Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Synthesis and Characterization of Group 13 Dichloride (M = Ga, In), Dimethyl (M = Al) and Cationic Methyl Aluminum Complexes Supported by Monoanionic *NNN*-Pincer Ligands

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Table of Contents

I. NMR Spectra

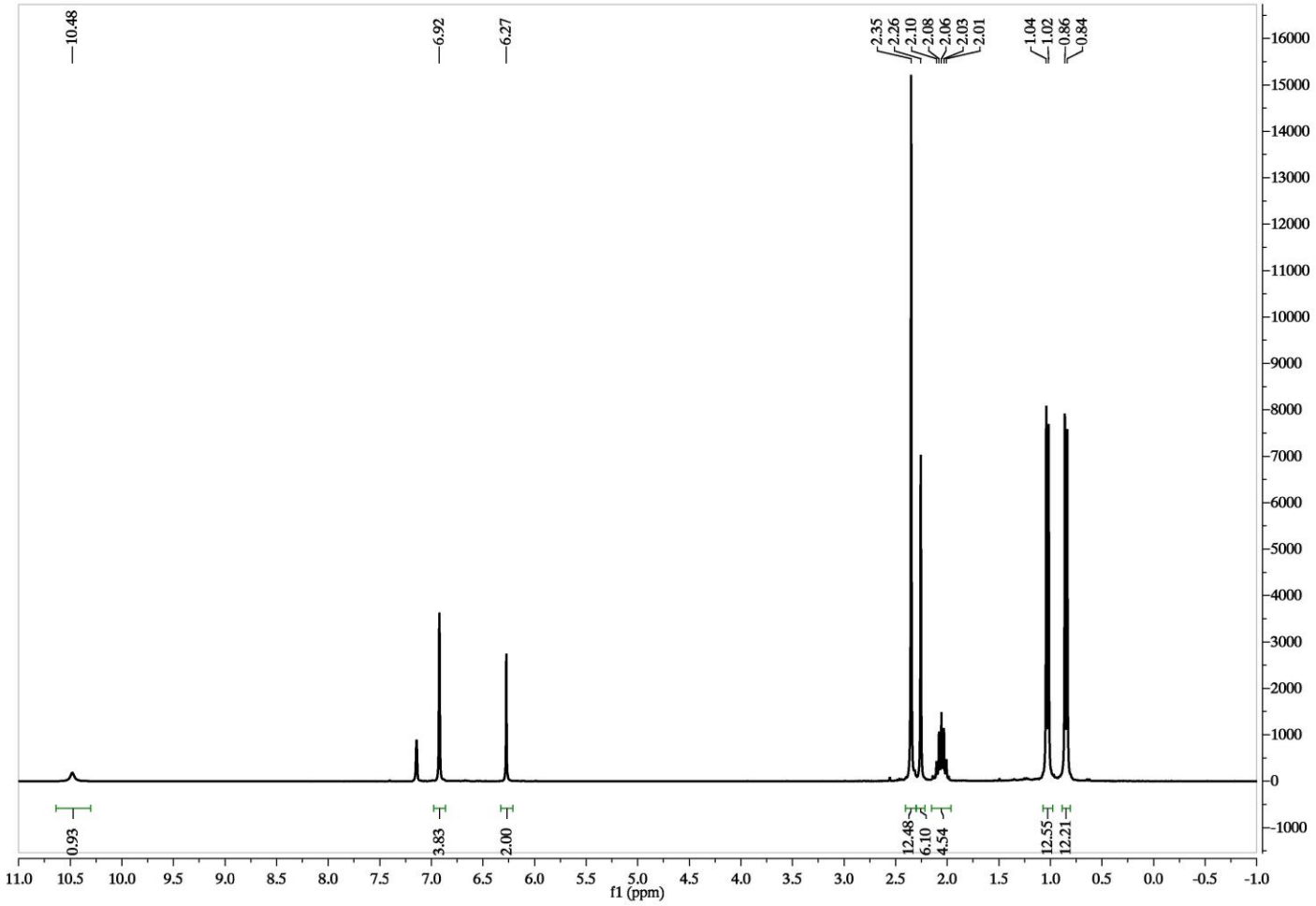

Figure S1. ^{1}H NMR spectrum of $\mathbf{L^{Mes}}$ in d_6-benzene.

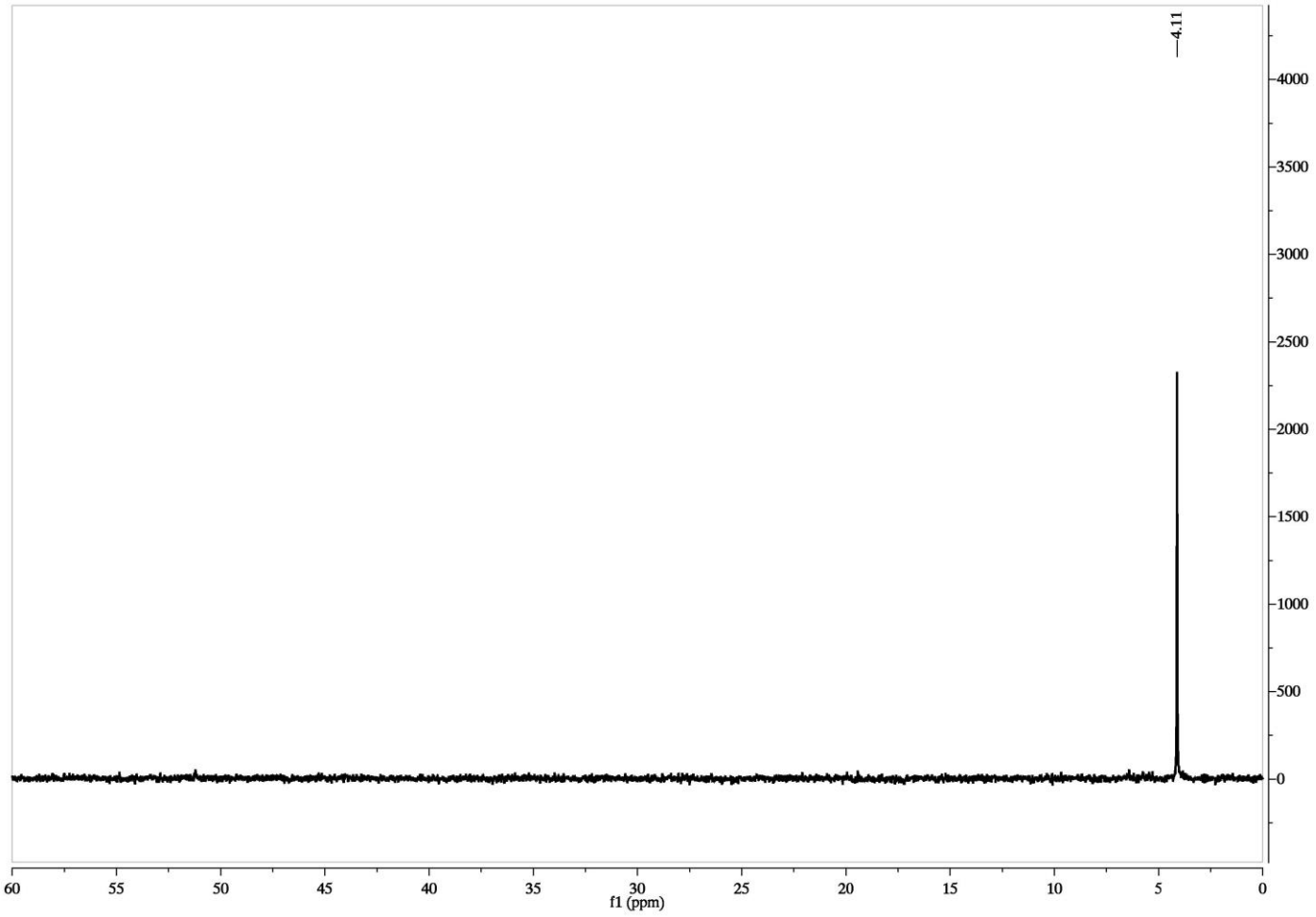

Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum of **L^{Mes}** in d_6-benzene.

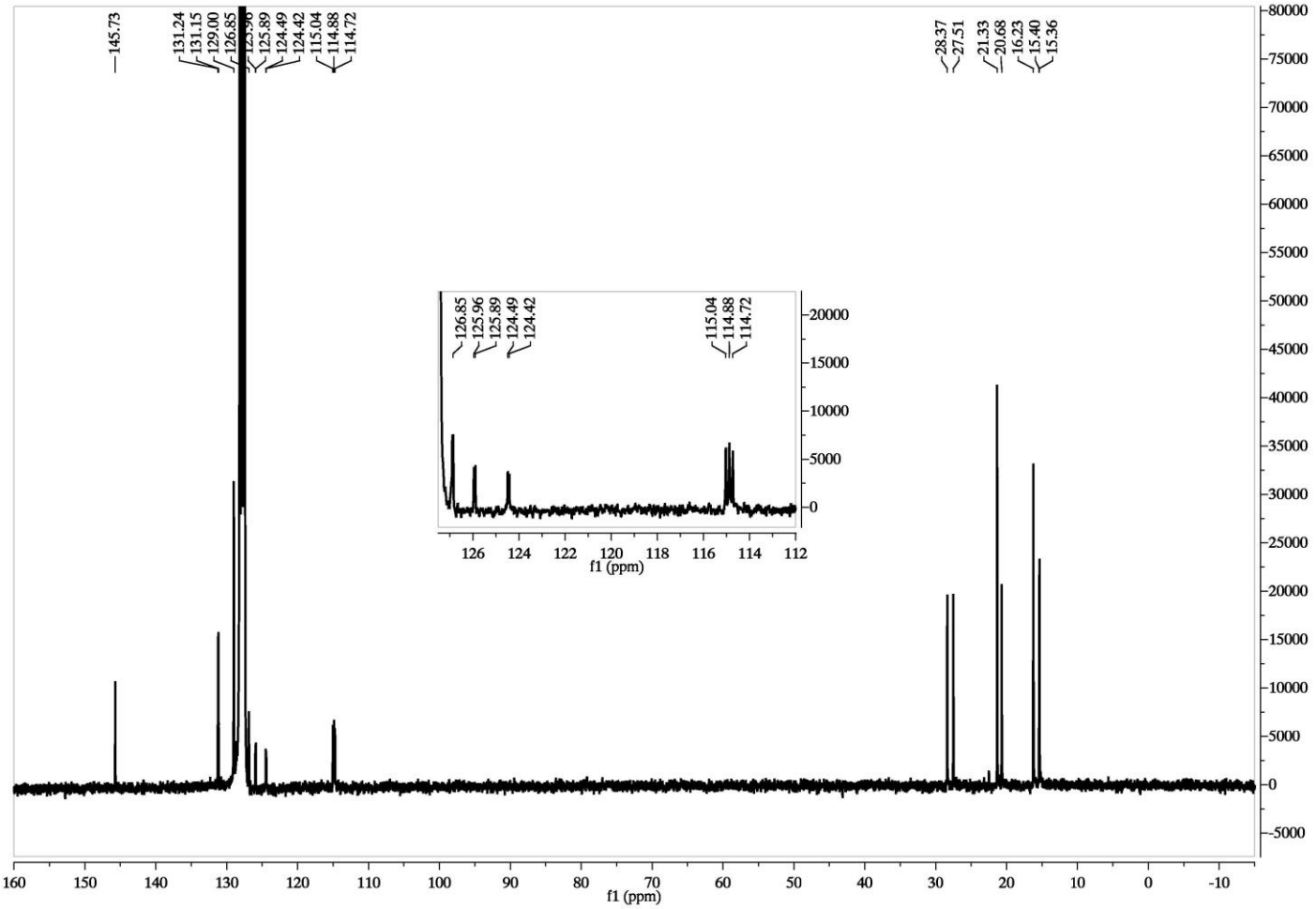

Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{L^{Mes}}$ in d_6-benzene.

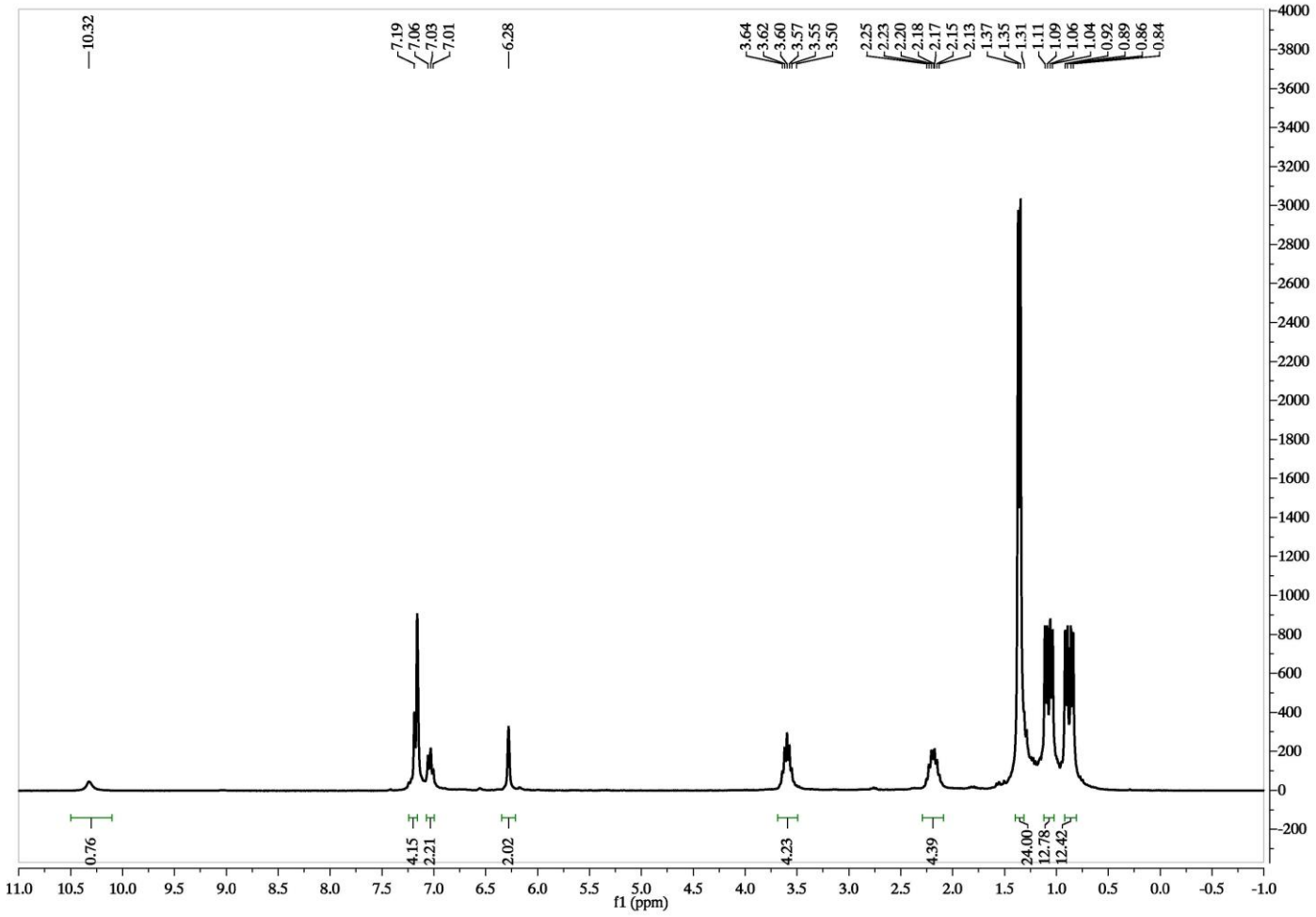

Figure S4. ^{1}H NMR spectrum of **L^{Dipp}** in d_6-benzene.

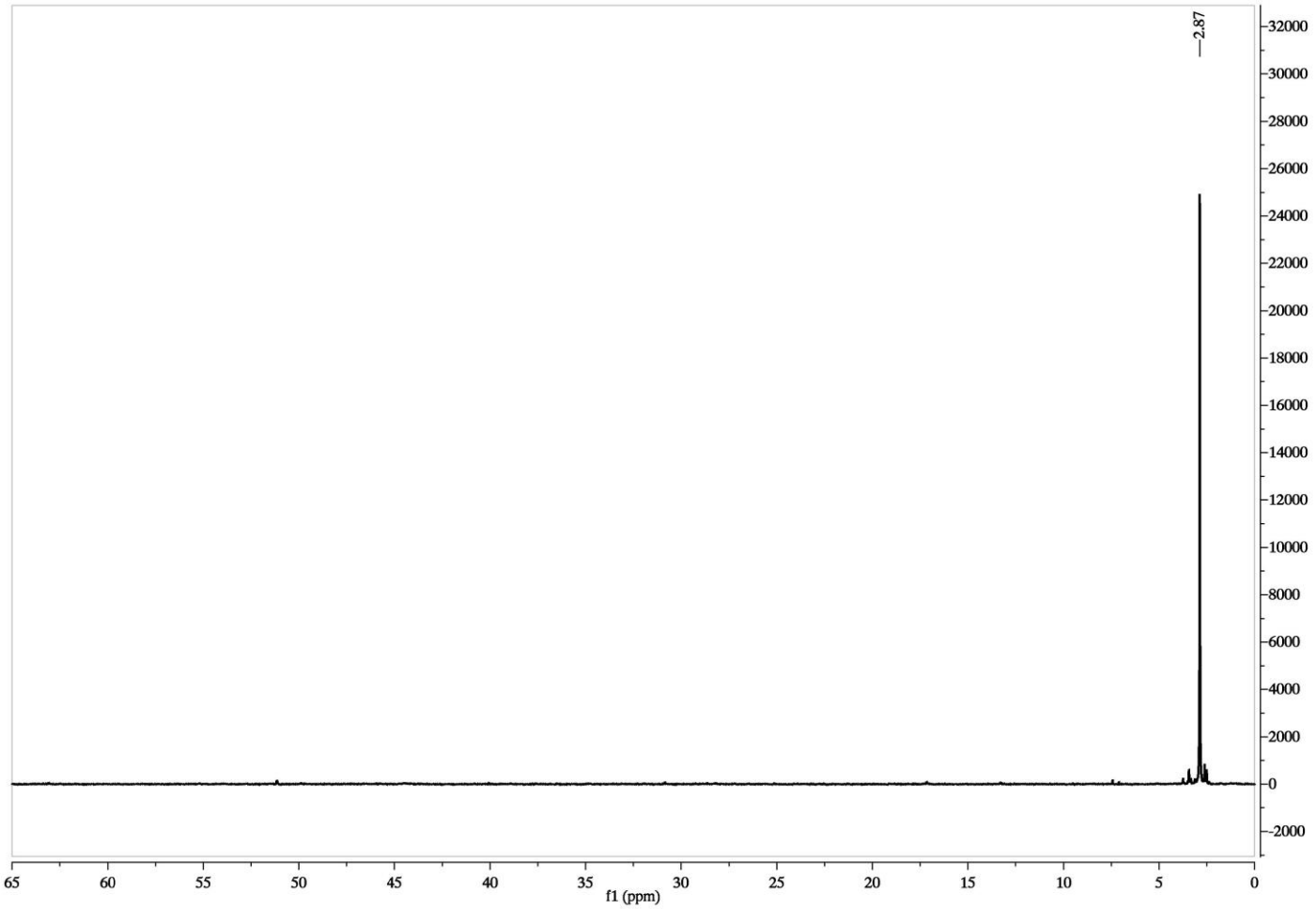

Figure S5. $^{31}P\{^{1}H\}$ NMR spectrum of $\mathbf{L^{Dipp}}$ in d_6-benzene

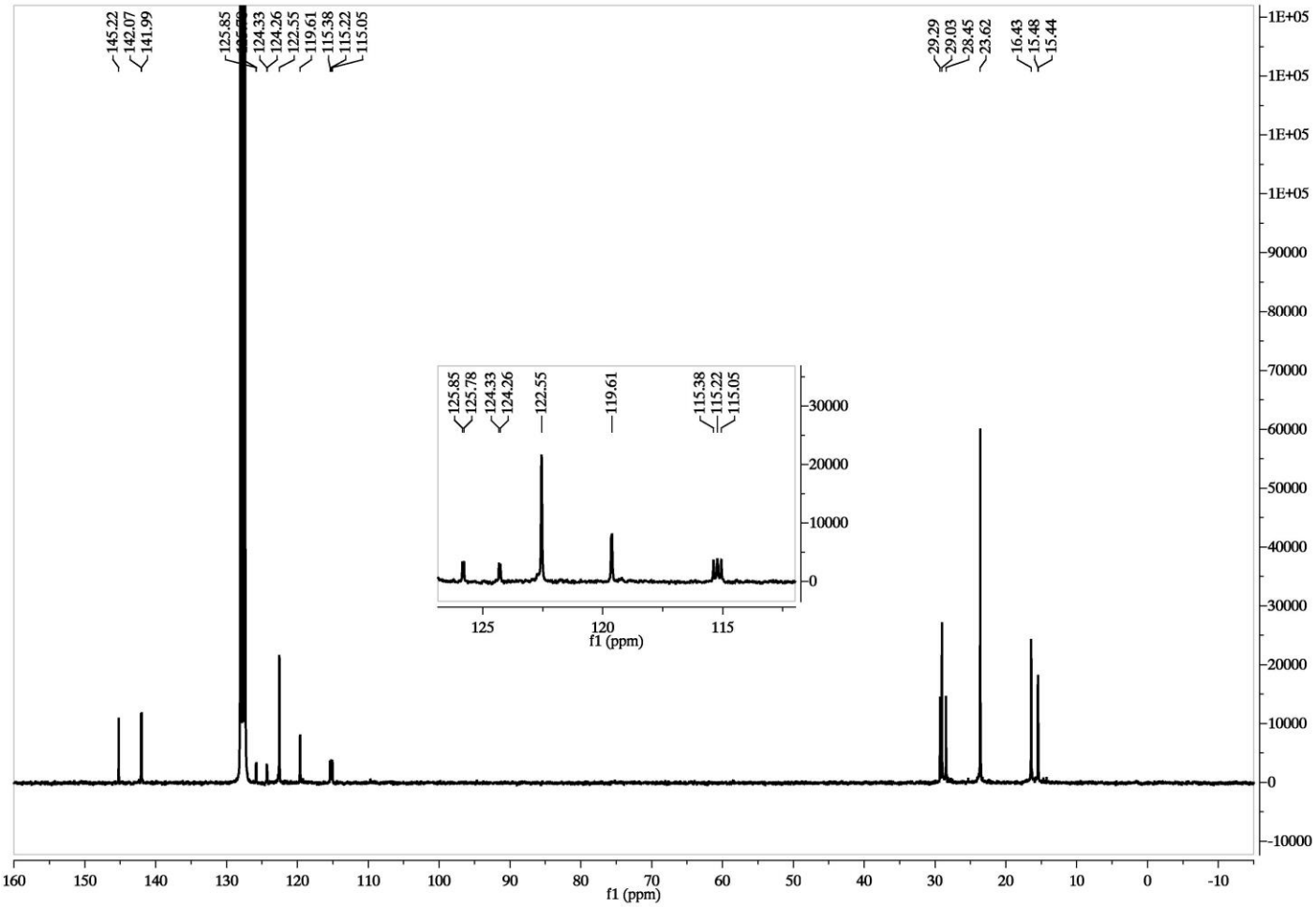

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{L^{Dipp}}$ in d_6-benzene.

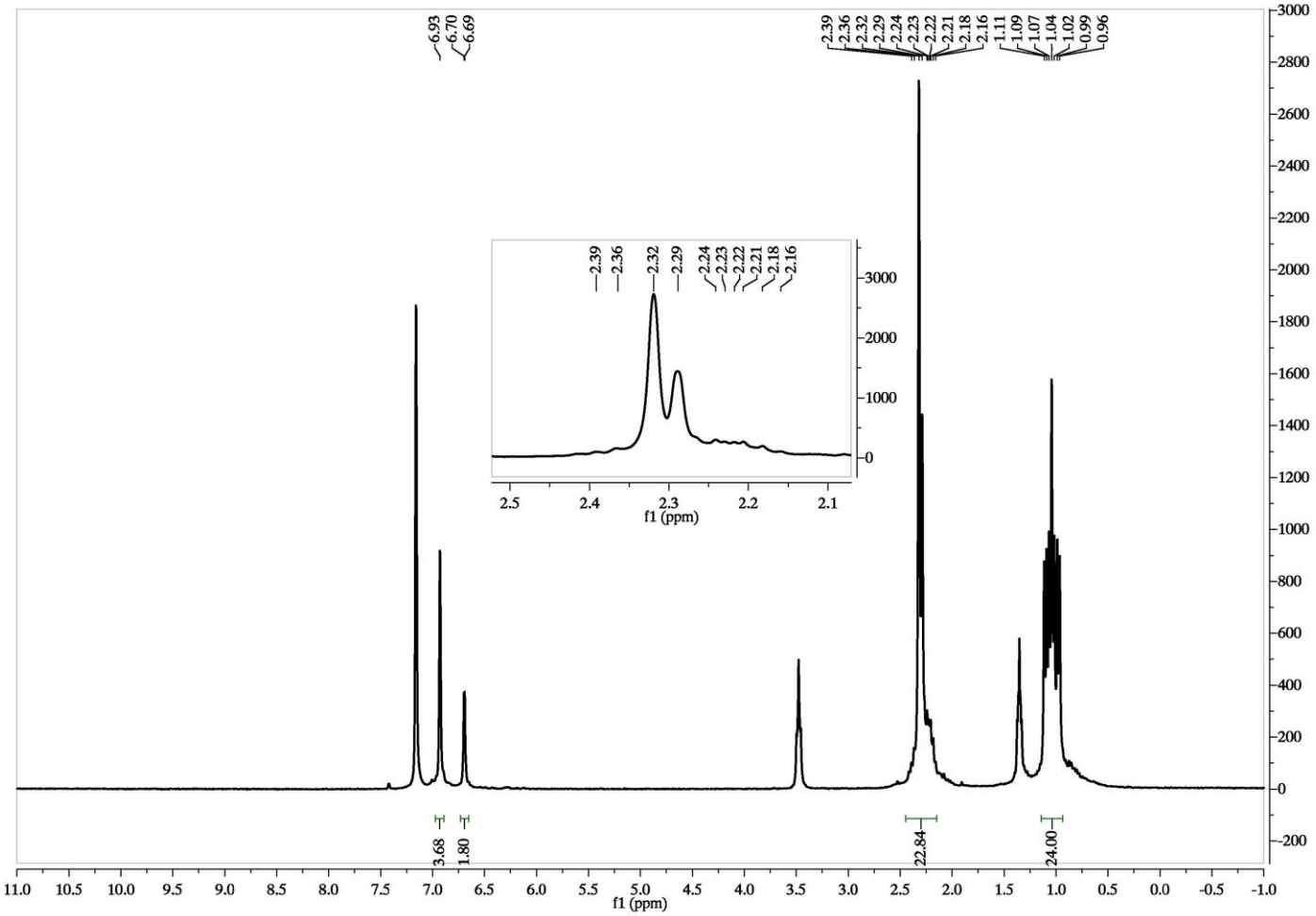

Figure S7. ^{1}H NMR spectrum of Na**L**$^{\mathbf{Mes}}$ in d_6-benzene. THF is present as a minor impurity.

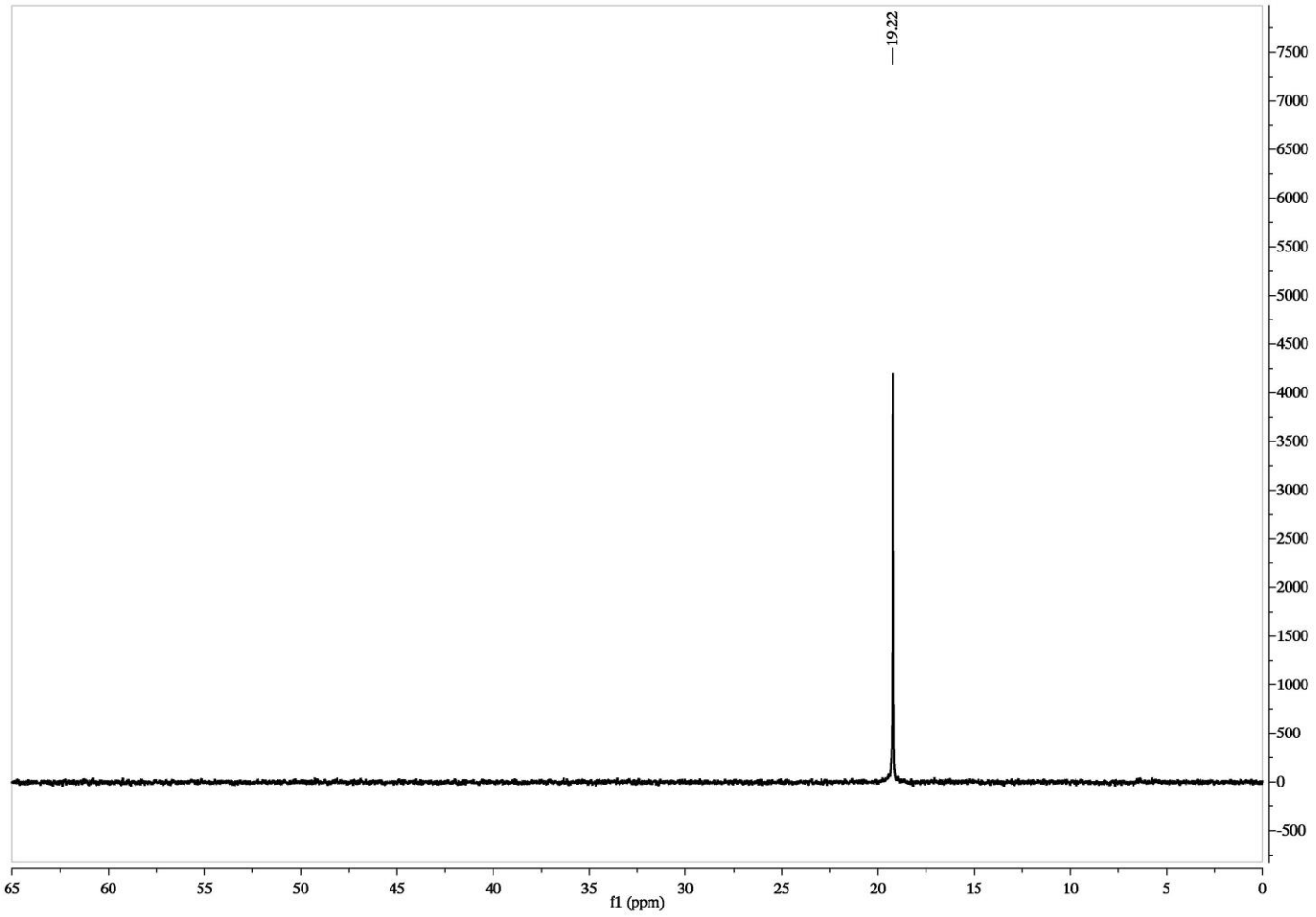

Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum of Na**L**$^{\mathbf{Mes}}$ in d_6-benzene.

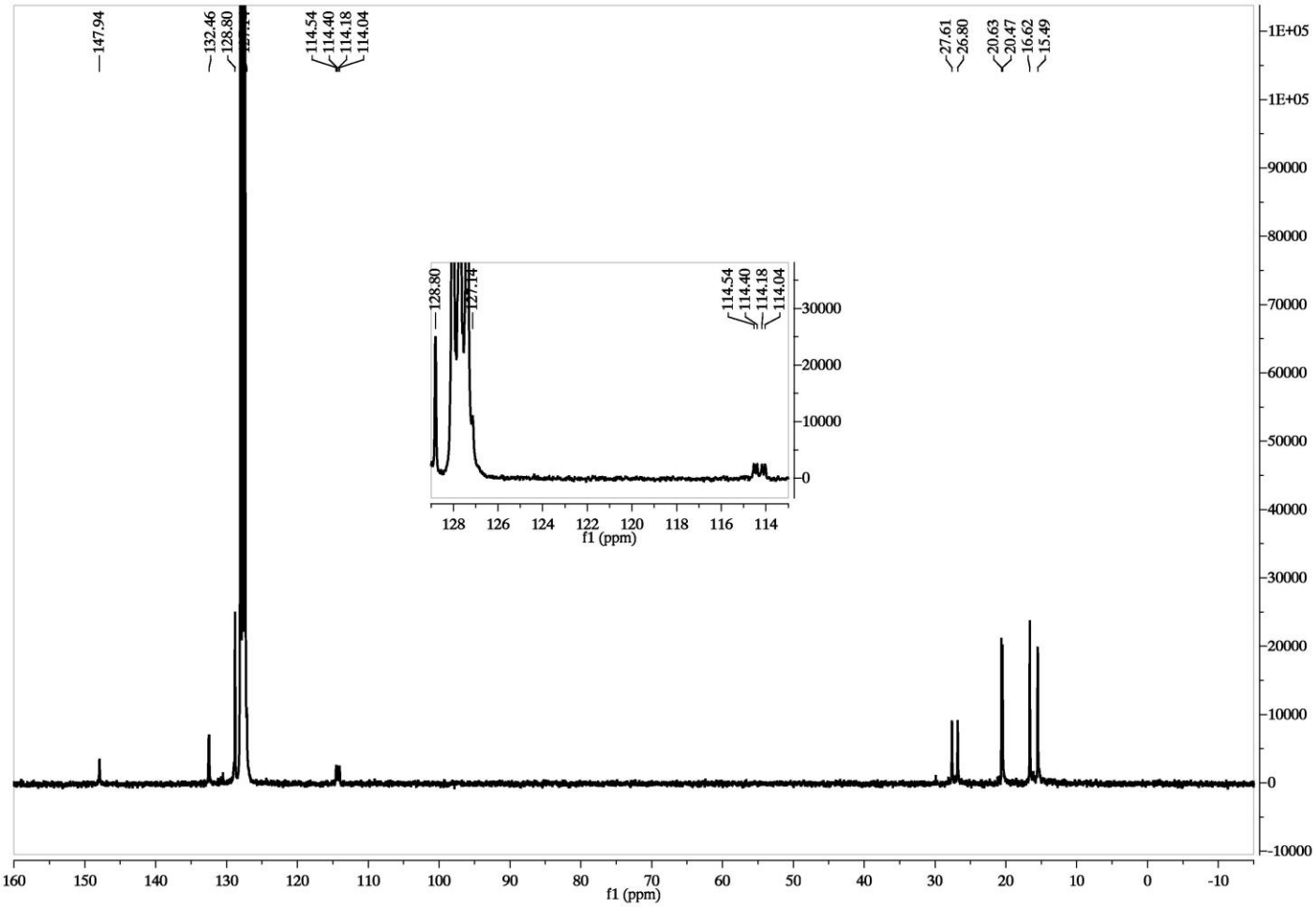

Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of Na**L**^{Mes} in d_6-benzene.

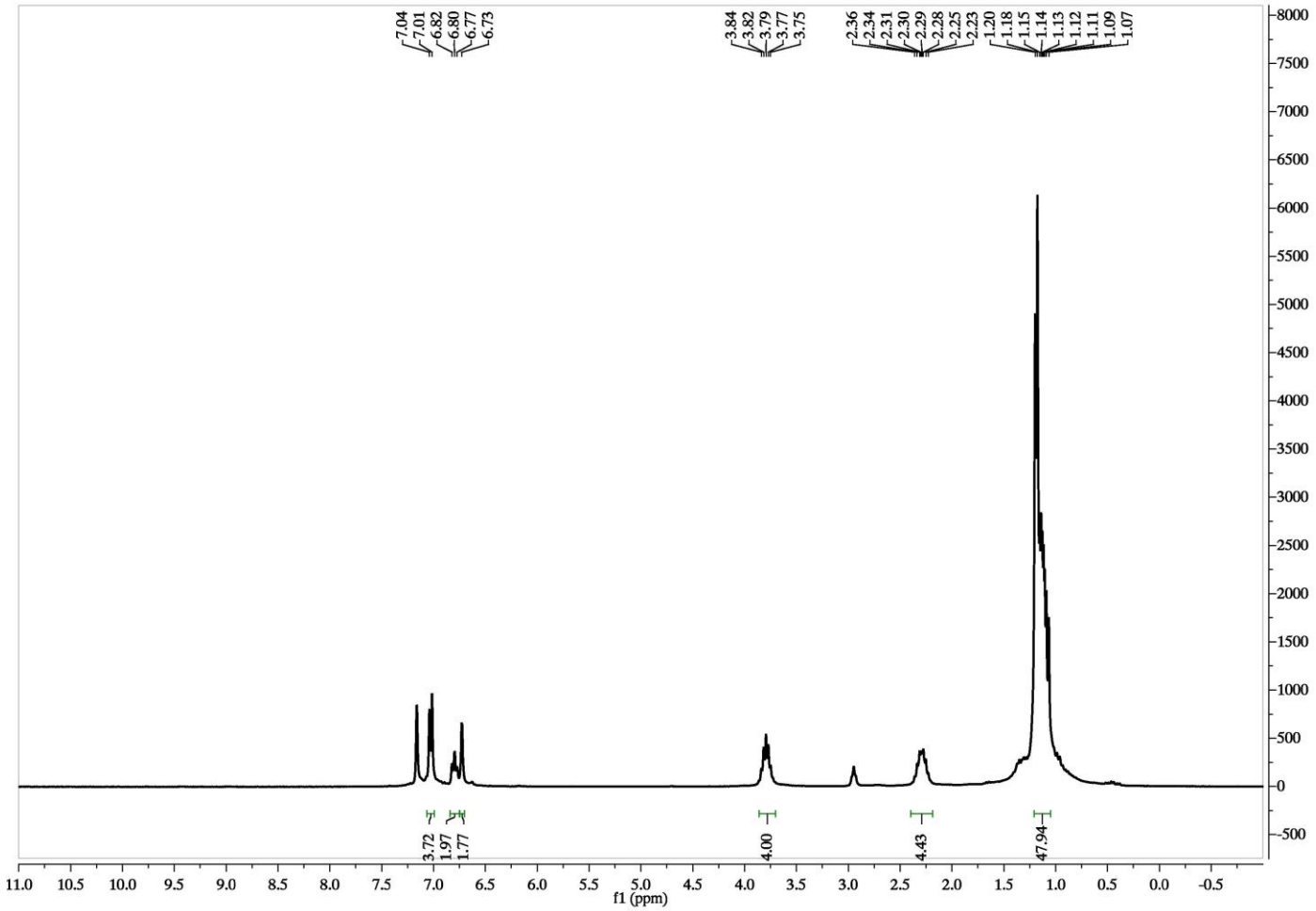

Figure S10. ^{1}H NMR spectrum of Na**L**$^{\mathbf{Dipp}}$ in d_6-benzene. THF is present as a minor impurity.

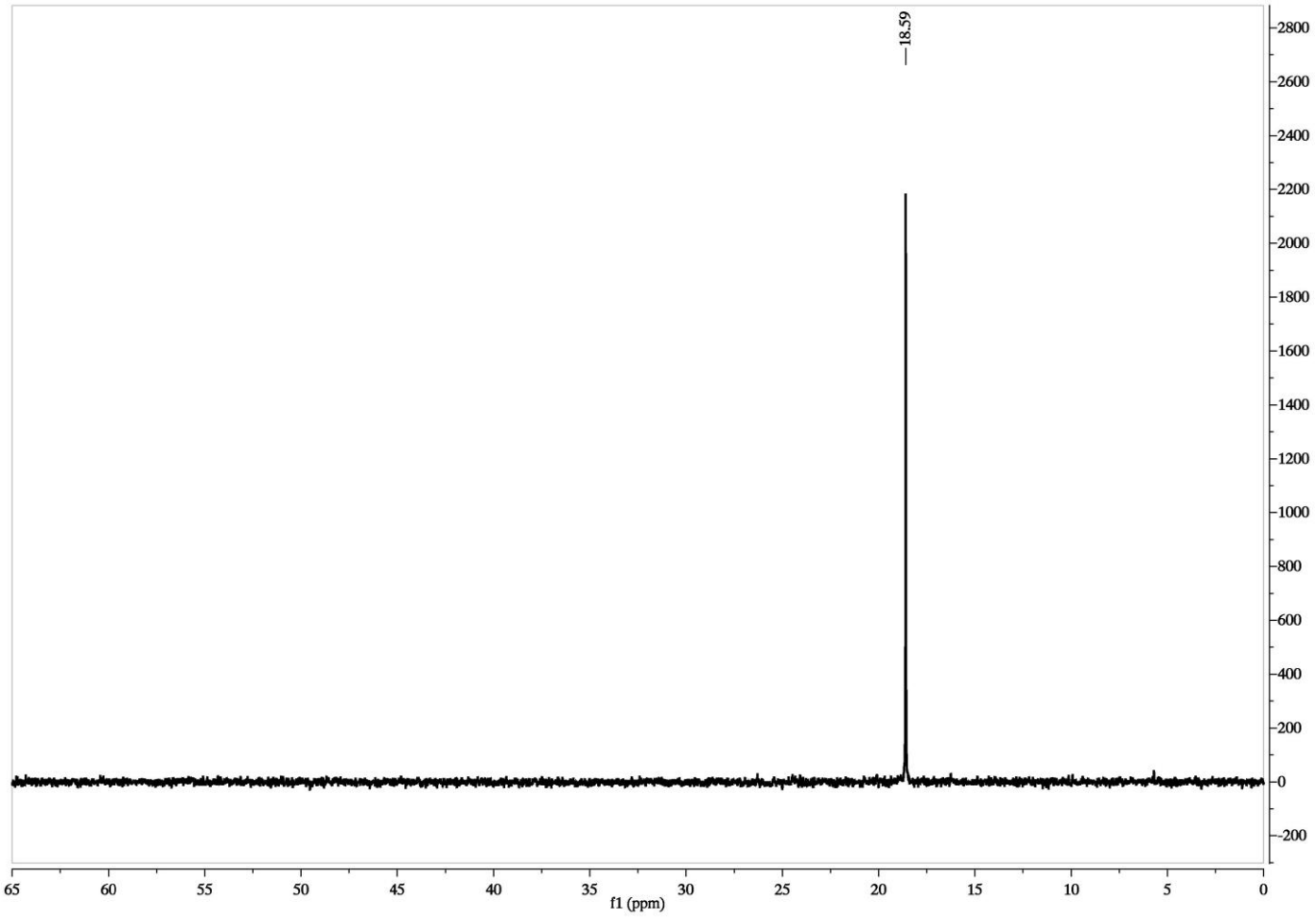

Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of Na**L**$^{\mathbf{Dipp}}$ in d_6-benzene.

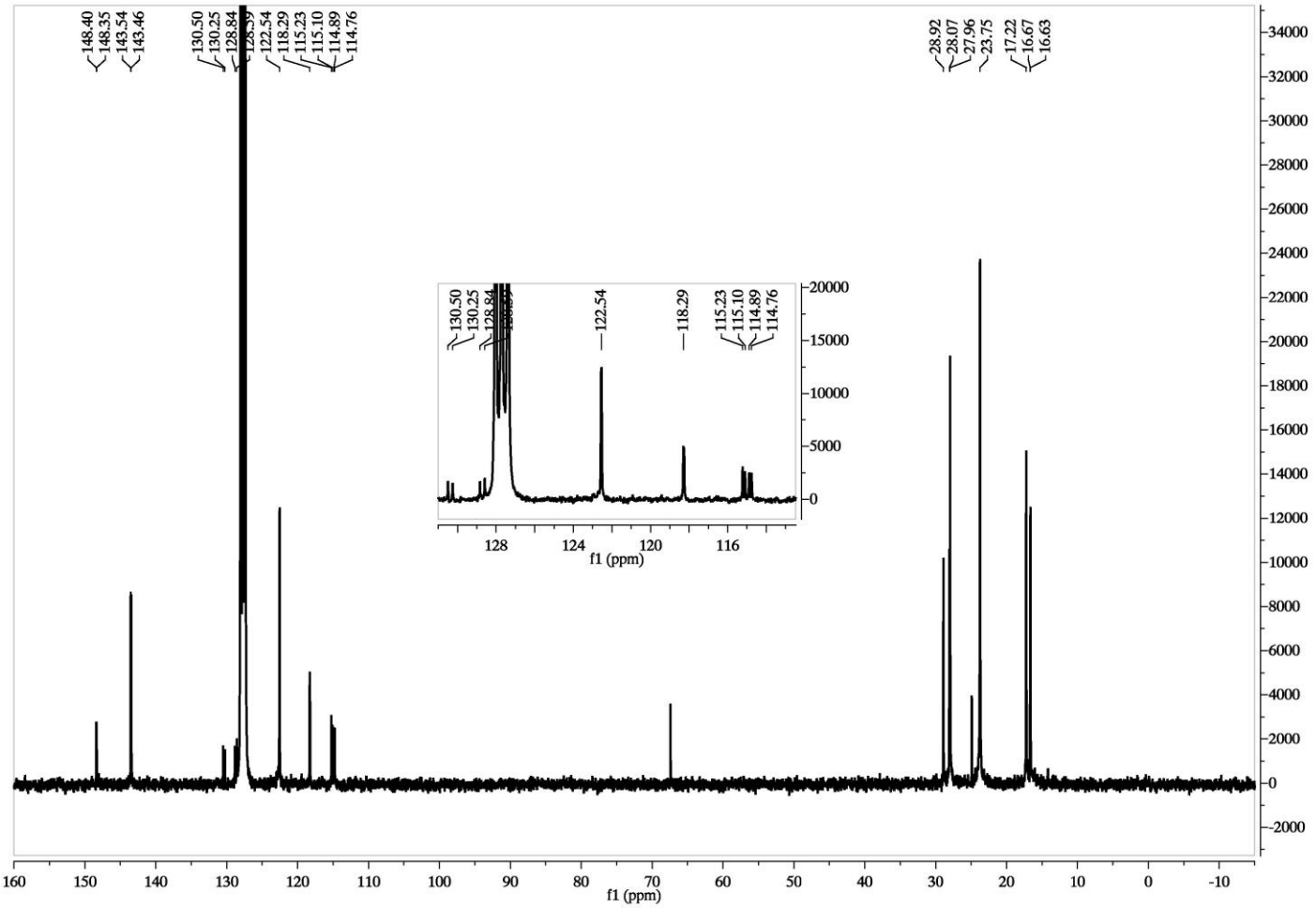

Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of Na**L**$^{\mathbf{Dipp}}$ in d_6-benzene. THF is present as a minor impurity.

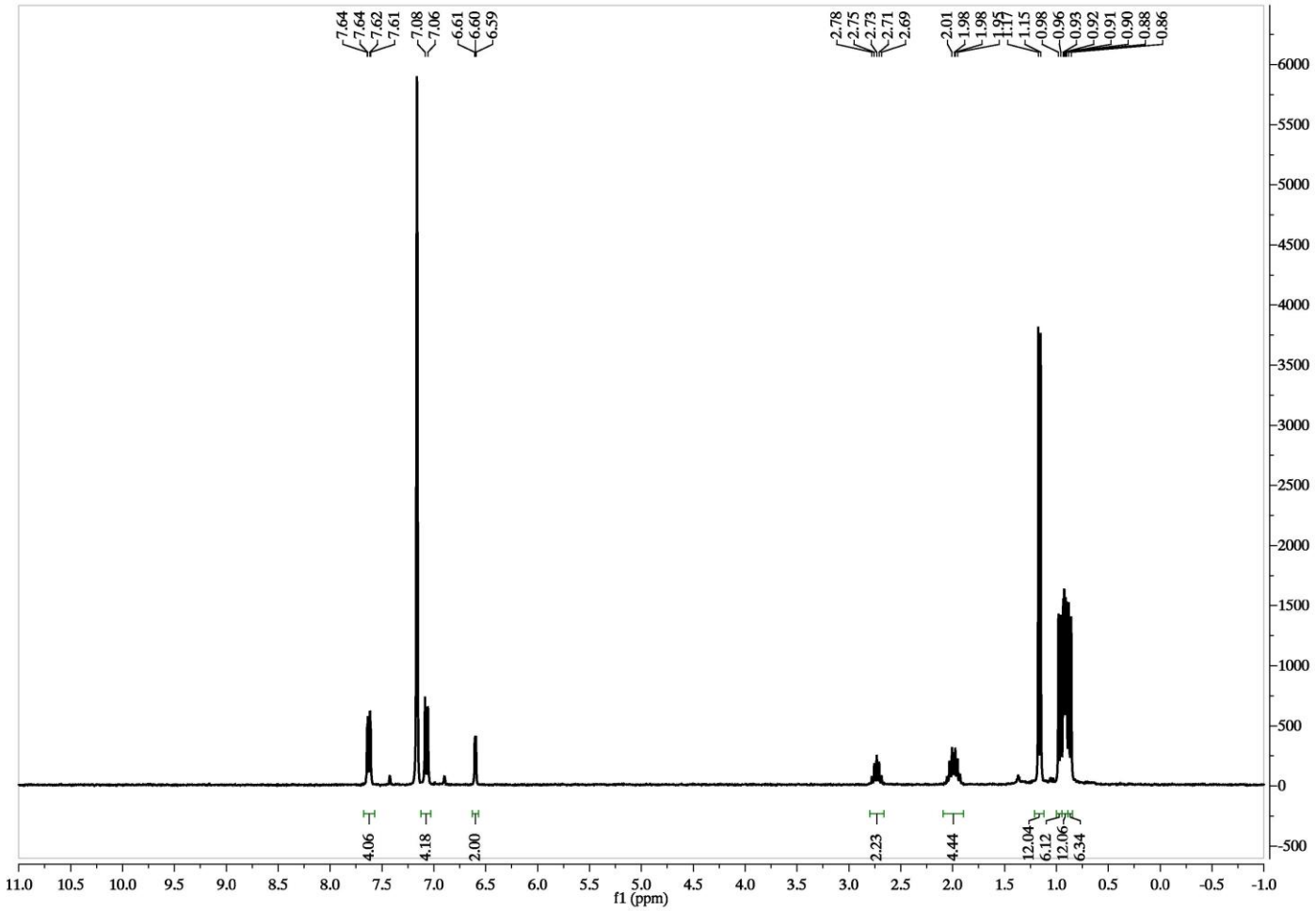

Figure S13. ^{1}H NMR spectrum of **1^{Pipp}** in d_6-benzene.

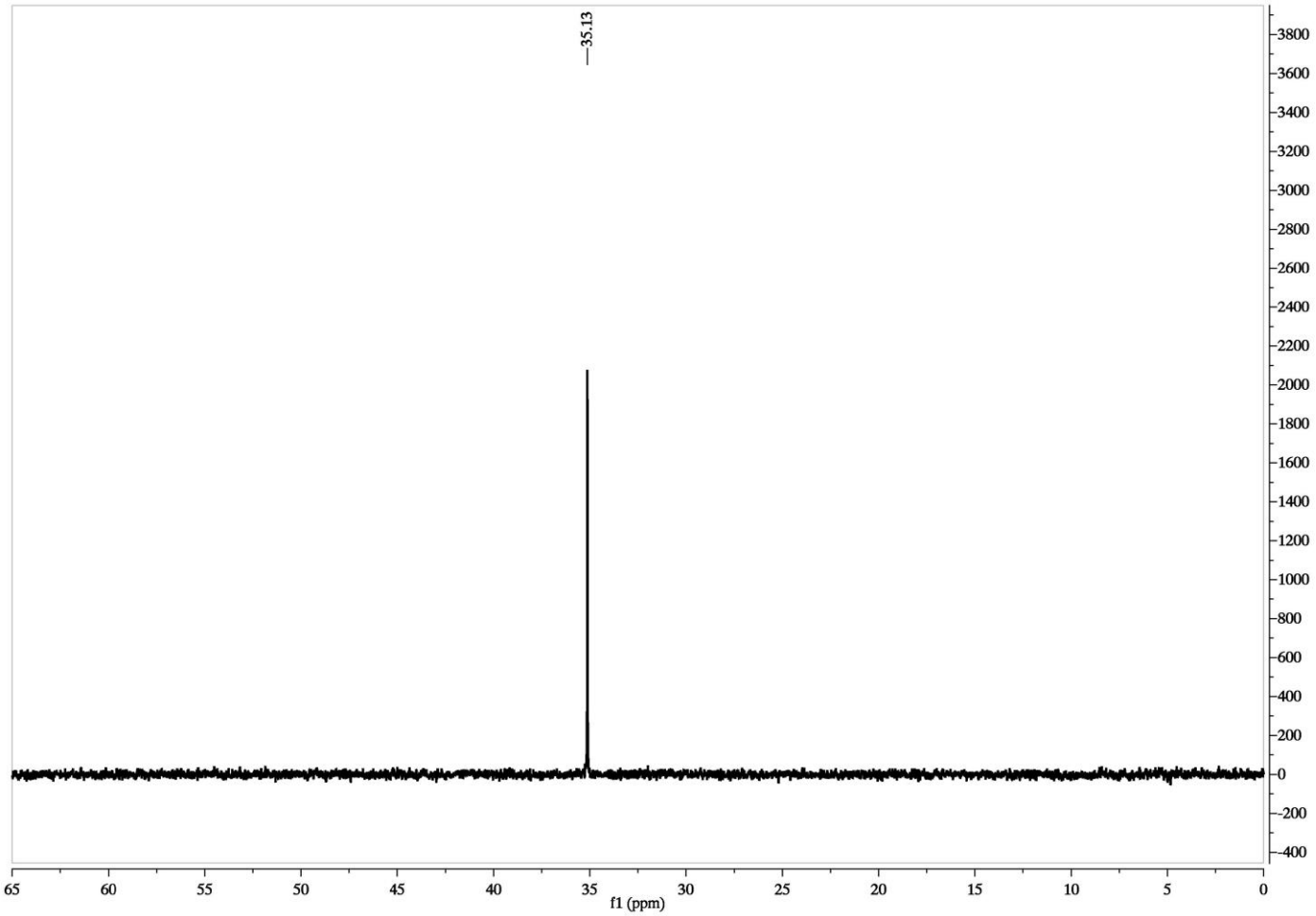

Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum of **1^{Pipp}** in d_6-benzene.

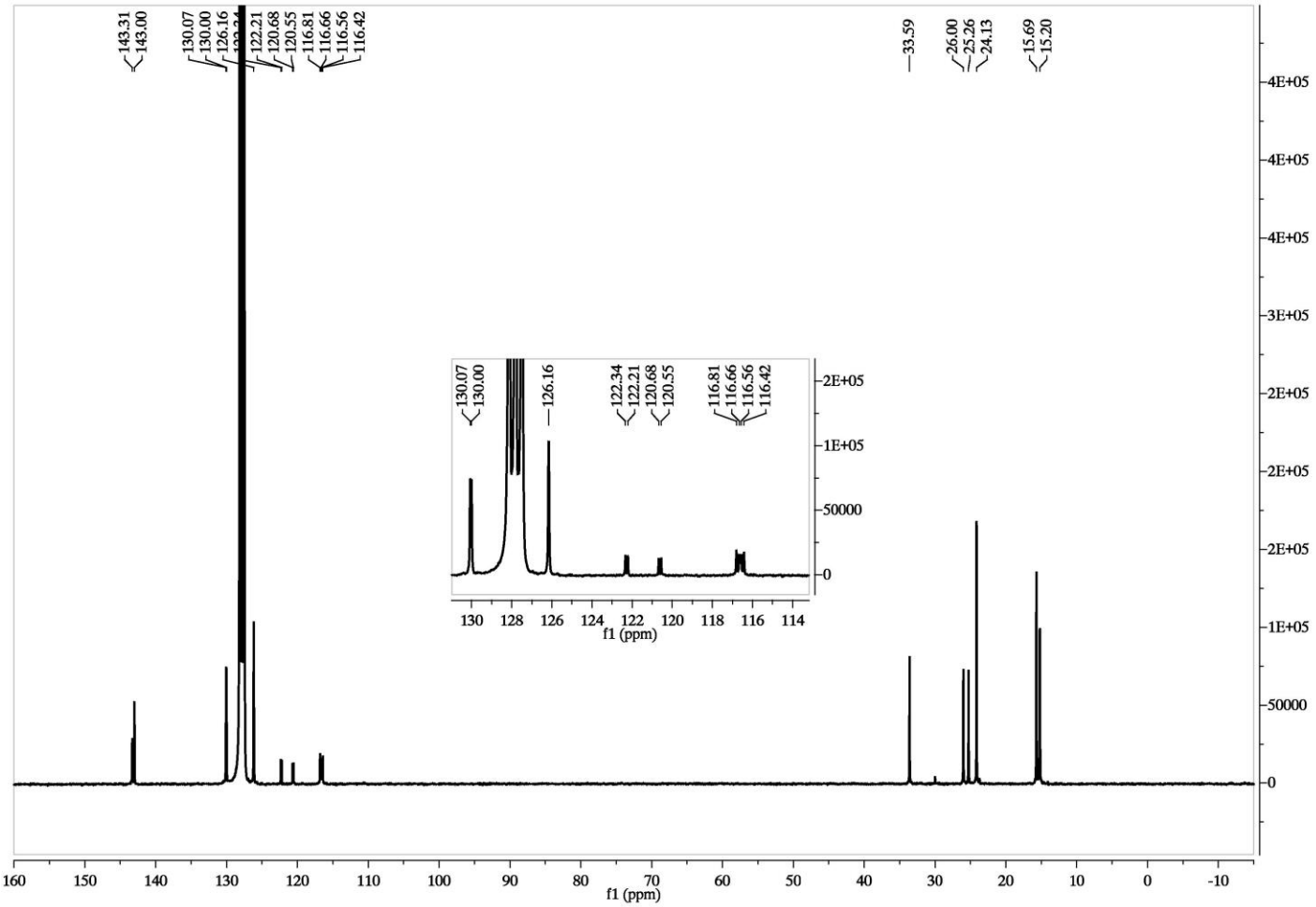

Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of **1^{Pipp}** in d_6-benzene.

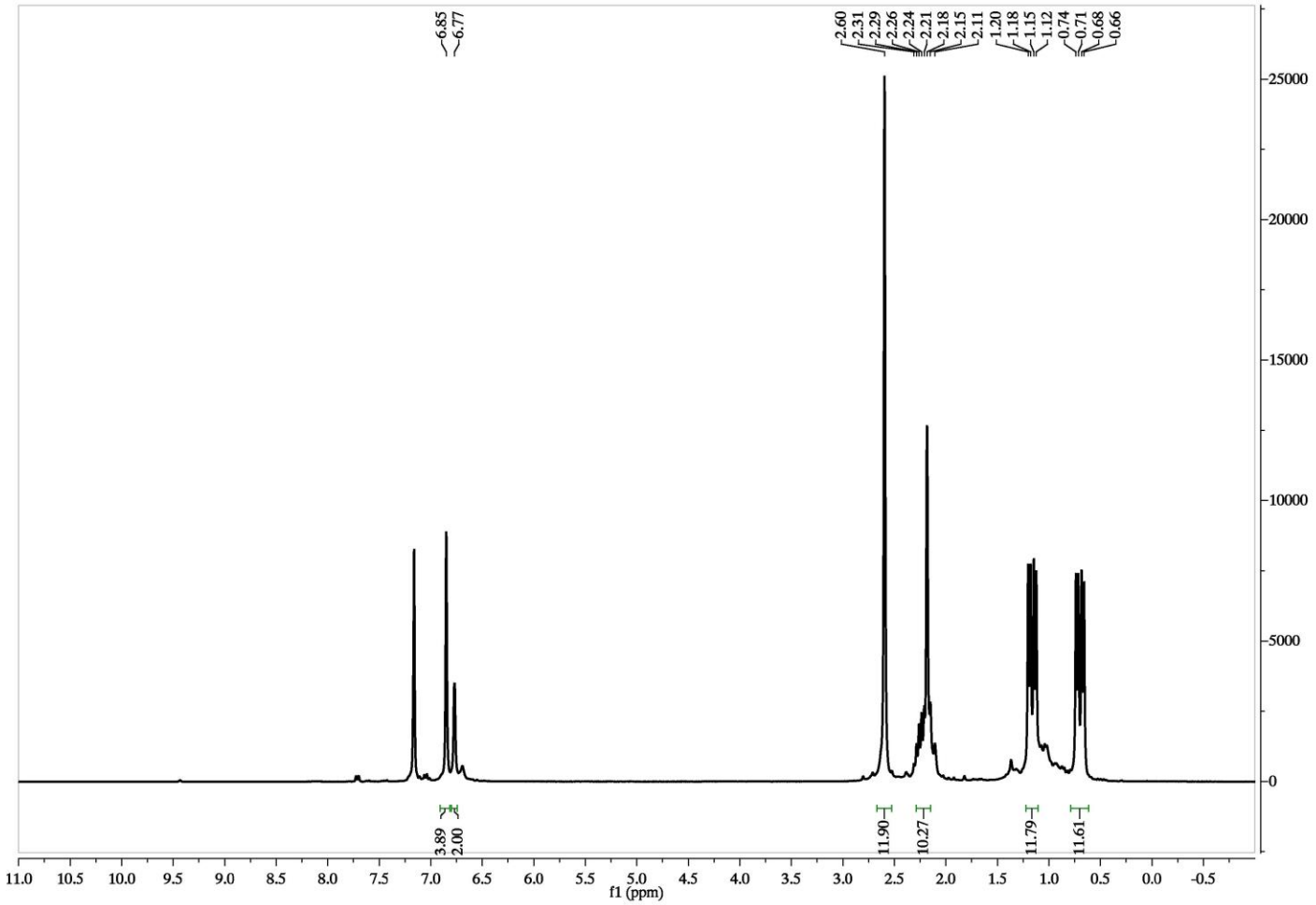

Figure S16. ^{1}H NMR spectrum of **1^{Mes}** in d_6-benzene.

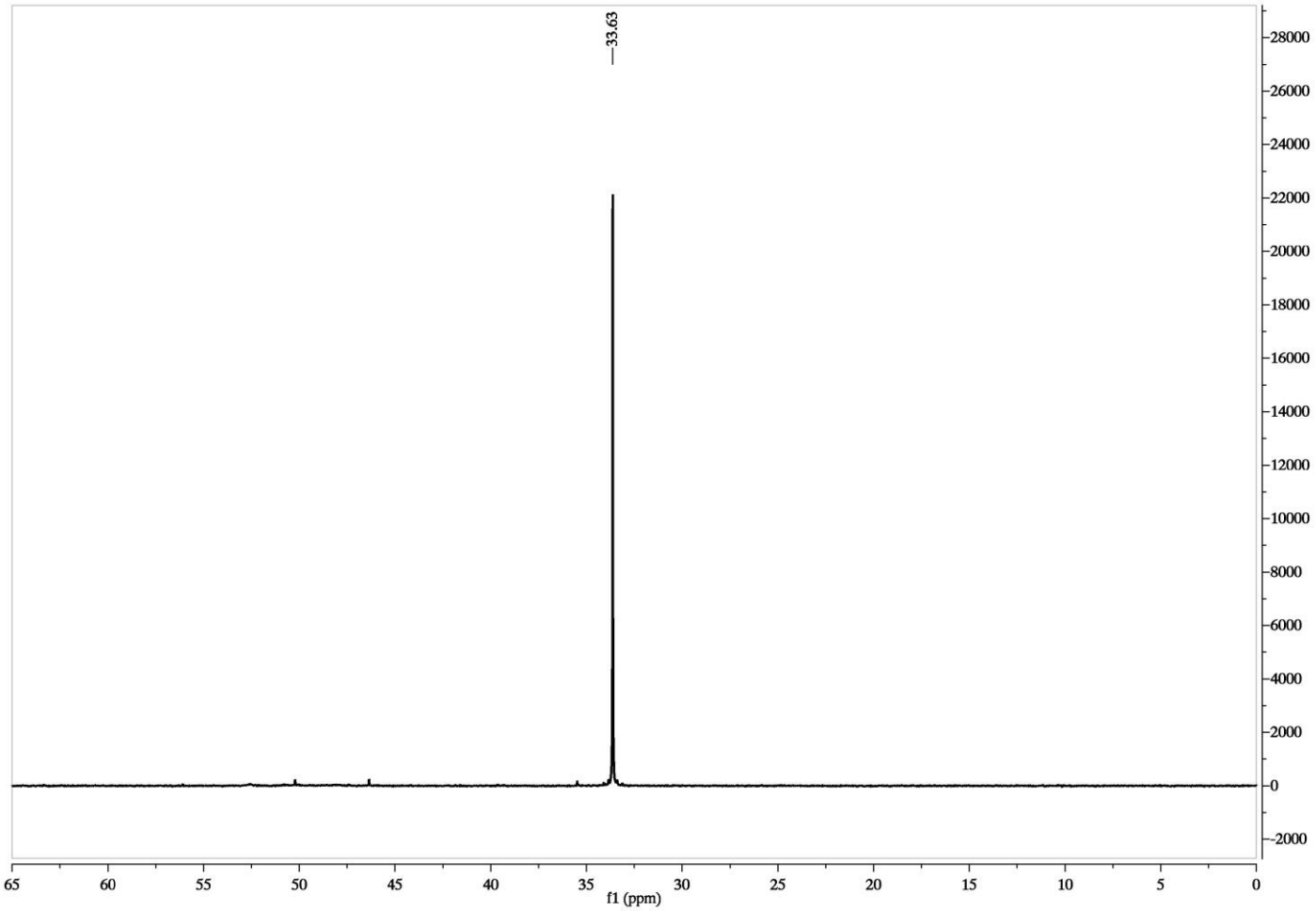

Figure S17. $^{31}P\{^{1}H\}$ NMR spectrum of **1^{Mes}** in d_6-benzene.

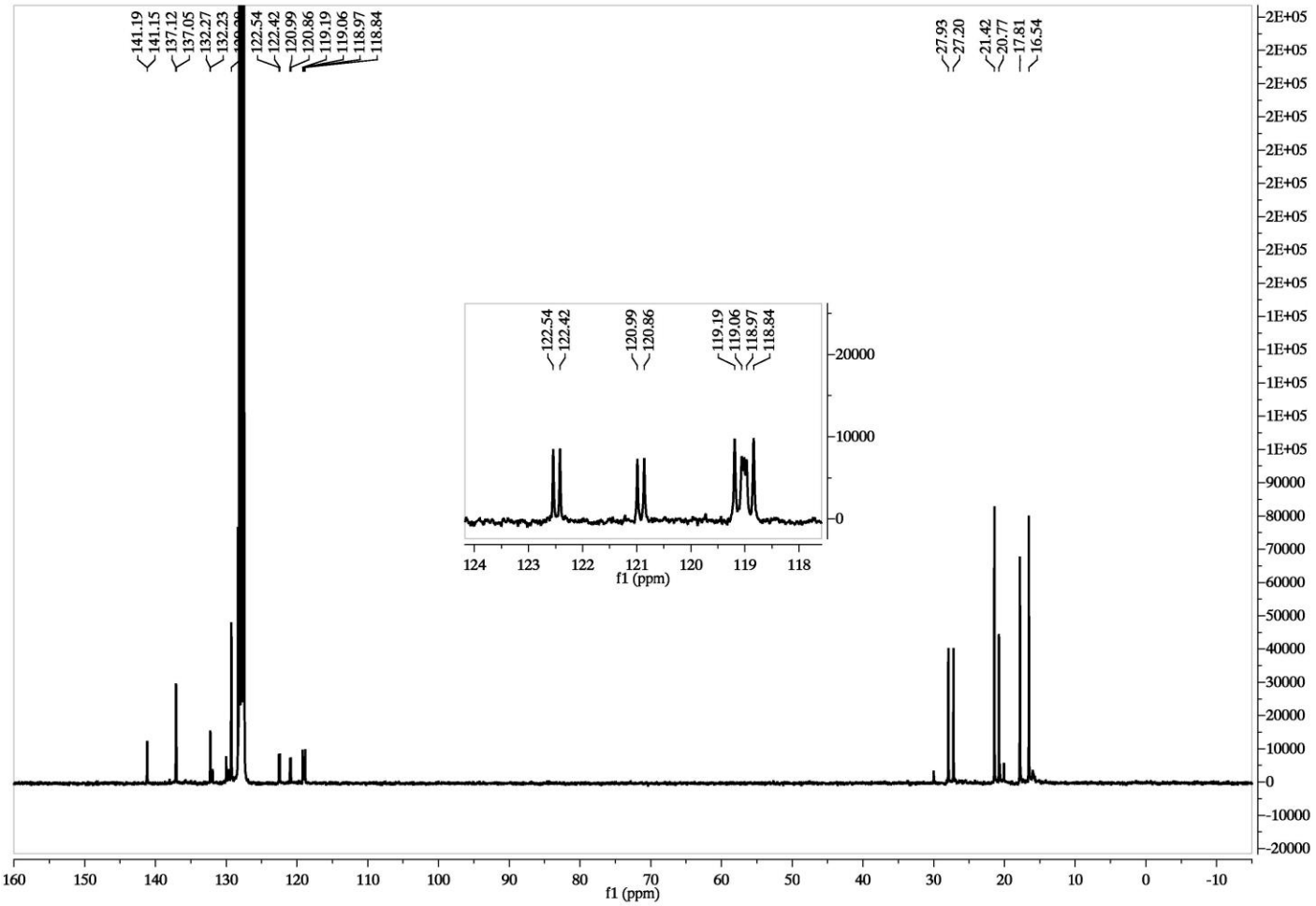

Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **1^{Mes}** in d_6-benzene.

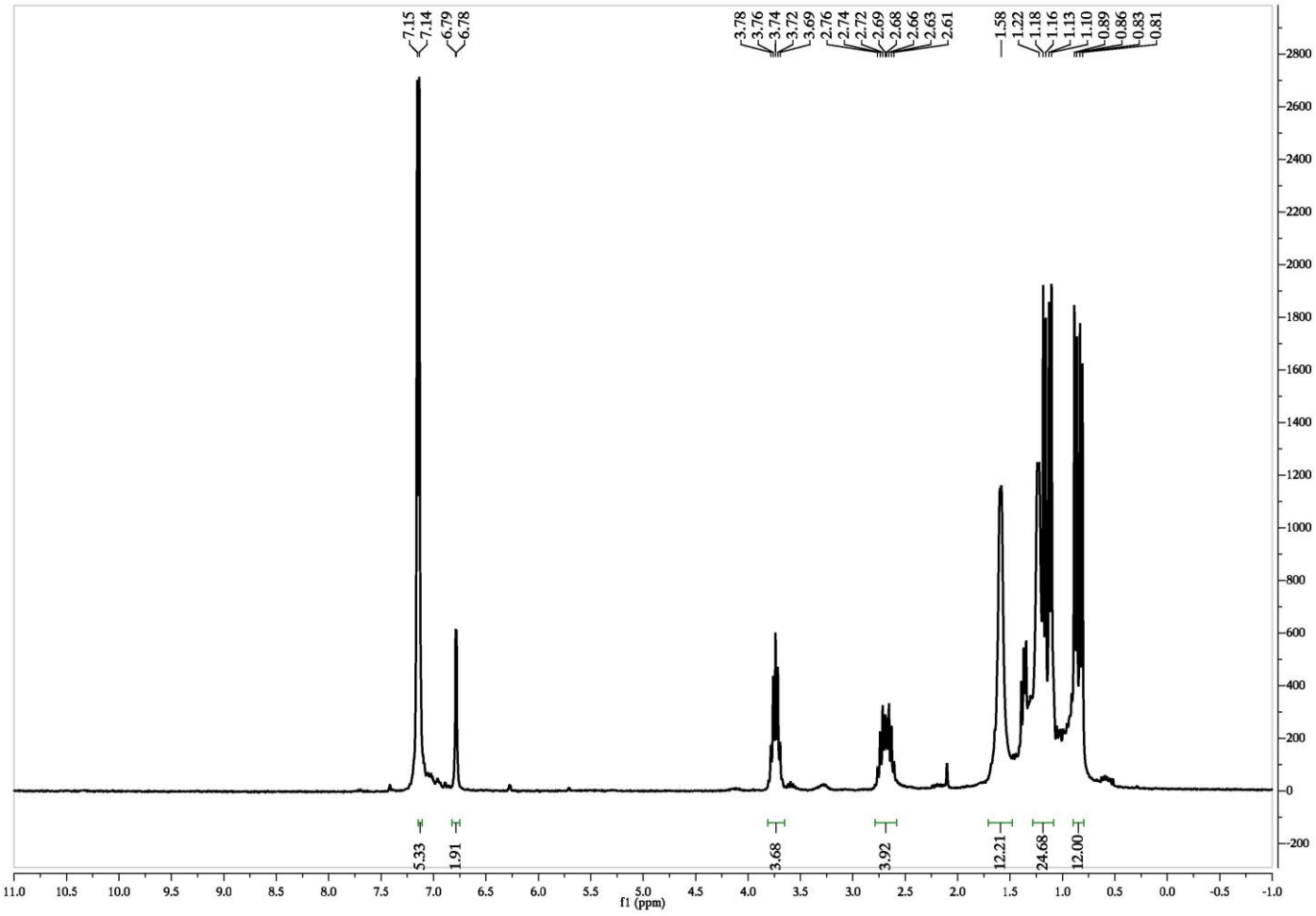

Figure S19. ^{1}H NMR spectrum of **1^{Dipp}** in d_6-benzene.

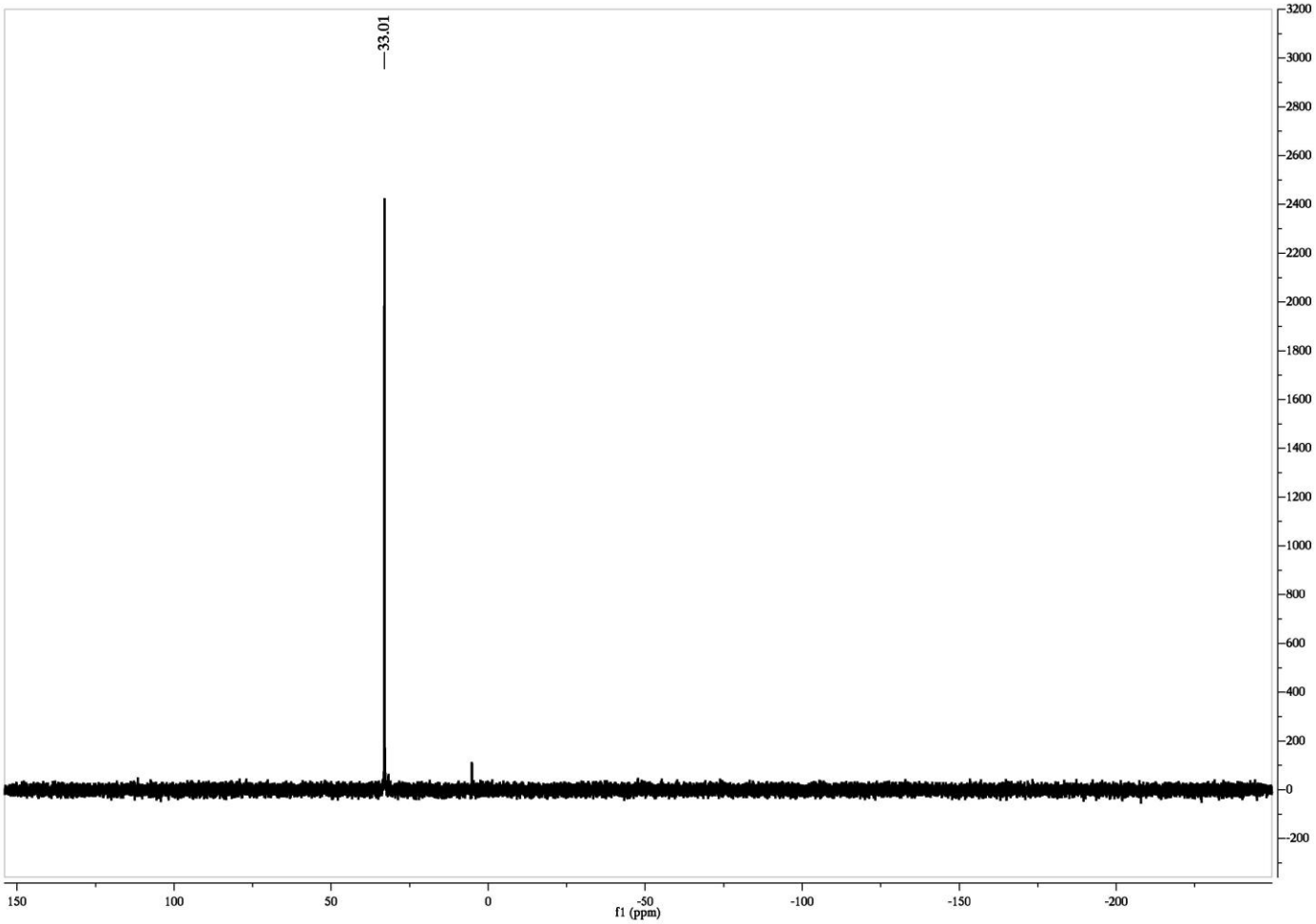

Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum of **1^{Dipp}** in d_6-benzene.

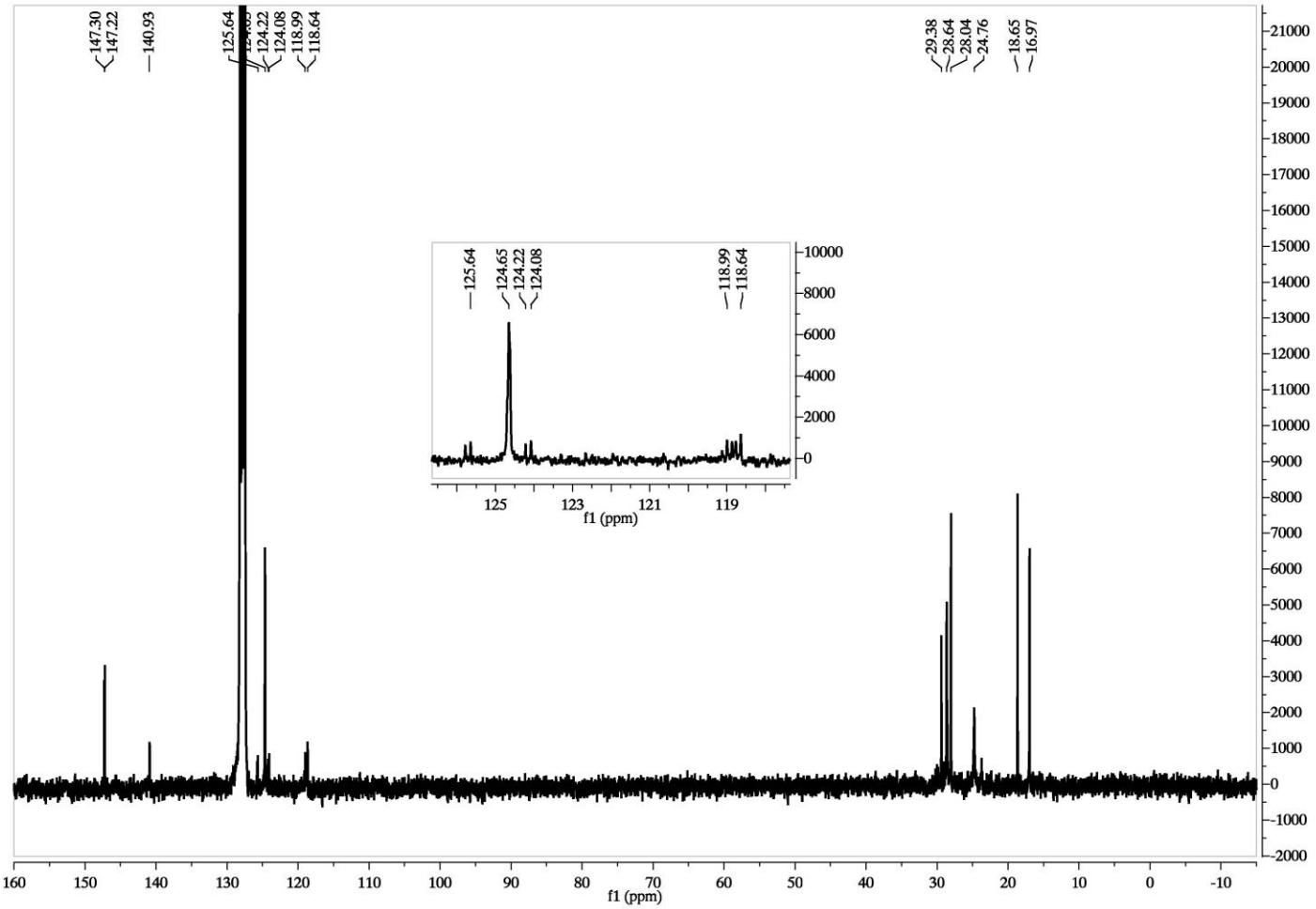

Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of **1^{Dipp}** in d_6-benzene.

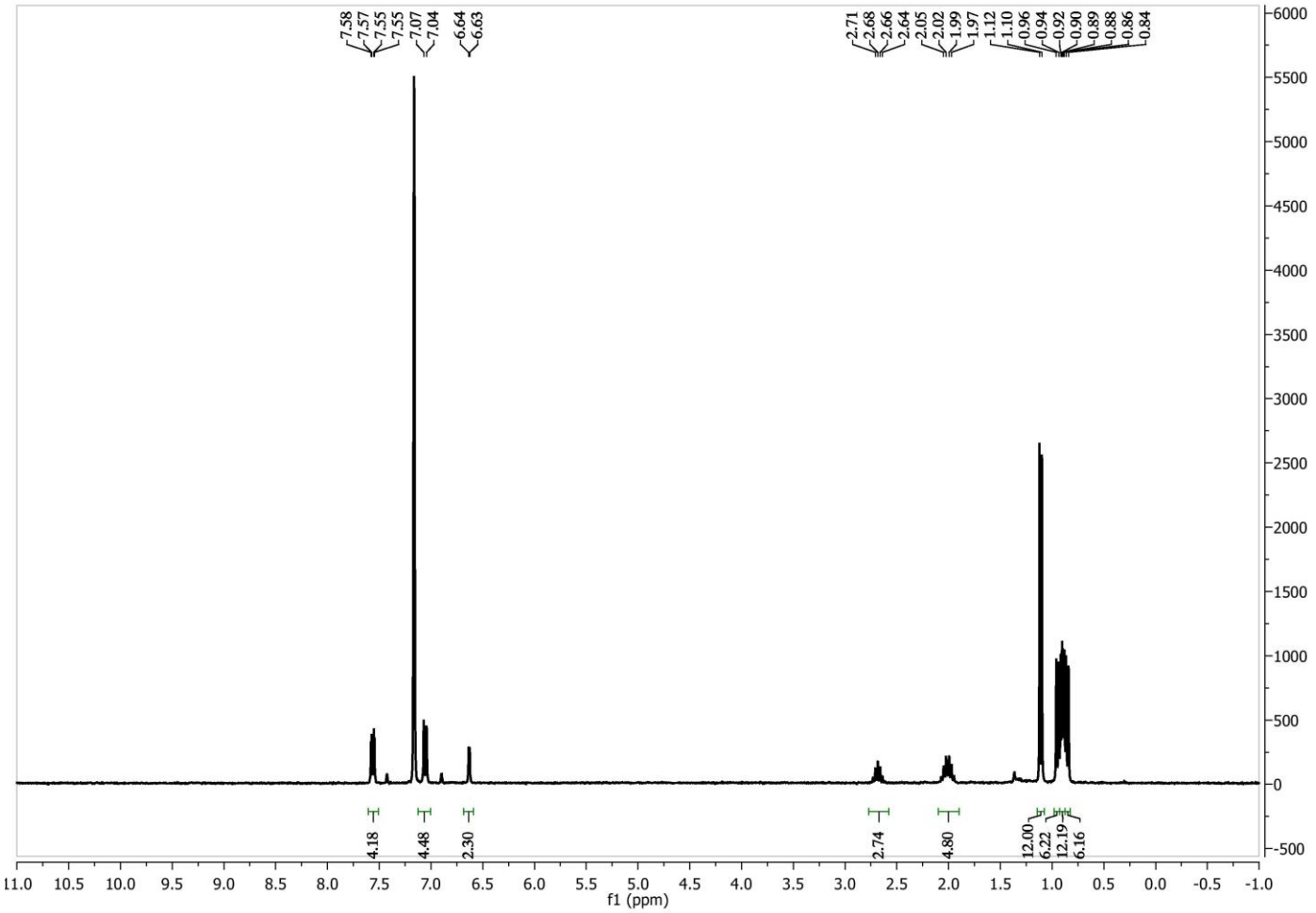

Figure S22. ^{1}H NMR spectrum of **2^{Pipp}** in d_6-benzene.

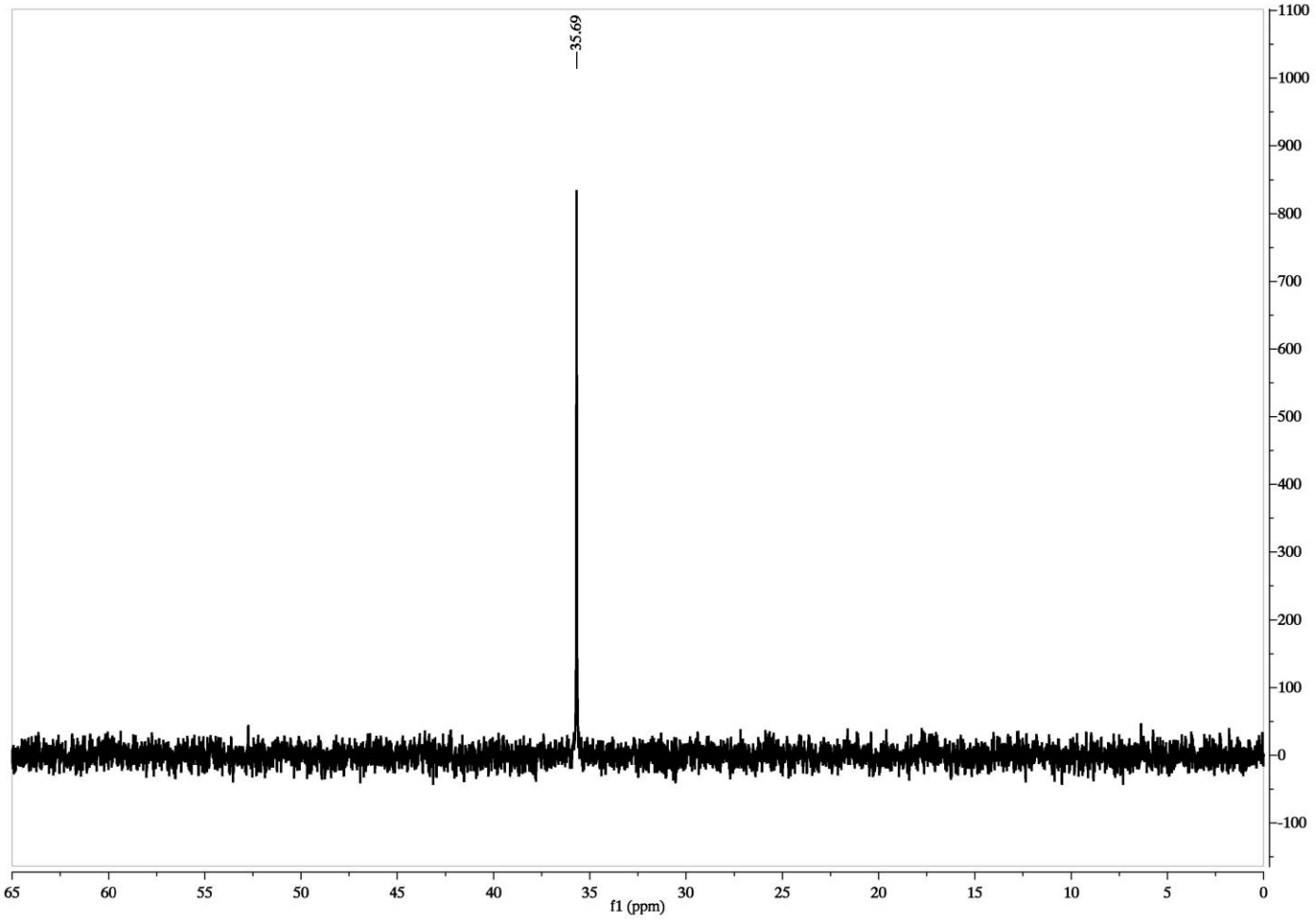

Figure S23. $^{31}P\{^{1}H\}$ NMR spectrum of **2^{Pipp}** in d_6-benzene.

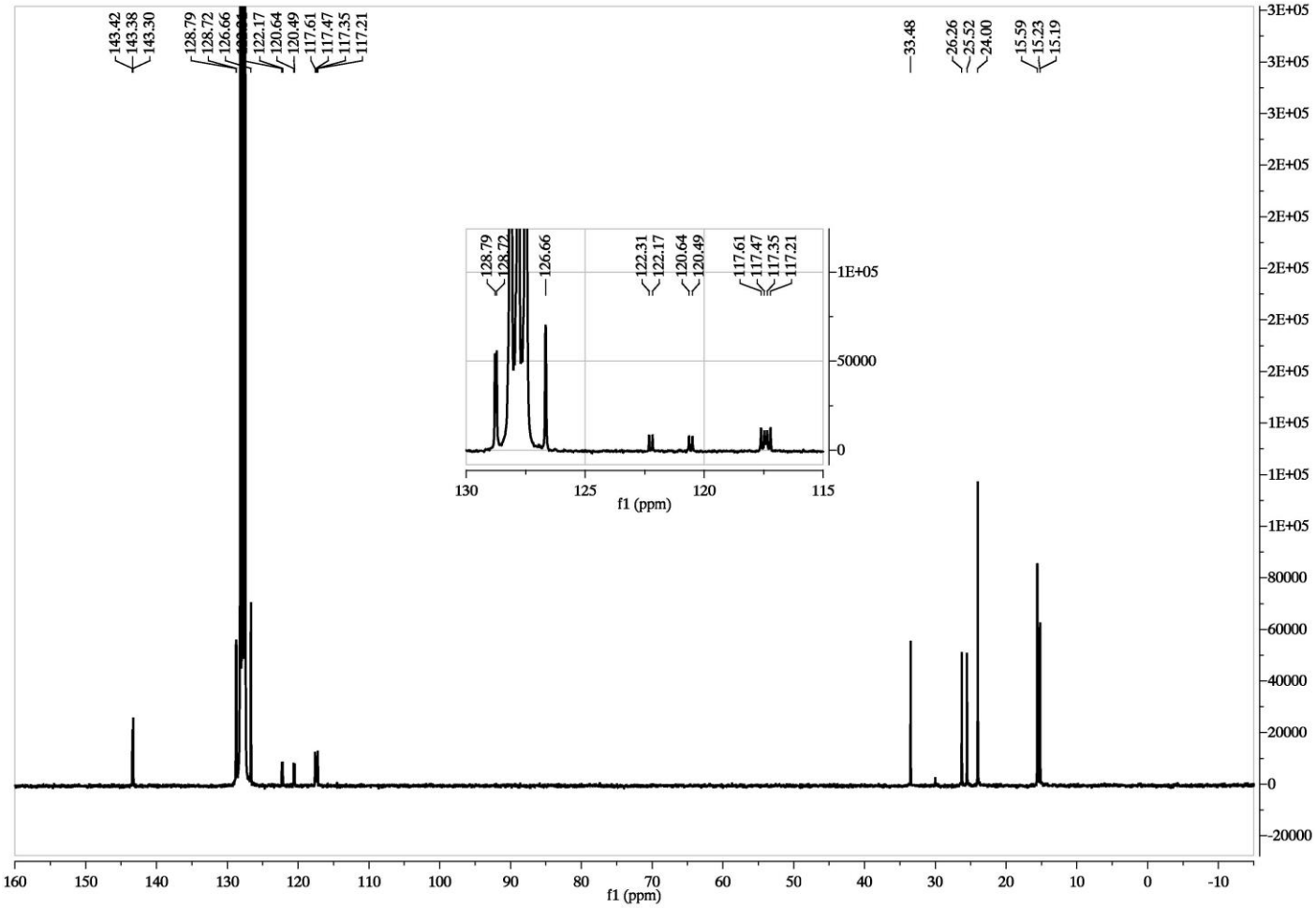

Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum of **2^{Pipp}** in d_6-benzene.

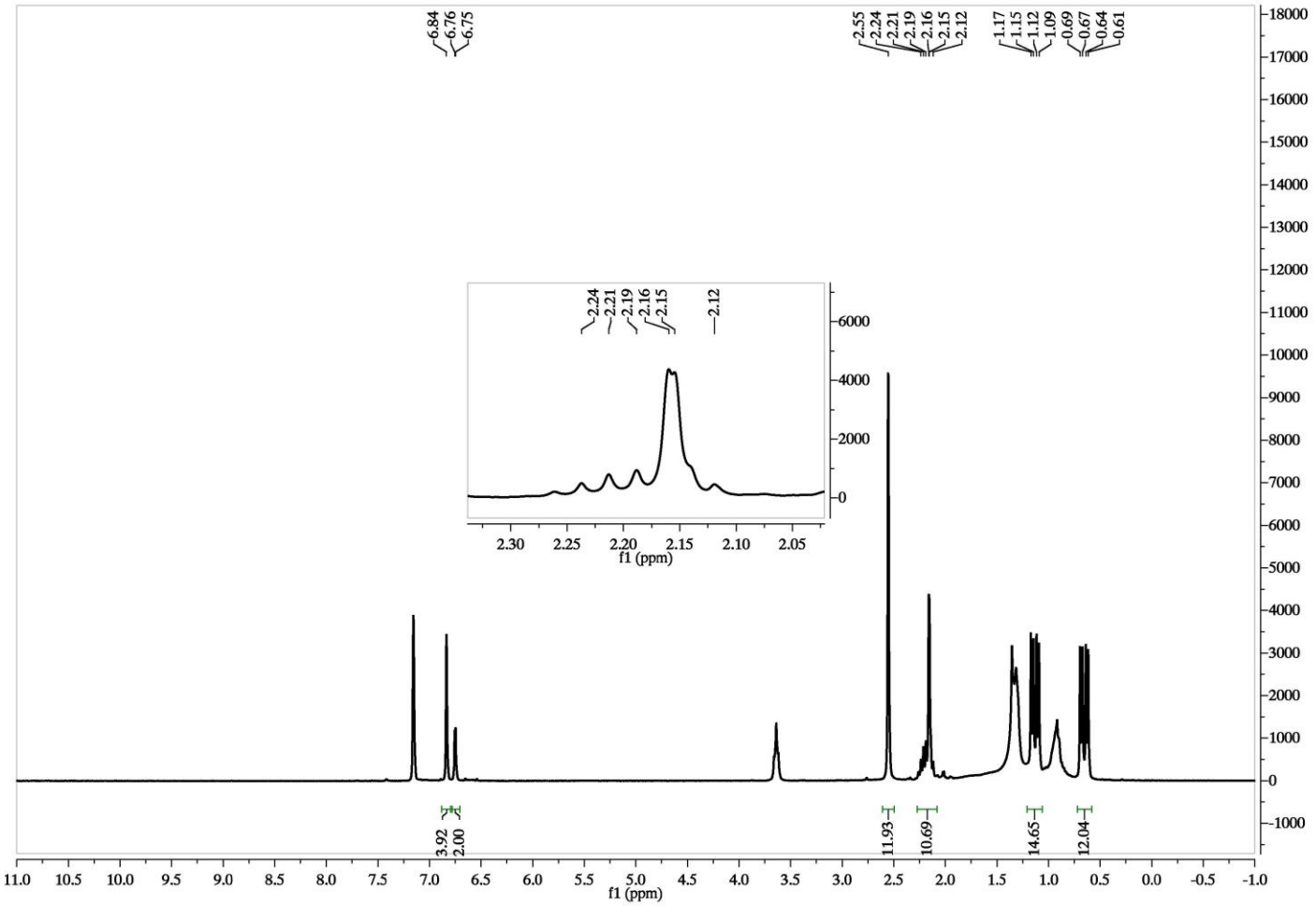

Figure S25. ^{1}H NMR spectrum of **2^{Mes}** in d_6-benzene.

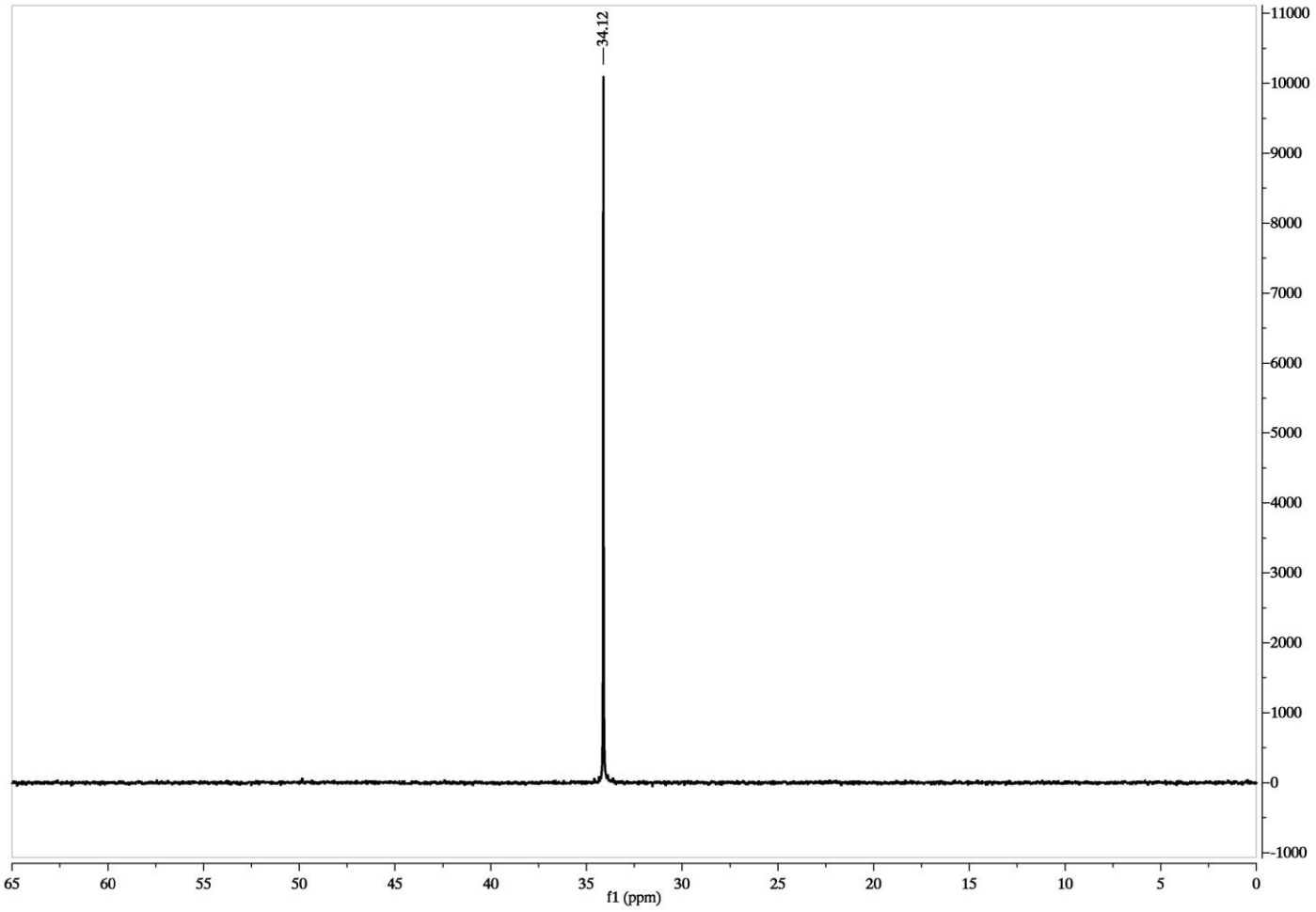

Figure S26. $^{31}P\{^{1}H\}$ NMR spectrum of **2^{Mes}** in d_6-benzene.

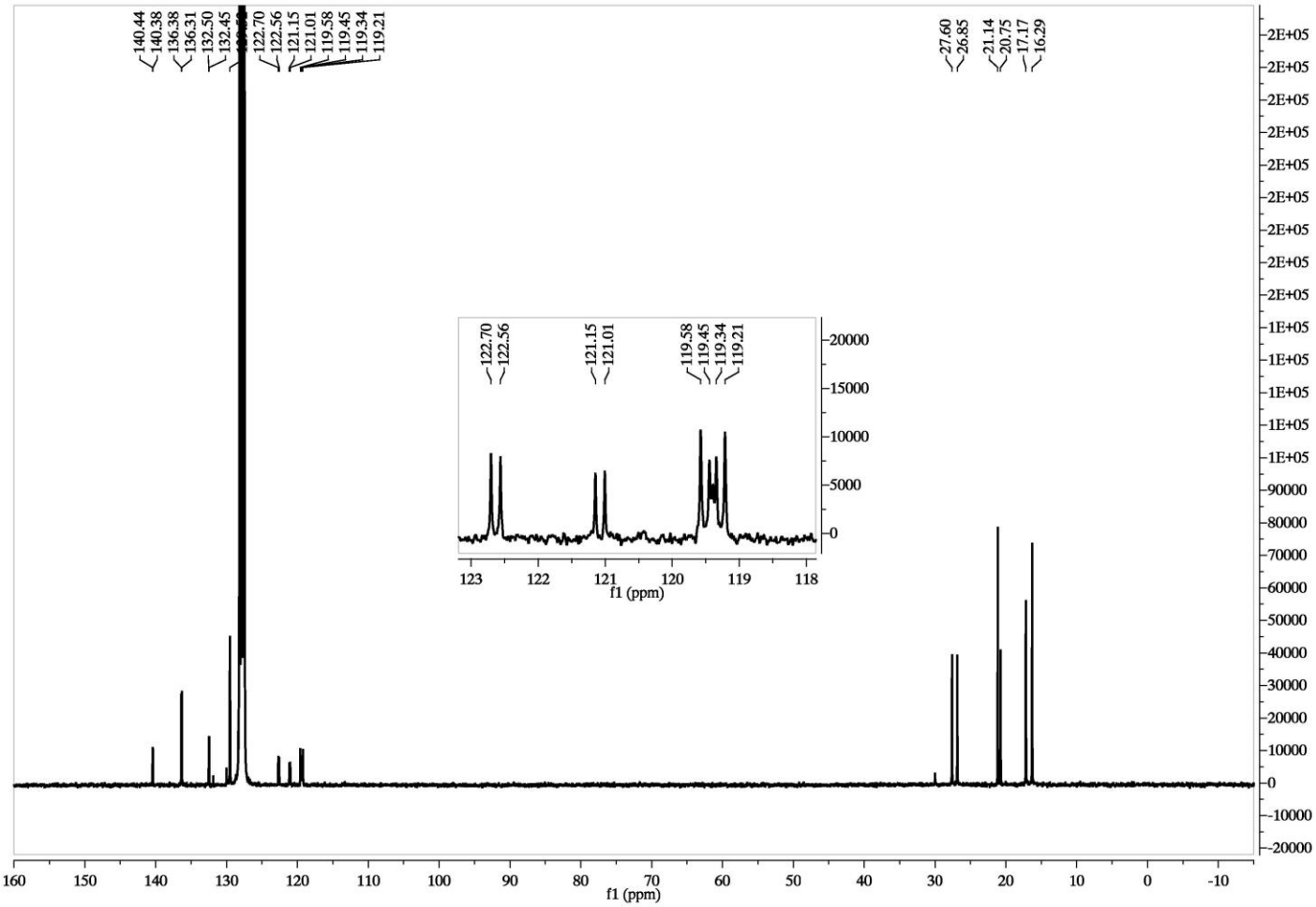

Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum of **2^{Mes}** in d_6-benzene.

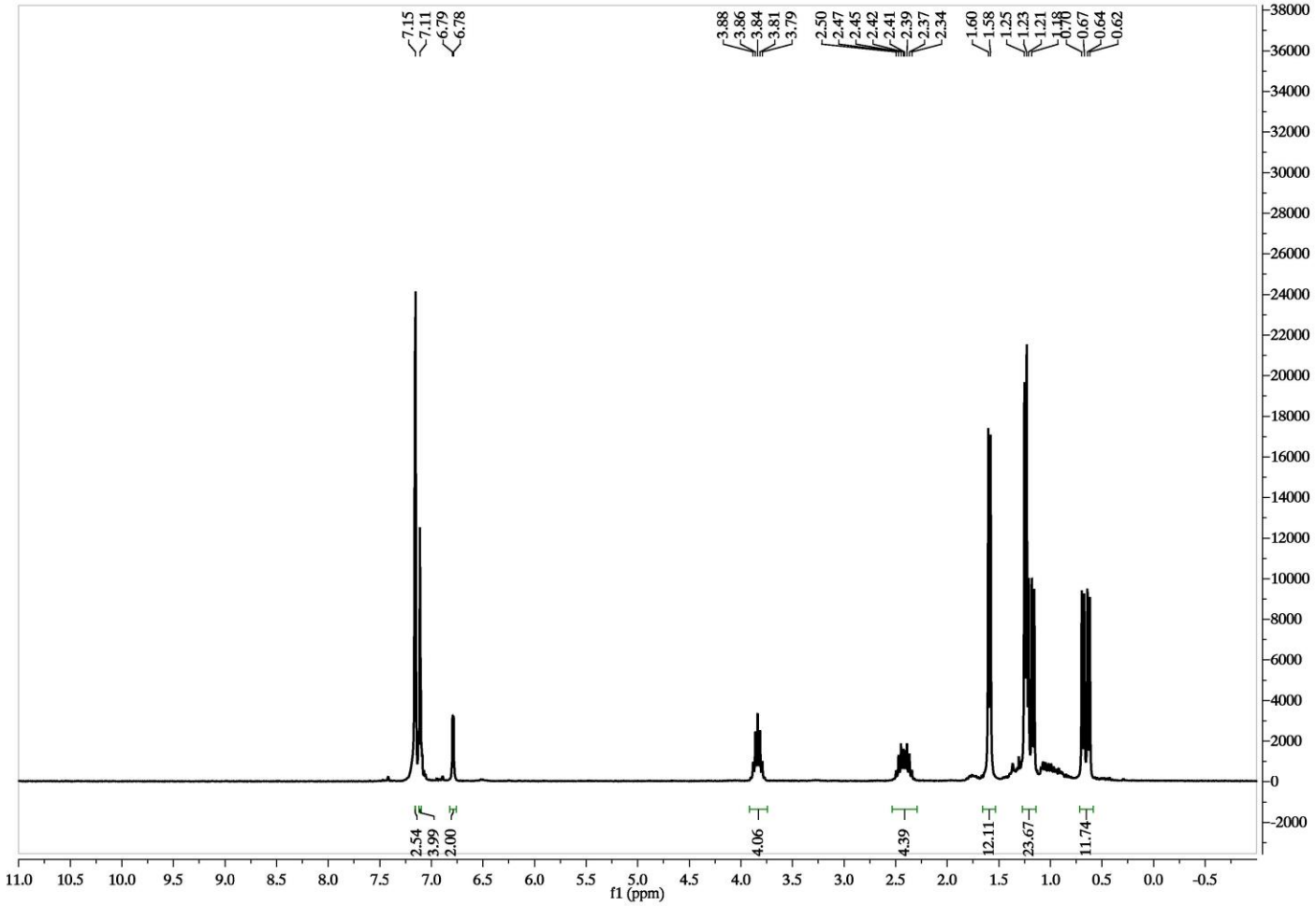

Figure S28.[1]H NMR spectrum of **2^{Dipp}** in d_6-benzene.

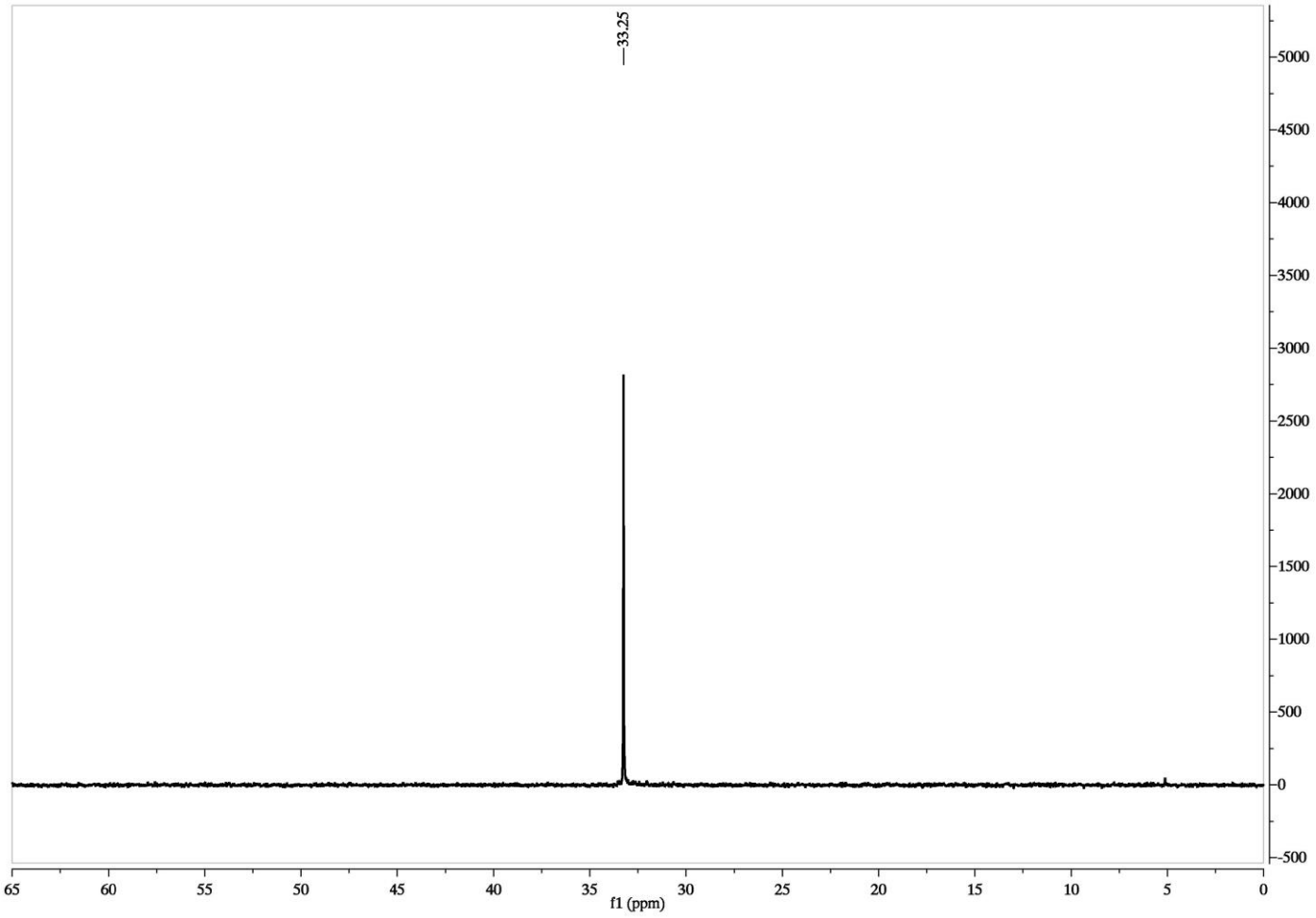

Figure S29. $^{31}P\{^{1}H\}$ NMR spectrum of **2^{Dipp}** in d_6-benzene.

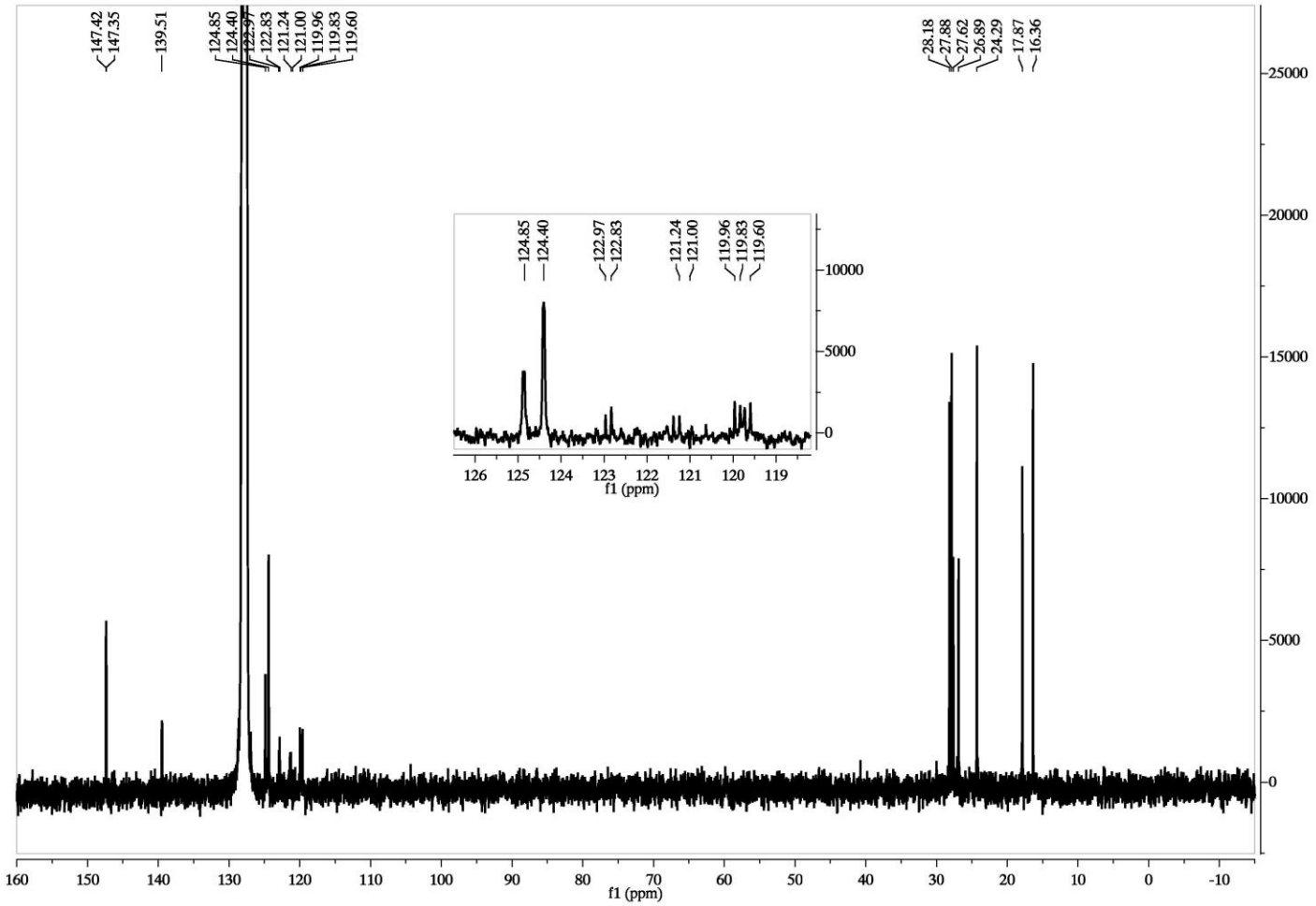

Figure S30. $^{13}C\{^{1}H\}$ NMR spectrum of **2^{Dipp}** in d_6-benzene.

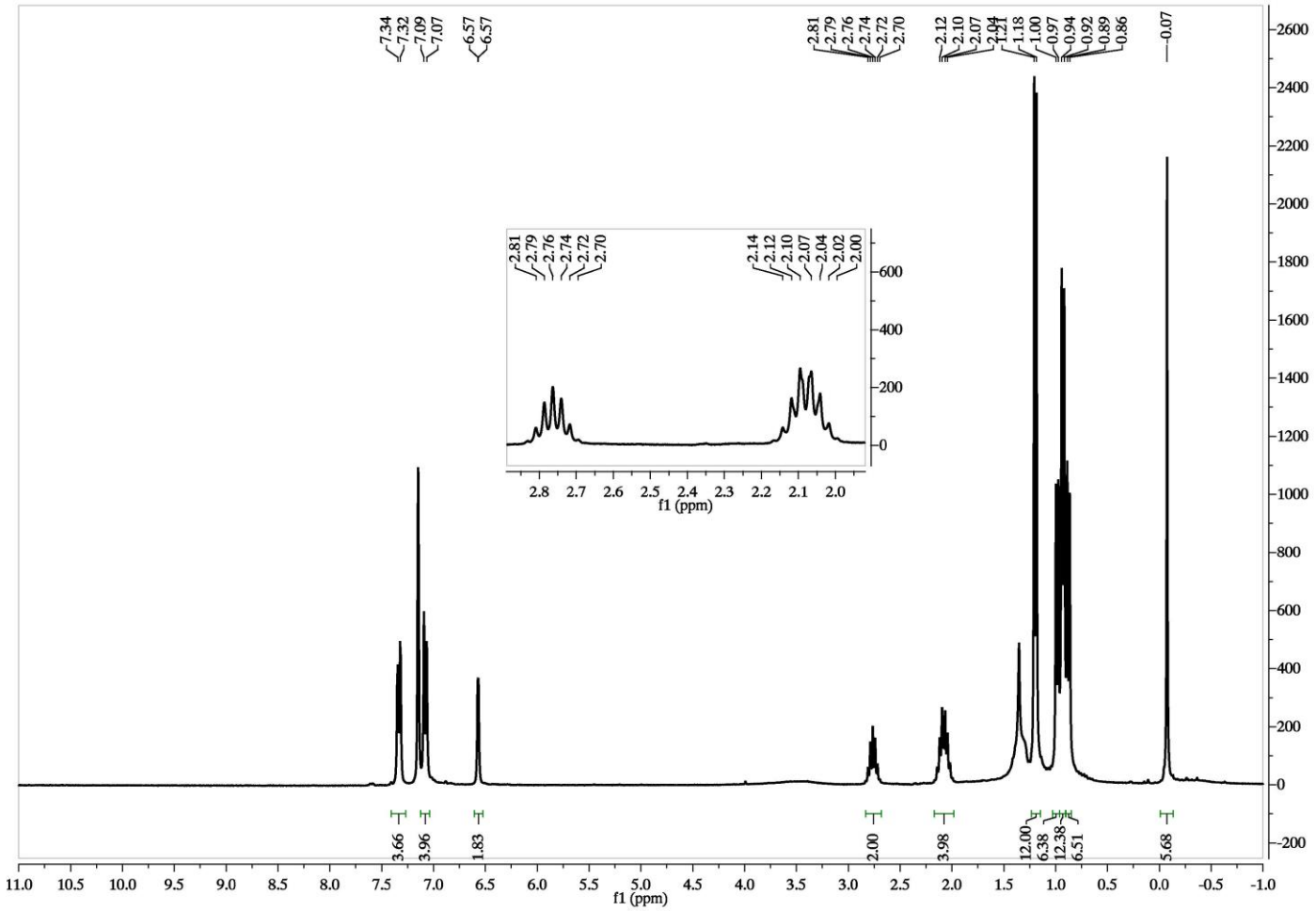

Figure S31.[1]H NMR spectrum of **3^{Pipp}** in d_6-benzene.

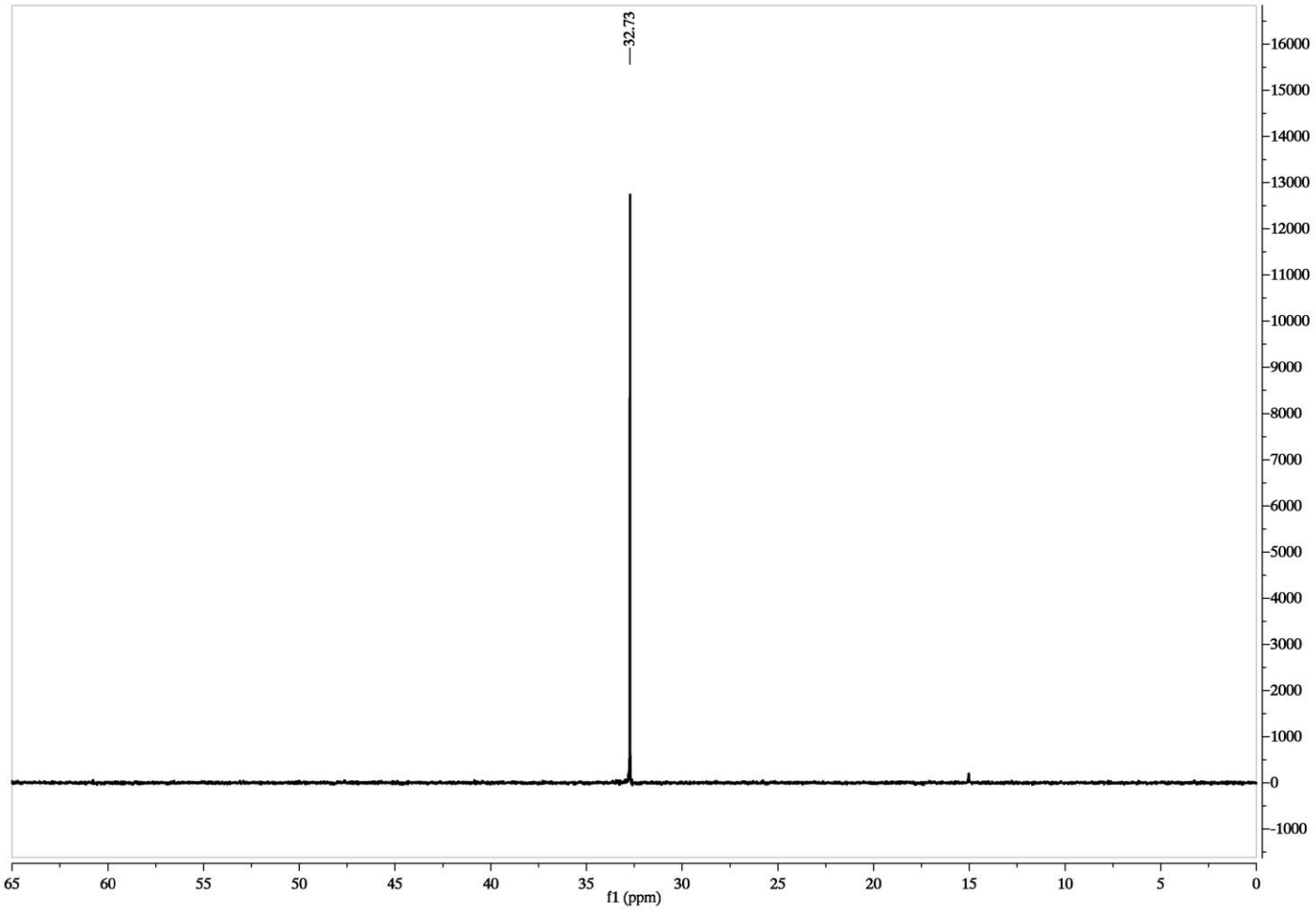

Figure S32. $^{31}P\{^{1}H\}$ NMR spectrum of **3^{Pipp}** in d_6-benzene.

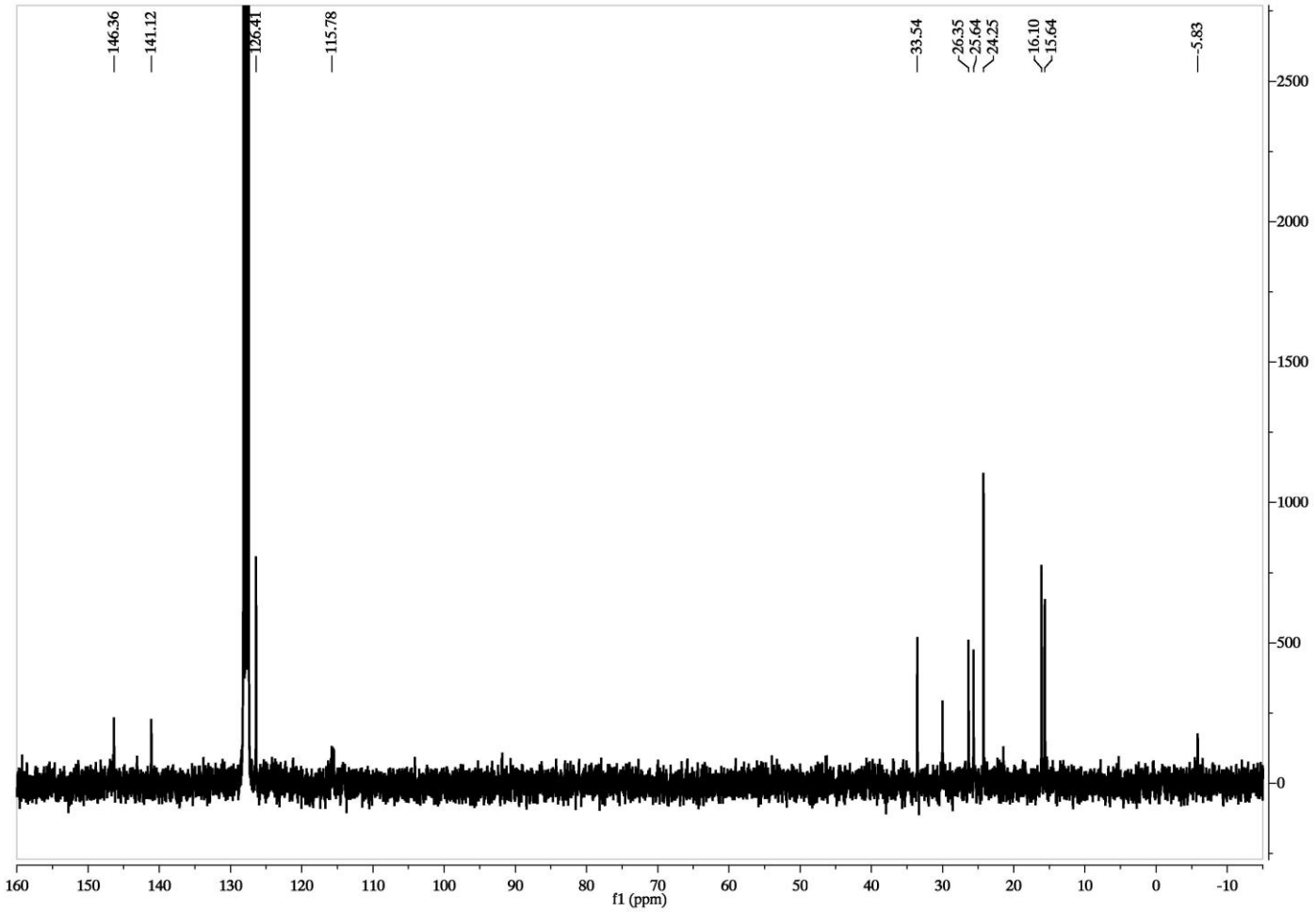

Figure S33. $^{13}C\{^{1}H\}$ NMR spectrum of **3^{Pipp}** in d_6-benzene.

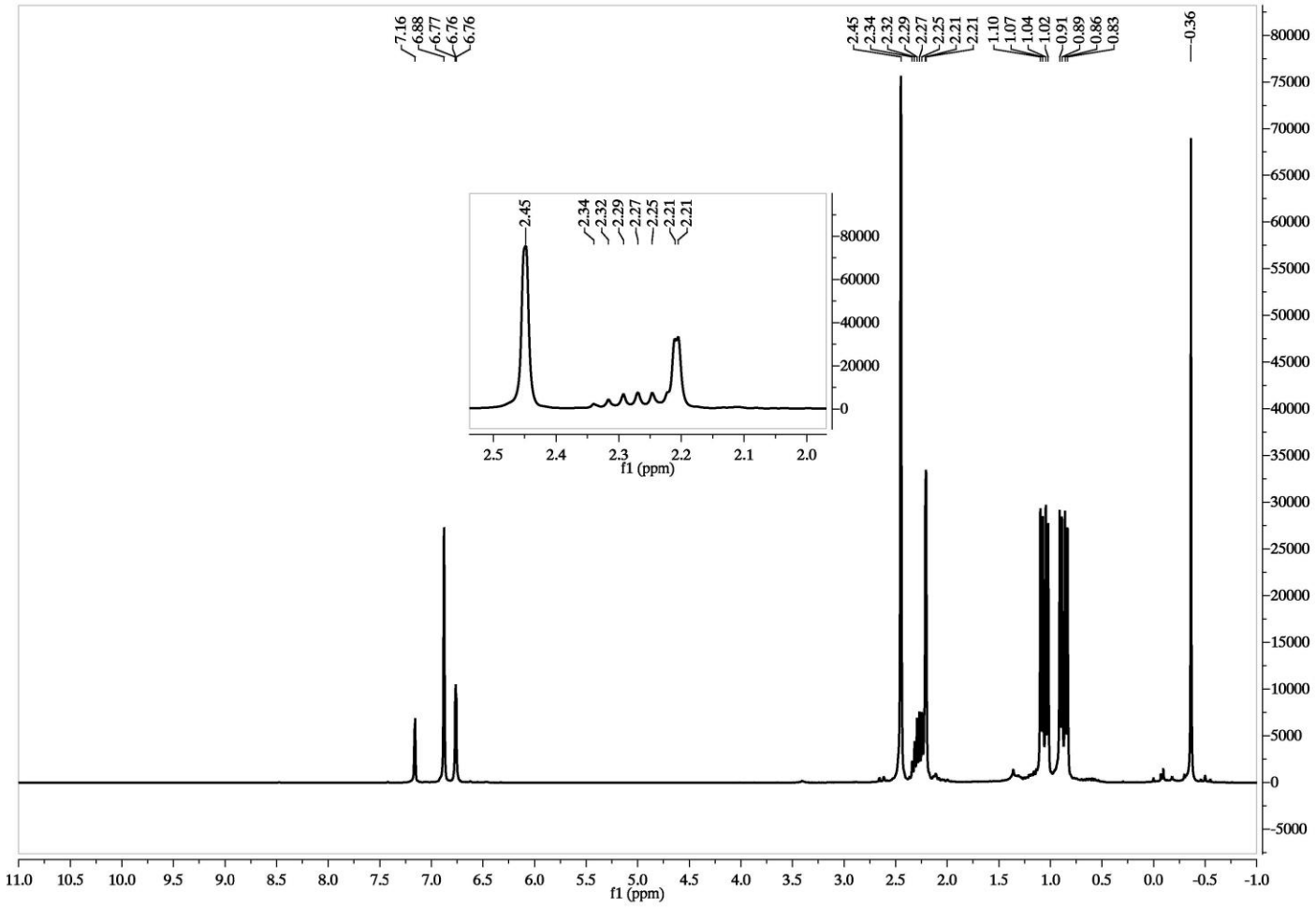

Figure S34. ^{1}H NMR spectrum of **3^{Mes}** in d_6-benzene.

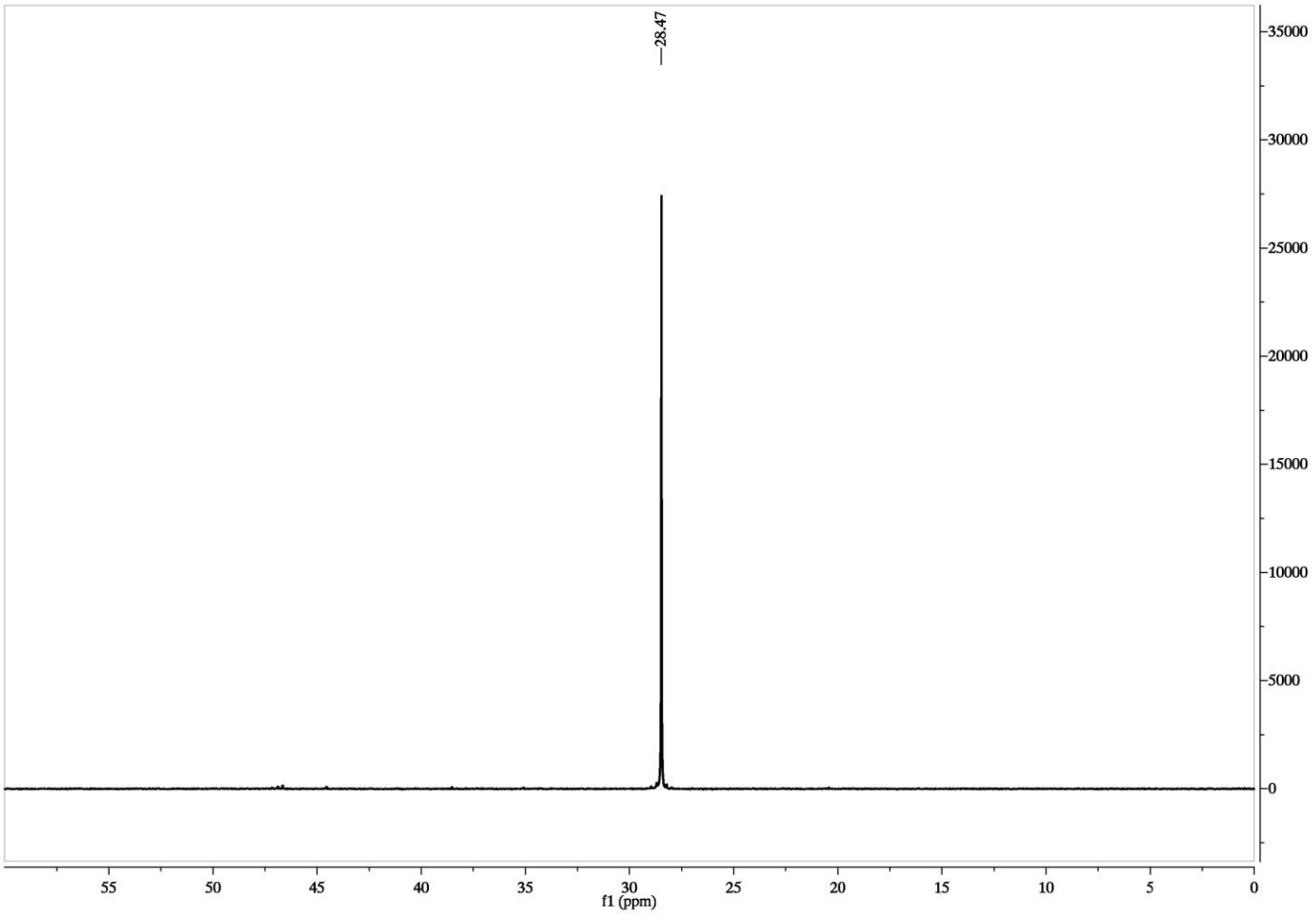

Figure S35. $^{31}P\{^{1}H\}$ NMR spectrum of **3^{Mes}** in d_6-benzene.

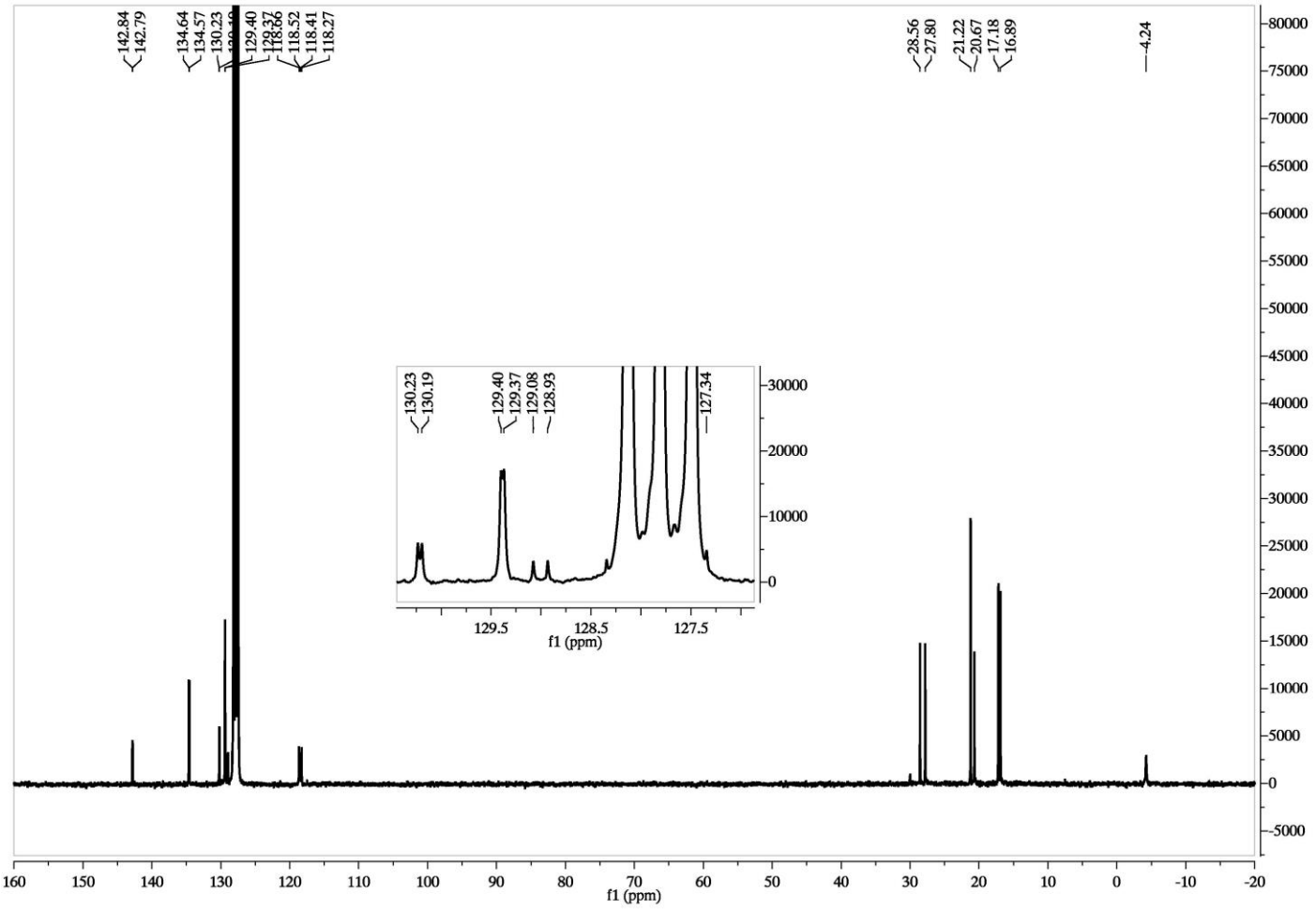

Figure S36. $^{13}C\{^{1}H\}$ NMR spectrum of **3^{Mes}** in d_6-benzene.

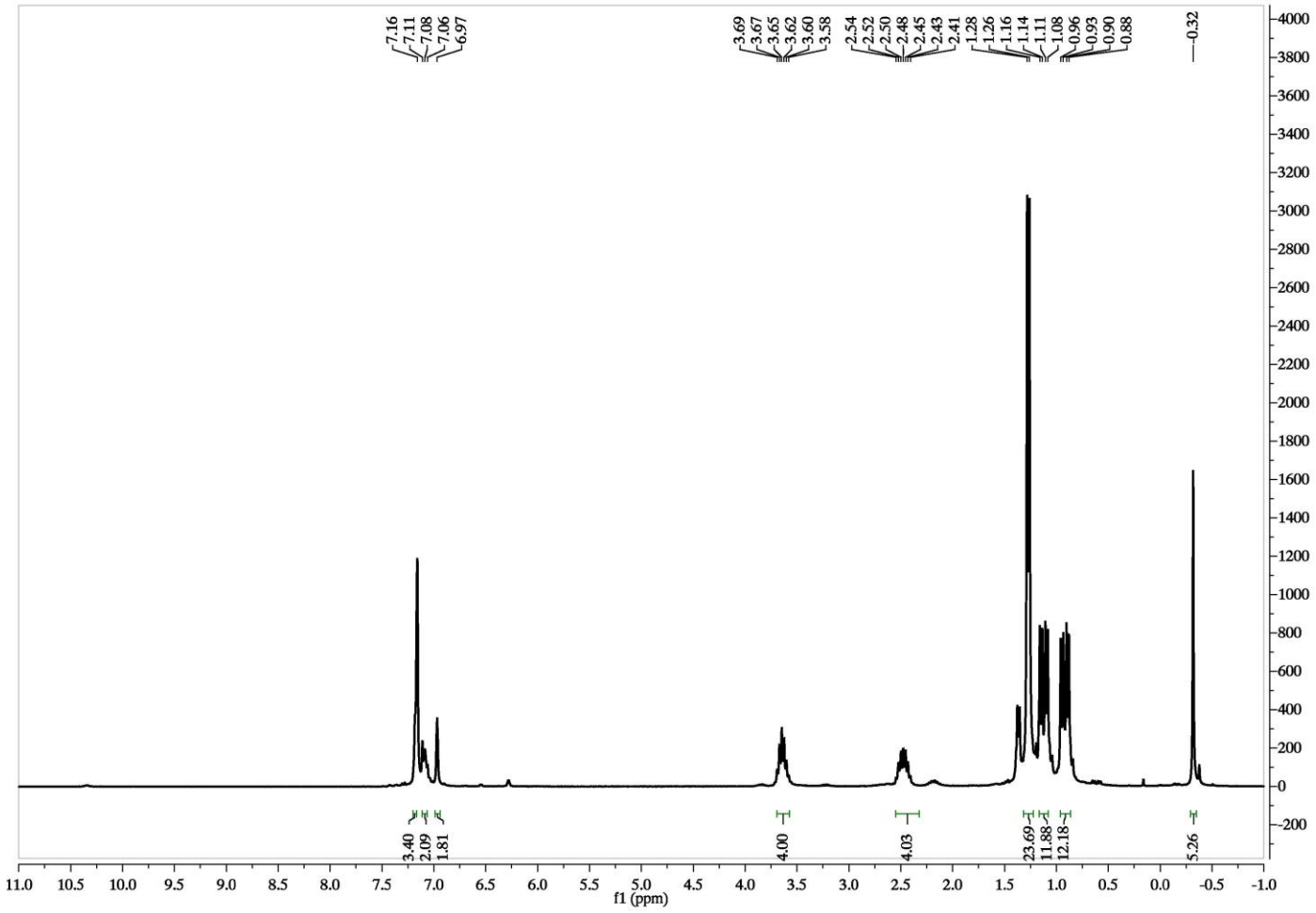

Figure S37.[1]H NMR spectrum of **3^{Dipp}** in d_6-benzene.

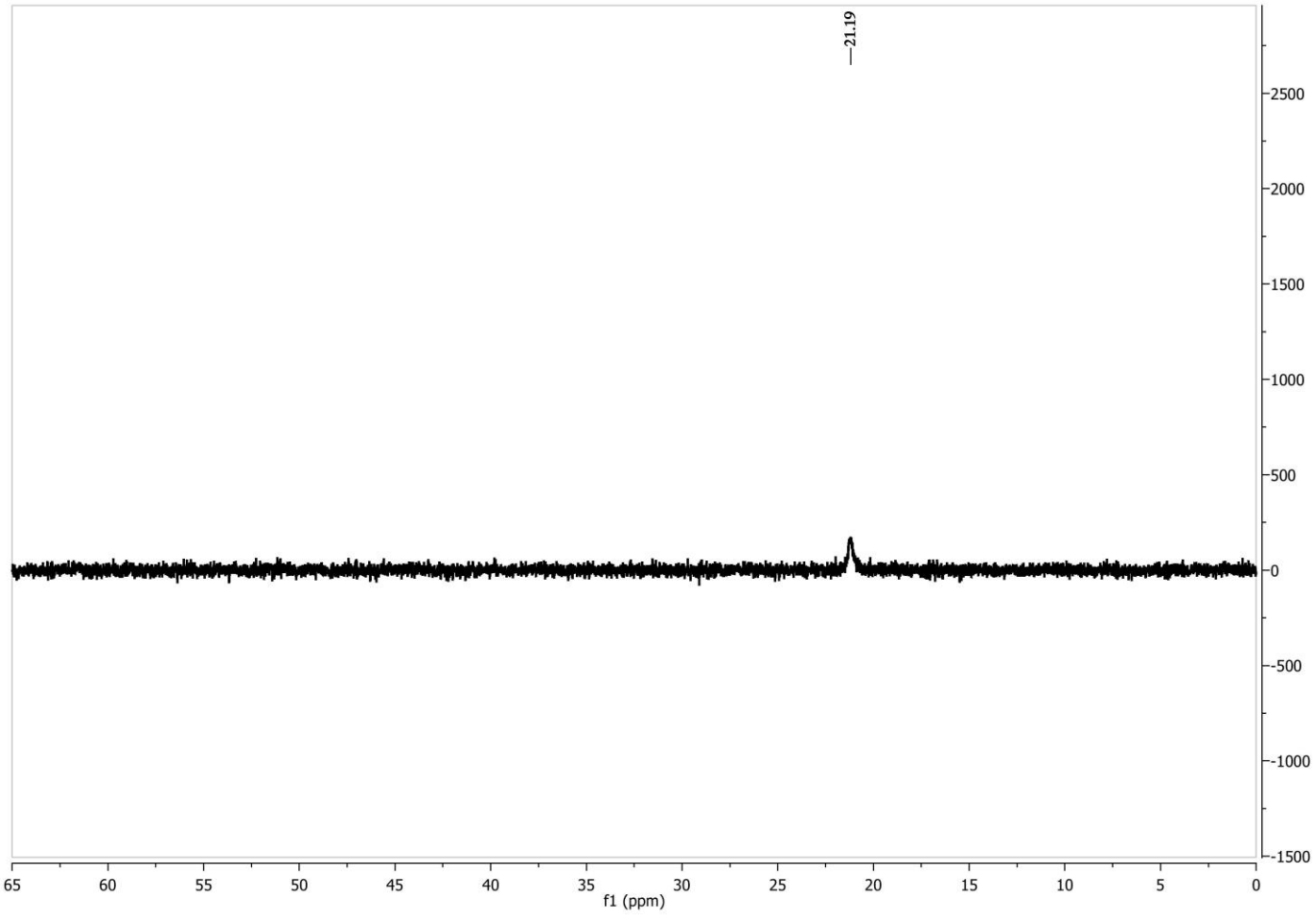

Figure S38. $^{31}P\{^{1}H\}$ NMR spectrum of **3^{Dipp}** in d_6-benzene.

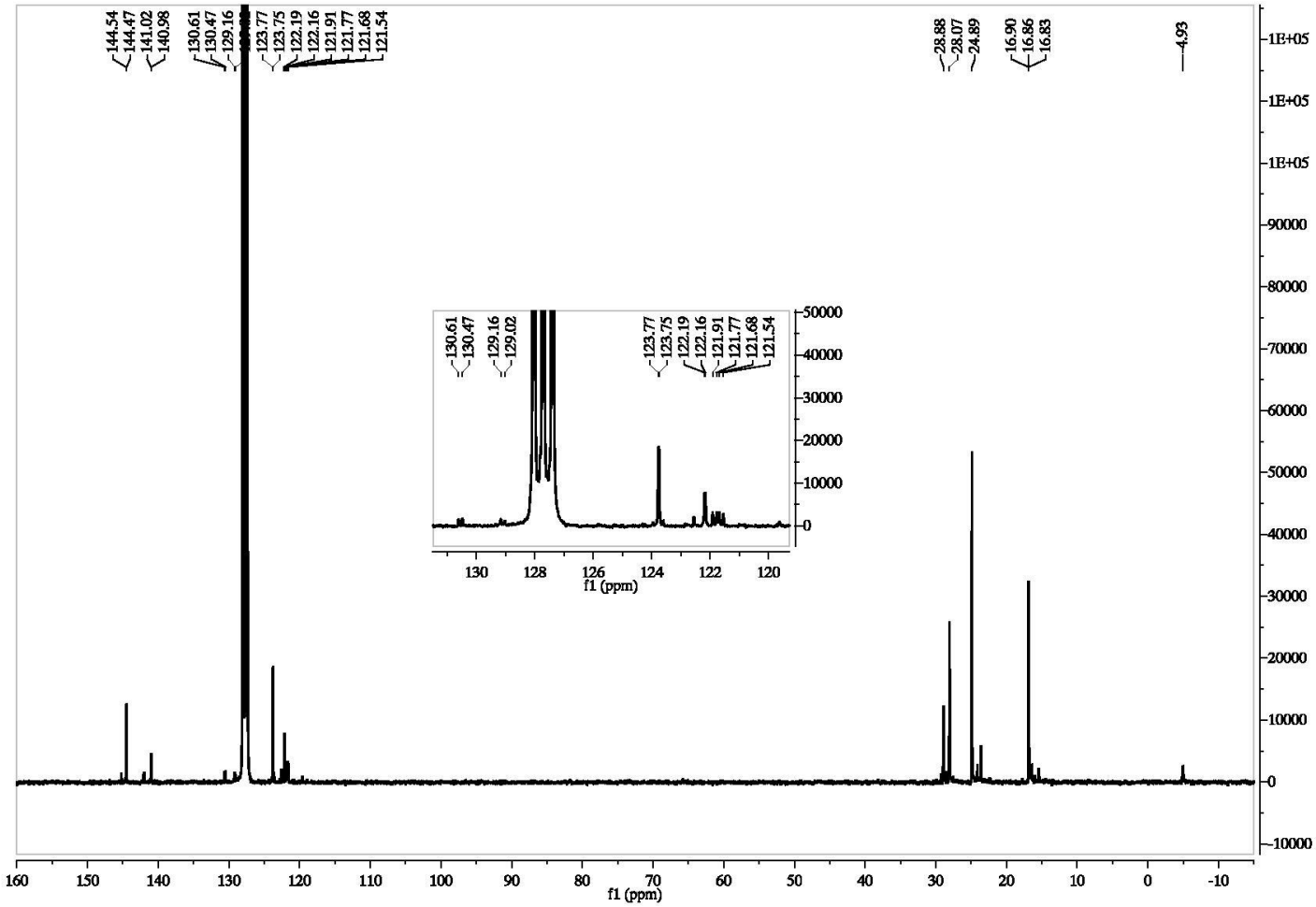

Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum of **3^{Dipp}** in d_6-benzene.

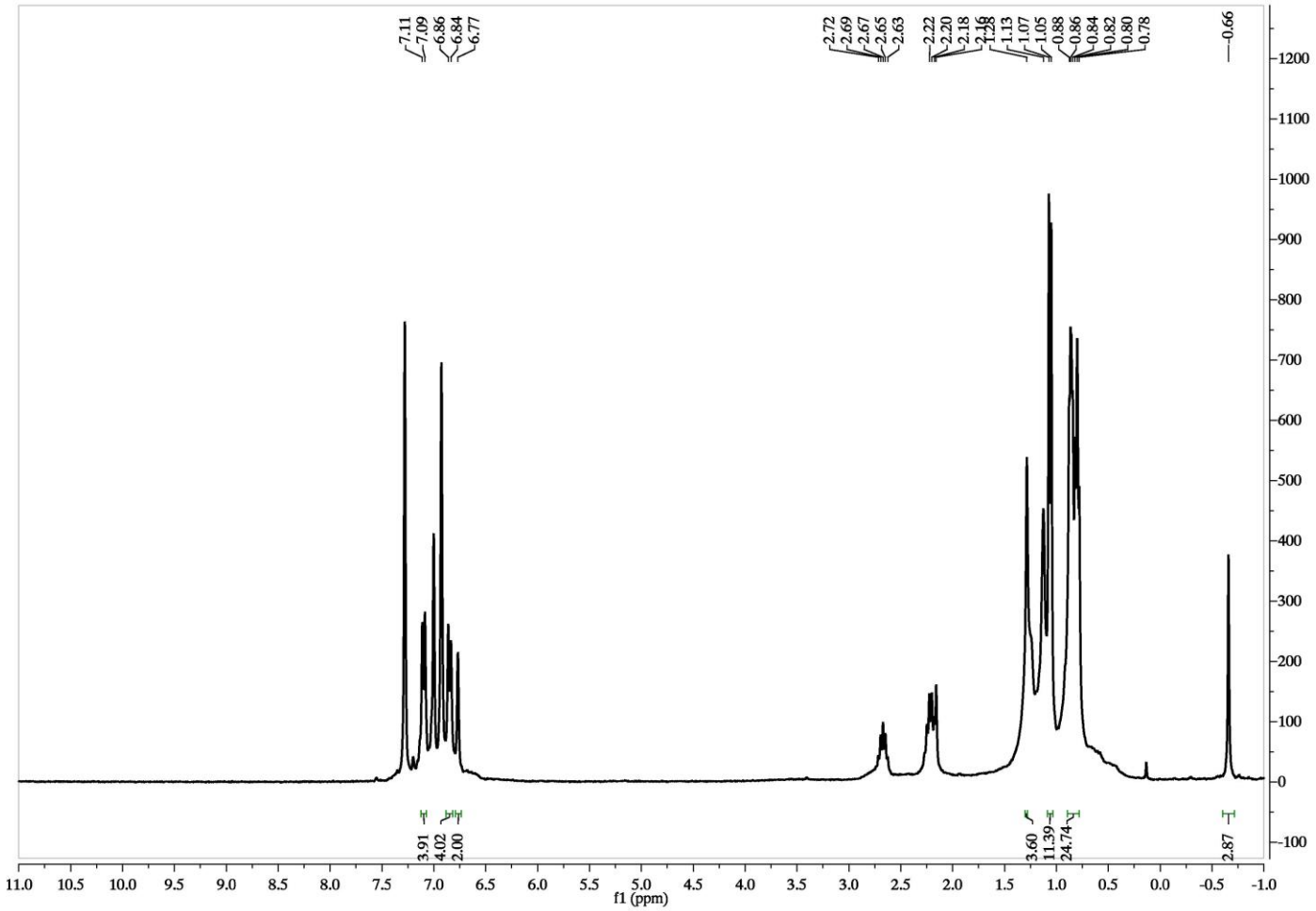

Figure S40. ^{1}H NMR spectrum of **4^{Pipp}** in d_5-bromobenzene.

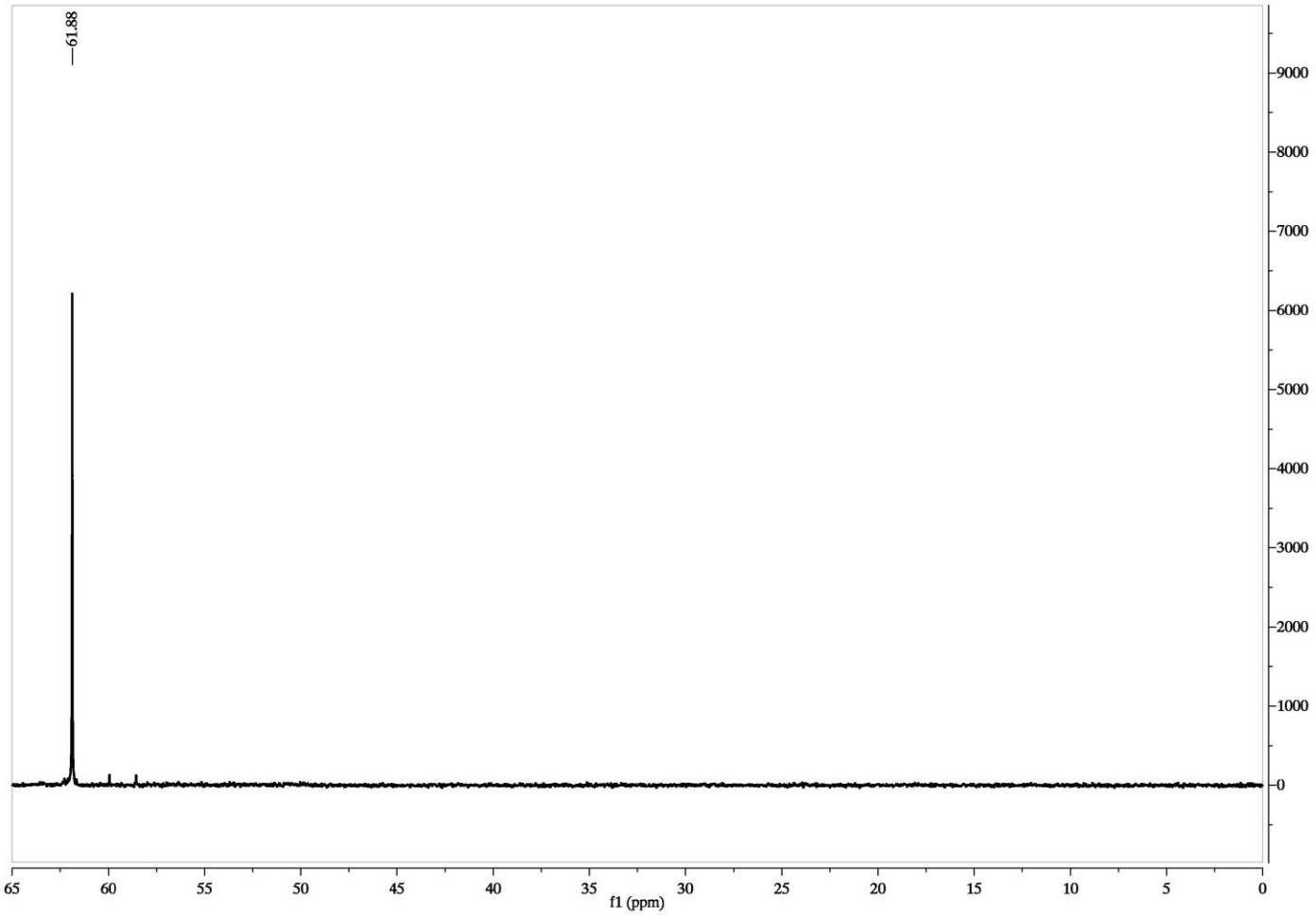

Figure S41. $^{31}P\{^{1}H\}$ NMR spectrum of **4^{Pipp}** in d_5-bromobenzene.

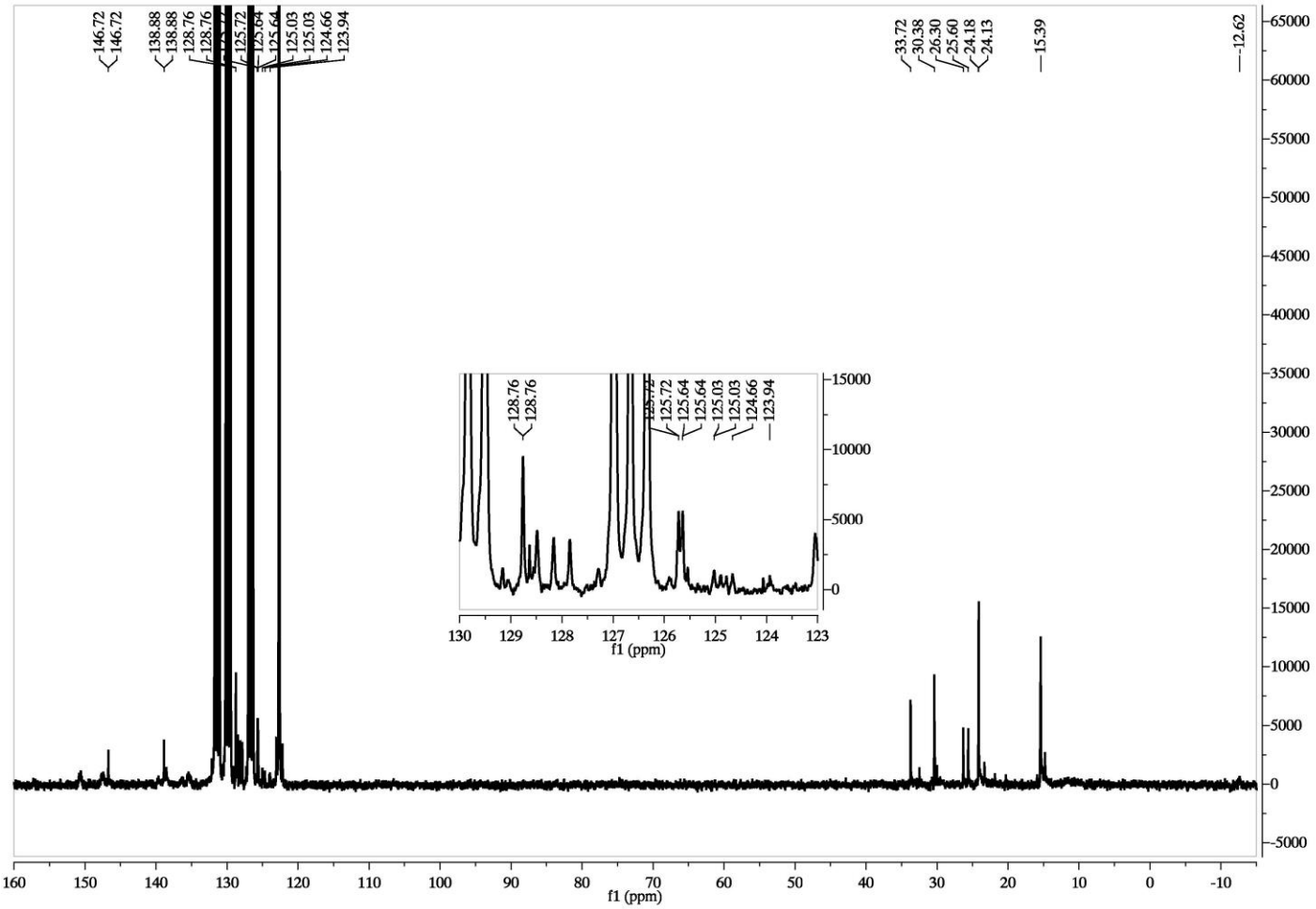

Figure S42. $^{13}C\{^{1}H\}$ NMR spectrum of **4^{Pipp}** in d_5-bromobenzene.

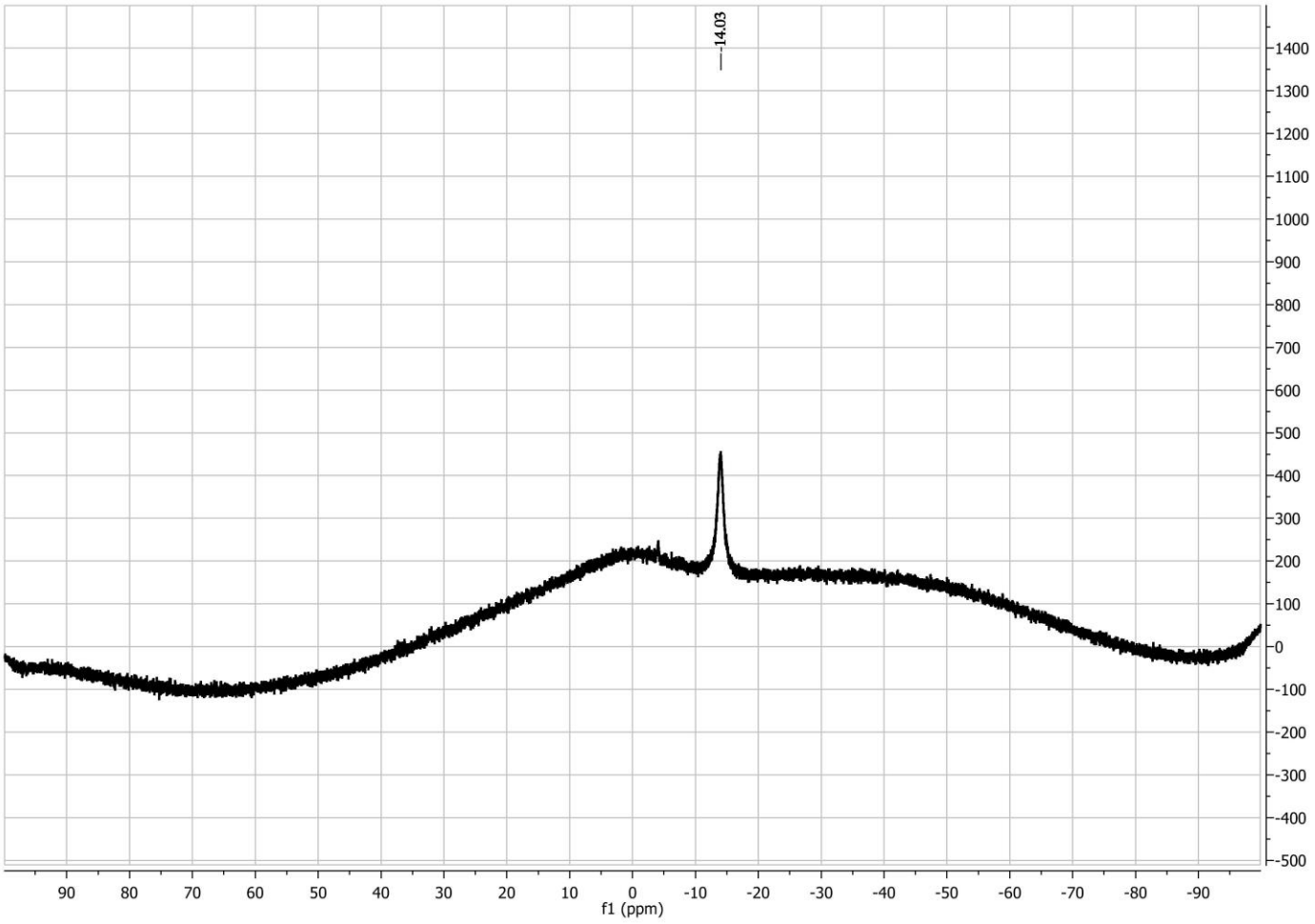

Figure S43. $^{11}B\{^{1}H\}$ NMR spectrum of **4^{Pipp}** in d_5-bromobenzene.

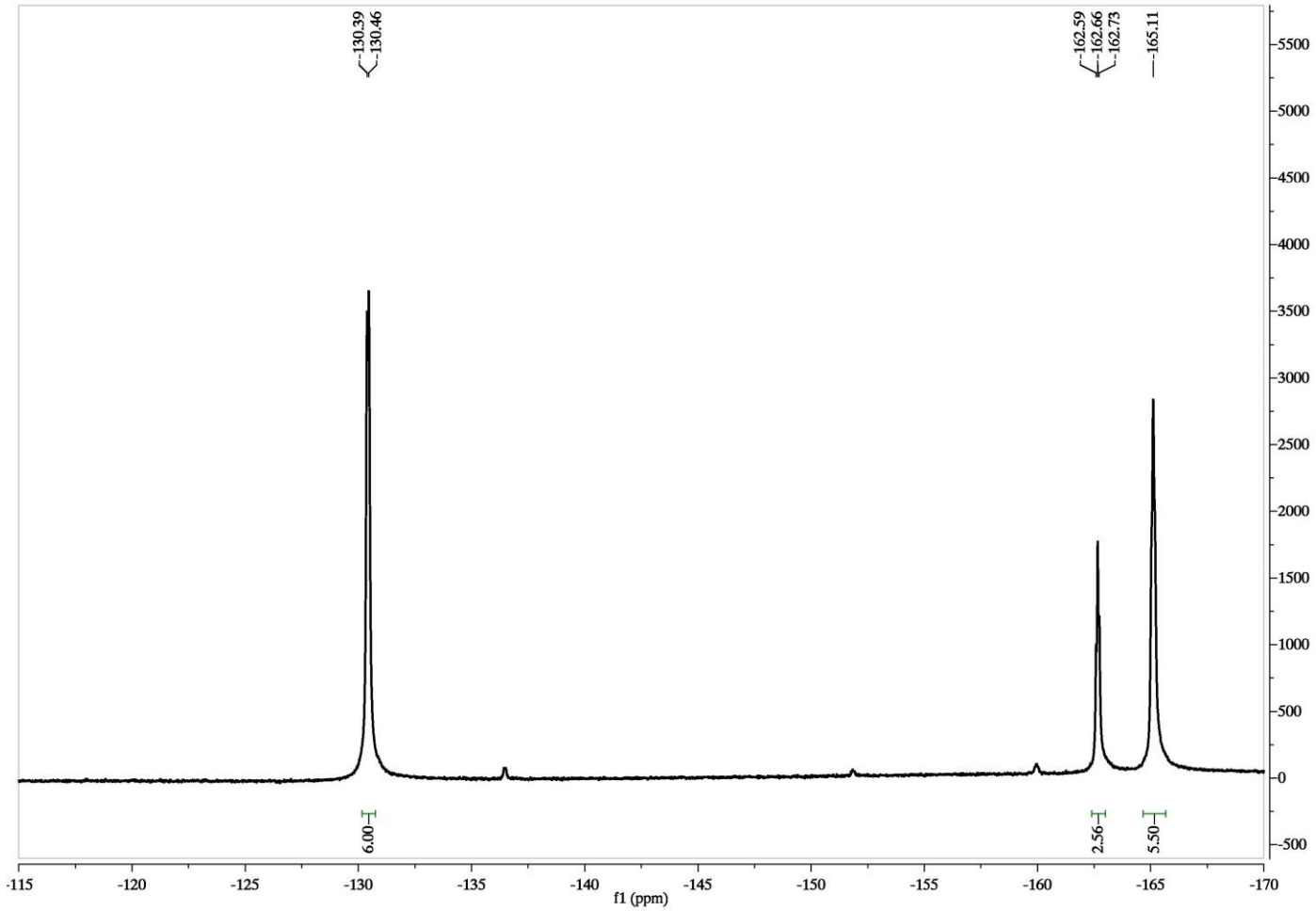

Figure S44. $^{19}F\{^{1}H\}$ NMR spectrum of **4^{Pipp}** in d_5-bromobenzene.

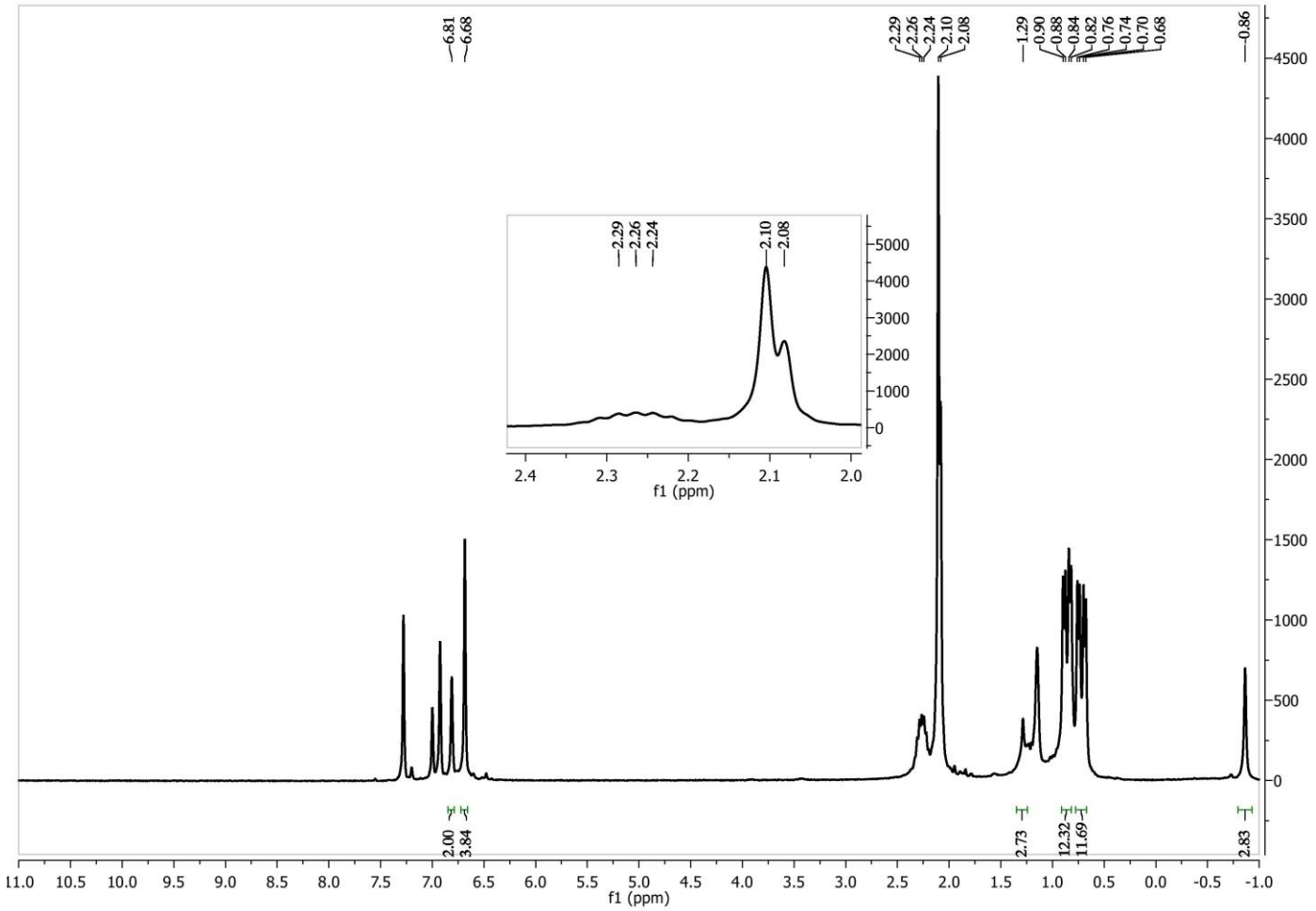

Figure S45. ^{1}H NMR spectrum **4^{Mes}** in d_5-bromobenzene. Pentane is present as a minor impurity.

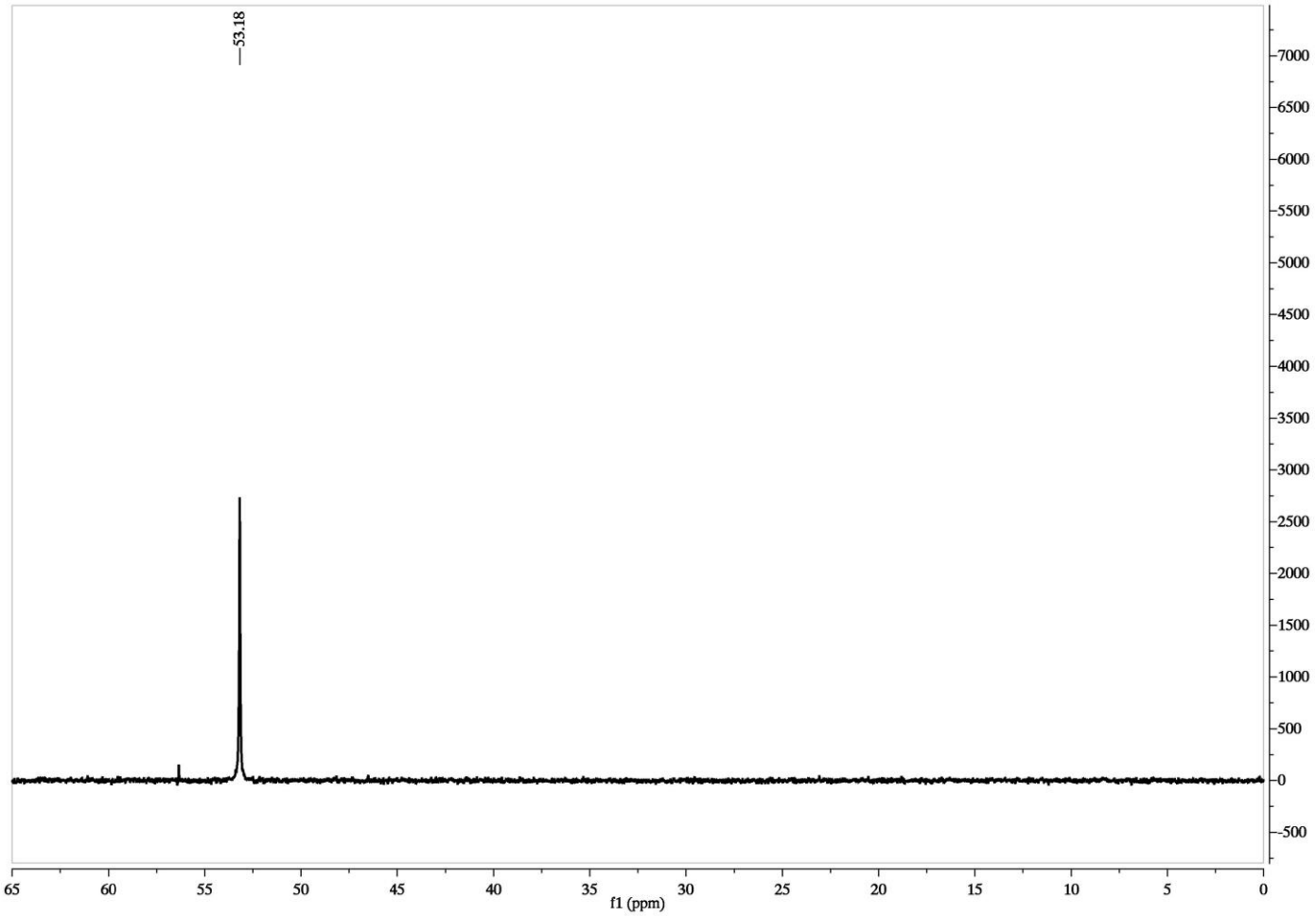

Figure S46. $^{31}P\{^{1}H\}$ NMR spectrum of **4^{Mes}** in d_5-bromobenzene.

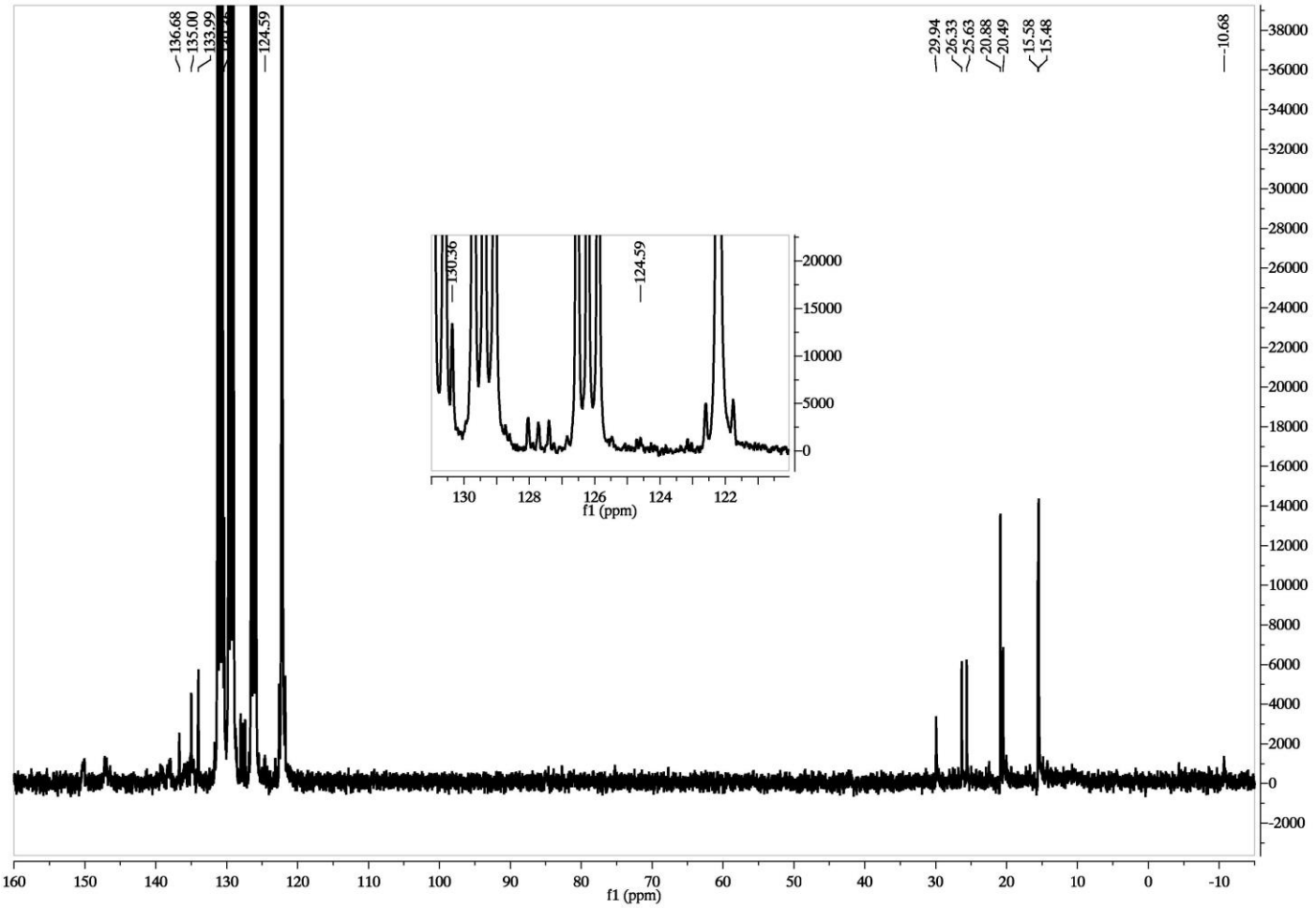

Figure S47. $^{13}C\{^{1}H\}$ NMR spectrum of **4^{Mes}** in d_5-bromobenzene.

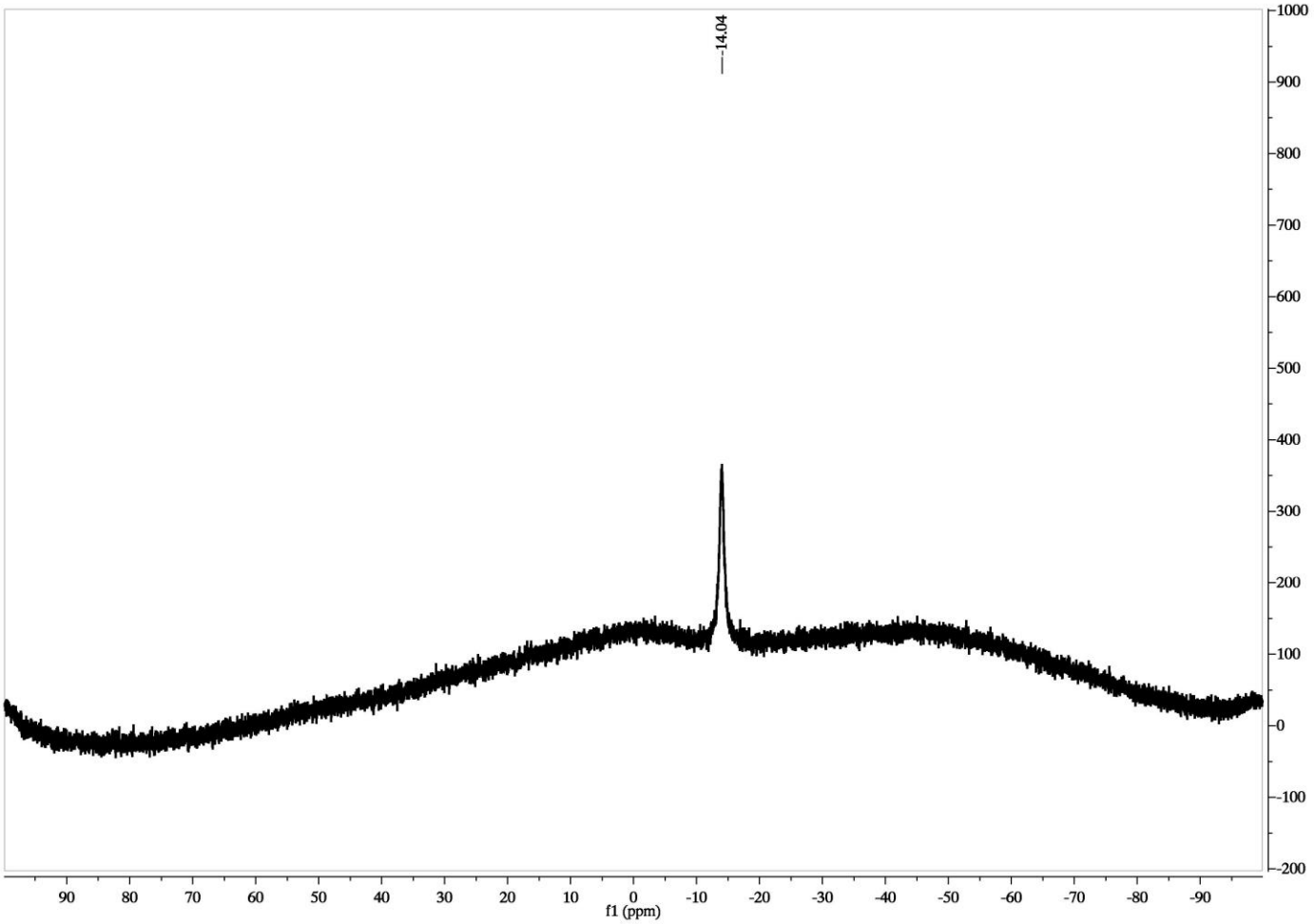

Figure S48. $^{11}B\{^{1}H\}$ NMR spectrum of **4^{Mes}** in d_5-bromobenzene.

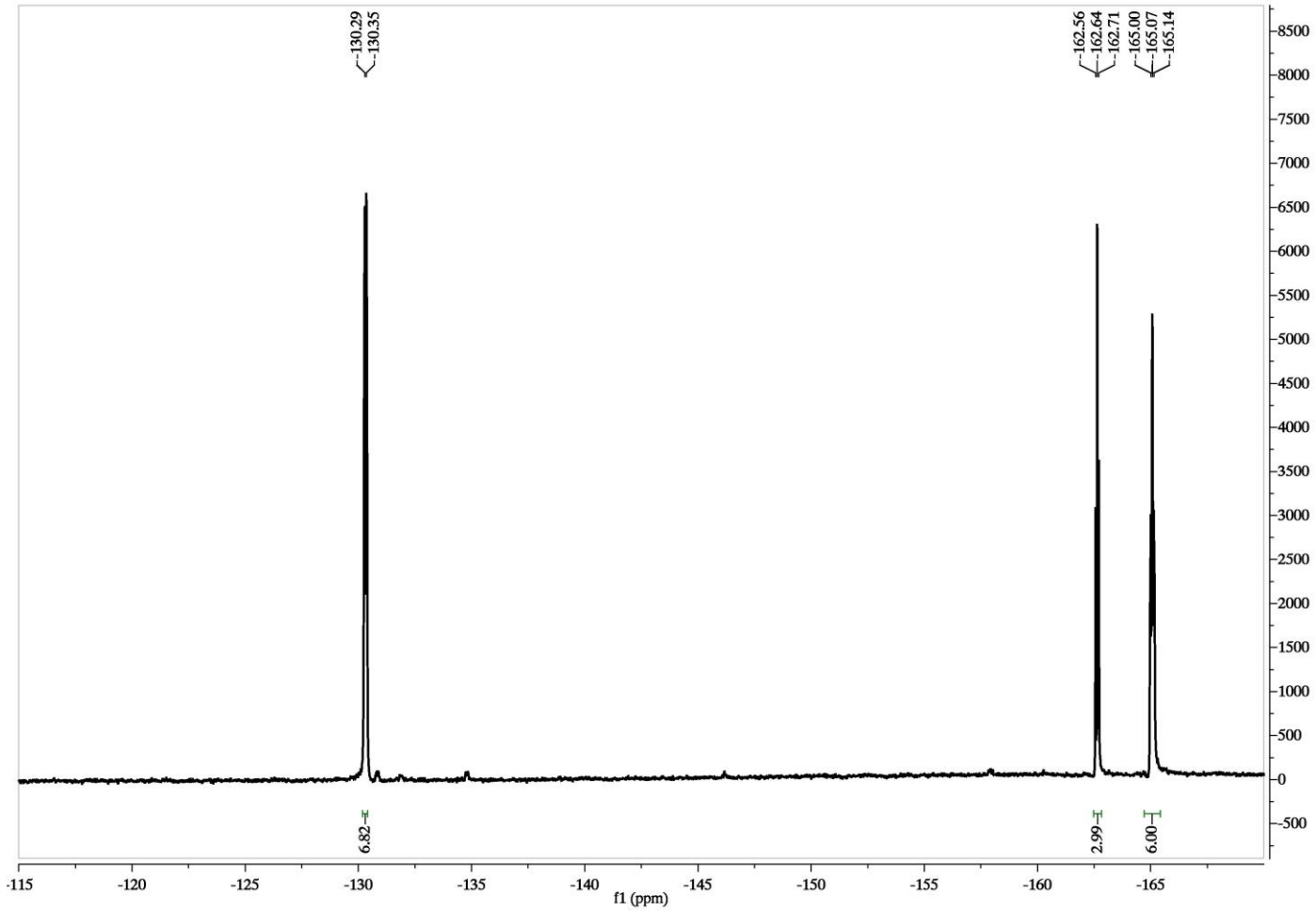

Figure S49. $^{19}F\{^{1}H\}$ NMR spectrum of **4^{Mes}** in d_5-bromobenzene.

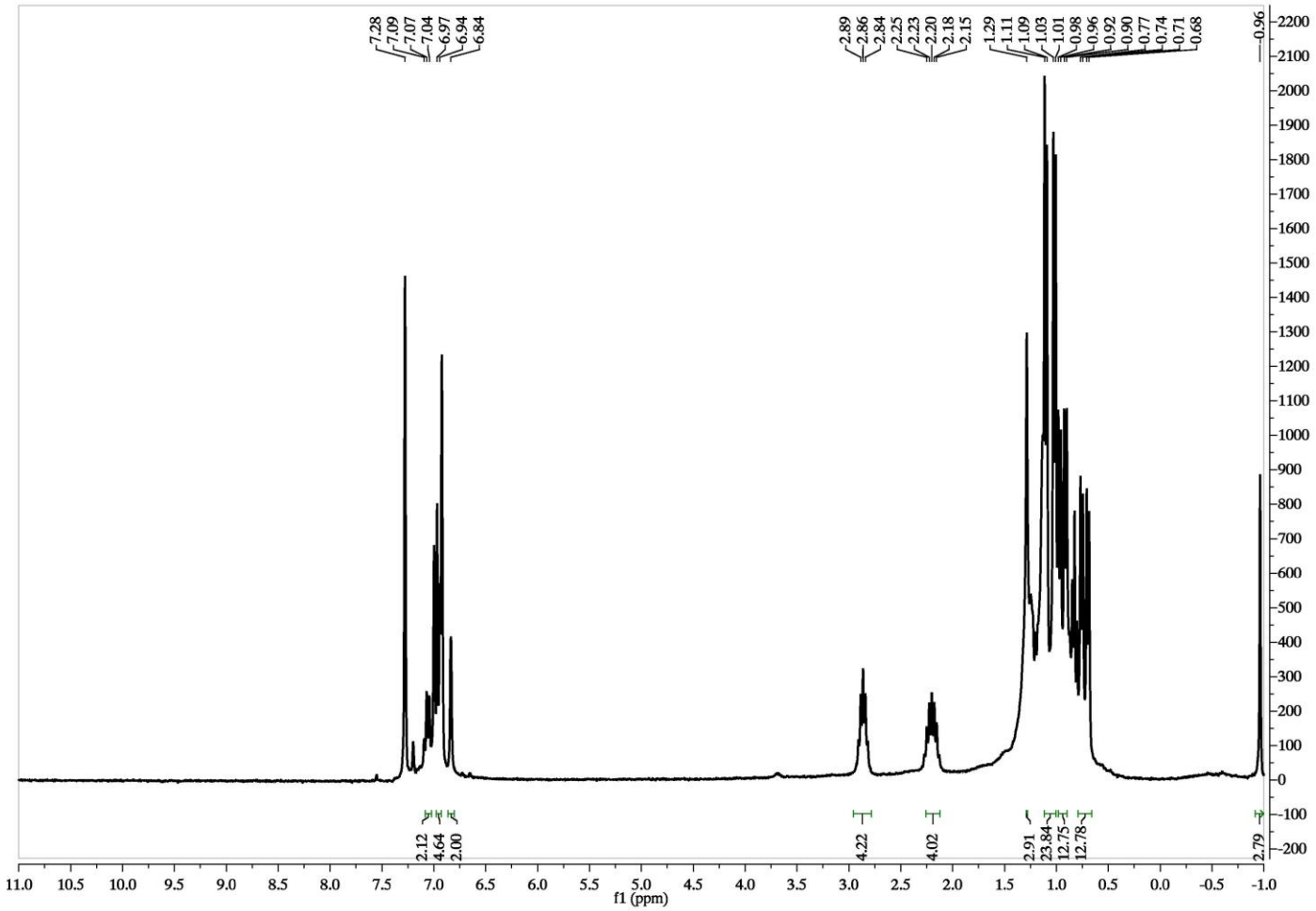

Figure S50. ^{1}H NMR spectrum of **4^{Dipp}** in d_5-bromobenzene.

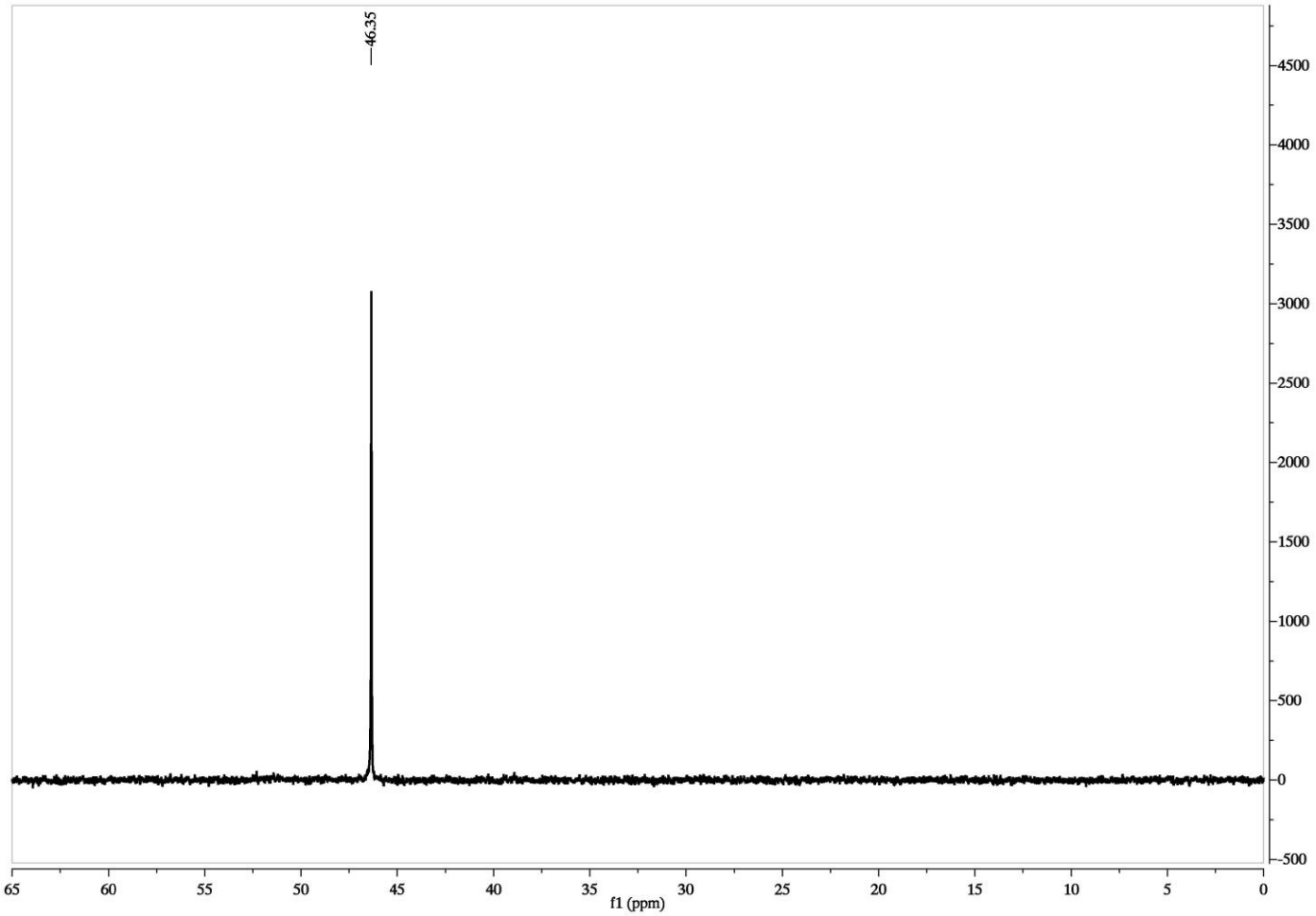

Figure S51. $^{31}P\{^{1}H\}$ NMR spectrum of **4^{Dipp}** in d_5-bromobenzene.

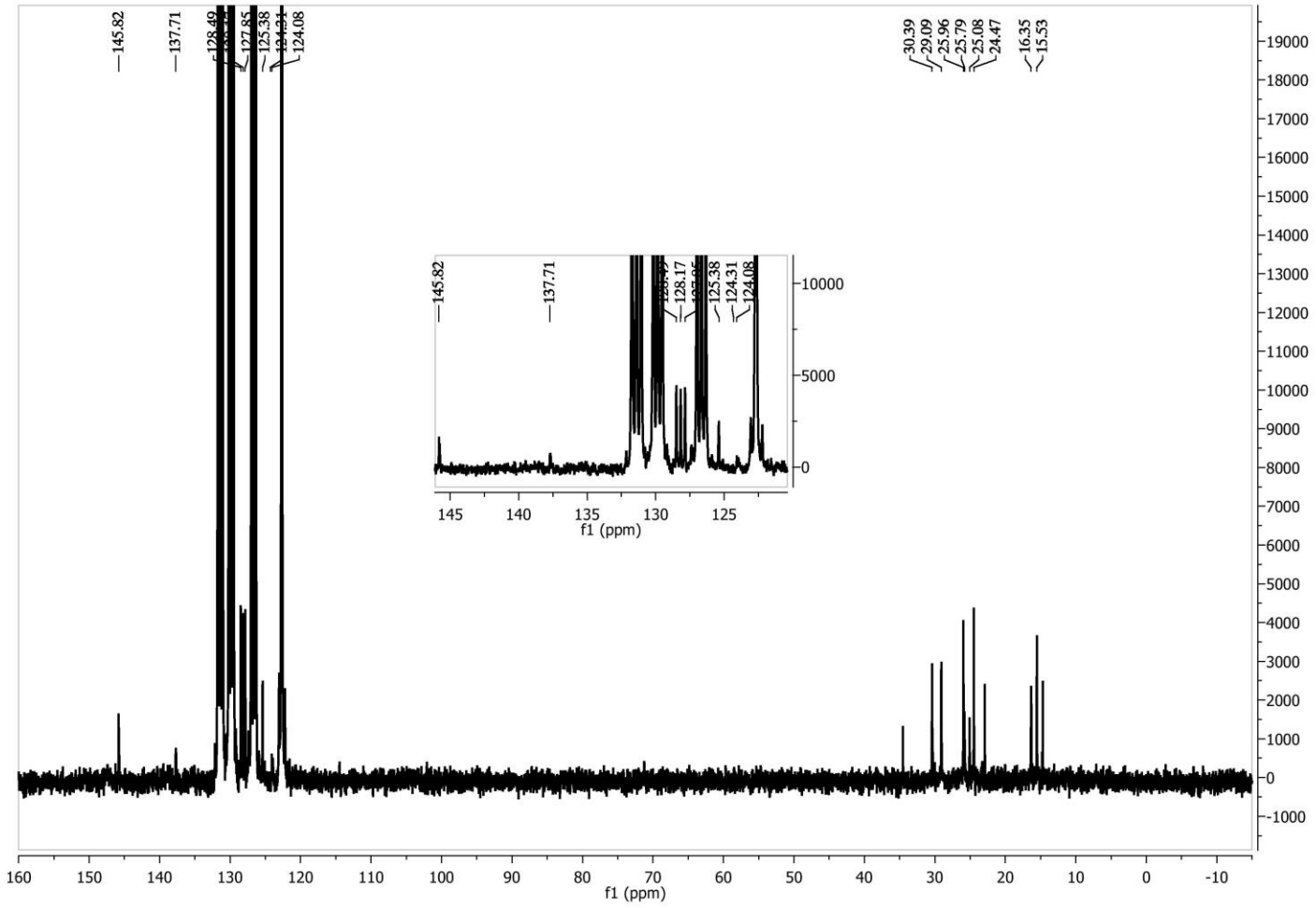

Figure S52. $^{13}C\{^{1}H\}$ NMR spectrum of **4^{Dipp}** in d_5-bromobenzene.

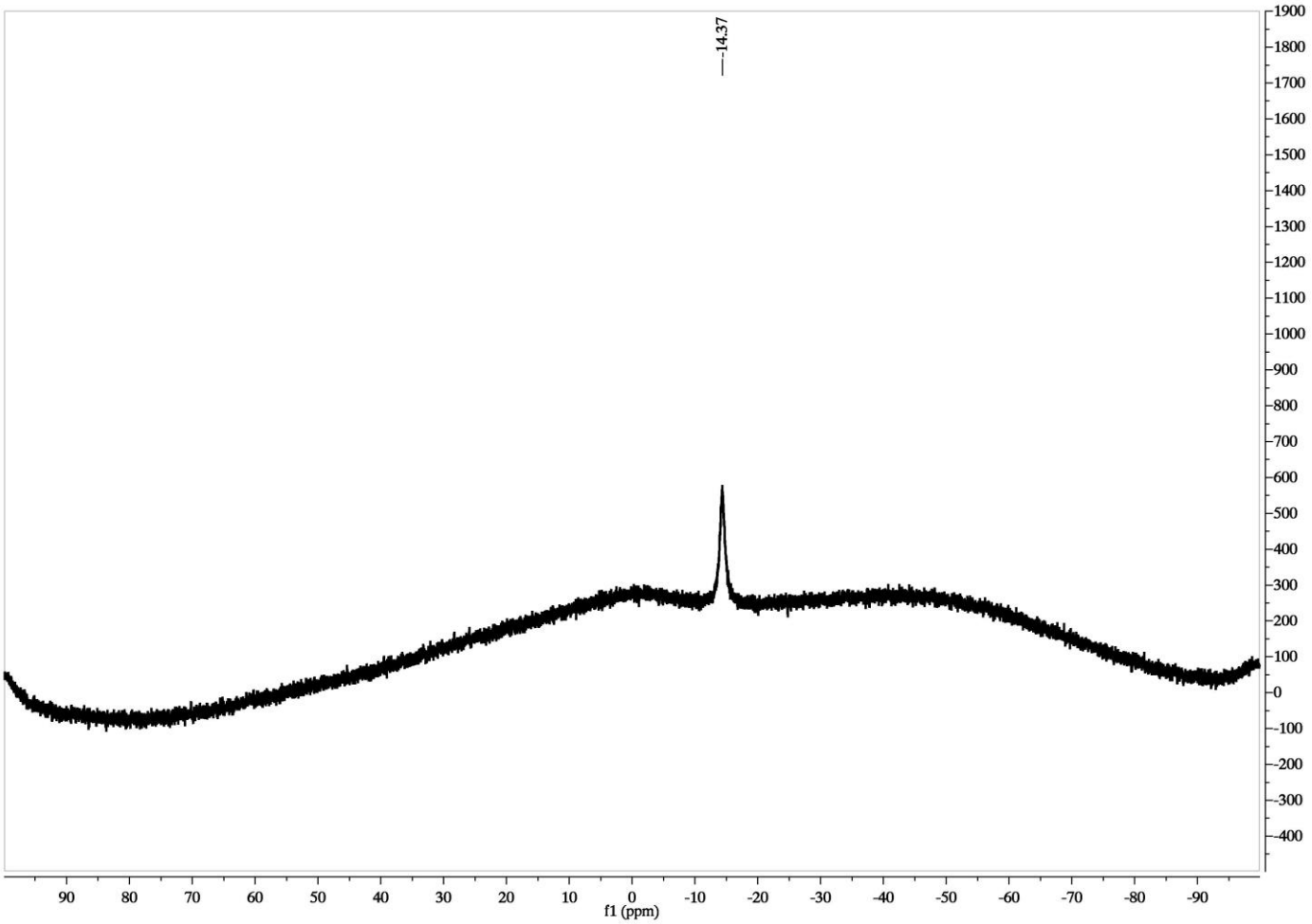

Figure S53. $^{11}B\{^{1}H\}$ NMR spectrum of **4^{Dipp}** in d_5-bromobenzene.

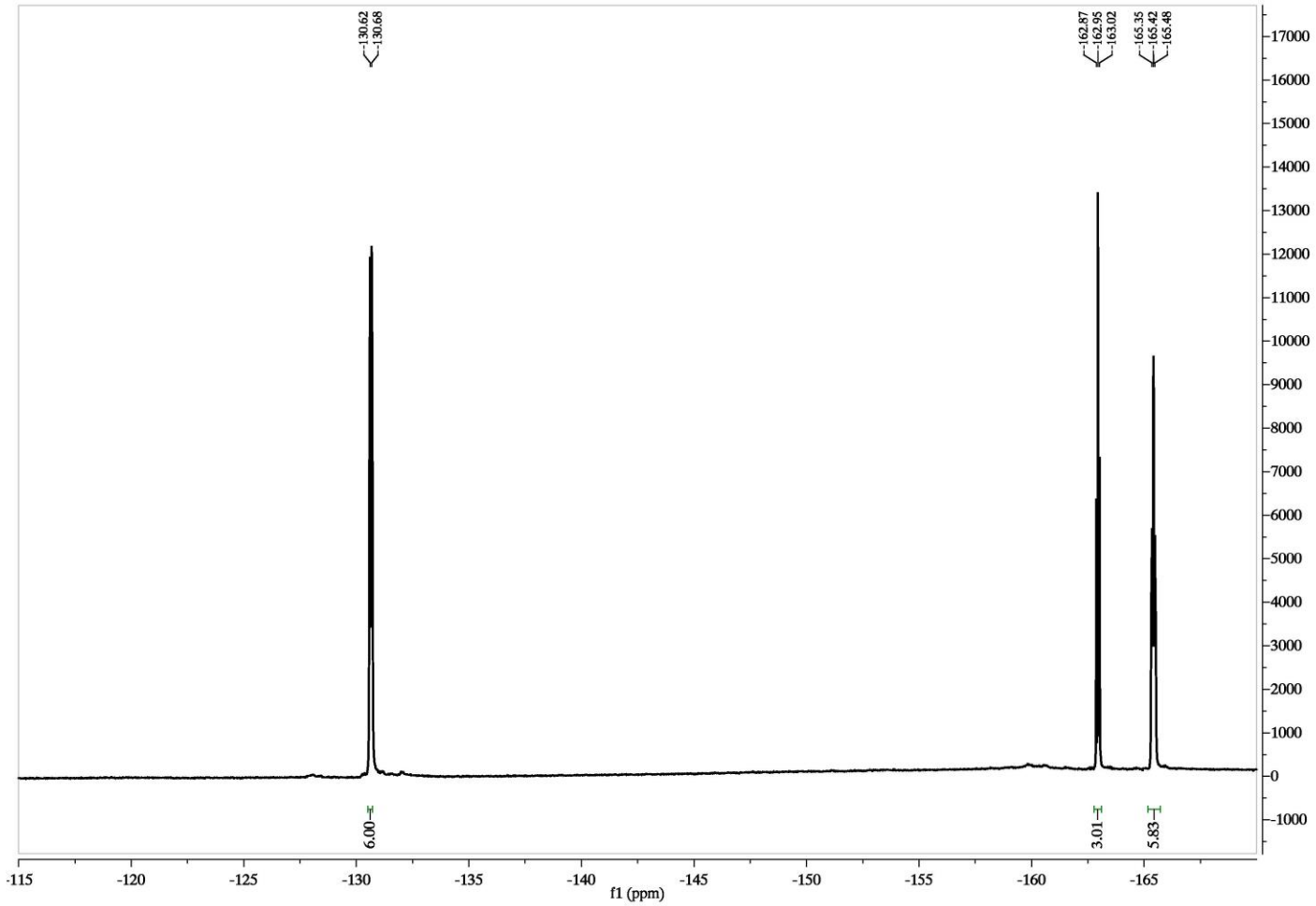

Figure S54. $^{19}F\{^{1}H\}$ NMR spectrum of **4^{Dipp}** in d_5-bromobenzene.

II. Crystallographic Details

X-Ray Diffraction Techniques. All structures were collected on a Rigaku SuperNova diffractometer equipped with a Dectris Pilatus 3R 200K-A hybrid-pixel-array detector, a four-circle κ goniometer, sealed graphite-monochromated Mo Kα (λ = 0.71073 Å) and Cu Kα (λ = 1.54178 Å) X-ray sources, and an Oxford cryostream-cooling device fixed at 100 K. Single crystals suitable for X-ray diffraction studies were mounted on a MiTiGen cryo-loop using desiccated Paratone–N oil stored in a glove box. Structures were solved by the Intrinsic Phasing methods and refined by least-squares methods using SHELXT-2014 and SHELXL-2014 through the OLEX2 interface.[1-3] The program PLATON served to prove the absence of higher symmetry space groups.[4] Non-H atoms were located in difference Fourier maps, and then refined anisotropically. Outlier reflections were omitted from refinement when appropriate. Hydrogen atoms on C atoms were placed at idealized positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the atoms they are linked to (1.5 times for methyl groups). Crystallographic refinement details, including disorder modeling and software employed, have been delineated within each crystallographic information file (*.cif). Molecular graphics were generated in the program Mercury.

Table S1: Single crystal X-ray diffraction details for $\mathbf{L^{Mes}}\cdot C_6H_6$, $\mathbf{L^{Dipp}}$, $\mathbf{1^{Dipp}}\cdot 0.5\ C_6H_6$ and $\mathbf{2^{Pipp}}$.

	$\mathbf{L^{Mes}}\cdot C_6H_6$	$\mathbf{L^{Dipp}}$	$\mathbf{1^{Dipp}}\cdot 0.5\ C_6H_6$	$\mathbf{2^{Pipp}}$
Crystal Size (mm)	0.19 x 0.18 x 0.09	0.086 x 0.068 x 0.035	0.32 x 0.16 x 0.07	0.17 x 0.03 x 0.03
Formula	$C_{40}H_{59}N_3P_2$	$C_{40}H_{65}N_3P_2$	$C_{43}H_{67}Cl_2GaN_3P_2$	$C_{34}H_{52}Cl_2InN_3P_2$
Formula Weight (g/mol)	643.84	649.89	828.55	750.44
λ (nm)	1.54184	1.54184	1.54184	1.54184
T (K)	100.02)	100.0(2)	100.01(13)	100.0(4)
Crystal System	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
Space Group	$P2_1/c$	$Pna2_1$	$P2_1/c$	$P2_1/c$
a (Å)	11.6933(2)	18.1046(3)	9.50090(10)	16.3379(2)
b (Å)	22.3999(3)	8.30160(10)	18.34940(10)	23.9920(2)
c (Å)	14.5398(2)	26.1934(4)	25.5029(2)	20.6103(2)
α (°)	90	90	90	90
β (°)	97.5960(10)	90	99.4290(10)	112.9950(10)
γ (°)	90	90	90	90
Z	4	4	4	8
Volume (Å^3)	3774.97(10)	3936.79(10)	4386.00(6)	7436.85(14)
Calc. ρ (g/cm^3)	1.133	1.096	1.255	1.341
μ (mm^{-1})	1.262	1.211	2.905	7.406
Independent Reflections	8034	7740	9471	15266
R_1, wR_2 [$I > 2\sigma(I)$]	0.0485, 0.1276	0.0358, 0.0890	0.0295, 0.0754	0.0422, 0.1183
GOF on F^2	1.059	1.064	1.066	1.040

Table S2: Single crystal X-ray diffraction details for **2**^{Mes}, **2**^{Dipp}·0.5 C_6H_6, **3**^{Pipp} and **3**^{Mes}.

	2^{Mes}	**2**^{Dipp}·0.5 C_6H_6	**3**^{Pipp}	**3**^{Mes}
Crystal Size (mm)	0.16 x 0.04 x 0.02	0.19 x 0.02 x 0.02	0.14 x 0.11 x 0.08	0.12 x 0.08 x 0.06
Formula	$C_{34}H_{52}Cl_2InN_3P_2$	$C_{43}H_{67}Cl_2InN_3P_2$	$C_{36}H_{58}AlN_3P_2$	$C_{36}H_{58}AlN_3P_2$
Formula Weight (g/mol)	750.44	873.65	621.77	621.77
λ (nm)	1.54184	1.54184	1.54184	1.54184
T (K)	293(2)	102.(3)	100.0(2)	100.0(3)
Crystal System	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space Group	$P2_1/c$	$P2_1/c$	$P2_1/n$	P-1
a (Å)	9.28430(10)	9.70160(10)	16.2453(2)	8.5179(4)
b (Å)	19.1068(3)	18.35830(10)	24.0373(2)	14.3557(4)
c (Å)	20.8295(3)	25.5187(2)	20.6341(3)	16.0481(4)
α (°)	90	90	90	66.419(4)
β (°)	92.3340(10)	99.6690(10)	112.9775(10)	82.147(3)
γ (°)	90	90	90	77.448(3)
Z	4	4	4	2
Volume (Å^3)	3691.95(9)	4480.44(6)	7418.18(18)	1752.81(11)
Calc. ρ (g/cm^3)	1.350	1.295	1.113	1.178
μ (mm^{-1})	7.459	6.220	1.485	1.572
Independent Reflections	7991	9708	13277	7267
R_1, wR_2 [$I > 2\sigma(I)$]	0.0326, 0.0875	0.0295, 0.0727	0.0337, 0.0851	0.0602, 0.1848
GOF on F^2	1.065	1.084	1.059	1.053

Table S3 Fractional Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **L^{Mes}**·C_6H_6. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	2627.1(4)	1784.4(2)	5019.4(3)	18.12(11)
P2	5871.1(4)	3406.4(2)	4359.2(3)	17.38(11)
N1	4311.2(12)	2553.9(6)	4698.0(9)	19.0(3)
N2	2283.7(13)	1897.0(6)	3957.5(10)	21.4(3)
N3	4937.8(13)	3541.6(7)	3516.2(10)	21.5(3)
C26	4451.6(15)	4066.4(8)	3116.8(11)	19.4(3)
C27	3316.2(15)	4227.5(8)	3257.3(11)	21.2(3)
C11	1867.4(16)	1534.7(7)	3209.5(11)	19.2(3)
C1	3989.7(15)	2153.5(7)	5326.0(11)	19.7(3)
C16	675.4(16)	1431.1(8)	2978.0(12)	21.4(3)
C15	271.6(16)	1097.8(8)	2195.5(12)	23.3(3)
C12	2629.9(15)	1303.6(8)	2616.8(11)	21.0(3)
C4	5314.9(15)	2832.8(8)	5041.7(11)	20.4(3)
C2	4816.9(16)	2175.5(8)	6100.2(12)	24.6(4)
C21	6291.2(15)	4001.8(8)	5196.7(12)	21.9(3)
C28	2808.1(16)	4737.5(8)	2833.7(12)	24.1(4)
C14	1016.0(17)	852.5(8)	1625.4(12)	23.9(4)
C13	2193.3(17)	958.7(8)	1856.3(12)	22.7(3)
C30	4485.3(17)	4933.8(8)	2117.2(12)	24.9(4)
C31	5022.3(16)	4421.0(8)	2510.2(11)	22.0(3)
C3	5647.3(16)	2601.5(9)	5921.6(12)	25.1(4)
C6	1657.7(16)	2146.4(8)	5739.4(12)	22.6(3)
C9	2807.1(16)	1015.4(8)	5439.6(12)	22.7(3)
C32	2661.5(16)	3849.2(9)	3866.3(12)	24.4(4)
C20	5211.4(16)	4253.5(8)	5554.0(12)	25.0(4)
C10	3637.5(19)	667.8(8)	4904.9(13)	28.4(4)
C24	7202.0(15)	3092.5(8)	4021.7(12)	23.2(4)
C29	3385.0(17)	5104.9(8)	2270.0(12)	26.1(4)
C7	2047.9(18)	2078.6(9)	6787.6(12)	29.1(4)
C34	6193.2(17)	4252.9(9)	2272.7(13)	27.8(4)
C17	3895.3(16)	1458.0(9)	2782.9(12)	25.6(4)
C23	8143.2(16)	2974.8(9)	4840.2(13)	28.9(4)
C5	1508.6(18)	2802.3(8)	5460.2(13)	28.4(4)
C22	6986.2(17)	4493.4(8)	4784.6(14)	27.7(4)
C8	1638.1(18)	703.2(9)	5390.5(14)	29.9(4)
C25	6894.6(19)	2524.5(10)	3454.1(14)	33.6(4)
C19	−164.4(17)	1699.1(9)	3564.5(14)	28.8(4)
C33	2847(2)	5675.9(9)	1859.7(15)	35.8(5)
C18	552(2)	515.6(10)	758.9(13)	33.5(4)
C014	8573(2)	4209.9(11)	1016.7(17)	40.0(5)
C015	9502(2)	4184.9(13)	2580.7(18)	47.2(6)
C016	8542(2)	3593.5(11)	997.4(16)	39.4(5)
C017	9478(2)	3568.4(13)	2565.2(17)	45.0(6)
C018	9048(2)	4508.7(11)	1808.5(19)	43.8(5)
C019	8997(2)	3269.3(11)	1772.7(17)	40.0(5)

Table S4 Anisotropic Displacement Parameters ($Å^2×10^3$) for $\mathbf{L^{Mes}}\cdot C_6H_6$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	25.0(2)	15.5(2)	13.5(2)	-0.94(14)	1.33(15)	-1.78(15)
P2	21.1(2)	16.2(2)	14.3(2)	0.12(14)	0.51(15)	-0.30(15)
N1	25.0(7)	17.3(7)	13.8(6)	1.1(5)	-0.3(5)	-1.1(5)
N2	30.4(8)	17.9(7)	15.5(7)	-1.2(5)	0.7(5)	-2.8(6)
N3	25.2(7)	19.0(7)	19.1(7)	-0.6(5)	-1.2(5)	0.2(6)
C26	25.8(8)	18.7(8)	12.7(7)	-1.0(6)	-1.2(6)	-0.4(6)
C27	25.5(8)	22.7(8)	14.2(7)	-1.5(6)	-1.6(6)	-0.9(7)
C11	28.8(9)	15.3(7)	13.2(7)	0.9(6)	0.8(6)	0.5(6)
C1	26.4(8)	17.6(8)	14.9(7)	1.0(6)	1.9(6)	-1.1(6)
C16	28.6(9)	17.3(8)	18.1(8)	-0.5(6)	2.0(6)	0.2(7)
C15	27.5(9)	20.0(8)	21.3(8)	-0.5(6)	-1.0(6)	-1.7(7)
C12	27.7(9)	18.8(8)	16.2(7)	3.5(6)	1.3(6)	2.8(6)
C4	23.5(8)	19.5(8)	17.4(7)	-0.8(6)	-0.2(6)	-0.9(6)
C2	31.0(9)	25.1(9)	16.3(8)	4.7(6)	-2.3(7)	-2.7(7)
C21	25.4(8)	20.9(8)	18.7(8)	-2.7(6)	0.1(6)	-3.1(7)
C28	26.3(8)	25.5(9)	19.3(8)	-2.9(7)	-1.1(6)	4.2(7)
C14	36.2(9)	17.3(8)	17.1(8)	-1.8(6)	-0.2(7)	-0.8(7)
C13	34.5(9)	17.2(8)	16.6(7)	0.8(6)	4.0(6)	3.2(7)
C30	35.9(9)	21.1(8)	16.6(8)	1.2(6)	0.2(7)	-4.6(7)
C31	27.3(8)	22.7(8)	15.4(7)	-1.2(6)	0.7(6)	-2.1(7)
C3	27.8(9)	27.8(9)	18.1(8)	3.5(7)	-3.1(6)	-3.5(7)
C6	28.1(9)	23.2(9)	17.0(8)	-4.2(6)	4.3(6)	-3.5(7)
C9	34.2(9)	14.5(8)	18.6(8)	2.3(6)	1.1(7)	-1.0(7)
C32	25.2(8)	29.7(9)	17.9(8)	1.2(7)	1.6(6)	0.5(7)
C20	29.6(9)	23.6(9)	21.6(8)	-4.5(7)	3.1(7)	-1.0(7)
C10	43.1(11)	20.5(9)	21.9(8)	0.2(7)	4.9(7)	5.1(8)
C24	23.3(8)	26.0(9)	20.0(8)	0.4(7)	2.4(6)	5.0(7)
C29	37.4(10)	20.2(8)	18.6(8)	0.2(6)	-3.9(7)	2.5(7)
C7	39.6(10)	31.9(10)	16.6(8)	-4.9(7)	6.3(7)	-3.3(8)
C34	30.2(9)	29.7(9)	24.3(9)	2.5(7)	6.1(7)	-1.8(8)
C17	28.7(9)	27.0(9)	21.0(8)	2.6(7)	3.1(7)	1.0(7)
C23	24.3(9)	32.9(10)	27.7(9)	-1.5(8)	-2.9(7)	5.0(7)
C5	35.9(10)	23.1(9)	26.9(9)	-4.1(7)	6.8(7)	0.6(8)
C22	30.7(9)	21.4(9)	31.2(9)	-3.9(7)	5.0(7)	-7.0(7)
C8	40.5(11)	20.2(8)	28.1(9)	2.9(7)	1.7(8)	-5.9(8)
C25	36.0(10)	35.1(11)	28.1(9)	-9.5(8)	-2.1(8)	12.1(9)
C19	27.1(9)	28.3(9)	30.8(10)	-8.7(8)	3.6(7)	0.6(7)
C33	49.3(12)	24.0(10)	31.3(10)	3.3(8)	-5.4(9)	7.7(9)
C18	44.9(11)	32.9(10)	21.9(9)	-10.3(8)	1.0(8)	-4.9(9)
C014	42.4(12)	38.2(12)	41.3(12)	-1.4(9)	12.3(9)	1.0(10)
C015	33.7(11)	59.2(16)	48.7(14)	-20.0(12)	4.9(10)	-5.6(11)
C016	43.7(12)	40.3(12)	35.4(11)	-7.5(9)	10.0(9)	-2.3(10)
C017	34.4(11)	59.6(15)	40.9(12)	1.5(11)	4.2(9)	3.2(11)
C018	36.6(12)	36.7(12)	60.0(15)	-12.9(11)	13.6(10)	-5.8(9)
C019	40.9(12)	34.8(11)	46.0(13)	-1.9(9)	11.6(10)	-0.8(9)

Table S5 Bond Lengths for $\mathbf{L^{Mes}}\cdot C_6H_6$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	N2	1.5636(14)	C4	C3	1.387(2)
P1	C1	1.7981(18)	C2	C3	1.410(3)
P1	C6	1.8309(18)	C21	C20	1.535(2)
P1	C9	1.8306(17)	C21	C22	1.537(2)
P2	N3	1.5592(15)	C28	C29	1.396(3)
P2	C4	1.7969(18)	C14	C13	1.394(3)
P2	C21	1.8288(17)	C14	C18	1.507(2)
P2	C24	1.8328(18)	C30	C31	1.395(3)
N1	C1	1.367(2)	C30	C29	1.388(3)
N1	C4	1.365(2)	C31	C34	1.504(3)
N2	C11	1.392(2)	C6	C7	1.539(2)
N3	C26	1.398(2)	C6	C5	1.528(3)
C26	C27	1.416(2)	C9	C10	1.534(3)
C26	C31	1.418(2)	C9	C8	1.529(3)
C27	C28	1.393(3)	C24	C23	1.533(2)
C27	C32	1.506(2)	C24	C25	1.533(3)
C11	C16	1.409(3)	C29	C33	1.513(3)
C11	C12	1.417(2)	C014	C016	1.381(3)
C1	C2	1.385(2)	C014	C018	1.383(3)
C16	C15	1.390(2)	C015	C017	1.381(4)
C16	C19	1.508(3)	C015	C018	1.382(4)
C15	C14	1.392(3)	C016	C019	1.387(4)
C12	C13	1.390(2)	C017	C019	1.386(4)
C12	C17	1.508(3)			

Table S6 Bond Angles for $\mathbf{L^{Mes}}\cdot C_6H_6$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	P1	C1	105.91(8)	N1	C4	C3	106.81(15)
N2	P1	C6	113.31(8)	C3	C4	P2	134.31(14)
N2	P1	C9	118.98(8)	C1	C2	C3	107.37(15)
C1	P1	C6	104.47(8)	C20	C21	P2	109.43(12)
C1	P1	C9	106.91(8)	C20	C21	C22	111.71(15)
C9	P1	C6	106.16(8)	C22	C21	P2	111.87(12)
N3	P2	C4	107.83(8)	C27	C28	C29	122.13(17)
N3	P2	C21	118.70(8)	C15	C14	C13	117.70(16)
N3	P2	C24	113.26(8)	C15	C14	C18	120.76(18)
C4	P2	C21	103.81(8)	C13	C14	C18	121.44(17)
C4	P2	C24	104.82(8)	C12	C13	C14	122.27(17)
C21	P2	C24	107.16(8)	C29	C30	C31	122.58(17)
C4	N1	C1	110.78(14)	C26	C31	C34	121.36(16)
C11	N2	P1	134.03(12)	C30	C31	C26	119.53(17)
C26	N3	P2	133.92(13)	C30	C31	C34	119.10(16)
N3	C26	C27	119.44(15)	C4	C3	C2	107.87(15)
N3	C26	C31	122.04(16)	C7	C6	P1	113.42(13)
C27	C26	C31	118.31(16)	C5	C6	P1	109.35(12)
C26	C27	C32	120.04(16)	C5	C6	C7	111.49(15)

C28	C27	C26	119.88(16)	C10	C9	P1	111.16(12)
C28	C27	C32	120.08(16)	C8	C9	P1	110.62(13)
N2	C11	C16	121.01(16)	C8	C9	C10	111.47(15)
N2	C11	C12	120.31(16)	C23	C24	P2	113.95(13)
C16	C11	C12	118.46(15)	C25	C24	P2	108.39(13)
N1	C1	P1	116.66(12)	C25	C24	C23	111.60(16)
N1	C1	C2	107.18(15)	C28	C29	C33	121.43(19)
C2	C1	P1	135.96(13)	C30	C29	C28	117.46(16)
C11	C16	C19	119.79(16)	C30	C29	C33	121.10(18)
C15	C16	C11	120.14(16)	C016	C014	C018	120.5(2)
C15	C16	C19	120.03(17)	C017	C015	C018	120.4(2)
C16	C15	C14	121.86(17)	C014	C016	C019	120.0(2)
C11	C12	C17	120.12(16)	C015	C017	C019	120.1(2)
C13	C12	C11	119.50(17)	C015	C018	C014	119.4(2)
C13	C12	C17	120.30(16)	C017	C019	C016	119.5(2)
N1	C4	P2	118.80(12)				

Table S7 Torsion Angles for **L**$^{\mathbf{Mes}}$·C_6H_6.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
P1	N2	C11	C16	87.0(2)	C15	C14	C13	C12	-1.0(3)
P1	N2	C11	C12	-98.4(2)	C12	C11	C16	C15	1.4(2)
P1	C1	C2	C3	-174.37(16)	C12	C11	C16	C19	-176.66(16)
P2	N3	C26	C27	-105.44(19)	C4	P2	N3	C26	132.26(17)
P2	N3	C26	C31	79.8(2)	C4	P2	C21	C20	-65.64(13)
P2	C4	C3	C2	176.39(15)	C4	P2	C21	C22	170.01(13)
N1	C1	C2	C3	0.1(2)	C4	P2	C24	C23	-64.50(15)
N1	C4	C3	C2	0.0(2)	C4	P2	C24	C25	60.41(14)
N2	P1	C1	N1	14.84(15)	C4	N1	C1	P1	175.60(12)
N2	P1	C1	C2	-171.12(19)	C4	N1	C1	C2	-0.1(2)
N2	P1	C6	C7	-175.38(13)	C21	P2	N3	C26	14.7(2)
N2	P1	C6	C5	-50.27(15)	C21	P2	C4	N1	135.32(14)
N2	P1	C9	C10	52.51(16)	C21	P2	C4	C3	-40.8(2)
N2	P1	C9	C8	-71.90(15)	C21	P2	C24	C23	45.39(16)
N2	C11	C16	C15	176.08(16)	C21	P2	C24	C25	170.29(13)
N2	C11	C16	C19	-2.0(2)	C31	C26	C27	C28	-2.6(2)
N2	C11	C12	C13	-177.92(15)	C31	C26	C27	C32	177.60(15)
N2	C11	C12	C17	-1.1(2)	C31	C30	C29	C28	-0.7(3)
N3	P2	C4	N1	8.55(16)	C31	C30	C29	C33	177.79(17)
N3	P2	C4	C3	-167.54(19)	C6	P1	N2	C11	-112.32(18)
N3	P2	C21	C20	53.96(15)	C6	P1	C1	N1	-105.07(14)
N3	P2	C21	C22	-70.38(15)	C6	P1	C1	C2	69.0(2)
N3	P2	C24	C23	178.22(13)	C6	P1	C9	C10	-178.33(13)
N3	P2	C24	C25	-56.87(15)	C6	P1	C9	C8	57.26(14)
N3	C26	C27	C28	-177.58(15)	C9	P1	N2	C11	13.5(2)
N3	C26	C27	C32	2.6(2)	C9	P1	C1	N1	142.66(13)
N3	C26	C31	C30	178.70(15)	C9	P1	C1	C2	-43.3(2)
N3	C26	C31	C34	-0.7(3)	C9	P1	C6	C7	52.23(15)
C26	C27	C28	C29	-0.4(3)	C9	P1	C6	C5	177.34(13)
C27	C26	C31	C30	3.9(2)	C32	C27	C28	C29	179.43(16)

C27	C26	C31	C34	-175.52(16)	C24	P2	N3	C26	-112.23(18)
C27	C28	C29	C30	2.0(3)	C24	P2	C4	N1	-112.39(14)
C27	C28	C29	C33	-176.46(17)	C24	P2	C4	C3	71.5(2)
C11	C16	C15	C14	0.7(3)	C24	P2	C21	C20	-176.22(12)
C11	C12	C13	C14	3.1(3)	C24	P2	C21	C22	59.43(15)
C1	P1	N2	C11	133.74(18)	C29	C30	C31	C26	-2.3(3)
C1	P1	C6	C7	-60.57(15)	C29	C30	C31	C34	177.15(17)
C1	P1	C6	C5	64.54(14)	C17	C12	C13	C14	-173.74(16)
C1	P1	C9	C10	-67.22(14)	C19	C16	C15	C14	178.73(17)
C1	P1	C9	C8	168.37(12)	C18	C14	C13	C12	175.43(17)
C1	N1	C4	P2	-177.01(12)	C014	C016	C019	C017	0.2(4)
C1	N1	C4	C3	0.1(2)	C015	C017	C019	C016	0.1(4)
C1	C2	C3	C4	0.0(2)	C016	C014	C018	C015	0.5(4)
C16	C11	C12	C13	-3.2(2)	C017	C015	C018	C014	-0.2(4)
C16	C11	C12	C17	173.61(15)	C018	C014	C016	C019	-0.5(4)
C16	C15	C14	C13	-0.9(3)	C018	C015	C017	C019	0.0(4)
C16	C15	C14	C18	-177.35(17)					

Table S8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **L^{Mes}**·C_6H_6.

Atom	*x*	*y*	*z*	U(eq)
H1	3923.58	2622.28	4147.2	23
H15	-535.23	1035.76	2045.57	28
H2	4823.68	1945.9	6650.23	30
H21	6794.18	3822.31	5735.78	26
H28	2044.45	4838.72	2931.46	29
H13	2715.28	789.51	1480.74	27
H30	4888.31	5175.4	1729.85	30
H3	6315.8	2710.84	6331.12	30
H6	885.81	1950.45	5599.48	27
H9	3153.42	1030.42	6105.95	27
H32A	2572.33	3444.78	3609.88	37
H32B	1898.54	4024.52	3892.16	37
H32C	3087.57	3832.23	4493.18	37
H20A	4705.82	4435.03	5038.1	37
H20B	5439.86	4556.31	6029.44	37
H20C	4799.1	3929.89	5822.79	37
H10A	3306.05	635.21	4251.6	43
H10B	3759.89	267.38	5171.3	43
H10C	4377.05	878.75	4950.05	43
H24	7515.92	3387.99	3604.33	28
H7A	2035.36	1655.64	6958.08	44
H7B	1523.79	2302.32	7133.01	44
H7C	2833.15	2234.82	6938.82	44
H34A	6326.62	4454.05	1697.78	42
H34B	6230.01	3819.66	2187.85	42
H34C	6786.14	4375.57	2777.48	42
H17A	4002.04	1875.2	2609.87	38
H17B	4320.33	1197.36	2405.88	38

H17C	4186	1401.89	3440.74	38
H23A	8388.48	3354.07	5139.36	43
H23B	8804.85	2781.81	4614.4	43
H23C	7837.75	2713.15	5289.99	43
H5A	2242.14	3012.86	5622.45	43
H5B	917.65	2984.35	5789.39	43
H5C	1270.41	2830.29	4789.57	43
H22A	7676.84	4318.68	4577.47	41
H22B	7215.48	4797.21	5258.27	41
H22C	6509.59	4677.96	4255.3	41
H8A	1141.17	925.54	5761.92	45
H8B	1749.28	296.41	5634.11	45
H8C	1274.35	687.4	4743.82	45
H25A	6685.01	2207.27	3864.95	50
H25B	7560.85	2397.33	3159.16	50
H25C	6241.33	2605.74	2975.47	50
H19A	-100.39	1491.34	4162.26	43
H19B	-951.59	1656.98	3243.58	43
H19C	12.96	2123.28	3668.86	43
H33A	2007.22	5627.89	1737.33	54
H33B	3149.64	5764.98	1277.86	54
H33C	3034.14	6004.8	2298.29	54
H18A	573.52	773.21	216.59	50
H18B	-245.16	393.85	795.86	50
H18C	1027.46	160.64	700.6	50
H014	8265.31	4430.22	482.39	48
H015	9832.53	4387.69	3125.66	57
H016	8208.24	3391.59	452.55	47
H017	9792	3348.98	3098.59	54
H018	9063.25	4932.66	1821.48	53
H019	8978.92	2845.35	1760.93	48

Table S9 Fractional Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **L^{Dipp}**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
P1	6245.6(3)	2739.0(8)	6088.0(3)	21.56(14)
P2	5984.4(3)	2536.3(9)	3962.7(3)	21.12(14)
N1	6099.7(13)	2762(2)	5025.8(10)	21.1(4)
N2	6533.2(12)	4496(3)	6053.6(10)	26.8(5)
N3	5851.5(11)	4380(3)	3940.2(11)	25.6(5)
C1	6111.9(15)	1865(3)	5463.5(11)	24.4(5)
C2	5999.1(19)	281(4)	5322.9(13)	34.7(7)
C3	5921(2)	240(4)	4789.5(12)	35.4(7)
C4	5986.3(15)	1790(3)	4611.0(11)	24.6(6)
C5	5322.2(15)	2647(4)	6380.6(11)	26.3(6)
C6	4799.5(15)	3763(4)	6090.7(14)	31.9(6)
C7	4999.2(17)	954(4)	6426.3(14)	37.2(7)
C8	6820.6(15)	1216(4)	6401.7(12)	28.6(6)

C9	7585.0(16)	1158(4)	6151.8(15)	36.1(7)
C10	6874.4(17)	1474(4)	6979.3(12)	33.6(7)
C11	5333.1(16)	1203(3)	3633.6(11)	26.7(6)
C12	4548.7(15)	1478(4)	3838.8(14)	35.3(7)
C13	5361.9(19)	1424(4)	3055.9(13)	35.8(7)
C14	6908.8(15)	2018(4)	3726.5(12)	30.5(6)
C15	7476.3(15)	3143(4)	3962.6(16)	42.8(8)
C16	7119.5(19)	266(4)	3818.4(15)	42.2(8)
C17	7160.6(14)	5312(3)	6241.6(11)	25.1(6)
C18	7769.8(15)	5592(3)	5913.3(13)	28.5(6)
C19	8381.9(15)	6434(3)	6103.1(15)	34.0(6)
C20	8405.3(17)	6991(4)	6595.3(16)	38.8(8)
C21	7800.9(17)	6767(4)	6911.1(14)	36.6(7)
C22	7166.6(16)	5949(4)	6741.7(13)	30.4(6)
C23	7732.8(15)	5073(4)	5362.5(13)	29.5(6)
C24	7261.1(18)	6286(4)	5059.1(15)	37.0(7)
C25	8486.0(17)	4841(5)	5107.1(15)	41.4(8)
C26	6489.3(18)	5830(4)	7076.9(12)	32.1(6)
C27	5912.3(18)	7070(4)	6905.7(14)	37.1(7)
C28	6638(2)	6010(5)	7649.8(14)	47.2(9)
C29	5298.6(15)	5361(3)	3729.3(11)	25.0(5)
C30	5385.6(16)	5986(3)	3231.8(12)	28.3(6)
C31	4843.7(19)	7006(4)	3033.0(13)	34.3(7)
C32	4220(2)	7410(4)	3313.9(13)	36.7(7)
C33	4142.5(16)	6824(4)	3803.4(13)	32.9(6)
C34	4668.0(14)	5801(3)	4022.8(12)	25.9(6)
C35	6082.1(17)	5589(4)	2929.8(12)	31.9(6)
C36	5994(2)	5736(4)	2353.4(14)	39.8(7)
C37	6726(2)	6643(5)	3107.3(14)	48.2(9)
C38	4608.6(14)	5244(3)	4570.6(12)	25.8(6)
C39	3815.1(16)	5069(4)	4767.3(14)	35.2(7)
C40	5054.6(17)	6388(4)	4909.3(12)	30.7(6)

Table S10 Anisotropic Displacement Parameters ($Å^2×10^3$) for **L^{Dipp}**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	18.1(3)	26.0(3)	20.6(3)	0.9(3)	-0.1(2)	-1.3(2)
P2	17.7(3)	25.3(3)	20.4(3)	-1.5(3)	1.6(3)	0.8(2)
N1	19.6(10)	20.9(10)	22.8(10)	-0.8(10)	0.8(7)	-0.2(9)
N2	20.5(10)	29.3(11)	30.7(13)	2.2(10)	-2.4(10)	-1.8(8)
N3	20.7(10)	27.0(11)	29.0(12)	-1.3(10)	0.3(10)	0.0(8)
C1	24.9(12)	24.2(13)	24.1(14)	1.2(11)	1.3(10)	-0.8(10)
C2	53.6(18)	25.1(14)	25.4(15)	2.1(12)	1.8(13)	-5.1(13)
C3	59(2)	23.2(14)	24.4(15)	-2.6(11)	3.5(14)	-6.7(13)
C4	26.1(13)	25.8(13)	21.9(14)	-1.3(11)	1.2(10)	-1.0(10)
C5	20.3(12)	32.6(14)	26.0(14)	1.1(11)	-0.3(10)	-2.8(10)
C6	20.1(12)	43.9(16)	31.6(15)	1.5(15)	0.8(12)	2.1(11)
C7	27.5(13)	39.5(17)	44.7(19)	4.2(14)	4.4(13)	-8.4(12)
C8	24.6(13)	32.6(15)	28.6(15)	2.6(12)	-0.7(11)	0.1(11)

C9	26.4(14)	39.8(15)	42.1(19)	11.0(15)	2.5(14)	7.2(12)
C10	35.7(15)	37.8(16)	27.4(16)	6.0(13)	-7.2(13)	2.3(13)
C11	26.8(13)	26.6(14)	26.8(15)	-4.0(11)	1.0(11)	-0.3(10)
C12	23.4(13)	36.1(15)	46(2)	-10.5(14)	1.8(13)	-5.5(11)
C13	40.6(17)	35.7(16)	31.2(17)	-2.8(13)	-5.8(13)	-7.0(13)
C14	21.6(13)	43.5(16)	26.5(14)	0.6(13)	4.1(11)	7.1(11)
C15	19.0(12)	56.0(19)	53(2)	-1.4(19)	4.5(14)	-1.2(12)
C16	35.6(15)	45.0(18)	46(2)	-4.1(15)	4.9(14)	17.6(14)
C17	18.4(12)	24.7(12)	32.3(16)	0.7(11)	-3.6(10)	0.1(10)
C18	19.6(12)	24.8(13)	41.3(17)	-1.3(12)	-4.1(11)	-0.2(10)
C19	19.3(12)	29.3(13)	53.3(19)	-6.2(15)	-2.3(13)	-2.1(10)
C20	24.5(13)	32.9(16)	59(2)	-10.6(15)	-9.0(14)	-2.8(12)
C21	34.5(15)	32.6(16)	42.7(19)	-7.6(14)	-12.2(14)	1.5(13)
C22	29.6(14)	25.6(13)	35.9(17)	1.0(12)	-6.7(12)	1.2(11)
C23	20.1(11)	31.6(14)	36.7(16)	0.9(12)	3.7(11)	-4.3(11)
C24	27.0(15)	40.5(17)	43.4(19)	3.8(16)	3.1(13)	-1.4(12)
C25	24.5(15)	52(2)	48(2)	-5.5(16)	5.7(14)	-4.3(13)
C26	39.3(15)	30.7(15)	26.5(16)	-3.5(12)	-2.4(13)	-4.6(12)
C27	34.9(15)	39.1(17)	37.4(17)	0.0(14)	7.0(13)	1.4(13)
C28	61(2)	52(2)	28.5(17)	-1.3(15)	-4.1(16)	-10.8(18)
C29	24.6(12)	22.7(12)	27.6(14)	-5.0(11)	-0.9(11)	-1.4(10)
C30	34.1(14)	24.1(13)	26.7(15)	-3.8(11)	-1.8(12)	-0.9(11)
C31	46.8(17)	28.8(14)	27.1(15)	-0.2(12)	-5.4(13)	5.4(13)
C32	44.0(17)	31.2(15)	34.8(16)	-3.5(14)	-7.9(14)	10.8(13)
C33	31.3(14)	29.2(14)	38.3(17)	-4.5(12)	-1.9(13)	6.5(11)
C34	24.5(12)	23.2(12)	29.9(15)	-2.2(11)	-2.0(11)	0.7(9)
C35	37.5(16)	33.6(15)	24.5(15)	-1.9(12)	3.1(12)	-2.4(13)
C36	44.6(17)	44.6(18)	30.2(17)	-5.7(14)	0.5(14)	-1.2(15)
C37	53(2)	61(2)	31.2(18)	-6.2(16)	7.1(15)	-21.0(18)
C38	19.0(12)	24.4(13)	34.0(16)	-2.2(11)	2.1(11)	2.0(10)
C39	23.0(13)	39.3(16)	43.3(18)	0.6(14)	5.1(13)	0.0(12)
C40	29.8(14)	31.8(14)	30.6(16)	-3.4(12)	-0.3(12)	-4.7(12)

Table S11 Bond Lengths for **L^{Dipp}**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	N2	1.552(2)	C17	C22	1.413(4)
P1	C1	1.806(3)	C18	C19	1.401(4)
P1	C5	1.841(3)	C18	C23	1.507(5)
P1	C8	1.832(3)	C19	C20	1.370(5)
P2	N3	1.550(2)	C20	C21	1.384(5)
P2	C4	1.808(3)	C21	C22	1.406(4)
P2	C11	1.833(3)	C22	C26	1.511(5)
P2	C14	1.835(3)	C23	C24	1.541(4)
N1	C1	1.367(4)	C23	C25	1.531(4)
N1	C4	1.369(4)	C26	C27	1.533(5)
N2	C17	1.411(3)	C26	C28	1.532(5)
N3	C29	1.404(4)	C29	C30	1.412(4)
C1	C2	1.381(4)	C29	C34	1.424(4)
C2	C3	1.405(4)	C30	C31	1.397(4)

C3	C4	1.374(4)	C30	C35	1.525(4)
C5	C6	1.526(4)	C31	C32	1.389(5)
C5	C7	1.527(4)	C32	C33	1.378(5)
C8	C9	1.532(4)	C33	C34	1.399(4)
C8	C10	1.531(4)	C34	C38	1.511(4)
C11	C12	1.536(4)	C35	C36	1.523(5)
C11	C13	1.525(4)	C35	C37	1.530(5)
C14	C15	1.520(5)	C38	C39	1.533(4)
C14	C16	1.523(5)	C38	C40	1.530(4)
C17	C18	1.418(4)			

Table S12 Bond Angles for **L^{Dipp}**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	P1	C1	111.73(14)	N2	C17	C22	120.6(3)
N2	P1	C5	111.58(13)	C22	C17	C18	119.7(3)
N2	P1	C8	118.95(13)	C17	C18	C23	120.0(2)
C1	P1	C5	103.82(13)	C19	C18	C17	118.8(3)
C1	P1	C8	101.85(14)	C19	C18	C23	121.2(3)
C8	P1	C5	107.50(13)	C20	C19	C18	121.8(3)
N3	P2	C4	111.98(14)	C19	C20	C21	119.5(3)
N3	P2	C11	118.59(13)	C20	C21	C22	121.5(3)
N3	P2	C14	111.10(14)	C17	C22	C26	120.5(3)
C4	P2	C11	103.66(13)	C21	C22	C17	118.7(3)
C4	P2	C14	103.56(14)	C21	C22	C26	120.7(3)
C11	P2	C14	106.65(14)	C18	C23	C24	109.4(3)
C1	N1	C4	110.3(2)	C18	C23	C25	114.5(3)
C17	N2	P1	134.5(2)	C25	C23	C24	110.5(3)
C29	N3	P2	134.3(2)	C22	C26	C27	109.8(3)
N1	C1	P1	122.9(2)	C22	C26	C28	114.9(3)
N1	C1	C2	107.0(3)	C28	C26	C27	109.9(3)
C2	C1	P1	130.1(2)	N3	C29	C30	119.8(2)
C1	C2	C3	107.6(3)	N3	C29	C34	120.5(3)
C4	C3	C2	107.9(3)	C30	C29	C34	119.6(3)
N1	C4	P2	122.9(2)	C29	C30	C35	119.4(3)
N1	C4	C3	107.2(3)	C31	C30	C29	119.3(3)
C3	C4	P2	129.8(2)	C31	C30	C35	121.3(3)
C6	C5	P1	109.3(2)	C32	C31	C30	121.3(3)
C6	C5	C7	111.1(2)	C33	C32	C31	119.4(3)
C7	C5	P1	114.7(2)	C32	C33	C34	121.8(3)
C9	C8	P1	110.1(2)	C29	C34	C38	119.4(2)
C10	C8	P1	112.5(2)	C33	C34	C29	118.6(3)
C10	C8	C9	111.7(3)	C33	C34	C38	121.8(3)
C12	C11	P2	109.9(2)	C30	C35	C37	110.4(3)
C13	C11	P2	111.8(2)	C36	C35	C30	114.2(3)
C13	C11	C12	111.2(3)	C36	C35	C37	109.5(3)
C15	C14	P2	109.6(2)	C34	C38	C39	114.5(2)
C15	C14	C16	110.7(3)	C34	C38	C40	108.8(2)
C16	C14	P2	113.5(2)	C40	C38	C39	111.0(3)
N2	C17	C18	119.5(3)				

Table S13 Torsion Angles for **L^{Dipp}**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
P1	N2	C17	C18	99.7(3)	C8	P1	C1	C2	38.5(3)
P1	N2	C17	C22	-84.7(4)	C8	P1	C5	C6	-173.7(2)
P1	C1	C2	C3	179.5(2)	C8	P1	C5	C7	-48.1(3)
P2	N3	C29	C30	-93.1(3)	C11	P2	N3	C29	3.0(4)
P2	N3	C29	C34	90.2(4)	C11	P2	C4	N1	-148.8(2)
N1	C1	C2	C3	0.2(4)	C11	P2	C4	C3	34.9(3)
N2	P1	C1	N1	-14.2(3)	C11	P2	C14	C15	176.9(2)
N2	P1	C1	C2	166.6(3)	C11	P2	C14	C16	-58.8(3)
N2	P1	C5	C6	54.2(2)	C14	P2	N3	C29	127.0(3)
N2	P1	C5	C7	179.8(2)	C14	P2	C4	N1	100.0(2)
N2	P1	C8	C9	-55.6(3)	C14	P2	C4	C3	-76.3(3)
N2	P1	C8	C10	69.7(3)	C14	P2	C11	C12	176.0(2)
N2	C17	C18	C19	178.7(3)	C14	P2	C11	C13	-60.1(2)
N2	C17	C18	C23	2.3(4)	C17	C18	C19	C20	0.0(4)
N2	C17	C22	C21	-179.4(3)	C17	C18	C23	C24	77.5(3)
N2	C17	C22	C26	-2.6(4)	C17	C18	C23	C25	-157.9(3)
N3	P2	C4	N1	-19.8(3)	C17	C22	C26	C27	-75.9(4)
N3	P2	C4	C3	163.9(3)	C17	C22	C26	C28	159.6(3)
N3	P2	C11	C12	-57.8(3)	C18	C17	C22	C21	-3.8(4)
N3	P2	C11	C13	66.2(3)	C18	C17	C22	C26	173.0(3)
N3	P2	C14	C15	46.3(3)	C18	C19	C20	C21	-2.2(5)
N3	P2	C14	C16	170.6(2)	C19	C18	C23	C24	-98.8(3)
N3	C29	C30	C31	-177.8(3)	C19	C18	C23	C25	25.8(4)
N3	C29	C30	C35	-0.1(4)	C19	C20	C21	C22	1.4(5)
N3	C29	C34	C33	177.9(3)	C20	C21	C22	C17	1.6(5)
N3	C29	C34	C38	1.8(4)	C20	C21	C22	C26	-175.1(3)
C1	P1	N2	C17	-122.6(3)	C21	C22	C26	C27	100.8(3)
C1	P1	C5	C6	-66.3(2)	C21	C22	C26	C28	-23.7(4)
C1	P1	C5	C7	59.3(3)	C22	C17	C18	C19	3.0(4)
C1	P1	C8	C9	67.7(3)	C22	C17	C18	C23	-173.4(3)
C1	P1	C8	C10	-167.1(2)	C23	C18	C19	C20	176.3(3)
C1	N1	C4	P2	-176.7(2)	C29	C30	C31	C32	-0.3(5)
C1	N1	C4	C3	0.3(3)	C29	C30	C35	C36	157.1(3)
C1	C2	C3	C4	0.0(4)	C29	C30	C35	C37	-79.0(4)
C2	C3	C4	P2	176.6(2)	C29	C34	C38	C39	-152.8(3)
C2	C3	C4	N1	-0.2(4)	C29	C34	C38	C40	82.4(3)
C4	P2	N3	C29	-117.7(3)	C30	C29	C34	C33	1.2(4)
C4	P2	C11	C12	67.0(2)	C30	C29	C34	C38	-174.9(2)
C4	P2	C11	C13	-169.0(2)	C30	C31	C32	C33	1.6(5)
C4	P2	C14	C15	-74.1(3)	C31	C30	C35	C36	-25.3(4)
C4	P2	C14	C16	50.3(3)	C31	C30	C35	C37	98.7(4)
C4	N1	C1	P1	-179.73(19)	C31	C32	C33	C34	-1.4(5)
C4	N1	C1	C2	-0.3(3)	C32	C33	C34	C29	0.0(4)
C5	P1	N2	C17	121.6(3)	C32	C33	C34	C38	176.0(3)
C5	P1	C1	N1	106.2(2)	C33	C34	C38	C39	31.3(4)
C5	P1	C1	C2	-73.1(3)	C33	C34	C38	C40	-93.5(3)
C5	P1	C8	C9	176.5(2)	C34	C29	C30	C31	-1.1(4)
C5	P1	C8	C10	-58.3(2)	C34	C29	C30	C35	176.6(3)

C8	P1	N2	C17	-4.4(4)	C35	C30	C31	C32	-177.9(3)
C8	P1	C1	N1	-142.2(2)					

Table S14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **L^{Dipp}**.

Atom	*x*	*y*	*z*	U(eq)
H1	6153(19)	3810(40)	5008(16)	25
H2	5978.31	-618.91	5546.46	42
H3	5837.16	-693.19	4587.85	42
H5	5369.17	3084.7	6734.83	32
H6A	5002.97	4856.75	6087.53	48
H6B	4316.24	3770.74	6259.32	48
H6C	4743.53	3377.51	5739.2	48
H7A	4943.22	486.09	6085.02	56
H7B	4515.43	1010.73	6593.16	56
H7C	5331.67	280	6629.93	56
H8	6581.09	146.07	6344.54	34
H9A	7529.34	1061.94	5780.9	54
H9B	7858.87	226.37	6282.18	54
H9C	7855.85	2147.71	6232.49	54
H10A	7137.07	2482.47	7048.71	50
H10B	7143.91	573.59	7133.83	50
H10C	6376.55	1530.06	7125.16	50
H11	5475.82	65.49	3711.71	32
H12A	4541.56	1286.39	4207.95	53
H12B	4206.43	733.9	3670.4	53
H12C	4397.49	2590.15	3769.06	53
H13A	5224.94	2533.36	2969.61	54
H13B	5015.73	676	2893.13	54
H13C	5863.63	1205.52	2933.7	54
H14	6912.22	2204.43	3349.37	37
H15A	7342.49	4262.21	3887.15	64
H15B	7964.98	2910.28	3819.55	64
H15C	7487.45	2983.24	4333.17	64
H16A	7157.21	67.16	4186.32	63
H16B	7596.32	41.56	3656.13	63
H16C	6740.67	-439.63	3671.93	63
H19	8791.57	6623.91	5884.62	41
H20	8833.18	7526.26	6718.91	47
H21	7815.04	7175.57	7249.81	44
H23	7471.3	4012.1	5352	35
H24A	6773.51	6383.42	5218.65	55
H24B	7204.33	5906.57	4707.02	55
H24C	7505.51	7339.19	5058.85	55
H25A	8746.73	5874.72	5094.77	62
H25B	8415.41	4435.01	4759.15	62
H25C	8778.01	4064.66	5303.85	62
H26	6270.75	4737.49	7022.47	39
H27A	6090.29	8157.08	6983.31	56

H27B	5447.21	6875.56	7086.98	56
H27C	5830.5	6967.92	6537.22	56
H28A	7009.81	5220.95	7755.94	71
H28B	6179.06	5824.19	7839.72	71
H28C	6818.9	7099.84	7720.39	71
H31	4902.91	7432.18	2698.82	41
H32	3850.69	8084.11	3170.16	44
H33	3720.49	7123.4	3996.98	39
H35	6214.51	4444.28	3006.31	38
H36A	5942.33	6874.4	2260.66	60
H36B	5553.29	5144.16	2244.43	60
H36C	6430.53	5285.57	2184.19	60
H37A	7184.59	6262.91	2949.55	72
H37B	6769.71	6579.35	3479.64	72
H37C	6635.27	7762.54	3006.33	72
H38	4846.49	4158.54	4592.31	31
H39A	3573.55	6125.04	4767.28	53
H39B	3823.27	4637.96	5115.65	53
H39C	3541.26	4330.99	4544.84	53
H40A	5563.52	6449.42	4783.39	46
H40B	5054.91	5985.17	5260.93	46
H40C	4830.81	7462.64	4900.35	46

Table S15 Fractional Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **1^{Dipp}**·0.5 C_6H_6. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Ga1	2012.6(2)	2674.8(2)	3564.2(2)	11.33(5)
Cl2	11.3(4)	2749.5(2)	3884.7(2)	17.95(8)
Cl1	1707.1(4)	1698.4(2)	3042.4(2)	17.85(8)
P2	2735.7(4)	3858.6(2)	2728.2(2)	12.65(8)
P1	4879.3(4)	2192.2(2)	4337.6(2)	12.37(8)
N1	3898.9(12)	3084.2(6)	3552.2(5)	12.5(2)
N3	1421.8(12)	3540.1(7)	3001.4(5)	12.9(2)
N2	3151.4(12)	2200.6(6)	4286.3(5)	12.1(2)
C29	50.0(15)	3875.6(8)	2808.1(6)	13.6(3)
C1	5135.4(15)	2815.4(8)	3830.2(6)	14.1(3)
C11	2470.6(15)	1913.1(8)	4708.5(6)	13.0(3)
C21	2187.9(16)	662.6(8)	4244.9(6)	15.2(3)
C33	-1963.1(16)	4012.7(9)	2095.0(6)	18.8(3)
C34	-829.4(15)	3591.3(8)	2351.8(6)	15.9(3)
C9	5688.4(16)	1319.7(8)	4192.7(7)	18.0(3)
C30	-396.5(16)	4513.6(8)	3049.2(6)	16.6(3)
C27	2870.1(16)	3515.0(9)	2060.4(6)	18.5(3)
C12	2156.1(16)	2372.0(8)	5122.4(6)	16.5(3)
C16	2068.0(16)	1170.6(8)	4705.2(6)	15.0(3)
C3	5720.3(16)	3545.1(8)	3194.8(6)	18.3(3)
C4	4245.7(15)	3528.1(8)	3164.6(6)	14.3(3)
C39	-654.8(16)	2819.4(8)	2161.6(6)	17.5(3)

C2	6286.4(16)	3088.8(8)	3619.8(6)	18.1(3)
C6	5782.6(16)	2516.4(9)	4985.5(6)	18.3(3)
C36	238.9(17)	4772.3(9)	3604.7(7)	20.3(3)
C20	701.5(17)	477.9(9)	3944.6(6)	20.2(3)
C18	2441.6(17)	3190.9(8)	5151.2(6)	18.4(3)
C7	5777.8(18)	1938.2(10)	5421.7(7)	24.1(3)
C10	5231.0(18)	1111.6(9)	3607.9(7)	23.4(3)
C24	2730.9(16)	4857.7(8)	2707.2(6)	18.5(3)
C32	-2279.5(16)	4683.9(9)	2291.0(7)	20.9(3)
C13	1523.6(19)	2069.0(9)	5526.8(7)	24.1(3)
C19	3408.0(19)	3420.7(9)	5673.4(7)	23.2(3)
C31	-1543.0(16)	4911.5(9)	2776.6(7)	20.1(3)
C8	7325.8(17)	1297.0(9)	4325.9(7)	24.8(3)
C28	3144(2)	2692.3(9)	2068.3(7)	24.9(4)
C15	1453.3(18)	894.2(9)	5124.9(7)	22.2(3)
C22	2991.5(18)	-43.7(9)	4418.9(7)	23.2(3)
C38	-793.1(19)	2746.7(10)	1558.7(7)	25.2(4)
C5	7279.6(18)	2841.1(9)	4999.6(7)	25.0(4)
C23	4208.6(18)	5216.7(9)	2796.4(7)	24.6(3)
C37	-855.4(19)	4645.5(9)	3979.0(7)	25.0(3)
C26	4042.1(19)	3896.5(10)	1813.0(7)	27.3(4)
C25	1754.2(18)	5167.3(9)	2219.3(7)	25.5(4)
C17	1045.5(19)	3622.1(9)	5110.5(7)	25.8(4)
C35	648(2)	5585.8(9)	3637.2(8)	29.2(4)
C14	1189(2)	1335.7(10)	5536.7(7)	26.9(4)
C40	-1757(2)	2329.6(10)	2365.9(8)	29.0(4)
C01D	4623(2)	5420.7(10)	5405.5(8)	35.4(4)
C01E	6382(2)	4753.8(10)	5029.6(9)	37.0(5)
C01F	6007(2)	5176.1(10)	5433.4(9)	37.3(5)

Table S16 Anisotropic Displacement Parameters ($Å^2×10^3$) for **1**^{Dipp}·0.5 C_6H_6. The Anisotropic displacement factor exponent takes the form: $–2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ga1	9.16(9)	12.04(9)	12.78(10)	0.53(6)	1.78(7)	-0.75(6)
Cl2	11.06(15)	23.41(18)	20.25(18)	4.54(13)	5.10(13)	2.10(12)
Cl1	22.60(17)	13.53(16)	16.22(17)	-0.95(12)	-0.38(13)	-0.56(12)
P2	10.39(16)	14.53(17)	12.87(17)	3.13(13)	1.48(13)	0.03(12)
P1	10.02(16)	12.06(16)	14.49(18)	2.49(13)	0.39(13)	0.90(12)
N1	10.6(5)	13.4(5)	13.8(6)	2.7(5)	2.1(4)	0.8(4)
N3	9.7(5)	14.8(6)	13.9(6)	3.7(5)	1.0(4)	0.4(4)
N2	9.9(5)	12.8(5)	13.2(6)	2.6(4)	1.0(4)	1.0(4)
C29	11.3(6)	15.1(7)	14.8(7)	3.7(5)	3.1(5)	0.4(5)
C1	9.8(6)	15.1(7)	16.7(7)	2.4(5)	0.4(5)	1.6(5)
C11	11.8(6)	15.2(7)	11.8(7)	1.8(5)	1.1(5)	-1.0(5)
C21	16.5(7)	11.8(6)	17.2(7)	-0.1(5)	2.6(6)	-0.8(5)
C33	11.7(7)	26.8(8)	17.1(7)	5.5(6)	-0.5(6)	-1.8(6)
C34	13.6(7)	18.4(7)	16.4(7)	3.8(6)	4.2(6)	-1.3(5)
C9	14.4(7)	14.0(7)	25.8(8)	3.5(6)	4.0(6)	3.5(5)

C30	14.6(7)	16.2(7)	19.3(7)	3.3(6)	3.8(6)	-0.2(5)
C27	16.3(7)	24.5(8)	15.1(7)	1.8(6)	3.6(6)	-2.3(6)
C12	17.6(7)	15.9(7)	15.9(7)	-0.3(6)	2.4(6)	-2.2(5)
C16	16.0(7)	14.8(7)	13.9(7)	1.5(5)	1.4(5)	-0.1(5)
C3	12.4(7)	20.5(7)	22.4(8)	6.2(6)	4.4(6)	-0.5(5)
C4	13.5(7)	14.8(7)	14.5(7)	3.1(5)	2.4(5)	-0.1(5)
C39	15.8(7)	20.3(7)	15.1(7)	0.3(6)	-1.3(6)	-1.1(6)
C2	11.4(6)	20.3(7)	22.7(8)	5.4(6)	3.2(6)	-0.1(5)
C6	16.8(7)	18.4(7)	18.1(7)	1.7(6)	-2.3(6)	1.7(6)
C36	20.2(7)	18.2(7)	22.2(8)	-3.0(6)	3.1(6)	2.5(6)
C20	19.7(7)	21.5(8)	19.3(8)	-1.9(6)	3.1(6)	-4.3(6)
C18	22.0(7)	15.3(7)	18.7(7)	-2.4(6)	5.8(6)	-1.0(6)
C7	23.1(8)	28.3(9)	18.9(8)	6.5(7)	-2.5(6)	1.1(6)
C10	21.0(8)	21.9(8)	28.2(9)	-4.8(7)	6.8(7)	2.9(6)
C24	17.0(7)	16.0(7)	22.7(8)	4.9(6)	3.4(6)	0.0(5)
C32	14.1(7)	25.3(8)	23.6(8)	11.2(6)	4.0(6)	4.6(6)
C13	32.0(9)	22.4(8)	19.9(8)	-4.8(6)	10.6(7)	-6.8(7)
C19	30.6(9)	18.4(7)	20.4(8)	-2.9(6)	2.9(7)	-3.5(6)
C31	16.7(7)	17.7(7)	27.3(8)	4.8(6)	7.4(6)	3.7(6)
C8	16.4(7)	24.3(8)	34.1(9)	6.4(7)	5.4(7)	6.7(6)
C28	28.7(9)	25.8(9)	22.2(8)	-2.5(7)	10.7(7)	-1.3(7)
C15	30.4(9)	17.0(7)	20.0(8)	1.1(6)	6.5(7)	-8.3(6)
C22	26.0(8)	14.3(7)	29.0(9)	3.1(6)	4.0(7)	2.4(6)
C38	27.4(9)	29.9(9)	17.5(8)	-3.5(7)	1.3(7)	-0.6(7)
C5	18.1(8)	24.1(8)	29.1(9)	2.5(7)	-7.0(7)	-3.3(6)
C23	21.3(8)	18.9(8)	32.8(9)	3.8(7)	2.0(7)	-4.4(6)
C37	31.6(9)	21.2(8)	23.7(8)	0.6(6)	8.5(7)	4.8(7)
C26	26.9(9)	34.9(9)	22.6(8)	0.5(7)	11.3(7)	-6.2(7)
C25	21.5(8)	22.7(8)	31.6(9)	11.9(7)	2.2(7)	2.7(6)
C17	27.7(9)	22.6(8)	27.5(9)	-6.1(7)	5.5(7)	4.1(7)
C35	31.9(9)	20.9(8)	36.5(10)	-6.4(7)	10.4(8)	-1.6(7)
C14	39.0(10)	25.5(8)	19.2(8)	-2.4(7)	13.2(7)	-12.1(7)
C40	33.4(10)	24.4(9)	30.4(10)	-0.5(7)	8.3(8)	-9.3(7)
C01D	48.2(12)	20.3(8)	37.4(11)	-0.3(7)	6.6(9)	-1.4(8)
C01E	29.1(9)	24.7(9)	55.8(13)	6.1(9)	2.5(9)	-1.3(7)
C01F	39.5(11)	25.0(9)	40.9(11)	3.6(8)	-12.6(9)	-8.4(8)

Table S17 Bond Lengths for **1**$^{\mathbf{Dipp}}$·0.5 C_6H_6.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ga1	Cl2	2.1935(4)	C9	C10	1.532(2)
Ga1	Cl1	2.2223(4)	C9	C8	1.538(2)
Ga1	N1	1.9481(12)	C30	C36	1.522(2)
Ga1	N3	2.1521(12)	C30	C31	1.398(2)
Ga1	N2	2.1601(12)	C27	C28	1.532(2)
P2	N3	1.6342(12)	C27	C26	1.536(2)
P2	C27	1.8399(16)	C12	C18	1.526(2)
P2	C4	1.7725(15)	C12	C13	1.392(2)
P2	C24	1.8340(16)	C16	C15	1.396(2)
P1	N2	1.6255(12)	C3	C4	1.391(2)

P1	C1	1.7732(15)	C3	C2	1.405(2)
P1	C9	1.8396(15)	C39	C38	1.527(2)
P1	C6	1.8318(16)	C39	C40	1.535(2)
N1	C1	1.3614(18)	C6	C7	1.538(2)
N1	C4	1.3623(18)	C6	C5	1.537(2)
N3	C29	1.4528(18)	C36	C37	1.540(2)
N2	C11	1.4436(18)	C36	C35	1.541(2)
C29	C34	1.416(2)	C18	C19	1.547(2)
C29	C30	1.419(2)	C18	C17	1.533(2)
C1	C2	1.388(2)	C24	C23	1.534(2)
C11	C12	1.420(2)	C24	C25	1.534(2)
C11	C16	1.415(2)	C32	C31	1.383(2)
C21	C16	1.518(2)	C13	C14	1.384(2)
C21	C20	1.530(2)	C15	C14	1.382(2)
C21	C22	1.533(2)	C01D	C01E[1]	1.377(3)
C33	C34	1.398(2)	C01D	C01F	1.380(3)
C33	C32	1.381(2)	C01E	C01F	1.381(3)
C34	C39	1.515(2)			

Table S18 Bond Angles for **1**^{Dipp}·0.5 C_6H_6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl2	Ga1	Cl1	103.731(15)	C33	C34	C29	119.11(14)
N1	Ga1	Cl2	146.89(4)	C33	C34	C39	118.91(14)
N1	Ga1	Cl1	109.37(4)	C10	C9	P1	110.57(11)
N1	Ga1	N3	81.09(5)	C10	C9	C8	108.89(13)
N1	Ga1	N2	80.51(5)	C8	C9	P1	114.84(11)
N3	Ga1	Cl2	93.16(3)	C29	C30	C36	124.02(13)
N3	Ga1	Cl1	101.61(3)	C31	C30	C29	118.62(14)
N3	Ga1	N2	154.85(5)	C31	C30	C36	117.26(14)
N2	Ga1	Cl2	92.94(3)	C28	C27	P2	111.29(11)
N2	Ga1	Cl1	100.59(3)	C28	C27	C26	108.75(14)
N3	P2	C27	116.48(7)	C26	C27	P2	112.90(11)
N3	P2	C4	101.89(6)	C11	C12	C18	124.21(13)
N3	P2	C24	111.81(7)	C13	C12	C11	118.88(14)
C4	P2	C27	106.99(7)	C13	C12	C18	116.90(14)
C4	P2	C24	110.99(7)	C11	C16	C21	122.79(13)
C24	P2	C27	108.41(7)	C15	C16	C11	119.47(14)
N2	P1	C1	101.11(6)	C15	C16	C21	117.63(13)
N2	P1	C9	116.22(7)	C4	C3	C2	106.51(13)
N2	P1	C6	112.79(7)	N1	C4	P2	113.15(10)
C1	P1	C9	107.63(7)	N1	C4	C3	109.54(13)
C1	P1	C6	110.41(7)	C3	C4	P2	137.01(12)
C6	P1	C9	108.33(7)	C34	C39	C38	114.08(13)
C1	N1	Ga1	124.73(10)	C34	C39	C40	108.80(13)
C1	N1	C4	107.69(12)	C38	C39	C40	109.85(14)
C4	N1	Ga1	125.06(10)	C1	C2	C3	106.69(13)
P2	N3	Ga1	114.47(6)	C7	C6	P1	111.84(11)
C29	N3	Ga1	131.34(9)	C5	C6	P1	116.23(12)
C29	N3	P2	114.15(9)	C5	C6	C7	111.27(13)

P1	N2	Ga1	115.51(6)	C30	C36	C37	108.95(13)
C11	N2	Ga1	124.05(9)	C30	C36	C35	114.21(14)
C11	N2	P1	120.43(10)	C37	C36	C35	107.64(13)
C34	C29	N3	119.90(13)	C12	C18	C19	112.67(13)
C34	C29	C30	118.81(13)	C12	C18	C17	111.09(13)
C30	C29	N3	121.18(13)	C17	C18	C19	107.60(13)
N1	C1	P1	113.82(10)	C23	C24	P2	115.29(11)
N1	C1	C2	109.57(13)	C23	C24	C25	112.24(13)
C2	C1	P1	136.55(12)	C25	C24	P2	113.09(11)
C12	C11	N2	120.82(13)	C33	C32	C31	119.03(14)
C16	C11	N2	120.08(13)	C14	C13	C12	122.03(15)
C16	C11	C12	119.07(13)	C32	C31	C30	121.74(15)
C16	C21	C20	110.06(12)	C14	C15	C16	121.39(15)
C16	C21	C22	113.10(13)	C15	C14	C13	119.04(15)
C20	C21	C22	109.44(13)	C01E[1]	C01D	C01F	119.6(2)
C32	C33	C34	121.35(15)	C01D[1]	C01E	C01F	120.12(19)
C29	C34	C39	121.77(13)	C01D	C01F	C01E	120.25(19)

Table S19 Torsion Angles for **1^{Dipp}**·0.5 C_6H_6.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ga1	N1	C1	P1	-14.84(16)	C9	P1	N2	Ga1	-101.14(8)
Ga1	N1	C1	C2	162.72(11)	C9	P1	N2	C11	79.65(13)
Ga1	N1	C4	P2	12.04(16)	C9	P1	C1	N1	120.44(11)
Ga1	N1	C4	C3	-162.72(11)	C9	P1	C1	C2	-56.21(19)
Ga1	N3	C29	C34	-90.11(16)	C9	P1	C6	C7	-53.73(13)
Ga1	N3	C29	C30	93.69(16)	C9	P1	C6	C5	75.55(13)
Ga1	N2	C11	C12	-87.67(15)	C30	C29	C34	C33	11.7(2)
Ga1	N2	C11	C16	90.40(15)	C30	C29	C34	C39	-162.99(13)
P2	N3	C29	C34	87.57(14)	C27	P2	N3	Ga1	99.16(8)
P2	N3	C29	C30	-88.63(15)	C27	P2	N3	C29	-78.92(12)
P1	N2	C11	C12	91.47(15)	C27	P2	C4	N1	-118.05(11)
P1	N2	C11	C16	-90.46(15)	C27	P2	C4	C3	54.70(19)
P1	C1	C2	C3	176.81(14)	C27	P2	C24	C23	-86.58(13)
N1	C1	C2	C3	0.07(18)	C27	P2	C24	C25	44.44(13)
N3	P2	C27	C28	-62.90(13)	C12	C11	C16	C21	172.04(13)
N3	P2	C27	C26	174.47(11)	C12	C11	C16	C15	-4.0(2)
N3	P2	C4	N1	4.68(12)	C12	C13	C14	C15	-1.9(3)
N3	P2	C4	C3	177.43(17)	C16	C11	C12	C18	-175.69(14)
N3	P2	C24	C23	143.68(12)	C16	C11	C12	C13	3.1(2)
N3	P2	C24	C25	-85.29(13)	C16	C15	C14	C13	0.9(3)
N3	C29	C34	C33	-164.57(13)	C4	P2	N3	Ga1	-16.85(8)
N3	C29	C34	C39	20.7(2)	C4	P2	N3	C29	165.07(10)
N3	C29	C30	C36	-19.0(2)	C4	P2	C27	C28	50.23(13)
N3	C29	C30	C31	164.79(13)	C4	P2	C27	C26	-72.39(13)
N2	P1	C1	N1	-1.89(12)	C4	P2	C24	C23	30.65(14)
N2	P1	C1	C2	-178.54(17)	C4	P2	C24	C25	161.67(11)
N2	P1	C9	C10	65.15(13)	C4	N1	C1	P1	-177.55(10)
N2	P1	C9	C8	-171.16(11)	C4	N1	C1	C2	0.01(17)

N2	P1	C6	C7	76.35(12)	C4	C3	C2	C1	-0.11(18)
N2	P1	C6	C5	-154.36(11)	C2	C3	C4	P2	-172.80(14)
N2	C11	C12	C18	2.4(2)	C2	C3	C4	N1	0.12(18)
N2	C11	C12	C13	-178.80(14)	C6	P1	N2	Ga1	132.91(7)
N2	C11	C16	C21	-6.1(2)	C6	P1	N2	C11	-46.30(13)
N2	C11	C16	C15	177.91(14)	C6	P1	C1	N1	-121.51(11)
C29	C34	C39	C38	-139.06(15)	C6	P1	C1	C2	61.84(19)
C29	C34	C39	C40	97.91(17)	C6	P1	C9	C10	-166.68(11)
C29	C30	C36	C37	-108.01(16)	C6	P1	C9	C8	-43.00(14)
C29	C30	C36	C35	131.61(16)	C36	C30	C31	C32	-173.94(14)
C29	C30	C31	C32	2.5(2)	C20	C21	C16	C11	-108.99(16)
C1	P1	N2	Ga1	15.01(8)	C20	C21	C16	C15	67.11(18)
C1	P1	N2	C11	-164.20(11)	C18	C12	C13	C14	178.69(16)
C1	P1	C9	C10	-47.29(12)	C24	P2	N3	Ga1	-135.44(7)
C1	P1	C9	C8	76.40(13)	C24	P2	N3	C29	46.48(12)
C1	P1	C6	C7	-171.35(11)	C24	P2	C27	C28	170.00(11)
C1	P1	C6	C5	-42.07(14)	C24	P2	C27	C26	47.37(14)
C1	N1	C4	P2	174.67(10)	C24	P2	C4	N1	123.86(11)
C1	N1	C4	C3	-0.08(17)	C24	P2	C4	C3	-63.40(19)
C11	C12	C18	C19	-123.16(16)	C32	C33	C34	C29	-3.0(2)
C11	C12	C18	C17	116.02(17)	C32	C33	C34	C39	171.88(14)
C11	C12	C13	C14	-0.2(3)	C13	C12	C18	C19	58.01(19)
C11	C16	C15	C14	2.0(3)	C13	C12	C18	C17	-62.81(19)
C21	C16	C15	C14	-174.26(16)	C31	C30	C36	C37	68.24(17)
C33	C34	C39	C38	46.21(19)	C31	C30	C36	C35	-52.14(19)
C33	C34	C39	C40	-76.81(18)	C22	C21	C16	C11	128.26(15)
C33	C32	C31	C30	6.3(2)	C22	C21	C16	C15	-55.63(19)
C34	C29	C30	C36	164.75(14)	C01D[1]	C01E	C01F	C01D	0.5(3)
C34	C29	C30	C31	-11.5(2)	C01E[1]	C01D	C01F	C01E	-0.5(3)
C34	C33	C32	C31	-6.0(2)					

Table S20 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **1^{Dipp}**·0.5 C_6H_6.

Atom	*x*	*y*	*z*	U(eq)
H21	2710.69	918.54	3999.58	18
H33	-2515.07	3837.28	1785.78	23
H9	5319.24	944.57	4407.71	22
H27	1955.73	3605.78	1830.06	22
H3	6231.21	3806.97	2976.62	22
H39	297.78	2648.96	2320.07	21
H2	7245.94	2989.15	3737.35	22
H6	5193.36	2917.51	5081.76	22
H36	1093.21	4482.56	3731.93	24
H20A	175.89	217.5	4175.76	30
H20B	789.64	180.53	3642.01	30
H20C	206.49	919.81	3827.78	30
H18	2914.88	3328.44	4852.02	22
H7A	4840.26	1731.79	5394.94	36
H7B	6041.34	2160.97	5764.32	36
H7C	6448.91	1560.76	5378.19	36

H10A	4223.15	1188.18	3508.03	35
H10B	5448.76	607.73	3559.15	35
H10C	5734.48	1408.58	3390	35
H24	2292.08	5008.75	3011.87	22
H32	-2977.63	4978.6	2099.41	25
H13	1319.73	2368.54	5798.85	29
H19A	2877.79	3390.94	5962.41	35
H19B	3727.93	3912.41	5640.83	35
H19C	4217.8	3101.38	5740.99	35
H31	-1817.78	5340.59	2925.61	24
H8A	7720.16	1678.31	4136.79	37
H8B	7661.91	833.61	4222.85	37
H8C	7617.76	1365.04	4701.19	37
H28A	4057.72	2591.54	2278.13	37
H28B	3133.74	2521.81	1711.8	37
H28C	2412.96	2447.72	2219.94	37
H15	1216.82	402.56	5127.34	27
H22A	3896.09	71.83	4629.89	35
H22B	3142.12	-313.79	4110.48	35
H22C	2439.72	-331.66	4625.34	35
H38A	-535.61	2261.33	1470.69	38
H38B	-169.89	3090.25	1429.02	38
H38C	-1760.88	2842.9	1397.6	38
H5A	7945.82	2456.45	4968.28	37
H5B	7563.4	3093.41	5329.74	37
H5C	7264.74	3176.07	4709.62	37
H23A	4755.81	5036.75	3120.43	37
H23B	4103.82	5735.43	2820.38	37
H23C	4691.18	5102.7	2504.08	37
H37A	-437.11	4773.51	4335.54	38
H37B	-1129.3	4141.41	3967.24	38
H37C	-1682.1	4942.51	3867.47	38
H26A	3844.1	4409.16	1783.11	41
H26B	4066.02	3697.62	1466.34	41
H26C	4948.91	3821.01	2034.71	41
H25A	2189.31	5096.12	1908.92	38
H25B	1611	5678.8	2269.77	38
H25C	851.08	4920.85	2173.77	38
H17A	427.71	3495.22	4786.78	39
H17B	1249.28	4134.52	5110.99	39
H17C	585.53	3506.44	5408.32	39
H35A	-196.62	5877.39	3549.59	44
H35B	1286.25	5687.16	3390.82	44
H35C	1109.73	5699.54	3991.26	44
H14	791.49	1142.93	5816.45	32
H40A	-2701.05	2496.37	2224.59	44
H40B	-1618.13	2349.12	2747.02	44
H40C	-1642.42	1836.77	2253.72	44
H01D	4369.76	5701.82	5678.88	42
H01E	7313.72	4586.97	5051.5	44
H01F	6689.86	5296.07	5725.13	45

Table S21 Fractional Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **2^{Pipp}**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
In2	6252.1(2)	6965.2(2)	2961.0(2)	16.80(6)
In1	8573.3(2)	4410.9(2)	6959.6(2)	17.63(6)
Cl3	7451.6(4)	6424.3(3)	3740.7(3)	24.72(13)
Cl4	6577.4(4)	7362.4(3)	2032.8(3)	24.78(13)
P2	8918.3(4)	5526.5(3)	6133.3(3)	17.15(13)
Cl1	8458.3(4)	4674.1(3)	8034.9(3)	25.89(13)
P1	10489.2(4)	3700.1(3)	7485.4(3)	17.83(13)
P3	4337.8(4)	6264.4(3)	2245.8(3)	17.79(13)
Cl2	7343.5(4)	3919.5(3)	6147.2(4)	28.49(14)
P4	5857.6(4)	7943.6(3)	3951.4(3)	18.17(13)
N4	5030.0(14)	7140.8(9)	3055.3(12)	18.9(4)
N1	9757.5(13)	4631.5(9)	6822.4(12)	18.4(4)
N5	5384.8(14)	6240.4(9)	2381.1(12)	19.5(4)
N2	9451.9(14)	3648.4(9)	7364.8(12)	20.3(4)
N3	8223.8(13)	5255.9(9)	6426.2(12)	18.9(4)
N6	6578.2(13)	7739.4(9)	3645.9(12)	19.4(4)
C1	10528.6(16)	4342.7(10)	7073.9(14)	18.3(5)
C35	4268.2(16)	6842.2(10)	2760.5(14)	18.8(5)
C4	9875.8(16)	5096.5(10)	6502.5(13)	17.0(4)
C31	6671.9(17)	5364.6(12)	5565.9(15)	23.0(5)
C3	10755.0(16)	5112.9(11)	6548.5(14)	19.3(5)
C12	8725.6(17)	2728.2(12)	7177.5(16)	23.4(5)
C23	8547.5(17)	5508.7(11)	5177.9(14)	20.1(5)
C5	11243.2(17)	3737.4(12)	8413.5(15)	24.6(5)
C2	11173.8(16)	4627.2(11)	6912.1(14)	19.3(5)
C15	8973.7(18)	2657.9(12)	8577.9(15)	24.6(5)
C11	9157.7(16)	3167.8(11)	7625.1(15)	20.7(5)
C42	3898.0(17)	5670.9(11)	2551.9(15)	22.0(5)
C46	6232.9(17)	5368.0(11)	2550.2(15)	21.5(5)
C24	9233.7(18)	5780.8(12)	4935.8(15)	25.7(5)
C48	6351.5(16)	4866.2(11)	1564.7(15)	22.9(5)
C14	8570.2(17)	2213.4(11)	8141.1(16)	23.3(5)
C47	6542.4(17)	4922.5(11)	2283.5(15)	22.9(5)
C30	5820.9(18)	5579.8(11)	5380.8(16)	24.1(5)
C44	4465(2)	5562.9(13)	3333.6(18)	29.8(6)
C16	9258.1(18)	3130.3(12)	8325.9(16)	23.6(5)
C26	7346.6(17)	5487.7(11)	6218.7(14)	20.3(5)
C65	8103.5(18)	7821.6(12)	4543.8(16)	25.4(5)
C58	5509(2)	8054.0(14)	5166.8(17)	31.5(6)
C60	7443.3(17)	7983.7(11)	3902.3(15)	20.7(5)
C64	8948.9(19)	8062.3(12)	4776.9(17)	27.5(6)
C38	4906.0(17)	7532.4(10)	3481.7(14)	19.6(5)
C39	3611.4(17)	6388.1(12)	1321.4(15)	23.4(5)
C7	12218.1(18)	3788.6(14)	8506.4(18)	31.8(6)
C49	5842.7(17)	5282.6(11)	1122.8(15)	23.2(5)

C43	3798(2)	5151.7(12)	2101.3(18)	30.6(6)
C36	3632.4(18)	7043.6(12)	2996.8(16)	23.8(5)
C57	6183.8(18)	7811.6(12)	4892.1(14)	24.0(5)
C55	5192.6(18)	8790.7(12)	2991.0(15)	25.4(5)
C21	9657.4(19)	6259.3(12)	7231.3(16)	27.6(6)
C50	5534.7(18)	5738.6(11)	1384.6(15)	22.7(5)
C45	5710.9(16)	5783.5(11)	2100.0(15)	19.8(5)
C51	6707.0(19)	4359.3(11)	1303.6(17)	25.9(6)
C8	10912.7(17)	3179.0(11)	7053.1(17)	24.8(5)
C20	9304.5(17)	6229.4(10)	6425.5(14)	21.0(5)
C40	3899(2)	6925.9(12)	1071.5(17)	27.8(6)
C13	8444.1(18)	2262.4(11)	7430.4(16)	24.2(5)
C6	10972(2)	4224.1(14)	8769.6(17)	31.7(6)
C29	5605.6(17)	5918.2(11)	5840.1(15)	22.0(5)
C25	8361.3(18)	4904.8(12)	4921.1(16)	26.8(6)
C54	5506.6(17)	8669.7(11)	3782.4(15)	21.6(5)
C62	8507.7(19)	8619.9(14)	3741.9(16)	30.0(6)
C59	6302(2)	7181.6(12)	5030.5(16)	28.4(6)
C37	4043.2(17)	7489.3(11)	3459.6(16)	23.9(5)
C10	10318(2)	3144.5(14)	6269.5(18)	33.8(7)
C63	9169.1(18)	8457.9(13)	4383.4(16)	26.9(6)
C28	6274.0(18)	6037.1(12)	6491.1(15)	26.5(6)
C9	11046(2)	2606.6(12)	7413(2)	36.0(7)
C61	7661.3(18)	8378.9(13)	3496.1(15)	26.6(6)
C22	8612.5(19)	6682.9(12)	6065.5(17)	28.4(6)
C27	7134.8(17)	5823.3(12)	6681.5(15)	24.7(5)
C41	2627.6(19)	6412.1(14)	1212.4(18)	32.5(6)
C17	8240.1(19)	1696.5(12)	8398.2(18)	28.8(6)
C32	4647.7(17)	6111.5(12)	5633.0(16)	26.5(6)
C56	6203(2)	9090.9(12)	4233.4(17)	29.8(6)
C19	7227(2)	1668.0(13)	8081.6(19)	34.5(7)
C66	10105.0(19)	8699.1(14)	4644.7(17)	31.4(6)
C34	4150.3(19)	5732.3(13)	5943.7(19)	32.1(6)
C33	4577(2)	6714.6(13)	5851(2)	39.2(8)
C53	7717(2)	4389.7(15)	1541(2)	39.4(8)
C52	6270(2)	4270.5(14)	513.4(18)	34.9(7)
C18	8582(2)	1650.1(15)	9193(2)	40.5(8)
C67	10624(2)	8445(2)	4248(2)	52.7(11)
C68	10109(3)	9327(2)	4616(5)	95(3)

Table S22 Anisotropic Displacement Parameters ($Å^2×10^3$) for **2**^{Pipp}. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
In2	13.62(9)	19.15(10)	18.92(10)	-0.05(6)	7.73(7)	1.13(5)
In1	13.97(9)	18.69(10)	21.72(10)	2.33(6)	8.59(7)	0.35(5)
Cl3	20.3(3)	25.5(3)	25.4(3)	3.5(2)	5.7(2)	4.9(2)
Cl4	24.0(3)	31.3(3)	21.6(3)	1.1(2)	11.7(2)	-2.6(2)
P2	15.3(3)	17.1(3)	19.8(3)	1.9(2)	7.6(2)	1.3(2)
Cl1	24.9(3)	31.5(3)	25.3(3)	-0.1(2)	14.2(2)	0.7(2)

P1	14.4(3)	17.3(3)	23.0(3)	3.4(2)	8.6(2)	1.0(2)
P3	14.7(3)	17.9(3)	21.9(3)	0.5(2)	8.4(2)	0.4(2)
Cl2	20.7(3)	26.7(3)	32.1(3)	1.5(3)	3.9(2)	-4.2(2)
P4	17.7(3)	19.5(3)	18.3(3)	-0.1(2)	8.1(2)	1.8(2)
N4	14.9(9)	21.2(10)	23.5(11)	-0.3(8)	10.6(8)	1.4(8)
N1	14.1(9)	20.4(10)	22.0(11)	3.1(8)	8.6(8)	-0.7(8)
N5	17.4(9)	18.4(9)	24.0(11)	-2.0(8)	9.6(8)	0.8(8)
N2	16.6(9)	20.8(10)	23.8(11)	4.4(9)	8.3(8)	-1.0(8)
N3	15.4(9)	19.6(10)	22.5(11)	4.6(8)	8.2(8)	4.2(8)
N6	15.5(9)	21.6(10)	21.1(10)	-3.3(8)	7.1(8)	-0.2(8)
C1	14.6(10)	17.4(11)	23.6(13)	2.3(9)	8.3(10)	2.2(8)
C35	17.0(11)	16.9(11)	23.4(13)	-0.1(10)	8.8(10)	1.1(9)
C4	16.4(11)	17.0(11)	17.9(11)	2.1(9)	7.1(9)	2.0(8)
C31	21.1(12)	25.7(13)	23.3(13)	-1.1(10)	9.9(10)	3.6(10)
C3	17.0(11)	20.4(11)	22.8(12)	-0.2(10)	10.1(9)	-1.7(9)
C12	21.6(12)	26.3(13)	25.5(13)	2.4(11)	12.5(10)	0.7(10)
C23	17.6(11)	24.7(12)	19.0(12)	1.1(10)	8.3(9)	1.8(9)
C5	19.0(12)	30.1(13)	22.2(13)	5.6(11)	5.3(10)	-0.2(10)
C2	16.1(11)	20.2(11)	22.5(12)	-0.6(10)	8.6(9)	-1.9(9)
C15	23.4(12)	27.2(13)	23.9(13)	6.2(11)	9.9(10)	0.5(10)
C11	16.2(11)	21.7(12)	26.7(13)	2.4(10)	11.1(10)	2.0(9)
C42	18.4(11)	20.8(12)	29.7(14)	2.5(10)	12.7(11)	-0.4(9)
C46	20.9(11)	21.6(12)	21.7(12)	-0.2(10)	8.0(10)	0.4(9)
C24	24.0(12)	31.8(14)	23.4(13)	4.0(11)	11.6(11)	1.3(10)
C48	15.9(11)	22.7(12)	30.9(14)	-4.0(11)	9.9(10)	-3.2(9)
C14	18.7(11)	20.8(12)	33.5(15)	6.7(11)	13.7(11)	2.1(9)
C47	16.8(11)	23.7(12)	27.9(13)	1.1(10)	8.3(10)	1.2(9)
C30	17.8(12)	28.4(13)	23.7(13)	-0.6(10)	5.5(10)	2.0(9)
C44	26.8(14)	31.2(15)	34.4(16)	9.9(12)	15.2(12)	2.9(11)
C16	22.2(12)	23.0(12)	26.2(14)	1.0(10)	10.1(11)	-1.8(10)
C26	18.7(11)	20.8(11)	23.5(13)	1.8(10)	10.5(10)	2.1(9)
C65	23.7(13)	24.4(13)	27.2(14)	2.3(11)	9.1(11)	-2.2(10)
C58	34.9(16)	39.3(16)	22.7(14)	2.6(12)	13.8(12)	11.0(12)
C60	19.5(12)	23.5(12)	20.7(13)	-2.0(10)	9.6(10)	0.7(9)
C64	18.8(12)	31.2(14)	27.9(15)	-1.8(11)	4.3(11)	0.4(10)
C38	19.9(11)	18.3(11)	22.1(12)	-1.1(9)	10.0(10)	2.8(9)
C39	19.1(11)	28.1(13)	22.1(13)	0.7(10)	7.0(10)	-1.5(10)
C7	16.3(12)	38.4(16)	35.0(16)	7.7(13)	3.9(11)	1.2(11)
C49	23.2(12)	24.0(12)	26.2(13)	-2.8(10)	13.7(11)	-1.2(10)
C43	31.1(14)	19.2(13)	46.6(18)	-3.0(12)	20.9(14)	-5.6(10)
C36	17.6(12)	22.8(12)	34.7(15)	-0.1(11)	14.1(11)	0.0(9)
C57	25.9(12)	28.1(13)	18.9(12)	0.8(10)	9.9(10)	5.5(10)
C55	25.7(13)	25.1(12)	26.0(14)	3.9(11)	10.8(11)	0.6(10)
C21	30.0(13)	24.6(13)	27.1(14)	-3.0(11)	9.8(11)	0.7(11)
C50	24.0(12)	22.5(12)	24.0(13)	4.4(10)	12.0(10)	2.2(10)
C45	16.6(11)	18.7(11)	27.4(13)	-0.9(10)	12.2(10)	-0.2(9)
C51	24.5(13)	21.5(12)	33.0(15)	-2.8(11)	12.5(12)	0.7(10)
C8	20.0(12)	19.9(12)	41.1(16)	0.8(11)	19.0(12)	0.9(9)
C20	22.7(12)	16.0(11)	25.6(13)	0.4(10)	10.7(10)	-0.8(9)
C40	26.1(13)	29.1(14)	29.6(15)	7.3(11)	12.6(12)	3.1(10)
C13	22.6(12)	20.1(12)	32.9(15)	-3.1(11)	14.1(11)	-2.7(9)

C6	26.4(13)	39.3(16)	27.3(15)	-2.8(13)	8.1(12)	-4.9(12)
C29	20.5(12)	21.0(12)	25.7(13)	3.4(10)	10.3(10)	3.5(9)
C25	24.1(12)	31.5(14)	26.9(14)	-8.8(11)	12.1(11)	-4.1(11)
C54	21.8(12)	19.2(11)	25.3(13)	0.6(10)	10.7(10)	1.8(9)
C62	25.9(13)	37.9(15)	26.9(14)	1.6(12)	11.0(12)	-6.3(11)
C59	30.3(14)	29.9(14)	27.9(15)	8.1(11)	14.3(12)	9.2(11)
C37	20.7(12)	22.8(12)	32.0(14)	0.1(11)	14.5(11)	3.4(9)
C10	41.9(17)	32.7(15)	36.2(17)	-10.3(13)	25.4(14)	-7.9(13)
C63	21.4(12)	31.3(14)	28.1(14)	-5.1(11)	9.9(11)	-2.6(11)
C28	23.4(12)	32.2(14)	25.5(14)	-4.7(11)	11.3(11)	8.1(11)
C9	31.0(15)	21.5(13)	63(2)	8.3(14)	27.0(15)	5.3(11)
C61	19.0(12)	37.1(15)	20.7(13)	1.6(11)	4.5(10)	-2.8(11)
C22	29.4(14)	21.7(12)	34.2(15)	5.0(11)	12.6(12)	6.9(10)
C27	17.1(11)	32.7(14)	22.1(13)	-1.9(11)	5.3(10)	2.6(10)
C41	21.1(13)	42.3(17)	33.1(16)	9.3(13)	9.6(12)	-0.5(11)
C17	26.8(13)	19.1(12)	45.3(18)	7.0(12)	19.3(13)	2.0(10)
C32	17.7(11)	31.4(14)	27.9(14)	1.6(11)	6.2(10)	5.4(10)
C56	36.5(15)	20.9(12)	30.5(15)	-5.7(11)	11.4(12)	-2.8(11)
C19	29.4(14)	30.7(15)	44.2(18)	7.4(13)	15.3(13)	-7.3(12)
C66	22.7(13)	38.8(16)	30.8(15)	-0.7(13)	8.3(12)	-7.8(11)
C34	22.0(13)	30.1(14)	44.9(18)	-4.5(13)	13.8(13)	0.0(11)
C33	30.7(15)	25.1(14)	65(2)	3.6(15)	22.7(16)	7.6(12)
C53	26.0(15)	39.2(17)	54(2)	-18.4(15)	17.3(15)	2.9(12)
C52	43.4(17)	29.6(15)	32.6(16)	-5.7(13)	15.9(14)	3.7(13)
C18	42.6(18)	34.9(16)	43.2(19)	18.3(15)	15.9(15)	-3.4(13)
C67	26.5(16)	85(3)	48(2)	-21(2)	16.9(16)	-16.0(17)
C68	37(2)	43(2)	177(7)	-7(3)	11(3)	-17.6(18)

Table S23 Bond Lengths for **2**^{Pipp}.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
In2	Cl3	2.3763(6)	C15	C14	1.385(4)
In2	Cl4	2.3757(6)	C15	C16	1.400(4)
In2	N4	2.123(2)	C11	C16	1.392(4)
In2	N5	2.267(2)	C42	C44	1.535(4)
In2	N6	2.267(2)	C42	C43	1.524(4)
In1	Cl1	2.3816(7)	C46	C47	1.385(4)
In1	Cl2	2.3669(6)	C46	C45	1.401(4)
In1	N1	2.129(2)	C48	C47	1.396(4)
In1	N2	2.273(2)	C48	C49	1.388(4)
In1	N3	2.270(2)	C48	C51	1.533(4)
P2	N3	1.615(2)	C14	C13	1.402(4)
P2	C4	1.778(2)	C14	C17	1.527(4)
P2	C23	1.821(3)	C30	C29	1.392(4)
P2	C20	1.819(3)	C26	C27	1.391(4)
P1	N2	1.619(2)	C65	C60	1.396(4)
P1	C1	1.773(3)	C65	C64	1.398(4)
P1	C5	1.829(3)	C58	C57	1.536(4)
P1	C8	1.821(3)	C60	C61	1.400(4)
P3	N5	1.623(2)	C64	C63	1.384(4)

P3	C35	1.776(3)	C38	C37	1.396(3)
P3	C42	1.815(3)	C39	C40	1.529(4)
P3	C39	1.833(3)	C39	C41	1.535(4)
P4	N6	1.613(2)	C49	C50	1.398(4)
P4	C38	1.775(3)	C36	C37	1.415(4)
P4	C57	1.826(3)	C57	C59	1.536(4)
P4	C54	1.825(3)	C55	C54	1.534(4)
N4	C35	1.357(3)	C21	C20	1.532(4)
N4	C38	1.355(3)	C50	C45	1.392(4)
N1	C1	1.351(3)	C51	C53	1.528(4)
N1	C4	1.348(3)	C51	C52	1.516(4)
N5	C45	1.436(3)	C8	C10	1.527(5)
N2	C11	1.432(3)	C8	C9	1.535(4)
N3	C26	1.438(3)	C20	C22	1.535(4)
N6	C60	1.427(3)	C29	C28	1.389(4)
C1	C2	1.401(3)	C29	C32	1.525(3)
C35	C36	1.395(4)	C54	C56	1.534(4)
C4	C3	1.403(3)	C62	C63	1.397(4)
C31	C30	1.390(4)	C62	C61	1.399(4)
C31	C26	1.398(4)	C63	C66	1.523(4)
C3	C2	1.409(4)	C28	C27	1.401(4)
C12	C11	1.397(4)	C17	C19	1.525(4)
C12	C13	1.386(4)	C17	C18	1.513(5)
C23	C24	1.539(4)	C32	C34	1.518(4)
C23	C25	1.532(4)	C32	C33	1.533(4)
C5	C7	1.533(4)	C66	C67	1.516(5)
C5	C6	1.534(4)	C66	C68	1.507(6)

Table S24 Bond Angles for **2**^{Pipp}.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl4	In2	Cl3	112.26(2)	C7	C5	P1	112.2(2)
N4	In2	Cl3	127.10(6)	C7	C5	C6	111.1(2)
N4	In2	Cl4	120.56(6)	C6	C5	P1	109.60(19)
N4	In2	N5	77.52(8)	C1	C2	C3	106.0(2)
N4	In2	N6	77.35(8)	C14	C15	C16	121.7(3)
N5	In2	Cl3	96.78(6)	C12	C11	N2	121.2(2)
N5	In2	Cl4	99.99(6)	C16	C11	N2	121.4(3)
N5	In2	N6	154.61(7)	C16	C11	C12	117.4(2)
N6	In2	Cl3	95.47(6)	C44	C42	P3	109.80(19)
N6	In2	Cl4	95.78(6)	C43	C42	P3	113.1(2)
Cl2	In1	Cl1	115.89(2)	C43	C42	C44	112.3(2)
N1	In1	Cl1	117.64(6)	C47	C46	C45	120.6(3)
N1	In1	Cl2	126.47(6)	C47	C48	C51	119.4(3)
N1	In1	N2	76.86(8)	C49	C48	C47	117.1(2)
N1	In1	N3	77.49(8)	C49	C48	C51	123.5(3)
N2	In1	Cl1	98.02(6)	C15	C14	C13	116.9(2)
N2	In1	Cl2	95.66(6)	C15	C14	C17	122.9(3)
N3	In1	Cl1	96.75(6)	C13	C14	C17	120.2(3)
N3	In1	Cl2	96.83(6)	C46	C47	C48	122.1(3)

N3	In1	N2	154.13(7)	C31	C30	C29	121.4(3)
N3	P2	C4	103.65(11)	C11	C16	C15	121.1(3)
N3	P2	C23	114.16(12)	C31	C26	N3	121.6(2)
N3	P2	C20	116.90(12)	C27	C26	N3	120.4(2)
C4	P2	C23	108.35(12)	C27	C26	C31	117.9(2)
C4	P2	C20	105.24(12)	C60	C65	C64	120.3(3)
C20	P2	C23	107.80(12)	C65	C60	N6	121.5(2)
N2	P1	C1	102.98(11)	C65	C60	C61	118.2(2)
N2	P1	C5	113.68(12)	C61	C60	N6	120.2(2)
N2	P1	C8	116.57(12)	C63	C64	C65	122.0(3)
C1	P1	C5	108.80(13)	N4	C38	P4	114.71(18)
C1	P1	C8	105.73(13)	N4	C38	C37	109.4(2)
C8	P1	C5	108.42(14)	C37	C38	P4	135.8(2)
N5	P3	C35	103.54(12)	C40	C39	P3	109.12(19)
N5	P3	C42	116.50(12)	C40	C39	C41	111.1(2)
N5	P3	C39	113.28(12)	C41	C39	P3	112.0(2)
C35	P3	C42	106.17(13)	C48	C49	C50	121.6(3)
C35	P3	C39	109.14(13)	C35	C36	C37	106.0(2)
C42	P3	C39	107.75(13)	C58	C57	P4	111.82(19)
N6	P4	C38	103.63(12)	C59	C57	P4	109.3(2)
N6	P4	C57	114.01(12)	C59	C57	C58	111.1(2)
N6	P4	C54	115.99(12)	C45	C50	C49	120.9(3)
C38	P4	C57	108.22(13)	C46	C45	N5	120.1(2)
C38	P4	C54	106.47(12)	C50	C45	N5	122.1(2)
C54	P4	C57	107.93(13)	C50	C45	C46	117.8(2)
C35	N4	In2	125.84(17)	C53	C51	C48	111.1(2)
C38	N4	In2	125.56(17)	C52	C51	C48	113.8(2)
C38	N4	C35	108.2(2)	C52	C51	C53	110.3(3)
C1	N1	In1	125.53(17)	C10	C8	P1	110.4(2)
C4	N1	In1	125.61(16)	C10	C8	C9	112.0(3)
C4	N1	C1	108.8(2)	C9	C8	P1	112.8(2)
P3	N5	In2	117.60(11)	C21	C20	P2	109.71(18)
C45	N5	In2	122.98(15)	C21	C20	C22	112.6(2)
C45	N5	P3	119.33(17)	C22	C20	P2	113.73(19)
P1	N2	In1	117.89(11)	C12	C13	C14	121.7(3)
C11	N2	In1	121.98(15)	C30	C29	C32	119.4(2)
C11	N2	P1	119.25(17)	C28	C29	C30	117.7(2)
P2	N3	In1	117.35(11)	C28	C29	C32	122.8(2)
C26	N3	In1	121.49(16)	C55	C54	P4	109.46(19)
C26	N3	P2	119.84(17)	C56	C54	P4	114.19(19)
P4	N6	In2	117.52(11)	C56	C54	C55	112.4(2)
C60	N6	In2	121.66(16)	C63	C62	C61	121.2(3)
C60	N6	P4	119.94(18)	C38	C37	C36	106.5(2)
N1	C1	P1	115.27(18)	C64	C63	C62	117.6(3)
N1	C1	C2	109.5(2)	C64	C63	C66	120.5(3)
C2	C1	P1	135.14(19)	C62	C63	C66	121.8(3)
N4	C35	P3	114.71(18)	C29	C28	C27	121.3(3)
N4	C35	C36	109.8(2)	C62	C61	C60	120.7(3)
C36	C35	P3	135.2(2)	C26	C27	C28	120.7(3)
N1	C4	P2	114.79(17)	C19	C17	C14	111.1(2)
N1	C4	C3	109.2(2)	C18	C17	C14	113.8(3)

C3	C4	P2	136.01(19)	C18	C17	C19	109.9(3)
C30	C31	C26	120.9(3)	C29	C32	C33	113.1(2)
C4	C3	C2	106.5(2)	C34	C32	C29	111.1(2)
C13	C12	C11	121.1(3)	C34	C32	C33	109.1(3)
C24	C23	P2	111.33(18)	C67	C66	C63	110.6(3)
C25	C23	P2	109.46(19)	C68	C66	C63	112.7(3)
C25	C23	C24	111.1(2)	C68	C66	C67	111.6(4)

Table S25 Torsion Angles for **2**^{Pipp}.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
In2	N4	C35	P3	-1.0(3)	C5	P1	C1	N1	-116.7(2)
In2	N4	C35	C36	173.61(19)	C5	P1	C1	C2	66.6(3)
In2	N4	C38	P4	3.5(3)	C5	P1	C8	C10	-178.34(19)
In2	N4	C38	C37	-173.82(18)	C5	P1	C8	C9	55.6(2)
In2	N5	C45	C46	76.5(3)	C15	C14	C13	C12	1.3(4)
In2	N5	C45	C50	-102.8(3)	C15	C14	C17	C19	110.9(3)
In2	N6	C60	C65	-89.5(3)	C15	C14	C17	C18	-13.8(4)
In2	N6	C60	C61	87.8(3)	C11	C12	C13	C14	0.7(4)
In1	N1	C1	P1	5.5(3)	C42	P3	N5	In2	-125.68(14)
In1	N1	C1	C2	-177.00(17)	C42	P3	N5	C45	57.6(2)
In1	N1	C4	P2	-3.5(3)	C42	P3	C35	N4	130.0(2)
In1	N1	C4	C3	176.67(17)	C42	P3	C35	C36	-42.8(3)
In1	N2	C11	C12	90.6(3)	C42	P3	C39	C40	173.46(19)
In1	N2	C11	C16	-86.8(3)	C42	P3	C39	C41	50.0(2)
In1	N3	C26	C31	-86.7(3)	C48	C49	C50	C45	-1.6(4)
In1	N3	C26	C27	90.3(3)	C14	C15	C16	C11	-1.0(4)
P2	N3	C26	C31	79.8(3)	C47	C46	C45	N5	179.3(2)
P2	N3	C26	C27	-103.2(3)	C47	C46	C45	C50	-1.5(4)
P2	C4	C3	C2	-179.3(2)	C47	C48	C49	C50	0.0(4)
P1	N2	C11	C12	-100.4(3)	C47	C48	C51	C53	-69.4(3)
P1	N2	C11	C16	82.2(3)	C47	C48	C51	C52	165.4(3)
P1	C1	C2	C3	177.2(2)	C30	C31	C26	N3	178.2(3)
P3	N5	C45	C46	-107.0(2)	C30	C31	C26	C27	1.2(4)
P3	N5	C45	C50	73.7(3)	C30	C29	C28	C27	-0.2(4)
P3	C35	C36	C37	173.1(2)	C30	C29	C32	C34	95.6(3)
P4	N6	C60	C65	79.5(3)	C30	C29	C32	C33	-141.3(3)
P4	N6	C60	C61	-103.2(3)	C16	C15	C14	C13	-1.2(4)
P4	C38	C37	C36	-176.1(2)	C16	C15	C14	C17	-179.0(2)
N4	C35	C36	C37	0.0(3)	C26	C31	C30	C29	-0.9(4)
N4	C38	C37	C36	0.4(3)	C65	C60	C61	C62	-2.5(4)
N1	C1	C2	C3	0.4(3)	C65	C64	C63	C62	1.1(4)
N1	C4	C3	C2	0.4(3)	C65	C64	C63	C66	-178.3(3)
N5	P3	C35	N4	6.8(2)	C60	C65	C64	C63	-1.1(5)
N5	P3	C35	C36	-166.0(3)	C64	C65	C60	N6	179.1(3)
N5	P3	C42	C44	53.5(2)	C64	C65	C60	C61	1.8(4)
N5	P3	C42	C43	-72.7(2)	C64	C63	C66	C67	103.6(4)
N5	P3	C39	C40	-56.2(2)	C64	C63	C66	C68	-130.7(5)
N5	P3	C39	C41	-179.6(2)	C38	P4	N6	In2	-10.83(16)
N2	P1	C1	N1	4.2(2)	C38	P4	N6	C60	179.7(2)

N2	P1	C1	C2	-172.5(3)	C38	P4	C57	C58	-69.7(2)
N2	P1	C5	C7	-179.8(2)	C38	P4	C57	C59	53.8(2)
N2	P1	C5	C6	-55.9(2)	C38	P4	C54	C55	-61.8(2)
N2	P1	C8	C10	51.9(2)	C38	P4	C54	C56	171.2(2)
N2	P1	C8	C9	-74.2(2)	C38	N4	C35	P3	-174.38(18)
N2	C11	C16	C15	-179.6(2)	C38	N4	C35	C36	0.2(3)
N3	P2	C4	N1	9.3(2)	C39	P3	N5	In2	108.50(14)
N3	P2	C4	C3	-171.0(3)	C39	P3	N5	C45	-68.2(2)
N3	P2	C23	C24	179.14(17)	C39	P3	C35	N4	-114.1(2)
N3	P2	C23	C25	-57.6(2)	C39	P3	C35	C36	73.1(3)
N3	P2	C20	C21	52.0(2)	C39	P3	C42	C44	-177.93(19)
N3	P2	C20	C22	-75.2(2)	C39	P3	C42	C43	55.8(2)
N3	C26	C27	C28	-178.1(3)	C49	C48	C47	C46	0.8(4)
N6	P4	C38	N4	5.1(2)	C49	C48	C51	C53	110.5(3)
N6	P4	C38	C37	-178.5(3)	C49	C48	C51	C52	-14.8(4)
N6	P4	C57	C58	175.6(2)	C49	C50	C45	N5	-178.5(2)
N6	P4	C57	C59	-60.9(2)	C49	C50	C45	C46	2.3(4)
N6	P4	C54	C55	52.9(2)	C57	P4	N6	In2	106.57(15)
N6	P4	C54	C56	-74.1(2)	C57	P4	N6	C60	-62.9(2)
N6	C60	C61	C62	-179.9(3)	C57	P4	C38	N4	-116.3(2)
C1	P1	N2	In1	-11.19(16)	C57	P4	C38	C37	60.1(3)
C1	P1	N2	C11	179.3(2)	C57	P4	C54	C55	-177.83(18)
C1	P1	C5	C7	-65.6(2)	C57	P4	C54	C56	55.2(2)
C1	P1	C5	C6	58.2(2)	C45	C46	C47	C48	-0.1(4)
C1	P1	C8	C10	-61.8(2)	C51	C48	C47	C46	-179.4(2)
C1	P1	C8	C9	172.1(2)	C51	C48	C49	C50	-179.8(2)
C1	N1	C4	P2	179.60(18)	C8	P1	N2	In1	-126.43(14)
C1	N1	C4	C3	-0.2(3)	C8	P1	N2	C11	64.1(2)
C35	P3	N5	In2	-9.57(16)	C8	P1	C1	N1	127.0(2)
C35	P3	N5	C45	173.7(2)	C8	P1	C1	C2	-49.7(3)
C35	P3	C42	C44	-61.1(2)	C8	P1	C5	C7	48.9(2)
C35	P3	C42	C43	172.6(2)	C8	P1	C5	C6	172.74(19)
C35	P3	C39	C40	58.6(2)	C20	P2	N3	In1	-126.46(13)
C35	P3	C39	C41	-64.9(2)	C20	P2	N3	C26	66.5(2)
C35	N4	C38	P4	176.94(18)	C20	P2	C4	N1	132.6(2)
C35	N4	C38	C37	-0.4(3)	C20	P2	C4	C3	-47.7(3)
C35	C36	C37	C38	-0.3(3)	C20	P2	C23	C24	47.5(2)
C4	P2	N3	In1	-11.21(16)	C20	P2	C23	C25	170.74(17)
C4	P2	N3	C26	-178.3(2)	C13	C12	C11	N2	179.8(2)
C4	P2	C23	C24	-65.9(2)	C13	C12	C11	C16	-2.8(4)
C4	P2	C23	C25	57.3(2)	C13	C14	C17	C19	-66.9(3)
C4	P2	C20	C21	-62.4(2)	C13	C14	C17	C18	168.4(3)
C4	P2	C20	C22	170.5(2)	C29	C28	C27	C26	0.5(5)
C4	N1	C1	P1	-177.67(18)	C54	P4	N6	In2	-127.11(13)
C4	N1	C1	C2	-0.1(3)	C54	P4	N6	C60	63.4(2)
C4	C3	C2	C1	-0.5(3)	C54	P4	C38	N4	127.9(2)
C31	C30	C29	C28	0.4(4)	C54	P4	C38	C37	-55.7(3)
C31	C30	C29	C32	-175.8(3)	C54	P4	C57	C58	45.2(2)
C31	C26	C27	C28	-1.0(4)	C54	P4	C57	C59	168.66(18)
C12	C11	C16	C15	2.9(4)	C62	C63	C66	C67	-75.7(4)
C23	P2	N3	In1	106.43(14)	C62	C63	C66	C68	49.9(5)

C23	P2	N3	C26	-60.6(2)	C63	C62	C61	C60	2.6(5)
C23	P2	C4	N1	-112.3(2)	C28	C29	C32	C34	-80.4(3)
C23	P2	C4	C3	67.4(3)	C28	C29	C32	C33	42.7(4)
C23	P2	C20	C21	-177.86(18)	C61	C62	C63	C64	-1.9(5)
C23	P2	C20	C22	55.0(2)	C61	C62	C63	C66	177.5(3)
C5	P1	N2	In1	106.34(15)	C17	C14	C13	C12	179.2(2)
C5	P1	N2	C11	-63.1(2)	C32	C29	C28	C27	175.9(3)

Table S26 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **2^{Pipp}**.

Atom	***x***	***y***	***z***	**U(eq)**
H31	6796.89	5130.54	5244.21	28
H3	11016.79	5395.73	6369.73	23
H12	8623.24	2749.07	6691.57	28
H23	7979.43	5723.53	4969.42	24
H5	11178.38	3384.78	8647.68	29
H2	11771.64	4515.61	7024.48	23
H15	9059.6	2641.68	9060.78	30
H42	3289.57	5775.76	2516.34	26
H46	6375.68	5392.24	3042.55	26
H24A	9263.61	6181.64	5033.85	39
H24B	9055.54	5721.13	4428.59	39
H24C	9819.02	5612.83	5190.98	39
H47	6895.73	4646.48	2599.62	27
H30	5376.3	5494.28	4931.19	29
H44A	4194.57	5263.9	3506.96	45
H44B	4496.03	5903.59	3604.61	45
H44C	5065.72	5452.27	3388.5	45
H16	9523.98	3430.18	8638.35	28
H65	7977.52	7546.4	4823.18	30
H58A	5468.36	8458.35	5093.44	47
H58B	5704.2	7973.39	5671.05	47
H58C	4925	7884.97	4911.09	47
H64	9385.69	7950.96	5218.93	33
H39	3690.42	6072.56	1034.21	28
H7A	12382.88	3464	8294.95	48
H7B	12598.26	3805.61	9009.78	48
H7C	12296.39	4128.8	8273.77	48
H49	5700.49	5256.97	630.61	28
H43A	4385.92	5026.77	2138.95	46
H43B	3429.67	5239.02	1608.39	46
H43C	3513.95	4855.51	2266.8	46
H36	3043.65	6909.16	2872.46	29
H57	6770.49	7996.09	5151.23	29
H55A	4893.64	9153.43	2886.06	38
H55B	4777.3	8499.36	2723.64	38
H55C	5706.44	8796.44	2857.72	38
H21A	9982.02	6609.53	7393.01	41

H21B	10057.98	5944.39	7434.74	41
H21C	9158.06	6243.02	7381.51	41
H50	5200.74	6021.59	1070.1	27
H51	6573.92	4022.76	1531.75	31
H8	11510.04	3309.88	7089.08	30
H20	9821.99	6300.45	6292.54	25
H40A	3779.61	7244.56	1319.13	42
H40B	3564.14	6969.13	562.92	42
H40C	4535.96	6908.56	1172.15	42
H13	8158.05	1968.52	7114.1	29
H6A	11078.14	4577.13	8576.21	48
H6B	11325.39	4213.73	9278.41	48
H6C	10339.6	4192.3	8681.87	48
H25A	8923.63	4699.92	5065.56	40
H25B	8063.21	4899.8	4405.97	40
H25C	7978.06	4728.15	5127.35	40
H54	4976.18	8712.78	3906.33	26
H62	8635.1	8898.72	3467.6	36
H59A	5724.05	6995.93	4811.96	43
H59B	6547.23	7112.97	5539.66	43
H59C	6709.75	7034.08	4828.13	43
H37	3782.98	7714.88	3706.83	29
H10A	10594.96	2899.92	6032.25	51
H10B	10241.84	3517.84	6061.16	51
H10C	9736.68	2993.59	6212.3	51
H28	6144.98	6267.94	6813.7	32
H9A	10475.25	2468.97	7399.28	54
H9B	11466.79	2641.28	7904.2	54
H9C	11282.83	2344.31	7165.04	54
H61	7229.94	8484.48	3048.99	32
H22A	8388.22	6635.56	5553	43
H22B	8889.2	7050.94	6193.38	43
H22C	8118.34	6651.74	6220.27	43
H27	7578.74	5908.53	7131.57	30
H41A	2448.02	6051.9	1338.79	49
H41B	2264.51	6494.83	717.06	49
H41C	2542.11	6704.74	1511.66	49
H17	8462.75	1363.74	8224.28	35
H32	4345.66	6089.44	5107.99	32
H56A	6387.61	8995.45	4732.82	45
H56B	5945.98	9466.24	4150.29	45
H56C	6720.88	9080.2	4105.25	45
H19A	6985.95	1982.7	8253.61	52
H19B	7033.86	1317.59	8221.23	52
H19C	7011	1685.34	7566.56	52
H66	10413.45	8589.27	5150.6	38
H34A	4169.36	5348.57	5787.26	48
H34B	3530.39	5854.78	5784.98	48
H34C	4430.21	5748.82	6459.29	48
H33A	4860.38	6746.65	6365.47	59
H33B	3948.88	6819.57	5691.68	59

H33C	4875.74	6963.14	5635.87	59
H53A	7872.29	4708.36	1314.23	59
H53B	7933.42	4045.45	1406.92	59
H53C	7991.73	4434.8	2054.01	59
H52A	5622.46	4259.16	367.23	52
H52B	6474.78	3917.36	390.8	52
H52C	6428.8	4577.63	271.6	52
H18A	9232.9	1670.77	9392.89	61
H18B	8394.17	1293.16	9320.52	61
H18C	8340.78	1956.25	9378.69	61
H67A	10659.7	8040.67	4317.74	79
H67B	11224.93	8602.9	4426.13	79
H67C	10322.19	8528.69	3744.7	79
H68A	9821.53	9449.58	4125.12	143
H68B	10724.15	9461.62	4815.59	143
H68C	9784.84	9476.95	4889.12	143

Table S27 Fractional Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **2^{Mes}**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
In1	2105.3(2)	3278.7(2)	3046.8(2)	39.82(7)
P1	1589.3(7)	3186.5(3)	4632.4(3)	41.57(14)
Cl2	2712.1(10)	2238.5(4)	2493.6(4)	62.73(19)
P2	4101(7)	4708(4)	2875(4)	40.8(7)
Cl1	-192.5(8)	3550.5(6)	2562.2(4)	71.7(2)
N1	2811(3)	4007.5(12)	3788.0(10)	45.1(5)
N3	3558(2)	4047.0(12)	2524.1(10)	42.2(4)
N2	1571(2)	2724.6(11)	3978.4(10)	42.1(4)
C26	4434(3)	3788.0(14)	2024.3(12)	41.8(5)
C12	2763(3)	1582.0(14)	4119.7(12)	45.1(5)
C31	5597(3)	3338.9(14)	2178.7(14)	47.1(6)
C13	2667(3)	861.1(15)	4210.9(14)	52.6(6)
C4	3469(3)	4627.6(15)	3689.6(12)	48.6(6)
C11	1500(3)	1975.6(14)	4027.3(12)	42.3(5)
C1	2548(3)	3956.1(14)	4423.6(12)	45.3(6)
C27	4122(3)	3962.0(15)	1375.8(12)	45.8(5)
C16	166(3)	1628.9(15)	3972.3(14)	48.8(6)
C17	4242(3)	1903.3(17)	4082.6(15)	54.7(7)
C2	3057(4)	4556.0(16)	4735.8(13)	53.5(7)
C28	4977(3)	3690.6(17)	904.6(13)	53.2(6)
C3	3644(4)	4985.8(16)	4269.7(14)	55.4(7)
C14	1354(4)	514.0(16)	4188.3(16)	58.3(7)
C15	130(4)	903.7(16)	4055.9(15)	56.9(7)
C6	-194(3)	3482.1(17)	4867.8(15)	55.2(7)
C30	6423(3)	3087.7(16)	1684.8(16)	53.3(6)
C29	6139(3)	3253.5(17)	1053.8(16)	55.8(7)
C32	2882(4)	4433.2(19)	1184.0(14)	61.8(8)
C19	-1202(3)	2015(2)	3798.8(19)	66.3(8)

C9	2438(3)	2726.9(16)	5325.0(13)	53.2(6)
C34	5967(3)	3097.5(19)	2854.1(16)	59.9(8)
C8	1373(4)	2267(2)	5674.6(18)	72.2(9)
C5	-958(4)	3871(2)	4315.1(18)	69.9(9)
C21	3094(15)	5494(6)	2588(8)	55.8(12)
C33	7061(4)	2960(3)	534(2)	80.8(11)
C18	1283(5)	-273.3(19)	4280(2)	86.9(12)
C10	3328(5)	3181(2)	5787.9(16)	70.2(9)
C7	-117(4)	3936(2)	5474.0(17)	76.9(10)
C23	6040(30)	5471(12)	2224(8)	70(5)
C20	1481(17)	5381(8)	2611(9)	63(3)
C24	6033(10)	4863(6)	2792(4)	49.6(19)
C22	3565(19)	6156(7)	2969(9)	76(4)
C25	6744(14)	5268(8)	3356(5)	76(4)
P0	3795(4)	4824.0(17)	2872.9(17)	40.8(5)
C21A	2559(8)	5523(3)	2599(3)	55.6(11)
C23A	6192(15)	5290(7)	2155(4)	95(4)
C20A	1011(8)	5294(5)	2667(6)	75(2)
C24A	5595(6)	5219(3)	2874(2)	55.8(12)
C22A	2843(10)	6226(3)	2940(5)	76.3(19)
C25A	6785(6)	4823(4)	3241(3)	73.3(16)

Table S28 Anisotropic Displacement Parameters ($Å^2×10^3$) for **2**^{Mes}. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
In1	45.54(10)	39.29(10)	34.99(9)	-0.41(6)	6.10(6)	-4.16(6)
P1	48.7(3)	40.7(3)	36.1(3)	3.6(2)	11.0(2)	0.1(3)
Cl2	92.2(5)	47.0(4)	50.1(4)	-8.3(3)	16.9(3)	-1.1(3)
P2	50.2(16)	36.8(14)	35.8(7)	3.8(10)	5.7(12)	-3.7(11)
Cl1	51.3(4)	94.3(6)	68.6(5)	17.0(4)	-7.9(3)	-6.4(4)
N1	59.7(13)	42.2(11)	33.8(9)	-1.9(8)	7.0(9)	-12.0(10)
N3	46.3(11)	42.9(11)	38.1(10)	4.3(8)	10.1(8)	-3.8(9)
N2	50.6(11)	38.2(10)	38.1(10)	2.8(8)	9.5(8)	-2.9(9)
C26	41.7(12)	43.0(13)	41.3(12)	2.8(10)	7.6(9)	-2.3(10)
C12	53.7(14)	44.3(13)	38.1(12)	0.2(10)	11.4(10)	0.0(11)
C31	41.6(13)	45.1(14)	55.1(15)	6.7(11)	6.5(11)	-0.3(10)
C13	68.4(17)	42.3(14)	48.1(14)	0.9(11)	15.9(12)	7.9(13)
C4	62.6(16)	45.2(14)	38.4(12)	1.5(10)	7.5(11)	-14.0(12)
C11	51.5(13)	39.9(12)	36.2(11)	2.4(9)	9.8(10)	-2.3(10)
C1	56.6(14)	45.2(13)	34.7(11)	-0.9(10)	10.1(10)	-5.4(11)
C27	48.9(13)	47.5(14)	41.5(12)	0.1(11)	6.2(10)	2.8(11)
C16	53.7(15)	47.9(14)	45.1(13)	-0.7(11)	7.6(11)	-5.8(11)
C17	51.8(15)	60.0(17)	52.9(15)	4.8(13)	10.2(12)	1.9(13)
C2	72.2(18)	50.8(15)	38.2(12)	-4.9(11)	10.4(12)	-7.0(13)
C28	58.5(16)	61.2(17)	40.6(13)	-1.3(12)	10.1(11)	1.4(13)
C3	74.1(19)	46.2(15)	46.3(14)	-4.1(12)	6.0(13)	-15.0(14)
C14	78(2)	39.8(14)	58.6(16)	0.5(12)	17.0(15)	-3.6(14)
C15	65.5(18)	48.3(15)	57.5(16)	-0.7(13)	10.5(13)	-15.5(13)
C6	57.1(16)	56.8(16)	53.1(15)	5.2(13)	17.8(13)	8.5(13)

C30	44.3(14)	48.1(15)	68.0(18)	2.1(13)	8.4(12)	3.4(11)
C29	52.0(15)	56.4(17)	60.1(17)	-9.2(13)	16.5(13)	0.8(13)
C32	71.2(19)	69(2)	44.8(15)	1.3(14)	-0.4(13)	19.3(16)
C19	50.1(16)	69(2)	80(2)	3.4(18)	1.7(15)	-6.6(15)
C9	64.4(17)	54.5(16)	41.3(13)	8.2(12)	9.9(12)	4.2(13)
C34	54.9(16)	62.8(18)	61.6(18)	20.5(15)	-0.2(13)	2.6(14)
C8	87(2)	70(2)	61.0(19)	23.8(17)	12.1(17)	-2.2(18)
C5	70(2)	70(2)	70(2)	-0.2(17)	4.7(16)	20.2(17)
C21	74(3)	42.0(17)	51.7(18)	4.0(14)	11(3)	6(3)
C33	72(2)	97(3)	75(2)	-20(2)	23.6(18)	16(2)
C18	111(3)	44.0(18)	108(3)	4.5(19)	23(3)	-4.1(19)
C10	86(2)	75(2)	48.7(16)	5.8(15)	-4.6(16)	1.2(18)
C7	85(2)	85(3)	61.6(19)	-7.5(18)	22.0(17)	25(2)
C23	102(10)	57(7)	54(5)	-1(5)	23(5)	-19(6)
C20	75(4)	52(6)	64(7)	-1(5)	17(6)	10(4)
C24	56(4)	52(5)	42(4)	-8(3)	16(3)	-12(3)
C22	104(9)	45(5)	79(7)	-4(4)	2(9)	4(6)
C25	92(8)	81(9)	55(4)	-18(5)	8(4)	-32(6)
P0	49.8(12)	36.3(10)	36.7(4)	3.2(6)	7.7(8)	-2.7(8)
C21A	74(3)	41.7(15)	51.6(17)	4.5(13)	11(3)	6(3)
C23A	116(7)	113(10)	58(3)	-2(4)	27(3)	-70(6)
C20A	70(3)	63(4)	92(5)	6(3)	16(4)	11(3)
C24A	62(2)	53(3)	54(2)	-0.5(19)	15.6(18)	-11(2)
C22A	104(5)	41(2)	84(4)	-5(2)	0(5)	13(3)
C25A	55(3)	80(4)	85(4)	4(3)	8(2)	-8(3)

Table S29 Bond Lengths for **2^{Mes}**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
In1	Cl2	2.3766(7)	C4	P0	1.780(4)
In1	Cl1	2.3801(8)	C11	C16	1.404(4)
In1	N1	2.161(2)	C1	C2	1.391(4)
In1	N3	2.298(2)	C27	C28	1.388(4)
In1	N2	2.283(2)	C27	C32	1.503(4)
P1	N2	1.623(2)	C16	C15	1.397(4)
P1	C1	1.782(3)	C16	C19	1.500(5)
P1	C6	1.835(3)	C2	C3	1.399(4)
P1	C9	1.839(3)	C28	C29	1.389(4)
P2	N3	1.534(8)	C14	C15	1.377(5)
P2	C4	1.824(8)	C14	C18	1.518(4)
P2	C21	1.856(11)	C6	C5	1.522(5)
P2	C24	1.834(9)	C6	C7	1.531(5)
N1	C4	1.353(3)	C30	C29	1.367(5)
N1	C1	1.359(3)	C29	C33	1.516(4)
N3	C26	1.435(3)	C9	C8	1.530(5)
N3	P0	1.663(4)	C9	C10	1.517(5)
N2	C11	1.436(3)	C21	C20	1.515(13)
C26	C31	1.406(4)	C21	C22	1.547(13)
C26	C27	1.410(4)	C23	C24	1.658(15)
C12	C13	1.394(4)	C24	C25	1.532(11)

C12	C11	1.400(4)	P0	C21A	1.836(6)
C12	C17	1.509(4)	P0	C24A	1.834(5)
C31	C30	1.393(4)	C21A	C20A	1.515(8)
C31	C34	1.507(4)	C21A	C22A	1.537(7)
C13	C14	1.387(5)	C23A	C24A	1.623(9)
C4	C3	1.392(4)	C24A	C25A	1.519(8)

Table S30 Bond Angles for **2**^{Mes}.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl2	In1	Cl1	101.71(4)	C12	C11	N2	120.3(2)
N1	In1	Cl2	144.53(7)	C12	C11	C16	119.2(3)
N1	In1	Cl1	113.76(7)	C16	C11	N2	120.5(2)
N1	In1	N3	76.12(8)	N1	C1	P1	114.10(19)
N1	In1	N2	76.21(8)	N1	C1	C2	109.0(2)
N3	In1	Cl2	98.58(6)	C2	C1	P1	136.8(2)
N3	In1	Cl1	101.13(6)	C26	C27	C32	121.4(2)
N2	In1	Cl2	95.06(6)	C28	C27	C26	119.2(3)
N2	In1	Cl1	103.87(6)	C28	C27	C32	119.3(3)
N2	In1	N3	148.34(8)	C11	C16	C19	121.5(3)
N2	P1	C1	103.43(11)	C15	C16	C11	118.9(3)
N2	P1	C6	114.40(14)	C15	C16	C19	119.5(3)
N2	P1	C9	112.85(13)	C1	C2	C3	107.1(2)
C1	P1	C6	106.05(14)	C27	C28	C29	121.8(3)
C1	P1	C9	112.53(14)	C4	C3	C2	106.2(2)
C6	P1	C9	107.45(14)	C13	C14	C18	120.8(3)
N3	P2	C4	105.2(4)	C15	C14	C13	117.7(3)
N3	P2	C21	111.1(6)	C15	C14	C18	121.5(3)
N3	P2	C24	113.1(5)	C14	C15	C16	122.5(3)
C4	P2	C21	101.0(6)	C5	C6	P1	110.2(2)
C4	P2	C24	117.0(5)	C5	C6	C7	110.6(3)
C24	P2	C21	108.7(6)	C7	C6	P1	112.4(2)
C4	N1	In1	125.59(17)	C29	C30	C31	122.6(3)
C4	N1	C1	108.1(2)	C28	C29	C33	121.2(3)
C1	N1	In1	126.03(18)	C30	C29	C28	118.2(3)
P2	N3	In1	119.2(3)	C30	C29	C33	120.6(3)
C26	N3	In1	118.98(16)	C8	C9	P1	112.6(2)
C26	N3	P2	116.4(3)	C10	C9	P1	115.5(2)
C26	N3	P0	123.8(2)	C10	C9	C8	111.9(3)
P0	N3	In1	115.65(15)	C20	C21	P2	111.1(9)
P1	N2	In1	117.78(11)	C20	C21	C22	111.0(11)
C11	N2	In1	122.33(16)	C22	C21	P2	111.6(10)
C11	N2	P1	118.77(17)	C23	C24	P2	102.3(11)
C31	C26	N3	119.8(2)	C25	C24	P2	113.7(8)
C31	C26	C27	119.3(2)	C25	C24	C23	100.4(11)
C27	C26	N3	120.9(2)	N3	P0	C4	101.8(2)
C13	C12	C11	119.4(3)	N3	P0	C21A	116.3(3)
C13	C12	C17	118.2(3)	N3	P0	C24A	118.2(3)
C11	C12	C17	122.3(3)	C4	P0	C21A	108.8(3)
C26	C31	C34	122.9(3)	C4	P0	C24A	106.0(3)

C30	C31	C26	118.8(3)	C24A	P0	C21A	105.0(3)
C30	C31	C34	118.2(3)	C20A	C21A	P0	110.2(5)
C14	C13	C12	122.0(3)	C20A	C21A	C22A	110.8(6)
N1	C4	P2	112.3(3)	C22A	C21A	P0	113.5(5)
N1	C4	C3	109.7(2)	C23A	C24A	P0	112.2(5)
N1	C4	P0	115.1(2)	C25A	C24A	P0	116.1(4)
C3	C4	P2	137.3(3)	C25A	C24A	C23A	103.7(7)
C3	C4	P0	135.0(2)				

Table S31 Torsion Angles for **2^{Mes}**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
In1	N1	C4	P2	-13.7(4)	C4	P2	C24	C23	-137.0(9)
In1	N1	C4	C3	174.4(2)	C4	P2	C24	C25	-29.7(11)
In1	N1	C4	P0	-1.6(4)	C4	N1	C1	P1	176.7(2)
In1	N1	C1	P1	2.6(3)	C4	N1	C1	C2	-0.3(3)
In1	N1	C1	C2	-174.4(2)	C4	P0	C21A	C20A	-58.9(6)
In1	N3	C26	C31	-68.4(3)	C4	P0	C21A	C22A	66.0(6)
In1	N3	C26	C27	109.8(2)	C4	P0	C24A	C23A	168.7(7)
In1	N3	P0	C4	24.6(3)	C4	P0	C24A	C25A	49.7(5)
In1	N3	P0	C21A	-93.4(3)	C11	C12	C13	C14	2.6(4)
In1	N3	P0	C24A	140.2(2)	C11	C16	C15	C14	-0.2(5)
In1	N2	C11	C12	81.1(3)	C1	P1	N2	In1	-16.19(16)
In1	N2	C11	C16	-97.8(3)	C1	P1	N2	C11	152.0(2)
P1	N2	C11	C12	-86.5(3)	C1	P1	C6	C5	59.2(3)
P1	N2	C11	C16	94.5(3)	C1	P1	C6	C7	-64.8(3)
P1	C1	C2	C3	-175.8(3)	C1	P1	C9	C8	156.6(2)
P2	N3	C26	C31	85.4(4)	C1	P1	C9	C10	26.4(3)
P2	N3	C26	C27	-96.4(4)	C1	N1	C4	P2	172.1(3)
P2	C4	C3	C2	-169.0(4)	C1	N1	C4	C3	0.2(4)
N1	C4	C3	C2	-0.1(4)	C1	N1	C4	P0	-175.8(2)
N1	C4	P0	N3	-15.2(3)	C1	C2	C3	C4	-0.1(4)
N1	C4	P0	C21A	108.1(4)	C27	C26	C31	C30	1.0(4)
N1	C4	P0	C24A	-139.4(3)	C27	C26	C31	C34	-177.0(3)
N1	C1	C2	C3	0.2(4)	C27	C28	C29	C30	0.5(5)
N3	P2	C4	N1	4.7(5)	C27	C28	C29	C33	179.9(3)
N3	P2	C4	C3	173.5(4)	C17	C12	C13	C14	-173.6(3)
N3	P2	C21	C20	51.8(11)	C17	C12	C11	N2	-8.4(4)
N3	P2	C21	C22	176.3(10)	C17	C12	C11	C16	170.5(3)
N3	P2	C24	C23	100.5(10)	C3	C4	P0	N3	170.1(3)
N3	P2	C24	C25	-152.3(10)	C3	C4	P0	C21A	-66.6(5)
N3	C26	C31	C30	179.3(2)	C3	C4	P0	C24A	45.9(5)
N3	C26	C31	C34	1.2(4)	C6	P1	N2	In1	98.68(15)
N3	C26	C27	C28	-178.8(3)	C6	P1	N2	C11	-93.2(2)
N3	C26	C27	C32	1.1(4)	C6	P1	C1	N1	-111.7(2)
N3	P0	C21A	C20A	55.3(6)	C6	P1	C1	C2	64.1(4)
N3	P0	C21A	C22A	-179.8(5)	C6	P1	C9	C8	40.2(3)
N3	P0	C24A	C23A	55.4(7)	C6	P1	C9	C10	-89.9(3)
N3	P0	C24A	C25A	-63.6(6)	C32	C27	C28	C29	179.9(3)
N2	P1	C1	N1	9.0(2)	C19	C16	C15	C14	177.2(3)

N2	P1	C1	C2	-175.2(3)	C9	P1	N2	In1	-138.07(14)
N2	P1	C6	C5	-54.1(3)	C9	P1	N2	C11	30.1(2)
N2	P1	C6	C7	-178.1(2)	C9	P1	C1	N1	131.1(2)
N2	P1	C9	C8	-86.8(3)	C9	P1	C1	C2	-53.1(4)
N2	P1	C9	C10	143.0(2)	C9	P1	C6	C5	179.8(3)
N2	C11	C16	C15	-176.7(2)	C9	P1	C6	C7	55.8(3)
N2	C11	C16	C19	6.0(4)	C34	C31	C30	C29	177.4(3)
C26	N3	P0	C4	-140.8(2)	C21	P2	N3	In1	-104.0(6)
C26	N3	P0	C21A	101.2(3)	C21	P2	N3	C26	102.3(6)
C26	N3	P0	C24A	-25.2(4)	C21	P2	C4	N1	120.5(5)
C26	C31	C30	C29	-0.8(5)	C21	P2	C4	C3	-70.8(7)
C26	C27	C28	C29	-0.3(5)	C21	P2	C24	C23	-23.4(11)
C12	C13	C14	C15	1.5(4)	C21	P2	C24	C25	83.8(11)
C12	C13	C14	C18	179.1(3)	C18	C14	C15	C16	179.7(3)
C12	C11	C16	C15	4.4(4)	C24	P2	N3	In1	133.5(4)
C12	C11	C16	C19	-173.0(3)	C24	P2	N3	C26	-20.3(6)
C31	C26	C27	C28	-0.5(4)	C24	P2	C4	N1	-121.8(5)
C31	C26	C27	C32	179.3(3)	C24	P2	C4	C3	47.0(7)
C31	C30	C29	C28	0.0(5)	C24	P2	C21	C20	176.9(9)
C31	C30	C29	C33	-179.3(3)	C24	P2	C21	C22	-58.6(12)
C13	C12	C11	N2	175.5(2)	P0	N3	C26	C31	96.5(3)
C13	C12	C11	C16	-5.5(4)	P0	N3	C26	C27	-85.3(3)
C13	C14	C15	C16	-2.7(5)	P0	C4	C3	C2	174.8(3)
C4	P2	N3	In1	4.6(4)	C21A	P0	C24A	C23A	-76.3(8)
C4	P2	N3	C26	-149.2(3)	C21A	P0	C24A	C25A	164.7(5)
C4	P2	C21	C20	-59.4(10)	C24A	P0	C21A	C20A	-172.0(5)
C4	P2	C21	C22	65.1(11)	C24A	P0	C21A	C22A	-47.1(6)

Table S32 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **2**^{Mes}.

Atom	***x***	***y***	***z***	**U(eq)**
H13	3507.55	605.26	4289.28	63
H17A	4914.85	1646.19	4353.77	82
H17B	4212.04	2381.27	4223.51	82
H17C	4540.74	1886.79	3647	82
H2	3015.13	4653.03	5172.14	64
H28	4766.48	3804.45	476.95	64
H3	4065.75	5422.92	4334.28	67
H15	-754.77	675.58	4020.82	68
H6	-767.17	3065.88	4960.1	66
H30	7199.5	2795.56	1788.49	64
H32A	2080.1	4333.21	1446	93
H32B	2606.48	4354.74	740.65	93
H32C	3167.03	4912.63	1242.99	93
H19A	-1504.69	2272.71	4165.27	99
H19B	-1938.41	1686.37	3667.65	99
H19C	-1037.42	2333.04	3452.59	99
H9	3125.85	2400.98	5142.17	64

H34A	5469.33	3383.39	3152.65	90
H34B	6987.63	3137.12	2939	90
H34C	5678.86	2618.29	2901.14	90
H8A	673.18	2557.18	5872.08	108
H8B	1884.42	1996.57	5998.93	108
H8C	893.63	1957.07	5372.33	108
H5A	-443.75	4294.96	4229.19	105
H5B	-1922.55	3983.84	4428.71	105
H5C	-988.96	3581.2	3938.56	105
H21	3321.56	5569.56	2137.5	67
H33A	6786.41	2483.86	445.96	121
H33B	8057.18	2975.63	675.55	121
H33C	6923.19	3234.05	149.8	121
H18A	1151.7	-496.99	3869.27	130
H18B	488.95	-386.79	4542.15	130
H18C	2165.14	-434	4487.16	130
H10A	4047.29	3426.11	5557.47	105
H10B	3789.1	2891.61	6112.09	105
H10C	2711.05	3512.9	5987.03	105
H7A	266.21	3664.12	5829.26	115
H7B	-1065.69	4096.71	5566.08	115
H7C	498.39	4330.64	5406.93	115
H23A	6888.74	5754.11	2280.66	106
H23B	5198.89	5760.95	2253.19	106
H23C	6030.75	5250.44	1810.15	106
H20A	1223.42	5316.3	3048.26	95
H20B	1213.52	4973.08	2364.48	95
H20C	985.35	5782.12	2433.52	95
H24	6564.91	4440.39	2680.57	59
H22A	3123.46	6560.81	2771.93	114
H22B	4594.17	6201.15	2967.69	114
H22C	3268.01	6115.61	3403.46	114
H25A	6537.64	5037.74	3751.97	114
H25B	6370.28	5736.06	3360.92	114
H25C	7767.41	5282.16	3309.32	114
H21A	2702.44	5595.7	2140.74	67
H23D	5578.82	5600.62	1906.15	142
H23E	6194.05	4837.55	1954.93	142
H23F	7154.9	5473.42	2179.98	142
H20D	833.53	4875.7	2420.61	112
H20E	374.37	5657.83	2511.77	112
H20F	843.04	5203.04	3110.9	112
H24A	5534.61	5689.85	3058.48	67
H22D	2869.04	6155.68	3397.05	114
H22E	2085.99	6548.61	2821.67	114
H22F	3750.05	6411.35	2815.15	114
H25D	7606.84	5123.21	3308.14	110
H25E	7052.87	4420.2	2998.54	110
H25F	6445.88	4676.59	3649.37	110

Table S33 Atomic Occupancy for **2**^{Mes}.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
P2	0.330(8)	C21	0.330(8)	H21	0.330(8)
C23	0.330(8)	H23A	0.330(8)	H23B	0.330(8)
H23C	0.330(8)	C20	0.330(8)	H20A	0.330(8)
H20B	0.330(8)	H20C	0.330(8)	C24	0.330(8)
H24	0.330(8)	C22	0.330(8)	H22A	0.330(8)
H22B	0.330(8)	H22C	0.330(8)	C25	0.330(8)
H25A	0.330(8)	H25B	0.330(8)	H25C	0.330(8)
P0	0.670(8)	C21A	0.670(8)	H21A	0.670(8)
C23A	0.670(8)	H23D	0.670(8)	H23E	0.670(8)
H23F	0.670(8)	C20A	0.670(8)	H20D	0.670(8)
H20E	0.670(8)	H20F	0.670(8)	C24A	0.670(8)
H24A	0.670(8)	C22A	0.670(8)	H22D	0.670(8)
H22E	0.670(8)	H22F	0.670(8)	C25A	0.670(8)
H25D	0.670(8)	H25E	0.670(8)	H25F	0.670(8)

Table S34 Fractional Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **2**^{Dipp}·0.5 C_6H_6. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
In1	3141.2(2)	7337.3(2)	6434.2(2)	12.92(5)
Cl2	3462.0(6)	8372.3(3)	7014.5(2)	20.06(11)
Cl1	5237.3(5)	7320.8(3)	6080.9(2)	21.33(11)
P1	2295.4(5)	6063.9(3)	7253.0(2)	14.59(10)
P2	126.5(6)	7780.4(3)	5657.6(2)	15.18(10)
N1	1139.4(17)	6857.6(10)	6430.3(7)	13.5(3)
N2	3621.3(18)	6377.9(10)	7006.9(7)	14.6(3)
N3	1811.8(19)	7807.5(10)	5684.4(7)	15.0(3)
C29	2440(2)	8112.5(12)	5259.7(8)	16.7(4)
C39	2767(2)	9345.2(12)	5747.4(9)	18.5(4)
C30	2732(2)	7663.9(12)	4839.9(9)	19.7(4)
C1	816(2)	6396.0(12)	6807.0(8)	16.0(4)
C4	-77(2)	7130.4(12)	6158.2(9)	16.7(4)
C21	4708(3)	5153.9(13)	6395.5(9)	22.9(5)
C13	7007(2)	5920.2(13)	7883.5(9)	21.4(5)
C27	-640(2)	8647.2(12)	5828.9(9)	19.4(4)
C9	2133(2)	6415.9(13)	7913.2(9)	20.8(4)
C12	5856(2)	6329.5(12)	7646.9(9)	18.2(4)
C14	7326(2)	5256.3(14)	7676.8(10)	23.7(5)
C3	-1205(2)	6839.9(13)	6365.3(9)	22.2(5)
C36	2473(3)	6845.2(12)	4807.9(9)	22.4(5)
C16	5396(2)	5410.3(12)	6945.4(9)	18.7(4)
C2	-631(2)	6367.8(13)	6779.6(9)	21.2(5)
C15	6561(2)	5025.6(13)	7199.4(10)	22.8(5)
C11	4970(2)	6041.2(12)	7197.2(8)	16.5(4)
C18	5674(2)	7093.3(13)	7848.0(9)	21.6(5)
C40	4249(3)	9534.4(14)	6027.8(10)	24.6(5)

C5	847(3)	4708.6(13)	7188.1(11)	27.0(5)
C34	2844(2)	8853.8(12)	5275.1(8)	18.1(4)
C28	-2243(2)	8694.6(14)	5707.7(11)	27.0(5)
C6	2304(2)	5065.4(12)	7280.2(9)	19.7(4)
C25	-834(3)	8058.4(15)	4580.5(10)	27.6(5)
C24	-803(3)	7469.7(13)	5012.6(9)	22.3(5)
C38	1956(3)	10049.2(13)	5593.6(10)	26.8(5)
C35	1534(3)	6614.1(14)	4285.1(10)	28.1(5)
C10	1876(3)	7240.4(14)	7892.7(10)	27.9(5)
C37	3851(3)	6428.0(15)	4856.7(11)	31.1(6)
C20	4378(3)	4333.5(14)	6363.4(11)	31.7(6)
C17	5771(3)	7142.3(16)	8452.1(10)	28.8(5)
C33	3421(3)	9141.7(14)	4855.2(10)	26.9(5)
C31	3323(3)	7981.7(15)	4432.0(10)	29.1(5)
C22	5688(3)	5330.4(14)	5994.6(10)	28.9(5)
C23	-2269(3)	7147.6(14)	5010.9(11)	28.3(5)
C8	962(3)	6048.0(15)	8157.7(10)	29.0(5)
C26	-141(3)	8822.9(14)	6416.0(10)	26.3(5)
C32	3649(3)	8712.7(16)	4432.0(10)	34.3(6)
C7	3249(3)	4765.1(14)	7777.2(10)	28.8(5)
C19	6773(3)	7591.9(14)	7667.3(11)	31.7(6)
C01D	-312(5)	5395.5(17)	5418.3(14)	52.3(9)
C01E	-1350(4)	5220.7(18)	5007.1(18)	56.1(10)
C01F	1026(4)	5180.3(17)	5412.1(15)	57.1(11)

Table S35 Anisotropic Displacement Parameters ($Å^2×10^3$) for **2**^{Dipp}·0.5 C_6H_6. The Anisotropic displacement factor exponent takes the form: $–2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
In1	12.39(7)	10.95(7)	15.26(7)	0.87(5)	1.88(5)	-0.32(5)
Cl2	25.5(3)	13.6(2)	19.8(2)	-1.71(18)	0.33(19)	-0.57(19)
Cl1	15.1(2)	22.7(3)	27.2(3)	3.1(2)	6.55(19)	1.06(19)
P1	14.7(2)	13.3(2)	15.4(2)	2.63(19)	1.37(18)	-0.25(19)
P2	15.0(2)	11.4(2)	18.3(2)	2.25(19)	0.47(19)	0.87(19)
N1	8.7(8)	13.3(8)	18.4(8)	1.4(7)	1.6(6)	-3.1(6)
N2	13.0(8)	12.4(8)	17.5(8)	4.1(7)	0.3(6)	1.8(7)
N3	17.2(8)	11.8(8)	15.5(8)	2.9(7)	1.4(7)	1.6(7)
C29	18.5(10)	16.3(10)	15.0(9)	0.1(8)	1.9(8)	-0.9(8)
C39	24.5(11)	11.8(10)	18.8(10)	0.1(8)	2.3(8)	-0.7(8)
C30	22.1(11)	15.6(11)	21.3(10)	-1.4(8)	3.4(9)	-2.1(9)
C1	17.0(10)	13.5(10)	17.3(9)	2.5(8)	1.8(8)	-0.4(8)
C4	12.6(9)	16.0(10)	20.9(10)	1.6(8)	1.7(8)	1.9(8)
C21	24.5(11)	18.4(11)	25.8(11)	-2.5(9)	3.8(9)	3.0(9)
C13	16.9(10)	24.8(12)	21.4(11)	8.4(9)	0.0(8)	-1.8(9)
C27	17.2(10)	12.3(10)	29.4(11)	4.1(9)	6.2(9)	2.4(8)
C9	21.7(11)	23.7(12)	17.3(10)	0.3(9)	3.7(8)	-2.7(9)
C12	16.3(10)	20.1(11)	18.6(10)	3.9(8)	4.3(8)	-1.5(8)
C14	16.0(10)	24.0(12)	30.5(12)	12.1(10)	2.3(9)	3.8(9)
C3	13.4(10)	23.6(12)	28.7(12)	8.8(9)	0.8(8)	1.2(9)
C36	31.6(12)	14.6(10)	21.3(11)	-1.7(9)	5.5(9)	-1.3(9)

C16	18.4(10)	15.7(10)	22.7(11)	3.7(8)	5.2(8)	-0.3(8)
C2	16.5(10)	22.0(11)	25.5(11)	6.9(9)	4.5(8)	0.0(9)
C15	21.2(11)	18.5(11)	29.8(12)	4.9(9)	7.6(9)	3.3(9)
C11	16.0(10)	16.1(10)	17.4(10)	4.3(8)	3.2(8)	0.1(8)
C18	19.9(11)	23.2(12)	20.2(11)	-0.1(9)	-0.7(8)	-1.4(9)
C40	26.3(12)	22.3(12)	24.5(11)	-1.3(9)	2.2(9)	-7.0(10)
C5	27.7(12)	17.3(11)	35.1(13)	4.0(10)	2.4(10)	-5.1(10)
C34	21.6(11)	15.7(10)	16.3(10)	0.8(8)	1.2(8)	-0.9(8)
C28	20.8(11)	22.2(12)	37.8(13)	5.0(10)	4.8(10)	4.2(9)
C6	21.3(11)	13.9(10)	24.4(11)	4.4(8)	4.9(9)	0.5(8)
C25	28.4(12)	28.1(13)	23.4(11)	5.4(10)	-3.7(9)	1.6(10)
C24	23.0(11)	18.6(11)	22.9(11)	1.4(9)	-2.9(9)	1.5(9)
C38	36.1(14)	13.6(11)	30.2(12)	2.2(9)	4.1(10)	1.5(10)
C35	40.3(14)	18.5(12)	24.2(12)	-3.5(9)	1.9(10)	-3.1(10)
C10	34.3(13)	26.2(13)	25.3(12)	-5.3(10)	11.4(10)	-1.0(11)
C37	36.2(14)	24.1(13)	33.5(13)	-7.5(10)	7.1(11)	5.4(11)
C20	35.6(14)	21.3(12)	39.7(14)	-7.4(11)	10.5(11)	-0.8(11)
C17	30.0(13)	34.3(14)	20.5(11)	-3.1(10)	-0.6(9)	-3.4(11)
C33	39.8(14)	17.4(11)	23.9(11)	1.6(9)	6.1(10)	-10.1(10)
C31	44.1(15)	26.4(13)	19.3(11)	-5.0(10)	12.9(10)	-8.4(11)
C22	40.6(14)	21.8(12)	25.6(12)	0.6(10)	9.5(10)	7.8(11)
C23	23.8(12)	24.0(12)	33.1(13)	2.0(10)	-7.1(10)	-2.6(10)
C8	32.2(13)	34.1(14)	23.3(11)	0.4(10)	11.7(10)	-5.5(11)
C26	23.9(12)	23.5(12)	32.8(13)	-4.8(10)	8.0(10)	0.3(10)
C32	54.8(17)	29.8(14)	21.5(12)	-2.5(10)	16.4(11)	-15.2(13)
C7	26.5(12)	25.1(12)	33.8(13)	11.5(10)	2.6(10)	2.3(10)
C19	37.3(15)	23.3(13)	34.2(14)	-1.3(10)	5.3(11)	-9.1(11)
C01D	98(3)	21.0(14)	40.3(17)	-0.9(12)	18.7(18)	1.4(17)
C01E	39.5(17)	29.6(16)	100(3)	13.6(18)	14.0(18)	1.3(14)
C01F	71(2)	24.6(15)	61(2)	8.4(15)	-31.3(18)	-12.9(16)

Table S36 Bond Lengths for **2**$^{\mathbf{Dipp}}$·0.5 C_6H_6.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
In1	Cl2	2.3969(5)	C21	C22	1.544(3)
In1	Cl1	2.3590(5)	C13	C12	1.396(3)
In1	N1	2.1309(17)	C13	C14	1.384(4)
In1	N2	2.2862(17)	C27	C28	1.536(3)
In1	N3	2.2891(17)	C27	C26	1.530(3)
P1	N2	1.6287(18)	C9	C10	1.534(3)
P1	C1	1.783(2)	C9	C8	1.541(3)
P1	C9	1.836(2)	C12	C11	1.416(3)
P1	C6	1.834(2)	C12	C18	1.514(3)
P2	N3	1.6256(19)	C14	C15	1.382(3)
P2	C4	1.783(2)	C3	C2	1.408(3)
P2	C27	1.840(2)	C36	C35	1.543(3)
P2	C24	1.830(2)	C36	C37	1.528(4)
N1	C1	1.357(3)	C16	C15	1.397(3)
N1	C4	1.360(3)	C16	C11	1.419(3)
N2	C11	1.455(3)	C18	C17	1.531(3)

N3	C29	1.443(3)	C18	C19	1.534(3)
C29	C30	1.417(3)	C5	C6	1.540(3)
C29	C34	1.415(3)	C34	C33	1.394(3)
C39	C40	1.534(3)	C6	C7	1.537(3)
C39	C34	1.517(3)	C25	C24	1.541(3)
C39	C38	1.530(3)	C24	C23	1.539(3)
C30	C36	1.524(3)	C33	C32	1.384(4)
C30	C31	1.397(3)	C31	C32	1.379(4)
C1	C2	1.395(3)	C01D	C01E	1.365(5)
C4	C3	1.399(3)	C01D	C01F	1.359(6)
C21	C16	1.524(3)	C01E	C01F[1]	1.378(6)
C21	C20	1.539(3)			

Table S37 Bond Angles for **2**^{Dipp}·0.5 C_6H_6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl1	In1	Cl2	102.44(2)	C3	C4	P2	135.52(17)
N1	In1	Cl2	110.74(5)	C16	C21	C20	114.0(2)
N1	In1	Cl1	146.76(5)	C16	C21	C22	108.8(2)
N1	In1	N2	76.83(6)	C20	C21	C22	108.4(2)
N1	In1	N3	76.52(7)	C14	C13	C12	121.6(2)
N2	In1	Cl2	102.97(5)	C28	C27	P2	115.92(17)
N2	In1	Cl1	97.95(5)	C26	C27	P2	109.94(16)
N2	In1	N3	148.26(6)	C26	C27	C28	109.16(19)
N3	In1	Cl2	102.35(5)	C10	C9	P1	110.77(16)
N3	In1	Cl1	94.95(5)	C10	C9	C8	108.7(2)
N2	P1	C1	103.66(9)	C8	C9	P1	113.59(17)
N2	P1	C9	115.12(10)	C13	C12	C11	118.8(2)
N2	P1	C6	111.68(10)	C13	C12	C18	118.8(2)
C1	P1	C9	106.34(10)	C11	C12	C18	122.12(19)
C1	P1	C6	111.35(10)	C15	C14	C13	119.0(2)
C6	P1	C9	108.51(11)	C4	C3	C2	106.40(19)
N3	P2	C4	102.81(9)	C30	C36	C35	112.67(19)
N3	P2	C27	114.05(10)	C30	C36	C37	110.9(2)
N3	P2	C24	112.81(10)	C37	C36	C35	108.3(2)
C4	P2	C27	108.11(10)	C15	C16	C21	117.8(2)
C4	P2	C24	109.80(11)	C15	C16	C11	118.5(2)
C24	P2	C27	108.98(11)	C11	C16	C21	123.6(2)
C1	N1	In1	125.01(14)	C1	C2	C3	106.43(19)
C1	N1	C4	107.91(17)	C14	C15	C16	121.8(2)
C4	N1	In1	124.19(14)	C12	C11	N2	120.08(19)
P1	N2	In1	115.46(9)	C12	C11	C16	119.3(2)
C11	N2	In1	128.02(13)	C16	C11	N2	120.63(19)
C11	N2	P1	116.44(14)	C12	C18	C17	113.9(2)
P2	N3	In1	116.44(9)	C12	C18	C19	108.9(2)
C29	N3	In1	121.62(13)	C17	C18	C19	109.8(2)
C29	N3	P2	121.95(14)	C29	C34	C39	122.94(19)
C30	C29	N3	120.37(19)	C33	C34	C29	119.2(2)
C34	C29	N3	120.15(19)	C33	C34	C39	117.7(2)
C34	C29	C30	119.4(2)	C5	C6	P1	114.90(16)

C34	C39	C40	109.75(19)	C7	C6	P1	112.84(17)
C34	C39	C38	112.97(19)	C7	C6	C5	112.23(19)
C38	C39	C40	109.27(19)	C25	C24	P2	111.86(17)
C29	C30	C36	124.2(2)	C23	C24	P2	115.96(18)
C31	C30	C29	118.6(2)	C23	C24	C25	111.2(2)
C31	C30	C36	117.1(2)	C32	C33	C34	121.5(2)
N1	C1	P1	114.12(15)	C32	C31	C30	122.0(2)
N1	C1	C2	109.77(18)	C31	C32	C33	119.1(2)
C2	C1	P1	135.63(17)	C01F	C01D	C01E	120.3(3)
N1	C4	P2	114.92(15)	C01D	C01E	C01F[1]	119.2(3)
N1	C4	C3	109.49(19)	C01D	C01F	C01E[1]	120.5(3)

Table S38 Torsion Angles for **2**^{Dipp}·0.5 C_6H_6.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
In1	N1	C1	P1	-11.9(2)	C21	C16	C11	N2	16.2(3)
In1	N1	C1	C2	161.36(15)	C21	C16	C11	C12	-165.6(2)
In1	N1	C4	P2	16.2(2)	C13	C12	C11	N2	167.60(19)
In1	N1	C4	C3	-161.36(16)	C13	C12	C11	C16	-10.6(3)
In1	N2	C11	C12	86.0(2)	C13	C12	C18	C17	-50.6(3)
In1	N2	C11	C16	-95.8(2)	C13	C12	C18	C19	72.3(3)
In1	N3	C29	C30	89.4(2)	C13	C14	C15	C16	-6.0(4)
In1	N3	C29	C34	-87.0(2)	C27	P2	N3	In1	99.83(12)
P1	N2	C11	C12	-90.6(2)	C27	P2	N3	C29	-80.04(19)
P1	N2	C11	C16	87.6(2)	C27	P2	C4	N1	-118.92(17)
P1	C1	C2	C3	171.0(2)	C27	P2	C4	C3	57.8(3)
P2	N3	C29	C30	-90.8(2)	C27	P2	C24	C25	53.9(2)
P2	N3	C29	C34	92.9(2)	C27	P2	C24	C23	-75.0(2)
P2	C4	C3	C2	-177.1(2)	C9	P1	N2	In1	-96.55(12)
N1	C1	C2	C3	-0.2(3)	C9	P1	N2	C11	80.44(18)
N1	C4	C3	C2	-0.3(3)	C9	P1	C1	N1	115.78(17)
N2	P1	C1	N1	-5.98(18)	C9	P1	C1	C2	-55.2(3)
N2	P1	C1	C2	-176.9(2)	C9	P1	C6	C5	85.86(19)
N2	P1	C9	C10	63.42(19)	C9	P1	C6	C7	-44.5(2)
N2	P1	C9	C8	-173.96(17)	C12	C13	C14	C15	5.8(3)
N2	P1	C6	C5	-146.20(17)	C14	C13	C12	C11	2.5(3)
N2	P1	C6	C7	83.40(18)	C14	C13	C12	C18	-172.0(2)
N3	P2	C4	N1	2.01(19)	C36	C30	C31	C32	-177.5(3)
N3	P2	C4	C3	178.7(2)	C15	C16	C11	N2	-167.78(19)
N3	P2	C27	C28	168.75(16)	C15	C16	C11	C12	10.4(3)
N3	P2	C27	C26	-66.87(18)	C11	C12	C18	C17	135.2(2)
N3	P2	C24	C25	-73.89(19)	C11	C12	C18	C19	-101.9(2)
N3	P2	C24	C23	157.22(17)	C11	C16	C15	C14	-2.1(3)
N3	C29	C30	C36	-2.4(3)	C18	C12	C11	N2	-18.2(3)
N3	C29	C30	C31	179.1(2)	C18	C12	C11	C16	163.6(2)
N3	C29	C34	C39	5.5(3)	C40	C39	C34	C29	110.8(2)
N3	C29	C34	C33	-178.6(2)	C40	C39	C34	C33	-65.1(3)
C29	C30	C36	C35	124.5(2)	C34	C29	C30	C36	174.0(2)
C29	C30	C36	C37	-113.9(3)	C34	C29	C30	C31	-4.5(3)

C29	C30	C31	C32	1.1(4)	C34	C33	C32	C31	-1.2(4)
C29	C34	C33	C32	-2.1(4)	C6	P1	N2	In1	139.13(10)
C39	C34	C33	C32	174.0(2)	C6	P1	N2	C11	-43.87(18)
C30	C29	C34	C39	-170.9(2)	C6	P1	C1	N1	-126.19(16)
C30	C29	C34	C33	5.0(3)	C6	P1	C1	C2	62.8(3)
C30	C31	C32	C33	1.8(5)	C6	P1	C9	C10	-170.62(17)
C1	P1	N2	In1	19.15(12)	C6	P1	C9	C8	-48.0(2)
C1	P1	N2	C11	-163.85(16)	C24	P2	N3	In1	-135.13(11)
C1	P1	C9	C10	-50.73(19)	C24	P2	N3	C29	45.0(2)
C1	P1	C9	C8	71.9(2)	C24	P2	C4	N1	122.30(17)
C1	P1	C6	C5	-30.9(2)	C24	P2	C4	C3	-61.0(3)
C1	P1	C6	C7	-161.24(17)	C24	P2	C27	C28	41.7(2)
C1	N1	C4	P2	177.73(15)	C24	P2	C27	C26	166.08(16)
C1	N1	C4	C3	0.2(3)	C38	C39	C34	C29	-127.0(2)
C4	P2	N3	In1	-16.94(12)	C38	C39	C34	C33	57.1(3)
C4	P2	N3	C29	163.19(17)	C20	C21	C16	C15	50.4(3)
C4	P2	C27	C28	-77.59(19)	C20	C21	C16	C11	-133.5(2)
C4	P2	C27	C26	46.79(18)	C31	C30	C36	C35	-56.9(3)
C4	P2	C24	C25	172.10(17)	C31	C30	C36	C37	64.7(3)
C4	P2	C24	C23	43.2(2)	C22	C21	C16	C15	-70.7(3)
C4	N1	C1	P1	-173.29(15)	C22	C21	C16	C11	105.4(2)
C4	N1	C1	C2	0.0(3)	C01E	C01D	C01F	C01E[1]	-0.4(6)
C4	C3	C2	C1	0.3(3)	C01F	C01D	C01E	C01F[1]	0.4(6)
C21	C16	C15	C14	174.2(2)					

Table S39 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **2^{Dipp}**·0.5 C_6H_6.

Atom	*x*	*y*	*z*	U(eq)
H39	2294.67	9078.17	5998.6	22
H21	3832.98	5423.86	6292.14	27
H13	7571.73	6097.86	8187.2	26
H27	-276.67	9029.63	5621.43	23
H9	3019.92	6326.62	8150.85	25
H14	8044.61	4969.76	7856.23	28
H3	-2148.04	6939	6251.75	27
H36	2008.63	6703.31	5104.89	27
H2	-1119.55	6091.65	6992.94	25
H15	6829.64	4602.54	7043.13	27
H18	4747.58	7268.31	7683.3	26
H40A	4752.77	9093.84	6133.97	37
H40B	4196.24	9826	6336.05	37
H40C	4726.29	9801.73	5788.84	37
H5A	367.96	4831.46	7476.03	41
H5B	945.98	4189.21	7170.9	41
H5C	319.13	4882.57	6859.96	41
H28A	-2554.6	8637.21	5332.63	40
H28B	-2538.15	9160.45	5819.13	40
H28C	-2637.23	8315.9	5895.69	40
H6	2742.27	4908.76	6979.84	24

H25A	-1487.91	8432.19	4634	41
H25B	-1113.24	7842.36	4236.47	41
H25C	81.15	8267.3	4601.82	41
H24	-239.93	7070.49	4905.67	27
H38A	1864.92	10317.01	5909.13	40
H38B	1043.45	9932.87	5402.54	40
H38C	2449.24	10339.35	5372.7	40
H35A	2039.45	6670.04	3994.9	42
H35B	712.95	6914.89	4225.19	42
H35C	1264.81	6113.77	4310.07	42
H10A	2616.96	7477.9	7752.56	42
H10B	1849.63	7418.21	8244.72	42
H10C	999.64	7341.36	7668.08	42
H37A	3668.59	5914.12	4858.52	47
H37B	4447.31	6562.41	5181.57	47
H37C	4304.08	6545.13	4560.58	47
H20A	5235.57	4061.78	6420.55	48
H20B	3860.03	4220.07	6018.6	48
H20C	3832.67	4207.04	6631.02	48
H17A	6703.32	7023.42	8621.32	43
H17B	5122.87	6805.77	8565.6	43
H17C	5546.42	7628.37	8548.1	43
H33	3657.69	9632.78	4859.39	32
H31	3500.71	7691.5	4152.2	35
H22A	5903.25	5841.18	6009.23	43
H22B	5234.45	5204.86	5642.47	43
H22C	6536.52	5054.9	6082.86	43
H23A	-2227.12	6795.97	5291.55	42
H23B	-2588.45	6915.32	4675.45	42
H23C	-2904.16	7530.52	5064.58	42
H8A	81.3	6121.07	7928.63	44
H8B	926.47	6258.01	8499.67	44
H8C	1148.1	5535.54	8197.03	44
H26A	-617.6	8514.62	6631.55	40
H26B	-341.53	9323.58	6481.84	40
H26C	847.83	8740.89	6503.16	40
H32	4018.56	8914.83	4151.42	41
H7A	4150.17	4993.48	7815.08	43
H7B	3352.11	4248.26	7741.33	43
H7C	2834.02	4865.8	8085.52	43
H19A	6646.36	8080.96	7783.65	48
H19B	6670.15	7582.17	7286.62	48
H19C	7691.64	7424.66	7818.75	48
H01D	-520.93	5663.35	5704.16	63
H01E	-2264.09	5370.41	5009.88	67
H01F	1727.57	5304.69	5692.78	69

Table S40 Fractional Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **3^{Pipp}**. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	7777.3(2)	5518.7(2)	3887.5(2)	13.66(8)
P3	3116.6(2)	2114.0(2)	3957.9(2)	15.29(9)
P4	2914.2(2)	3774.4(2)	2236.0(2)	14.90(9)
P2	7991.9(2)	3704.4(2)	2522.5(2)	17.19(9)
Al2	1828.4(3)	3086.7(2)	3009.0(2)	16.84(10)
Al1	6702.8(3)	4416.8(2)	3095.0(2)	17.72(10)
N6	2030.0(8)	3790.8(5)	2407.0(7)	17.3(3)
N2	6807.9(8)	5235.0(5)	3598.5(7)	16.8(3)
N1	7905.8(8)	4617.9(5)	3202.7(6)	15.2(2)
N5	2105.1(8)	2332.4(5)	3653.7(7)	17.7(3)
N3	7088.9(8)	3660.5(5)	2660.9(7)	18.3(3)
N4	3026.3(8)	2922.6(5)	3073.2(6)	15.1(2)
C21	8357.9(10)	5528.2(6)	4844.0(8)	18.1(3)
C26	6122.1(10)	5465.2(6)	3792.7(8)	16.6(3)
C4	8362.5(10)	5083.3(6)	3524.5(8)	14.9(3)
C40	3486.3(10)	3197.8(6)	2741.1(8)	15.8(3)
C1	8436.4(10)	4342.7(6)	2934.8(8)	16.1(3)
C3	9183.6(10)	5107.6(6)	3458.4(8)	16.7(3)
C38	4405.4(10)	2543.3(6)	3407.8(8)	19.1(3)
C37	3588.4(10)	2521.9(6)	3478.7(8)	16.3(3)
C2	9232.4(10)	4630.6(6)	3082.5(8)	17.2(3)
C47	1481.5(10)	2085.8(6)	3904.0(8)	18.3(3)
C39	4339.6(10)	2976.4(6)	2933.1(8)	19.0(3)
C64	753.9(10)	5104.8(6)	2286.2(9)	20.4(3)
C42	3752.5(11)	2234.2(7)	4897.3(8)	21.3(3)
C66	252.9(10)	4705.6(7)	1143.3(9)	22.5(3)
C27	6097.2(10)	5369.5(6)	4450.3(8)	18.5(3)
C31	5432.5(10)	5785.4(7)	3315.6(8)	19.3(3)
C15	5388.0(11)	2683.9(7)	1444.8(9)	22.6(3)
C52	1486.7(11)	2208.4(7)	4565.5(8)	20.8(3)
C67	835.0(10)	4258.0(7)	1415.0(9)	20.6(3)
C63	1340.5(10)	4664.2(6)	2557.2(8)	19.2(3)
C11	6523.9(10)	3186.9(6)	2399.0(8)	18.2(3)
C29	4726.0(10)	5900.2(6)	4152.6(8)	18.7(3)
C62	1403.1(10)	4233.1(6)	2123.2(8)	17.9(3)
C65	203.6(10)	5141.1(6)	1571.5(9)	20.8(3)
C28	5416.9(10)	5584.2(6)	4627.9(8)	19.1(3)
C57	3678.3(10)	4362.0(6)	2534.3(8)	20.0(3)
C46	2799.7(11)	1266.4(7)	2998.2(9)	23.0(3)
C45	3288.3(10)	1386.8(6)	3784.2(8)	19.7(3)
C49	224.8(11)	1473.1(7)	3717.3(9)	26.7(4)
C60	2706.2(10)	3659.7(7)	1307.0(8)	20.4(3)
C14	5433.6(10)	2228.4(6)	1868.8(9)	21.3(3)
C48	828.5(11)	1718.4(7)	3479.5(9)	24.1(3)
C72	801.3(10)	2769.1(7)	2217.3(8)	22.9(3)
C30	4752.8(10)	5998.8(7)	3495.3(8)	20.9(3)
C24	7868.4(10)	6217.3(6)	3573.9(8)	18.4(3)

C50	235.1(11)	1588.5(7)	4382.0(9)	23.4(3)
C33	3959.9(10)	6095.1(7)	4346.6(9)	22.5(3)
C12	6552.6(10)	2736.2(7)	2838.5(9)	21.1(3)
C22	9267.9(10)	5821.4(7)	5086.2(8)	23.7(3)
C35	6478.0(12)	3994.8(7)	3830.4(9)	24.7(3)
C13	6025.2(10)	2268.5(7)	2576.7(9)	21.9(3)
C36	5740.0(10)	4657.4(7)	2202.3(8)	22.5(3)
C23	7425.9(11)	6232.6(7)	2772.2(9)	23.0(3)
C16	5916.7(11)	3154.0(7)	1702.0(9)	22.0(3)
C61	2207.3(11)	3109.8(7)	1066.5(9)	26.0(4)
C69	-414.3(11)	5641.1(7)	1300.1(9)	24.8(3)
C51	878.8(11)	1961.6(7)	4798.5(9)	23.6(3)
C18	4861.2(11)	1709.8(7)	1603.7(10)	25.9(4)
C9	7821.9(11)	3734.3(8)	1591.1(9)	27.5(4)
C58	3305.3(11)	4889.7(7)	2103.6(10)	28.6(4)
C71	1631.7(12)	3562.8(7)	3718.2(9)	25.4(3)
C32	3149.0(11)	5713.0(7)	4021.9(10)	26.2(4)
C25	7511.5(12)	6671.3(7)	3916.6(9)	26.5(4)
C20	8460.4(10)	4932.0(7)	5126.2(9)	23.0(3)
C43	4699.7(11)	1994.8(7)	5154.5(9)	27.5(4)
C54	-441.4(12)	1331.6(8)	4638.4(9)	29.8(4)
C56	3934.1(11)	4452.6(7)	3322.9(9)	27.5(4)
C8	8707.1(13)	3775.9(9)	1488.6(11)	38.7(5)
C41	3778.2(11)	2859.8(7)	5048.6(9)	26.9(4)
C6	8858.4(11)	3185.2(7)	2938.4(10)	28.2(4)
C59	3562.5(12)	3672.4(9)	1164.3(10)	33.0(4)
C19	4420.0(14)	1667.2(8)	806.8(11)	37.8(5)
C10	7207.6(13)	4221.7(9)	1233.1(9)	34.0(4)
C70	-758.8(14)	5719.6(8)	507.5(10)	36.8(4)
C17	4151.4(12)	1665.5(7)	1917.2(11)	31.6(4)
C34	3675.2(12)	6697.5(7)	4133.7(11)	33.0(4)
C44	3038.9(13)	969.8(7)	4239.7(9)	29.2(4)
C5	9048.8(12)	3142.8(8)	3721.0(11)	36.4(4)
C68	-1188.4(13)	5621.5(9)	1546.9(12)	41.3(5)
C7	8630.0(13)	2617.6(7)	2568.5(13)	40.6(5)
C55	-1367.7(14)	1564.3(13)	4240.0(12)	56.8(7)
C53	-421(2)	702.7(11)	4625.4(19)	76.7(10)

Table S41 Anisotropic Displacement Parameters ($Å^2×10^3$) for **3^{Pipp}**. The Anisotropic displacement factor exponent takes the form: $–2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	13.99(17)	13.46(17)	13.87(18)	-1.07(13)	5.80(14)	0.22(13)
P3	16.02(18)	15.67(18)	12.95(18)	-0.42(14)	4.32(14)	0.83(13)
P4	13.53(17)	15.06(18)	16.52(18)	-0.09(14)	6.30(14)	0.46(13)
P2	15.84(18)	15.94(18)	21.4(2)	-5.73(15)	9.04(15)	-1.98(14)
Al2	13.7(2)	21.1(2)	16.2(2)	-1.68(17)	6.28(17)	1.79(16)
Al1	14.4(2)	21.3(2)	18.3(2)	-0.56(17)	7.24(18)	-2.94(16)
N6	14.9(6)	18.2(6)	19.6(6)	0.9(5)	7.6(5)	1.8(5)
N2	13.7(6)	19.3(6)	17.8(6)	-2.8(5)	6.6(5)	-0.3(5)

N1	15.2(6)	14.7(6)	16.5(6)	-1.2(5)	7.1(5)	0.2(5)
N5	16.4(6)	21.1(6)	15.6(6)	0.8(5)	6.2(5)	0.7(5)
N3	16.9(6)	17.6(6)	21.1(7)	-5.2(5)	8.2(5)	-2.5(5)
N4	14.9(6)	14.3(6)	16.2(6)	-1.4(5)	6.1(5)	-0.2(5)
C21	16.5(7)	23.2(8)	14.4(7)	-1.9(6)	5.8(6)	-0.2(6)
C26	15.3(7)	17.0(7)	17.4(7)	-3.8(6)	6.3(6)	-1.8(5)
C4	16.3(7)	12.6(7)	14.8(7)	0.1(5)	4.9(6)	0.1(5)
C40	16.3(7)	15.1(7)	16.0(7)	-1.5(6)	6.3(6)	-1.2(5)
C1	16.9(7)	14.1(7)	18.3(7)	-0.9(6)	7.9(6)	1.8(5)
C3	16.1(7)	14.9(7)	18.2(7)	0.9(6)	5.8(6)	-1.2(5)
C38	16.1(7)	17.3(7)	23.0(8)	-1.1(6)	6.6(6)	2.9(6)
C37	16.6(7)	14.8(7)	15.1(7)	-1.9(6)	3.7(6)	1.1(5)
C2	15.6(7)	18.6(7)	19.6(7)	0.7(6)	9.2(6)	1.4(6)
C47	17.7(7)	19.4(7)	17.7(7)	2.2(6)	6.9(6)	2.2(6)
C39	15.7(7)	19.1(7)	23.4(8)	-1.8(6)	8.9(6)	-1.1(6)
C64	23.3(8)	18.3(8)	24.2(8)	-0.3(6)	14.1(7)	0.3(6)
C42	22.2(8)	24.5(8)	14.9(7)	-1.5(6)	4.7(6)	0.7(6)
C66	19.2(7)	27.1(8)	19.7(8)	2.1(6)	6.1(6)	1.8(6)
C27	17.5(7)	20.8(8)	16.9(7)	2.4(6)	6.2(6)	1.8(6)
C31	20.2(7)	22.9(8)	15.4(7)	2.3(6)	7.6(6)	1.5(6)
C15	22.2(8)	24.3(8)	21.5(8)	-5.7(7)	8.8(6)	-3.9(6)
C52	23.1(8)	21.3(8)	18.5(8)	-2.3(6)	8.7(6)	-2.7(6)
C67	19.1(7)	20.9(8)	22.5(8)	-3.0(6)	8.7(6)	1.1(6)
C63	18.4(7)	21.2(8)	18.9(8)	0.3(6)	8.1(6)	0.3(6)
C11	17.0(7)	18.0(7)	23.0(8)	-4.1(6)	11.4(6)	-1.5(6)
C29	17.7(7)	18.2(7)	20.4(8)	-3.3(6)	7.7(6)	-0.6(6)
C62	14.7(7)	17.5(7)	23.5(8)	0.9(6)	9.6(6)	0.6(6)
C65	19.2(7)	19.7(8)	26.5(8)	3.7(6)	12.1(6)	2.1(6)
C28	21.7(7)	20.5(8)	16.5(7)	0.5(6)	9.0(6)	-0.2(6)
C57	17.7(7)	17.2(7)	25.0(8)	-0.9(6)	8.2(6)	-1.6(6)
C46	26.0(8)	19.6(8)	22.7(8)	-4.4(6)	8.8(7)	-1.8(6)
C45	20.0(7)	16.5(7)	21.1(8)	0.3(6)	6.3(6)	0.7(6)
C49	24.7(8)	32.8(9)	22.6(8)	-4.7(7)	9.3(7)	-9.5(7)
C60	18.6(7)	26.3(8)	17.6(7)	0.1(6)	8.5(6)	1.9(6)
C14	18.5(7)	18.5(8)	31.0(9)	-5.5(7)	14.2(7)	-0.1(6)
C48	24.1(8)	31.9(9)	17.7(8)	-4.6(7)	9.7(7)	-4.0(7)
C72	17.7(7)	29.4(9)	20.9(8)	2.3(7)	6.9(6)	-2.4(6)
C30	18.1(7)	22.0(8)	19.8(8)	2.9(6)	4.4(6)	4.6(6)
C24	20.2(7)	13.9(7)	21.5(8)	-0.9(6)	8.6(6)	0.6(6)
C50	23.6(8)	26.0(8)	21.8(8)	3.1(7)	10.3(7)	-0.4(6)
C33	21.3(8)	25.5(8)	22.5(8)	0.1(7)	10.4(7)	4.2(6)
C12	17.6(7)	21.6(8)	23.6(8)	-1.5(6)	7.4(6)	1.0(6)
C22	18.7(8)	30.2(9)	18.8(8)	-2.6(7)	3.5(6)	-3.1(6)
C35	31.2(9)	21.0(8)	28.1(9)	-3.8(7)	18.2(7)	-5.5(7)
C13	20.9(8)	18.7(8)	28.9(9)	1.6(6)	12.7(7)	1.0(6)
C36	18.2(7)	25.8(8)	22.0(8)	-4.4(7)	6.1(6)	0.6(6)
C23	27.6(8)	19.4(8)	22.6(8)	4.1(6)	10.5(7)	1.9(6)
C16	23.9(8)	21.5(8)	22.7(8)	-0.8(6)	11.4(7)	-2.8(6)
C61	24.8(8)	29.1(9)	22.1(8)	-6.9(7)	7.0(7)	-0.4(7)
C69	27.2(8)	21.0(8)	29.0(9)	6.0(7)	14.0(7)	5.2(7)
C51	28.9(8)	26.6(8)	17.6(8)	-0.6(6)	11.8(7)	-0.7(7)

C18	26.0(8)	17.2(8)	36.6(10)	-7.6(7)	14.6(7)	-2.9(6)
C9	27.9(9)	34.9(9)	24.8(9)	-11.9(7)	15.8(7)	-9.6(7)
C58	24.6(8)	16.9(8)	42.5(10)	4.5(7)	11.1(8)	0.1(6)
C71	32.8(9)	23.5(8)	24.0(8)	3.4(7)	15.8(7)	7.0(7)
C32	23.8(8)	26.7(9)	33.6(9)	5.2(7)	17.0(7)	2.5(7)
C25	34.3(9)	18.7(8)	27.9(9)	-3.3(7)	13.8(7)	3.1(7)
C20	19.5(7)	28.2(9)	20.2(8)	6.2(7)	6.7(6)	1.8(6)
C43	24.5(8)	30.6(9)	18.6(8)	-2.8(7)	-1.1(7)	4.1(7)
C54	33.6(9)	36.3(10)	23.5(9)	-1.8(7)	15.6(8)	-10.5(8)
C56	26.2(8)	25.7(9)	28.5(9)	-8.0(7)	8.3(7)	-4.7(7)
C8	37.1(11)	52.9(12)	36.3(11)	-15.1(9)	25.4(9)	-9.8(9)
C41	24.1(8)	28.9(9)	24.0(8)	-9.5(7)	5.4(7)	1.3(7)
C6	17.7(8)	16.8(8)	48.8(11)	-4.7(7)	11.6(8)	-0.7(6)
C59	25.6(9)	52.4(12)	25.4(9)	-5.2(8)	14.5(7)	-3.8(8)
C19	41.1(11)	31.4(10)	42.3(11)	-16.9(9)	17.8(9)	-14.2(8)
C10	34.5(10)	45.8(11)	22.6(9)	1.6(8)	12.4(8)	-10.2(8)
C70	46.3(11)	30.7(10)	31.2(10)	9.1(8)	12.7(9)	13.8(8)
C17	29.8(9)	23.9(9)	43.1(11)	-4.0(8)	16.2(8)	-9.2(7)
C34	28.1(9)	23.4(9)	52.0(12)	-5.1(8)	20.5(9)	2.2(7)
C44	38.0(10)	20.5(8)	27.6(9)	3.3(7)	11.0(8)	-1.0(7)
C5	24.7(9)	25.7(9)	46.7(12)	9.5(8)	0.9(8)	-1.1(7)
C68	35.9(10)	38.0(11)	58.7(13)	21.7(10)	27.9(10)	18.7(8)
C7	30.6(10)	17.7(9)	80.9(16)	-12.8(9)	29.6(10)	-4.0(7)
C55	28.2(10)	106(2)	39.1(12)	21.6(13)	16.4(9)	-6.9(12)
C53	111(2)	41.9(14)	118(3)	-2.2(15)	89(2)	-24.4(15)

Table S42 Bond Lengths for **3**$^{\mathbf{Pipp}}$

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	N2	1.6023(12)	C64	C63	1.388(2)
P1	C21	1.8256(15)	C64	C65	1.397(2)
P1	C4	1.7652(15)	C42	C43	1.531(2)
P1	C24	1.8264(15)	C42	C41	1.533(2)
P3	N5	1.6013(13)	C66	C67	1.397(2)
P3	C37	1.7659(16)	C66	C65	1.392(2)
P3	C42	1.8289(16)	C27	C28	1.392(2)
P3	C45	1.8275(15)	C31	C30	1.393(2)
P4	N6	1.6076(13)	C15	C14	1.385(2)
P4	C40	1.7649(15)	C15	C16	1.393(2)
P4	C57	1.8214(15)	C52	C51	1.389(2)
P4	C60	1.8329(16)	C67	C62	1.392(2)
P2	N3	1.6037(13)	C63	C62	1.399(2)
P2	C1	1.7663(15)	C11	C12	1.402(2)
P2	C9	1.8333(17)	C11	C16	1.393(2)
P2	C6	1.8253(17)	C29	C28	1.392(2)
Al2	N6	2.1984(13)	C29	C30	1.394(2)
Al2	N5	2.1892(13)	C29	C33	1.523(2)
Al2	N4	1.9389(13)	C65	C69	1.525(2)
Al2	C72	1.9768(16)	C57	C58	1.532(2)
Al2	C71	1.9794(17)	C57	C56	1.530(2)

Al1	N2	2.1995(13)	C46	C45	1.529(2)
Al1	N1	1.9400(13)	C45	C44	1.533(2)
Al1	N3	2.2225(13)	C49	C48	1.388(2)
Al1	C35	1.9742(17)	C49	C50	1.393(2)
Al1	C36	1.9810(16)	C60	C61	1.528(2)
N6	C62	1.4299(19)	C60	C59	1.530(2)
N2	C26	1.4341(19)	C14	C13	1.404(2)
N1	C4	1.3630(19)	C14	C18	1.523(2)
N1	C1	1.3632(19)	C24	C23	1.525(2)
N5	C47	1.433(2)	C24	C25	1.532(2)
N3	C11	1.4294(19)	C50	C51	1.391(2)
N4	C40	1.3656(19)	C50	C54	1.524(2)
N4	C37	1.3656(19)	C33	C32	1.529(2)
C21	C22	1.535(2)	C33	C34	1.531(2)
C21	C20	1.531(2)	C12	C13	1.389(2)
C26	C27	1.392(2)	C69	C70	1.520(2)
C26	C31	1.398(2)	C69	C68	1.531(2)
C4	C3	1.394(2)	C18	C19	1.519(3)
C40	C39	1.390(2)	C18	C17	1.530(2)
C1	C2	1.391(2)	C9	C8	1.536(2)
C3	C2	1.404(2)	C9	C10	1.529(3)
C38	C37	1.392(2)	C54	C55	1.512(3)
C38	C39	1.405(2)	C54	C53	1.513(3)
C47	C52	1.393(2)	C6	C5	1.524(3)
C47	C48	1.395(2)	C6	C7	1.537(2)

Table S43 Bond Angles for **3**$^{\mathbf{Pipp}}$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	P1	C21	115.19(7)	C4	C3	C2	106.40(13)
N2	P1	C4	101.75(7)	C37	C38	C39	106.53(13)
N2	P1	C24	117.60(7)	N4	C37	P3	113.71(11)
C21	P1	C24	107.00(7)	N4	C37	C38	110.28(13)
C4	P1	C21	109.24(7)	C38	C37	P3	136.01(12)
C4	P1	C24	105.27(7)	C1	C2	C3	106.21(13)
N5	P3	C37	101.64(7)	C52	C47	N5	122.07(14)
N5	P3	C42	115.60(7)	C52	C47	C48	117.46(14)
N5	P3	C45	116.65(7)	C48	C47	N5	120.46(14)
C37	P3	C42	108.46(7)	C40	C39	C38	106.17(13)
C37	P3	C45	106.77(7)	C63	C64	C65	121.92(15)
C45	P3	C42	107.02(7)	C43	C42	P3	112.55(11)
N6	P4	C40	101.49(7)	C43	C42	C41	110.76(14)
N6	P4	C57	117.15(7)	C41	C42	P3	109.28(11)
N6	P4	C60	114.67(7)	C65	C66	C67	121.47(15)
C40	P4	C57	106.09(7)	C28	C27	C26	121.55(14)
C40	P4	C60	109.82(7)	C30	C31	C26	121.05(14)
C57	P4	C60	107.05(7)	C14	C15	C16	121.84(15)
N3	P2	C1	101.64(7)	C51	C52	C47	121.04(15)
N3	P2	C9	114.54(7)	C62	C67	C66	121.46(15)
N3	P2	C6	117.55(8)	C64	C63	C62	121.15(15)

C1	P2	C9	109.68(8)	C12	C11	N3	121.11(14)
C1	P2	C6	105.79(7)	C16	C11	N3	121.80(14)
C6	P2	C9	107.02(9)	C16	C11	C12	117.09(14)
N5	Al2	N6	160.13(5)	C28	C29	C30	117.08(14)
N4	Al2	N6	80.11(5)	C28	C29	C33	119.97(14)
N4	Al2	N5	80.06(5)	C30	C29	C33	122.86(14)
N4	Al2	C72	118.60(6)	C67	C62	N6	122.43(14)
N4	Al2	C71	120.97(7)	C67	C62	C63	117.13(14)
C72	Al2	N6	95.41(6)	C63	C62	N6	120.44(14)
C72	Al2	N5	95.12(6)	C64	C65	C69	119.67(14)
C72	Al2	C71	120.43(7)	C66	C65	C64	116.82(14)
C71	Al2	N6	94.32(6)	C66	C65	C69	123.51(15)
C71	Al2	N5	94.81(6)	C27	C28	C29	121.42(14)
N2	Al1	N3	160.00(5)	C58	C57	P4	112.52(11)
N1	Al1	N2	80.45(5)	C56	C57	P4	109.65(11)
N1	Al1	N3	79.62(5)	C56	C57	C58	112.39(14)
N1	Al1	C35	121.35(7)	C46	C45	P3	109.46(11)
N1	Al1	C36	115.36(6)	C46	C45	C44	111.99(13)
C35	Al1	N2	95.73(6)	C44	C45	P3	114.08(12)
C35	Al1	N3	93.18(6)	C48	C49	C50	121.67(15)
C35	Al1	C36	123.29(7)	C61	C60	P4	109.12(11)
C36	Al1	N2	93.77(6)	C61	C60	C59	111.19(14)
C36	Al1	N3	96.24(6)	C59	C60	P4	112.82(11)
P4	N6	Al2	116.63(7)	C15	C14	C13	116.68(14)
C62	N6	P4	118.87(10)	C15	C14	C18	123.04(15)
C62	N6	Al2	124.36(9)	C13	C14	C18	120.25(15)
P1	N2	Al1	116.11(7)	C49	C48	C47	121.07(15)
C26	N2	P1	119.32(10)	C31	C30	C29	121.69(14)
C26	N2	Al1	123.47(9)	C23	C24	P1	109.71(10)
C4	N1	Al1	126.35(10)	C23	C24	C25	112.36(13)
C1	N1	Al1	126.92(10)	C25	C24	P1	113.20(11)
C1	N1	C4	106.60(12)	C49	C50	C54	121.87(15)
P3	N5	Al2	116.46(7)	C51	C50	C49	116.99(15)
C47	N5	P3	119.01(10)	C51	C50	C54	121.12(15)
C47	N5	Al2	123.73(9)	C29	C33	C32	110.66(13)
P2	N3	Al1	116.08(7)	C29	C33	C34	113.70(14)
C11	N3	P2	118.82(10)	C32	C33	C34	109.28(14)
C11	N3	Al1	124.28(9)	C13	C12	C11	120.95(15)
C40	N4	Al2	126.75(10)	C12	C13	C14	121.88(15)
C37	N4	Al2	126.76(10)	C11	C16	C15	121.48(15)
C37	N4	C40	106.45(12)	C65	C69	C68	111.22(14)
C22	C21	P1	112.54(11)	C70	C69	C65	113.96(14)
C20	C21	P1	109.45(11)	C70	C69	C68	110.90(16)
C20	C21	C22	110.99(13)	C52	C51	C50	121.75(15)
C27	C26	N2	122.00(13)	C14	C18	C17	111.11(13)
C27	C26	C31	117.20(14)	C19	C18	C14	114.06(15)
C31	C26	N2	120.78(14)	C19	C18	C17	109.75(15)
N1	C4	P1	114.35(10)	C8	C9	P2	112.39(13)
N1	C4	C3	110.27(13)	C10	C9	P2	109.83(12)
C3	C4	P1	135.32(12)	C10	C9	C8	110.68(16)
N4	C40	P4	114.31(10)	C55	C54	C50	111.15(15)

N4	C40	C39	110.58(13)	C55	C54	C53	112.6(2)
C39	C40	P4	134.87(12)	C53	C54	C50	112.03(17)
N1	C1	P2	114.37(11)	C5	C6	P2	110.13(12)
N1	C1	C2	110.52(13)	C5	C6	C7	112.13(16)
C2	C1	P2	135.05(12)	C7	C6	P2	112.41(13)

Table S44 Torsion Angles for **3**^{Pipp}.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
P1	N2	C26	C27	-78.01(17)	C37	P3	C45	C46	-61.86(12)
P1	N2	C26	C31	103.75(15)	C37	P3	C45	C44	171.77(11)
P1	C4	C3	C2	-177.40(13)	C37	N4	C40	P4	-175.32(10)
P3	N5	C47	C52	75.55(17)	C37	N4	C40	C39	-0.14(16)
P3	N5	C47	C48	-105.79(15)	C37	C38	C39	C40	0.19(17)
P4	N6	C62	C67	73.88(17)	C47	C52	C51	C50	-0.8(3)
P4	N6	C62	C63	-106.01(15)	C39	C38	C37	P3	-179.92(13)
P4	C40	C39	C38	173.76(13)	C39	C38	C37	N4	-0.29(17)
P2	N3	C11	C12	98.83(15)	C64	C63	C62	N6	178.12(14)
P2	N3	C11	C16	-81.82(17)	C64	C63	C62	C67	-1.8(2)
P2	C1	C2	C3	-177.02(13)	C64	C65	C69	C70	162.62(16)
Al2	N6	C62	C67	-101.57(16)	C64	C65	C69	C68	-71.1(2)
Al2	N6	C62	C63	78.54(16)	C42	P3	N5	Al2	105.64(8)
Al2	N5	C47	C52	-93.79(16)	C42	P3	N5	C47	-64.47(14)
Al2	N5	C47	C48	84.87(17)	C42	P3	C37	N4	-115.69(11)
Al2	N4	C40	P4	2.58(16)	C42	P3	C37	C38	63.93(18)
Al2	N4	C40	C39	177.75(10)	C42	P3	C45	C46	-177.85(11)
Al2	N4	C37	P3	2.10(16)	C42	P3	C45	C44	55.78(13)
Al2	N4	C37	C38	-177.63(10)	C66	C67	C62	N6	-177.37(14)
Al1	N2	C26	C27	89.51(16)	C66	C67	C62	C63	2.5(2)
Al1	N2	C26	C31	-88.73(16)	C66	C65	C69	C70	-17.8(2)
Al1	N1	C4	P1	1.76(16)	C66	C65	C69	C68	108.48(19)
Al1	N1	C4	C3	-175.84(10)	C27	C26	C31	C30	0.1(2)
Al1	N1	C1	P2	-6.38(17)	C31	C26	C27	C28	-0.2(2)
Al1	N1	C1	C2	176.09(10)	C15	C14	C13	C12	-1.2(2)
Al1	N3	C11	C12	-91.93(16)	C15	C14	C18	C19	15.1(2)
Al1	N3	C11	C16	87.42(16)	C15	C14	C18	C17	-109.60(18)
N6	P4	C40	N4	4.03(12)	C52	C47	C48	C49	-1.8(2)
N6	P4	C40	C39	-169.59(16)	C67	C66	C65	C64	-0.9(2)
N6	P4	C57	C58	-72.10(14)	C67	C66	C65	C69	179.47(15)
N6	P4	C57	C56	53.77(13)	C63	C64	C65	C66	1.6(2)
N6	P4	C60	C61	-58.36(13)	C63	C64	C65	C69	-178.71(14)
N6	P4	C60	C59	177.52(12)	C11	C12	C13	C14	-1.0(2)
N2	P1	C21	C22	-178.19(11)	C65	C64	C63	C62	-0.3(2)
N2	P1	C21	C20	57.91(12)	C65	C66	C67	C62	-1.2(2)
N2	P1	C4	N1	-7.89(12)	C28	C29	C30	C31	0.9(2)
N2	P1	C4	C3	168.91(16)	C28	C29	C33	C32	-98.83(17)
N2	P1	C24	C23	-50.71(13)	C28	C29	C33	C34	137.74(16)
N2	P1	C24	C25	75.67(13)	C57	P4	N6	Al2	-123.04(8)
N2	C26	C27	C28	-178.48(14)	C57	P4	N6	C62	61.16(14)
N2	C26	C31	C30	178.43(14)	C57	P4	C40	N4	126.93(11)

N1	C4	C3	C2	-0.51(17)	C57	P4	C40	C39	-46.69(18)
N1	C1	C2	C3	-0.19(17)	C57	P4	C60	C61	169.87(11)
N5	P3	C37	N4	6.58(12)	C57	P4	C60	C59	45.75(14)
N5	P3	C37	C38	-173.79(16)	C45	P3	N5	Al2	-127.22(8)
N5	P3	C42	C43	177.81(11)	C45	P3	N5	C47	62.67(13)
N5	P3	C42	C41	-58.70(13)	C45	P3	C37	N4	129.29(11)
N5	P3	C45	C46	50.90(13)	C45	P3	C37	C38	-51.08(18)
N5	P3	C45	C44	-75.47(13)	C45	P3	C42	C43	45.98(14)
N5	C47	C52	C51	-179.61(14)	C45	P3	C42	C41	169.47(11)
N5	C47	C48	C49	179.47(15)	C49	C50	C51	C52	-0.1(2)
N3	P2	C1	N1	-3.30(13)	C49	C50	C54	C55	-69.4(2)
N3	P2	C1	C2	173.44(16)	C49	C50	C54	C53	57.5(3)
N3	P2	C9	C8	-179.99(13)	C60	P4	N6	Al2	110.22(8)
N3	P2	C9	C10	56.33(14)	C60	P4	N6	C62	-65.58(13)
N3	P2	C6	C5	-50.40(14)	C60	P4	C40	N4	-117.71(11)
N3	P2	C6	C7	75.41(16)	C60	P4	C40	C39	68.66(17)
N3	C11	C12	C13	-177.75(14)	C60	P4	C57	C58	58.29(13)
N3	C11	C16	C15	177.97(14)	C60	P4	C57	C56	-175.84(11)
N4	C40	C39	C38	-0.04(17)	C14	C15	C16	C11	0.5(2)
C21	P1	N2	Al1	-107.67(8)	C48	C47	C52	C51	1.7(2)
C21	P1	N2	C26	60.74(13)	C48	C49	C50	C51	0.0(3)
C21	P1	C4	N1	114.33(11)	C48	C49	C50	C54	178.41(17)
C21	P1	C4	C3	-68.87(17)	C30	C29	C28	C27	-0.9(2)
C21	P1	C24	C23	177.83(11)	C30	C29	C33	C32	77.75(19)
C21	P1	C24	C25	-55.79(13)	C30	C29	C33	C34	-45.7(2)
C26	C27	C28	C29	0.6(2)	C24	P1	N2	Al1	124.70(8)
C26	C31	C30	C29	-0.5(2)	C24	P1	N2	C26	-66.88(13)
C4	P1	N2	Al1	10.35(9)	C24	P1	C21	C22	-45.41(13)
C4	P1	N2	C26	178.77(11)	C24	P1	C21	C20	-169.31(10)
C4	P1	C21	C22	68.06(13)	C24	P1	C4	N1	-131.07(11)
C4	P1	C21	C20	-55.84(12)	C24	P1	C4	C3	45.73(17)
C4	P1	C24	C23	61.68(12)	C50	C49	C48	C47	1.0(3)
C4	P1	C24	C25	-171.94(11)	C33	C29	C28	C27	175.84(14)
C4	N1	C1	P2	177.42(10)	C33	C29	C30	C31	-175.81(15)
C4	N1	C1	C2	-0.12(17)	C12	C11	C16	C15	-2.7(2)
C4	C3	C2	C1	0.42(16)	C13	C14	C18	C19	-166.70(15)
C40	P4	N6	Al2	-8.08(9)	C13	C14	C18	C17	68.6(2)
C40	P4	N6	C62	176.12(11)	C16	C15	C14	C13	1.4(2)
C40	P4	C57	C58	175.52(12)	C16	C15	C14	C18	179.71(15)
C40	P4	C57	C56	-58.61(12)	C16	C11	C12	C13	2.9(2)
C40	P4	C60	C61	55.13(12)	C51	C50	C54	C55	109.0(2)
C40	P4	C60	C59	-68.99(14)	C51	C50	C54	C53	-124.1(2)
C40	N4	C37	P3	179.99(10)	C18	C14	C13	C12	-179.53(14)
C40	N4	C37	C38	0.27(16)	C9	P2	N3	Al1	-108.34(9)
C1	P2	N3	Al1	9.83(9)	C9	P2	N3	C11	61.77(14)
C1	P2	N3	C11	179.94(12)	C9	P2	C1	N1	118.31(12)
C1	P2	C9	C8	66.50(15)	C9	P2	C1	C2	-64.95(18)
C1	P2	C9	C10	-57.18(13)	C9	P2	C6	C5	179.10(12)
C1	P2	C6	C5	62.19(13)	C9	P2	C6	C7	-55.10(15)
C1	P2	C6	C7	-172.01(13)	C54	C50	C51	C52	-178.54(16)
C1	N1	C4	P1	178.00(10)	C6	P2	N3	Al1	124.72(8)

C1	N1	C4	C3	0.39(16)	C6	P2	N3	C11	-65.17(14)
C37	P3	N5	Al2	-11.57(9)	C6	P2	C1	N1	-126.59(12)
C37	P3	N5	C47	178.32(11)	C6	P2	C1	C2	50.15(18)
C37	P3	C42	C43	-68.87(13)	C6	P2	C9	C8	-47.82(15)
C37	P3	C42	C41	54.62(13)	C6	P2	C9	C10	-171.49(12)

Table S45 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **3**^{Pipp}.

Atom	*x*	*y*	*z*	U(eq)
H21	7984.61	5732.98	5038.23	22
H3	9613.84	5384.98	3629.38	20
H38	4898.12	2315.45	3630.93	23
H2	9702.34	4527.63	2957.23	21
H39	4778.43	3091.8	2778.4	23
H64	726.3	5383.97	2589.06	25
H42	3437.4	2050.21	5157.52	26
H66	-109.71	4712.79	665.83	27
H27	6545.58	5157.12	4778.67	22
H31	5427.76	5856.94	2871.19	23
H15	4993.44	2675.55	975.36	27
H52	1903.77	2459.44	4855.66	25
H67	843.14	3970.38	1116.07	25
H63	1698.27	4655.49	3035.67	23
H28	5424.03	5515.2	5073.52	23
H57	4225.3	4261.79	2468.48	24
H46A	2166.55	1261.11	2879.81	34
H46B	2986.4	911.47	2890.6	34
H46C	2939.39	1550.93	2730.79	34
H45	3928.67	1340.45	3895.91	24
H49	-197.27	1225.42	3425.55	32
H60	2315.88	3959.27	1032.96	24
H48	797.25	1636.61	3029.98	29
H72A	501.7	3059.01	1890.23	34
H72B	392.76	2602.49	2393.55	34
H72C	1010.71	2491.47	1983.58	34
H30	4305.29	6212.68	3168.36	25
H24	8506.3	6291.61	3704.35	22
H33	4160.81	6070.26	4859.51	27
H12	6930.39	2750.59	3312.2	25
H22A	9624.93	5651.07	4864.18	36
H22B	9567.98	5789.29	5588.02	36
H22C	9179.93	6207.4	4957.99	36
H35A	7037.57	3883.15	4189.47	37
H35B	6127.68	3670.82	3625.1	37
H35C	6159.34	4225.29	4034.17	37
H13	6065.03	1973.47	2879.06	26
H36A	5295.86	4860.7	2304.01	34
H36B	5469.72	4336.53	1923.31	34
H36C	5987.69	4891.46	1947.02	34

H23A	7647.36	5930.74	2581.34	34
H23B	7561.84	6579.33	2605.14	34
H23C	6790.12	6197.37	2625.54	34
H16	5863.12	3452.58	1401.52	26
H61A	2600.63	2806.04	1287	39
H61B	2006.53	3077.8	564.46	39
H61C	1701.21	3100.25	1196.95	39
H69	-60.69	5972.26	1513.94	30
H51	902.66	2048.13	5244.78	28
H18	5257.38	1387.46	1771.04	31
H9	7522.36	3390.22	1365.78	33
H58A	3171.63	4816.62	1615.49	43
H58B	3740.88	5182.06	2265.56	43
H58C	2769.49	5001.31	2159.7	43
H71A	2176.78	3752.52	3992.91	38
H71B	1449.22	3335.89	4021.38	38
H71C	1173.65	3830.88	3484.12	38
H32A	2926.51	5737.5	3518.08	39
H32B	2689.76	5825.31	4178.33	39
H32C	3321.7	5336.27	4165.56	39
H25A	6874.14	6636.67	3758.17	40
H25B	7657.12	7030.38	3787.19	40
H25C	7779.59	6631.29	4419.13	40
H20A	7894.19	4744.97	4929.04	34
H20B	8661.78	4940.03	5629.73	34
H20C	8889.4	4737.36	4996.66	34
H43A	4668.52	1598.29	5093.65	41
H43B	5014.54	2081.86	5643.82	41
H43C	5010.14	2153.95	4887.38	41
H54	-264.08	1442.53	5131.5	36
H56A	3408.81	4542.9	3407.2	41
H56B	4355.6	4752.73	3482.54	41
H56C	4198.6	4119.13	3573.81	41
H8A	9031.01	4098.25	1730.66	58
H8B	8584.86	3806.86	995.69	58
H8C	9058.46	3448.59	1675.27	58
H41A	4112.56	3046.34	4819.04	40
H41B	4058.67	2921.39	5547.13	40
H41C	3179.37	3003.36	4874.54	40
H6	9406.62	3317.77	2897.63	34
H59A	3822.99	4036.95	1265.16	50
H59B	3422.68	3583.8	679.14	50
H59C	3978.95	3404.33	1459.15	50
H19A	3977.79	1954.39	628.14	57
H19B	4139.24	1309.99	677.48	57
H19C	4864.1	1710.42	611.19	57
H10A	6665.01	4193.66	1312.74	51
H10B	7069.47	4211.86	736.46	51
H10C	7502.71	4565.44	1425.44	51
H70A	-265.37	5712.57	361.7	55
H70B	-1061.08	6070.84	382.44	55

H70C	-1167.6	5425	277.59	55
H17A	4437.49	1660.58	2421.57	47
H17B	3815.5	1328.73	1756.59	47
H17C	3755.94	1979.28	1770.14	47
H34A	4187.24	6936.81	4322.63	49
H34B	3238.06	6806.78	4315.4	49
H34C	3421.81	6726.58	3629.75	49
H44A	3366.67	1054.83	4728.03	44
H44B	3184.44	600.09	4143.68	44
H44C	2409.37	993.4	4132.78	44
H5A	9165.31	3507.06	3927.88	55
H5B	9561.1	2909.57	3947.31	55
H5C	8539.96	2985.08	3780.6	55
H68A	-1578.34	5317.72	1320.48	62
H68B	-1516.32	5964.4	1427.16	62
H68C	-955.98	5569.95	2047.83	62
H7A	8082.93	2481.12	2584.66	61
H7B	9104.14	2359.34	2802.72	61
H7C	8560.13	2657.56	2086.86	61
H55A	-1356.32	1961.04	4296.62	85
H55B	-1776.6	1404.61	4420.92	85
H55C	-1558.29	1475.07	3749.48	85
H53A	-678.56	575.24	4146.82	115
H53B	-758.28	557.19	4879.58	115
H53C	186.51	576.41	4841.7	115

Table S46 Fractional Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **3^{Mes}**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
P1	5912.1(8)	2041.1(5)	6048.1(5)	22.51(18)
P2	3786.0(8)	3154.6(5)	8921.6(5)	23.04(18)
Al1	2723.1(10)	2520.3(6)	7062.1(6)	24.1(2)
N1	4735(3)	2631.8(18)	7423.6(15)	23.7(5)
N2	3965(3)	2259.9(18)	6012.4(15)	23.2(5)
N3	2181(3)	2792.4(18)	8902.8(16)	26.1(5)
C11	3248(3)	2407(2)	5194.4(18)	23.8(5)
C4	5206(3)	2820(2)	8120.7(18)	24.8(5)
C1	6138(3)	2450(2)	6925.0(19)	25.3(6)
C26	987(3)	2566(2)	9622.8(19)	26.1(6)
C9	6888(4)	2743(2)	4949.8(19)	28.3(6)
C13	2245(4)	3525(2)	3708.6(19)	29.1(6)
C28	-141(4)	1319(2)	10982(2)	28.7(6)
C27	934(3)	1531(2)	10220.2(19)	26.7(6)
C12	2893(3)	3406(2)	4506.2(19)	25.9(6)
C32	2002(4)	622(2)	10066(2)	29.6(6)
C16	2875(3)	1567(2)	5069.3(19)	25.9(6)
C6	6855(3)	672(2)	6415.9(19)	26.4(6)
C35	1750(3)	1287(2)	7772.0(19)	27.3(6)

C2	7469(4)	2503(2)	7301(2)	30.0(6)
C24	3674(4)	4565(2)	8557(2)	30.2(6)
C29	-1229(4)	2094(2)	11173(2)	30.2(6)
C17	3145(4)	4372(2)	4590(2)	30.5(6)
C8	7153(4)	2148(2)	4318(2)	33.1(7)
C3	6874(4)	2746(2)	8060(2)	29.6(6)
C7	8698(4)	488(2)	6439(2)	32.0(6)
C10	8422(4)	3093(2)	5022(2)	33.6(7)
C15	2211(3)	1727(2)	4265(2)	27.3(6)
C31	-219(3)	3346(2)	9760(2)	28.2(6)
C14	1901(4)	2700(2)	3568(2)	30.6(6)
C21	4817(4)	2615(2)	9989(2)	29.0(6)
C36	1108(4)	3796(2)	6604(2)	30.8(6)
C22	3775(4)	2951(3)	10714(2)	36.4(7)
C19	3142(4)	485(2)	5791(2)	29.2(6)
C33	-2301(4)	1850(3)	12034(2)	35.6(7)
C30	-1284(4)	3103(2)	10532(2)	30.0(6)
C34	-404(4)	4449(2)	9089(2)	34.0(7)
C5	6133(4)	60(2)	7354(2)	32.5(6)
C25	5234(4)	4888(3)	8629(3)	41.8(8)
C18	1156(4)	2858(3)	2711(2)	37.2(7)
C20	5326(4)	1440(2)	10338(2)	36.0(7)
C23	3110(4)	5116(2)	7589(2)	38.9(7)

Table S47 Anisotropic Displacement Parameters ($Å^2×10^3$) for **3^{Mes}**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	23.9(3)	21.5(3)	20.3(3)	-7.0(3)	1.4(2)	-3.9(3)
P2	24.8(3)	22.4(3)	21.4(3)	-8.3(3)	0.5(3)	-4.7(3)
Al1	22.1(4)	22.3(4)	25.1(4)	-7.0(3)	0.8(3)	-3.9(3)
N1	24.3(11)	24.5(11)	23.2(11)	-11.2(9)	2.5(9)	-3.9(9)
N2	26.2(11)	23.8(11)	17.5(10)	-6.6(9)	1.2(8)	-4.0(9)
N3	26.5(12)	23.5(11)	25.4(12)	-6.2(9)	-1.0(9)	-5.5(9)
C11	24.0(12)	24.1(13)	21.6(12)	-8.8(10)	1.1(10)	-2.0(10)
C4	26.7(13)	27.3(14)	21.1(13)	-11.0(11)	1.5(10)	-4.7(10)
C1	23.6(13)	28.5(14)	23.1(13)	-11.1(11)	3.4(10)	-3.8(10)
C26	27.9(14)	24.7(13)	25.6(13)	-8.4(11)	-2.1(11)	-6.5(11)
C9	31.8(15)	23.4(13)	25.2(14)	-6.5(11)	5.0(11)	-5.9(11)
C13	31.7(14)	26.2(14)	21.9(13)	-4.4(11)	1.7(11)	-1.7(11)
C28	31.2(14)	26.8(14)	27.0(14)	-7.5(11)	-1.2(11)	-8.6(11)
C27	28.2(13)	22.8(13)	27.7(14)	-7.3(11)	-4.3(11)	-4.9(10)
C12	24.2(13)	25.2(13)	23.8(13)	-7.0(11)	1.4(10)	-2.2(10)
C32	36.2(15)	22.0(13)	26.8(14)	-7.0(11)	-0.7(11)	-3.1(11)
C16	24.9(13)	25.6(14)	26.3(14)	-10.5(11)	1.1(10)	-3.1(10)
C6	27.0(14)	23.4(13)	25.7(13)	-6.8(11)	-1.1(10)	-3.7(10)
C35	26.7(13)	30.2(14)	25.1(13)	-10.5(11)	2.6(10)	-7.8(11)
C2	25.3(14)	35.1(16)	32.2(15)	-16.5(13)	2.3(11)	-5.9(11)
C24	30.2(14)	24.6(14)	35.6(15)	-11.2(12)	3.3(12)	-8.1(11)
C29	27.8(14)	34.9(16)	29.3(14)	-12.6(12)	-1.2(11)	-7.9(12)

C17	34.9(15)	22.1(13)	28.8(14)	-4.8(11)	-0.4(12)	-3.9(11)
C8	41.3(17)	33.3(16)	23.5(14)	-11.8(12)	6.6(12)	-7.8(13)
C3	29.7(14)	36.1(16)	28.1(14)	-16.9(12)	-2.0(11)	-6.7(12)
C7	26.9(14)	26.9(14)	38.4(16)	-9.6(12)	-3.2(12)	-2.2(11)
C10	33.2(15)	29.7(15)	36.3(16)	-12.8(13)	11.8(12)	-10.6(12)
C15	27.4(13)	28.2(14)	29.4(14)	-15.7(12)	0.5(11)	-3.1(11)
C31	27.0(14)	24.2(13)	33.0(15)	-9.8(11)	-1.8(11)	-6.0(11)
C14	29.0(14)	35.2(16)	25.2(14)	-10.9(12)	1.0(11)	-3.5(12)
C21	31.5(14)	32.5(15)	26.6(14)	-15.4(12)	-0.7(11)	-5.9(12)
C36	29.7(14)	29.5(15)	30.1(15)	-10.1(12)	-1.4(11)	-1.8(11)
C22	34.3(16)	50(2)	28.4(15)	-21.1(14)	-0.2(12)	-3.5(14)
C19	33.3(15)	23.1(13)	29.9(14)	-8.4(11)	-2.1(11)	-5.5(11)
C33	35.0(16)	42.5(18)	29.6(15)	-14.9(13)	3.6(12)	-9.2(13)
C30	26.4(14)	28.8(14)	36.7(16)	-15.4(12)	0.7(12)	-4.9(11)
C34	29.9(15)	26.1(14)	40.7(17)	-9.6(13)	2.6(12)	-3.7(11)
C5	35.4(16)	24.2(14)	29.0(15)	-2.6(11)	-1.5(12)	-2.4(12)
C25	36.9(17)	29.8(16)	60(2)	-14.4(15)	-3.5(15)	-12.7(13)
C18	39.7(17)	43.3(18)	26.4(15)	-13.4(13)	-3.0(12)	-1.9(14)
C20	44.8(18)	29.6(15)	29.3(15)	-6.0(12)	-10.1(13)	-3.3(13)
C23	40.9(17)	25.1(15)	40.9(18)	-1.7(13)	-2.2(14)	-7.5(13)

Table S48 Bond Lengths for **3**$^{\mathbf{Mes}}$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	N2	1.624(2)	C9	C10	1.532(4)
P1	C1	1.773(3)	C13	C12	1.396(4)
P1	C9	1.832(3)	C13	C14	1.387(4)
P1	C6	1.836(3)	C28	C27	1.394(4)
P2	N3	1.573(2)	C28	C29	1.392(4)
P2	C4	1.778(3)	C27	C32	1.508(4)
P2	C24	1.853(3)	C12	C17	1.508(4)
P2	C21	1.833(3)	C16	C15	1.395(4)
Al1	N1	1.940(2)	C16	C19	1.512(4)
Al1	N2	1.986(2)	C6	C7	1.537(4)
Al1	C35	1.972(3)	C6	C5	1.529(4)
Al1	C36	1.972(3)	C2	C3	1.399(4)
N1	C4	1.378(4)	C24	C25	1.532(4)
N1	C1	1.381(3)	C24	C23	1.526(5)
N2	C11	1.443(3)	C29	C33	1.507(4)
N3	C26	1.413(4)	C29	C30	1.396(4)
C11	C12	1.415(4)	C15	C14	1.394(4)
C11	C16	1.404(4)	C31	C30	1.402(4)
C4	C3	1.394(4)	C31	C34	1.505(4)
C1	C2	1.385(4)	C14	C18	1.507(4)
C26	C27	1.416(4)	C21	C22	1.535(4)
C26	C31	1.411(4)	C21	C20	1.530(4)
C9	C8	1.534(4)			

Table S49 Bond Angles for **3**^{Mes}.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	P1	C1	101.42(13)	C8	C9	P1	111.6(2)
N2	P1	C9	112.09(13)	C10	C9	P1	114.3(2)
N2	P1	C6	114.60(13)	C10	C9	C8	112.2(2)
C1	P1	C9	113.89(13)	C14	C13	C12	122.4(3)
C1	P1	C6	106.88(13)	C29	C28	C27	122.3(3)
C9	P1	C6	107.91(13)	C26	C27	C32	122.5(3)
N3	P2	C4	107.72(13)	C28	C27	C26	120.2(3)
N3	P2	C24	116.24(14)	C28	C27	C32	117.3(3)
N3	P2	C21	118.84(13)	C11	C12	C17	123.5(3)
C4	P2	C24	104.07(14)	C13	C12	C11	119.4(3)
C4	P2	C21	105.38(13)	C13	C12	C17	117.1(3)
C21	P2	C24	103.18(14)	C11	C16	C19	122.1(3)
N1	Al1	N2	87.49(10)	C15	C16	C11	119.7(3)
N1	Al1	C35	119.25(12)	C15	C16	C19	118.2(3)
N1	Al1	C36	117.36(12)	C7	C6	P1	113.5(2)
C35	Al1	N2	106.26(12)	C5	C6	P1	109.9(2)
C35	Al1	C36	112.95(13)	C5	C6	C7	109.7(2)
C36	Al1	N2	109.12(12)	C1	C2	C3	106.0(3)
C4	N1	Al1	136.02(19)	C25	C24	P2	114.9(2)
C4	N1	C1	105.3(2)	C23	C24	P2	109.5(2)
C1	N1	Al1	118.57(19)	C23	C24	C25	110.4(3)
P1	N2	Al1	115.70(13)	C28	C29	C33	121.2(3)
C11	N2	P1	119.95(18)	C28	C29	C30	117.1(3)
C11	N2	Al1	123.67(18)	C30	C29	C33	121.7(3)
C26	N3	P2	125.4(2)	C4	C3	C2	107.3(3)
C12	C11	N2	120.4(2)	C14	C15	C16	122.2(3)
C16	C11	N2	120.8(2)	C26	C31	C34	121.5(3)
C16	C11	C12	118.8(3)	C30	C31	C26	120.2(3)
N1	C4	P2	121.8(2)	C30	C31	C34	118.3(3)
N1	C4	C3	110.1(2)	C13	C14	C15	117.4(3)
C3	C4	P2	128.0(2)	C13	C14	C18	121.1(3)
N1	C1	P1	115.0(2)	C15	C14	C18	121.4(3)
N1	C1	C2	111.3(3)	C22	C21	P2	110.5(2)
C2	C1	P1	133.1(2)	C20	C21	P2	112.9(2)
N3	C26	C27	120.5(3)	C20	C21	C22	111.3(3)
C31	C26	N3	122.0(3)	C29	C30	C31	122.1(3)
C31	C26	C27	117.5(3)				

Table S50 Torsion Angles for **3**^{Mes}.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
P1	N2	C11	C12	-89.3(3)	C1	N1	C4	P2	177.2(2)
P1	N2	C11	C16	91.3(3)	C1	N1	C4	C3	-0.6(3)
P1	C1	C2	C3	-171.4(2)	C1	C2	C3	C4	0.5(3)
P2	N3	C26	C27	-98.7(3)	C26	C31	C30	C29	-1.9(4)
P2	N3	C26	C31	83.4(3)	C9	P1	N2	Al1	-135.94(14)
P2	C4	C3	C2	-177.6(2)	C9	P1	N2	C11	34.9(2)

Al1	N1	C4	P2	-5.9(4)	C9	P1	C1	N1	132.1(2)
Al1	N1	C4	C3	176.4(2)	C9	P1	C1	C2	-57.7(3)
Al1	N1	C1	P1	-4.3(3)	C9	P1	C6	C7	54.1(2)
Al1	N1	C1	C2	-176.6(2)	C9	P1	C6	C5	177.4(2)
Al1	N2	C11	C12	80.9(3)	C28	C29	C30	C31	-4.4(4)
Al1	N2	C11	C16	-98.5(3)	C27	C26	C31	C30	8.3(4)
N1	C4	C3	C2	0.0(3)	C27	C26	C31	C34	-171.5(3)
N1	C1	C2	C3	-1.0(3)	C27	C28	C29	C33	-175.8(3)
N2	P1	C1	N1	11.5(2)	C27	C28	C29	C30	4.3(4)
N2	P1	C1	C2	-178.3(3)	C12	C11	C16	C15	1.8(4)
N2	P1	C9	C8	-84.6(2)	C12	C11	C16	C19	-177.0(3)
N2	P1	C9	C10	146.7(2)	C12	C13	C14	C15	0.6(4)
N2	P1	C6	C7	179.7(2)	C12	C13	C14	C18	178.2(3)
N2	P1	C6	C5	-57.0(2)	C16	C11	C12	C13	-2.6(4)
N2	C11	C12	C13	178.0(2)	C16	C11	C12	C17	176.2(3)
N2	C11	C12	C17	-3.2(4)	C16	C15	C14	C13	-1.4(4)
N2	C11	C16	C15	-178.8(2)	C16	C15	C14	C18	-178.9(3)
N2	C11	C16	C19	2.4(4)	C6	P1	N2	Al1	100.64(16)
N3	P2	C4	N1	20.4(3)	C6	P1	N2	C11	-88.5(2)
N3	P2	C4	C3	-162.3(3)	C6	P1	C1	N1	-108.8(2)
N3	P2	C24	C25	177.0(2)	C6	P1	C1	C2	61.4(3)
N3	P2	C24	C23	-58.1(3)	C6	P1	C9	C8	42.5(3)
N3	P2	C21	C22	-65.2(3)	C6	P1	C9	C10	-86.2(2)
N3	P2	C21	C20	60.1(3)	C24	P2	N3	C26	-87.9(3)
N3	C26	C27	C28	173.6(3)	C24	P2	C4	N1	-103.6(2)
N3	C26	C27	C32	-6.9(4)	C24	P2	C4	C3	73.7(3)
N3	C26	C31	C30	-173.7(3)	C24	P2	C21	C22	65.1(2)
N3	C26	C31	C34	6.5(4)	C24	P2	C21	C20	-169.6(2)
C11	C16	C15	C14	0.2(4)	C29	C28	C27	C26	2.2(4)
C4	P2	N3	C26	155.9(2)	C29	C28	C27	C32	-177.4(3)
C4	P2	C24	C25	-64.7(3)	C31	C26	C27	C28	-8.4(4)
C4	P2	C24	C23	60.2(2)	C31	C26	C27	C32	171.1(3)
C4	P2	C21	C22	174.0(2)	C14	C13	C12	C11	1.4(4)
C4	P2	C21	C20	-60.7(2)	C14	C13	C12	C17	-177.4(3)
C4	N1	C1	P1	173.31(19)	C21	P2	N3	C26	36.3(3)
C4	N1	C1	C2	1.0(3)	C21	P2	C4	N1	148.2(2)
C1	P1	N2	Al1	-14.08(16)	C21	P2	C4	C3	-34.5(3)
C1	P1	N2	C11	156.8(2)	C21	P2	C24	C25	45.1(3)
C1	P1	C9	C8	161.0(2)	C21	P2	C24	C23	170.0(2)
C1	P1	C9	C10	32.3(3)	C19	C16	C15	C14	179.1(3)
C1	P1	C6	C7	-68.8(2)	C33	C29	C30	C31	175.7(3)
C1	P1	C6	C5	54.5(2)	C34	C31	C30	C29	177.9(3)

Table S51 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **3^{Mes}**.

Atom	*x*	*y*	*z*	U(eq)
H9	6102.68	3388.95	4651.02	34
H13	2033.13	4196.72	3244.74	35
H28	-131.37	620.72	11385.36	34

H32A	1362.5	280.37	9850.05	44
H32B	2471.08	131.52	10638.57	44
H32C	2866.52	862.77	9608.53	44
H6	6598.51	402.48	5973.79	32
H35A	2586.03	711.98	8095.26	41
H35B	1251.54	1097.89	7360.01	41
H35C	927.15	1436.75	8213.66	41
H2	8563.5	2397.2	7087.21	36
H24	2829.84	4801.59	8962.99	36
H17A	2101.02	4819.3	4601.04	46
H17B	3824.85	4739.09	4068.92	46
H17C	3673.4	4184.62	5154.95	46
H8A	7975.99	1527.53	4557.02	50
H8B	7511.37	2589.24	3707.49	50
H8C	6141.24	1946.99	4286.21	50
H3	7491.41	2841.81	8460.61	36
H7A	9163.11	827.09	5824.45	48
H7B	9121.79	-255.35	6661.47	48
H7C	8982.47	775.95	6846.92	48
H10A	8193.62	3479.03	5421.32	50
H10B	8792.47	3536.66	4415.08	50
H10C	9262.19	2486.26	5274.64	50
H15	1961.74	1152.15	4190.05	33
H21	5821.13	2914.78	9863.63	35
H36A	315.98	3834.14	7098.43	46
H36B	561.99	3790.9	6107.09	46
H36C	1645.05	4396.85	6379.1	46
H22A	3546.32	3707.36	10492.46	55
H22B	4353.84	2670.94	11275.36	55
H22C	2761.19	2690.46	10838.24	55
H19A	2357.53	103.25	5741.53	44
H19B	3006.74	518.02	6394.95	44
H19C	4234.99	130.57	5702.93	44
H33A	-1645.43	1629.47	12558.9	53
H33B	-2859.01	1293.16	12097.78	53
H33C	-3095.82	2466.76	12004.97	53
H30	-2067.01	3641.2	10622.32	36
H34A	290.57	4812.08	9242.65	51
H34B	-1529.19	4789.92	9113.54	51
H34C	-95.45	4462.95	8473.36	51
H5A	6491.54	243.22	7814.36	49
H5B	6490.82	-681.14	7497.1	49
H5C	4955.16	226.04	7350.91	49
H25A	5499.77	4606.25	9269.08	63
H25B	5088.06	5643.34	8388.75	63
H25C	6111.55	4620.44	8276.51	63
H18A	1378.17	2207.78	2616.38	56
H18B	1616.24	3387.34	2190.8	56
H18C	-11.29	3083.27	2769.11	56
H20A	4376.64	1114.96	10592.94	54
H20B	6098.32	1212.09	10811.2	54

H20C	5830.35	1239.8	9833.19	54
H23A	3949.71	4945.07	7164.37	58
H23B	2893.5	5864.33	7429.7	58
H23C	2122.65	4892.89	7550.07	58

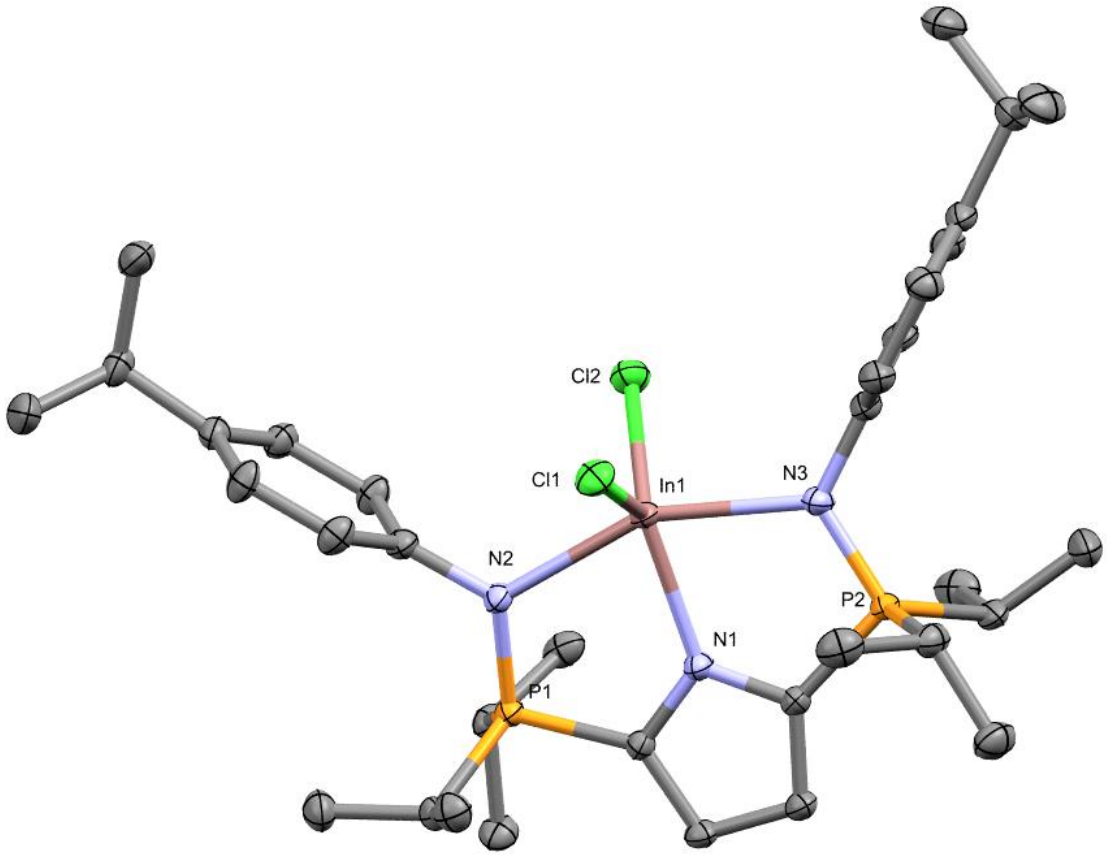

Figure S55. X-ray crystal structure of **2**^{Pipp}. Thermal Ellipsoids are drawn at 50% probability. Hydrogen atoms have been omitted for clarity.

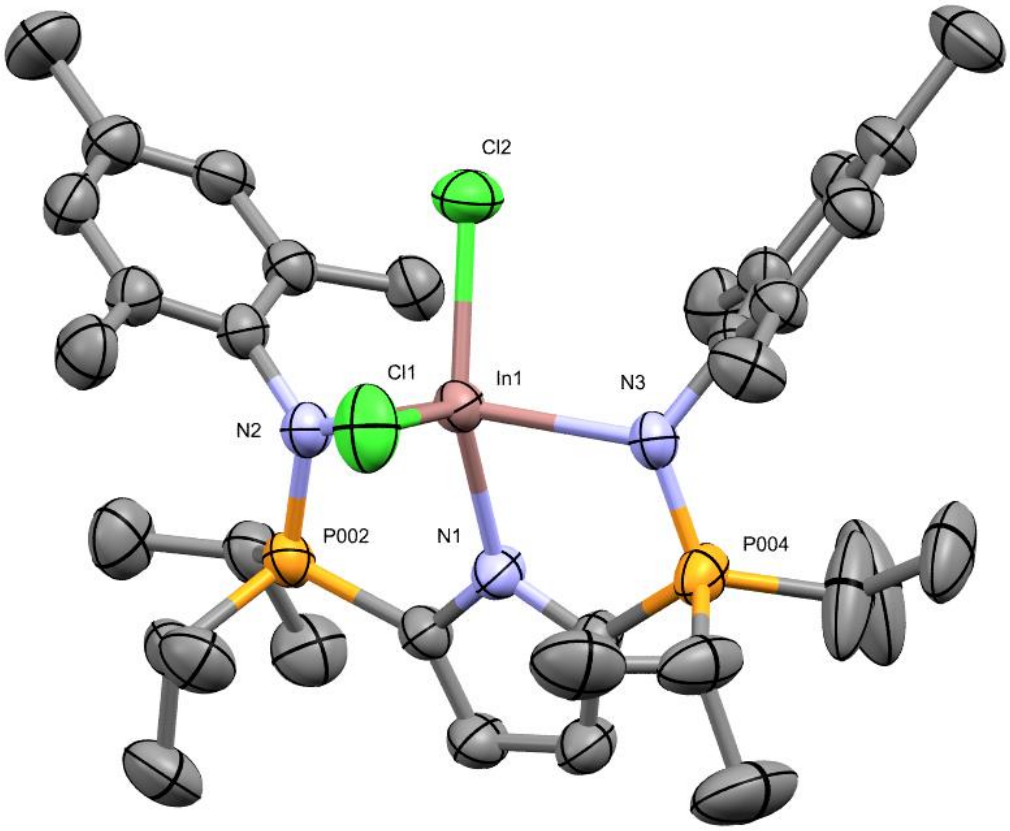

Figure S56. X-ray crystal structure of **2**^{Mes}. Thermal Ellipsoids are drawn at 50% probability. Hydrogen atoms have been omitted for clarity.

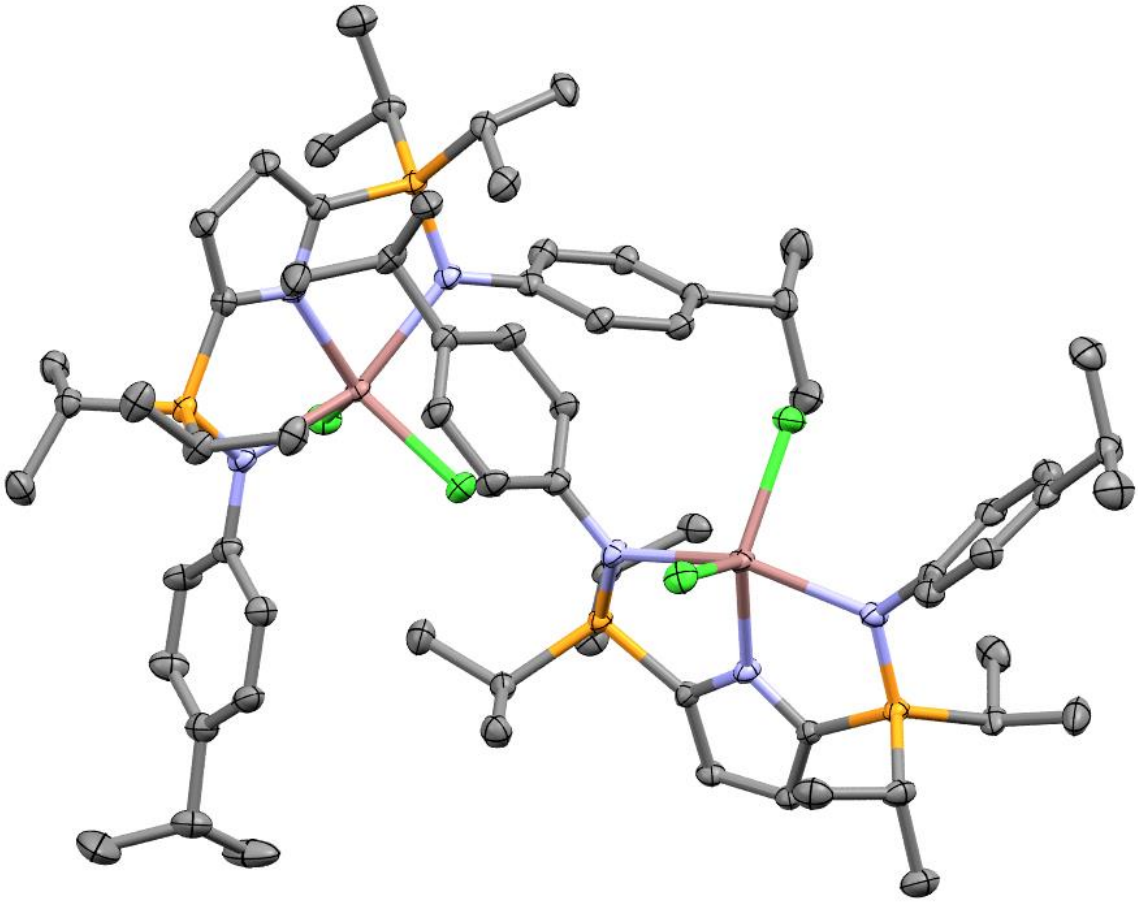

Figure S57. Asymmetric unit of **2**^{Mes}.Thermal Ellipsoids are drawn at 50% probability. Hydrogen atoms have been omitted for clarity.

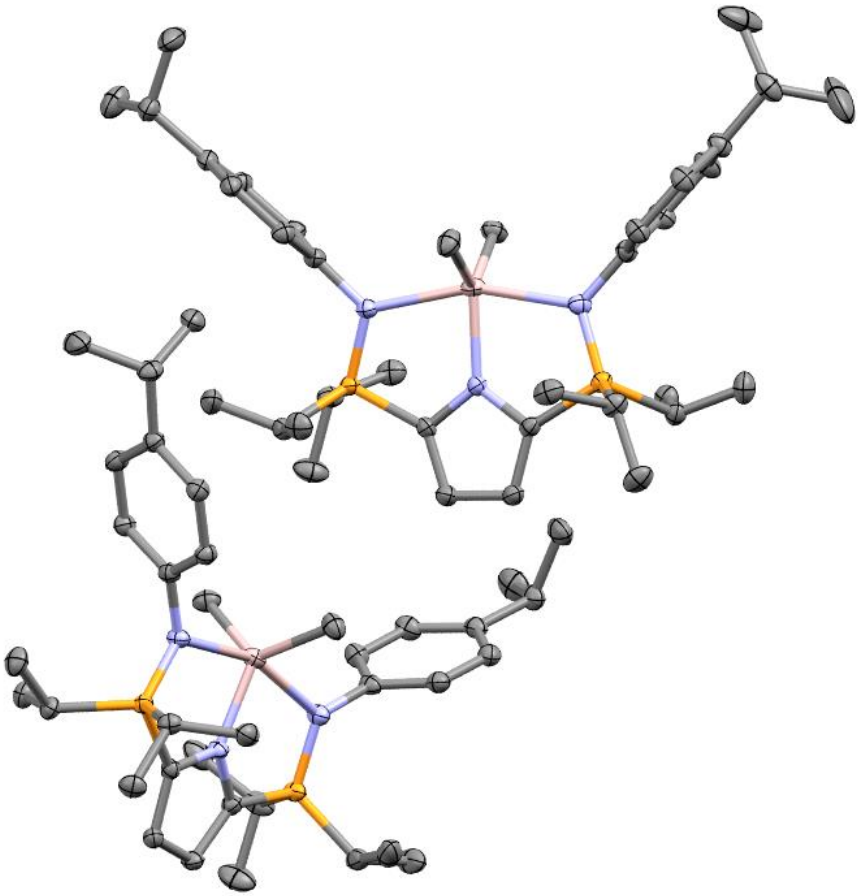

Figure S58. Asymmetric unit of **3**$^{\mathbf{Pipp}}$.Thermal Ellipsoids are drawn at 50% probability. Hydrogen atoms have been omitted for clarity.

III. References

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