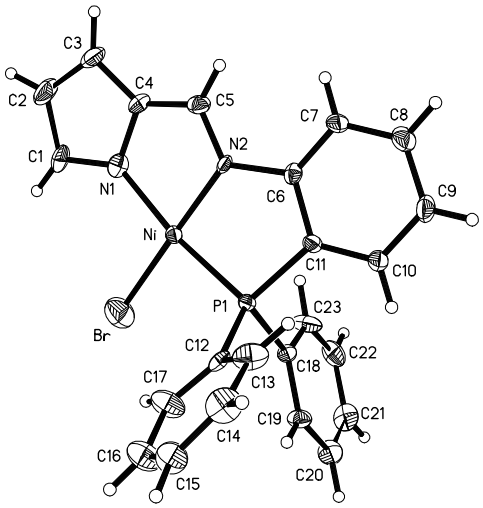


Table 1. Crystal data and structure refinement for cd2728.

Identification code	cd2728
Empirical formula	C23 H18 Br N2 Ni P
Formula weight	491.98
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pna2(1)
Unit cell dimensions	a = 18.8941(17) A alpha = 90 deg.
	b = 8.8776(8) A beta = 90 deg.
	c = 11.9195(11) A gamma = 90 deg.
Volume	1999.3(3) A^3
Z, Calculated density	4, 1.634 Mg/m^3
Absorption coefficient	3.060 mm^-1
F(000)	992
Crystal size	0.316 x 0.127 x 0.065 mm
Theta range for data collection	2.16 to 25.99 deg
Limiting indices	-23<=h<=22, -7<=k<=10, -14<=l<=14
Reflections collected / unique	10491 / 3843 [R(int) = 0.0824]
Completeness to theta = 25.99	99.9 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.77672
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3843 / 1 / 254
Goodness-of-fit on F^2	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0777, wR2 = 0.2321
R indices (all data)	R1 = 0.0886, wR2 = 0.2415
Absolute structure parameter	0.00(5)
Largest diff. peak and hole	1.814 and -1.914 e.A^-3

X-Ray of the complex 4 (cat. 4):

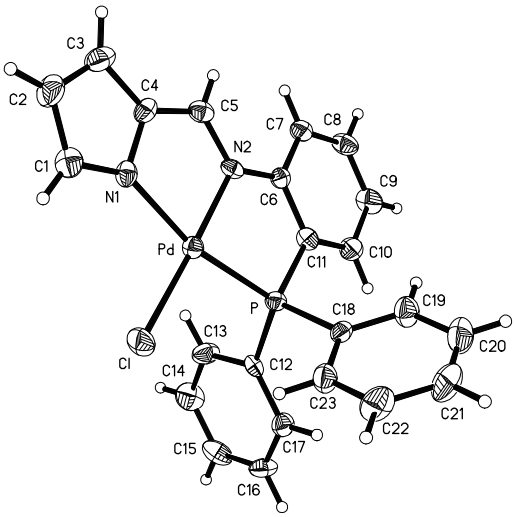


Table 1. Crystal data and structure refinement for cd22321.

Identification code	cd22321
Empirical formula	C23 H18 N2 P Cl Pd
Formula weight	495.21
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pna2(1)
Unit cell dimensions	a = 18.8885(13) A alpha = 90 deg. b = 8.9493(7) A beta = 90 deg. c = 11.9998(9) A gamma = 90 deg.
Volume	2028.4(3) A^3
Z, Calculated density	4, 1.622 Mg/m^3
Absorption coefficient	1.136 mm^-1
F(000)	992
Crystal size	0.255 x 0.196 x 0.193 mm
Theta range for data collection	2.16 to 28.28 deg.
Limiting indices	-24<=h<=25, -11<=k<=11, -8<=l<=16
Reflections collected / unique	11928 / 3614 [R(int) = 0.0611]
Completeness to theta = 28.28	96.6 %
Absorption correction	Sadabs
Max. and min. transmission	1.00000 and 0.81868
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3614 / 1 / 257
Goodness-of-fit on F^2	0.773
Final R indices [I>2sigma(I)]	R1 = 0.0362, wR2 = 0.0496
R indices (all data)	R1 = 0.0555, wR2 = 0.0527
Absolute structure parameter	0.01(3)
Largest diff. peak and hole	1.079 and -0.498 e.A^-3