Supporting Information (SI) File

Tailoring the Fe→Pd interaction in cationic Pd (II) complexes via structural variation of the ligand scaffold of sterically demanding dppf-analogs and their P, N-counterparts

Subhayan Dey,[a] Fabian Roesler,[a] Clemens Bruhn,[a] Zsolt Kelemen,*[b] Rudolf Pietschnig*[a]

[a] Institut für Chemie und CINSaT, University of Kassel, Heinrich Plett-Straße 40, 34132 Kassel, Germany. E-mail: pietschnig@uni-kassel.de

[b] Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Műegyetem Rkp 3, 1111 Budapest, Hungary.

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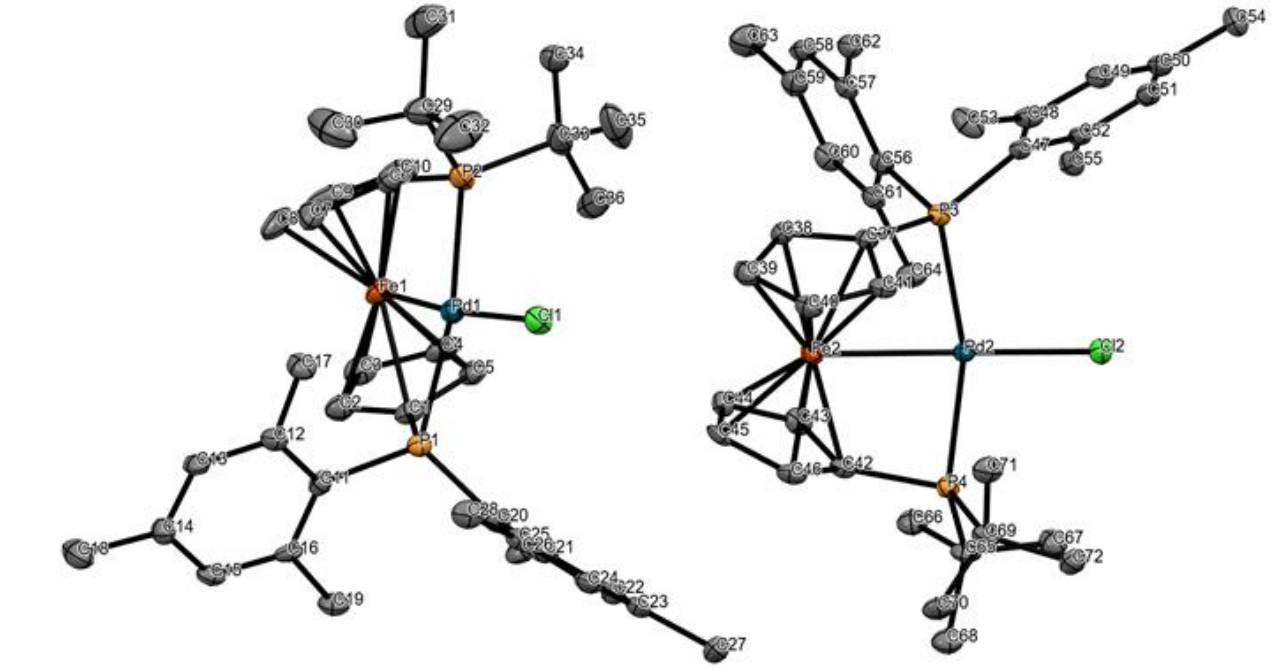
Table S1. Molecular parameters of cationic Pd(II) complexes of dppf and its diphospha- and azaphospha-analogs with Fe→Pd bonding interactions.

Entry	DPPF Analogs	Square-planar Pd(II) complexes	Avg. $C^{ipso,Cp}$-E Bond Length (Å)[#]	Avg. Pd-P/N Bond Length (Å)[#]	Pd-PR_3/anion Bond Length (Å)[#]	Pd-Fe distance (Å)	Tilt Angle α (°)*	Bite Angle β_n (°)	Torsion Angle τ (°)*
1	dppf	[dppf·Pd(PPh_3)][BF_4]$_2$[1, 2]	1.787[a] (E = P)[1, 2]	2.2958 (E = P)	2.2783 (PR_3 = PPh_3)[1, 2]	2.8934[a]	19.7[a]	156.79[a]	41.1
		[dppf·PdP(C_5H_4-*p*-F)$_3$][BF_4]$_2$[3]	1.784 (E = P)[3]	2.293 (E = P)	2.2835(7) (PR_3 = P(C_5H_4-*p*-F)$_3$)[3]	3.0014(4)[3]	22.1	157.54(3)[3]	26.9
2	Fc'(P^tBu_2)(PPh_2)	[Fc'(P^tBu_2)(PPh_2)·Pd(PPh_3)][BF_4]$_2$[1]	1.785(3) (E = P^{tBu}), 1.777(3) (E = P^{Ph})[1]	2.342(1) (E = P^{tBu}), 2.307(1) (E = P^{Ph})[1]	2.2953(9) (PR_3 = PPh_3)[1]	2.9310(5)[1]	19.7	156.11(3)[1]	42.6
3	Fc'(P^tBu_2)$_2$	[Fc'(P^tBu_2)$_2$·PdCl][$SbCl_6$][1]	1.797 (E = P)[1]	2.275 (E = P)[1]	2.316(2) (anion = Cl^-)[1]	2.9389(4)[1]	19.8	162.34(2)[1]	30.5
		[Fc'(P^tBu_2)$_2$·PdI][I][1, 4]	1.823[a] (E = P)[1, 4]	2.3296[a] (E = P)	2.6402[a] (anion = I^-)	2.9390[a]	18.0[a]	161.88[a]	34.6
		[Fc'(P^tBu_2)$_2$·PdBr][TFAB][ǂ4]	1.829 (E = P)[4]	2.296 (E = P)	2.449(1) (anion = Br^-)	2.9395(18)	19.2	163.04(5)	31.0
		[Fc'(P^tBu_2)$_2$·Pd(C_6H_4-*p*-CN)][BF_4]$_2$[5]	1.808 (E = P)[5]	2.307 (E = P)	2.001 (anion = (C_6H_4-*p*-CN)$^-$)	2.9988(8)	16.3	159.75(4)	35.9
4	Fc'[P(C_6H_{11})$_2$]$_2$	[Fc'[P(C_6H_{11})$_2$]$_2$·Pd(PPh_3)][BF_4]$_2$[1]	1.782 (E = P)[1]	2.3134 (E = P)	2.2860(7) (PR_3 = PPh_3)[1]	2.9339(5)[1]	18.9	156.63(3)[1]	38.2
		[Fc'[P(C_6H_{11})$_2$]$_2$·Pd(PMe_3)][BF_4]$_2$[1]	1.783 (E = P)[1]	2.302 (E = P)	2.271(2) (PR_3 = PMe_3)[1]	2.9567(10)[1]	20.4	157.20(6)[1]	41.7
5	Fc'(CpP^iPr_2)$_2$	[Fc'(CpP^iPr_2)$_2$·Pd(PMe_3)][BF_4]$_2$[1]	1.786 (E = P)[1]	2.2924 (E = P)	2.2590(5) (PR_3 = PMe_3)[1]	3.0168(4)[1]	19.1	158.09(2)[1]	32.6
6	Fc'($PMes_2$)(P^tBu_2) (**8**)	[Fc'($PMes_2$)(P^tBu_2)·PdCl][SbF_6] (**10^A** and **10^B**)[a]	1.792(5) (E = P^{tBu}) and 1.785(5) (E = P^{Mes}) for **10^A**; 1.797(5) (E = P^{tBu}) and 1.790(5) (E = P^{Mes}) for **10^B**	2.2751(16) (E = P^{tBu}) and 2.3404(14) (E = P^{Mes}) for **10^A**; 2.2931(15) (E = P^{tBu}) and 2.3289(15) (E = P^{Mes}) for **10^B**	2.3278(13) (**10^A**) and 2.3278(13) (**10^B**)	2.8369(10) (**10^A**) and 2.7974(10) (**10^B**)	21.5[a]	161.60(5)° (**10^A**) and 161.46(5)° (**10^B**)	40.5 (**10^A**) and 46.2 (**10^B**)
7	Fc'[NC(NHR)$_2$](PPh_2)	[Fc'[NC(NH^{i}Pr)$_2$](PPh_2)·PdCl][SbF_6][6]	1.775(2) (E = P) and 1.379(3) (E = N)[6]	2.1947(6) (E = P) and 2.084(2) (E = N)[6]	2.3755(7)[6]	2.7590(5)[6]	24.6	163.01(5)[6]	1.9
		[Fc'[NC(NHCy)$_2$](PPh_2)·PdCl][SbF_6][c6]	1.773(2) (E = P) and 1.388(2) (E = N)[6]	2.1822(7) (E = P) and 2.051(2) (E = N)[6]	2.3352(5)[6]	2.7956(5)[6]	22.8	162.46(5)[6]	5.7
		[Fc'[NC(NHXyl)$_2$](PPh_2)·PdCl][SbF_6][d6]	1.770(2) (E = P) and 1.384(2) (E = N)[6]	2.1850(6) (E = P) and 2.065(2) (E = N)[6]	2.3514(5)[6]	2.7821(4)[6]	23.0	163.15(5)[6]	5.9
8	Fc'[NH(CH_2)$_2$$PPh_2$]($PPh_2$)	[Fc'[NH(CH_2)$_2$$PPh_2$]($PPh_2$)· Pd][$SbF_6$]$_2$[7]	1.790(7) (E = P) and 1.419(9) (E = N)[7]	2.212(2) (E = P) and 2.083(4) (E = N)[7]	2.261(2) (PR_3 = $PPh_2C_2H_4Fc$)[7]	2.7889(9)[7]	21.3	164.4(2)[7]	9.8
9	Fc'(NMe_2)(PPh_2) (**3a**)	[Fc'(PPh_2)(NMe_2)·PdCl][SbF_6]$_2$ (**11**)	1.783(11) (E = P) and 1.389(15) (E = N)	2.190(3) (E = P) and 2.118(8) (E = N)	2.315(3) (anion = Cl^-)	2.738(2)	22.9	163.6(3)	1.7
		[Fc'(PPh_2)(NMe_2)·Pd($PPh_2C_5H_5$)][SbF_6]$_2$ (**12**)	1.788(8) (E = P) and 1.420(9) (E = N)	2.236(3) (E = P) and 2.140(6) (E = N)	2.310(3) (PR_3 = $PPh_2C_5H_5$)	2.811(3)	21.9	159.11(19)	22.3
		[Fc'(PPh_2)(NMe_2)·Pd(PPh_3)][BF_4]$_2$ (**13**)	1.773(12) (E = P) and 1.427(15) (E = N)	2.253(3) (E = P) and 2.157(9) (E = N)	2.298(3) (PR_3 = PPh_3)	2.8289(19)	20.9	158.9(3)	20.4
		[Fc'(PPh_2)(NMe_2)·Pd(PPh_2)Fc'(NMe_2)][BF_4]$_2$ (**14**)	1.766(6) (E = P) and 1.427(7) (E = N)	2.2297(15) (E = P) and 2.138(5) (E = N)	2.3022(14) (PR_3 = (PPh_2)Fc'(NMe_2))	2.8184(9)	19.5	158.79(13)	30.7
		[Fc'(PPh_2)(NMe_2)·PdP(*p*-OMe-C_6H_4)$_3$][BF_4]$_2$ (**15**)	1.770(7) (E = P) and 1.408(9) (E = N)	2.2468(14) (E = P) and 2.146(5) (E = N)	2.2996(17) (PR_3 = P(*p*-OMe-C_6H_4)$_3$)	2.8349(11)	22.5	160.45(16)	11.1

[#] Averages of two identical bonds from a single molecule (standard deviations are excluded)
* Angles were calculated using Mercury as crystallographic software[8, 9]
[ǂ] TFAB = tetrakis(pentafluorophenyl)borate, [$B(C_6F_5)_4$]$^-$

[a] Averages from all crystallographically independent entities in the unit cell (standard deviations are excluded)
[b] Im = 1,3-di(propan-2-yl)-1,3-dihydro-2H-imidazol-2-ylidene
[c] Cy = C_6H_{11}; [d] Xyl = 2,4,6-Me_3-C_6H_2

Table S2. Molecular parameters for two independent molecules of **10**^{A} and **10**^{B} in the unit cell of **10**



Parameters	Molecule 1 (10^{A})	Molecule 2 (10^{B})
Fe-Pd distance	2.8369(10) Å	2.7974(10) Å
Pd-Cl	2.3278(13) Å	2.3278(13) Å
P^{Mes}-$C^{ipso,Cp,Fc}$	1.785(5) Å	1.790(5) Å
P^{tBu}-$C^{ipso,Cp,Fc}$	1.792(5) Å	1.797(5) Å
P-$C^{ipso,Mes}$	1.828(5) Å, 1.829(5) Å	1.828(5) Å, 1.832(5) Å
P-$C^{ipso,tBu}$	1.888(6) Å, 1.868(6) Å	1.887(5) Å, 1.873(5) Å
Pd-P^{Mes}	2.3404(14) Å	2.3289(15) Å
Pd-P^{tBu}	2.2751(16) Å	2.2931(15) Å
Tilt Angle	21.32°	21.63°
Torsion Angle	40.46°	46.17°
$C^{ipso,Mes}$-P-$C^{ipso,Mes}$	113.2(2)°	108.7(2)°
$C^{ipso,tBu}$-P-$C^{ipso,tBu}$	111.8(3)°	111.7(2)°
Bite angle	161.60(5)°	161.46(5)
Pd-P-$C^{ipso,tBu}$	117.84(19)° and 115.7(2)°	117.66(16)° and 117.96(16)°
Pd-P-$C^{ipso,Mes}$	120.16(16)° and 118.34(17)°	117.18(16)° and 123.59(16)°
$C^{ipso,tBu}$-P-$C^{ipso,tBu}$	111.8(3)°	111.7(2)°
$C^{ipso,Fc}$-P-$C^{ipso,tBu}$	108.6(3)° and 110.3(3)°	109.6(2)° and 109.7(2)°
Cumulative Angle around P^{tBu}	330.7(3)°	331.0(2)°
$C^{ipso,Mes}$-P-$C^{ipso,Mes}$	113.2(2)°	108.7(2)°
$C^{ipso,Fc}$-P-$C^{ipso,Mes}$	105.0(2) and 111.3(2)°	115.3(2)° and 104.2(2)°
Cumulative Angle around P^{Mes}	329.5(2)°	328.2(2)°

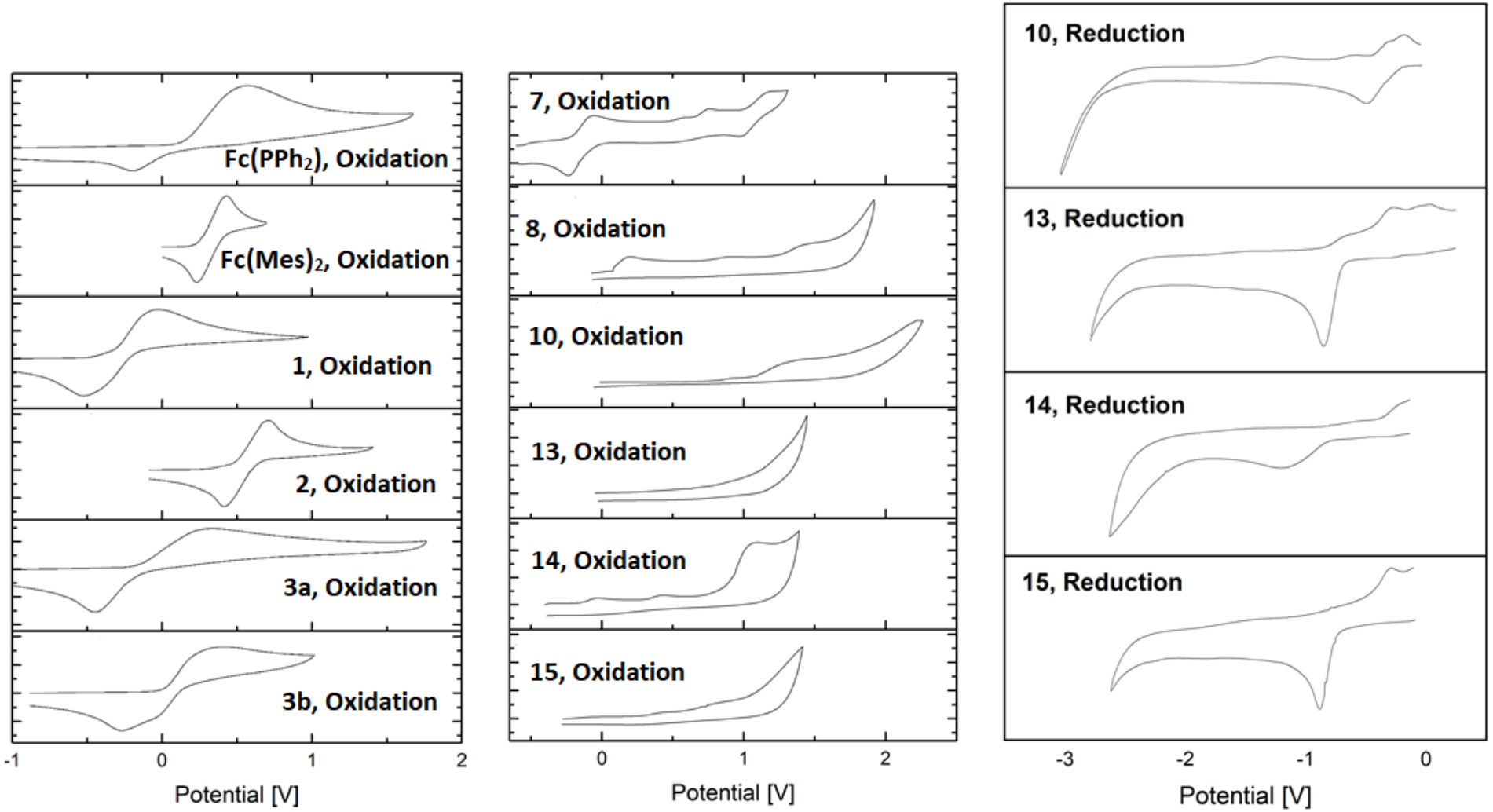


Fig S1. Cyclic voltammetry of $Fc(PPh_2)$, $Fc(PMes_2)$, **1**-**3**, **7**, **8**, **10** and **13**-**15**.

The oxidation and reduction potentials were measured with voltage sweep 250 mV/s in DCM and thf, respectively. The oxidation and reduction potentials are 0.573 and -0.202 V for $Fc(PPh_2)$;[10] 0.434 and 0.230 V for $Fc(PMes_2)$; 0.022 and -0.522 V for **1**; 0.712 and -0.413 V for **2**; 0.340 and -0.454 V for **3a**; 0.408 and -0.267 V for **3b**; -0.085 and -0.239 V for **7**. The potential for irreversible oxidation for compounds **8** and **14** are 0.147 V and 1.102 V, respectively. The reductions potentials for **10**, **13**, **14**, and **15** are -0.495 V, -0.849 V, -1.204 V and -0.885 V, respectively. All the measurements were referenced versus $FcMe_{10}/FcMe_{10}^{+}$. As compounds **11** and **12** could not be obtained as analytically pure forms no cyclovoltammetry were performed on them.

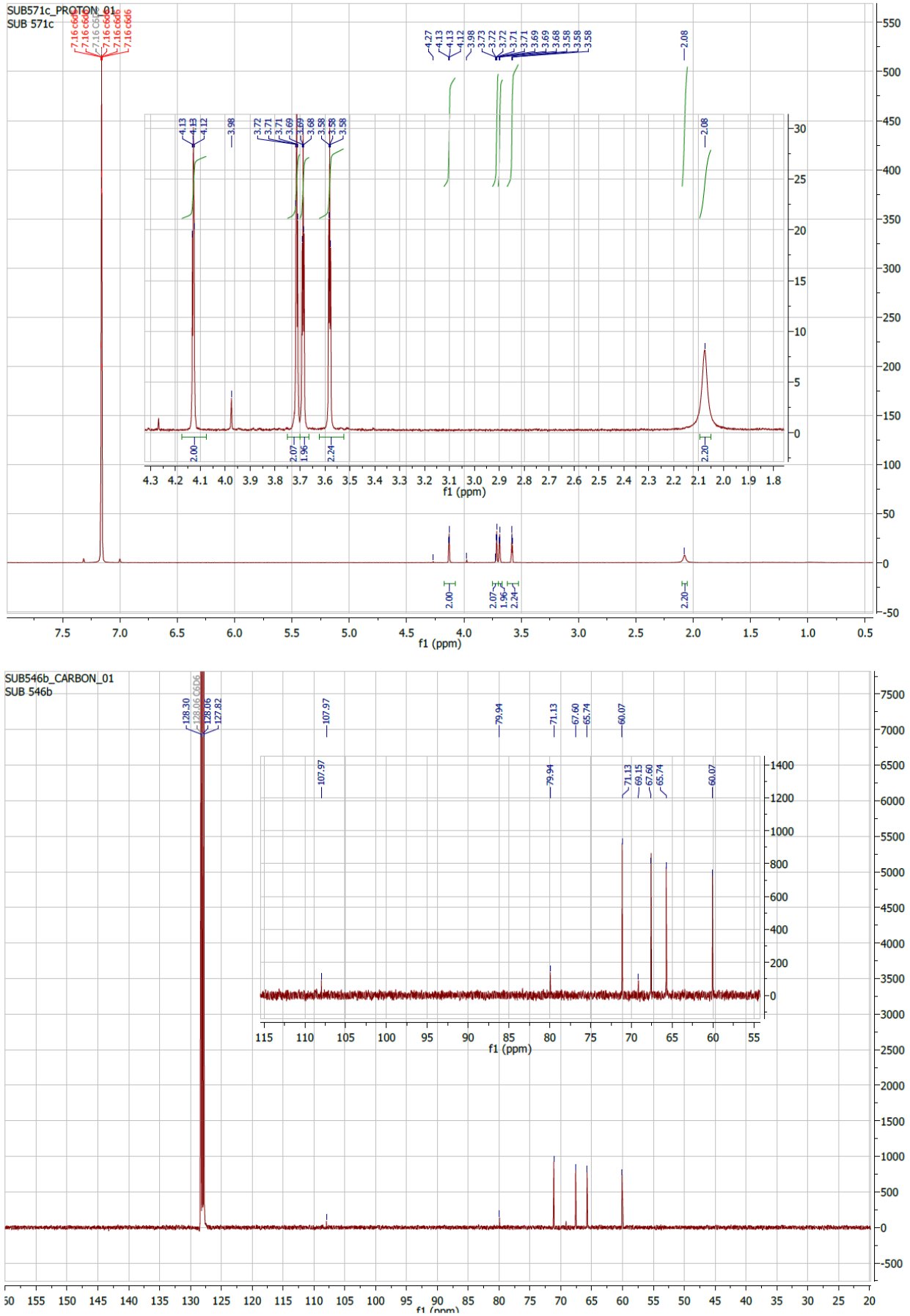


Fig S2. ^{1}H and ^{13}C NMR of Fc'(NH_2)Br (**1**), measured in C_6D_6.

The peak at δ 3.98 ppm is resulting from free cyclopentadienyl (Cp) ring of aminoferrocene, which is an impurity (varies between ca. 1-3%) present in this compound.

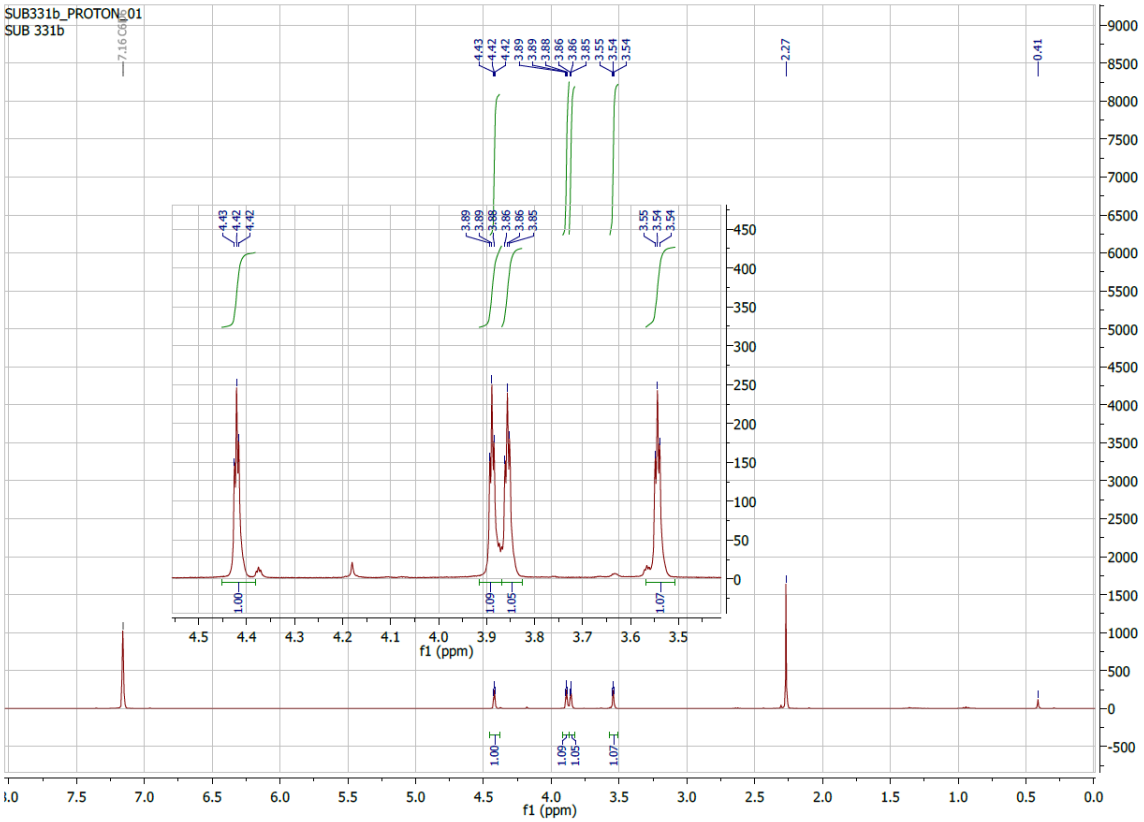


Fig S3. ^{1}H NMR of Fc'(NMe_2)Br (**2**), measured in C_6D_6.

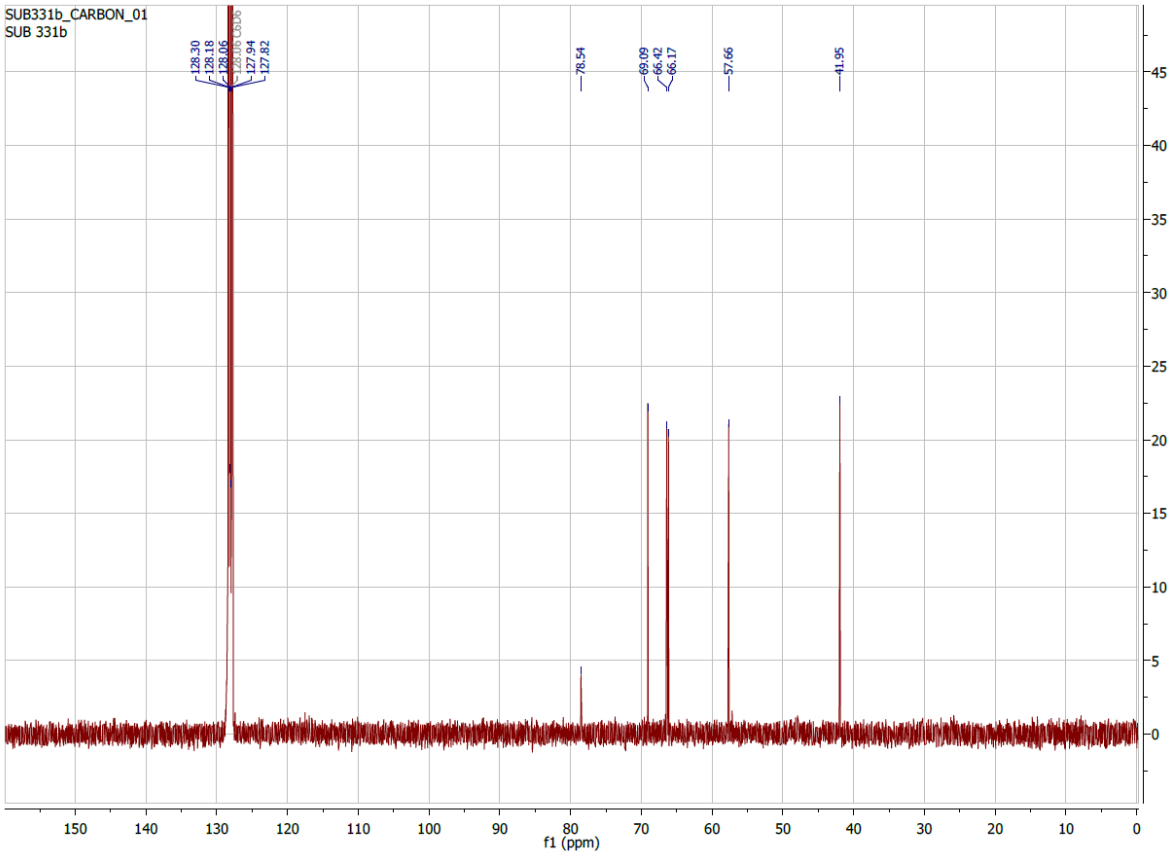


Fig S4. ^{13}C NMR of Fc'(NMe_2)Br (**2**), measured in C_6D_6.

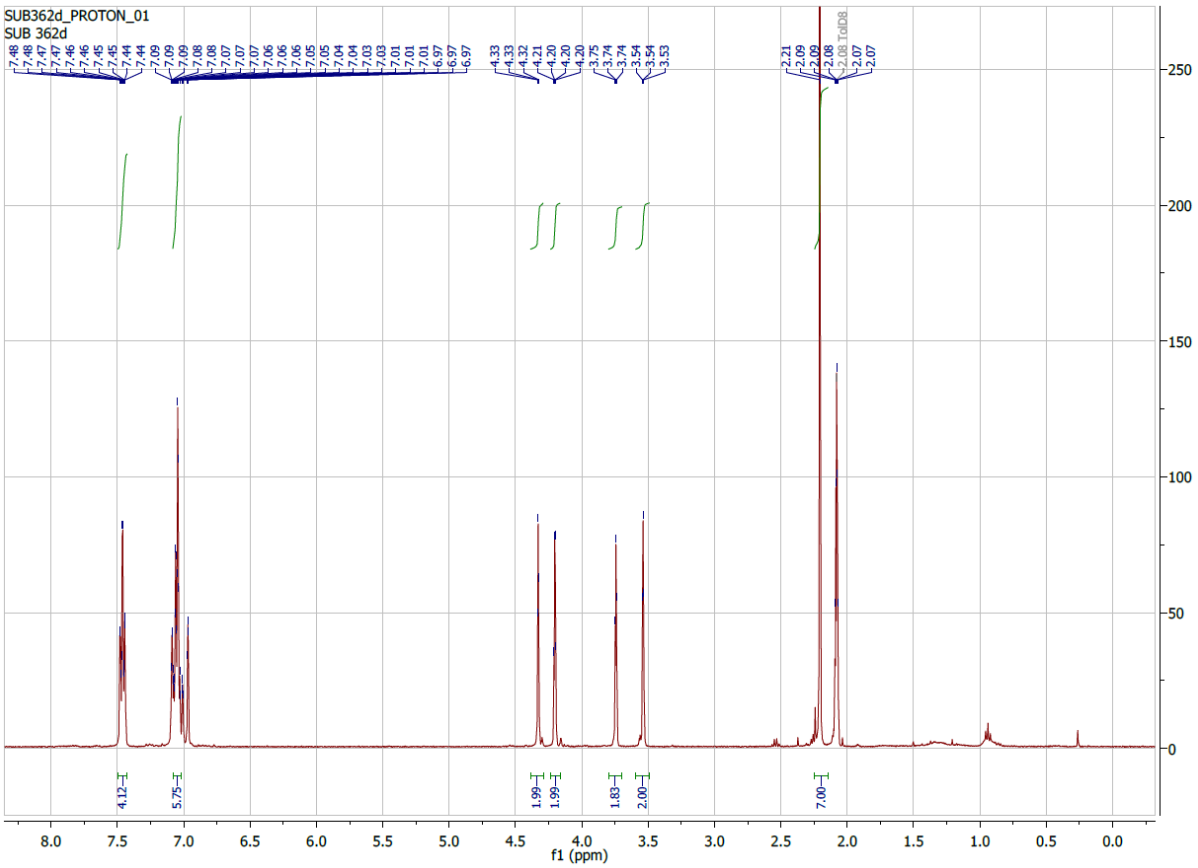


Fig S5. ^{1}H NMR of Fc'(NMe_2)(PPh_2) (**3a**), measured in TolueneD_8.

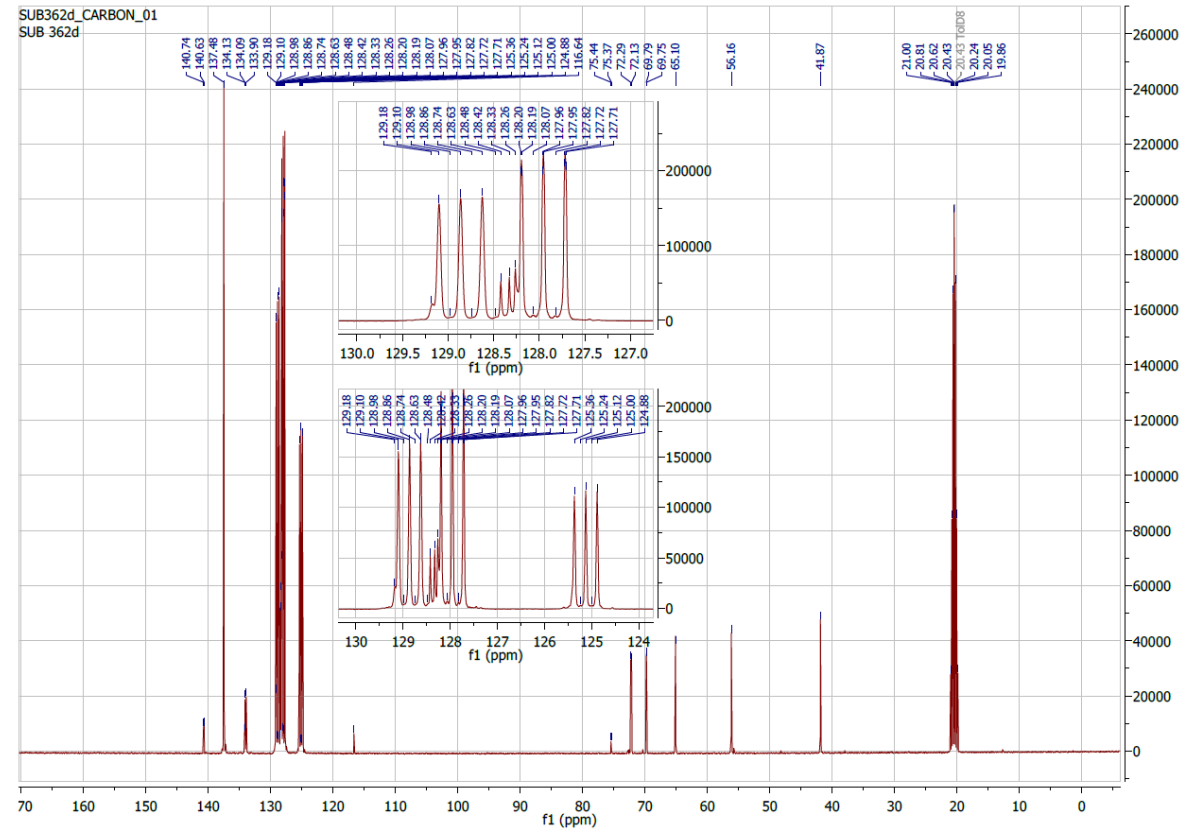


Fig S6. ^{13}C NMR of Fc'(NMe_2)(PPh_2) (**3a**), measured in Toluene D_8.

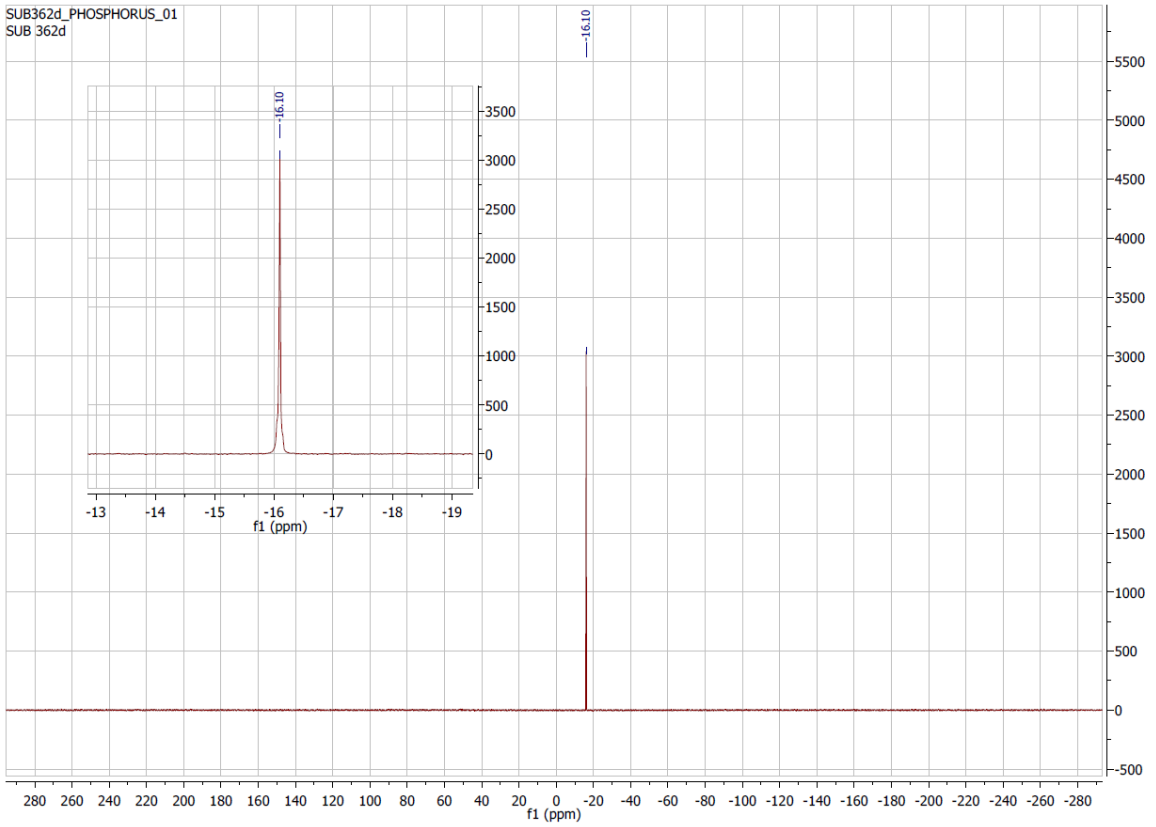


Fig S7. ^{31}P {^{1}H} NMR of Fc'(NMe_2)(PPh_2) (**3a**), measured in Toluene D_8.

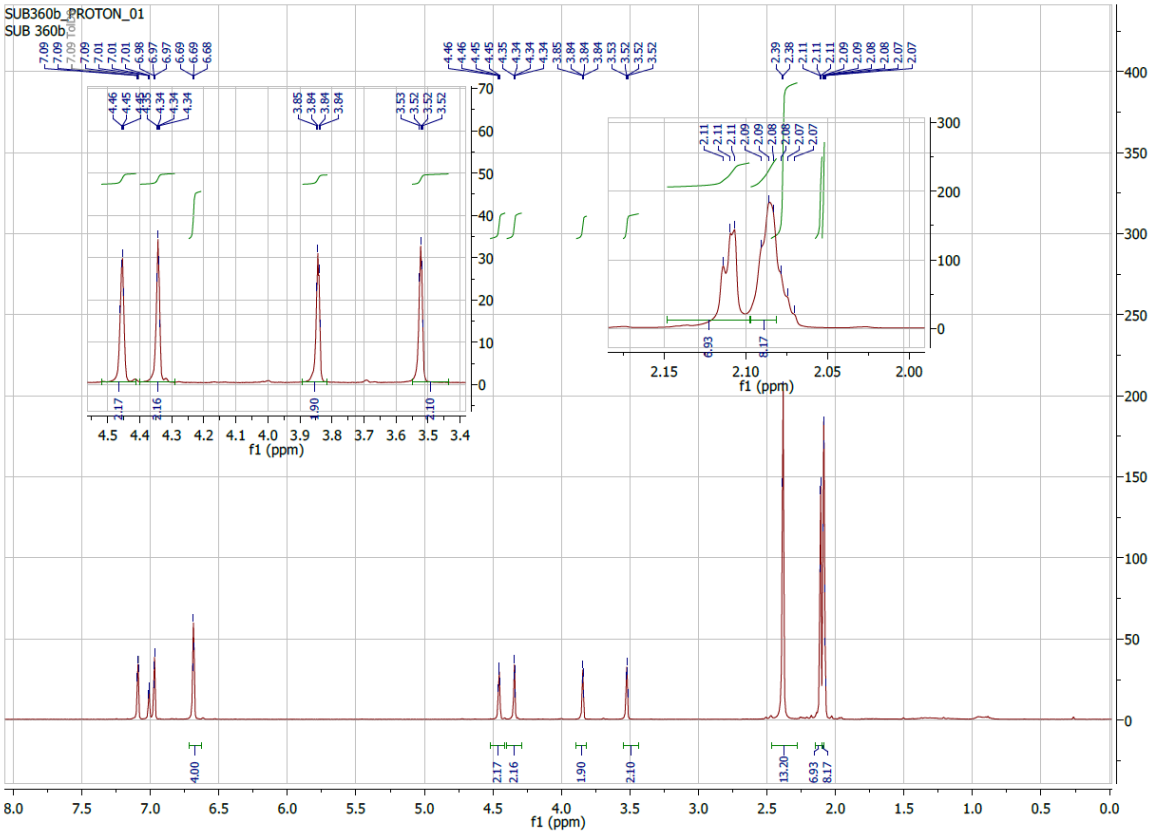


Fig S8. ^{1}H NMR of Fc'(NMe_2)($PMes_2$) (**3b**), measured in Toluene D_8.

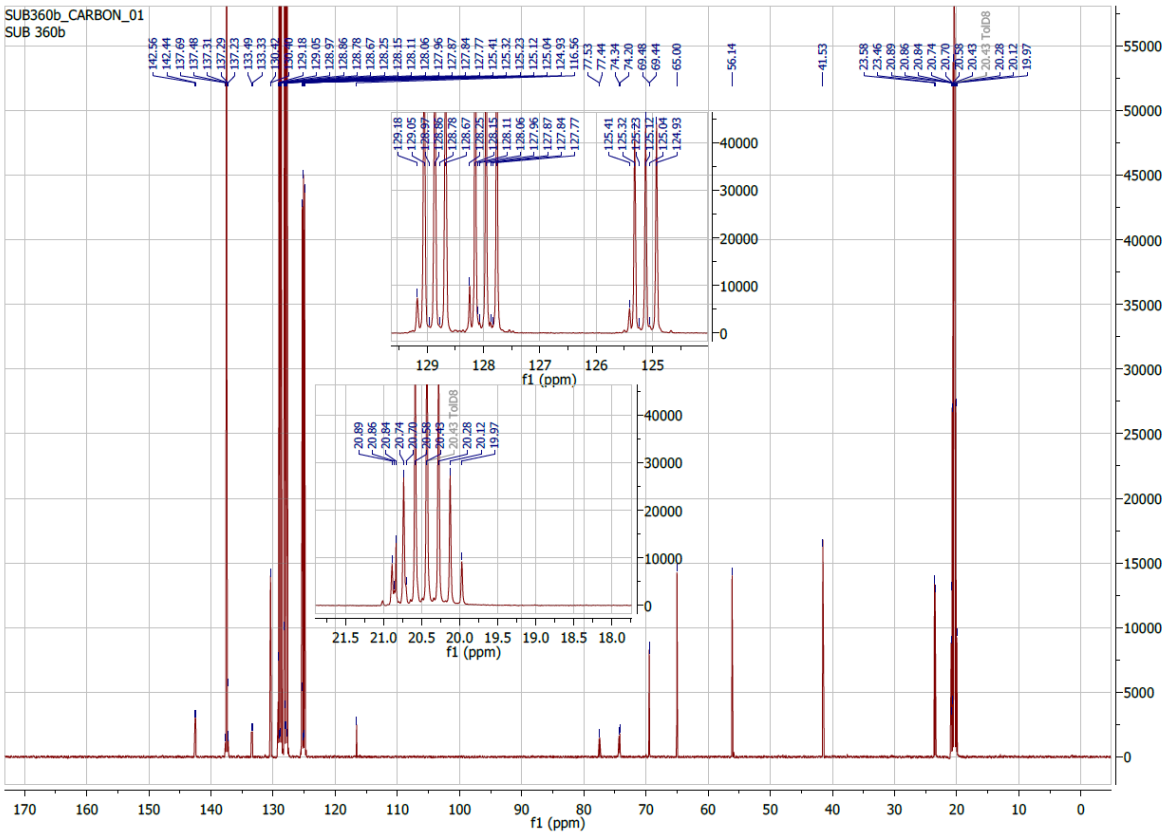


Fig S9. ^{13}C NMR of Fc'(NMe_2)($PMes_2$) (**3b**), measured in Toluene D_8.

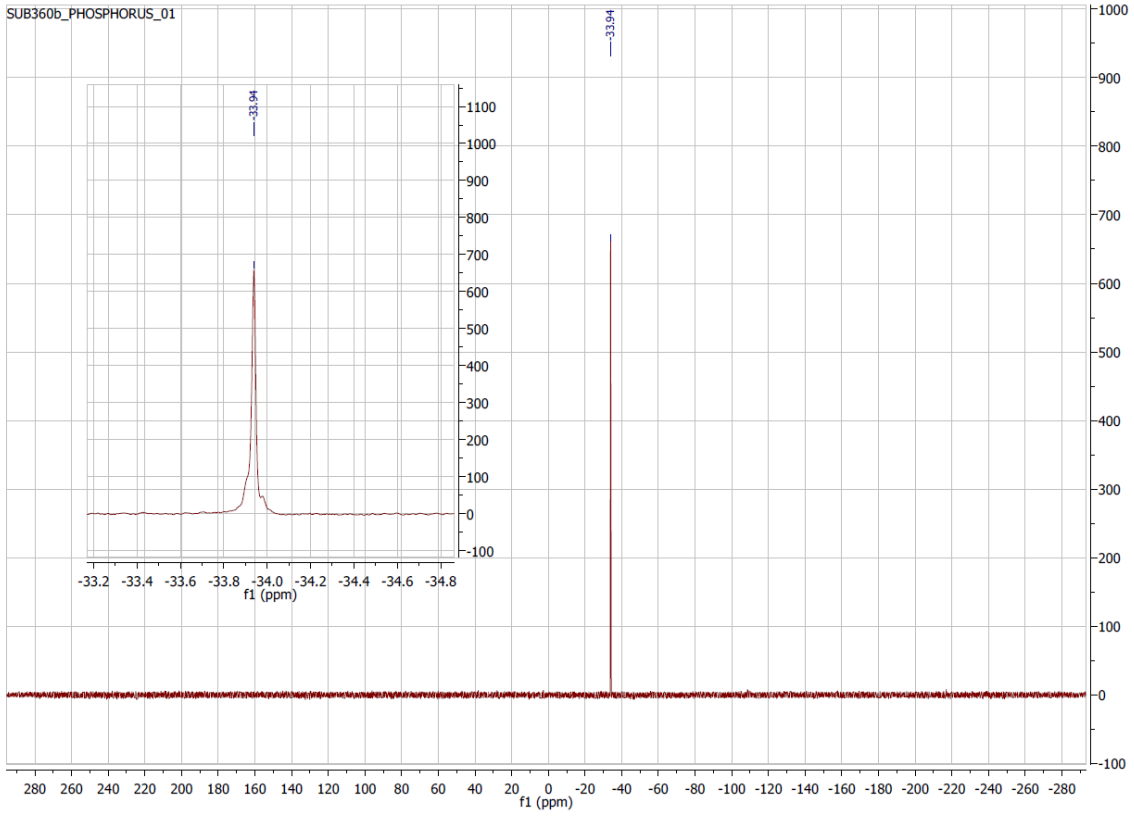


Fig S10. ^{31}P NMR of Fc'(NMe_2)($PMes_2$) (**3b**), measured in Toluene D_8.

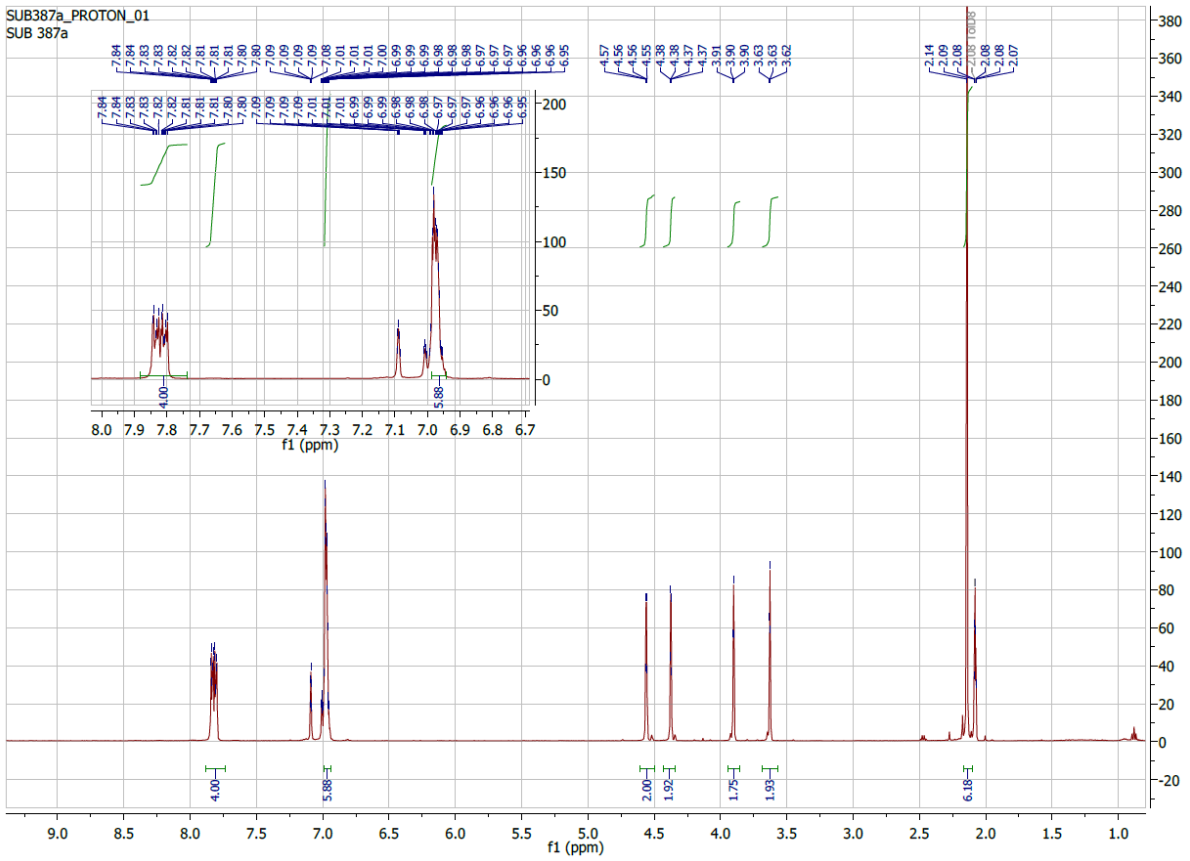


Fig S11. ^{1}H NMR of Fc'(NMe_2)($PSePh_2$) (**4a**), measured in Toluene D_8.

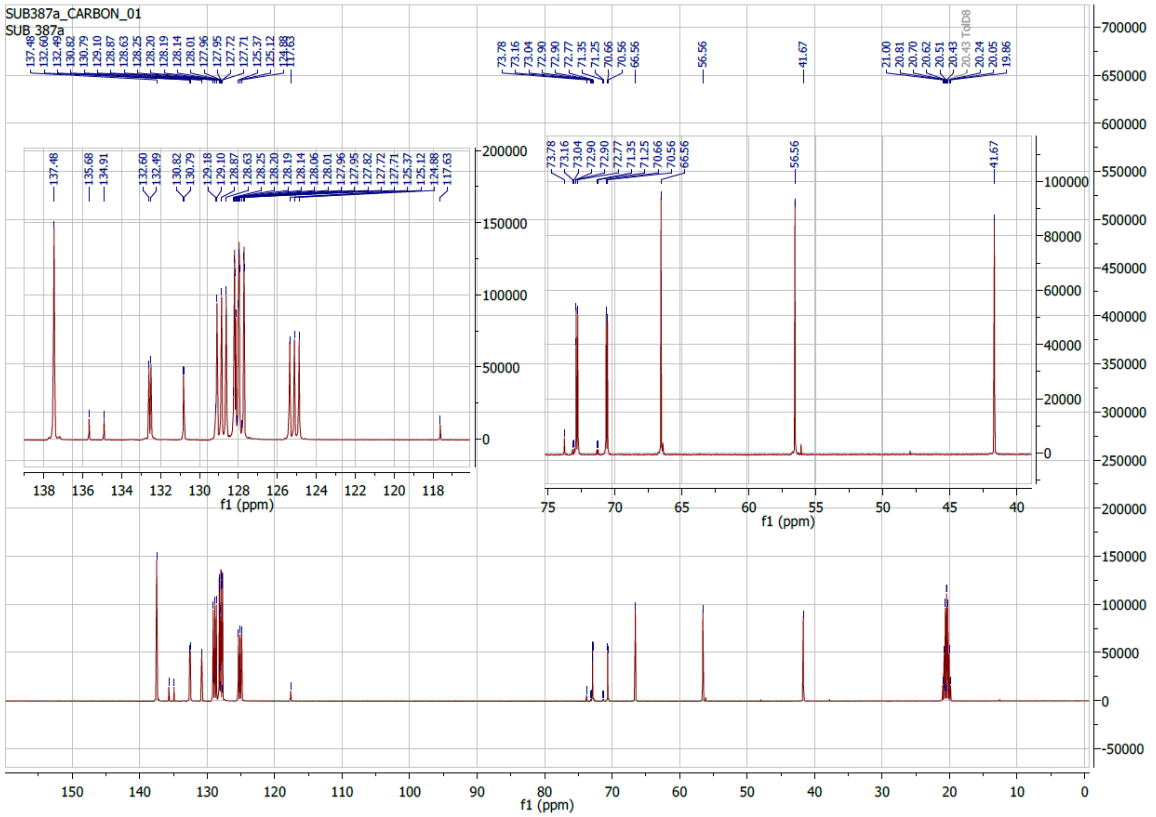


Fig S12. ^{13}C NMR of Fc'(NMe_2)($PSePh_2$) (**4a**), measured in Toluene D_8.

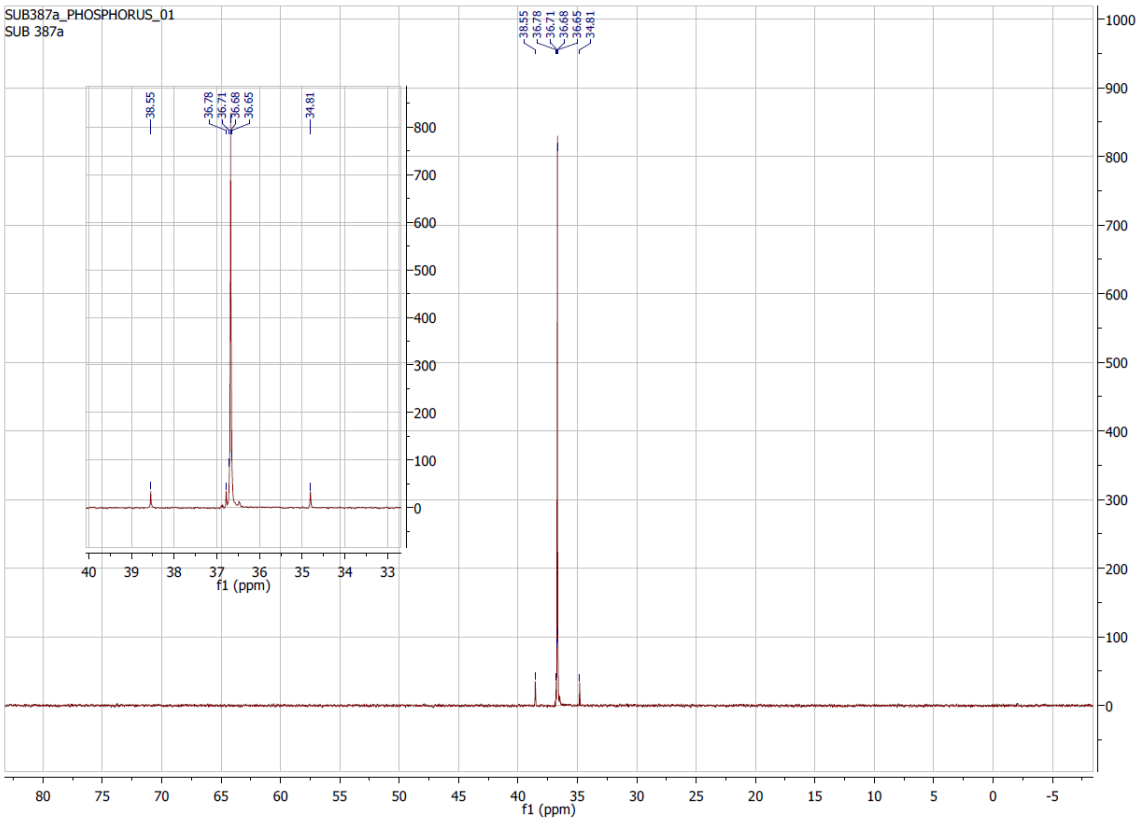


Fig S13. ^{31}P NMR of Fc'(NMe_2)($PSePh_2$) (**4a**), measured in Toluene D_8.

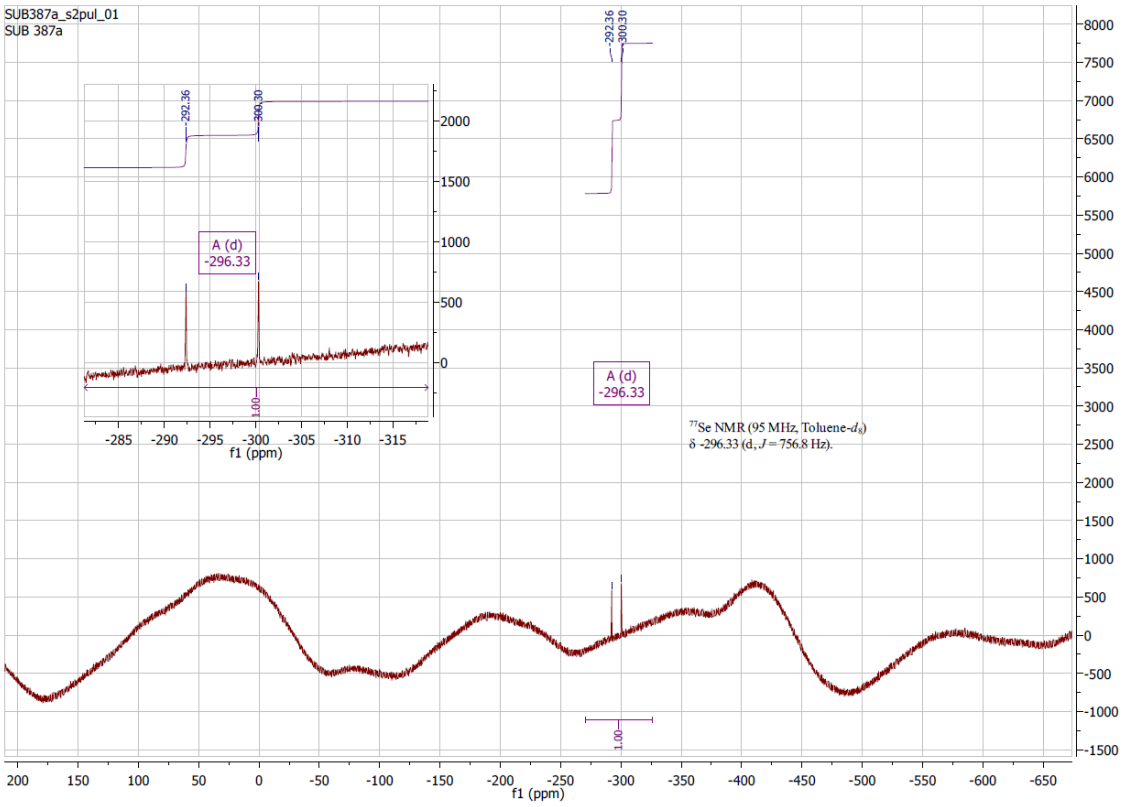


Fig S14. ^{77}Se NMR of Fc'(NMe_2)($PSePh_2$) (**4a**), measured in Toluene D_8.

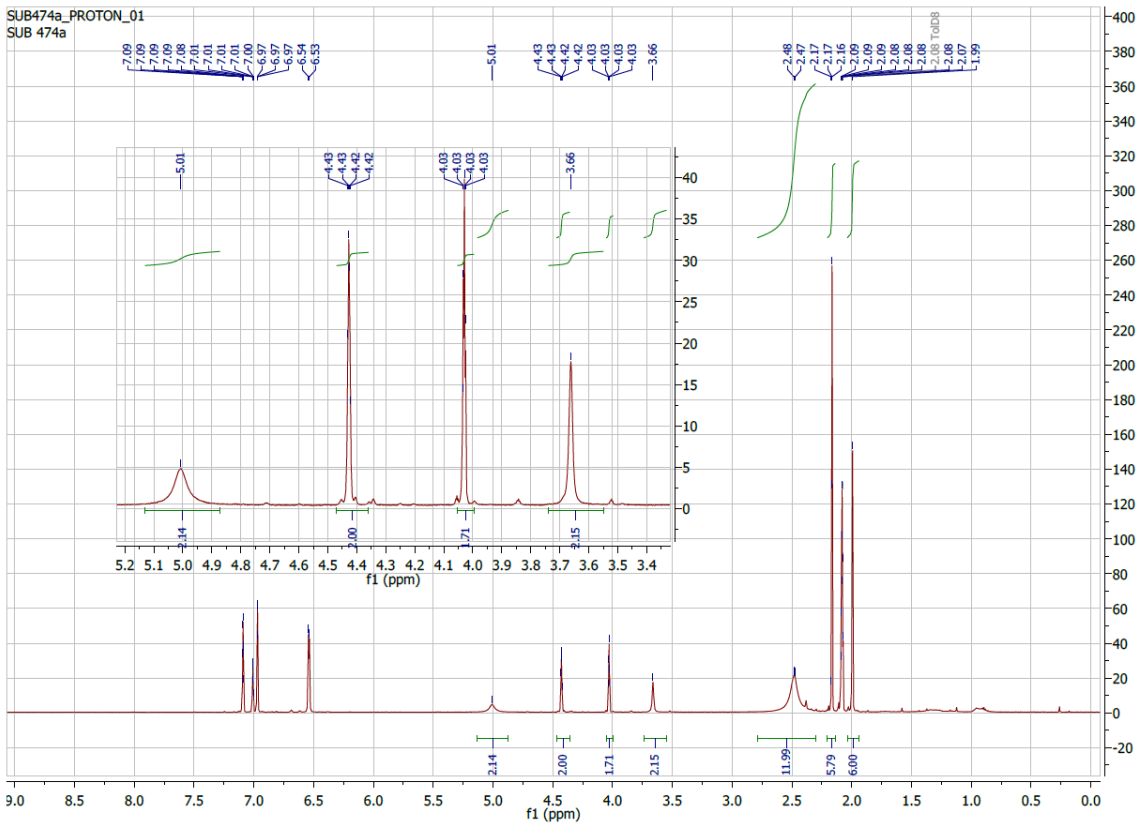


Fig S15. ^{1}H NMR of Fc'(NMe_2)($PSeMes_2$) (**4b**), measured in Toluene D_8.

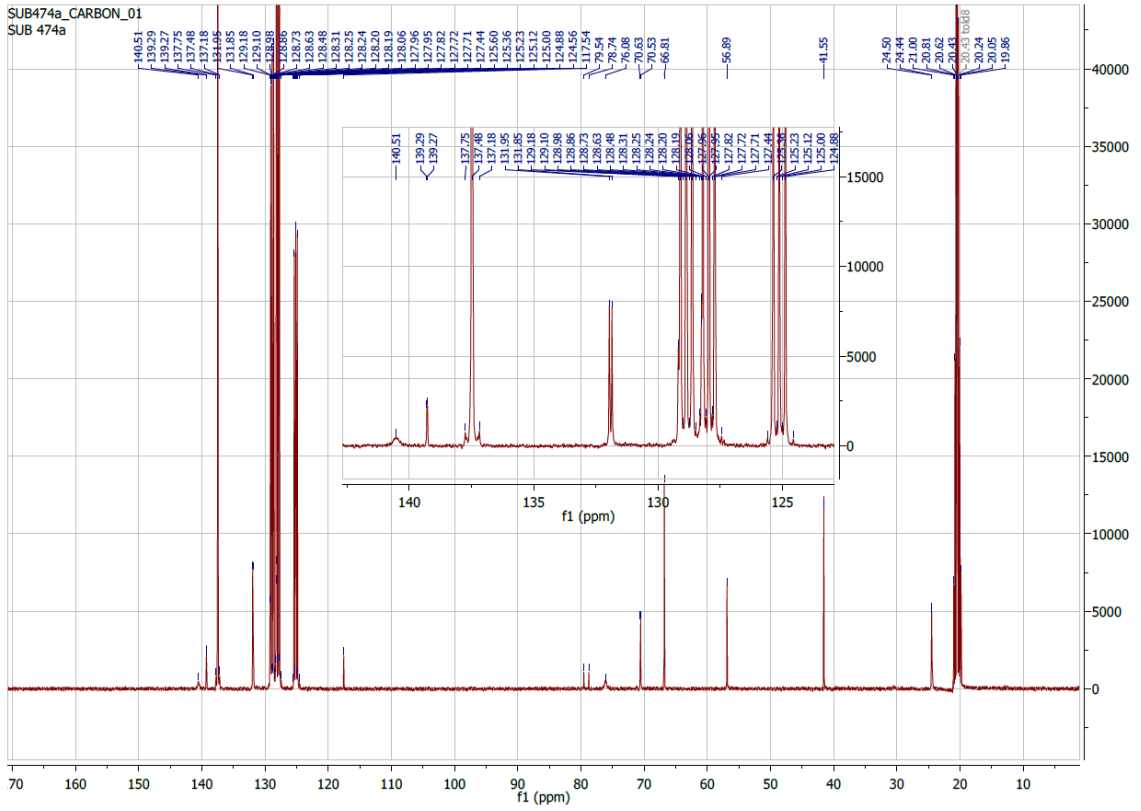


Fig S16. ^{13}C NMR of Fc'(NMe_2)($PSeMes_2$) (**4b**), measured in Toluene D_8.

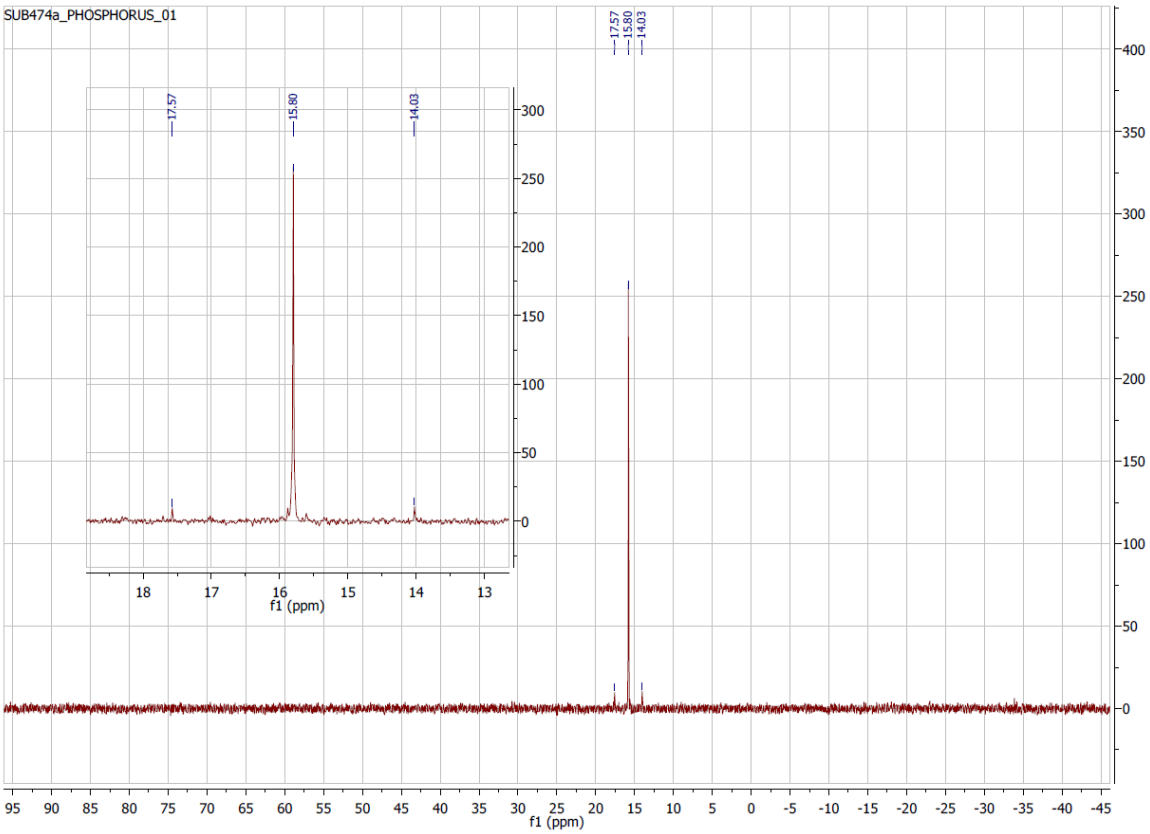


Fig S17. ^{31}P NMR of Fc'(NMe_2)($PSeMes_2$) (**4b**), measured in Toluene D_8.

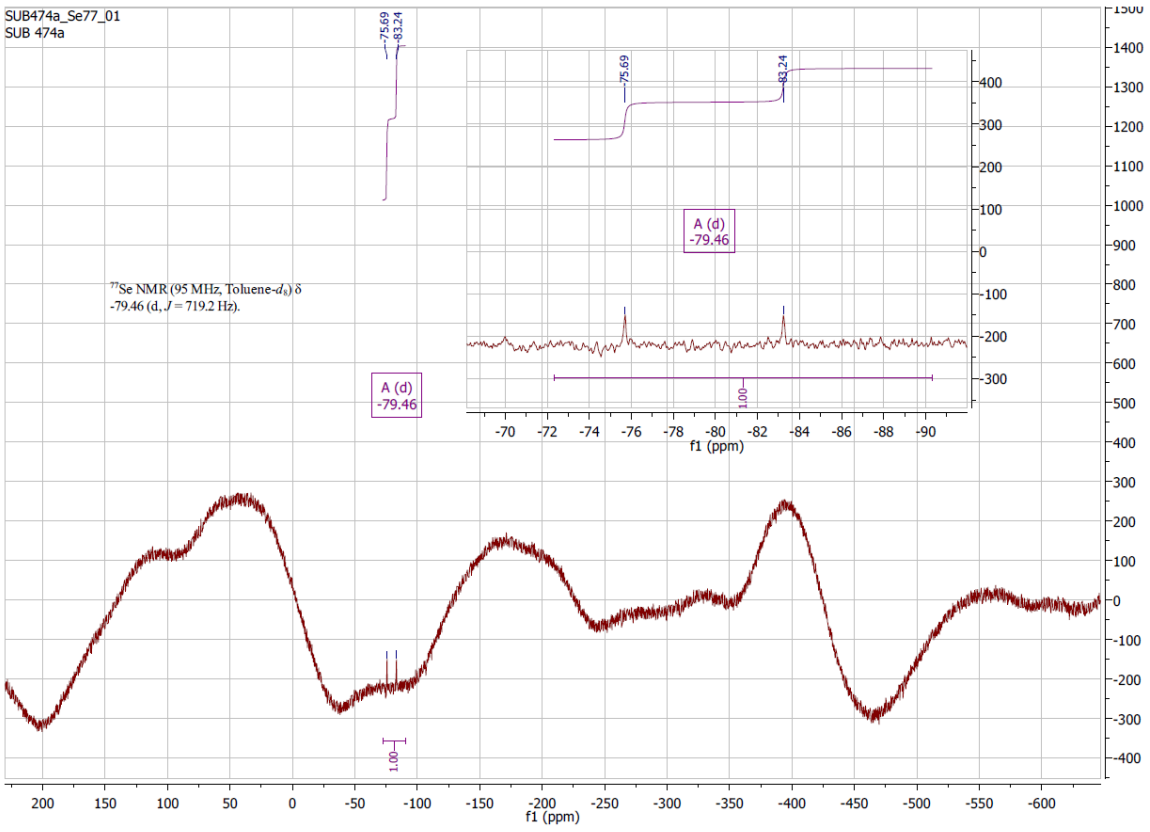


Fig S18. ^{77}Se NMR of Fc'(NMe_2)($PSeMes_2$) (**4b**), measured in Toluene D_8.

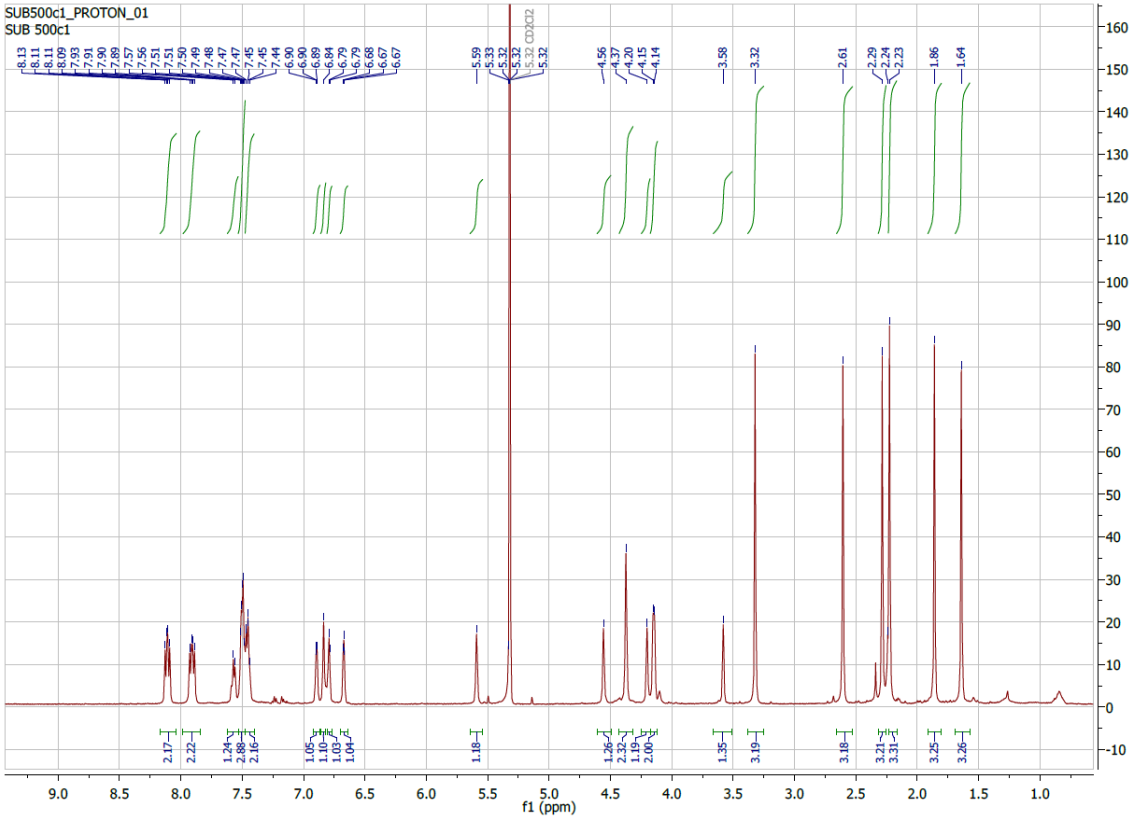


Fig S19. ^{1}H NMR of [Fc'(PMes$_2$)(PPh$_2$)·PdCl$_2$] (**7**), measured in CD_2Cl_2.

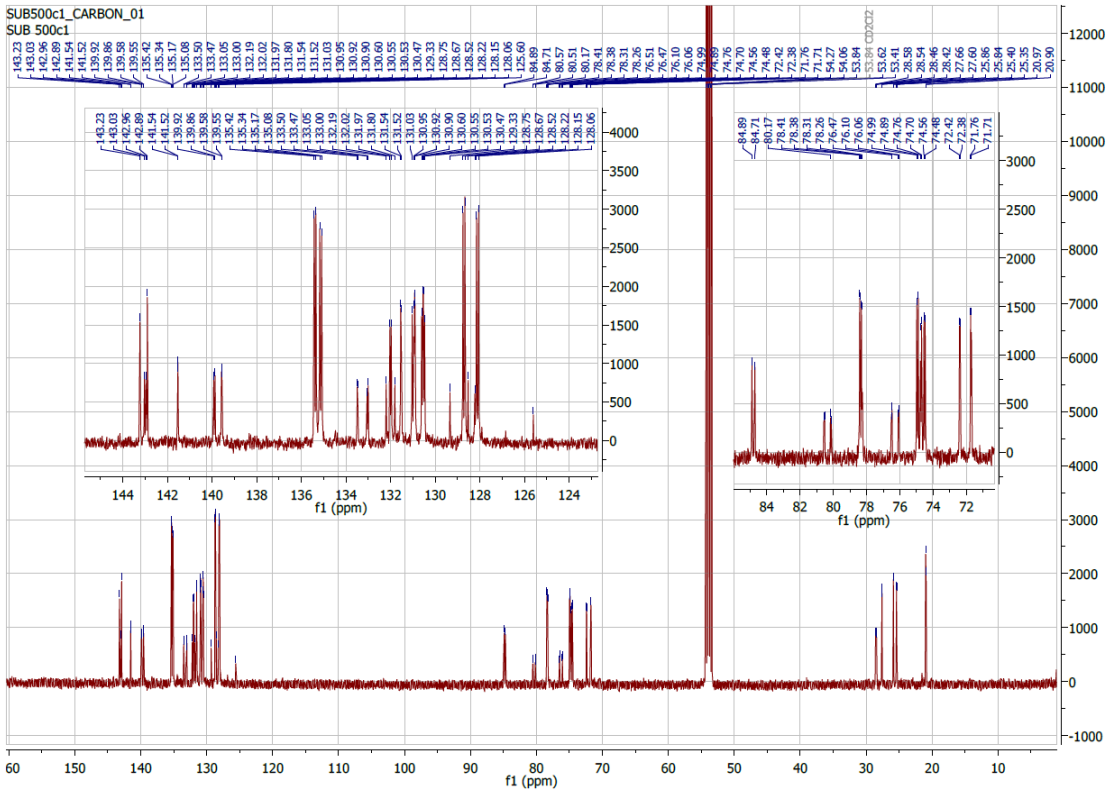


Fig S20. ^{13}C NMR of [Fc'(PMes$_2$)(PPh$_2$)·PdCl$_2$] (**7**), measured in CD_2Cl_2.

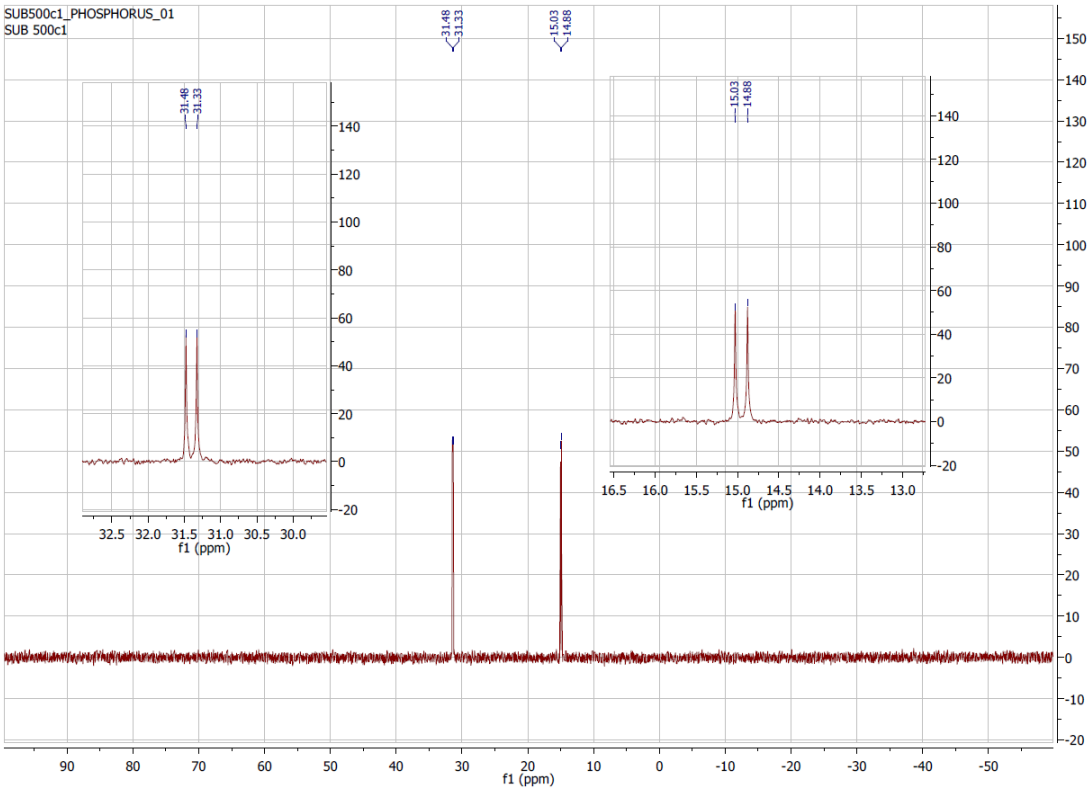


Fig S21. $^{31}P\{^{1}H\}$ NMR of [Fc'($PMes_2$)(PPh_2)·$PdCl_2$] (**7**), measured in CD_2Cl_2.

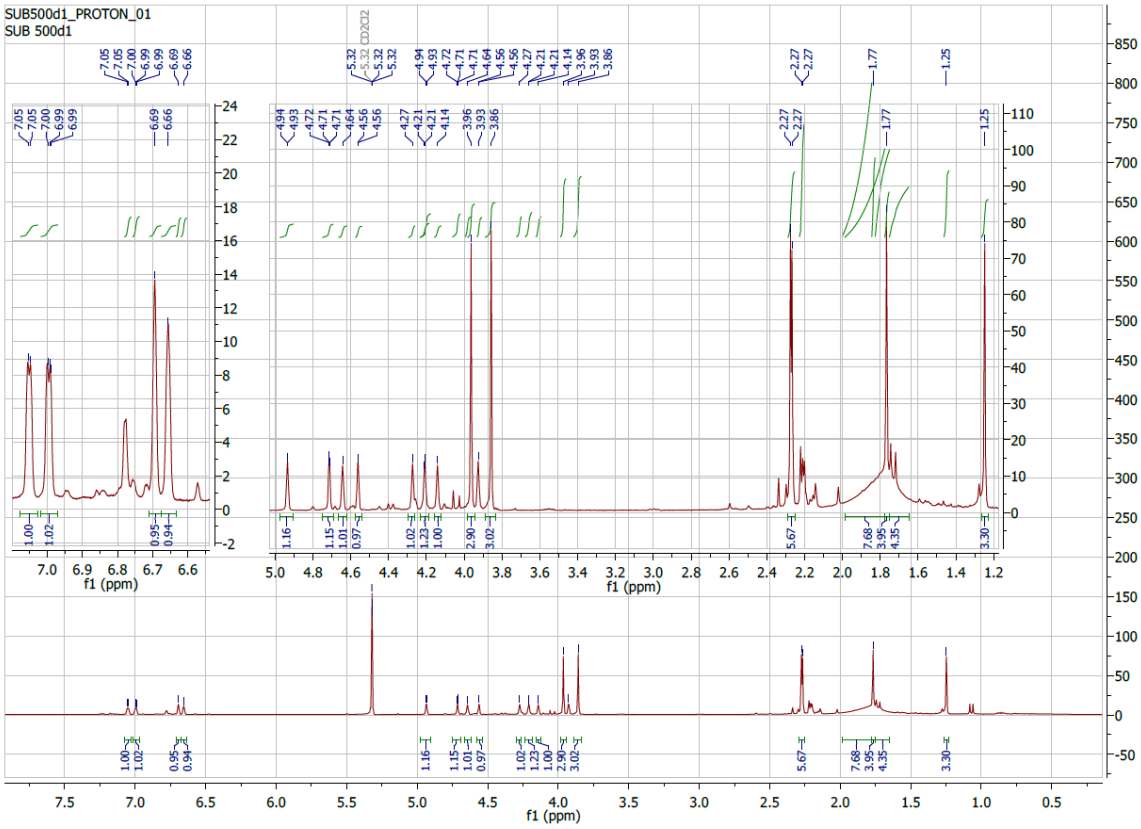


Fig S22. ^{1}H NMR of [Fc'($PMes_2$)(P^tBu_2)·$PdCl_2$] (**8**), measured in CD_2Cl_2.

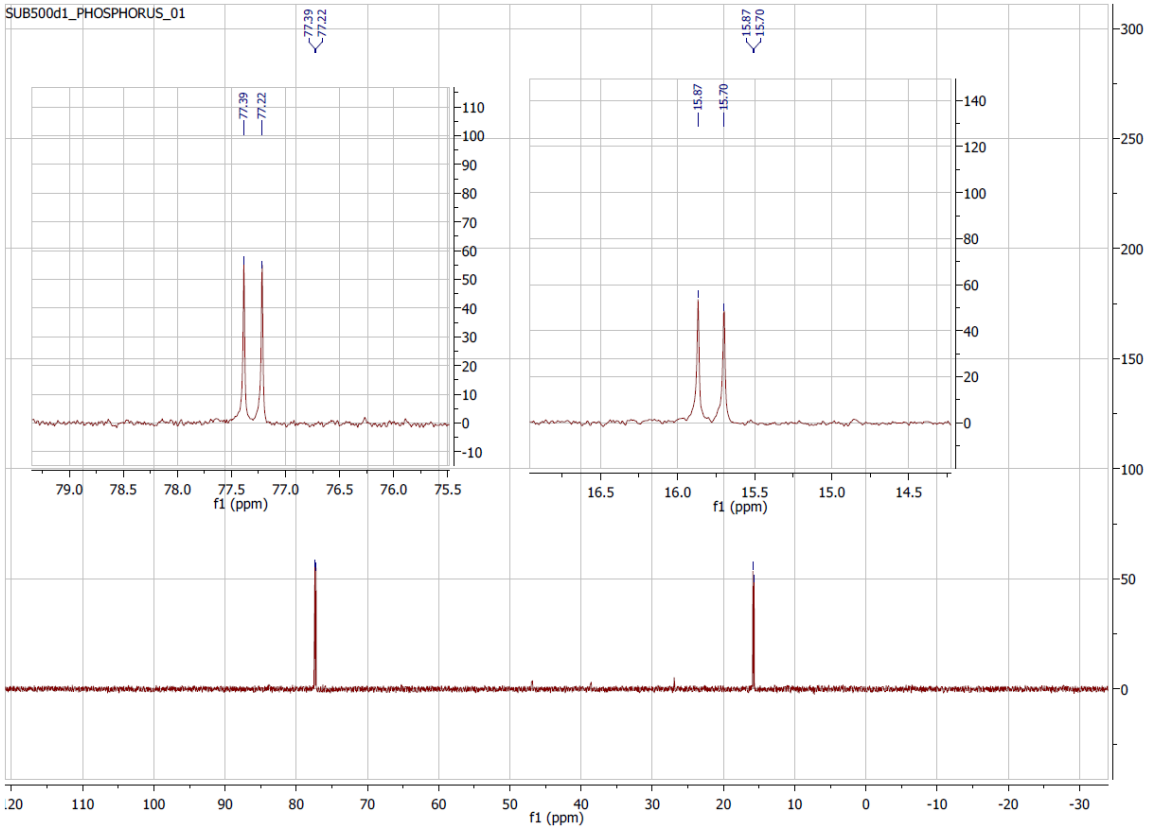


Fig S23. ^{31}P NMR{^{1}H} of [Fc'($PMes_2$)(P^tBu_2)·$PdCl_2$] (**8**), measured in CD_2Cl_2.

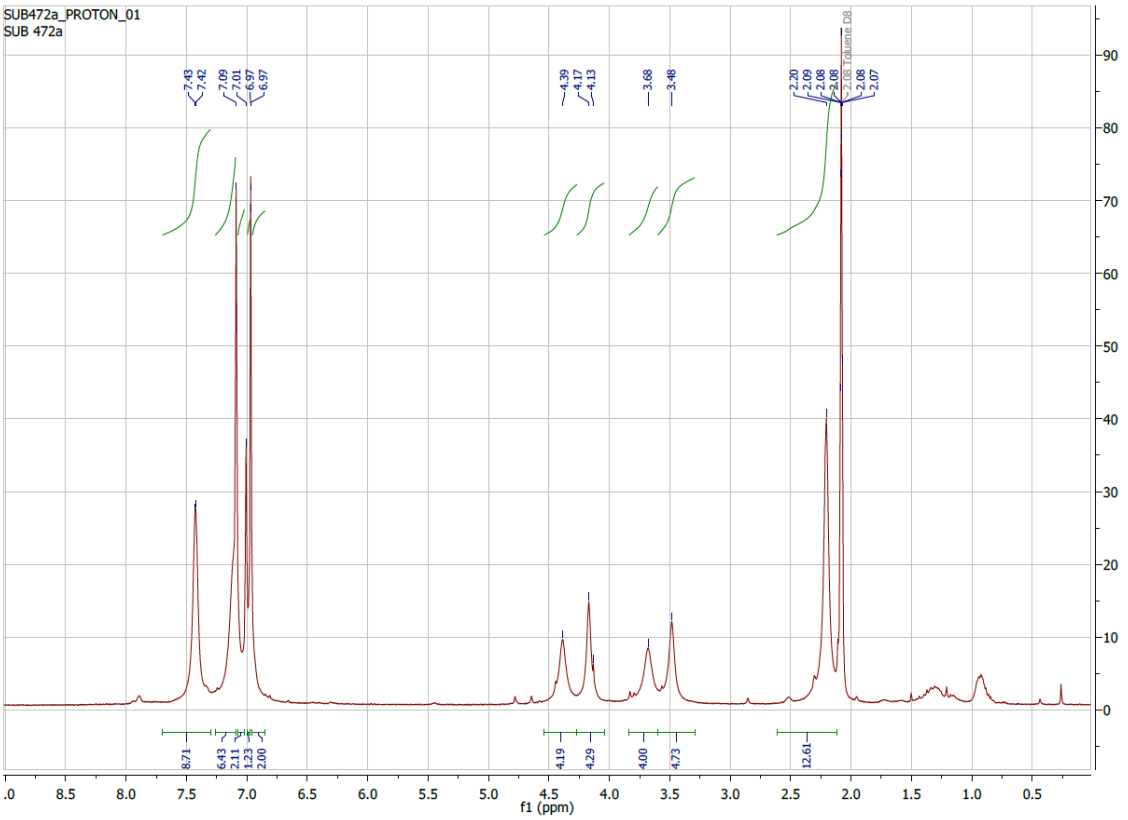


Fig S24. ^{1}H NMR of [Fc'(NMe_2)(PPh_2)·0.5$PdCl_2$] (**9**), measured in Toluene D_8.

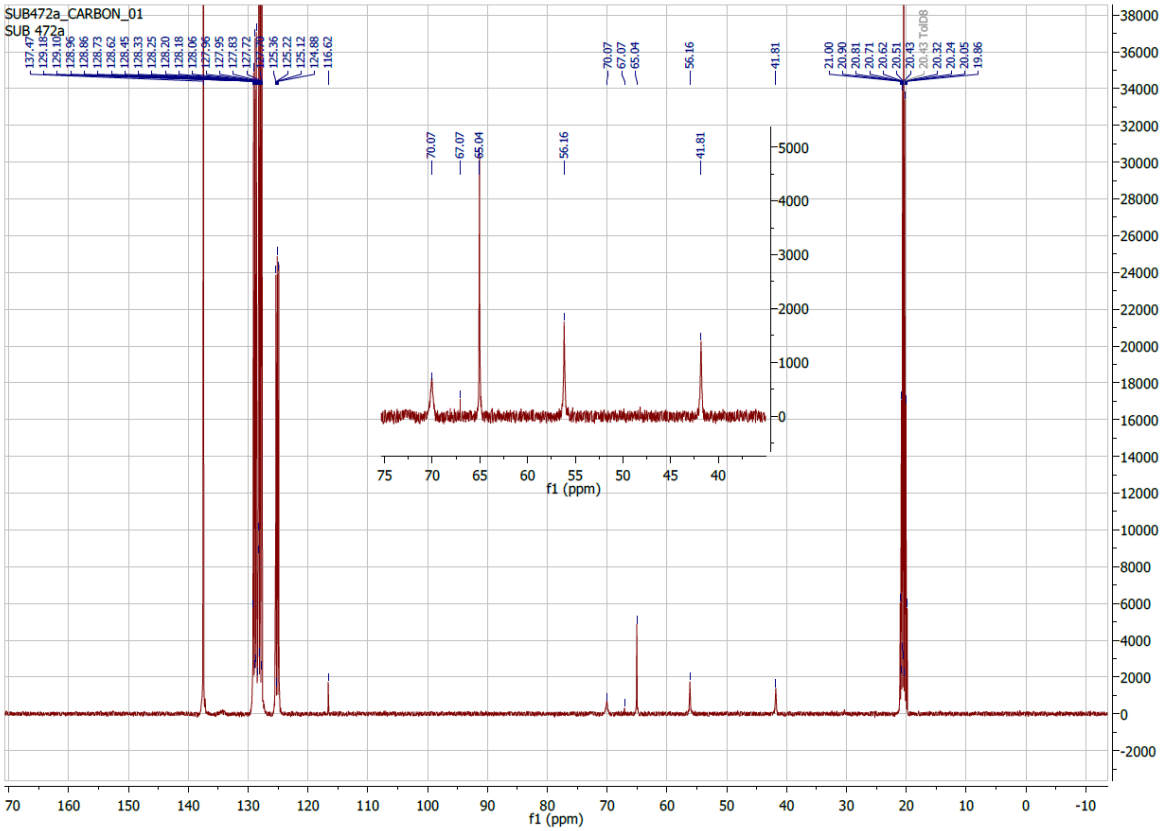


Fig S25. ^{13}C NMR of [Fc'(NMe_2)(PPh_2)·0.5$PdCl_2$] (**9**), measured in Toluene D_8.

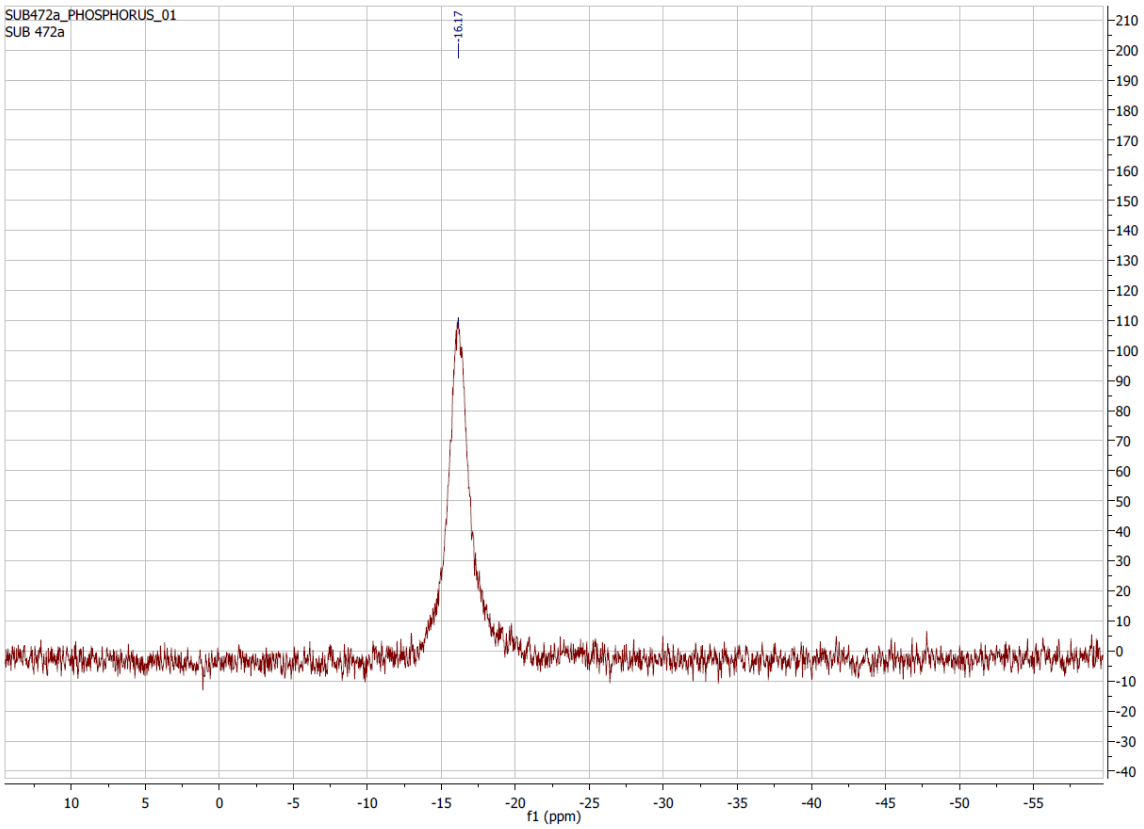


Fig S26. $^{31}P\{^1H\}$ NMR of [Fc'(NMe_2)(PPh_2)·0.5$PdCl_2$] (**9**), measured in Toluene D_8.

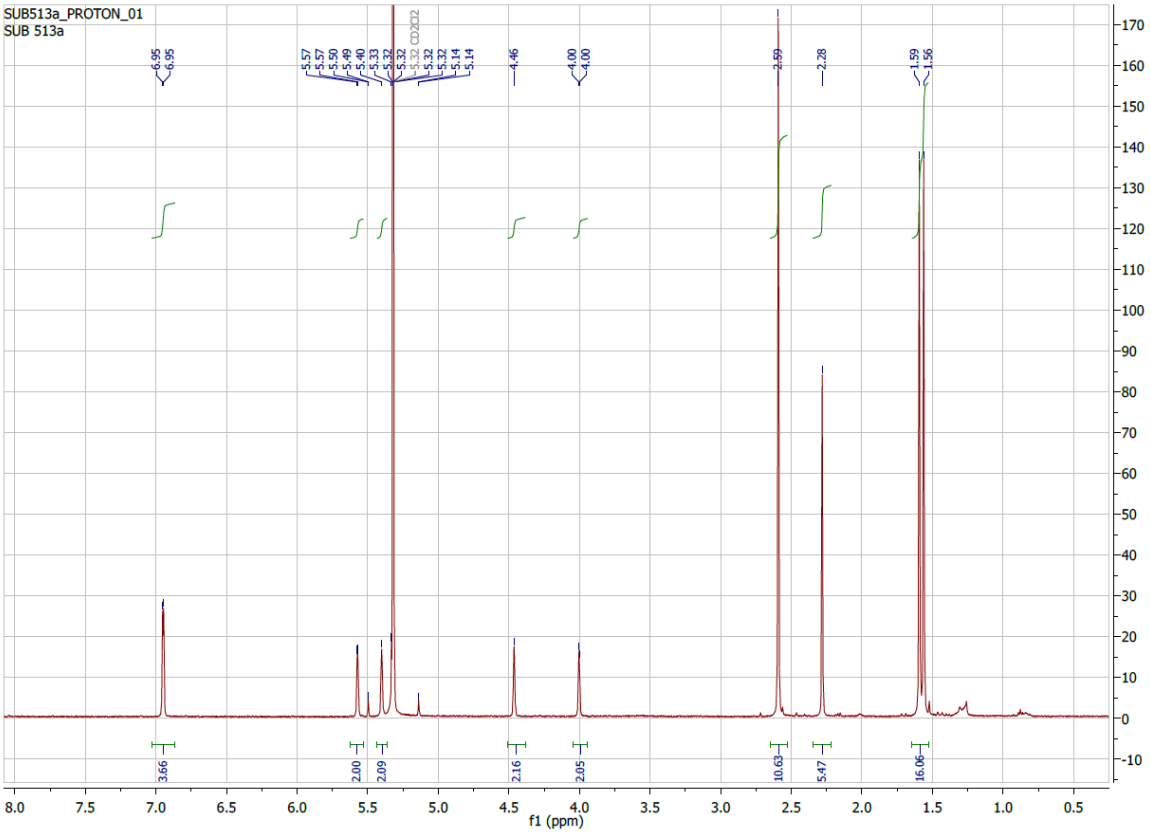


Fig S27. ^{1}H NMR of [Fc'(PMes$_2$)(P^{t}Bu$_2$)·PdCl][SbF$_6$] (**10**), measured in CD_2Cl_2.

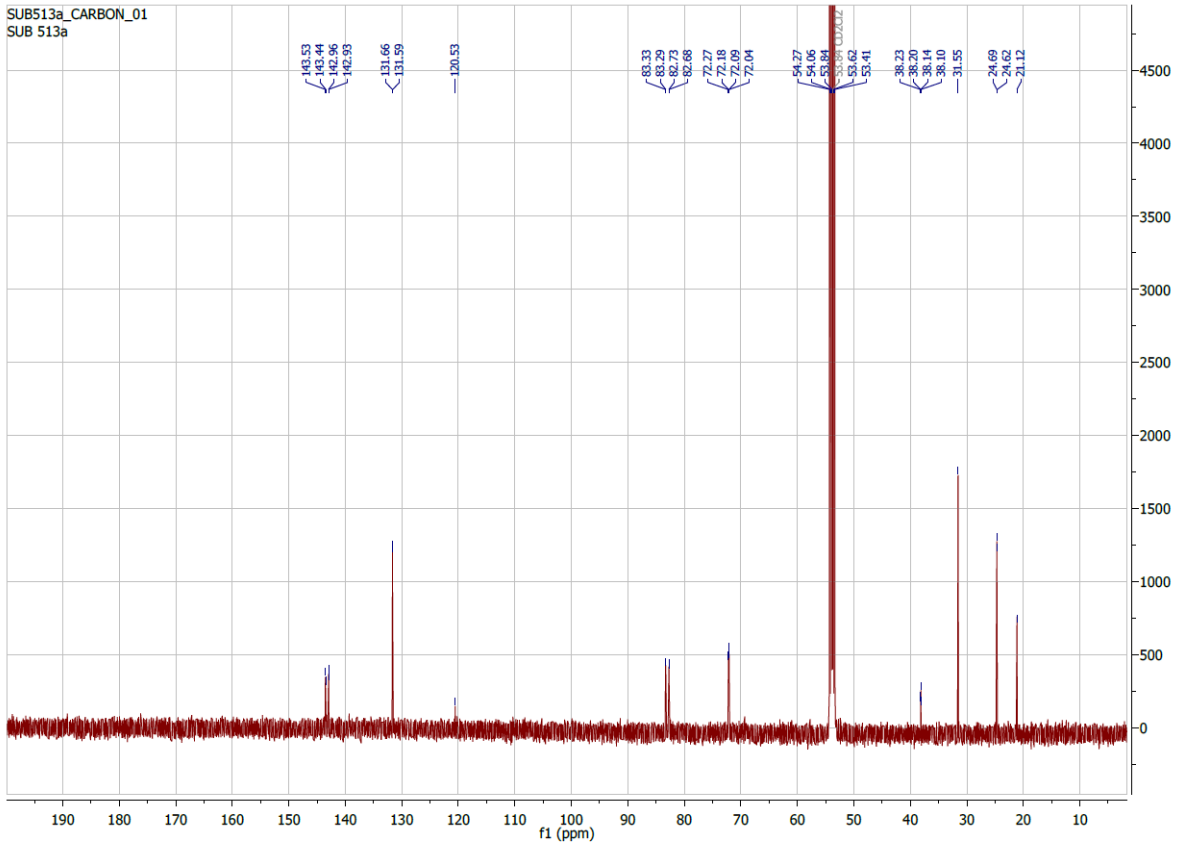


Fig S28. ^{13}C NMR of [Fc'(PMes$_2$)(P^{t}Bu$_2$)·PdCl][SbF$_6$] (**10**), measured in CD_2Cl_2.

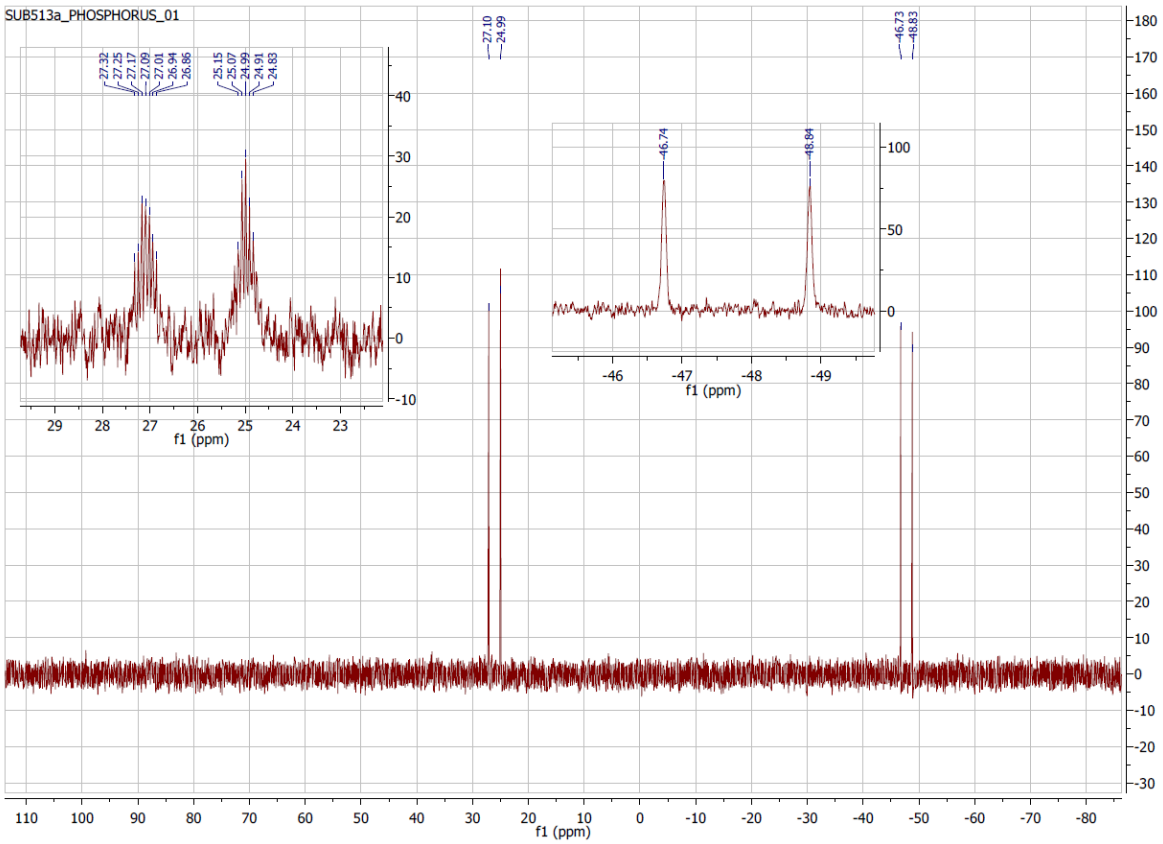


Fig S29. $^{31}P\{^{1}H\}$ NMR of Fc'($PMes_2$)(P^tBu_2)[PdCl][SbF_6] (**10**), measured in CD_2Cl_2. Corresponding peaks in ^{1}H coupled ^{31}P NMR are shown in insets.

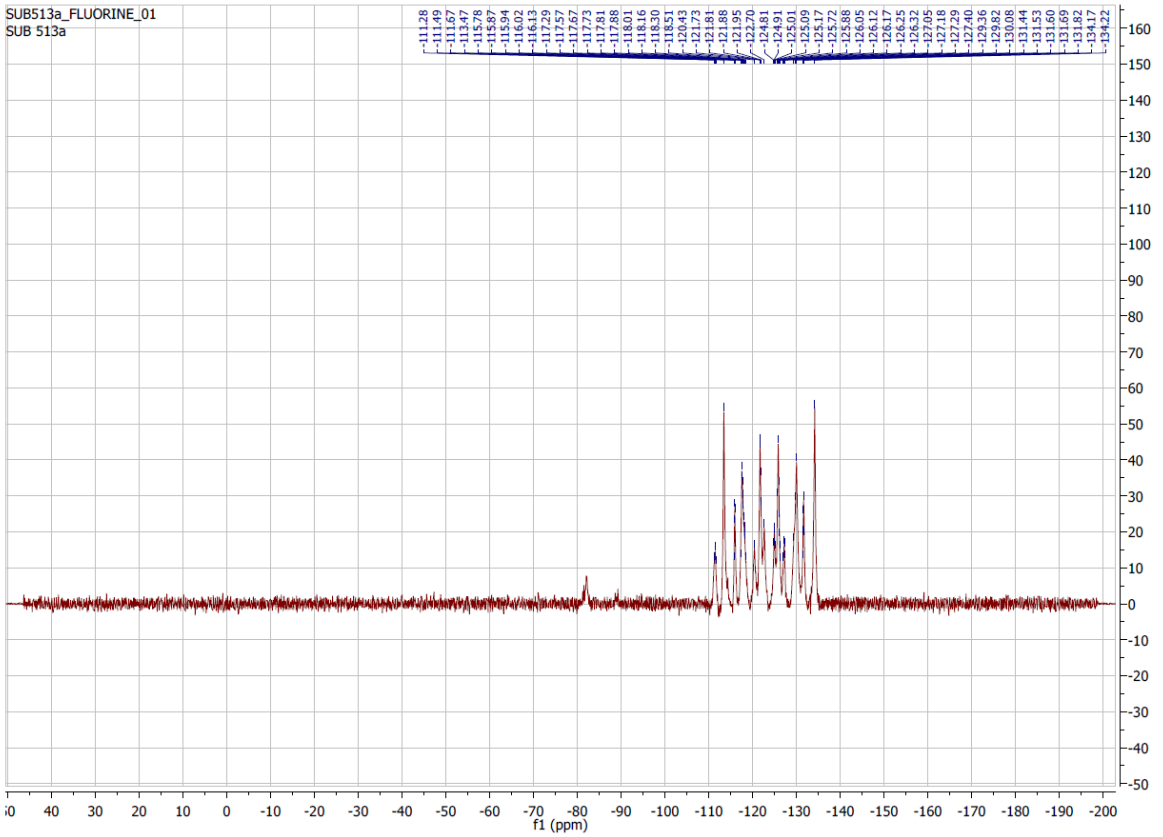


Fig S30. ^{19}F NMR of [Fc'($PMes_2$)(P^tBu_2)·PdCl][SbF_6] (**10**), measured in CD_2Cl_2.

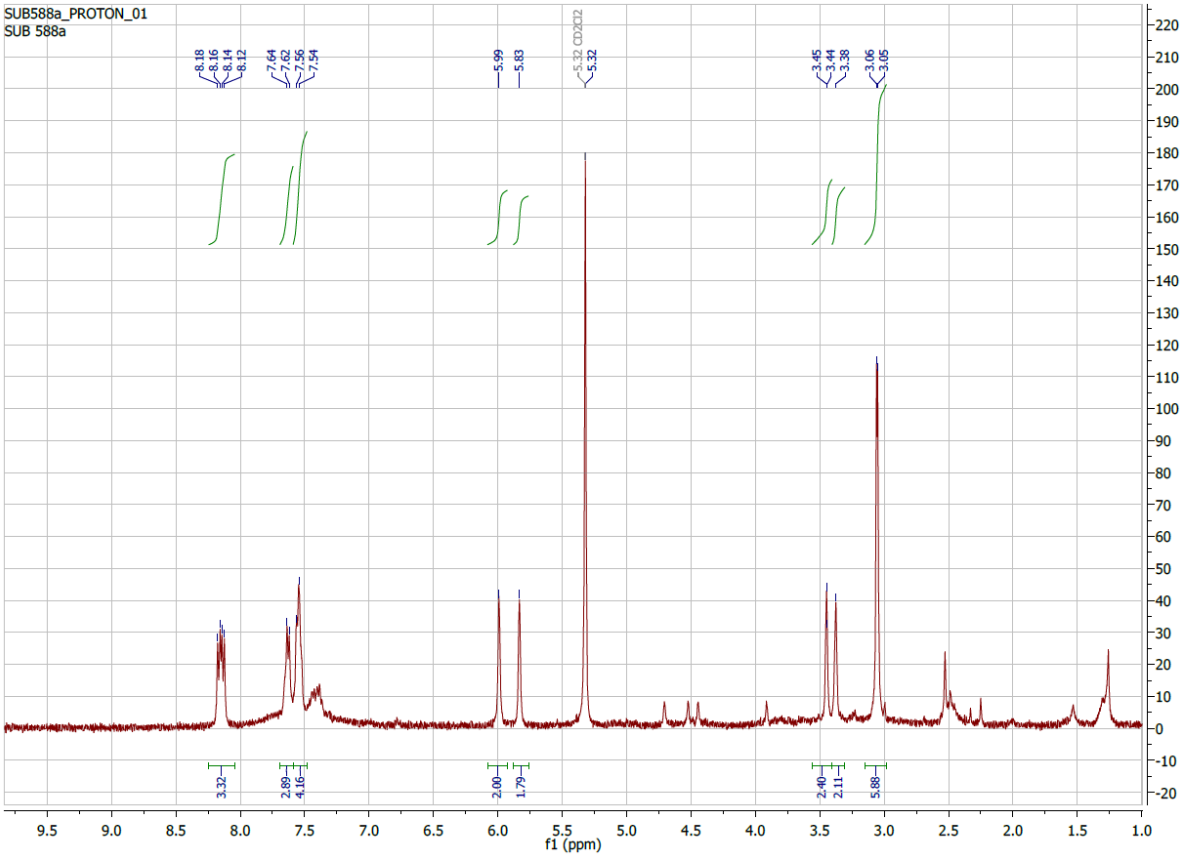


Fig S31. ^{1}H NMR of [Fc'(NMe$_2$)(PPh$_2$)·PdCl][SbF$_6$]$_2$ (**11**), measured in CD_2Cl_2.
Compound **11** contains impurities which could not be removed after several recrystallization attempts.

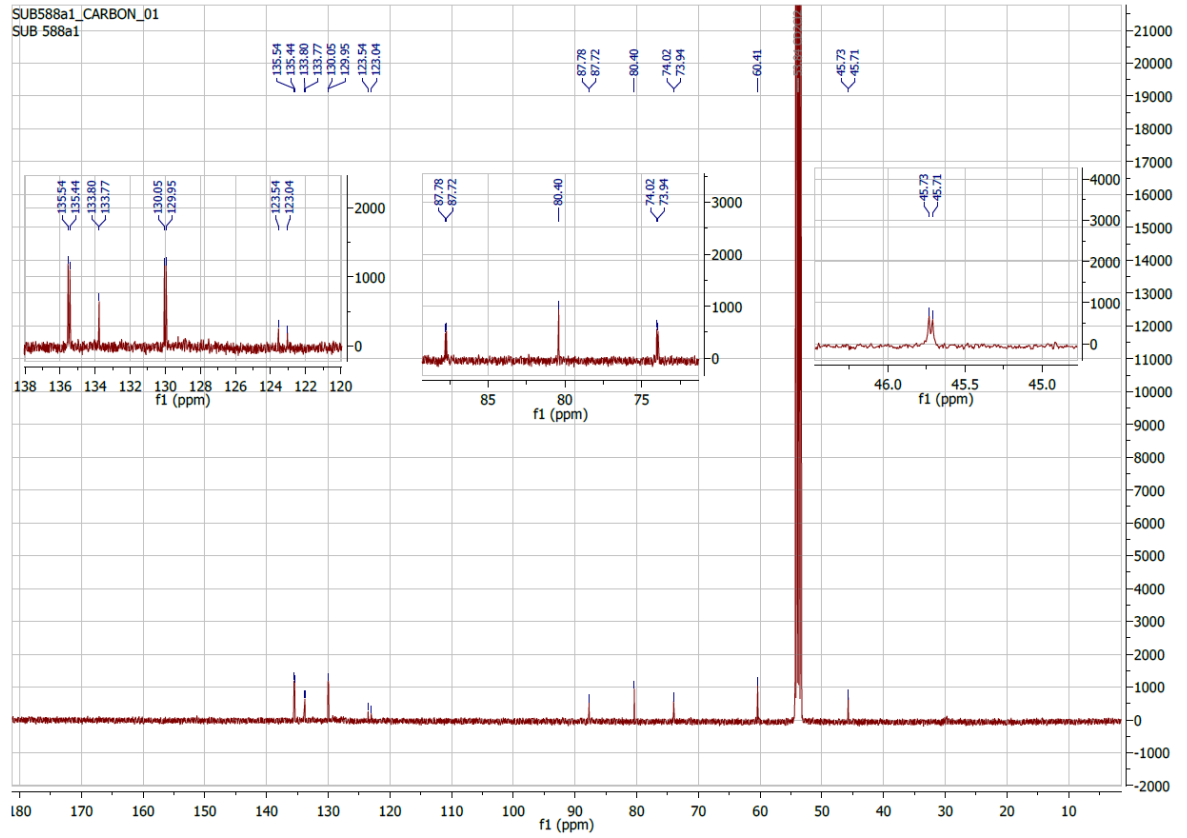


Fig S32. ^{13}C NMR of [Fc'(NMe$_2$)(PPh$_2$)·PdCl][SbF$_6$]$_2$ (**11**), measured in CD_2Cl_2.

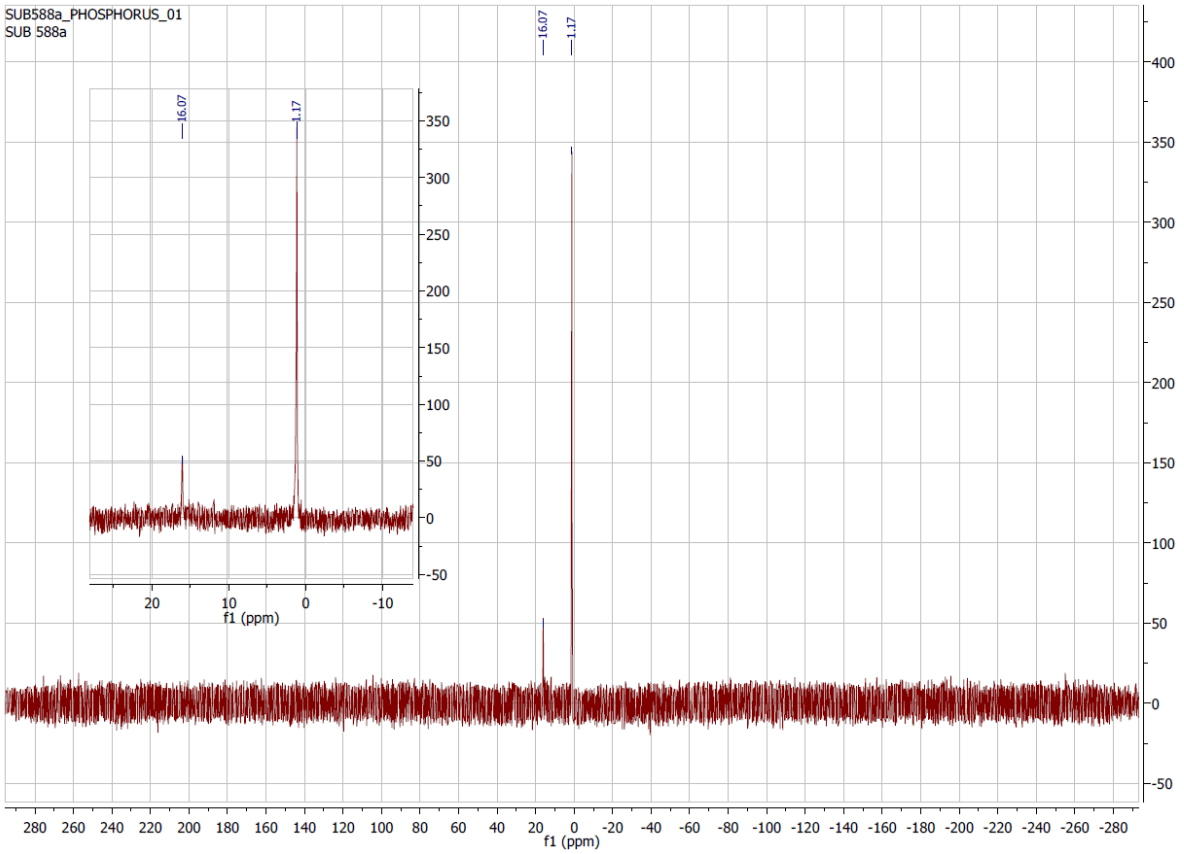


Fig S33. $^{31}P\{^{1}H\}$ NMR of [Fc'(NMe_2)(PPh_2)·PdCl][SbF_6]$_2$ (**11**), measured in CD_2Cl_2.

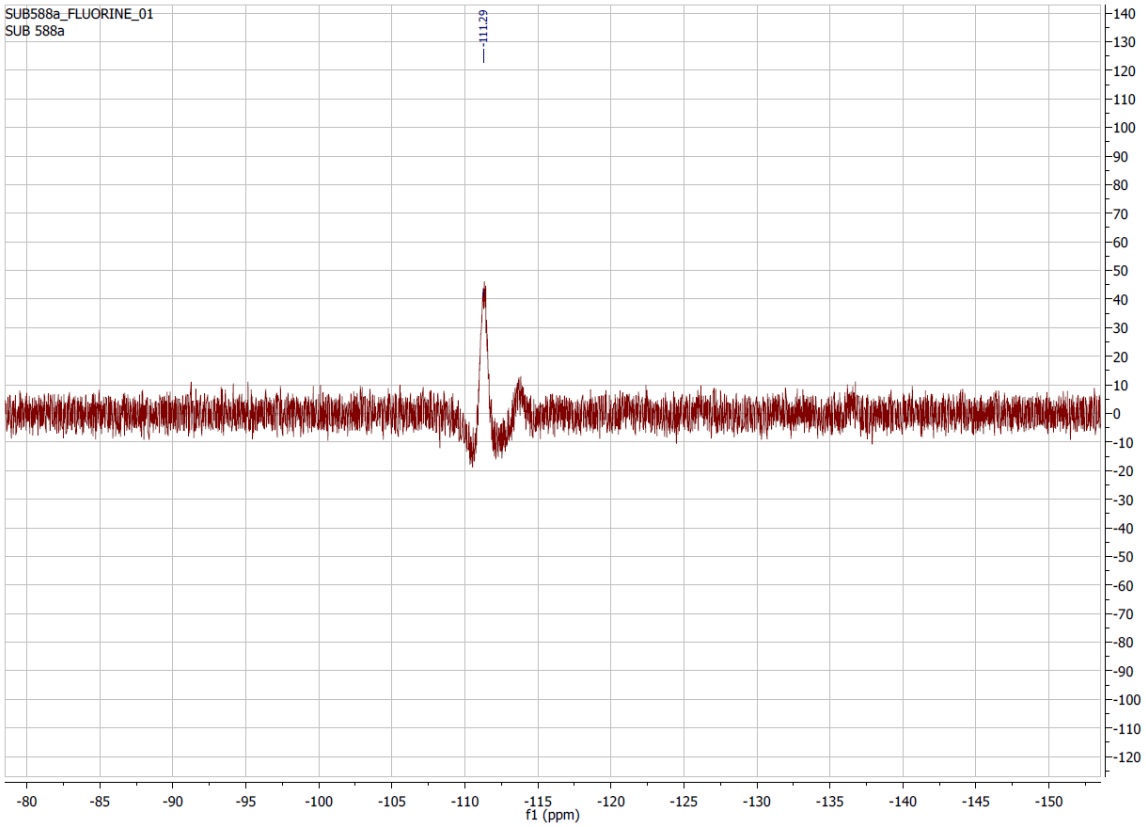


Fig S34. ^{19}F NMR of [Fc'(NMe_2)(PPh_2)·PdCl][SbF_6]$_2$ (**11**), measured in CD_2Cl_2.

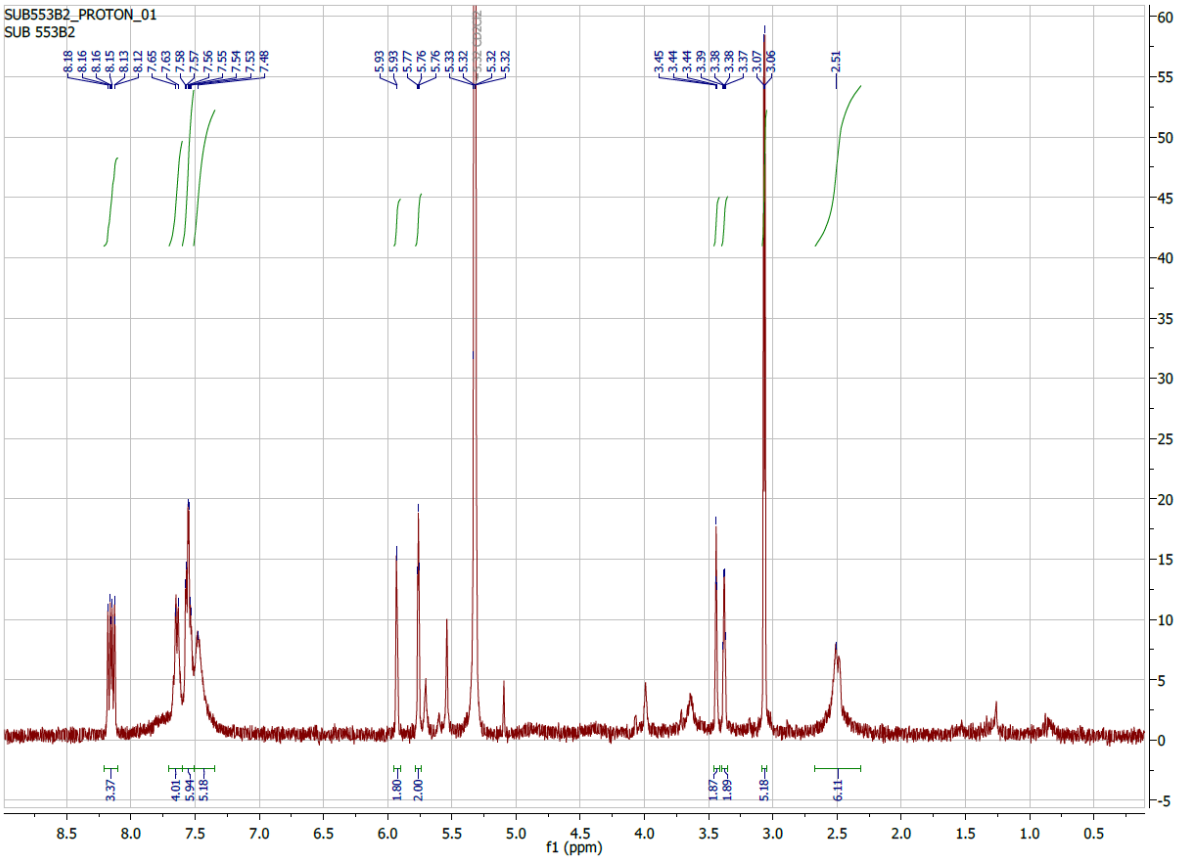


Fig S35. ^{1}H NMR of [Fc'(NMe$_2$)(PPh$_2$)·PdPPh$_2$(C$_5$H$_5$)][SbF$_6$]$_2$ (**12**), measured in CD$_2$Cl$_2$.

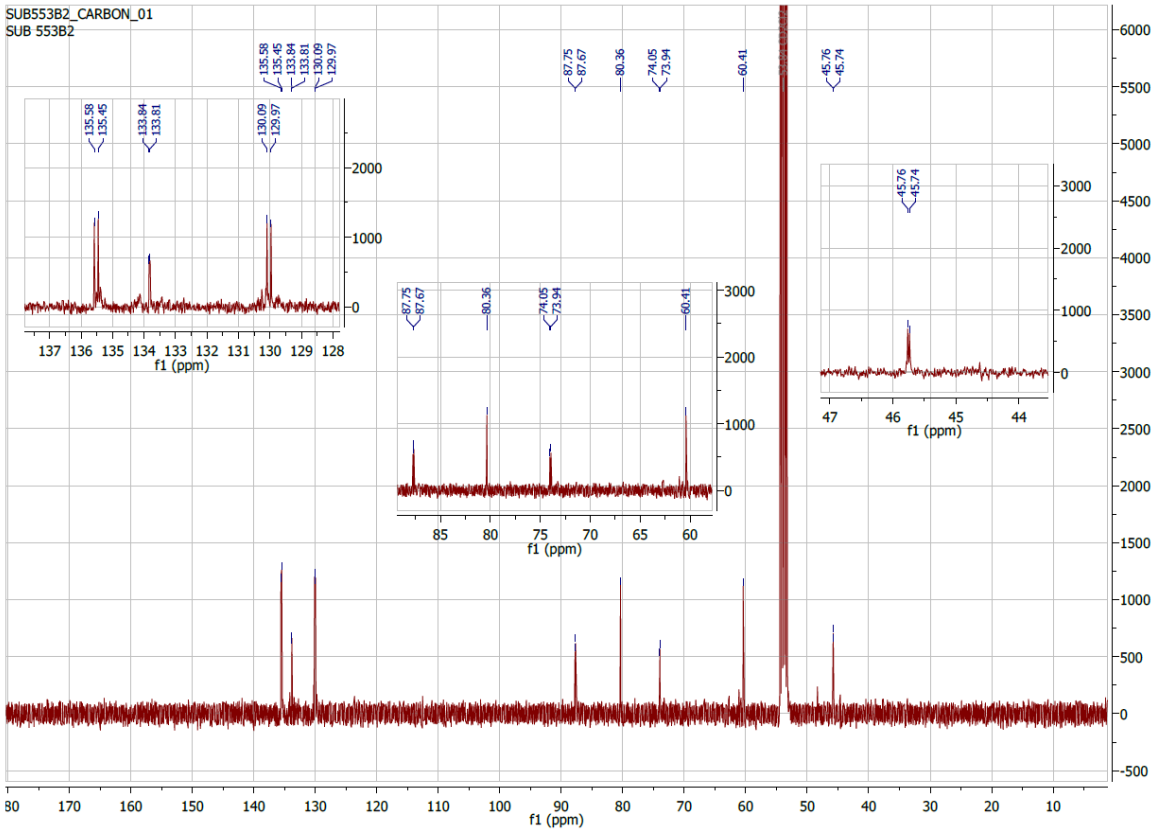


Fig S36. ^{13}C NMR of [Fc'(NMe$_2$)(PPh$_2$)·PdPPh$_2$(C$_5$H$_5$)][SbF$_6$]$_2$ (**12**), measured in CD$_2$Cl$_2$.

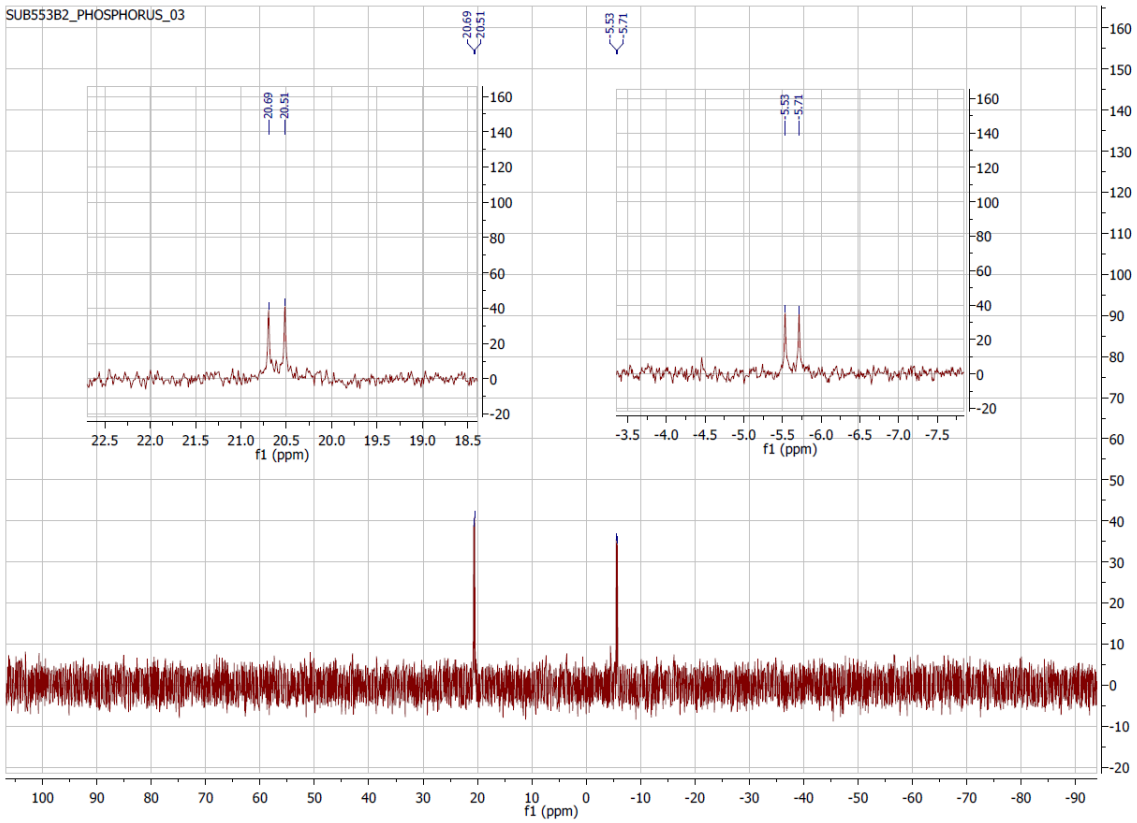


Fig S37. $^{31}P\{^{1}H\}$ NMR of $[Fc'(NMe_2)(PPh_2)\cdot PdPPh_2(C_5H_5)][SbF_6]_2$ (**12**), measured in CD_2Cl_2.

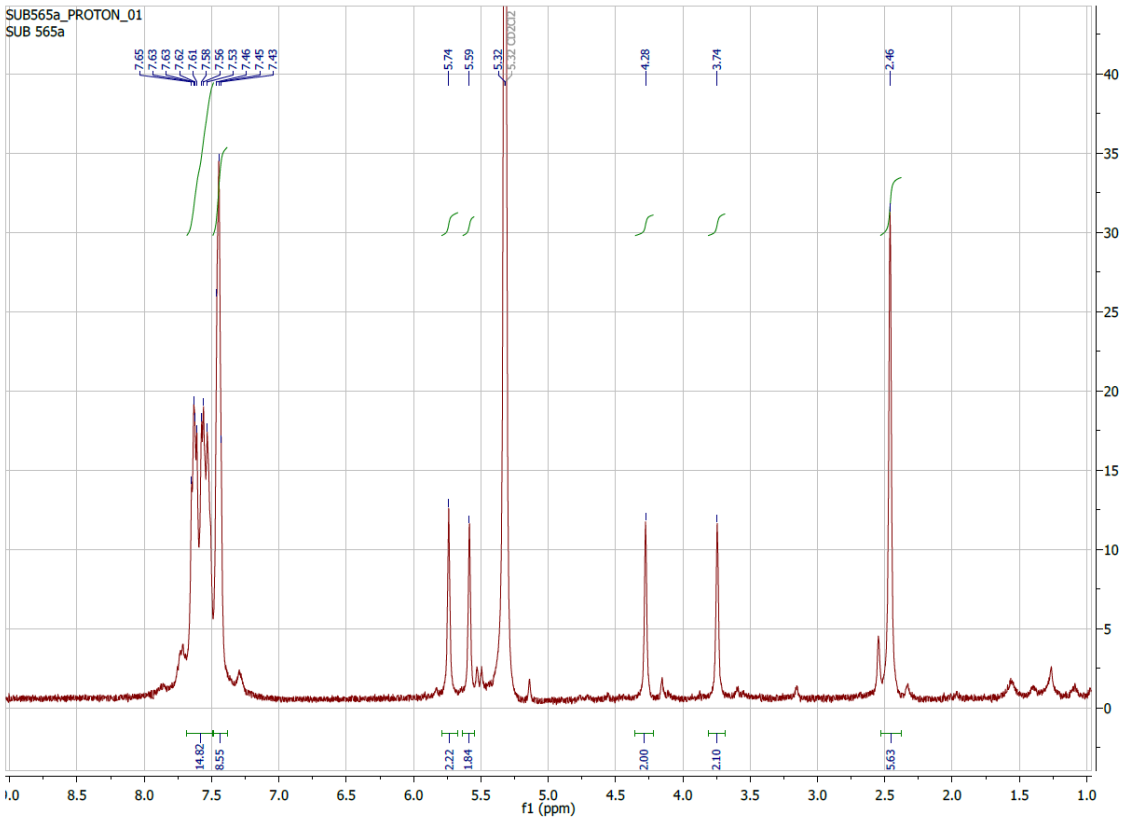


Fig S38. ^{1}H NMR of $[Fc'(NMe_2)(PPh_2)\cdot PdPPh_3][BF_4]_2$ (**13**), measured in CD_2Cl_2.

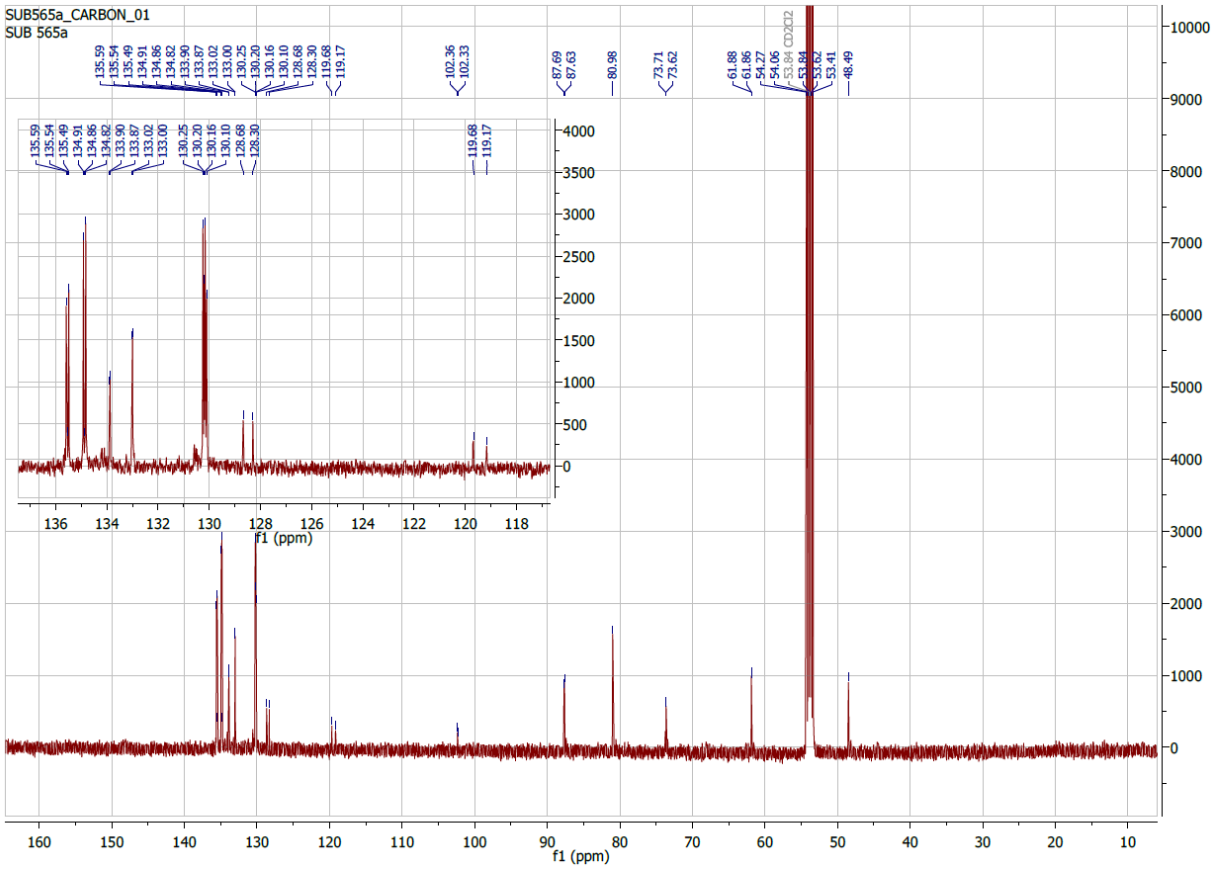


Fig S39. ^{13}C NMR of $[Fc'(NMe_2)(PPh_2)\cdot PdPPh_3][BF_4]_2$ (**13**), measured in CD_2Cl_2.

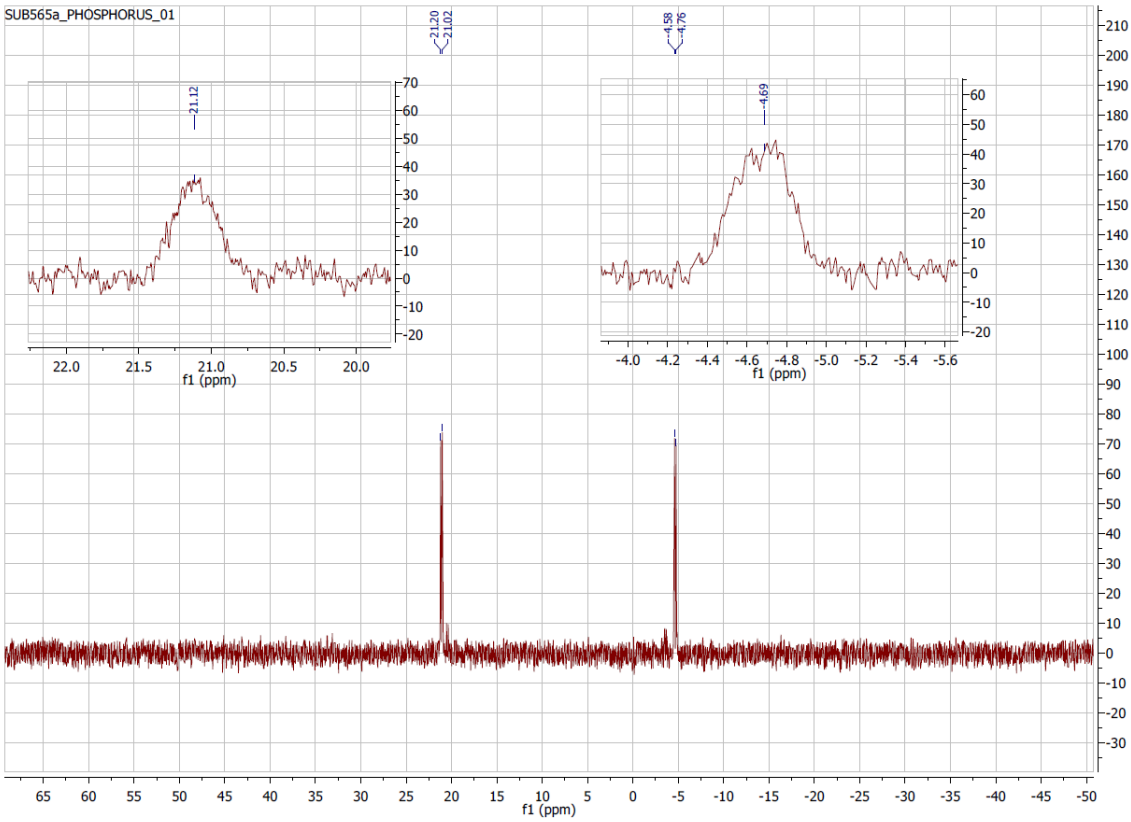


Fig S40. $^{31}P\{^1H\}$ NMR of $[Fc'(NMe_2)(PPh_2)\cdot PdPPh_3][BF_4]_2$ (**13**), measured in CD_2Cl_2.
Corresponding peaks in ^1H coupled ^{31}P NMR are shown in insets.

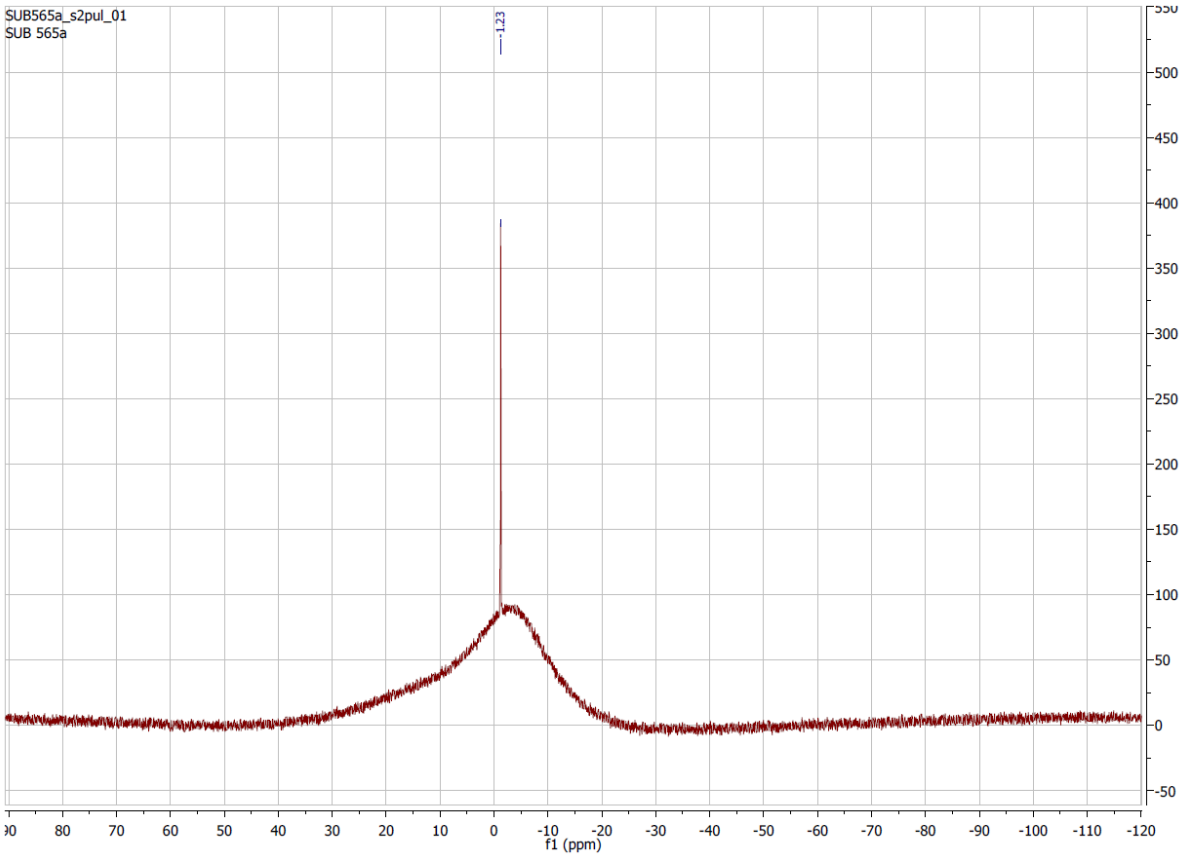


Fig S41. ^{11}B NMR of $[Fc'(NMe_2)(PPh_2)\cdot PdPPh_3][BF_4]_2$ (**13**), measured in CD_2Cl_2.

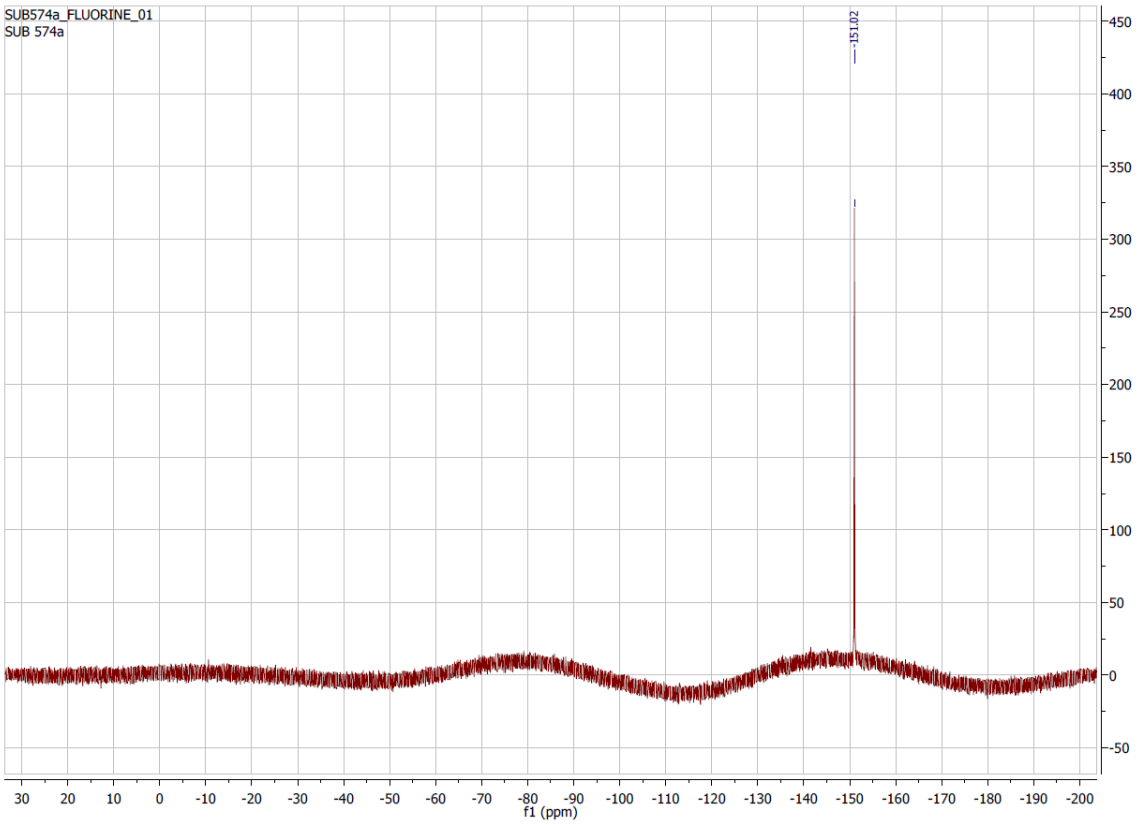


Fig S42. ^{19}F NMR of $[Fc'(NMe_2)(PPh_2)\cdot PdPPh_3][BF_4]_2$ (**13**), measured in CD_2Cl_2.

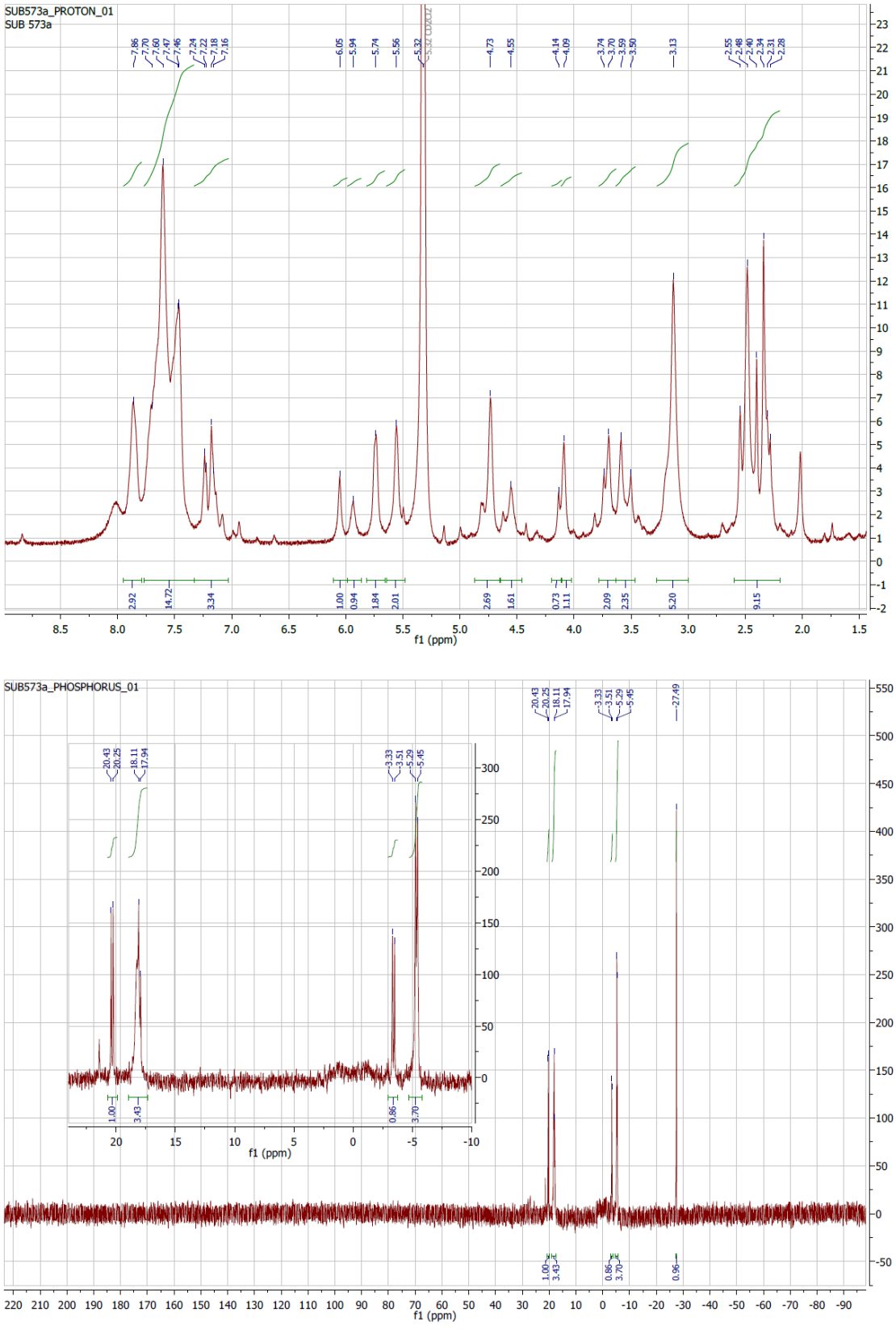


Fig S43. ^{1}H and ^{31}P NMR for failed synthesis of $[Fc'(NMe_2)(PPh_2)\cdot PdMes_3][BF_4]_2$, measured in CD_2Cl_2. The peak at δ -27.49 ppm are resulting from $PMes_3$, which could not be removed after several washing with toluene and Et_2O. This reaction mixture contains multiple rotamers of $[Fc'(NMe_2)(PPh_2)\cdot Pd(PPh_2)Fc'(NMe_2)][BF_4]_2$ (**14**) (ca. 74:26) as major products. HRMS (MALDI) of this species shows major peak at 769.0980 which corresponds to [M] for $[C_{41}H_{39}FeNP_2Pd]^{2+}$ (or $Fc'(NMe_2)(PPh_2)\cdot Pd(PPh_2Cp)^{2+}$). Anal found: C, 50.09; H, 4.04; N, 2.50 (Anal. Calcd. for $C_{48}H_{48}B_2F_8Fe_2N_2P_2Pd$: C, 52.10; H, 4.37; N, 2.53).

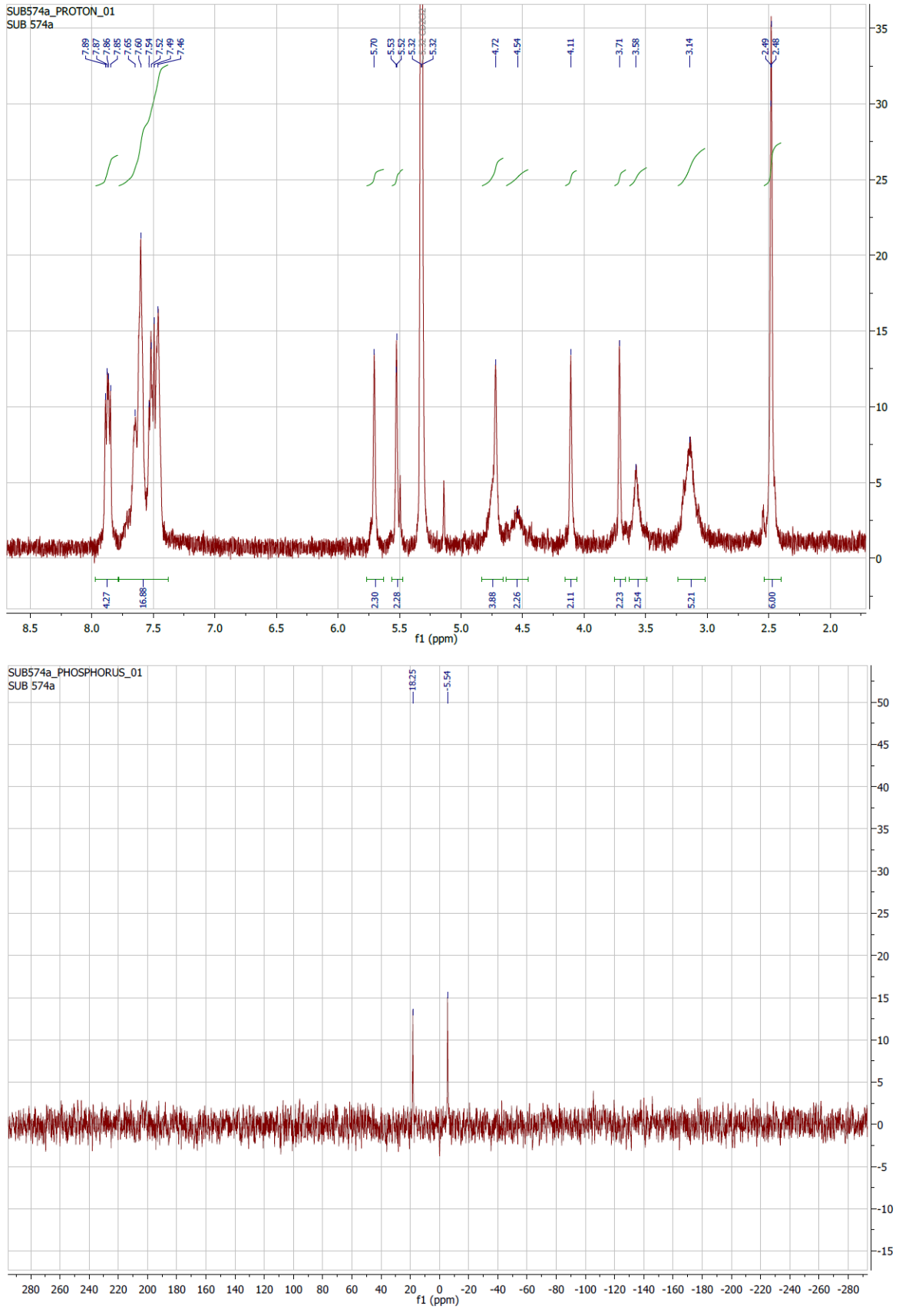


Fig S44. ^{1}H and $^{31}P\{^{1}H\}$ NMR for failed synthesis of $[Fc'(NMe_2)(PPh_2)\cdot Pd(o\text{-}Tol)_3][BF_4]_2$, measured in CD_2Cl_2. This reaction mixture contains $[Fc'(NMe_2)(PPh_2)\cdot Pd(PPh_2)Fc'(NMe_2)][BF_4]_2$ (**14**). HRMS (MALDI) of this species shows major peak at 769.0980, which corresponds to $[C_{41}H_{39}FeNP_2Pd]^{2+}$ (or $Fc'(NMe_2)(PPh_2)\cdot Pd(PPh_2Cp)^{2+}$) and minor peak at 519.0080, which corresponds to $[C_{24}H_{24}FeNPPd]^{2+}$ (or $Fc'(NMe_2)(PPh_2)\cdot Pd^{2+}$). Anal found: C, 51.65; H, 4.44; N, 2.45 (Anal. Calcd. for $C_{48}H_{48}B_2F_8Fe_2N_2P_2Pd$: C, 52.10; H, 4.37; N, 2.53).

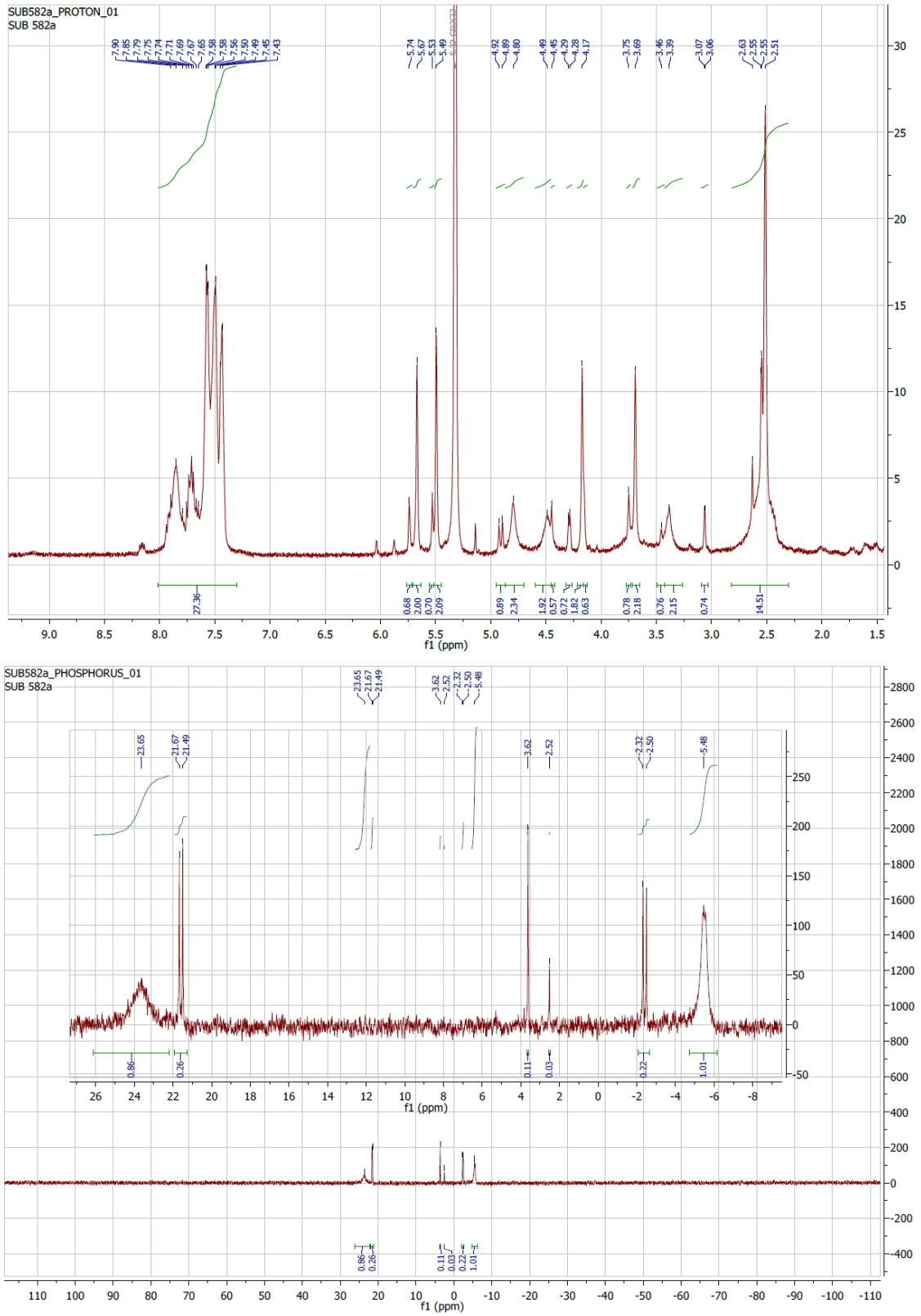


Fig S45. ^{1}H and ^{31}P NMR for selective synthesis of $[Fc'(NMe_2)(PPh_2)\cdot Pd(PPh_2)Fc'(NMe_2)][BF_4]_2$ (**14**), measured in CD_2Cl_2.

This reaction mixture contains multiple rotamers of $[Fc'(NMe_2)(PPh_2)\cdot Pd(PPh_2)Fc'(NMe_2)][BF_4]_2$ (**14**) (ca. 74:26) as major products. HRMS (MALDI) of this species shows major peak at 769.0980, which corresponds to $[C_{41}H_{39}FeNP_2Pd]^{2+}$ (or $Fc'(NMe_2)(PPh_2)\cdot Pd(PPh_2Cp)^{2+}$) and minor peak at 932.0970, which corresponds to $[C_{24}H_{24}FeNPPd]^{2+}$ (or $Fc'(NMe_2)(PPh_2)\cdot Pd(PPh_2)Fc'(NMe_2)^{2+}$). Anal found: C, 50.88; H, 4.62; N, 2.45 (Anal. Calcd. for $C_{48}H_{48}B_2F_8Fe_2N_2P_2Pd$: C, 52.10; H, 4.37; N, 2.53).

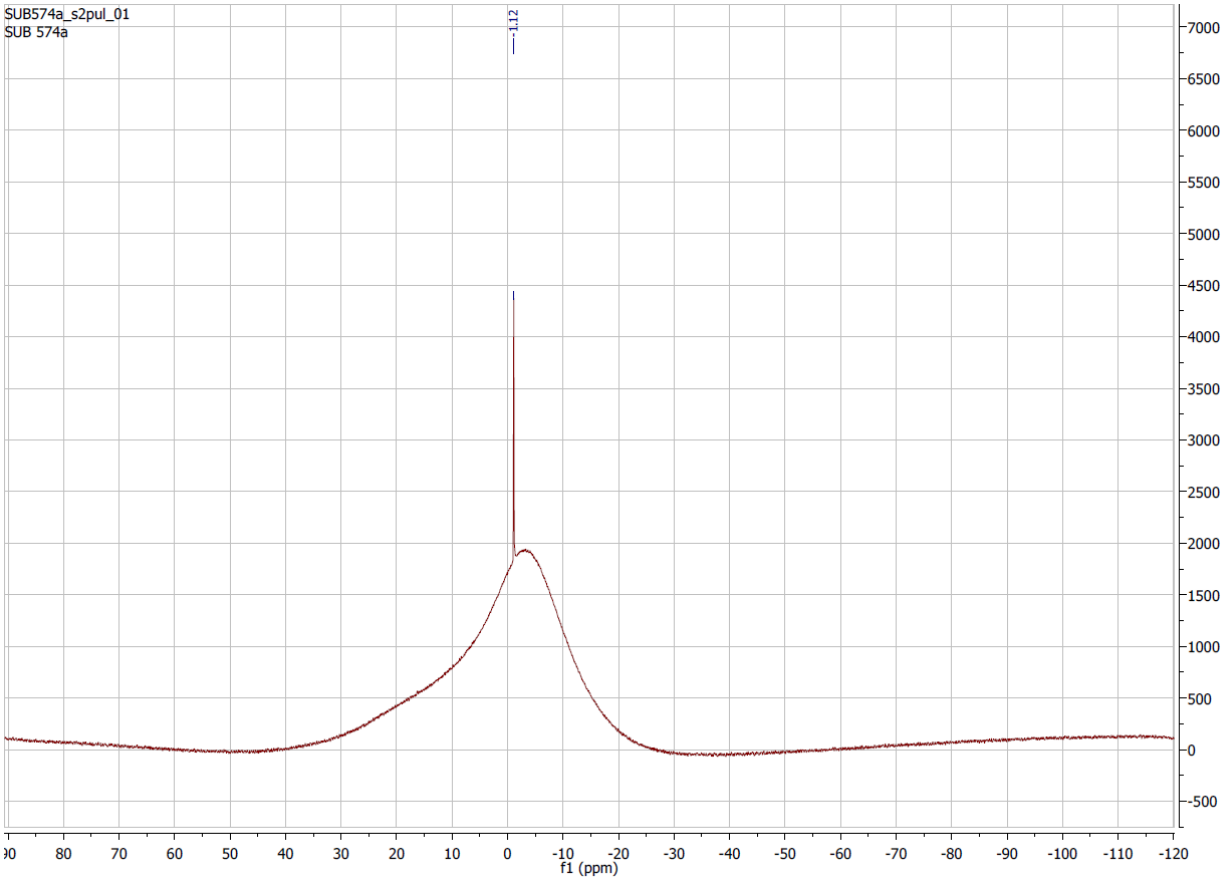


Fig S46. ^{11}B NMR of [Fc'(NMe$_2$)(PPh$_2$)·Pd(PPh$_2$)Fc'(NMe$_2$)][BF$_4$]$_2$ (**14**), measured in CD_2Cl_2.

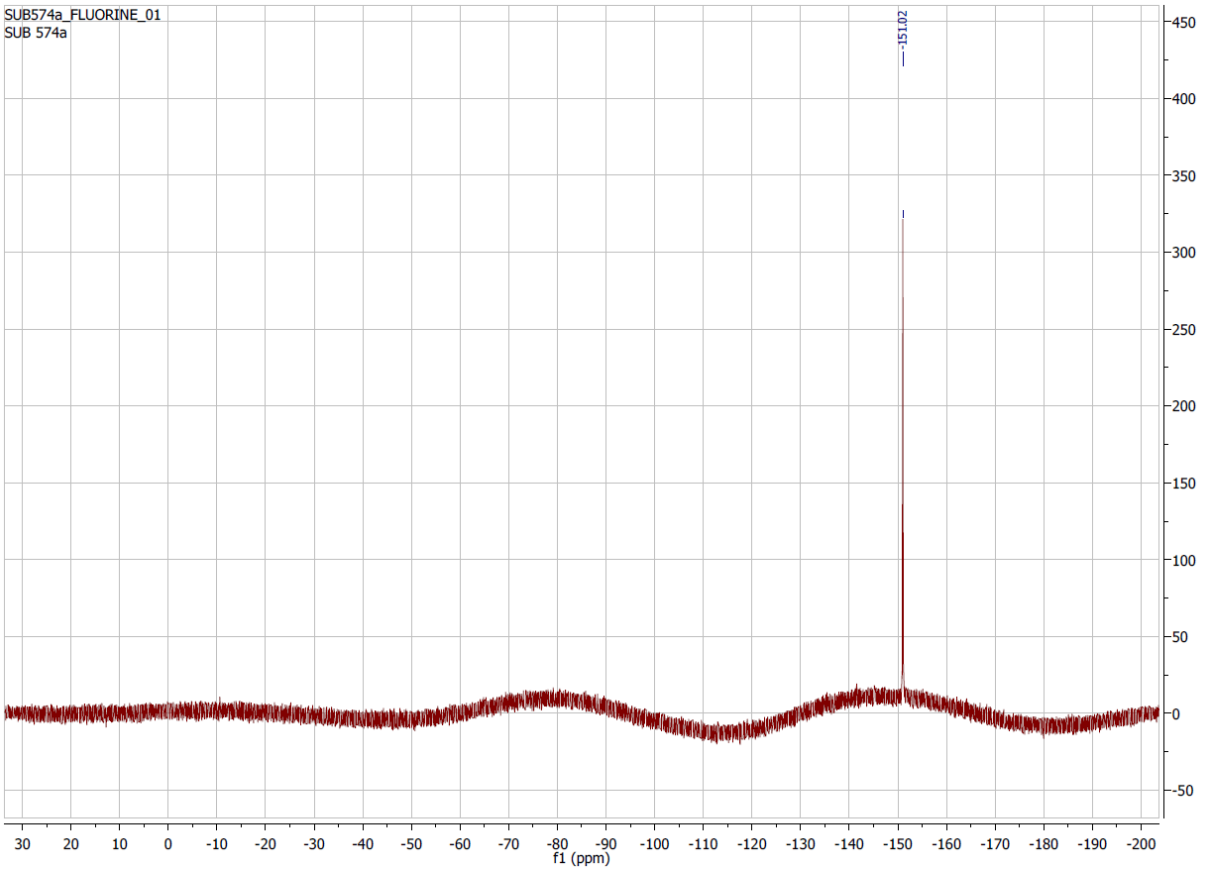


Fig S47. ^{19}F NMR of [Fc'(NMe$_2$)(PPh$_2$)·Pd(PPh$_2$)Fc'(NMe$_2$)][BF$_4$]$_2$ (**14**), measured in CD_2Cl_2.

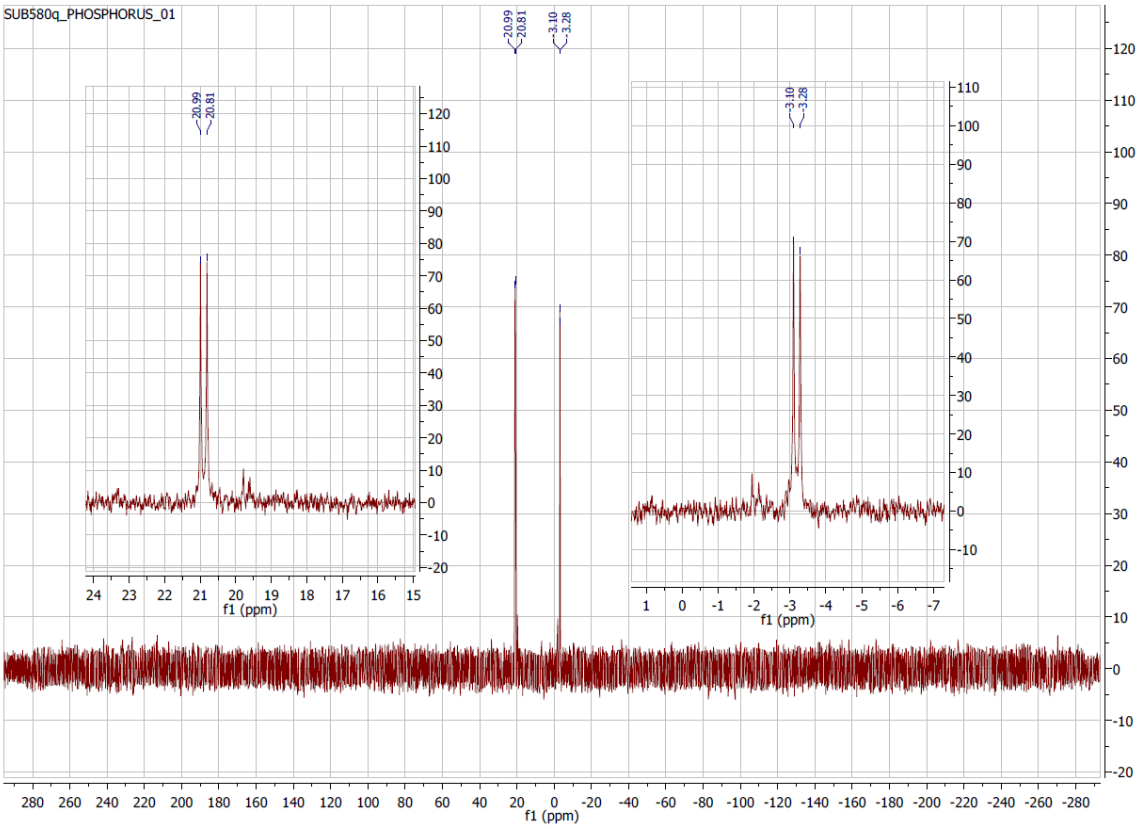


Fig S48. $^{31}P\{^{1}H\}$ NMR of the reaction mixture of **13** and P(p-OMe-C_6H_4)$_3$, measured after 5 mins at RT in non-deuterated Acetone.

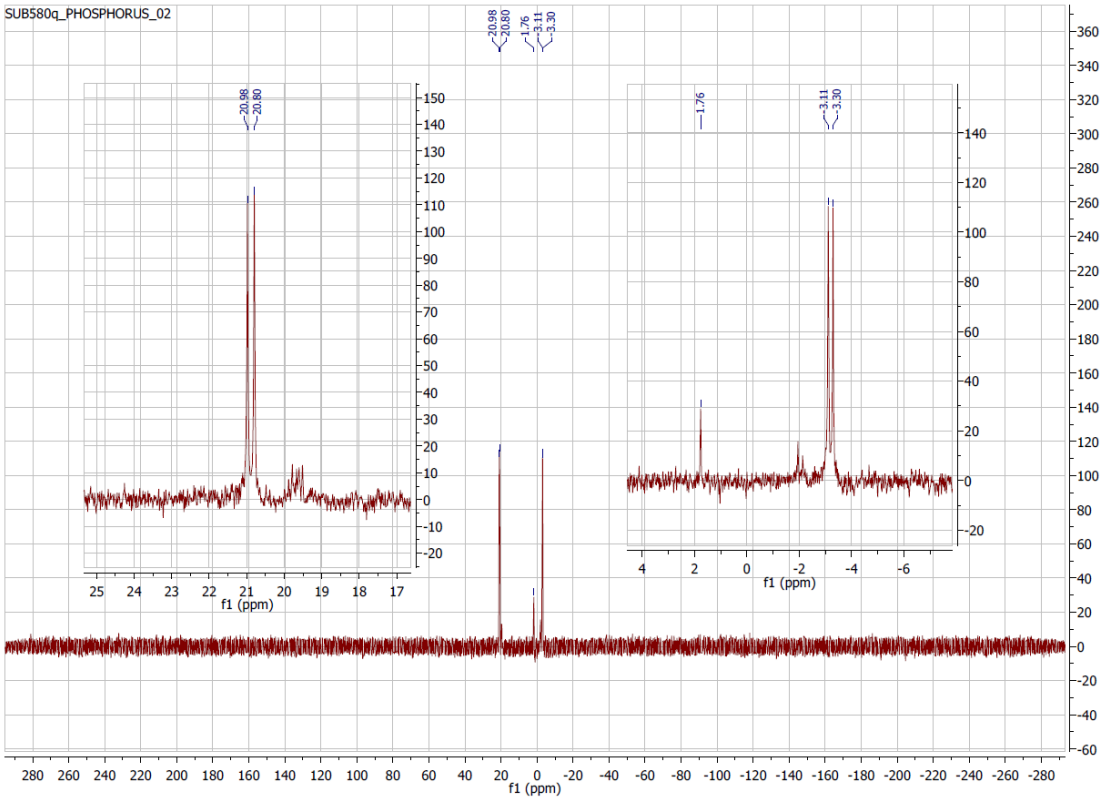


Fig S49. $^{31}P\{^{1}H\}$ NMR of the reaction mixture of **13** and P(*p*-OMe-C_6H_4)$_3$, measured after 1 hr at 50 °C in non-deuterated Acetone.

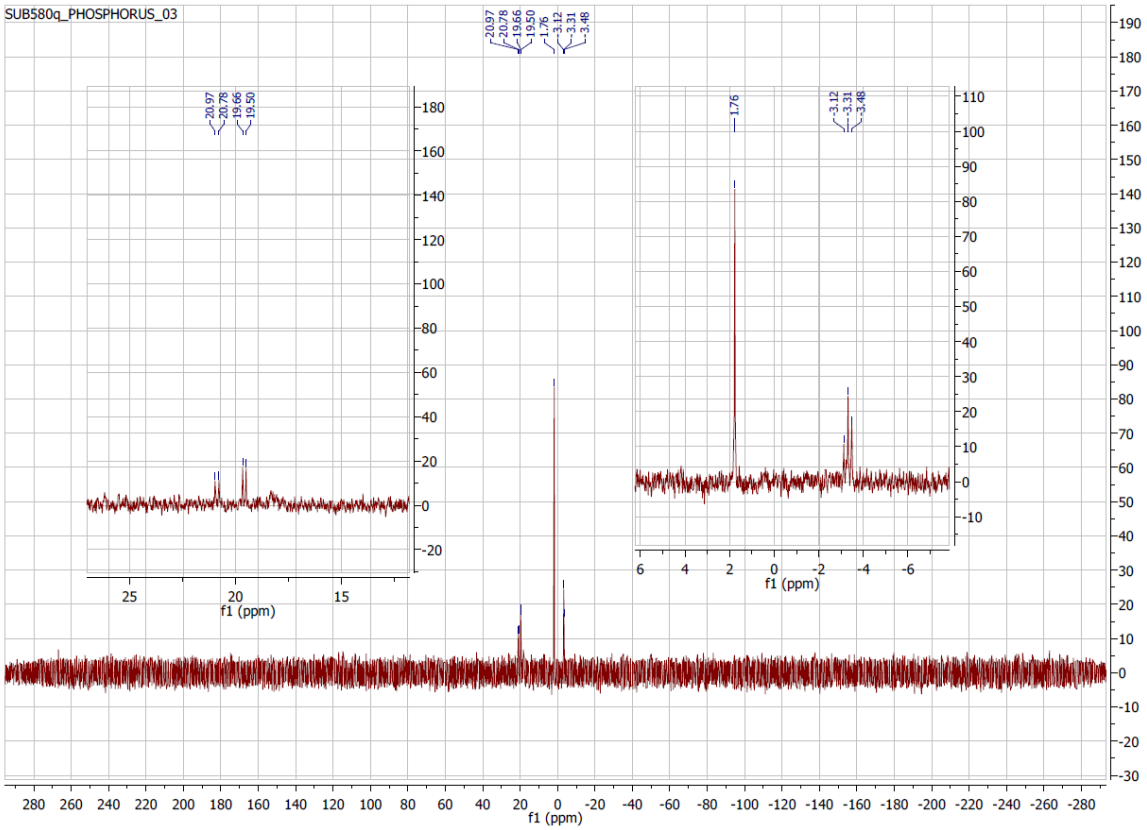


Fig S50. $^{31}P\{^{1}H\}$ NMR of the reaction mixture of **13** and P(*p*-OMe-$C_6H_4)_3$, measured after 15 hrs at 50 °C in non-deuterated Acetone.

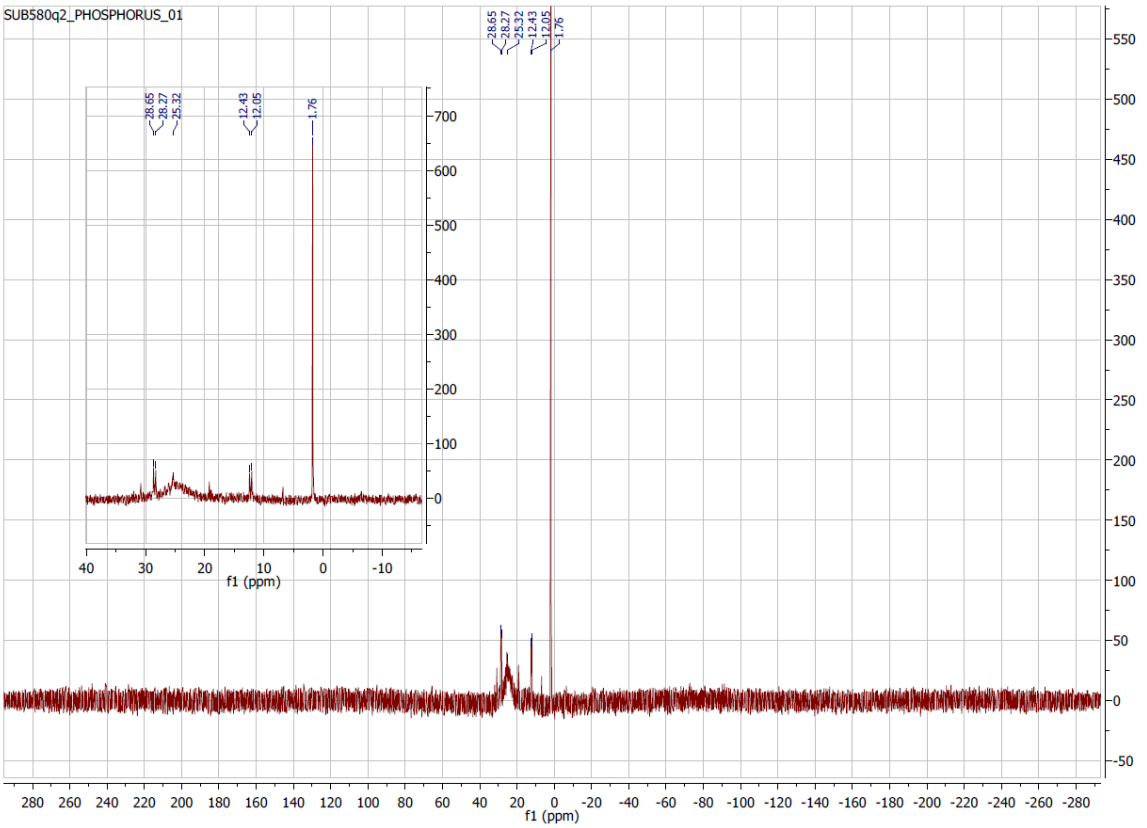


Fig S51. $^{31}P\{^{1}H\}$ NMR of the reaction mixture of **13** and P(*p*-OMe-$C_6H_4)_3$, measured after 39 hrs at 50 °C in non-deuterated Acetone.

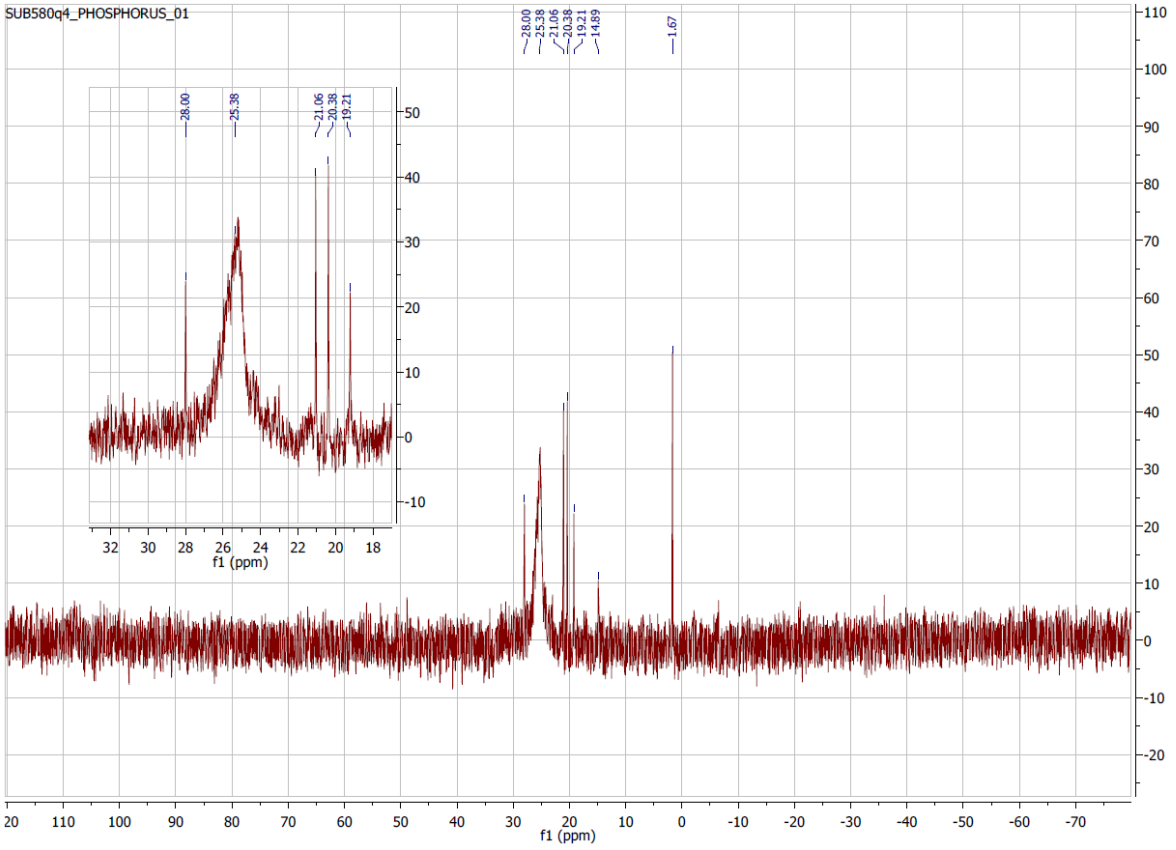


Fig S52. $^{31}P\{^{1}H\}$ NMR of the reaction mixture of **13** and P(*p*-OMe-C_6H_4)$_3$, measured after 50 hrs at 50 °C in non-deuterated Acetone.

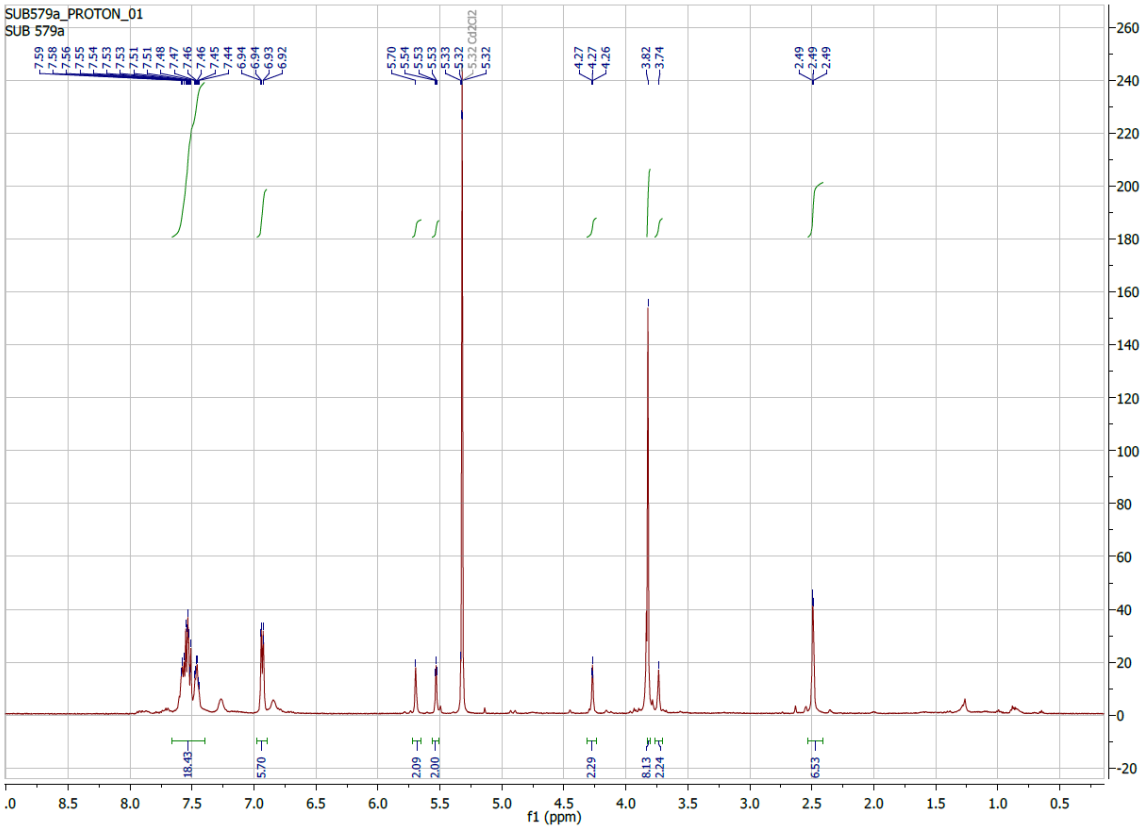


Fig S53. ^{1}H NMR of [Fc'(NMe_2)(PPh_2)]Pd[P(*p*-OMe-C_6H_4)$_3$][BF_4]$_2$ (**15**), measured in CD_2Cl_2.

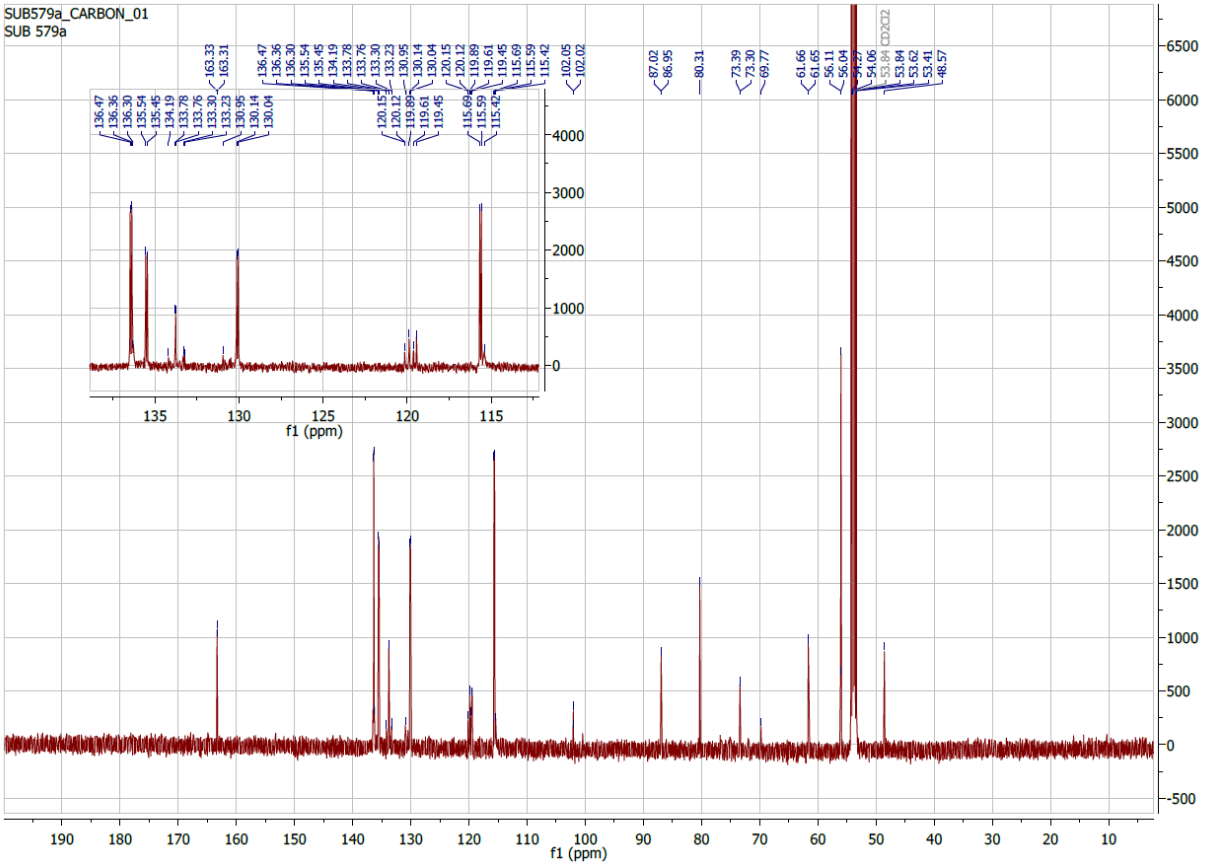


Fig S54. ^{13}C NMR of [Fc'(NMe_2)(PPh_2)]Pd[P(*p*-OMe-C_6H_4)$_3$][BF_4]$_2$ (**15**), measured in CD_2Cl_2.

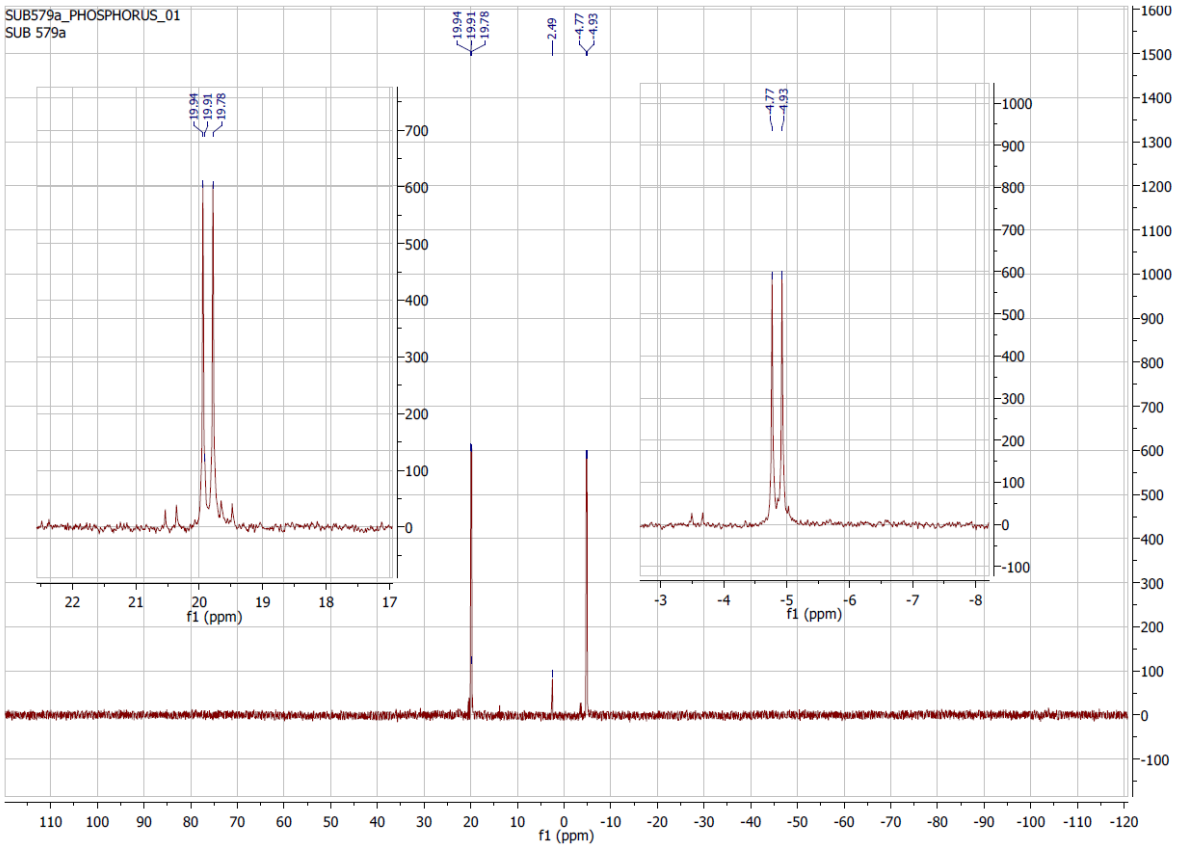


Fig S55. $^{31}P\{^1H\}$ NMR of [Fc'(NMe_2)(PPh_2)]Pd[P(*p*-OMe-C_6H_4)$_3$][BF_4]$_2$ (**15**), measured in CD_2Cl_2.

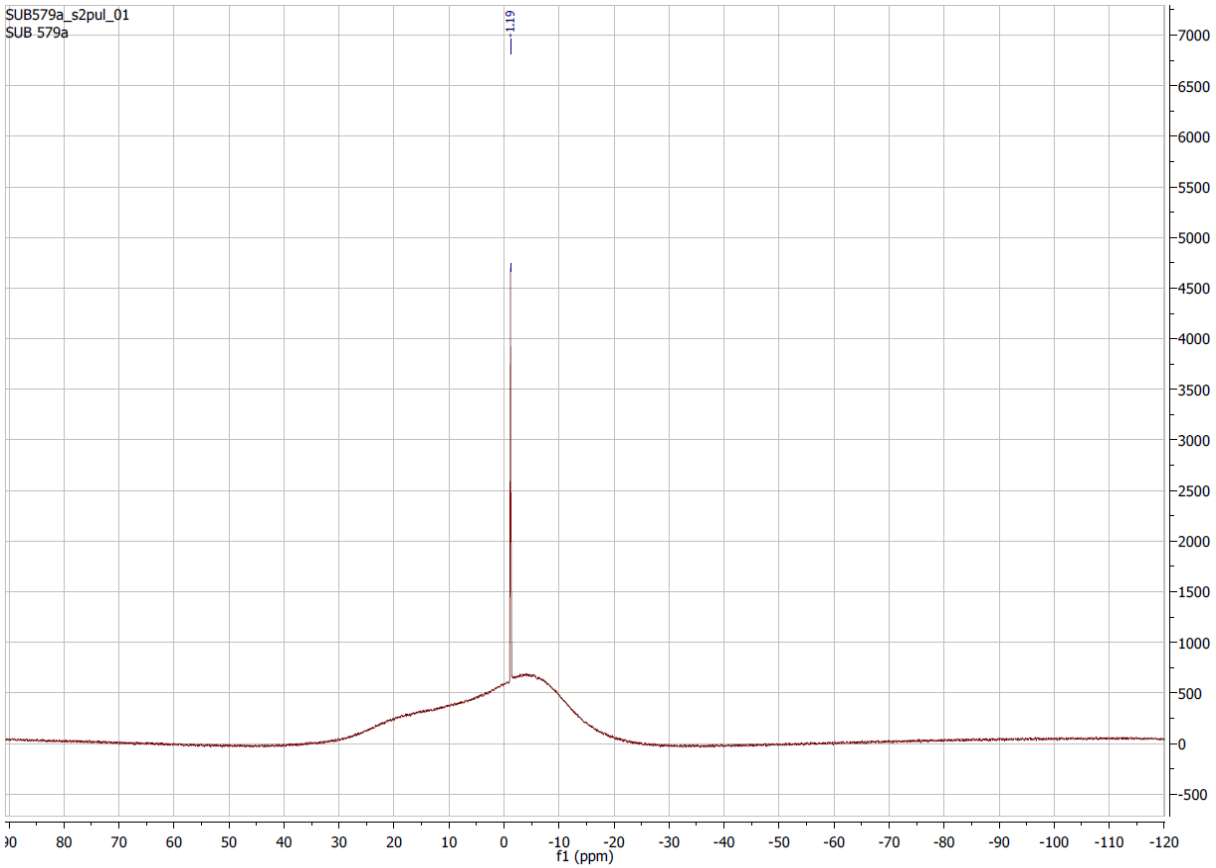


Fig S56. ^{11}B NMR of [Fc'(NMe$_2$)(PPh$_2$)]Pd[P(*p*-OMe-C$_6$H$_4$)$_3$][BF$_4$]$_2$ (**15**), measured in CD_2Cl_2.

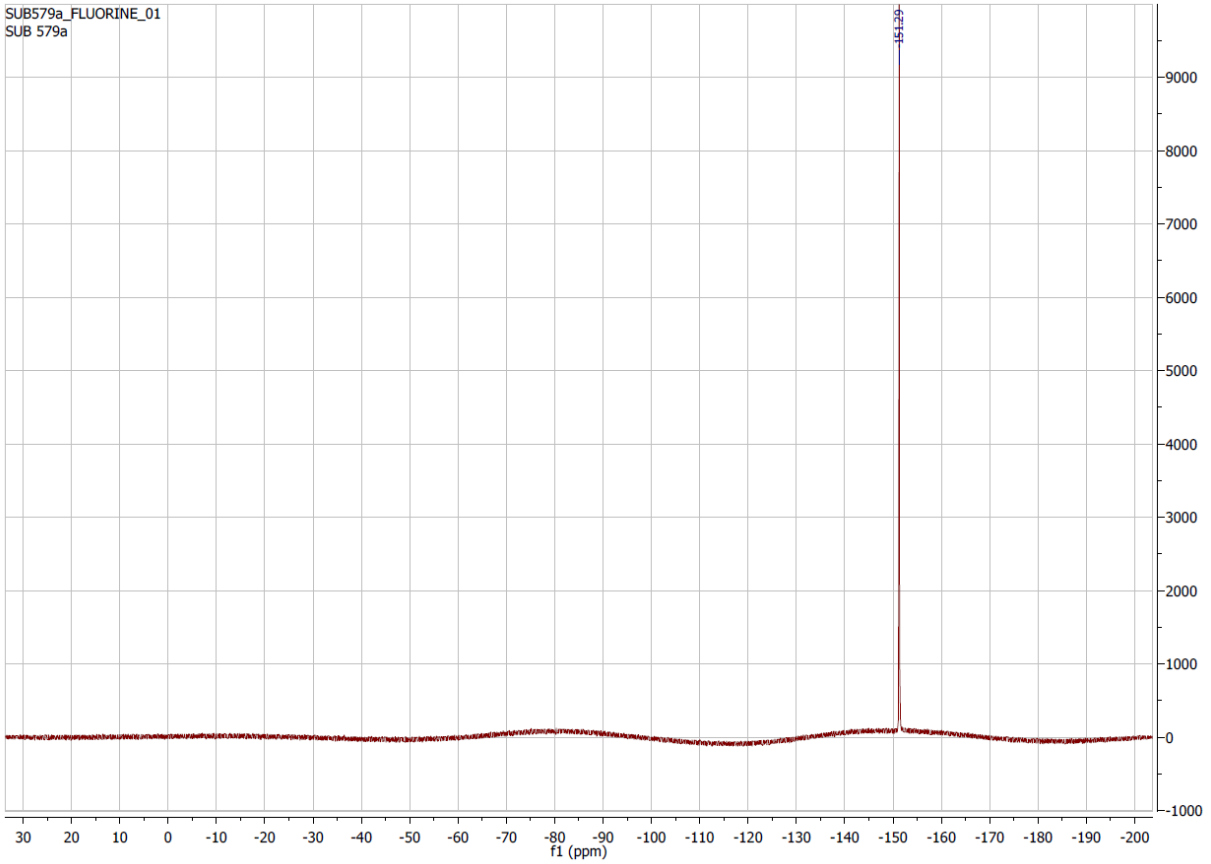


Fig S57. ^{19}F NMR of [Fc'(NMe$_2$)(PPh$_2$)]Pd[P(*p*-OMe-C$_6$H$_4$)$_3$][BF$_4$]$_2$ (**15**), measured in CD_2Cl_2.

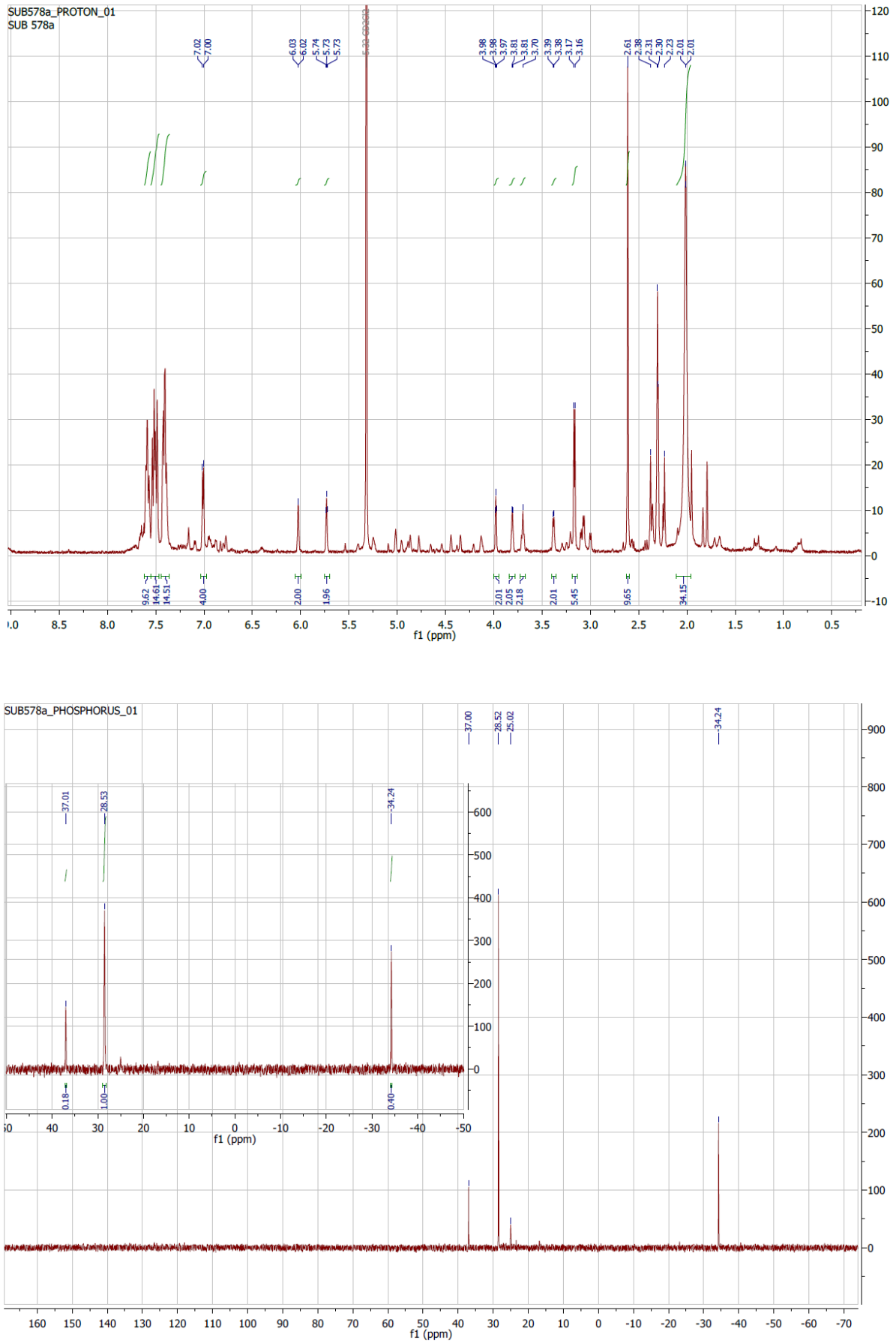


Fig S58. ^{1}H and $^{31}P\{^{1}H\}$ NMR for unsuccessful synthesis of $[Fc'(NMe_2)(PMes_2)\cdot Pd][BF_4]_2$, measured in CD_2Cl_2. The signal at -34.00 ppm is resulting from the unreacted $Fc'(NMe_2)(PMes_2)$.

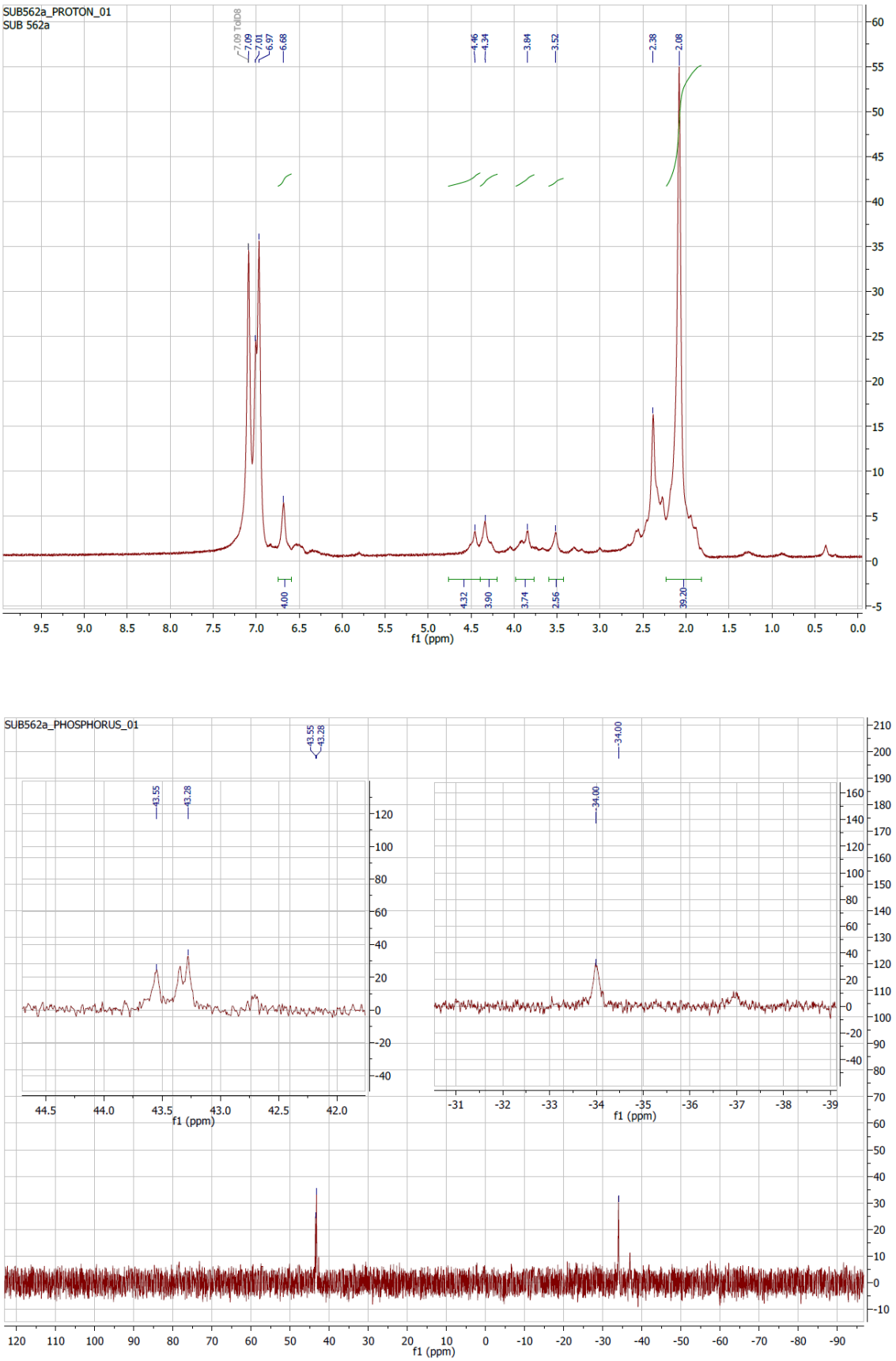


Fig S59. ^{1}H and $^{31}P\{^{1}H\}$ NMR for unsuccessful synthesis of [Fc'(NMe_2)($PMes_2$)·$PdCl_2$], measured in Toluene D8.

The signal at -34.00 ppm is resulting from the unreacted Fc'(NMe_2)($PMes_2$).

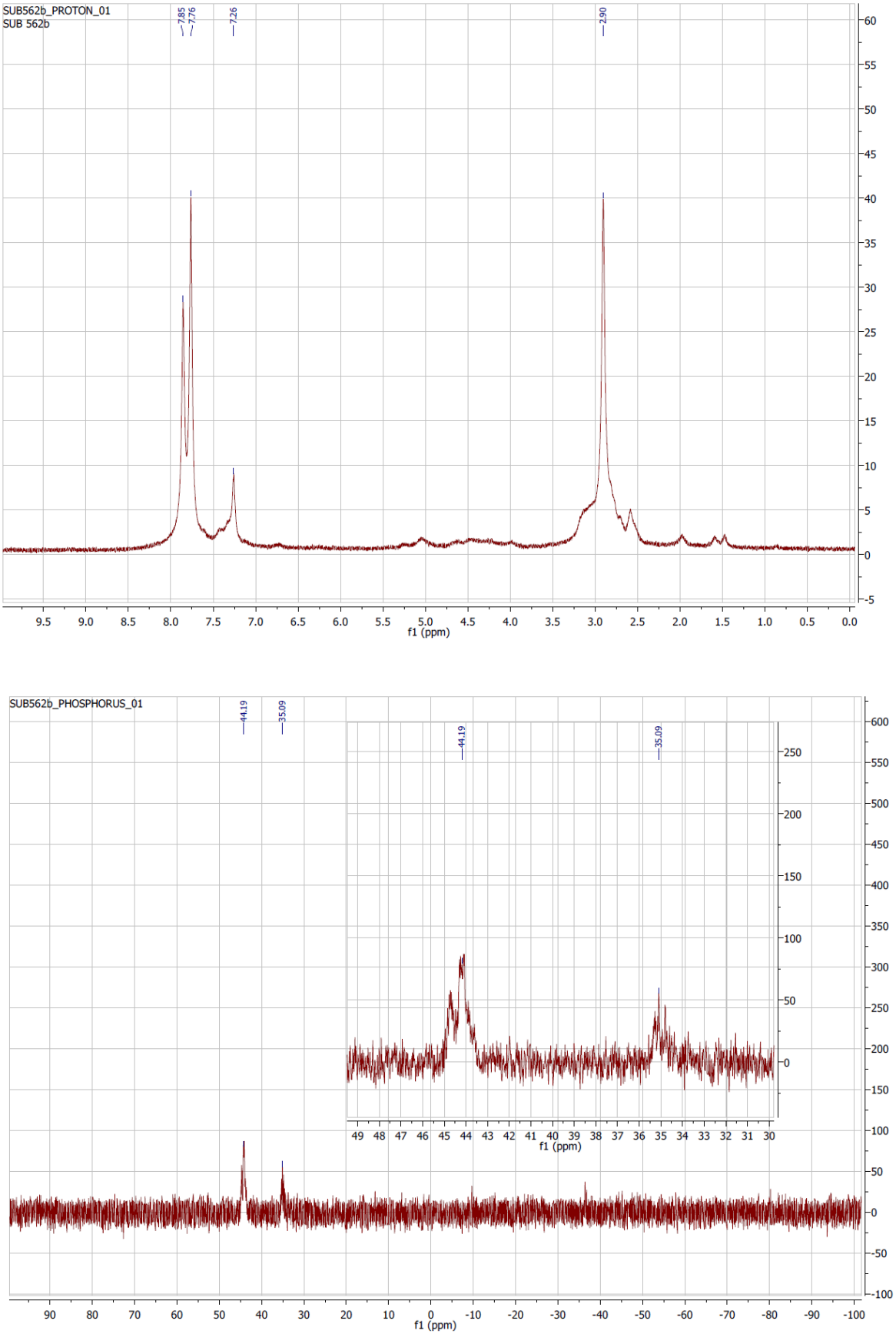


Fig S60. ^{1}H and $^{31}P\{^{1}H\}$ NMR for unsuccessful synthesis of $[Fc'(NMe_2)(PMes_2)\cdot PdCl_2]$, measured in Toluene D8 after heating at 50°C for 2 hrs.

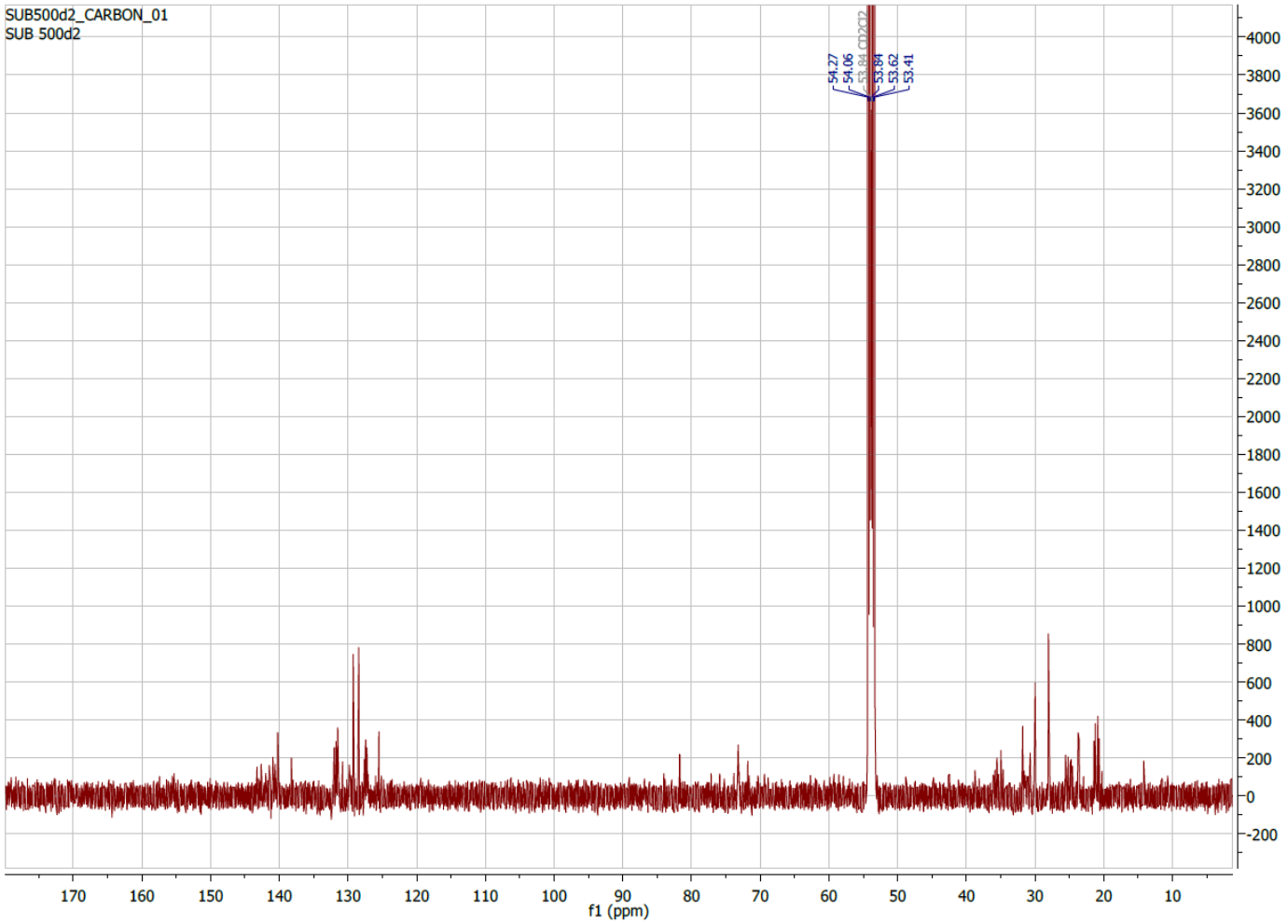


Fig S61. ^{13}C NMR of [Fc'($PMes_2$)(P^tBu_2)·$PdCl_2$] (**8**), measured in CD_2Cl_2.

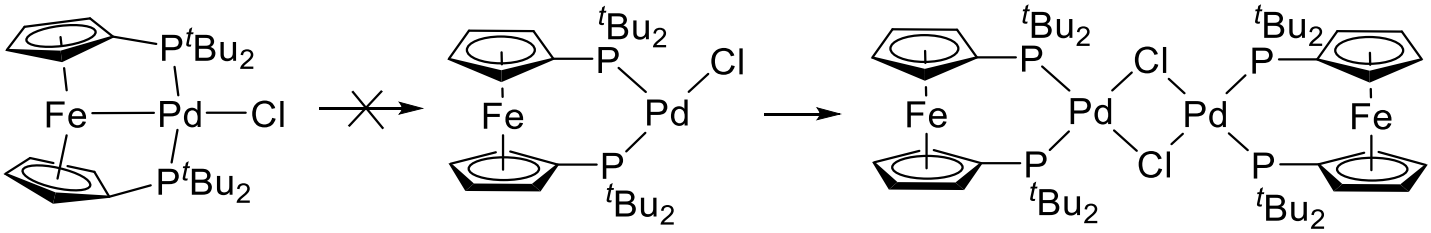


Fig S62. Isomer of [d*t*bpf·PdCl]$^+$ with Fe-Pd interaction and dimer with T-shaped geometry around Pd center.

Table S3. Crystal Refinement data of Compounds **1**, **3** and **4a**.

Acronym	**1**	**3a**	**3b**	**4a**
CCDC Deposition Number	2243451	217930	2243452	2243453
Empirical formula	$C_{10}H_{10}BrFeN$	$C_{24}H_{24}FeNP$	$C_{30}H_{36}FeNP$	$C_{24}H_{24}FeNPSe$
Formula weight	279.95	413.26	497.42	492.22
Temperature/K	100(2)	100(2)	100(2)	100
Crystal system	monoclinic	monoclinic	triclinic	triclinic
Space group	$P2_1/c$	$P2_1/c$	P-1	P-1
a/Å	12.3649(8)	8.4135(7)	9.2998(6)	8.6171(9)
b/Å	7.4650(4)	16.8152(15)	9.8582(6)	9.6018(13)
c/Å	10.4750(6)	28.089(2)	14.4614(9)	13.2757(19)
α/°	90	90	80.415(5)	89.994(11)
β/°	99.832(5)	90.863(6)	74.260(5)	100.144(10)
γ/°	90	90	78.804(5)	106.456(10)
Volume/$Å^3$	952.68(10)	3973.5(6)	1242.68(14)	1035.5(2)
Z	4	8	2	2
$\rho_{calc}g/cm^3$	1.952	1.382	1.329	1.579
μ/mm^{-1}	5.723	6.891	0.690	8.638
F(000)	552.0	1728.0	528.0	500.0
Crystal size/mm^3	0.17 × 0.107 × 0.02	0.089 × 0.075 × 0.048	0.36 × 0.233 × 0.05	0.322 × 0.243 × 0.129
Radiation	MoKα (λ = 0.71073)	Cu Kα (λ = 1.54186)	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54186)
2Θ range for data collection/°	3.342 to 51.448	6.126 to 142.006	2.948 to 51.466	6.774 to 143.67
Index ranges	-15 ≤ h ≤ 15, -9 ≤ k ≤ 7, -12 ≤ l ≤ 10	-10 ≤ h ≤ 8, -14 ≤ k ≤ 20, -20 ≤ l ≤ 33	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -17 ≤ l ≤ 17	-5 ≤ h ≤ 10, -11 ≤ k ≤ 10, -16 ≤ l ≤ 15
Reflections collected	3771	17195	8697	8726
Independent reflections	1793 [R_{int} = 0.0215, R_{sigma} = 0.0216]	7308 [R_{int} = 0.0303, R_{sigma} = 0.0407]	4677 [R_{int} = 0.0465, R_{sigma} = 0.0416]	3917 [R_{int} = 0.0272, R_{sigma} = 0.0268]
Data/restraints/parameters	1793/2/124	7308/0/491	4677/0/306	3917/0/255
Goodness-of-fit on F^2	1.077	1.070	1.116	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0364, wR_2 = 0.0960	R_1 = 0.0410, wR_2 = 0.0831	R_1 = 0.0598, wR_2 = 0.1653	R_1 = 0.0386, wR_2 = 0.0990
Final R indexes [all data]	R_1 = 0.0453, wR_2 = 0.1012	R_1 = 0.0606, wR_2 = 0.0904	R_1 = 0.0668, wR_2 = 0.1755	R_1 = 0.0410, wR_2 = 0.1008
Largest diff. peak/hole / e $Å^{-3}$	0.62/-0.80	0.41/-0.27	0.72/-0.95	0.71/-1.10

Table S4. Crystal Refinement data of Compounds **7**-**9**.

Acronym	**7**	**8**	**9**
CCDC Deposition Number	2243454	2243455	2243456
Empirical formula	$C_{41}H_{42}Cl_4FeP_2Pd$	$C_{38}H_{52}Cl_6FeP_2Pd$	$C_{48}H_{48}Cl_2Fe_2N_2P_2Pd$
Formula weight	900.73	945.68	1003.82
Temperature/K	100	100	100
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	$P2_1/c$	$P2_1/n$
a/Å	10.8066(6)	19.0610(9)	10.135(3)
b/Å	11.6528(7)	10.2156(3)	14.632(14)
c/Å	17.1079(9)	21.9718(10)	14.651(3)
α/°	75.563(4)	90	90
β/°	78.165(4)	110.152(4)	100.75(2)
γ/°	62.693(4)	90	90
Volume/$Å^3$	1843.49(19)	4016.4(3)	2134(2)
Z	2	4	2
$\rho_{calc}g/cm^3$	1.623	1.564	1.562
μ/mm^{-1}	1.289	1.315	10.882
F(000)	916.0	1936.0	1024.0
Crystal size/mm^3	0.34 × 0.173 × 0.05	0.24 × 0.107 × 0.02	0.16 × 0.07 × 0.02
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54186)
2Θ range for data collection/°	2.472 to 51.504	3.818 to 51.648	8.618 to 141.91
Index ranges	-13 ≤ h ≤ 11, -14 ≤ k ≤ 14, -20 ≤ l ≤ 19	-23 ≤ h ≤ 23, -12 ≤ k ≤ 12, -26 ≤ l ≤ 26	-11 ≤ h ≤ 12, -17 ≤ k ≤ 17, -10 ≤ l ≤ 17
Reflections collected	13347	22037	13111
Independent reflections	6971 [R_{int} = 0.0204, R_{sigma} = 0.0212]	7641 [R_{int} = 0.0749, R_{sigma} = 0.0647]	3944 [R_{int} = 0.0453, R_{sigma} = 0.0440]
Data/restraints/parameters	6971/0/448	7641/0/445	3944/0/261
Goodness-of-fit on F^2	1.064	1.067	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0273, wR_2 = 0.0707	R_1 = 0.0562, wR_2 = 0.1322	R_1 = 0.0524, wR_2 = 0.1203
Final R indexes [all data]	R_1 = 0.0314, wR_2 = 0.0722	R_1 = 0.0787, wR_2 = 0.1480	R_1 = 0.0763, wR_2 = 0.1348
Largest diff. peak/hole / e $Å^{-3}$	0.40/-0.49	1.04/-1.36	0.96/-1.77

Table S5. Crystal Refinement data of Compounds **10**-**15**.

Acronym	**10**	**11**	**12**	**13**	**14**	**15**
CCDC Deposition Number	2243457	2243458	2243459	2243460	2243461	2243462
Empirical formula	$C_{36}H_{48}ClF_6FeP_2PdSb$	$C_{24}H_{24}ClF_6FeNPPdSb$	$C_{41}H_{39}F_{12}FeNP_2PdSb_2$	$C_{43}H_{41}B_2Cl_2F_8FeNP_2Pd$	$C_{48}H_{48}B_2F_8Fe_2N_2P_2Pd$	$C_{45}H_{45}B_2F_8FeNO_3P_2Pd$
Formula weight	976.13	790.86	1241.42	1040.48	1106.54	1045.63
Temperature/K	100	100	100	100	100	100
Crystal system	triclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P-1	$P2_1/n$	$P2_1/c$	$P2_1/n$	C2/c	P2/c
a/Å	12.667(3)	12.9682(7)	16.508(16)	9.4973(17)	30.8242(14)	22.1592(9)
b/Å	16.343(2)	10.3965(4)	14.757(6)	31.289(15)	13.9370(4)	9.5811(3)
c/Å	20.387(6)	19.4858(11)	17.421(16)	14.506(4)	25.8720(10)	21.0726(9)
α/°	92.695(18)	90	90	90	90	90
β/°	107.49(2)	103.946(4)	93.66(8)	98.711(18)	102.787(3)	93.274(3)
γ/°	107.202(14)	90	90	90	90	90
Volume/$Å^3$	3802.0(15)	2549.7(2)	4235(6)	4261(2)	10838.9(7)	4466.6(3)
Z	4	4	4	4	8	4
$\rho_{calc}g/cm^3$	1.705	2.060	1.947	1.622	1.356	1.555
μ/mm^{-1}	1.759	20.576	2.176	8.596	7.951	7.181
F(000)	1952.0	1536.0	2416.0	2096.0	4480.0	2120.0
Crystal size/mm^3	0.12 × 0.07 × 0.03	0.15 × 0.083 × 0.02	0.12 × 0.083 × 0.06	0.15 × 0.073 × 0.01	0.25 × 0.107 × 0.03	0.192 × 0.091 × 0.015
Radiation	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54186)	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54186)	Cu Kα (λ = 1.54186)	Cu Kα (λ = 1.54186)
2Θ range for data collection/°	4.622 to 52	9.354 to 141.404	4.468 to 65.432	6.78 to 141.722	6.992 to 142.75	7.992 to 142.956
Index ranges	-15 ≤ h ≤ 12, -19 ≤ k ≤ 20, -22 ≤ l ≤ 25	-15 ≤ h ≤ 13, -12 ≤ k ≤ 5, -23 ≤ l ≤ 21	-24 ≤ h ≤ 17, -21 ≤ k ≤ 14, -26 ≤ l ≤ 22	-11 ≤ h ≤ 5, -37 ≤ k ≤ 30, -17 ≤ l ≤ 16	-37 ≤ h ≤ 30, -16 ≤ k ≤ 7, -31 ≤ l ≤ 30	-26 ≤ h ≤ 26, -4 ≤ k ≤ 11, -18 ≤ l ≤ 25
Reflections collected	29707	10456	29678	18315	22334	19338
Independent reflections	14665 [R_{int} = 0.0332, R_{sigma} = 0.0591]	4707 [R_{int} = 0.0765, R_{sigma} = 0.0678]	13195 [R_{int} = 0.0996, R_{sigma} = 0.1798]	7779 [R_{int} = 0.0821, R_{sigma} = 0.0806]	10214 [R_{int} = 0.0637, R_{sigma} = 0.0610]	8418 [R_{int} = 0.0588, R_{sigma} = 0.0622]
Data/restraints/parameters	14665/0/889	4707/0/327	13195/0/543	7779/0/543	10214/0/590	8418/9/574
Goodness-of-fit on F^2	1.006	1.025	0.994	1.023	1.044	1.016
Final R indexes [I>=2σ (I)]	R_1 = 0.0411, wR_2 = 0.0808	R_1 = 0.0832, wR_2 = 0.2208	R_1 = 0.0706, wR_2 = 0.1291	R_1 = 0.0945, wR_2 = 0.2395	R_1 = 0.0653, wR_2 = 0.1717	R_1 = 0.0726, wR_2 = 0.1831
Final R indexes [all data]	R_1 = 0.0726, wR_2 = 0.0916	R_1 = 0.1001, wR_2 = 0.2427	R_1 = 0.1884, wR_2 = 0.1689	R_1 = 0.1272, wR_2 = 0.2730	R_1 = 0.0892, wR_2 = 0.1902	R_1 = 0.0959, wR_2 = 0.2033
Largest diff. peak/hole / e $Å^{-3}$	3.50/-0.91	1.75/-2.94	1.13/-1.34	1.89/-1.82	0.79/-1.81	1.44/-2.00

Table S6: Bond lengths and angles for compound **1**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C6	1.477(6)	Fe1	C8	2.021(4)
Br1	C1	1.883(4)	Fe1	C9	2.011(4)
C1	Fe1	2.018(4)	Fe1	C10	2.043(4)
C1	C2	1.415(6)	C2	C3	1.419(6)
C1	C5	1.411(6)	C3	C4	1.416(6)
Fe1	C2	2.028(4)	C4	C5	1.428(6)
Fe1	C3	2.034(4)	C6	C7	1.396(7)
Fe1	C4	2.045(4)	C6	C10	1.421(7)
Fe1	C5	2.041(4)	C7	C8	1.418(7)
Fe1	C6	2.082(4)	C8	C9	1.391(7)
Fe1	C7	2.043(4)	C9	C10	1.409(7)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Br1	C1	Fe1	127.7(2)	C9	Fe1	C3	107.85(17)
C2	C1	Br1	124.2(3)	C9	Fe1	C4	123.28(18)
C2	C1	Fe1	69.9(2)	C9	Fe1	C5	159.2(2)
C5	C1	Br1	126.0(3)	C9	Fe1	C6	67.68(18)
C5	C1	Fe1	70.6(2)	C9	Fe1	C7	68.13(19)
C5	C1	C2	109.8(4)	C9	Fe1	C8	40.4(2)
C1	Fe1	C2	40.95(17)	C9	Fe1	C10	40.7(2)
C1	Fe1	C3	68.30(17)	C10	Fe1	C4	159.6(2)
C1	Fe1	C4	68.20(17)	C10	Fe1	C6	40.30(19)
C1	Fe1	C5	40.66(17)	C10	Fe1	C7	67.77(19)
C1	Fe1	C6	108.33(17)	C1	C2	Fe1	69.2(2)
C1	Fe1	C7	122.92(18)	C1	C2	C3	106.7(4)
C1	Fe1	C8	159.2(2)	C3	C2	Fe1	69.8(2)
C1	Fe1	C10	122.83(19)	C2	C3	Fe1	69.3(2)
C2	Fe1	C3	40.91(18)	C4	C3	Fe1	70.1(2)
C2	Fe1	C4	68.84(17)	C4	C3	C2	108.6(4)
C2	Fe1	C5	69.25(17)	C3	C4	Fe1	69.3(2)
C2	Fe1	C6	123.43(18)	C3	C4	C5	108.1(4)
C2	Fe1	C7	158.71(19)	C5	C4	Fe1	69.4(2)
C2	Fe1	C10	107.26(18)	C1	C5	Fe1	68.8(2)
C3	Fe1	C4	40.62(17)	C1	C5	C4	106.8(4)
C3	Fe1	C5	68.79(18)	C4	C5	Fe1	69.7(2)
C3	Fe1	C6	159.78(19)	N1	C6	Fe1	129.5(3)
C3	Fe1	C7	159.14(19)	C7	C6	N1	127.2(5)
C3	Fe1	C10	123.45(18)	C7	C6	Fe1	68.7(2)
C4	Fe1	C6	158.47(19)	C7	C6	C10	107.9(4)
C5	Fe1	C4	40.90(17)	C10	C6	N1	124.8(5)
C5	Fe1	C6	122.55(18)	C10	C6	Fe1	68.4(2)
C5	Fe1	C7	107.28(18)	C6	C7	Fe1	71.7(2)
C5	Fe1	C10	158.3(2)	C6	C7	C8	108.1(4)
C7	Fe1	C4	123.12(18)	C8	C7	Fe1	68.7(2)
C7	Fe1	C6	39.53(19)	C7	C8	Fe1	70.4(2)
C8	Fe1	C2	158.58(19)	C9	C8	Fe1	69.4(2)
C8	Fe1	C3	122.85(18)	C9	C8	C7	107.9(4)

C8	Fe1	C4	107.80(18)	C8	C9	Fe1	70.2(2)
C8	Fe1	C5	122.96(19)	C8	C9	C10	108.7(4)
C8	Fe1	C6	67.45(18)	C10	C9	Fe1	70.9(3)
C8	Fe1	C7	40.85(19)	C6	C10	Fe1	71.3(2)
C8	Fe1	C10	68.1(2)	C9	C10	Fe1	68.4(2)
C9	Fe1	C1	158.92(19)	C9	C10	C6	107.3(4)
C9	Fe1	C2	122.53(19)				

Table S7: Bond lengths and angles for compound **3a**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	C1	2.040(3)	Fe2	C25	2.038(3)
Fe1	C2	2.048(3)	Fe2	C26	2.035(3)
Fe1	C3	2.057(3)	Fe2	C27	2.045(3)
Fe1	C4	2.051(3)	Fe2	C28	2.055(3)
Fe1	C5	2.049(3)	Fe2	C29	2.044(3)
Fe1	C6	2.112(3)	Fe2	C30	2.088(3)
Fe1	C7	2.061(3)	Fe2	C31	2.046(3)
Fe1	C8	2.033(3)	Fe2	C32	2.029(3)
Fe1	C9	2.028(3)	Fe2	C33	2.031(3)
Fe1	C10	2.050(3)	Fe2	C34	2.044(3)
P1	C1	1.814(3)	P2	C25	1.814(3)
P1	C11	1.837(3)	P2	C35	1.835(3)
P1	C17	1.844(3)	P2	C41	1.840(3)
N1	C6	1.391(4)	N2	C30	1.400(4)
N1	C23	1.453(4)	N2	C47	1.469(4)
N1	C24	1.459(4)	N2	C48	1.453(4)
C1	C2	1.436(4)	C25	C26	1.438(4)
C1	C5	1.435(4)	C25	C29	1.430(4)
C2	C3	1.437(4)	C26	C27	1.419(4)
C3	C4	1.420(4)	C27	C28	1.425(4)
C4	C5	1.426(4)	C28	C29	1.419(4)
C6	C7	1.439(4)	C30	C31	1.431(4)
C6	C10	1.433(4)	C30	C34	1.421(4)
C7	C8	1.431(4)	C31	C32	1.429(4)
C8	C9	1.404(5)	C32	C33	1.418(4)
C9	C10	1.424(4)	C33	C34	1.422(4)
C11	C12	1.390(4)	C35	C36	1.396(4)
C11	C16	1.402(4)	C35	C40	1.396(4)
C12	C13	1.386(4)	C36	C37	1.391(4)
C13	C14	1.382(5)	C37	C38	1.387(5)
C14	C15	1.392(5)	C38	C39	1.382(4)
C15	C16	1.385(4)	C39	C40	1.390(4)
C17	C18	1.396(4)	C41	C42	1.395(4)
C17	C22	1.397(4)	C41	C46	1.399(4)
C18	C19	1.385(4)	C42	C43	1.382(5)
C19	C20	1.388(4)	C43	C44	1.376(5)
C20	C21	1.391(4)	C44	C45	1.387(5)
C21	C22	1.382(4)	C45	C46	1.390(4)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	Fe1	C2	41.13(11)	C25	Fe2	C27	69.13(11)
C1	Fe1	C3	69.15(11)	C25	Fe2	C28	68.95(11)
C1	Fe1	C4	68.95(11)	C25	Fe2	C29	41.00(11)
C1	Fe1	C5	41.09(11)	C25	Fe2	C30	124.27(12)
C1	Fe1	C6	124.17(11)	C25	Fe2	C31	160.43(12)
C1	Fe1	C7	160.81(11)	C25	Fe2	C34	107.67(11)
C1	Fe1	C10	106.72(11)	C26	Fe2	C25	41.35(11)
C2	Fe1	C3	40.97(11)	C26	Fe2	C27	40.71(12)
C2	Fe1	C4	68.52(11)	C26	Fe2	C28	68.58(12)
C2	Fe1	C5	68.77(11)	C26	Fe2	C29	68.72(12)
C2	Fe1	C6	109.17(11)	C26	Fe2	C30	107.13(12)
C2	Fe1	C7	124.63(12)	C26	Fe2	C31	122.99(12)
C2	Fe1	C10	122.48(12)	C26	Fe2	C34	121.29(12)
C3	Fe1	C6	123.90(12)	C27	Fe2	C28	40.68(12)
C3	Fe1	C7	108.38(12)	C27	Fe2	C30	120.80(12)
C4	Fe1	C3	40.44(12)	C27	Fe2	C31	106.33(12)
C4	Fe1	C6	158.73(12)	C28	Fe2	C30	156.17(12)
C4	Fe1	C7	122.31(12)	C29	Fe2	C27	68.39(12)
C5	Fe1	C3	68.51(12)	C29	Fe2	C28	40.51(11)
C5	Fe1	C4	40.69(11)	C29	Fe2	C30	161.80(12)
C5	Fe1	C6	159.94(11)	C29	Fe2	C31	156.70(12)
C5	Fe1	C7	157.25(11)	C31	Fe2	C28	120.78(12)
C5	Fe1	C10	122.78(12)	C31	Fe2	C30	40.49(11)
C7	Fe1	C6	40.33(11)	C32	Fe2	C25	157.19(12)
C8	Fe1	C1	156.37(12)	C32	Fe2	C26	160.02(13)
C8	Fe1	C2	160.93(12)	C32	Fe2	C27	123.47(13)
C8	Fe1	C3	123.73(12)	C32	Fe2	C28	107.17(12)
C8	Fe1	C4	106.96(12)	C32	Fe2	C29	121.56(12)
C8	Fe1	C5	120.70(12)	C32	Fe2	C30	68.43(12)
C8	Fe1	C6	67.92(11)	C32	Fe2	C31	41.07(12)
C8	Fe1	C7	40.90(12)	C32	Fe2	C33	40.88(12)
C8	Fe1	C10	68.37(12)	C32	Fe2	C34	68.73(12)
C9	Fe1	C1	120.76(12)	C33	Fe2	C25	121.68(12)
C9	Fe1	C2	157.70(12)	C33	Fe2	C26	157.37(12)
C9	Fe1	C3	159.17(12)	C33	Fe2	C27	160.97(12)
C9	Fe1	C4	122.48(12)	C33	Fe2	C28	124.81(12)
C9	Fe1	C5	105.99(12)	C33	Fe2	C29	108.47(12)
C9	Fe1	C6	67.93(11)	C33	Fe2	C30	68.13(11)
C9	Fe1	C7	68.48(13)	C33	Fe2	C31	68.71(12)
C9	Fe1	C8	40.44(13)	C33	Fe2	C34	40.84(11)
C9	Fe1	C10	40.87(12)	C34	Fe2	C27	156.17(12)
C10	Fe1	C3	158.93(12)	C34	Fe2	C28	162.09(12)
C10	Fe1	C4	159.13(12)	C34	Fe2	C29	125.60(12)
C10	Fe1	C6	40.23(11)	C34	Fe2	C30	40.20(11)
C10	Fe1	C7	68.36(12)	C34	Fe2	C31	68.36(12)
C1	P1	C11	101.63(12)	C25	P2	C35	100.68(13)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	P1	C17	102.64(12)	C25	P2	C41	99.55(13)
C11	P1	C17	98.98(12)	C35	P2	C41	101.47(13)
C6	N1	C23	115.1(2)	C30	N2	C47	114.9(3)
C6	N1	C24	115.0(2)	C30	N2	C48	114.8(3)
C23	N1	C24	113.2(3)	C48	N2	C47	113.3(3)
P1	C1	Fe1	125.27(14)	P2	C25	Fe2	125.58(14)
C2	C1	Fe1	69.73(15)	C26	C25	Fe2	69.19(16)
C2	C1	P1	122.5(2)	C26	C25	P2	125.0(2)
C5	C1	Fe1	69.78(16)	C29	C25	Fe2	69.73(16)
C5	C1	P1	130.1(2)	C29	C25	P2	128.2(2)
C5	C1	C2	107.4(2)	C29	C25	C26	106.8(3)
C1	C2	Fe1	69.14(15)	C25	C26	Fe2	69.46(16)
C1	C2	C3	108.1(2)	C27	C26	Fe2	70.04(16)
C3	C2	Fe1	69.84(15)	C27	C26	C25	108.4(3)
C2	C3	Fe1	69.19(15)	C26	C27	Fe2	69.24(16)
C4	C3	Fe1	69.55(16)	C26	C27	C28	108.2(3)
C4	C3	C2	107.8(2)	C28	C27	Fe2	70.05(16)
C3	C4	Fe1	70.00(16)	C27	C28	Fe2	69.28(16)
C3	C4	C5	108.6(2)	C29	C28	Fe2	69.33(15)
C5	C4	Fe1	69.58(15)	C29	C28	C27	107.8(3)
C1	C5	Fe1	69.13(16)	C25	C29	Fe2	69.26(15)
C4	C5	Fe1	69.73(16)	C28	C29	Fe2	70.16(16)
C4	C5	C1	108.1(2)	C28	C29	C25	108.8(3)
N1	C6	Fe1	131.8(2)	N2	C30	Fe2	130.3(2)
N1	C6	C7	126.6(3)	N2	C30	C31	127.1(3)
N1	C6	C10	126.3(3)	N2	C30	C34	125.5(3)
C7	C6	Fe1	67.91(15)	C31	C30	Fe2	68.17(16)
C10	C6	Fe1	67.54(15)	C34	C30	Fe2	68.21(16)
C10	C6	C7	107.0(3)	C34	C30	C31	107.3(3)
C6	C7	Fe1	71.76(16)	C30	C31	Fe2	71.34(16)
C8	C7	Fe1	68.52(16)	C32	C31	Fe2	68.82(16)
C8	C7	C6	107.7(3)	C32	C31	C30	108.1(3)
C7	C8	Fe1	70.58(16)	C31	C32	Fe2	70.11(16)
C9	C8	Fe1	69.59(17)	C33	C32	Fe2	69.66(16)
C9	C8	C7	108.5(3)	C33	C32	C31	107.8(3)
C8	C9	Fe1	69.97(17)	C32	C33	Fe2	69.47(17)
C8	C9	C10	108.4(3)	C32	C33	C34	108.1(3)
C10	C9	Fe1	70.38(16)	C34	C33	Fe2	70.05(16)
C6	C10	Fe1	72.22(16)	C30	C34	Fe2	71.59(16)
C9	C10	Fe1	68.75(16)	C30	C34	C33	108.6(3)
C9	C10	C6	108.2(3)	C33	C34	Fe2	69.11(16)
C12	C11	P1	124.6(2)	C36	C35	P2	118.3(2)
C12	C11	C16	118.3(3)	C36	C35	C40	118.6(3)
C16	C11	P1	117.0(2)	C40	C35	P2	123.0(2)
C13	C12	C11	120.5(3)	C37	C36	C35	120.7(3)
C14	C13	C12	120.8(3)	C38	C37	C36	120.0(3)
C13	C14	C15	119.4(3)	C39	C38	C37	119.9(3)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C16	C15	C14	119.9(3)	C38	C39	C40	120.2(3)
C15	C16	C11	121.0(3)	C39	C40	C35	120.6(3)
C18	C17	P1	122.8(2)	C42	C41	P2	118.5(2)
C18	C17	C22	118.3(3)	C42	C41	C46	118.1(3)
C22	C17	P1	118.8(2)	C46	C41	P2	123.4(2)
C19	C18	C17	121.1(3)	C43	C42	C41	120.9(3)
C18	C19	C20	120.2(3)	C44	C43	C42	120.6(3)
C19	C20	C21	119.0(3)	C43	C44	C45	119.5(3)
C22	C21	C20	120.9(3)	C44	C45	C46	120.3(3)
C21	C22	C17	120.5(3)	C45	C46	C41	120.5(3)

Table S8: Bond lengths and angles for compound **3b**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	C1	2.072(3)	C6	C10	1.424(4)
Fe1	C2	2.040(3)	C7	C8	1.432(5)
Fe1	C3	2.050(3)	C8	C9	1.424(5)
Fe1	C4	2.047(3)	C9	C10	1.420(5)
Fe1	C5	2.042(3)	C11	C12	1.412(4)
Fe1	C6	2.119(3)	C11	C16	1.409(4)
Fe1	C7	2.045(3)	C12	C13	1.397(4)
Fe1	C8	2.034(3)	C12	C17	1.505(4)
Fe1	C9	2.042(3)	C13	C14	1.375(4)
Fe1	C10	2.062(3)	C14	C15	1.394(4)
P1	C1	1.813(3)	C14	C18	1.502(4)
P1	C11	1.843(3)	C15	C16	1.394(4)
P1	C20	1.852(3)	C16	C19	1.502(4)
N1	C6	1.386(4)	C20	C21	1.423(4)
N1	C29	1.460(4)	C20	C25	1.412(4)
N1	C30	1.462(4)	C21	C22	1.393(4)
C1	C2	1.437(4)	C21	C26	1.507(4)
C1	C5	1.433(4)	C22	C23	1.378(5)
C2	C3	1.425(4)	C23	C24	1.388(4)
C3	C4	1.416(5)	C23	C27	1.505(4)
C4	C5	1.417(4)	C24	C25	1.394(4)
C6	C7	1.422(4)	C25	C28	1.513(4)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	Fe1	C6	132.86(12)	C3	C2	Fe1	69.98(18)
C2	Fe1	C1	40.90(11)	C3	C2	C1	108.1(3)
C2	Fe1	C3	40.79(12)	C2	C3	Fe1	69.23(17)
C2	Fe1	C4	68.56(12)	C4	C3	Fe1	69.65(17)
C2	Fe1	C5	68.68(12)	C4	C3	C2	108.2(3)
C2	Fe1	C6	108.20(12)	C3	C4	Fe1	69.90(18)
C2	Fe1	C7	127.32(13)	C3	C4	C5	108.1(3)
C2	Fe1	C9	151.64(13)	C5	C4	Fe1	69.54(16)
C2	Fe1	C10	118.13(12)	C1	C5	Fe1	70.77(17)
C3	Fe1	C1	68.43(11)	C4	C5	Fe1	69.91(17)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C3	Fe1	C6	113.96(12)	C4	C5	C1	108.7(3)
C3	Fe1	C10	147.74(13)	N1	C6	Fe1	131.9(2)
C4	Fe1	C1	68.43(11)	N1	C6	C7	126.5(3)
C4	Fe1	C3	40.44(13)	N1	C6	C10	126.5(3)
C4	Fe1	C6	145.18(12)	C7	C6	Fe1	67.24(17)
C4	Fe1	C10	171.80(12)	C7	C6	C10	106.9(3)
C5	Fe1	C1	40.75(12)	C10	C6	Fe1	67.94(16)
C5	Fe1	C3	68.19(12)	C6	C7	Fe1	72.88(17)
C5	Fe1	C4	40.55(11)	C6	C7	C8	108.7(3)
C5	Fe1	C6	172.92(11)	C8	C7	Fe1	69.03(17)
C5	Fe1	C7	147.09(12)	C7	C8	Fe1	69.86(17)
C5	Fe1	C9	111.82(12)	C9	C8	Fe1	69.87(18)
C5	Fe1	C10	135.34(11)	C9	C8	C7	107.6(3)
C7	Fe1	C1	167.81(13)	C8	C9	Fe1	69.25(18)
C7	Fe1	C3	104.24(12)	C10	C9	Fe1	70.52(18)
C7	Fe1	C4	112.83(12)	C10	C9	C8	107.6(3)
C7	Fe1	C6	39.87(12)	C6	C10	Fe1	72.26(17)
C7	Fe1	C10	67.63(12)	C9	C10	Fe1	69.00(18)
C8	Fe1	C1	151.06(13)	C9	C10	C6	109.2(3)
C8	Fe1	C2	165.94(13)	C12	C11	P1	115.4(2)
C8	Fe1	C3	127.14(13)	C16	C11	P1	125.5(2)
C8	Fe1	C4	106.50(13)	C16	C11	C12	119.1(3)
C8	Fe1	C5	116.76(13)	C11	C12	C17	122.6(3)
C8	Fe1	C6	67.84(12)	C13	C12	C11	119.2(3)
C8	Fe1	C7	41.11(13)	C13	C12	C17	118.2(3)
C8	Fe1	C9	40.88(13)	C14	C13	C12	122.5(3)
C8	Fe1	C10	68.14(13)	C13	C14	C15	117.8(3)
C9	Fe1	C1	120.34(12)	C13	C14	C18	121.5(3)
C9	Fe1	C3	167.49(13)	C15	C14	C18	120.7(3)
C9	Fe1	C4	131.48(13)	C16	C15	C14	122.2(3)
C9	Fe1	C6	67.66(12)	C11	C16	C19	123.6(3)
C9	Fe1	C7	68.62(13)	C15	C16	C11	119.1(3)
C9	Fe1	C10	40.48(13)	C15	C16	C19	117.2(3)
C10	Fe1	C1	112.99(11)	C21	C20	P1	114.5(2)
C10	Fe1	C6	39.80(11)	C25	C20	P1	127.0(2)
C1	P1	C11	101.72(13)	C25	C20	C21	117.9(3)
C1	P1	C20	109.10(13)	C20	C21	C26	122.4(3)
C11	P1	C20	105.18(13)	C22	C21	C20	119.8(3)
C6	N1	C29	115.4(3)	C22	C21	C26	117.8(3)
C6	N1	C30	116.0(2)	C23	C22	C21	122.7(3)
C29	N1	C30	112.8(3)	C22	C23	C24	117.1(3)
P1	C1	Fe1	129.47(15)	C22	C23	C27	122.0(3)
C2	C1	Fe1	68.34(16)	C24	C23	C27	120.9(3)
C2	C1	P1	133.0(2)	C23	C24	C25	123.1(3)
C5	C1	Fe1	68.49(16)	C20	C25	C28	124.8(3)
C5	C1	P1	120.3(2)	C24	C25	C20	119.4(3)
C5	C1	C2	106.7(2)	C24	C25	C28	115.8(3)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	C2	Fe1	70.75(17)				

Table S9: Bond lengths and angles for compound **4a**

Se1	P1	2.1076(8)	C3	C4	1.427(4)
N1	C6	1.389(4)	C4	C5	1.425(4)
N1	C11	1.456(4)	C6	C7	1.433(4)
N1	C12	1.459(4)	C6	C10	1.432(4)
Fe1	C1	2.028(3)	C7	C8	1.424(5)
Fe1	C2	2.056(3)	C8	C9	1.407(5)
Fe1	C3	2.063(3)	C9	C10	1.427(4)
Fe1	C4	2.051(3)	C13	C14	1.396(4)
Fe1	C5	2.023(3)	C13	C18	1.393(4)
Fe1	C6	2.135(3)	C14	C15	1.383(4)
Fe1	C7	2.069(3)	C15	C16	1.385(4)
Fe1	C8	2.023(3)	C16	C17	1.391(4)
Fe1	C9	2.023(3)	C17	C18	1.387(4)
Fe1	C10	2.048(3)	C19	C20	1.394(4)
P1	C1	1.788(3)	C19	C24	1.405(4)
P1	C13	1.816(3)	C20	C21	1.393(4)
P1	C19	1.806(3)	C21	C22	1.391(4)
C1	C2	1.440(4)	C22	C23	1.378(4)
C1	C5	1.436(4)	C23	C24	1.389(4)
C2	C3	1.417(4)			

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C6	N1	C11	115.9(3)	C19	P1	C13	104.42(12)
C6	N1	C12	116.7(3)	P1	C1	Fe1	129.33(15)
C11	N1	C12	114.2(3)	C2	C1	Fe1	70.41(15)
C1	Fe1	C2	41.28(11)	C2	C1	P1	125.7(2)
C1	Fe1	C3	68.80(11)	C5	C1	Fe1	69.09(15)
C1	Fe1	C4	69.08(11)	C5	C1	P1	126.6(2)
C1	Fe1	C6	139.10(11)	C5	C1	C2	107.5(2)
C1	Fe1	C7	178.88(12)	C1	C2	Fe1	68.32(15)
C1	Fe1	C10	111.07(11)	C3	C2	Fe1	70.14(17)
C2	Fe1	C3	40.25(11)	C3	C2	C1	108.0(3)
C2	Fe1	C6	113.48(11)	C2	C3	Fe1	69.61(16)
C2	Fe1	C7	138.05(12)	C2	C3	C4	108.4(3)
C3	Fe1	C6	114.79(12)	C4	C3	Fe1	69.28(17)
C3	Fe1	C7	111.21(12)	C3	C4	Fe1	70.14(17)
C4	Fe1	C2	68.34(12)	C5	C4	Fe1	68.47(16)
C4	Fe1	C3	40.58(13)	C5	C4	C3	108.2(2)
C4	Fe1	C6	141.76(12)	C1	C5	Fe1	69.40(15)
C4	Fe1	C7	111.71(12)	C4	C5	Fe1	70.59(17)
C5	Fe1	C1	41.51(11)	C4	C5	C1	107.9(2)
C5	Fe1	C2	69.29(12)	N1	C6	Fe1	132.8(2)
C5	Fe1	C3	68.84(12)	N1	C6	C7	126.1(3)
C5	Fe1	C4	40.94(12)	N1	C6	C10	126.5(3)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C5	Fe1	C6	176.37(11)	C7	C6	Fe1	67.63(16)
C5	Fe1	C7	139.60(12)	C10	C6	Fe1	66.76(16)
C5	Fe1	C10	137.16(12)	C10	C6	C7	107.4(3)
C7	Fe1	C6	39.80(12)	C6	C7	Fe1	72.57(16)
C8	Fe1	C1	140.04(12)	C8	C7	Fe1	67.90(17)
C8	Fe1	C2	177.02(12)	C8	C7	C6	107.6(3)
C8	Fe1	C3	136.78(13)	C7	C8	Fe1	71.40(17)
C8	Fe1	C4	109.22(13)	C9	C8	Fe1	69.64(17)
C8	Fe1	C5	110.13(13)	C9	C8	C7	108.9(3)
C8	Fe1	C6	67.24(12)	C8	C9	Fe1	69.64(18)
C8	Fe1	C7	40.70(13)	C8	C9	C10	107.9(3)
C8	Fe1	C10	68.51(13)	C10	C9	Fe1	70.44(16)
C9	Fe1	C1	111.54(12)	C6	C10	Fe1	73.26(17)
C9	Fe1	C2	142.25(12)	C9	C10	Fe1	68.52(17)
C9	Fe1	C3	176.29(13)	C9	C10	C6	108.0(3)
C9	Fe1	C4	135.81(13)	C14	C13	P1	118.5(2)
C9	Fe1	C5	108.82(13)	C18	C13	P1	122.4(2)
C9	Fe1	C6	67.56(12)	C18	C13	C14	119.2(3)
C9	Fe1	C7	68.52(12)	C15	C14	C13	120.6(3)
C9	Fe1	C8	40.71(13)	C14	C15	C16	120.1(3)
C9	Fe1	C10	41.03(13)	C15	C16	C17	119.7(3)
C10	Fe1	C2	114.00(12)	C18	C17	C16	120.4(3)
C10	Fe1	C3	142.59(13)	C17	C18	C13	120.1(3)
C10	Fe1	C4	176.82(12)	C20	C19	P1	120.4(2)
C10	Fe1	C6	39.98(11)	C20	C19	C24	119.5(2)
C10	Fe1	C7	68.20(12)	C24	C19	P1	120.0(2)
C1	P1	Se1	116.28(9)	C21	C20	C19	120.1(3)
C1	P1	C13	104.87(12)	C22	C21	C20	119.8(3)
C1	P1	C19	104.00(13)	C23	C22	C21	120.5(3)
C13	P1	Se1	111.30(9)	C22	C23	C24	120.2(3)
C19	P1	Se1	114.79(9)	C23	C24	C19	119.9(3)

Table S10: Bond lengths and angles for compound **7**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	Cl1	2.3599(6)	C11	C16	1.413(3)
Pd1	P1	2.3470(6)	C12	C13	1.390(3)
Pd1	Cl2	2.3461(6)	C12	C17	1.511(3)
Pd1	P2	2.2899(6)	C13	C14	1.379(4)
Fe1	C1	2.033(2)	C14	C15	1.381(4)
Fe1	C2	2.039(2)	C14	C18	1.511(4)
Fe1	C3	2.047(2)	C15	C16	1.391(4)
Fe1	C4	2.043(3)	C16	C19	1.497(4)
Fe1	C5	2.013(2)	C20	C21	1.411(3)
Fe1	C6	1.996(2)	C20	C25	1.424(3)
Fe1	C7	2.030(2)	C21	C22	1.394(3)
Fe1	C8	2.066(2)	C21	C26	1.499(3)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	C9	2.071(3)	C22	C23	1.384(4)
Fe1	C10	2.032(3)	C23	C24	1.388(4)
P1	C1	1.812(2)	C23	C27	1.494(3)
P1	C11	1.852(2)	C24	C25	1.388(4)
P1	C20	1.853(2)	C25	C28	1.515(3)
C1	C2	1.454(3)	C29	C30	1.392(3)
C1	C5	1.437(3)	C29	C34	1.408(3)
P2	C6	1.804(2)	C30	C31	1.381(3)
P2	C29	1.828(2)	C31	C32	1.378(4)
P2	C35	1.825(2)	C32	C33	1.379(4)
C2	C3	1.408(4)	C33	C34	1.386(4)
C3	C4	1.422(4)	C35	C36	1.389(3)
C4	C5	1.414(3)	C35	C40	1.394(3)
C6	C7	1.443(3)	C36	C37	1.384(4)
C6	C10	1.431(3)	C37	C38	1.376(4)
C7	C8	1.419(4)	C38	C39	1.379(4)
C8	C9	1.403(4)	C39	C40	1.386(4)
C9	C10	1.416(3)	Cl3	C41	1.749(3)
C11	C12	1.413(3)	Cl4	C41	1.741(3)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
P1	Pd1	Cl1	177.77(2)	C2	C3	Fe1	69.52(14)
Cl2	Pd1	Cl1	86.11(2)	C2	C3	C4	108.4(2)
Cl2	Pd1	P1	91.68(2)	C4	C3	Fe1	69.50(14)
P2	Pd1	Cl1	80.49(2)	C3	C4	Fe1	69.81(14)
P2	Pd1	P1	101.73(2)	C5	C4	Fe1	68.46(14)
P2	Pd1	Cl2	165.68(2)	C5	C4	C3	108.4(2)
C1	Fe1	C2	41.84(9)	C1	C5	Fe1	69.96(13)
C1	Fe1	C3	69.29(10)	C4	C5	Fe1	70.76(14)
C1	Fe1	C4	69.16(10)	C4	C5	C1	108.5(2)
C1	Fe1	C8	142.05(10)	P2	C6	Fe1	123.99(13)
C1	Fe1	C9	177.93(10)	C7	C6	Fe1	70.26(13)
C2	Fe1	C3	40.32(10)	C7	C6	P2	127.23(19)
C2	Fe1	C4	68.44(10)	C10	C6	Fe1	70.54(14)
C2	Fe1	C8	113.38(10)	C10	C6	P2	125.79(19)
C2	Fe1	C9	140.01(10)	C10	C6	C7	107.0(2)
C3	Fe1	C8	111.76(10)	C6	C7	Fe1	67.75(13)
C3	Fe1	C9	111.62(10)	C8	C7	Fe1	71.09(15)
C4	Fe1	C3	40.69(11)	C8	C7	C6	107.4(2)
C4	Fe1	C8	137.63(10)	C7	C8	Fe1	68.39(13)
C4	Fe1	C9	110.22(11)	C9	C8	Fe1	70.37(15)
C5	Fe1	C1	41.59(10)	C9	C8	C7	109.0(2)
C5	Fe1	C2	69.64(10)	C8	C9	Fe1	69.98(15)
C5	Fe1	C3	69.02(10)	C8	C9	C10	108.3(2)
C5	Fe1	C4	40.78(10)	C10	C9	Fe1	68.35(14)
C5	Fe1	C7	141.04(10)	C6	C10	Fe1	67.86(13)
C5	Fe1	C8	176.35(11)	C9	C10	Fe1	71.29(15)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C5	Fe1	C9	136.70(11)	C9	C10	C6	108.3(2)
C5	Fe1	C10	109.18(10)	C12	C11	P1	116.63(17)
C6	Fe1	C1	109.95(9)	C12	C11	C16	118.3(2)
C6	Fe1	C2	139.41(10)	C16	C11	P1	125.01(19)
C6	Fe1	C3	179.07(10)	C11	C12	C17	125.0(2)
C6	Fe1	C4	138.67(10)	C13	C12	C11	119.7(2)
C6	Fe1	C5	110.07(10)	C13	C12	C17	115.3(2)
C6	Fe1	C7	41.99(10)	C14	C13	C12	122.6(2)
C6	Fe1	C8	69.16(10)	C13	C14	C15	117.2(2)
C6	Fe1	C9	69.12(10)	C13	C14	C18	121.2(3)
C6	Fe1	C10	41.61(10)	C15	C14	C18	121.6(2)
C7	Fe1	C1	112.51(10)	C14	C15	C16	123.1(2)
C7	Fe1	C2	112.14(10)	C11	C16	C19	125.0(2)
C7	Fe1	C3	138.68(10)	C15	C16	C11	119.0(2)
C7	Fe1	C4	178.14(10)	C15	C16	C19	116.0(2)
C7	Fe1	C8	40.52(10)	C21	C20	P1	122.65(17)
C7	Fe1	C9	68.14(11)	C21	C20	C25	118.5(2)
C7	Fe1	C10	69.31(10)	C25	C20	P1	118.75(17)
C8	Fe1	C9	39.65(11)	C20	C21	C26	123.9(2)
C10	Fe1	C1	137.76(10)	C22	C21	C20	119.7(2)
C10	Fe1	C2	178.55(10)	C22	C21	C26	116.4(2)
C10	Fe1	C3	138.65(11)	C23	C22	C21	122.3(2)
C10	Fe1	C4	110.12(11)	C22	C23	C24	117.6(2)
C10	Fe1	C8	67.76(10)	C22	C23	C27	121.8(2)
C10	Fe1	C9	40.36(10)	C24	C23	C27	120.6(2)
C1	P1	Pd1	111.86(8)	C25	C24	C23	122.9(2)
C1	P1	C11	111.22(11)	C20	C25	C28	126.3(2)
C1	P1	C20	100.62(10)	C24	C25	C20	119.0(2)
C11	P1	Pd1	109.08(7)	C24	C25	C28	114.6(2)
C11	P1	C20	101.61(11)	C30	C29	P2	122.21(18)
C20	P1	Pd1	121.78(8)	C30	C29	C34	118.4(2)
P1	C1	Fe1	126.62(12)	C34	C29	P2	119.09(18)
C2	C1	Fe1	69.29(13)	C31	C30	C29	120.5(2)
C2	C1	P1	127.03(19)	C32	C31	C30	120.6(2)
C5	C1	Fe1	68.44(13)	C31	C32	C33	120.0(2)
C5	C1	P1	126.63(18)	C32	C33	C34	120.2(2)
C5	C1	C2	106.3(2)	C33	C34	C29	120.3(2)
C6	P2	Pd1	124.22(8)	C36	C35	P2	122.71(19)
C6	P2	C29	99.73(11)	C36	C35	C40	119.0(2)
C6	P2	C35	100.18(11)	C40	C35	P2	118.06(18)
C29	P2	Pd1	115.02(8)	C37	C36	C35	119.8(2)
C35	P2	Pd1	106.86(8)	C38	C37	C36	120.8(2)
C35	P2	C29	109.43(11)	C37	C38	C39	119.9(3)
C1	C2	Fe1	68.87(13)	C38	C39	C40	119.8(2)
C3	C2	Fe1	70.16(14)	C39	C40	C35	120.6(2)
C3	C2	C1	108.3(2)	Cl4	C41	Cl3	113.83(18)

Table S11: Bond lengths and angles for compound **8**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	Cl1	2.3792(12)	C9	C10	1.428(7)
Pd1	P1	2.3167(13)	C11	C12	1.414(7)
Pd1	Cl2	2.3285(13)	C11	C16	1.409(7)
Pd1	P2	2.3518(13)	C12	C13	1.403(7)
Fe1	C1	2.023(5)	C12	C17	1.494(7)
Fe1	C2	2.053(5)	C13	C14	1.379(8)
Fe1	C3	2.069(5)	C14	C15	1.380(8)
Fe1	C4	2.047(5)	C14	C18	1.508(7)
Fe1	C5	2.007(5)	C15	C16	1.394(7)
Fe1	C6	2.019(5)	C16	C19	1.502(8)
Fe1	C7	2.019(5)	C20	C21	1.425(7)
Fe1	C8	2.060(6)	C20	C25	1.422(7)
Fe1	C9	2.063(5)	C21	C22	1.382(8)
Fe1	C10	2.032(5)	C21	C26	1.501(7)
P1	C1	1.835(5)	C22	C23	1.394(8)
P1	C11	1.861(5)	C23	C24	1.361(8)
P1	C20	1.851(5)	C23	C27	1.510(8)
C1	C2	1.435(7)	C24	C25	1.393(8)
C1	C5	1.419(7)	C25	C28	1.517(7)
P2	C6	1.818(5)	C29	C30	1.529(8)
P2	C29	1.888(5)	C29	C31	1.539(7)
P2	C33	1.913(6)	C29	C32	1.539(7)
C2	C3	1.424(7)	C33	C34	1.537(7)
C3	C4	1.407(8)	C33	C35	1.552(7)
C4	C5	1.433(7)	C33	C36	1.534(7)
C6	C7	1.439(7)	Cl5	C38	1.752(7)
C6	C10	1.449(7)	Cl6	C38	1.750(6)
C7	C8	1.423(7)	Cl3	C37	1.761(6)
C8	C9	1.413(8)	Cl4	C37	1.756(6)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
P1	Pd1	Cl1	81.99(5)	C3	C2	C1	108.0(5)
P1	Pd1	Cl2	167.48(5)	C2	C3	Fe1	69.2(3)
P1	Pd1	P2	103.37(5)	C4	C3	Fe1	69.2(3)
Cl2	Pd1	Cl1	85.62(5)	C4	C3	C2	108.4(5)
Cl2	Pd1	P2	88.94(5)	C3	C4	Fe1	70.9(3)
P2	Pd1	Cl1	174.17(5)	C3	C4	C5	108.1(5)
C1	Fe1	C2	41.2(2)	C5	C4	Fe1	67.8(3)
C1	Fe1	C3	68.8(2)	C1	C5	Fe1	70.0(3)
C1	Fe1	C4	69.2(2)	C1	C5	C4	108.2(5)
C1	Fe1	C8	148.7(2)	C4	C5	Fe1	70.8(3)
C1	Fe1	C9	170.3(2)	P2	C6	Fe1	133.1(3)
C1	Fe1	C10	131.1(2)	C7	C6	Fe1	69.1(3)
C2	Fe1	C3	40.4(2)	C7	C6	P2	123.6(4)
C2	Fe1	C8	116.2(2)	C7	C6	C10	106.3(4)
C2	Fe1	C9	147.4(2)	C10	C6	Fe1	69.5(3)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C4	Fe1	C2	68.1(2)	C10	C6	P2	129.4(4)
C4	Fe1	C3	40.0(2)	C6	C7	Fe1	69.1(3)
C4	Fe1	C8	130.0(2)	C8	C7	Fe1	71.1(3)
C4	Fe1	C9	107.9(2)	C8	C7	C6	109.0(5)
C5	Fe1	C1	41.2(2)	C7	C8	Fe1	68.0(3)
C5	Fe1	C2	69.0(2)	C9	C8	Fe1	70.1(3)
C5	Fe1	C3	68.6(2)	C9	C8	C7	107.9(5)
C5	Fe1	C4	41.4(2)	C8	C9	Fe1	69.9(3)
C5	Fe1	C6	114.8(2)	C8	C9	C10	108.8(5)
C5	Fe1	C7	148.6(2)	C10	C9	Fe1	68.4(3)
C5	Fe1	C8	169.1(2)	C6	C10	Fe1	68.6(3)
C5	Fe1	C9	130.6(2)	C9	C10	Fe1	70.7(3)
C5	Fe1	C10	107.4(2)	C9	C10	C6	107.9(5)
C6	Fe1	C1	107.7(2)	C12	C11	P1	124.6(4)
C6	Fe1	C2	131.6(2)	C16	C11	P1	116.8(4)
C6	Fe1	C3	170.9(2)	C16	C11	C12	118.6(4)
C6	Fe1	C4	147.8(2)	C11	C12	C17	125.9(5)
C6	Fe1	C8	69.7(2)	C13	C12	C11	118.4(5)
C6	Fe1	C9	69.5(2)	C13	C12	C17	115.6(5)
C6	Fe1	C10	41.9(2)	C14	C13	C12	122.7(5)
C7	Fe1	C1	116.2(2)	C13	C14	C15	117.6(5)
C7	Fe1	C2	109.1(2)	C13	C14	C18	120.4(5)
C7	Fe1	C3	131.3(2)	C15	C14	C18	121.9(5)
C7	Fe1	C4	169.2(2)	C14	C15	C16	122.4(5)
C7	Fe1	C6	41.7(2)	C11	C16	C19	123.4(4)
C7	Fe1	C8	40.8(2)	C15	C16	C11	119.2(5)
C7	Fe1	C9	68.4(2)	C15	C16	C19	117.2(5)
C7	Fe1	C10	69.6(2)	C21	C20	P1	118.3(4)
C8	Fe1	C3	108.6(2)	C25	C20	P1	123.5(4)
C8	Fe1	C9	40.1(2)	C25	C20	C21	118.0(5)
C9	Fe1	C3	115.4(2)	C20	C21	C26	125.8(5)
C10	Fe1	C2	171.4(2)	C22	C21	C20	119.2(5)
C10	Fe1	C3	146.6(2)	C22	C21	C26	115.0(5)
C10	Fe1	C4	114.8(2)	C21	C22	C23	122.8(5)
C10	Fe1	C8	68.7(2)	C22	C23	C27	121.0(5)
C10	Fe1	C9	40.8(2)	C24	C23	C22	117.4(5)
C1	P1	Pd1	120.90(17)	C24	C23	C27	121.6(5)
C1	P1	C11	101.9(2)	C23	C24	C25	123.3(5)
C1	P1	C20	97.5(2)	C20	C25	C28	125.0(5)
C11	P1	Pd1	108.18(16)	C24	C25	C20	119.1(5)
C20	P1	Pd1	116.54(16)	C24	C25	C28	115.7(5)
C20	P1	C11	110.6(2)	C30	C29	P2	107.5(3)
P1	C1	Fe1	130.6(3)	C30	C29	C31	108.4(5)
C2	C1	Fe1	70.5(3)	C30	C29	C32	108.9(4)
C2	C1	P1	128.7(4)	C31	C29	P2	108.9(4)
C5	C1	Fe1	68.8(3)	C31	C29	C32	108.0(4)
C5	C1	P1	123.7(4)	C32	C29	P2	115.0(4)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C5	C1	C2	107.4(4)	C34	C33	P2	114.3(4)
C6	P2	Pd1	115.91(17)	C34	C33	C35	106.8(4)
C6	P2	C29	107.2(2)	C35	C33	P2	110.2(4)
C6	P2	C33	98.4(2)	C36	C33	P2	108.4(4)
C29	P2	Pd1	108.12(17)	C36	C33	C34	108.6(4)
C29	P2	C33	109.3(2)	C36	C33	C35	108.3(5)
C33	P2	Pd1	117.20(17)	Cl6	C38	Cl5	110.3(3)
C1	C2	Fe1	68.3(3)	Cl4	C37	Cl3	111.8(3)
C3	C2	Fe1	70.4(3)				

Table S12: Bond lengths and angles for compound **9**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	$Cl1^1$	2.2933(18)	C1	C5	1.437(8)
Pd1	Cl1	2.2933(18)	C2	C3	1.397(8)
Pd1	P1	2.3361(17)	C3	C4	1.425(9)
Pd1	$P1^1$	2.3361(17)	C4	C5	1.426(8)
Fe1	C1	2.052(6)	C6	C7	1.437(8)
Fe1	C2	2.034(6)	C6	C10	1.432(8)
Fe1	C3	2.044(6)	C7	C8	1.418(9)
Fe1	C4	2.060(6)	C8	C9	1.432(9)
Fe1	C5	2.048(6)	C9	C10	1.453(9)
Fe1	C6	2.103(6)	C11	C12	1.387(8)
Fe1	C7	2.055(6)	C11	C16	1.388(8)
Fe1	C8	2.045(6)	C12	C13	1.389(8)
Fe1	C9	2.053(6)	C13	C14	1.387(9)
Fe1	C10	2.067(6)	C14	C15	1.373(9)
P1	C1	1.789(6)	C15	C16	1.390(8)
P1	C11	1.826(6)	C17	C18	1.386(8)
P1	C17	1.829(6)	C17	C22	1.410(8)
N1	C6	1.393(8)	C18	C19	1.381(8)
N1	C23	1.446(8)	C19	C20	1.383(9)
N1	C24	1.465(8)	C20	C21	1.374(9)
C1	C2	1.445(8)	C21	C22	1.394(9)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
$Cl1^1$	Pd1	Cl1	180.0	C17	P1	Pd1	120.09(19)
$Cl1^1$	Pd1	$P1^1$	93.06(7)	C6	N1	C23	115.9(5)
$Cl1^1$	Pd1	P1	86.94(7)	C6	N1	C24	115.6(5)
Cl1	Pd1	P1	93.06(7)	C23	N1	C24	113.5(5)
Cl1	Pd1	$P1^1$	86.94(7)	P1	C1	Fe1	131.2(3)
P1	Pd1	$P1^1$	180.0	C2	C1	Fe1	68.6(3)
C1	Fe1	C4	68.5(2)	C2	C1	P1	126.3(4)
C1	Fe1	C6	155.9(2)	C5	C1	Fe1	69.3(3)
C1	Fe1	C7	163.5(2)	C5	C1	P1	126.5(5)
C1	Fe1	C9	111.2(2)	C5	C1	C2	107.0(5)
C1	Fe1	C10	123.2(2)	C1	C2	Fe1	70.0(3)
C2	Fe1	C1	41.4(2)	C3	C2	Fe1	70.3(3)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	Fe1	C3	40.1(2)	C3	C2	C1	108.2(5)
C2	Fe1	C4	68.3(2)	C2	C3	Fe1	69.6(3)
C2	Fe1	C5	69.2(2)	C2	C3	C4	109.1(5)
C2	Fe1	C6	160.0(2)	C4	C3	Fe1	70.3(3)
C2	Fe1	C7	123.7(2)	C3	C4	Fe1	69.0(3)
C2	Fe1	C8	107.6(2)	C3	C4	C5	107.7(5)
C2	Fe1	C9	122.0(2)	C5	C4	Fe1	69.2(3)
C2	Fe1	C10	158.4(2)	C1	C5	Fe1	69.6(3)
C3	Fe1	C1	68.4(2)	C4	C5	Fe1	70.2(3)
C3	Fe1	C4	40.6(2)	C4	C5	C1	107.9(5)
C3	Fe1	C5	68.5(3)	N1	C6	Fe1	131.3(4)
C3	Fe1	C6	123.1(2)	N1	C6	C7	126.5(5)
C3	Fe1	C7	104.3(2)	N1	C6	C10	126.1(5)
C3	Fe1	C8	117.6(3)	C7	C6	Fe1	68.0(3)
C3	Fe1	C9	154.1(3)	C10	C6	Fe1	68.6(3)
C3	Fe1	C10	161.0(2)	C10	C6	C7	107.3(5)
C4	Fe1	C6	105.5(2)	C6	C7	Fe1	71.6(3)
C4	Fe1	C10	125.5(2)	C8	C7	Fe1	69.4(3)
C5	Fe1	C1	41.0(2)	C8	C7	C6	108.9(5)
C5	Fe1	C4	40.6(2)	C7	C8	Fe1	70.1(3)
C5	Fe1	C6	119.3(2)	C7	C8	C9	108.3(5)
C5	Fe1	C7	151.8(2)	C9	C8	Fe1	69.9(3)
C5	Fe1	C9	129.4(3)	C8	C9	Fe1	69.2(3)
C5	Fe1	C10	109.4(2)	C8	C9	C10	107.3(5)
C7	Fe1	C4	116.3(2)	C10	C9	Fe1	69.9(3)
C7	Fe1	C6	40.4(2)	C6	C10	Fe1	71.3(3)
C7	Fe1	C10	68.2(2)	C6	C10	C9	108.0(5)
C8	Fe1	C1	128.4(2)	C9	C10	Fe1	68.8(3)
C8	Fe1	C4	151.0(3)	C12	C11	P1	118.3(4)
C8	Fe1	C5	167.1(2)	C12	C11	C16	120.3(5)
C8	Fe1	C6	68.1(2)	C16	C11	P1	121.5(4)
C8	Fe1	C7	40.5(2)	C11	C12	C13	119.8(6)
C8	Fe1	C9	40.9(3)	C14	C13	C12	119.6(6)
C8	Fe1	C10	68.8(2)	C15	C14	C13	120.7(6)
C9	Fe1	C4	165.1(3)	C14	C15	C16	120.0(6)
C9	Fe1	C6	68.3(2)	C11	C16	C15	119.6(5)
C9	Fe1	C7	68.5(2)	C18	C17	P1	120.8(5)
C9	Fe1	C10	41.3(2)	C18	C17	C22	117.9(6)
C10	Fe1	C6	40.2(2)	C22	C17	P1	121.2(5)
C1	P1	Pd1	111.7(2)	C19	C18	C17	121.1(6)
C1	P1	C11	105.8(3)	C18	C19	C20	120.4(6)
C1	P1	C17	104.9(3)	C21	C20	C19	120.0(6)
C11	P1	Pd1	109.95(19)	C20	C21	C22	120.0(6)
C11	P1	C17	103.3(3)	C21	C22	C17	120.6(6)

Table S13: Bond lengths and angles for compound **10**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	Pd1	2.3278(13)	Fe2	C42	2.110(5)
P1	Pd1	2.3404(14)	Fe2	C43	2.071(5)
P1	C1	1.785(5)	Fe2	C44	2.092(5)
P1	C11	1.829(5)	Fe2	C45	2.074(5)
P1	C20	1.828(5)	Fe2	C46	2.077(5)
Fe1	Pd1	2.8369(10)	Cl2	Pd2	2.3278(13)
Fe1	C1	2.133(5)	Pd2	P3	2.3289(15)
Fe1	C2	2.079(5)	Pd2	P4	2.2931(15)
Fe1	C3	2.054(5)	P3	C37	1.790(5)
Fe1	C4	2.074(5)	P3	C47	1.828(5)
Fe1	C5	2.088(5)	P3	C56	1.832(5)
Fe1	C6	2.109(5)	P4	C42	1.797(5)
Fe1	C7	2.067(5)	P4	C65	1.887(5)
Fe1	C8	2.071(6)	P4	C69	1.873(5)
Fe1	C9	2.077(6)	C37	C38	1.414(7)
Fe1	C10	2.084(6)	C37	C41	1.459(7)
Pd1	P2	2.2751(16)	C38	C39	1.416(7)
C1	C2	1.407(7)	C39	C40	1.430(7)
C1	C5	1.457(7)	C40	C41	1.410(7)
C2	C3	1.424(7)	C42	C43	1.460(7)
P2	C6	1.792(5)	C42	C46	1.423(7)
P2	C29	1.888(6)	C43	C44	1.398(7)
P2	C33	1.868(6)	C44	C45	1.419(7)
C3	C4	1.418(8)	C45	C46	1.417(7)
C4	C5	1.396(7)	C47	C48	1.415(7)
C6	C7	1.459(7)	C47	C52	1.416(6)
C6	C10	1.416(7)	C48	C49	1.397(7)
C7	C8	1.415(8)	C48	C53	1.503(7)
C8	C9	1.391(9)	C49	C50	1.377(7)
C9	C10	1.393(9)	C50	C51	1.379(7)
C11	C12	1.417(7)	C50	C54	1.512(7)
C11	C16	1.411(7)	C51	C52	1.389(7)
C12	C13	1.392(7)	C52	C55	1.506(7)
C12	C17	1.502(6)	C56	C57	1.421(7)
C13	C14	1.392(7)	C56	C61	1.418(7)
C14	C15	1.384(7)	C57	C58	1.392(7)
C14	C18	1.503(7)	C57	C62	1.511(7)
C15	C16	1.386(7)	C58	C59	1.387(7)
C16	C19	1.516(7)	C59	C60	1.385(7)
C20	C21	1.411(7)	C59	C63	1.518(7)
C20	C25	1.424(7)	C60	C61	1.394(7)
C21	C22	1.387(7)	C61	C64	1.505(7)
C21	C26	1.521(7)	C65	C66	1.533(7)
C22	C23	1.390(8)	C65	C67	1.534(7)
C23	C24	1.385(8)	C65	C68	1.542(7)
C23	C27	1.512(7)	C69	C70	1.537(7)
C24	C25	1.390(7)	C69	C71	1.556(7)
C25	C28	1.505(7)	C69	C72	1.535(7)
C29	C30	1.541(9)	Sb2	F7	1.861(3)
C29	C31	1.528(8)	Sb2	F8	1.871(3)
C29	C32	1.533(9)	Sb2	F9	1.876(3)
C33	C34	1.547(8)	Sb2	F10	1.874(3)
C33	C35	1.564(9)	Sb2	F11	1.869(3)
C33	C36	1.505(9)	Sb2	F12	1.873(3)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe2	Pd2	2.7974(10)	F1	Sb1	1.861(3)
Fe2	C37	2.128(5)	Sb1	F2	1.870(3)
Fe2	C38	2.076(5)	Sb1	F3	1.868(3)
Fe2	C39	2.056(5)	Sb1	F4	1.878(4)
Fe2	C40	2.079(5)	Sb1	F5	1.871(3)
Fe2	C41	2.093(5)	Sb1	F6	1.869(3)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	P1	Pd1	82.94(17)	C39	Fe2	C44	101.5(2)
C1	P1	C11	105.0(2)	C39	Fe2	C45	90.4(2)
C1	P1	C20	111.3(2)	C39	Fe2	C46	116.5(2)
C11	P1	Pd1	120.16(16)	C40	Fe2	Pd2	113.05(14)
C20	P1	Pd1	118.34(17)	C40	Fe2	C37	66.88(18)
C20	P1	C11	113.2(2)	C40	Fe2	C41	39.52(18)
C1	Fe1	Pd1	65.80(14)	C40	Fe2	C42	132.21(19)
C2	Fe1	Pd1	99.46(14)	C40	Fe2	C44	132.2(2)
C2	Fe1	C1	39.00(19)	C41	Fe2	Pd2	74.39(14)
C2	Fe1	C5	67.2(2)	C41	Fe2	C37	40.45(18)
C2	Fe1	C6	157.5(2)	C41	Fe2	C42	123.87(19)
C2	Fe1	C10	157.4(2)	C42	Fe2	Pd2	69.06(13)
C3	Fe1	Pd1	131.71(15)	C42	Fe2	C37	136.91(18)
C3	Fe1	C1	66.3(2)	C43	Fe2	Pd2	76.36(14)
C3	Fe1	C2	40.3(2)	C43	Fe2	C37	126.09(19)
C3	Fe1	C4	40.2(2)	C43	Fe2	C38	120.7(2)
C3	Fe1	C5	66.8(2)	C43	Fe2	C40	167.0(2)
C3	Fe1	C6	157.5(2)	C43	Fe2	C41	150.7(2)
C3	Fe1	C7	136.8(2)	C43	Fe2	C42	40.86(18)
C3	Fe1	C8	100.0(2)	C43	Fe2	C44	39.26(19)
C3	Fe1	C9	91.9(2)	C43	Fe2	C45	66.7(2)
C3	Fe1	C10	119.1(2)	C43	Fe2	C46	67.4(2)
C4	Fe1	Pd1	111.99(15)	C44	Fe2	Pd2	114.74(14)
C4	Fe1	C1	66.5(2)	C44	Fe2	C37	134.62(19)
C4	Fe1	C2	67.5(2)	C44	Fe2	C41	168.6(2)
C4	Fe1	C5	39.20(19)	C44	Fe2	C42	67.21(19)
C4	Fe1	C6	134.5(2)	C45	Fe2	Pd2	135.60(15)
C4	Fe1	C9	100.0(2)	C45	Fe2	C37	155.8(2)
C4	Fe1	C10	102.3(2)	C45	Fe2	C38	117.5(2)
C5	Fe1	Pd1	73.36(14)	C45	Fe2	C40	100.8(2)
C5	Fe1	C1	40.36(19)	C45	Fe2	C41	138.0(2)
C5	Fe1	C6	124.8(2)	C45	Fe2	C42	67.0(2)
C6	Fe1	Pd1	70.00(14)	C45	Fe2	C44	39.84(19)
C6	Fe1	C1	135.80(19)	C45	Fe2	C46	39.9(2)
C7	Fe1	Pd1	79.28(16)	C46	Fe2	Pd2	103.60(14)
C7	Fe1	C1	126.3(2)	C46	Fe2	C37	158.3(2)
C7	Fe1	C2	119.1(2)	C46	Fe2	C40	100.9(2)
C7	Fe1	C4	166.6(2)	C46	Fe2	C41	118.9(2)
C7	Fe1	C5	152.6(2)	C46	Fe2	C42	39.73(18)
C7	Fe1	C6	40.9(2)	C46	Fe2	C44	67.0(2)
C7	Fe1	C8	40.0(2)	Cl2	Pd2	Fe2	166.94(4)
C7	Fe1	C9	66.7(3)	Cl2	Pd2	P3	100.02(5)
C7	Fe1	C10	67.1(2)	P3	Pd2	Fe2	80.83(4)
C8	Fe1	Pd1	118.77(19)	P4	Pd2	Fe2	80.66(4)
C8	Fe1	C1	136.8(2)	P4	Pd2	Cl2	98.26(5)
C8	Fe1	C2	103.8(2)	P4	Pd2	P3	161.46(5)
C8	Fe1	C4	129.2(2)	C37	P3	Pd2	84.75(16)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C8	Fe1	C5	166.8(2)	C37	P3	C47	115.3(2)
C8	Fe1	C6	67.2(2)	C37	P3	C56	104.2(2)
C8	Fe1	C9	39.2(3)	C47	P3	Pd2	117.18(16)
C8	Fe1	C10	66.1(3)	C47	P3	C56	108.7(2)
C9	Fe1	Pd1	136.29(17)	C56	P3	Pd2	123.59(16)
C9	Fe1	C1	157.8(2)	C42	P4	Pd2	87.02(16)
C9	Fe1	C2	120.5(2)	C42	P4	C65	109.6(2)
C9	Fe1	C5	136.0(2)	C42	P4	C69	109.7(2)
C9	Fe1	C6	66.3(2)	C65	P4	Pd2	117.66(16)
C9	Fe1	C10	39.1(2)	C69	P4	Pd2	117.96(16)
C10	Fe1	Pd1	103.10(16)	C69	P4	C65	111.7(2)
C10	Fe1	C1	156.9(2)	P3	C37	Fe2	116.8(2)
C10	Fe1	C5	118.4(2)	C38	C37	Fe2	68.4(3)
C10	Fe1	C6	39.5(2)	C38	C37	P3	127.0(4)
Cl1	Pd1	P1	102.25(5)	C38	C37	C41	107.2(4)
Cl1	Pd1	Fe1	166.91(4)	C41	C37	Fe2	68.5(3)
P1	Pd1	Fe1	82.29(4)	C41	C37	P3	124.2(4)
P2	Pd1	Cl1	96.02(5)	C37	C38	Fe2	72.3(3)
P2	Pd1	P1	161.60(5)	C37	C38	C39	108.6(5)
P2	Pd1	Fe1	79.39(4)	C39	C38	Fe2	69.2(3)
P1	C1	Fe1	121.7(3)	C38	C39	Fe2	70.7(3)
C2	C1	P1	128.7(4)	C38	C39	C40	108.4(5)
C2	C1	Fe1	68.4(3)	C40	C39	Fe2	70.6(3)
C2	C1	C5	107.3(4)	C39	C40	Fe2	68.9(3)
C5	C1	P1	123.4(4)	C41	C40	Fe2	70.8(3)
C5	C1	Fe1	68.1(3)	C41	C40	C39	108.0(4)
C1	C2	Fe1	72.6(3)	C37	C41	Fe2	71.1(3)
C1	C2	C3	107.9(5)	C40	C41	Fe2	69.7(3)
C3	C2	Fe1	68.9(3)	C40	C41	C37	107.8(4)
C6	P2	Pd1	90.11(17)	P4	C42	Fe2	116.0(2)
C6	P2	C29	108.6(3)	C43	C42	Fe2	68.1(3)
C6	P2	C33	110.3(3)	C43	C42	P4	122.0(4)
C29	P2	Pd1	117.84(19)	C46	C42	Fe2	68.9(3)
C33	P2	Pd1	115.7(2)	C46	C42	P4	130.4(4)
C33	P2	C29	111.8(3)	C46	C42	C43	105.8(4)
C2	C3	Fe1	70.8(3)	C42	C43	Fe2	71.0(3)
C4	C3	Fe1	70.7(3)	C44	C43	Fe2	71.2(3)
C4	C3	C2	108.5(5)	C44	C43	C42	108.9(4)
C3	C4	Fe1	69.1(3)	C43	C44	Fe2	69.6(3)
C5	C4	Fe1	71.0(3)	C43	C44	C45	107.9(5)
C5	C4	C3	108.2(5)	C45	C44	Fe2	69.4(3)
C1	C5	Fe1	71.5(3)	C44	C45	Fe2	70.7(3)
C4	C5	Fe1	69.8(3)	C46	C45	Fe2	70.1(3)
C4	C5	C1	107.9(5)	C46	C45	C44	108.5(5)
P2	C6	Fe1	114.9(3)	C42	C46	Fe2	71.4(3)
C7	C6	Fe1	68.0(3)	C45	C46	Fe2	70.0(3)
C7	C6	P2	122.2(4)	C45	C46	C42	108.8(4)
C10	C6	Fe1	69.3(3)	C48	C47	P3	125.8(4)
C10	C6	P2	130.0(4)	C48	C47	C52	119.5(4)
C10	C6	C7	105.9(5)	C52	C47	P3	114.6(3)
C6	C7	Fe1	71.1(3)	C47	C48	C53	125.6(4)
C8	C7	Fe1	70.2(3)	C49	C48	C47	117.7(5)
C8	C7	C6	107.3(5)	C49	C48	C53	116.7(4)
C7	C8	Fe1	69.8(3)	C50	C49	C48	123.5(5)
C9	C8	Fe1	70.7(4)	C49	C50	C51	117.7(5)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C9	C8	C7	108.6(5)	C49	C50	C54	121.3(5)
C8	C9	Fe1	70.2(3)	C51	C50	C54	121.1(5)
C8	C9	C10	109.0(5)	C50	C51	C52	122.4(5)
C10	C9	Fe1	70.7(3)	C47	C52	C55	122.2(4)
C6	C10	Fe1	71.2(3)	C51	C52	C47	119.1(4)
C9	C10	Fe1	70.2(3)	C51	C52	C55	118.7(4)
C9	C10	C6	109.3(6)	C57	C56	P3	120.5(4)
C12	C11	P1	118.9(4)	C61	C56	P3	120.4(4)
C16	C11	P1	121.7(4)	C61	C56	C57	119.2(5)
C16	C11	C12	119.3(4)	C56	C57	C62	123.8(4)
C11	C12	C17	125.4(4)	C58	C57	C56	118.9(4)
C13	C12	C11	118.8(4)	C58	C57	C62	117.3(4)
C13	C12	C17	115.8(4)	C59	C58	C57	122.7(5)
C14	C13	C12	122.3(5)	C58	C59	C63	121.6(5)
C13	C14	C18	120.2(5)	C60	C59	C58	117.7(5)
C15	C14	C13	117.6(5)	C60	C59	C63	120.7(5)
C15	C14	C18	122.2(5)	C59	C60	C61	122.7(5)
C14	C15	C16	122.7(5)	C56	C61	C64	124.1(5)
C11	C16	C19	123.2(4)	C60	C61	C56	118.8(5)
C15	C16	C11	119.1(4)	C60	C61	C64	117.0(4)
C15	C16	C19	117.7(4)	C66	C65	P4	108.4(3)
C21	C20	P1	126.0(4)	C66	C65	C67	107.8(4)
C21	C20	C25	118.8(5)	C66	C65	C68	109.4(4)
C25	C20	P1	114.6(4)	C67	C65	P4	108.8(3)
C20	C21	C26	125.8(5)	C67	C65	C68	110.0(4)
C22	C21	C20	118.3(5)	C68	C65	P4	112.3(3)
C22	C21	C26	115.8(5)	C70	C69	P4	115.8(3)
C21	C22	C23	123.3(5)	C70	C69	C71	109.5(4)
C22	C23	C27	121.0(5)	C71	C69	P4	107.0(3)
C24	C23	C22	117.9(5)	C72	C69	P4	108.6(3)
C24	C23	C27	121.1(5)	C72	C69	C70	108.7(4)
C23	C24	C25	121.3(5)	C72	C69	C71	106.8(4)
C20	C25	C28	121.1(5)	F7	Sb2	F8	179.46(17)
C24	C25	C20	119.9(5)	F7	Sb2	F9	90.77(18)
C24	C25	C28	118.9(5)	F7	Sb2	F10	90.88(18)
C30	C29	P2	110.4(4)	F7	Sb2	F11	89.13(19)
C31	C29	P2	114.3(5)	F7	Sb2	F12	90.43(17)
C31	C29	C30	104.7(5)	F8	Sb2	F9	88.80(17)
C31	C29	C32	111.5(6)	F8	Sb2	F10	89.53(17)
C32	C29	P2	111.9(4)	F8	Sb2	F12	89.24(16)
C32	C29	C30	103.2(6)	F10	Sb2	F9	177.97(16)
C34	C33	P2	114.1(4)	F11	Sb2	F8	91.21(18)
C34	C33	C35	107.1(5)	F11	Sb2	F9	90.49(16)
C35	C33	P2	107.7(4)	F11	Sb2	F10	90.70(16)
C36	C33	P2	107.7(4)	F11	Sb2	F12	179.55(19)
C36	C33	C34	110.5(5)	F12	Sb2	F9	89.46(15)
C36	C33	C35	109.8(6)	F12	Sb2	F10	89.36(16)
C37	Fe2	Pd2	67.86(13)	F1	Sb1	F2	179.23(19)
C38	Fe2	Pd2	102.03(14)	F1	Sb1	F3	91.52(19)
C38	Fe2	C37	39.28(18)	F1	Sb1	F4	90.56(19)
C38	Fe2	C40	67.5(2)	F1	Sb1	F5	89.48(17)
C38	Fe2	C41	67.4(2)	F1	Sb1	F6	90.25(16)
C38	Fe2	C42	160.02(19)	F2	Sb1	F4	88.72(19)
C38	Fe2	C44	103.0(2)	F2	Sb1	F5	90.28(16)
C38	Fe2	C46	154.3(2)	F3	Sb1	F2	89.21(18)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C39	Fe2	Pd2	134.03(14)	F3	Sb1	F4	177.74(19)
C39	Fe2	C37	66.61(19)	F3	Sb1	F5	89.79(17)
C39	Fe2	C38	40.06(19)	F3	Sb1	F6	89.26(15)
C39	Fe2	C40	40.5(2)	F5	Sb1	F4	91.11(18)
C39	Fe2	C41	67.2(2)	F6	Sb1	F2	90.00(16)
C39	Fe2	C42	155.63(19)	F6	Sb1	F4	89.84(17)
C39	Fe2	C43	138.7(2)	F6	Sb1	F5	179.01(17)

Table S14: Bond lengths and angles for compound **11**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	Pd1	2.190(3)	C4	C5	1.433(14)
P1	C1	1.783(11)	C6	C7	1.431(15)
P1	C11	1.798(10)	C6	C10	1.451(14)
P1	C17	1.803(10)	C7	C8	1.425(17)
Pd1	Cl1	2.315(3)	C8	C9	1.412(17)
Pd1	Fe1	2.7384(18)	C9	C10	1.407(16)
Pd1	N1	2.118(8)	C11	C12	1.396(14)
Pd1	C6	2.459(10)	C11	C16	1.420(14)
Fe1	C1	2.124(10)	C12	C13	1.384(14)
Fe1	C2	2.100(10)	C13	C14	1.414(16)
Fe1	C3	2.062(11)	C14	C15	1.365(16)
Fe1	C4	2.067(10)	C15	C16	1.363(16)
Fe1	C5	2.072(10)	C17	C18	1.400(13)
Fe1	C6	2.169(10)	C17	C22	1.387(14)
Fe1	C7	2.117(11)	C18	C19	1.411(14)
Fe1	C8	2.052(11)	C19	C20	1.361(16)
Fe1	C9	2.040(11)	C20	C21	1.387(15)
Fe1	C10	2.086(10)	C21	C22	1.418(14)
N1	C6	1.394(15)	F1	Sb1	1.868(6)
N1	C23	1.510(13)	Sb1	F2	1.882(6)
N1	C24	1.506(14)	Sb1	F3	1.878(6)
C1	C2	1.423(14)	Sb1	F4	1.870(6)
C1	C5	1.424(14)	Sb1	F5	1.874(7)
C2	C3	1.417(16)	Sb1	F6	1.884(6)
C3	C4	1.403(15)			

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	P1	Pd1	92.6(3)	C23	N1	Pd1	115.9(6)
C1	P1	C11	108.8(5)	C24	N1	Pd1	108.8(6)
C1	P1	C17	108.3(5)	C24	N1	C23	109.1(8)
C11	P1	Pd1	113.5(3)	P1	C1	Fe1	113.4(6)
C11	P1	C17	108.9(4)	C2	C1	P1	126.5(7)
C17	P1	Pd1	122.8(3)	C2	C1	Fe1	69.4(6)
P1	Pd1	Cl1	98.15(10)	C2	C1	C5	108.8(9)
P1	Pd1	Fe1	82.35(8)	C5	C1	P1	121.9(7)
P1	Pd1	C6	131.1(3)	C5	C1	Fe1	68.2(5)
Cl1	Pd1	Fe1	176.03(8)	C1	C2	Fe1	71.2(6)
Cl1	Pd1	C6	130.8(3)	C3	C2	Fe1	68.7(6)
N1	Pd1	P1	163.9(2)	C3	C2	C1	106.6(9)
N1	Pd1	Cl1	96.6(3)	C2	C3	Fe1	71.5(6)
N1	Pd1	Fe1	83.4(3)	C4	C3	Fe1	70.3(6)
N1	Pd1	C6	34.5(4)	C4	C3	C2	109.8(10)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C6	Pd1	Fe1	49.0(3)	C3	C4	Fe1	70.0(6)
C1	Fe1	Pd1	71.6(3)	C3	C4	C5	107.6(9)
C1	Fe1	C6	130.2(4)	C5	C4	Fe1	69.9(6)
C2	Fe1	Pd1	95.4(3)	C1	C5	Fe1	72.2(6)
C2	Fe1	C1	39.4(4)	C1	C5	C4	107.1(9)
C2	Fe1	C6	137.8(4)	C4	C5	Fe1	69.6(6)
C2	Fe1	C7	112.7(4)	Fe1	C6	Pd1	72.2(3)
C3	Fe1	Pd1	134.2(3)	N1	C6	Pd1	59.2(5)
C3	Fe1	C1	65.9(4)	N1	C6	Fe1	131.4(7)
C3	Fe1	C2	39.8(4)	N1	C6	C7	125.3(9)
C3	Fe1	C4	39.7(4)	N1	C6	C10	125.9(9)
C3	Fe1	C5	67.2(4)	C7	C6	Pd1	111.6(7)
C3	Fe1	C6	155.9(4)	C7	C6	Fe1	68.5(6)
C3	Fe1	C7	117.0(5)	C7	C6	C10	108.8(10)
C3	Fe1	C10	144.6(5)	C10	C6	Pd1	103.9(6)
C4	Fe1	Pd1	130.8(3)	C10	C6	Fe1	67.0(6)
C4	Fe1	C1	66.5(4)	C6	C7	Fe1	72.5(6)
C4	Fe1	C2	67.2(4)	C8	C7	Fe1	67.6(6)
C4	Fe1	C5	40.5(4)	C8	C7	C6	105.9(10)
C4	Fe1	C6	155.0(4)	C7	C8	Fe1	72.5(6)
C4	Fe1	C7	145.5(4)	C9	C8	Fe1	69.3(6)
C4	Fe1	C10	115.2(4)	C9	C8	C7	109.6(10)
C5	Fe1	Pd1	90.3(3)	C8	C9	Fe1	70.3(6)
C5	Fe1	C1	39.6(4)	C10	C9	Fe1	71.9(6)
C5	Fe1	C2	67.4(4)	C10	C9	C8	108.8(10)
C5	Fe1	C6	136.9(4)	C6	C10	Fe1	73.2(6)
C5	Fe1	C7	174.0(4)	C9	C10	Fe1	68.3(6)
C5	Fe1	C10	111.6(4)	C9	C10	C6	106.6(10)
C6	Fe1	Pd1	58.8(3)	C12	C11	P1	119.4(7)
C7	Fe1	Pd1	83.6(3)	C12	C11	C16	118.7(9)
C7	Fe1	C1	136.8(4)	C16	C11	P1	121.7(8)
C7	Fe1	C6	39.0(4)	C13	C12	C11	120.4(9)
C8	Fe1	Pd1	121.5(3)	C12	C13	C14	119.8(9)
C8	Fe1	C1	155.6(4)	C15	C14	C13	119.0(10)
C8	Fe1	C2	116.3(5)	C16	C15	C14	122.4(10)
C8	Fe1	C3	93.9(5)	C15	C16	C11	119.5(10)
C8	Fe1	C4	107.1(4)	C18	C17	P1	119.5(8)
C8	Fe1	C5	145.9(4)	C22	C17	P1	118.4(7)
C8	Fe1	C6	65.3(4)	C22	C17	C18	122.0(9)
C8	Fe1	C7	39.9(5)	C17	C18	C19	118.0(9)
C8	Fe1	C10	67.3(5)	C20	C19	C18	120.5(10)
C9	Fe1	Pd1	119.1(3)	C19	C20	C21	121.5(10)
C9	Fe1	C1	155.5(4)	C20	C21	C22	119.5(10)
C9	Fe1	C2	144.8(5)	C17	C22	C21	118.4(9)
C9	Fe1	C3	106.7(5)	F1	Sb1	F2	177.5(3)
C9	Fe1	C4	92.6(4)	F1	Sb1	F3	89.7(3)
C9	Fe1	C5	115.9(4)	F1	Sb1	F4	89.3(3)
C9	Fe1	C6	65.9(4)	F1	Sb1	F5	90.7(3)
C9	Fe1	C7	67.8(5)	F1	Sb1	F6	89.2(3)
C9	Fe1	C8	40.4(5)	F2	Sb1	F6	89.2(3)
C9	Fe1	C10	39.9(5)	F3	Sb1	F2	92.2(3)
C10	Fe1	Pd1	80.0(3)	F3	Sb1	F6	89.2(3)
C10	Fe1	C1	137.1(4)	F4	Sb1	F2	88.8(3)
C10	Fe1	C2	175.3(4)	F4	Sb1	F3	179.0(3)
C10	Fe1	C6	39.8(4)	F4	Sb1	F5	90.8(3)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C10	Fe1	C7	67.8(4)	F4	Sb1	F6	90.9(3)
C6	N1	Pd1	86.3(6)	F5	Sb1	F2	90.9(3)
C6	N1	C23	117.3(8)	F5	Sb1	F3	89.2(3)
C6	N1	C24	117.6(8)	F5	Sb1	F6	178.3(3)

Table S15: Bond lengths and angles for compound **12**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	Fe1	2.103(7)	C16	C17	1.390(12)
C1	P2	1.766(8)	C17	C18	1.376(11)
C1	C2	1.447(10)	C19	C20	1.376(12)
C1	C5	1.439(11)	C19	C24	1.378(12)
Fe1	Pd1	2.811(3)	C20	C21	1.417(12)
Fe1	C2	2.059(7)	C21	C22	1.358(13)
Fe1	C3	2.062(8)	C22	C23	1.355(14)
Fe1	C4	2.062(8)	C23	C24	1.399(12)
Fe1	C5	2.086(8)	C25	C26	1.419(12)
Fe1	C6	2.143(8)	C25	C30	1.398(12)
Fe1	C7	2.078(7)	C26	C27	1.346(12)
Fe1	C8	2.051(7)	C27	C28	1.394(13)
Fe1	C9	2.045(8)	C28	C29	1.341(14)
Fe1	C10	2.092(7)	C29	C30	1.373(12)
P1	Pd1	2.310(3)	C31	C32	1.412(11)
P1	C25	1.795(8)	C31	C35	1.375(11)
P1	C31	1.811(8)	C32	C33	1.383(12)
P1	C36	1.800(9)	C33	C41	1.347(13)
Pd1	N1	2.140(6)	C34	C35	1.392(12)
Pd1	P2	2.236(3)	C34	C41	1.364(13)
Pd1	C6	2.522(9)	C36	C37	1.334(11)
N1	C6	1.388(10)	C36	C40	1.482(12)
N1	C11	1.491(10)	C37	C38	1.484(15)
N1	C12	1.480(10)	C38	C39	1.375(15)
P2	C13	1.802(8)	C39	C40	1.482(13)
P2	C19	1.816(8)	Sb2	F7	1.876(5)
C2	C3	1.409(11)	Sb2	F8	1.877(5)
C3	C4	1.426(11)	Sb2	F9	1.884(5)
C4	C5	1.416(12)	Sb2	F10	1.874(5)
C6	C7	1.448(11)	Sb2	F11	1.866(5)
C6	C10	1.431(11)	Sb2	F12	1.860(5)
C7	C8	1.415(12)	Sb1	F1	1.893(5)
C8	C9	1.407(12)	Sb1	F2	1.864(6)
C9	C10	1.424(11)	Sb1	F3	1.874(5)
C13	C14	1.373(11)	Sb1	F4	1.854(5)
C13	C18	1.376(11)	Sb1	F5	1.864(6)
C14	C15	1.396(11)	Sb1	F6	1.879(5)
C15	C16	1.386(12)			

Atom	Atom	Atom	Angle/˚
P2	C1	Fe1	114.4(4)
C2	C1	Fe1	68.0(4)
C2	C1	P2	125.4(6)
C5	C1	Fe1	69.3(4)
C5	C1	P2	124.3(6)
C5	C1	C2	107.9(7)
C1	Fe1	Pd1	70.8(2)
C1	Fe1	C6	130.2(3)
C2	Fe1	C1	40.7(3)
C2	Fe1	Pd1	85.5(2)
C2	Fe1	C3	40.0(3)
C2	Fe1	C4	68.2(3)
C2	Fe1	C5	68.5(3)
C2	Fe1	C6	128.4(3)
C2	Fe1	C7	163.1(3)
C2	Fe1	C10	111.5(3)
C3	Fe1	C1	66.9(3)
C3	Fe1	Pd1	125.5(2)
C3	Fe1	C4	40.5(3)
C3	Fe1	C5	67.5(3)
C3	Fe1	C6	145.1(3)
C3	Fe1	C7	156.8(3)
C3	Fe1	C10	107.2(3)
C4	Fe1	C1	67.1(3)
C4	Fe1	Pd1	137.0(2)
C4	Fe1	C5	39.9(3)
C4	Fe1	C6	161.4(3)
C4	Fe1	C7	125.9(3)
C4	Fe1	C10	132.4(3)
C5	Fe1	C1	40.2(3)
C5	Fe1	Pd1	99.7(3)
C5	Fe1	C6	146.8(3)
C5	Fe1	C10	172.2(3)
C6	Fe1	Pd1	59.4(2)
C7	Fe1	C1	131.0(3)
C7	Fe1	Pd1	77.5(2)
C7	Fe1	C5	114.9(3)
C7	Fe1	C6	40.1(3)
C7	Fe1	C10	67.6(3)
C8	Fe1	C1	147.7(3)
C8	Fe1	Pd1	117.5(3)
C8	Fe1	C2	156.6(3)
C8	Fe1	C3	116.7(3)
C8	Fe1	C4	94.7(3)
C8	Fe1	C5	109.1(3)
C8	Fe1	C6	66.9(3)
C8	Fe1	C7	40.1(3)
C8	Fe1	C10	67.7(3)
C9	Fe1	C1	160.7(3)
C9	Fe1	Pd1	125.0(3)
C9	Fe1	C2	123.7(3)
C9	Fe1	C3	93.8(4)
C9	Fe1	C4	97.9(3)

Atom	Atom	Atom	Angle/˚
C5	C4	Fe1	71.0(5)
C5	C4	C3	108.4(8)
C1	C5	Fe1	70.5(4)
C4	C5	C1	107.5(7)
C4	C5	Fe1	69.1(5)
Fe1	C6	Pd1	73.6(2)
N1	C6	Fe1	130.8(6)
N1	C6	Pd1	58.0(4)
N1	C6	C7	125.8(7)
N1	C6	C10	126.8(7)
C7	C6	Fe1	67.5(4)
C7	C6	Pd1	99.8(5)
C10	C6	Fe1	68.4(4)
C10	C6	Pd1	118.8(5)
C10	C6	C7	107.3(7)
C6	C7	Fe1	72.4(4)
C8	C7	Fe1	68.9(4)
C8	C7	C6	107.8(7)
C7	C8	Fe1	71.0(4)
C9	C8	Fe1	69.7(4)
C9	C8	C7	108.2(7)
C8	C9	Fe1	70.2(5)
C8	C9	C10	109.2(8)
C10	C9	Fe1	71.7(4)
C6	C10	Fe1	72.2(4)
C9	C10	Fe1	68.1(4)
C9	C10	C6	107.3(7)
C14	C13	P2	119.8(6)
C14	C13	C18	119.4(8)
C18	C13	P2	120.8(6)
C13	C14	C15	121.0(8)
C16	C15	C14	119.5(8)
C15	C16	C17	118.8(8)
C18	C17	C16	121.1(8)
C13	C18	C17	120.2(8)
C20	C19	P2	118.7(6)
C20	C19	C24	120.4(8)
C24	C19	P2	120.8(7)
C19	C20	C21	119.2(8)
C22	C21	C20	120.2(10)
C23	C22	C21	119.7(9)
C22	C23	C24	121.8(9)
C19	C24	C23	118.5(9)
C26	C25	P1	122.9(7)
C30	C25	P1	119.7(6)
C30	C25	C26	117.4(7)
C27	C26	C25	121.1(9)
C26	C27	C28	119.3(9)
C29	C28	C27	121.5(9)
C28	C29	C30	120.0(10)
C29	C30	C25	120.7(9)
C32	C31	P1	118.5(6)
C35	C31	P1	121.9(7)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C9	Fe1	C5	132.8(3)	C35	C31	C32	119.6(8)
C9	Fe1	C6	66.6(3)	C33	C32	C31	118.6(8)
C9	Fe1	C7	67.4(3)	C41	C33	C32	120.4(9)
C9	Fe1	C8	40.2(3)	C41	C34	C35	118.9(9)
C9	Fe1	C10	40.2(3)	C31	C35	C34	120.3(9)
C10	Fe1	C1	144.2(3)	C37	C36	P1	125.4(7)
C10	Fe1	Pd1	88.0(2)	C37	C36	C40	109.0(8)
C10	Fe1	C6	39.5(3)	C40	C36	P1	125.6(7)
C25	P1	Pd1	108.3(3)	C36	C37	C38	109.5(9)
C25	P1	C31	105.2(4)	C39	C38	C37	108.2(9)
C25	P1	C36	108.0(4)	C38	C39	C40	107.9(9)
C31	P1	Pd1	115.6(3)	C36	C40	C39	105.5(8)
C36	P1	Pd1	115.5(3)	C33	C41	C34	122.2(9)
C36	P1	C31	103.7(4)	F7	Sb2	F8	179.4(2)
P1	Pd1	Fe1	169.81(6)	F7	Sb2	F9	89.5(2)
P1	Pd1	C6	137.3(2)	F8	Sb2	F9	90.0(2)
N1	Pd1	Fe1	80.08(19)	F10	Sb2	F7	91.2(2)
N1	Pd1	P1	104.0(2)	F10	Sb2	F8	89.3(2)
N1	Pd1	P2	159.11(19)	F10	Sb2	F9	178.7(2)
N1	Pd1	C6	33.4(2)	F11	Sb2	F7	88.9(2)
P2	Pd1	Fe1	79.49(9)	F11	Sb2	F8	90.8(2)
P2	Pd1	P1	96.88(10)	F11	Sb2	F9	89.6(3)
P2	Pd1	C6	125.8(2)	F11	Sb2	F10	89.3(2)
C6	Pd1	Fe1	46.99(19)	F12	Sb2	F7	89.4(2)
C6	N1	Pd1	88.6(4)	F12	Sb2	F8	90.9(2)
C6	N1	C11	114.4(6)	F12	Sb2	F9	90.3(2)
C6	N1	C12	113.6(6)	F12	Sb2	F10	90.8(2)
C11	N1	Pd1	114.8(5)	F12	Sb2	F11	178.3(2)
C12	N1	Pd1	114.9(5)	F2	Sb1	F1	176.2(3)
C12	N1	C11	109.4(6)	F2	Sb1	F3	89.0(2)
C1	P2	Pd1	92.4(3)	F2	Sb1	F5	92.3(3)
C1	P2	C13	106.4(4)	F2	Sb1	F6	89.5(3)
C1	P2	C19	111.3(4)	F3	Sb1	F1	87.8(2)
C13	P2	Pd1	114.1(3)	F3	Sb1	F6	89.0(2)
C13	P2	C19	108.0(4)	F4	Sb1	F1	90.8(3)
C19	P2	Pd1	122.7(3)	F4	Sb1	F2	92.4(3)
C1	C2	Fe1	71.3(4)	F4	Sb1	F3	178.0(2)
C3	C2	C1	107.1(7)	F4	Sb1	F5	92.2(3)
C3	C2	Fe1	70.1(4)	F4	Sb1	F6	89.5(2)
C2	C3	Fe1	69.9(4)	F5	Sb1	F1	89.7(3)
C2	C3	C4	109.1(7)	F5	Sb1	F3	89.3(2)
C4	C3	Fe1	69.8(4)	F5	Sb1	F6	177.5(3)
C3	C4	Fe1	69.7(4)	F6	Sb1	F1	88.4(3)

Table S16: Bond lengths and angles for compound **13**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	N1	2.123(8)	C15	C16	1.398(17)
Pd1	Fe1	2.8289(19)	C16	C17	1.363(16)
Pd1	P1	2.305(2)	C17	C18	1.408(14)
Pd1	P2	2.252(2)	C19	C20	1.386(13)
Pd1	C6	2.526(9)	C19	C24	1.422(14)
N1	C6	1.415(12)	C20	C21	1.384(15)
N1	C11	1.482(13)	C21	C22	1.376(15)

N1	C12	1.499(12)	C22	C23	1.379(14)
Fe1	C1	2.114(10)	C23	C24	1.399(14)
Fe1	C2	2.071(10)	C25	C26	1.366(15)
Fe1	C3	2.057(10)	C25	C30	1.410(14)
Fe1	C4	2.068(10)	C26	C27	1.425(17)
Fe1	C5	2.086(11)	C27	C28	1.39(2)
Fe1	C6	2.124(10)	C28	C29	1.341(19)
Fe1	C7	2.058(11)	C29	C30	1.403(15)
Fe1	C8	2.063(10)	C31	C32	1.394(14)
Fe1	C9	2.072(11)	C31	C36	1.398(14)
Fe1	C10	2.075(11)	C32	C33	1.383(15)
P1	C13	1.818(10)	C33	C34	1.387(17)
P1	C19	1.805(10)	C34	C35	1.362(17)
P1	C25	1.802(10)	C35	C36	1.384(15)
C1	P2	1.758(10)	C37	C38	1.400(13)
C1	C2	1.441(13)	C37	C42	1.389(13)
C1	C5	1.436(13)	C38	C39	1.400(14)
P2	C31	1.811(10)	C39	C40	1.381(16)
P2	C37	1.791(10)	C40	C41	1.383(16)
C2	C3	1.399(14)	C41	C42	1.392(15)
C3	C4	1.402(16)	B2	F5	1.276(17)
C4	C5	1.396(14)	B2	F6	1.335(18)
C6	C7	1.413(14)	B2	F7	1.294(17)
C6	C10	1.426(15)	B2	F8	1.49(2)
C7	C8	1.400(16)	F1	B1	1.386(14)
C8	C9	1.436(18)	B1	F2	1.375(15)
C9	C10	1.388(16)	B1	F3	1.367(14)
C13	C14	1.386(14)	B1	F4	1.405(13)
C13	C18	1.409(13)	Cl1	C43	1.786(16)
C14	C15	1.397(14)	Cl2	C43	1.787(15)

Atom	**Atom**	**Atom**	**Angle/˚**	**Atom**	**Atom**	**Atom**	**Angle/˚**
N1	Pd1	Fe1	79.8(2)	C37	P2	C31	107.7(4)
N1	Pd1	P1	99.5(2)	C1	C2	Fe1	71.4(6)
N1	Pd1	P2	158.9(2)	C3	C2	Fe1	69.7(6)
N1	Pd1	C6	34.0(3)	C3	C2	C1	108.2(9)
P1	Pd1	Fe1	177.64(7)	C2	C3	Fe1	70.7(6)
P1	Pd1	C6	133.3(2)	C2	C3	C4	108.1(9)
P2	Pd1	Fe1	79.47(7)	C4	C3	Fe1	70.6(6)
P2	Pd1	P1	100.98(9)	C3	C4	Fe1	69.7(6)
P2	Pd1	C6	125.7(2)	C5	C4	Fe1	71.0(6)
C6	Pd1	Fe1	46.3(2)	C5	C4	C3	109.7(9)
C6	N1	Pd1	88.8(5)	C1	C5	Fe1	71.1(6)
C6	N1	C11	112.9(8)	C4	C5	Fe1	69.7(6)
C6	N1	C12	110.7(7)	C4	C5	C1	107.4(9)
C11	N1	Pd1	112.4(6)	N1	C6	Pd1	57.2(4)
C11	N1	C12	109.3(8)	N1	C6	Fe1	130.2(6)
C12	N1	Pd1	121.4(6)	N1	C6	C10	125.6(9)
C1	Fe1	Pd1	70.9(3)	Fe1	C6	Pd1	74.4(3)
C1	Fe1	C6	130.1(4)	C7	C6	Pd1	120.6(7)
C2	Fe1	Pd1	87.8(3)	C7	C6	N1	126.8(9)
C2	Fe1	C1	40.3(4)	C7	C6	Fe1	67.7(6)
C2	Fe1	C5	67.4(4)	C7	C6	C10	107.6(9)
C2	Fe1	C6	128.6(4)	C10	C6	Pd1	98.2(6)
C2	Fe1	C9	156.8(4)	C10	C6	Fe1	68.3(6)
C2	Fe1	C10	163.6(4)	C6	C7	Fe1	72.8(6)
C3	Fe1	Pd1	127.4(3)	C8	C7	Fe1	70.3(6)
C3	Fe1	C1	66.9(4)	C8	C7	C6	107.9(10)
C3	Fe1	C2	39.6(4)	C7	C8	Fe1	69.9(6)
C3	Fe1	C4	39.7(4)	C7	C8	C9	108.2(10)

C3	Fe1	C5	67.0(4)	C9	C8	Fe1	70.0(6)
C3	Fe1	C6	144.6(4)	C8	C9	Fe1	69.3(6)
C3	Fe1	C7	106.6(4)	C10	C9	Fe1	70.5(6)
C3	Fe1	C8	93.7(5)	C10	C9	C8	107.5(10)
C3	Fe1	C9	117.4(5)	C6	C10	Fe1	72.0(6)
C3	Fe1	C10	156.5(4)	C9	C10	Fe1	70.3(6)
C4	Fe1	Pd1	135.7(3)	C9	C10	C6	108.6(10)
C4	Fe1	C1	66.2(4)	C14	C13	P1	122.0(8)
C4	Fe1	C2	66.4(4)	C14	C13	C18	118.7(9)
C4	Fe1	C5	39.3(4)	C18	C13	P1	119.2(7)
C4	Fe1	C6	162.9(4)	C13	C14	C15	121.3(10)
C4	Fe1	C9	97.2(5)	C14	C15	C16	119.2(10)
C4	Fe1	C10	127.6(5)	C17	C16	C15	120.4(10)
C5	Fe1	Pd1	98.5(3)	C16	C17	C18	120.7(10)
C5	Fe1	C1	40.0(4)	C17	C18	C13	119.6(9)
C5	Fe1	C6	147.6(4)	C20	C19	P1	124.3(8)
C6	Fe1	Pd1	59.3(2)	C20	C19	C24	118.6(9)
C7	Fe1	Pd1	88.9(3)	C24	C19	P1	117.0(7)
C7	Fe1	C1	142.9(4)	C21	C20	C19	121.2(10)
C7	Fe1	C2	110.8(4)	C22	C21	C20	119.4(10)
C7	Fe1	C4	133.0(4)	C21	C22	C23	121.8(10)
C7	Fe1	C5	172.3(4)	C22	C23	C24	119.0(10)
C7	Fe1	C6	39.5(4)	C23	C24	C19	120.0(9)
C7	Fe1	C8	39.7(5)	C26	C25	P1	120.8(8)
C7	Fe1	C9	67.6(5)	C26	C25	C30	120.7(10)
C7	Fe1	C10	67.3(4)	C30	C25	P1	118.4(8)
C8	Fe1	Pd1	124.6(4)	C25	C26	C27	118.6(11)
C8	Fe1	C1	160.6(4)	C28	C27	C26	119.4(12)
C8	Fe1	C2	123.1(5)	C29	C28	C27	122.1(11)
C8	Fe1	C4	99.7(5)	C28	C29	C30	119.4(11)
C8	Fe1	C5	134.3(5)	C29	C30	C25	119.8(10)
C8	Fe1	C6	65.8(4)	C32	C31	P2	119.5(7)
C8	Fe1	C9	40.6(5)	C32	C31	C36	119.7(9)
C8	Fe1	C10	66.8(5)	C36	C31	P2	120.8(7)
C9	Fe1	Pd1	115.0(3)	C33	C32	C31	120.3(10)
C9	Fe1	C1	149.1(5)	C32	C33	C34	119.7(11)
C9	Fe1	C5	110.8(5)	C35	C34	C33	119.9(10)
C9	Fe1	C6	66.0(4)	C34	C35	C36	122.0(11)
C9	Fe1	C10	39.1(4)	C35	C36	C31	118.5(10)
C10	Fe1	Pd1	75.9(3)	C38	C37	P2	121.1(7)
C10	Fe1	C1	132.1(4)	C42	C37	P2	120.6(7)
C10	Fe1	C5	116.6(4)	C42	C37	C38	118.1(9)
C10	Fe1	C6	39.7(4)	C37	C38	C39	120.7(9)
C13	P1	Pd1	116.4(3)	C40	C39	C38	119.8(10)
C19	P1	Pd1	114.9(3)	C39	C40	C41	120.0(10)
C19	P1	C13	102.9(4)	C40	C41	C42	120.0(10)
C25	P1	Pd1	109.4(3)	C37	C42	C41	121.2(10)
C25	P1	C13	104.0(5)	F5	B2	F6	119.3(13)
C25	P1	C19	108.4(5)	F5	B2	F7	119.4(15)
P2	C1	Fe1	115.4(5)	F5	B2	F8	96.5(14)
C2	C1	Fe1	68.3(6)	F6	B2	F8	99.0(14)
C2	C1	P2	125.2(7)	F7	B2	F6	118.2(13)
C5	C1	Fe1	68.9(6)	F7	B2	F8	92.4(13)
C5	C1	P2	126.3(7)	F1	B1	F4	109.2(9)
C5	C1	C2	106.6(9)	F2	B1	F1	109.0(10)
C1	P2	Pd1	92.9(3)	F2	B1	F4	109.7(10)
C1	P2	C31	107.5(4)	F3	B1	F1	111.6(10)
C1	P2	C37	105.4(4)	F3	B1	F2	109.6(10)
C31	P2	Pd1	122.2(3)	F3	B1	F4	107.7(10)
C37	P2	Pd1	118.1(3)	Cl1	C43	Cl2	107.6(8)

Table S17: Bond lengths and angles for compound **14**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	Fe1	2.8184(9)	C22	C17	1.401(8)
Pd1	P2	2.2297(15)	C22	C21	1.365(9)
Pd1	P1	2.3022(14)	C5	C4	1.402(10)
Pd1	N1	2.138(5)	N2	C40	1.485(8)
Pd1	C6	2.514(5)	N2	C48	1.501(8)
Fe1	C1	2.118(6)	N2	C47	1.493(9)
Fe1	C5	2.052(7)	C38	C37	1.406(10)
Fe1	C9	2.044(6)	C38	C39	1.424(9)
Fe1	C8	2.067(6)	C9	C8	1.430(8)
Fe1	C7	2.084(6)	C9	C10	1.399(9)
Fe1	C10	2.080(6)	C35	C36	1.423(8)
Fe1	C6	2.103(6)	C35	C39	1.435(9)
Fe1	C2	2.088(6)	C36	C37	1.442(9)
Fe1	C4	2.056(6)	C8	C7	1.410(8)
Fe1	C3	2.069(7)	C23	C28	1.379(8)
Fe2	C38	2.040(6)	C23	C24	1.383(9)
Fe2	C35	2.061(6)	C7	C6	1.428(9)
Fe2	C36	2.064(5)	C10	C6	1.426(7)
Fe2	C37	2.054(6)	C17	C18	1.401(8)
Fe2	C40	2.001(6)	C21	C20	1.365(9)
Fe2	C44	2.065(7)	F7	B2	1.356(10)
Fe2	C39	2.035(6)	C30	C31	1.377(9)
Fe2	C41	2.054(6)	C2	C3	1.422(8)
Fe2	C42	2.062(6)	C34	C33	1.394(10)
Fe2	C43	2.053(6)	C28	C27	1.385(8)
P2	C1	1.766(6)	C11	C16	1.399(8)
P2	C29	1.802(6)	C11	C12	1.399(10)
P2	C23	1.804(6)	C40	C44	1.424(9)
P1	C35	1.795(6)	C40	C41	1.414(9)
P1	C17	1.813(6)	C27	C26	1.382(10)
P1	C11	1.810(5)	C32	C33	1.388(11)
F1	B1	1.391(8)	C32	C31	1.386(10)
F4	B1	1.405(8)	C44	C43	1.420(10)
F2	B1	1.378(8)	C16	C15	1.380(9)
F3	B1	1.393(7)	C18	C19	1.356(9)
F8	B2	1.372(10)	C41	C42	1.436(10)
N1	C6	1.427(7)	C20	C19	1.383(10)
N1	C45	1.477(8)	C12	C13	1.385(8)
N1	C46	1.495(8)	C42	C43	1.413(11)
C1	C5	1.462(8)	C24	C25	1.381(9)
C1	C2	1.444(10)	C4	C3	1.378(11)
F5	B2	1.361(8)	C26	C25	1.396(10)
F6	B2	1.358(10)	C14	C13	1.389(11)
C29	C30	1.405(8)	C14	C15	1.393(11)
C29	C34	1.398(9)			

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
P2	Pd1	Fe1	79.74(4)	C45	N1	C46	110.7(5)
P2	Pd1	P1	98.14(5)	C46	N1	Pd1	110.7(4)
P2	Pd1	C6	125.53(14)	P2	C1	Fe1	114.3(3)
P1	Pd1	Fe1	176.43(5)	C5	C1	Fe1	67.1(3)
P1	Pd1	C6	136.30(14)	C5	C1	P2	127.8(5)
N1	Pd1	Fe1	79.50(13)	C2	C1	Fe1	68.8(3)
N1	Pd1	P2	158.79(13)	C2	C1	P2	123.8(4)
N1	Pd1	P1	102.37(13)	C2	C1	C5	105.8(5)
N1	Pd1	C6	34.54(18)	C30	C29	P2	119.1(5)
C6	Pd1	Fe1	46.02(14)	C34	C29	P2	121.4(5)
C1	Fe1	Pd1	70.28(17)	C34	C29	C30	119.0(6)
C5	Fe1	Pd1	86.01(19)	C21	C22	C17	120.1(6)
C5	Fe1	C1	41.0(2)	C1	C5	Fe1	71.9(4)
C5	Fe1	C8	161.7(2)	C4	C5	Fe1	70.2(4)
C5	Fe1	C7	158.3(3)	C4	C5	C1	107.8(7)
C5	Fe1	C10	111.3(3)	C40	N2	C48	109.8(5)
C5	Fe1	C6	125.2(3)	C40	N2	C47	112.4(5)
C5	Fe1	C2	68.1(3)	C47	N2	C48	113.1(5)
C5	Fe1	C4	39.9(3)	C37	C38	Fe2	70.5(4)
C5	Fe1	C3	66.8(3)	C37	C38	C39	107.6(6)
C9	Fe1	Pd1	125.63(18)	C39	C38	Fe2	69.4(4)
C9	Fe1	C1	162.8(2)	C8	C9	Fe1	70.5(3)
C9	Fe1	C5	126.9(2)	C10	C9	Fe1	71.5(3)
C9	Fe1	C8	40.7(2)	C10	C9	C8	109.8(5)
C9	Fe1	C7	67.1(2)	P1	C35	Fe2	133.9(3)
C9	Fe1	C10	39.7(3)	C36	C35	Fe2	69.9(3)
C9	Fe1	C6	66.3(2)	C36	C35	P1	126.9(5)
C9	Fe1	C2	131.0(3)	C36	C35	C39	107.4(5)
C9	Fe1	C4	95.8(2)	C39	C35	Fe2	68.5(3)
C9	Fe1	C3	97.8(3)	C39	C35	P1	125.0(4)
C8	Fe1	Pd1	112.23(17)	C35	C36	Fe2	69.7(3)
C8	Fe1	C1	145.5(2)	C35	C36	C37	107.5(6)
C8	Fe1	C7	39.7(2)	C37	C36	Fe2	69.1(3)
C8	Fe1	C10	67.8(3)	C9	C8	Fe1	68.8(3)
C8	Fe1	C6	66.8(3)	C7	C8	Fe1	70.8(3)
C8	Fe1	C2	108.9(3)	C7	C8	C9	107.0(6)
C8	Fe1	C3	98.9(3)	C38	C37	Fe2	69.4(3)
C7	Fe1	Pd1	72.53(16)	C38	C37	C36	108.9(6)
C7	Fe1	C1	128.8(2)	C36	C37	Fe2	69.9(3)
C7	Fe1	C6	39.9(2)	C28	C23	P2	120.7(4)
C7	Fe1	C2	117.5(3)	C28	C23	C24	120.4(6)
C10	Fe1	Pd1	91.87(17)	C24	C23	P2	118.5(4)
C10	Fe1	C1	145.8(3)	C8	C7	Fe1	69.5(3)
C10	Fe1	C7	67.6(2)	C8	C7	C6	108.0(5)
C10	Fe1	C6	39.9(2)	C6	C7	Fe1	70.8(3)
C10	Fe1	C2	168.6(2)	C9	C10	Fe1	68.8(3)
C6	Fe1	Pd1	59.34(14)	C9	C10	C6	106.9(5)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C6	Fe1	C1	129.3(2)	C6	C10	Fe1	71.0(3)
C2	Fe1	Pd1	99.38(17)	C22	C17	P1	118.6(5)
C2	Fe1	C1	40.2(3)	C18	C17	P1	123.7(5)
C2	Fe1	C6	150.2(2)	C18	C17	C22	117.8(6)
C4	Fe1	Pd1	125.9(2)	Fe1	C6	Pd1	74.64(16)
C4	Fe1	C1	67.4(2)	N1	C6	Pd1	58.1(3)
C4	Fe1	C8	121.8(3)	N1	C6	Fe1	130.0(4)
C4	Fe1	C7	161.2(2)	N1	C6	C7	124.8(5)
C4	Fe1	C10	104.9(3)	C7	C6	Pd1	93.2(3)
C4	Fe1	C6	141.7(3)	C7	C6	Fe1	69.3(3)
C4	Fe1	C2	66.9(3)	C10	C6	Pd1	126.8(4)
C4	Fe1	C3	39.0(3)	C10	C6	Fe1	69.2(3)
C3	Fe1	Pd1	136.56(18)	C10	C6	N1	126.8(6)
C3	Fe1	C1	67.0(3)	C10	C6	C7	108.4(5)
C3	Fe1	C7	131.9(3)	C20	C21	C22	121.3(6)
C3	Fe1	C10	128.7(2)	C31	C30	C29	121.3(7)
C3	Fe1	C6	163.6(3)	C1	C2	Fe1	71.0(4)
C3	Fe1	C2	40.0(2)	C3	C2	Fe1	69.3(4)
C38	Fe2	C35	69.0(2)	C3	C2	C1	107.5(7)
C38	Fe2	C36	68.7(3)	C33	C34	C29	119.0(7)
C38	Fe2	C37	40.2(3)	C23	C28	C27	120.1(6)
C38	Fe2	C44	158.8(3)	C16	C11	P1	123.7(5)
C38	Fe2	C41	103.7(3)	C16	C11	C12	118.9(5)
C38	Fe2	C42	120.3(3)	C12	C11	P1	117.4(5)
C38	Fe2	C43	157.3(3)	N2	C40	Fe2	126.6(4)
C35	Fe2	C36	40.4(2)	C44	C40	Fe2	71.9(3)
C35	Fe2	C44	123.6(3)	C44	C40	N2	121.5(6)
C35	Fe2	C42	126.2(3)	C41	C40	Fe2	71.6(3)
C36	Fe2	C44	108.8(3)	C41	C40	N2	127.0(6)
C37	Fe2	C35	68.3(2)	C41	C40	C44	111.4(6)
C37	Fe2	C36	41.0(2)	C26	C27	C28	119.3(6)
C37	Fe2	C44	124.3(3)	C31	C32	C33	119.7(7)
C37	Fe2	C42	154.7(3)	C40	C44	Fe2	67.1(3)
C40	Fe2	C38	121.1(3)	C43	C44	Fe2	69.4(4)
C40	Fe2	C35	158.3(3)	C43	C44	C40	105.1(6)
C40	Fe2	C36	121.8(2)	C38	C39	Fe2	69.7(3)
C40	Fe2	C37	106.1(2)	C38	C39	C35	108.7(6)
C40	Fe2	C44	41.0(3)	C35	C39	Fe2	70.5(3)
C40	Fe2	C39	158.2(3)	C32	C33	C34	121.3(7)
C40	Fe2	C41	40.8(3)	C15	C16	C11	119.5(7)
C40	Fe2	C42	67.8(3)	C30	C31	C32	119.6(7)
C40	Fe2	C43	67.7(3)	C19	C18	C17	121.1(6)
C39	Fe2	C38	40.9(2)	C40	C41	Fe2	67.6(3)
C39	Fe2	C35	41.0(2)	C40	C41	C42	105.3(7)
C39	Fe2	C36	68.4(2)	C42	C41	Fe2	69.9(4)
C39	Fe2	C37	67.9(3)	C21	C20	C19	119.6(6)
C39	Fe2	C44	159.4(3)	C13	C12	C11	121.2(7)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C39	Fe2	C41	122.0(3)	C41	C42	Fe2	69.3(3)
C39	Fe2	C42	108.1(3)	C43	C42	Fe2	69.6(3)
C39	Fe2	C43	123.9(3)	C43	C42	C41	108.5(6)
C41	Fe2	C35	160.6(3)	C25	C24	C23	120.4(6)
C41	Fe2	C36	155.4(3)	C5	C4	Fe1	69.9(4)
C41	Fe2	C37	118.4(3)	C3	C4	Fe1	71.0(4)
C41	Fe2	C44	69.4(3)	C3	C4	C5	109.4(6)
C41	Fe2	C42	40.8(3)	C18	C19	C20	120.2(6)
C42	Fe2	C36	163.0(3)	C27	C26	C25	121.0(6)
C42	Fe2	C44	68.2(3)	C44	C43	Fe2	70.3(3)
C43	Fe2	C35	111.0(3)	C42	C43	Fe2	70.3(4)
C43	Fe2	C36	127.0(3)	C42	C43	C44	109.6(6)
C43	Fe2	C37	162.4(3)	C2	C3	Fe1	70.7(4)
C43	Fe2	C44	40.3(3)	C4	C3	Fe1	70.0(4)
C43	Fe2	C41	68.5(3)	C4	C3	C2	109.4(7)
C43	Fe2	C42	40.2(3)	C13	C14	C15	119.3(6)
C1	P2	Pd1	92.3(2)	C12	C13	C14	119.6(7)
C1	P2	C29	110.5(3)	C16	C15	C14	121.4(7)
C1	P2	C23	103.7(3)	C24	C25	C26	118.8(7)
C29	P2	Pd1	119.4(2)	F1	B1	F4	109.1(5)
C29	P2	C23	109.0(3)	F1	B1	F3	109.1(5)
C23	P2	Pd1	119.0(2)	F2	B1	F1	110.7(6)
C35	P1	Pd1	112.11(19)	F2	B1	F4	108.5(5)
C35	P1	C17	106.3(3)	F2	B1	F3	109.3(6)
C35	P1	C11	104.4(3)	F3	B1	F4	110.0(6)
C17	P1	Pd1	110.47(19)	F5	B2	F8	109.9(6)
C11	P1	Pd1	113.6(2)	F6	B2	F8	112.0(7)
C11	P1	C17	109.5(3)	F6	B2	F5	107.1(8)
C6	N1	Pd1	87.3(3)	F7	B2	F8	111.8(8)
C6	N1	C45	111.1(5)	F7	B2	F5	108.3(7)
C6	N1	C46	113.6(5)	F7	B2	F6	107.4(7)
C45	N1	Pd1	121.6(3)				

Table S18: Bond lengths and angles for compound **15**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	Fe1	2.8349(11)	C11	C16	1.381(9)
Pd1	P1	2.2996(17)	C12	C13	1.381(9)
Pd1	P2	2.2468(14)	C13	C14	1.390(10)
Pd1	N1	2.146(5)	C14	C15	1.375(10)
Pd1	C6	2.528(6)	C15	C16	1.387(9)
Fe1	C1	2.104(6)	C18	C19	1.389(10)
Fe1	C2	2.087(7)	C18	C23	1.383(10)
Fe1	C3	2.053(7)	C19	C20	1.387(10)
Fe1	C4	2.055(7)	C20	C21	1.407(10)
Fe1	C5	2.069(7)	C21	C22	1.385(10)
Fe1	C6	2.132(6)	C22	C23	1.384(10)
Fe1	C7	2.078(7)	C25	C26	1.390(10)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	C8	2.045(7)	C25	C30	1.395(9)
Fe1	C9	2.043(7)	C26	C27	1.375(9)
Fe1	C10	2.082(7)	C27	C28	1.409(10)
P1	C11	1.821(6)	C28	C29	1.377(11)
P1	C18	1.814(7)	C29	C30	1.384(9)
P1	C25	1.823(7)	C32	C33	1.379(9)
P2	C1	1.770(7)	C32	C37	1.399(9)
P2	C32	1.800(7)	C33	C34	1.395(10)
P2	C38	1.815(6)	C34	C35	1.379(11)
O1	C14	1.359(8)	C35	C36	1.380(12)
O1	C17	1.441(9)	C36	C37	1.377(10)
O2	C21	1.349(8)	C38	C39	1.372(9)
O2	C24	1.434(9)	C38	C43	1.396(9)
O3	C28	1.370(8)	C39	C40	1.387(10)
O3	C31	1.443(9)	C40	C41	1.367(12)
N1	C6	1.408(9)	C41	C42	1.378(12)
N1	C44	1.491(9)	C42	C43	1.400(10)
N1	C45	1.496(8)	F6	B2	1.356(9)
C1	C2	1.424(9)	F5	B2	1.373(10)
C1	C5	1.446(9)	B2	F6[1]	1.356(9)
C2	C3	1.414(10)	B2	F5[1]	1.373(10)
C3	C4	1.422(11)	F3	B1	1.376(10)
C4	C5	1.425(10)	F4	B1	1.387(10)
C6	C7	1.427(11)	F1	B1	1.376(12)
C6	C10	1.429(10)	F2	B1	1.383(12)
C7	C8	1.435(11)	F7	B3	1.306(13)
C8	C9	1.413(13)	F8	B3	1.306(11)
C9	C10	1.422(12)	B3	F7[2]	1.306(13)
C11	C12	1.405(9)	B3	F8[2]	1.306(11)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
P1	Pd1	Fe1	173.55(5)	C2	C3	Fe1	71.3(4)
P1	Pd1	C6	132.98(15)	C2	C3	C4	108.9(6)
P2	Pd1	Fe1	80.39(5)	C4	C3	Fe1	69.8(4)
P2	Pd1	P1	100.13(6)	C3	C4	Fe1	69.7(4)
P2	Pd1	C6	126.74(15)	C3	C4	C5	108.1(6)
N1	Pd1	Fe1	80.08(16)	C5	C4	Fe1	70.3(4)
N1	Pd1	P1	99.19(16)	C1	C5	Fe1	71.0(4)
N1	Pd1	P2	160.45(16)	C4	C5	Fe1	69.3(4)
N1	Pd1	C6	33.8(2)	C4	C5	C1	107.0(6)
C6	Pd1	Fe1	46.41(15)	Fe1	C6	Pd1	74.39(17)
C1	Fe1	Pd1	70.24(17)	N1	C6	Pd1	58.0(3)
C1	Fe1	C6	129.4(2)	N1	C6	Fe1	132.0(4)
C2	Fe1	Pd1	96.57(18)	N1	C6	C7	126.1(6)
C2	Fe1	C1	39.7(3)	N1	C6	C10	125.9(7)
C2	Fe1	C6	143.4(3)	C7	C6	Pd1	103.9(4)
C3	Fe1	Pd1	135.1(2)	C7	C6	Fe1	68.2(4)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C3	Fe1	C1	66.9(3)	C7	C6	C10	107.9(6)
C3	Fe1	C2	39.9(3)	C10	C6	Pd1	115.8(5)
C3	Fe1	C4	40.5(3)	C10	C6	Fe1	68.3(4)
C3	Fe1	C5	68.0(3)	C6	C7	Fe1	72.2(4)
C3	Fe1	C6	160.5(3)	C6	C7	C8	107.6(7)
C3	Fe1	C7	122.7(3)	C8	C7	Fe1	68.4(4)
C3	Fe1	C10	137.0(3)	C7	C8	Fe1	70.9(4)
C4	Fe1	Pd1	128.3(2)	C9	C8	Fe1	69.7(4)
C4	Fe1	C1	67.4(3)	C9	C8	C7	108.1(7)
C4	Fe1	C2	67.7(3)	C8	C9	Fe1	69.9(4)
C4	Fe1	C5	40.4(3)	C8	C9	C10	108.5(7)
C4	Fe1	C6	148.5(3)	C10	C9	Fe1	71.3(4)
C4	Fe1	C7	152.4(3)	C6	C10	Fe1	72.1(4)
C4	Fe1	C10	109.3(3)	C9	C10	Fe1	68.4(4)
C5	Fe1	Pd1	87.9(2)	C9	C10	C6	107.9(7)
C5	Fe1	C1	40.5(3)	C12	C11	P1	118.0(5)
C5	Fe1	C2	68.0(3)	C16	C11	P1	123.7(5)
C5	Fe1	C6	130.8(3)	C16	C11	C12	118.3(6)
C5	Fe1	C7	167.1(3)	C13	C12	C11	120.8(6)
C5	Fe1	C10	110.6(3)	C12	C13	C14	119.6(6)
C6	Fe1	Pd1	59.20(17)	O1	C14	C13	115.2(6)
C7	Fe1	Pd1	79.3(2)	O1	C14	C15	124.6(7)
C7	Fe1	C1	133.3(3)	C15	C14	C13	120.2(6)
C7	Fe1	C2	114.6(3)	C14	C15	C16	119.9(7)
C7	Fe1	C6	39.6(3)	C11	C16	C15	121.2(7)
C7	Fe1	C10	67.4(3)	C19	C18	P1	120.3(5)
C8	Fe1	Pd1	119.5(2)	C23	C18	P1	121.2(5)
C8	Fe1	C1	151.3(3)	C23	C18	C19	118.5(6)
C8	Fe1	C2	112.1(3)	C20	C19	C18	120.2(7)
C8	Fe1	C3	93.6(3)	C19	C20	C21	120.7(7)
C8	Fe1	C4	111.8(3)	O2	C21	C20	115.5(6)
C8	Fe1	C5	151.6(3)	O2	C21	C22	125.5(6)
C8	Fe1	C6	67.1(3)	C22	C21	C20	119.0(6)
C8	Fe1	C7	40.7(3)	C23	C22	C21	119.4(6)
C8	Fe1	C10	67.7(4)	C18	C23	C22	122.3(6)
C9	Fe1	Pd1	124.2(2)	C26	C25	P1	121.6(5)
C9	Fe1	C1	158.5(3)	C26	C25	C30	117.6(6)
C9	Fe1	C2	137.6(3)	C30	C25	P1	120.6(5)
C9	Fe1	C3	100.7(3)	C27	C26	C25	121.3(6)
C9	Fe1	C4	91.6(3)	C26	C27	C28	119.8(7)
C9	Fe1	C5	119.4(3)	O3	C28	C27	116.1(6)
C9	Fe1	C6	67.0(3)	O3	C28	C29	123.9(6)
C9	Fe1	C7	68.0(3)	C29	C28	C27	119.9(6)
C9	Fe1	C8	40.4(4)	C28	C29	C30	119.0(6)
C9	Fe1	C10	40.3(3)	C29	C30	C25	122.3(7)
C10	Fe1	Pd1	86.1(2)	C33	C32	P2	123.2(5)
C10	Fe1	C1	140.8(3)	C33	C32	C37	118.5(6)

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C10	Fe1	C2	176.9(3)	C37	C32	P2	118.3(5)
C10	Fe1	C6	39.6(3)	C32	C33	C34	120.9(7)
C11	P1	Pd1	114.7(2)	C35	C34	C33	119.5(7)
C11	P1	C25	105.4(3)	C34	C35	C36	120.4(7)
C18	P1	Pd1	109.9(2)	C37	C36	C35	119.7(7)
C18	P1	C11	107.4(3)	C36	C37	C32	121.0(7)
C18	P1	C25	104.9(3)	C39	C38	P2	121.7(5)
C25	P1	Pd1	113.8(2)	C39	C38	C43	120.0(6)
C1	P2	Pd1	91.80(19)	C43	C38	P2	118.3(5)
C1	P2	C32	104.3(3)	C38	C39	C40	120.4(7)
C1	P2	C38	106.5(3)	C41	C40	C39	119.5(7)
C32	P2	Pd1	123.4(2)	C40	C41	C42	121.6(7)
C32	P2	C38	107.3(3)	C41	C42	C43	118.9(7)
C38	P2	Pd1	119.5(2)	C38	C43	C42	119.5(7)
C14	O1	C17	117.4(6)	F6[1]	B2	F6	112.4(11)
C21	O2	C24	117.0(6)	F6[1]	B2	F5	108.2(3)
C28	O3	C31	116.5(6)	F6	B2	F5	111.3(5)
C6	N1	Pd1	88.2(3)	F6	B2	F5[1]	108.2(3)
C6	N1	C44	113.3(6)	F6[1]	B2	F5[1]	111.3(5)
C6	N1	C45	112.5(5)	F5[1]	B2	F5	105.4(12)
C44	N1	Pd1	111.6(4)	F3	B1	F4	108.8(7)
C44	N1	C45	110.8(5)	F3	B1	F1	109.2(8)
C45	N1	Pd1	118.7(4)	F3	B1	F2	110.1(8)
P2	C1	Fe1	117.2(3)	F1	B1	F4	108.9(8)
C2	C1	Fe1	69.5(4)	F1	B1	F2	109.0(7)
C2	C1	P2	128.1(5)	F2	B1	F4	110.8(7)
C2	C1	C5	108.2(6)	F7	B3	F7[2]	125(2)
C5	C1	Fe1	68.4(3)	F8	B3	F7	103.4(8)
C5	C1	P2	122.3(5)	F8[2]	B3	F7	101.0(7)
C1	C2	Fe1	70.8(4)	F8	B3	F7[2]	101.0(7)
C3	C2	Fe1	68.7(4)	F8[2]	B3	F7[2]	103.4(8)
C3	C2	C1	107.7(6)	F8	B3	F8[2]	125.7(19)

Computational details

All the geometry optimizations and DFT computations were carried out with the Gaussian 16 suite of programs.[11] Harmonic vibrational analysis was obtained at the same level, and in the case of minima, all eigenvalues of the Hessian matrix were positive. For the determination of bond critical points and for Wiberg indices, Multiwfn program was used.[12]

Table S19: Experimental and DFT calculated Fe-Pd distances (in Å). For C, N, O, H, Cl, P 6-311+G** and for Pd Def2TZVP basis sets were applied

	10	11	12	13	14	15
experimental	2.837	2.7384	2.811	2.8289	2.8184	2.8349
B3LYP	2.998	2.863	2.993	3.000	3.042	3.021
B3LYP-D3	3.033	2.9	2.965	2.978	3.002	3.002
ωB97X-D	2.945	2.832	2.87	2.883	2.895	2.896
M06-2X	3.028	2.911	2.974	2.985	2.998	3.010

BP86	2.951	2.824	2.968	2.972	3.020	3.000
PBEh1PBE	2.932	2.818	2.915	2.921	2.965	2.940

Table S20: Electron density in the bond critical point and Wiberg index for Fe-Pd bond at ωB97X-D/6-311+G** (for Pd Def2TZVP)

Fe-Pd bond	**10**	**11**	**12**	**13**	**14**	**15**
Electron density in the bond critical point [a.u.]	0.027	0.033	0.032	0.031	0.03	0.03
Wiberg bond index	0.243	0.313	0.267	0.264	0.256	0.252

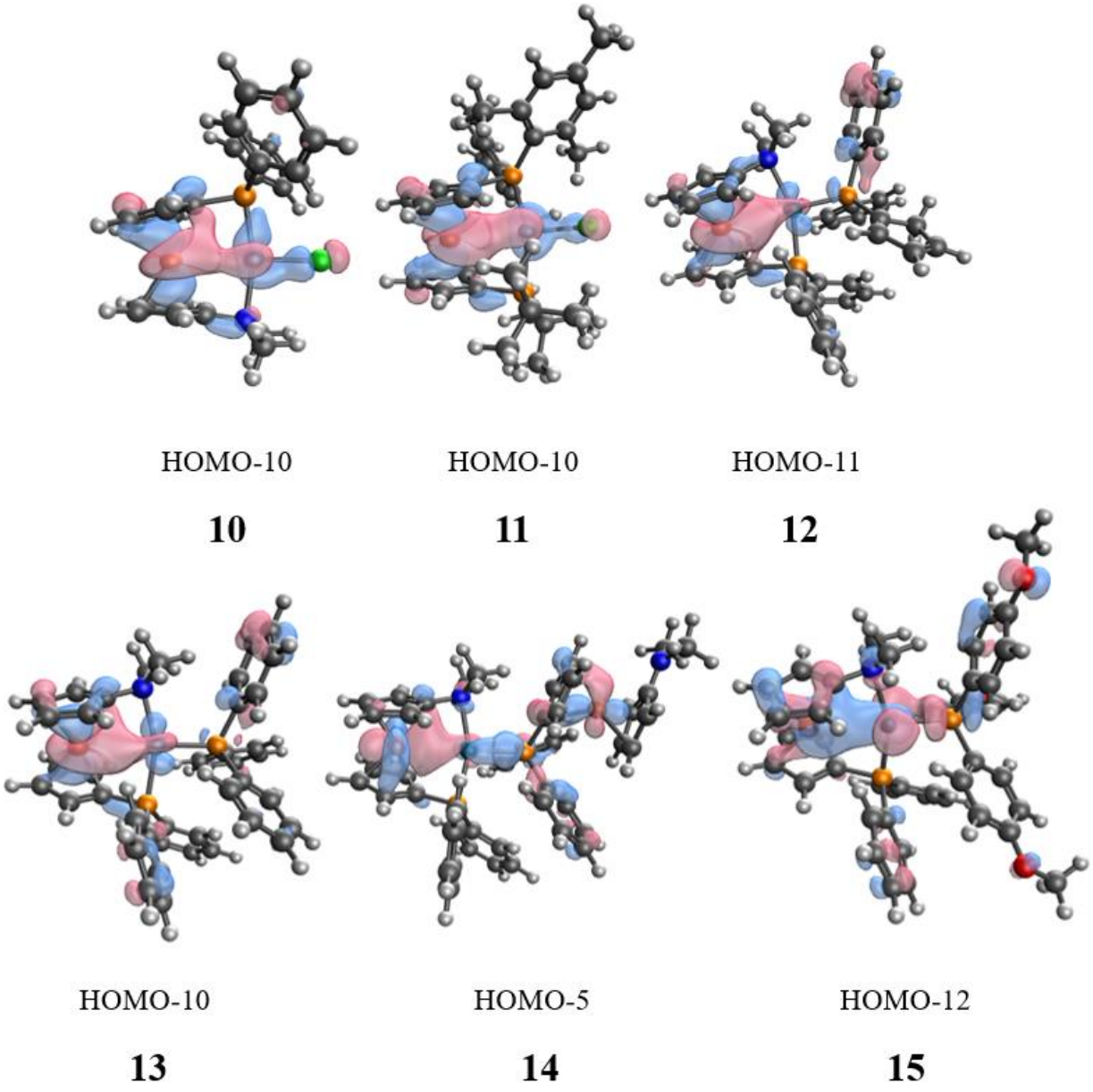


Fig S63 Selected Kohn-Sham orbitals of the investigated systems. These orbitals can be responsible for the Fe->Pd interaction

Table S21. Tabulated data of the PES scans of compounds **10**-**15**

10		**11**		**12**		**13**		**14**		**15**	
Pd-Fe distance (Å)	relative E (kcal/mol)	Pd-Fe distance (Å)	relative E (kcal/mol)	Pd-Fe distance (Å)	relative E (kcal/mol)	Pd-Fe distance (Å)	relative E (kcal/mol)	Pd-Fe distance (Å)	relative E (kcal/mol)	Pd-Fe distance (Å)	relative E (kcal/mol)
2.695	2.6	2.582	4.5	2.57	6.0	2.583	5.8	2.595	5.6	2.596	5.6
2.745	1.5	2.632	2.7	2.67	2.4	2.683	2.3	2.645	3.6	2.696	2.2
2.795	0.7	2.682	1.4	2.77	0.5	2.783	0.5	2.695	2.2	2.796	0.4
2.845	0.3	2.732	0.6	**2.87**	**0.0**	**2.883**	**0.0**	2.745	1.1	**2.896**	**0.0**
2.895	0.1	2.782	0.1	2.97	0.6	2.983	0.6	2.795	0.4	2.996	0.6
2.945	**0.0**	**2.832**	**0.0**	3.07	2.2	3.083	2.2	**2.845**	**0.0**	3.096	2.1
2.995	0.1	2.882	0.2	3.087	2.6	3.183	4.5	**2.895**	**0.0**	3.196	4.3
3.045	0.5	2.932	0.8	3.187	5.1	3.283	7.4	2.995	0.7	3.296	7.1
3.095	1.1	2.982	1.6	3.287	8.1	3.383	10.8	3.095	2.3	3.396	10.2
3.145	1.8	3.032	2.7	3.387	11.6	3.483	14.2	3.195	4.7	3.496	13.0
3.195	2.7	3.082	4.0	3.487	14.9	3.583	16.4	3.295	7.8	3.596	12.6
3.245	3.9	3.132	5.5	3.587	16.1	3.683	14.9	3.395	11.2	3.696	10.8
3.345	6.6	3.232	9.1	3.687	14.8	3.783	13.3	3.495	14.5	3.796	8.8
3.445	10.0	3.332	13.3	3.787	13.2	3.883	12.4	3.595	15.7	3.896	7.9
3.545	13.9	3.432	17.9	3.887	12.3	3.983	11.8	3.695	11.4	3.996	7.4
3.645	12.5	3.532	22.4	3.987	11.9	4.083	12.0	3.795	10.2	4.096	7.6
3.745	14.2	3.632	25.5	4.087	12.2	4.183	13.0	3.895	9.4	4.196	8.6
3.845	16.2	3.732	12.9	4.187	13.2	4.283	14.8	3.995	9.3	4.296	10.4
3.945	18.6	3.832	12.0	4.287	15.1			4.095	9.9	4.396	13.0
4.045	21.3	3.932	11.5	4.387	17.8			4.195	11.2		
4.145	24.2	4.032	11.9	4.487	21.2			4.295	13.2		
4.245	27.2	4.132	13.2					4.395	15.9		
		4.232	15.4					4.495	19.3		
		4.332	18.4								
		4.432	22.3								

Table S22. Results of the PES scan of **16** and the electron density in the bond critical points and Wiberg bond indices

Fe-Pd distance [Å]	relative energy at ωB97X-D/6-311+G**// ωB97X-D/6-31G* (for Pd Def2TZVP) [kcal/mol]	relative energy at ωB97X-D/6-31G* (for Pd Def2TZVP) [kcal/mol]	electron density in the bond critical point [a.u.]	Wiberg bond index
2.377	11.5	10.3	0.071	0.555
2.427	7.7	7.5	0.065	0.519
2.477	4.8	4.6	0.060	0.486
2.527	2.7	2.5	0.055	0.454
2.577	1.2	1.1	0.050	0.425
2.627	0.3	0.3	0.046	0.397
2.677	0.0	0.0	0.043	0.371
2.727	0.2	0.2	0.040	0.348
2.777	0.8	0.9	0.037	0.326
2.827	1.8	2.0	0.034	0.305
2.877	3.1	3.4	0.032	0.286
2.927	4.8	5.2	0.029	0.268
2.977	6.8	7.2	0.027	0.251

Table S23. Results of the PES scan of **17** and the electron density in the bond critical points and Wiberg bond indices

Fe-Pd distance [Å]	relative energy at ωB97X-D/6-311+G**// ωB97X-D/6-31G* (for Pd Def2TZVP) [kcal/mol]	relative energy at ωB97X-D/6-31G* (for Pd Def2TZVP) [kcal/mol]	electron density in the bond critical point [a.u.]	Wiberg bond index
2.506	7.7	7.5	0.056	0.475
2.556	5.2	5.0	0.052	0.445
2.606	3.2	3.0	0.047	0.417
2.656	1.7	1.6	0.044	0.391
2.706	0.8	0.7	0.04	0.367
2.756	0.2	0.2	0.037	0.343
2.806	0.0	0.0	0.035	0.321
2.856	0.1	0.2	no_bp	0.301
2.906	0.6	0.6	no_bp	0.281
2.956	1.3	1.4	no_bp	0.262
3.006	2.2	2.4	no_bp	0.245
3.056	3.4	3.6	no_bp	0.229
3.106	4.8	5.1	no_bp	0.214

Table S24. Results of the PES scan of **18** and the electron density in the bond critical points and Wiberg bond indices

Fe-Pd distance [Å]	relative energy at ωB97X-D/6-311+G**// ωB97X-D/6-31G* (for Pd Def2TZVP) [kcal/mol]	relative energy at ωB97X-D/6-31G* (for Pd Def2TZVP) [kcal/mol]	electron density in the bond critical point (bp) [a.u.]	Wiberg bond index
2.69	3.6	3.8	0.041	0.363
2.74	2.4	2.5	0.038	0.341

2.79	1.5	1.5	0.034	0.320
2.84	0.8	0.8	0.032	0.300
2.89	0.4	0.3	0.029	0.281
2.94	0.1	0.1	0.027	0.265
2.99	0.0	0.0	0.025	0.248
3.04	0.0	0.1	0.023	0.232
3.09	0.3	0.4	0.021	0.217
3.14	0.4	0.8	0.020	0.205
3.19	1.0	1.4	no_bp	0.191
3.24	1.7	2.2	no_bp	0.178
3.29	2.5	3.2	no_bp	0.165

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