Tuning of Metal Complex Electronics and Reactivity by Remote Lewis Acid Binding to π-Coordinated-Pyridine Diphosphine Ligands

Kyle T. Horak, David VanderVelde, and Theodor Agapie*

Division of Chemistry and Chemical Engineering, California Institute of Technology, 1200 East California Boulevard, MC 127-72, Pasadena, California 91125, United States

Supporting Information

NMR Spectra

Figure S1. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **mP_2NBr_2** 3
Figure S2. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **mP_2NBr_2** 3
Figure S3. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **1** 3
Figure S4. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **1** 4
Figure S5. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **1** 4
Figure S6. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **1-$B(C_6F_5)_3$** 4
Figure S7. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **1-$B(C_6F_5)_3$** 5
Figure S8. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **1-$B(C_6F_5)_3$** 5
Figure S9. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **1-$B(C_6F_5)_3$** 5
Figure S10. ^{1}H NMR (300 MHz, C_6D_6) spectrum of **2Ni** 6
Figure S11. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **2Ni** 6
Figure S12. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **2Ni** 6
Figure S13. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **2Pd** 7
Figure S14. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **2Pd** 7
Figure S15. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **2Pd** 7
Figure S16. ^{1}H NMR (300 MHz, C_6D_6) spectrum of **2Ni-$B(C_6F_5)_3$** 8
Figure S17. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **2Ni-$B(C_6F_5)_3$** 8
Figure S18. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **2Ni-$B(C_6F_5)_3$** 8
Figure S19. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **2Ni-$B(C_6F_5)_3$** 9
Figure S20. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **2Pd-$B(C_6F_5)_3$** 9
Figure S21. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **2Pd-$B(C_6F_5)_3$** 9
Figure S22. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **2Pd-$B(C_6F_5)_3$** 10
Figure S23. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **2Pd-$B(C_6F_5)_3$** 10
Figure S24. ^{1}H NMR (300 MHz, C_6D_6) spectrum of **2Ni-Me** 10
Figure S25. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **2Ni-Me** 11
Figure S26. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **2Ni-Me** 11
Figure S27. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **2Ni-Me** 11
Figure S28. ^{1}H NMR (300 MHz, C_6D_6) spectrum of **2Ni-BCy_2OTf** 12
Figure S29. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **2Ni-BCy_2OTf** 12
Figure S30. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **2Ni-BCy_2OTf** 12
Figure S31. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **2Ni-BCy_2OTf** 13
Figure S32. ^{1}H NMR (500 MHz, CD_3CN) spectrum of **2Pd-H** 13

Figure S33. ^{31}P NMR (121 MHz, CD_3CN) spectrum of **2Pd-H** 13
Figure S34. ^{13}C NMR (126 MHz, CD_3CN) spectrum of **2Pd-H** 14
Figure S35. ^{19}F NMR (282 MHz, CD_3CN) spectrum of **2Pd-H** 14
Figure S36. ^{1}H NMR (300 MHz, d_8-THF) spectrum of **3Ni** 14
Figure S37. ^{31}P NMR (121 MHz, d_8-THF) spectrum of **3Ni** 15
Figure S38. ^{19}F NMR (282 MHz, d_8-THF) spectrum of **3Ni** 15
Figure S39. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **4Ni** 15
Figure S40. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **4Ni** 16
Figure S41 ^{13}C NMR (126 MHz, C_6D_6) spectrum of **4Ni** 16
Figure S42. ^{1}H NMR (300 MHz, C_6D_6) spectrum of **4Ni- $B(C_6F_5)_3$** 16
Figure S43. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **4Ni- $B(C_6F_5)_3$** 17
Figure S44. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **4Ni- $B(C_6F_5)_3$** 17
Figure S45. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **4Ni- $B(C_6F_5)_3$** 17
Figure S46. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **4Ni-Me** 18
Figure S47. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **4Ni-Me** 18
Figure S48. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **4Ni-Me** 18
Figure S49. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **4Ni-Me** 19
Figure S50. ^{1}H NMR (500 MHz, CD_3CN) spectrum of **4Ni-H** 19
Figure S51 ^{31}P NMR (121 MHz, CD_3CN) spectrum of **4Ni-H** 19
Figure S52. ^{13}C NMR (126 MHz, CD_3CN) spectrum of **4Ni-H** 20
Figure S53. ^{19}F NMR (282 MHz, CD_3CN) spectrum of **4Ni-H** 20
Figure S54. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **5Ni** 20
Figure S55. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **5Ni** 21
Figure S56. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **5Ni** 21
Figure S57. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **5Ni** 21
Figure S58. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **6Ni** 22
Figure S59. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **6Ni** 22
Figure S60. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **6Ni** 22
Figure S61. gHSQCAD NMR (^{1}H 500 MHz, C_6D_6) spectrum of **6Ni** 23
Figure S62. gHMBCAD NMR (^{1}H 500 MHz, C_6D_6) spectrum of **6Ni** 23
Figure S63. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **7Ni** 24
Figure S64. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **7Ni** 24
Figure S65. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **7Ni** 24
Figure S66. gHSQCAD NMR (^{1}H 500 MHz, C_6D_6) spectrum of **7Ni** 25
Figure S67. gHMBCAD NMR (^{1}H 500 MHz, C_6D_6) spectrum of **7Ni** 25
Figure S68. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **8Ni** 26
Figure S69. ^{31}P NMR (121 MHz, C_6D_6) spectrum of **8Ni** 26
Figure S70. ^{13}C NMR (126 MHz, C_6D_6) spectrum of **8Ni** 26
Figure S71. gHSQCAD NMR (^{1}H 500 MHz, C_6D_6) spectrum of **8Ni** 27
Figure S72. gHMBCAD NMR (^{1}H 500 MHz, C_6D_6) spectrum of **8Ni** 27
Figure S73. Variable temperature NMR (202 MHz ^{31}P, d_8-toluene) data for **2Ni** 28

Crystallographic Information
Refinement Details 29
Table S1. Crystal and refinement data for reported complexes 29
Table S2. Crystal and refinement data for reported complexes 30

References 30

Experimental Details

Nuclear Magnetic Resonance Spectra

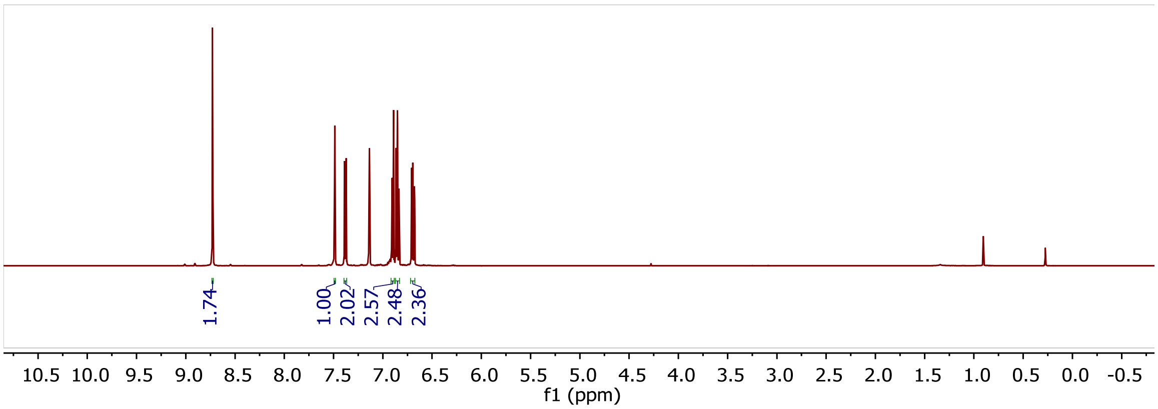

Figure S1. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **mBr$_2$N**

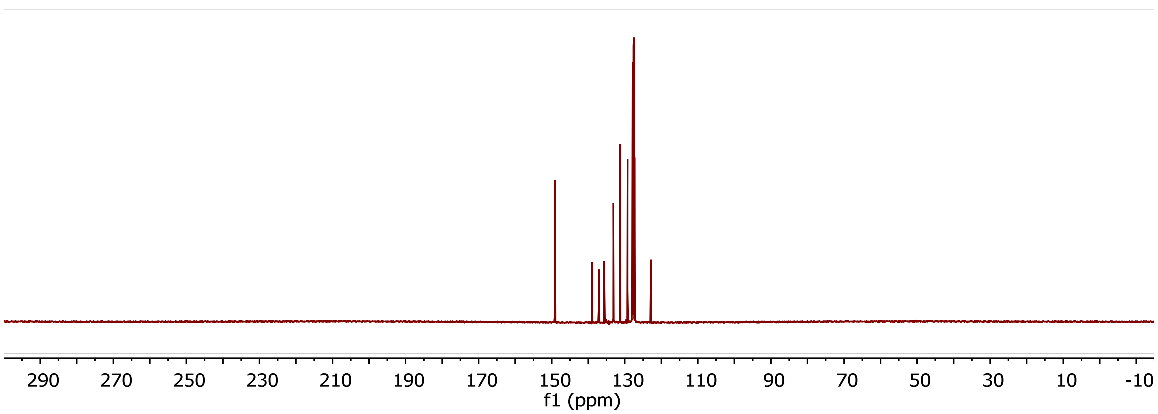

Figure S2. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **mBr$_2$N**

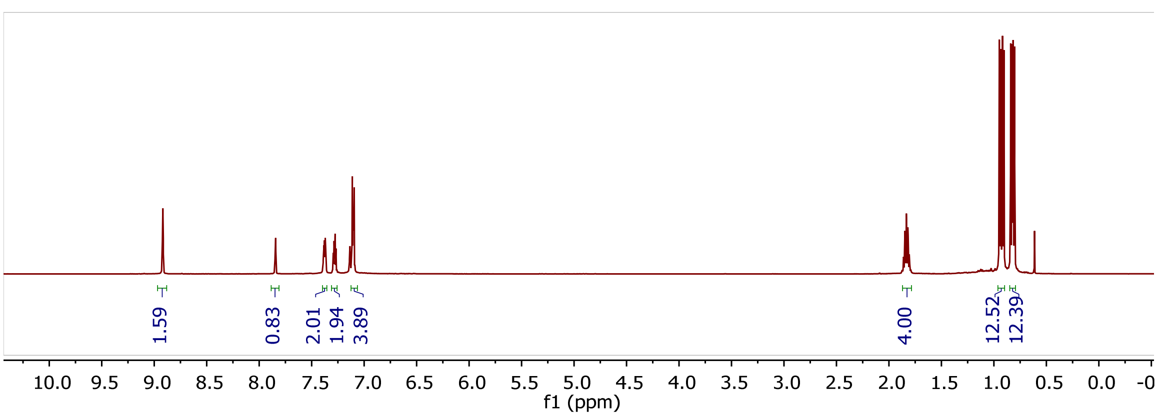

Figure S3. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **1**

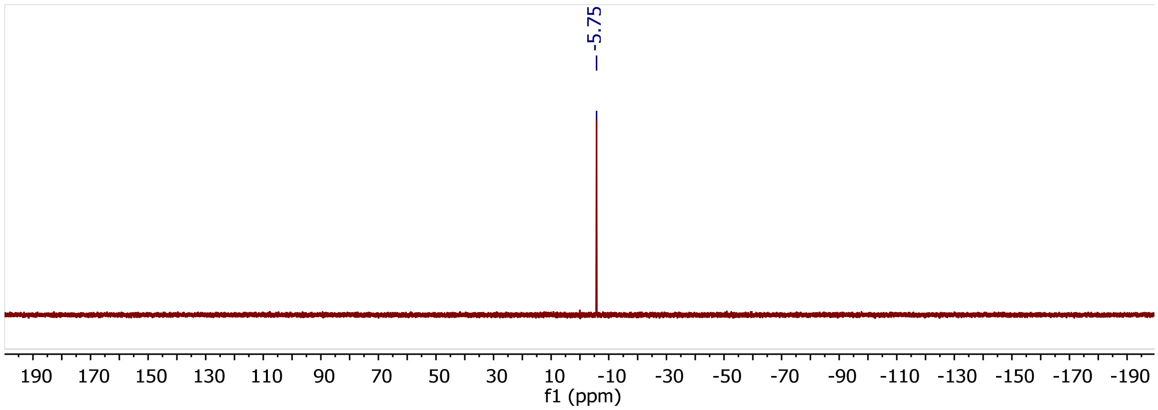

Figure S4. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **1**

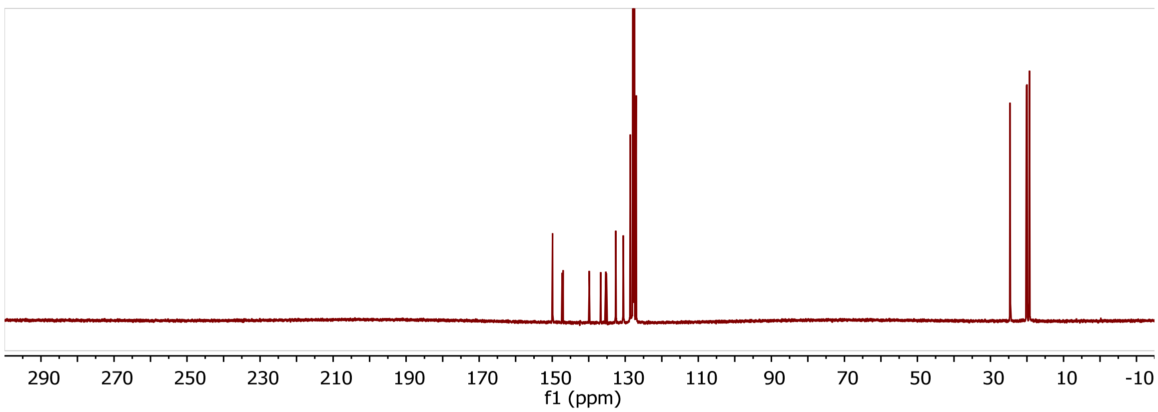

Figure S5. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **1**

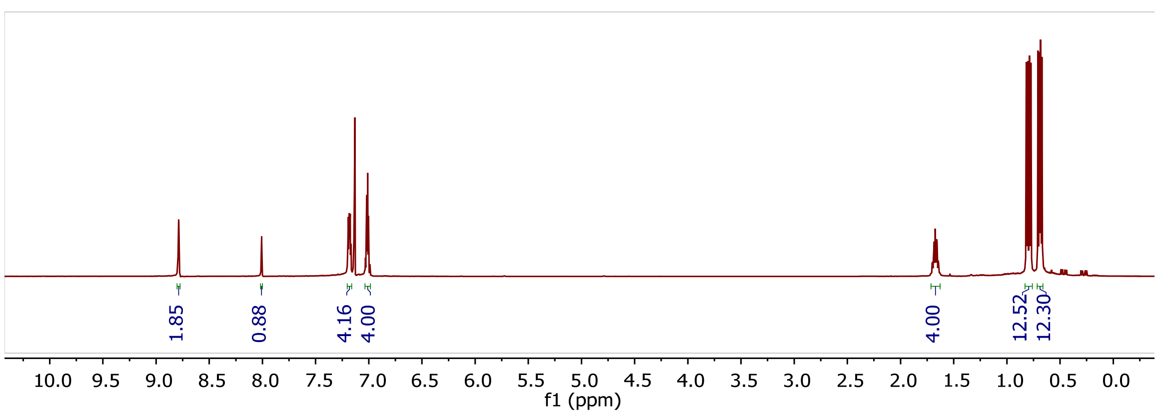

Figure S6. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **1-B(C_6F_5)$_3$**

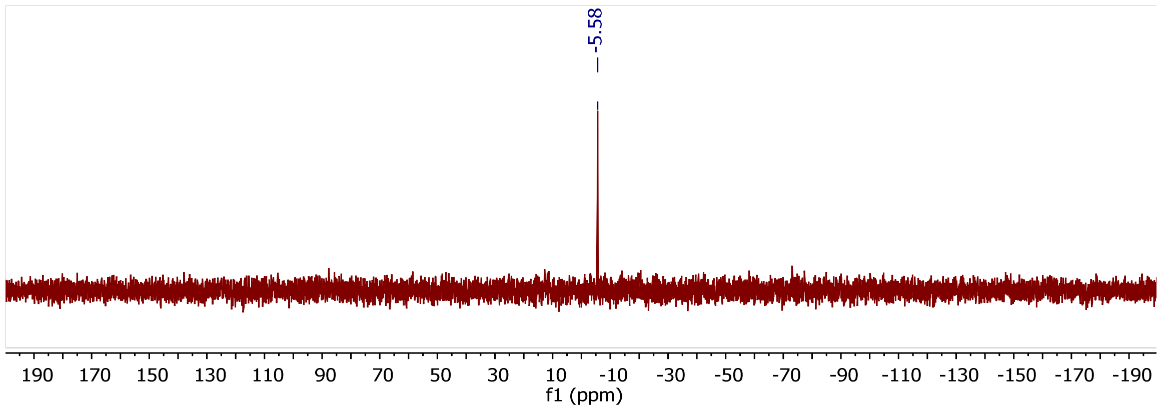

Figure S7. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **1-B(C_6F_5)$_3$**

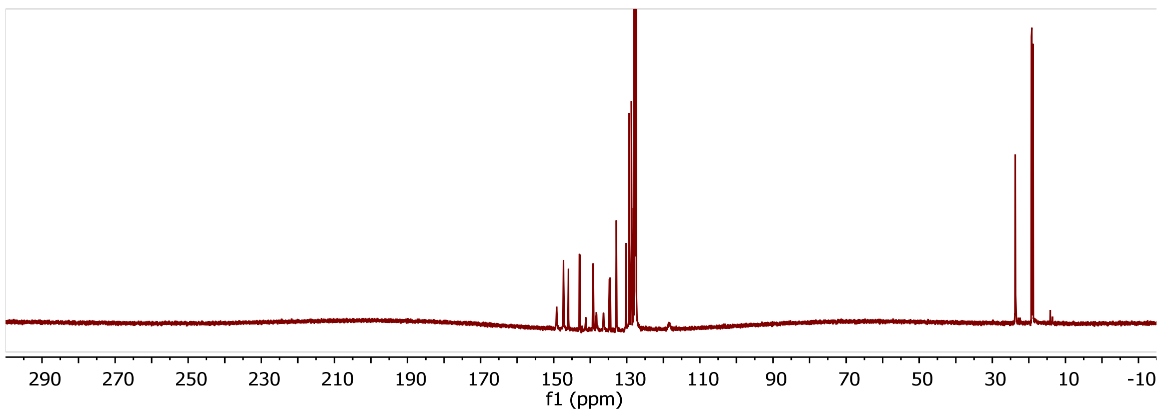

Figure S8. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **1-B(C_6F_5)$_3$**

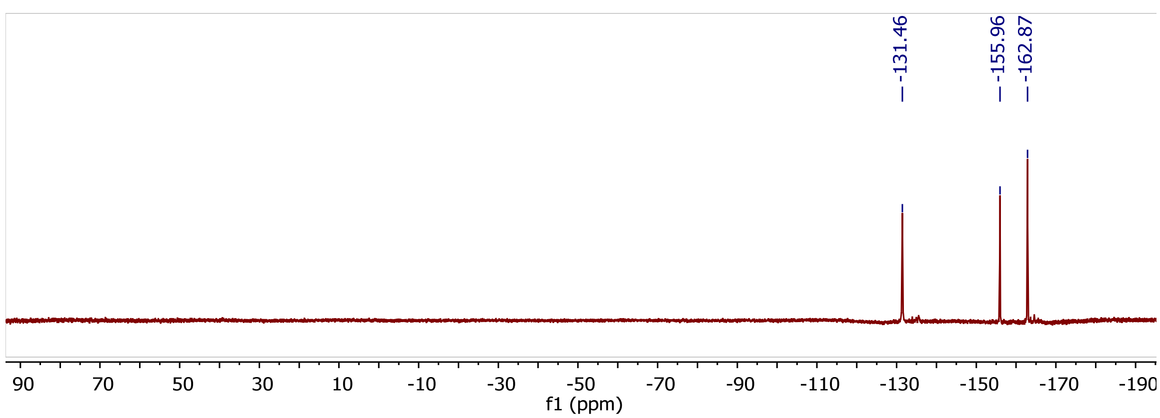

Figure S9. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **1-B(C_6F_5)$_3$**

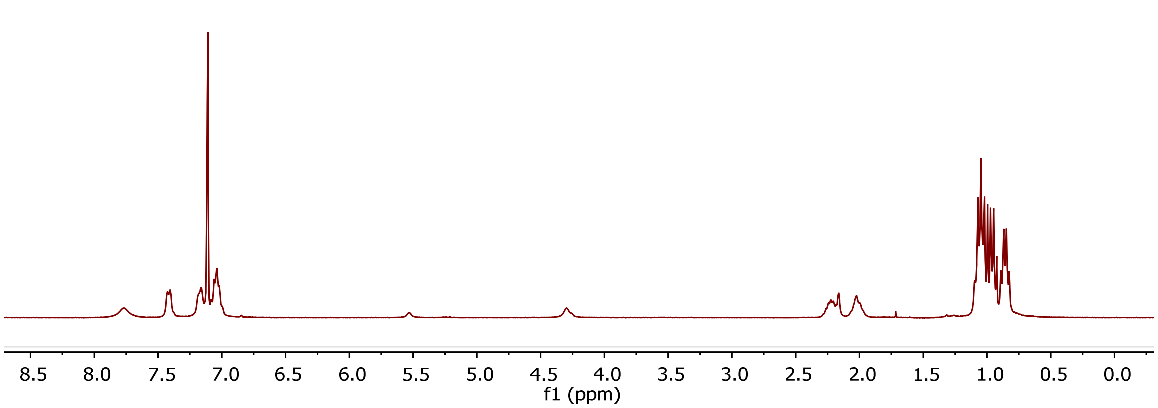

Figure S10. ^{1}H NMR (300 MHz, C_6D_6) spectrum of **2Ni**

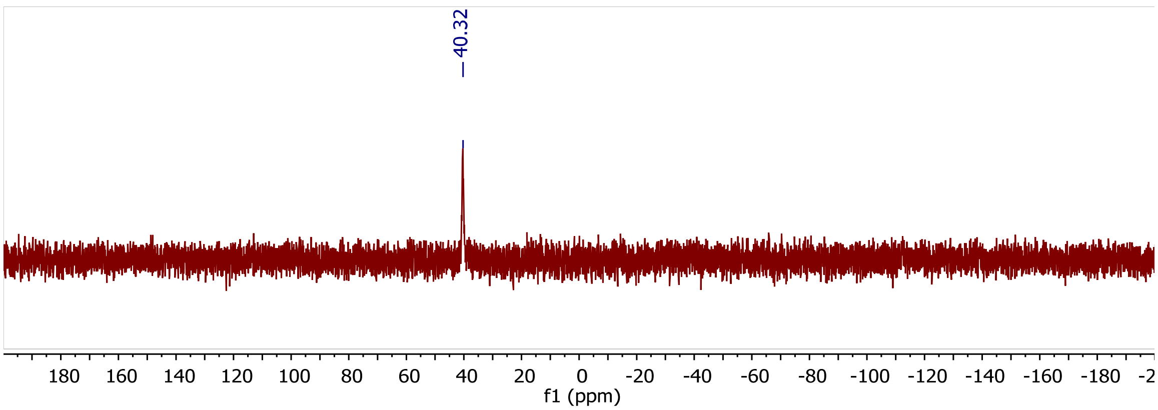

Figure S11. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **2Ni**

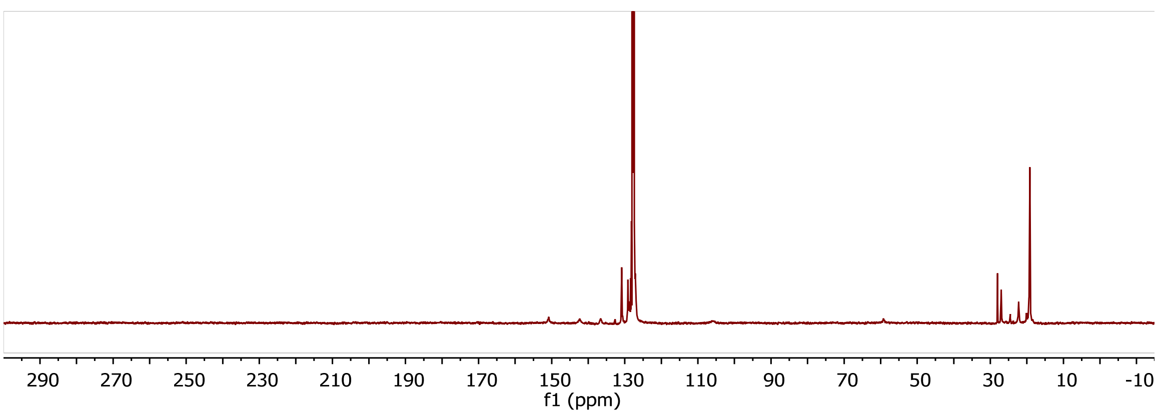

Figure S12. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **2Ni**

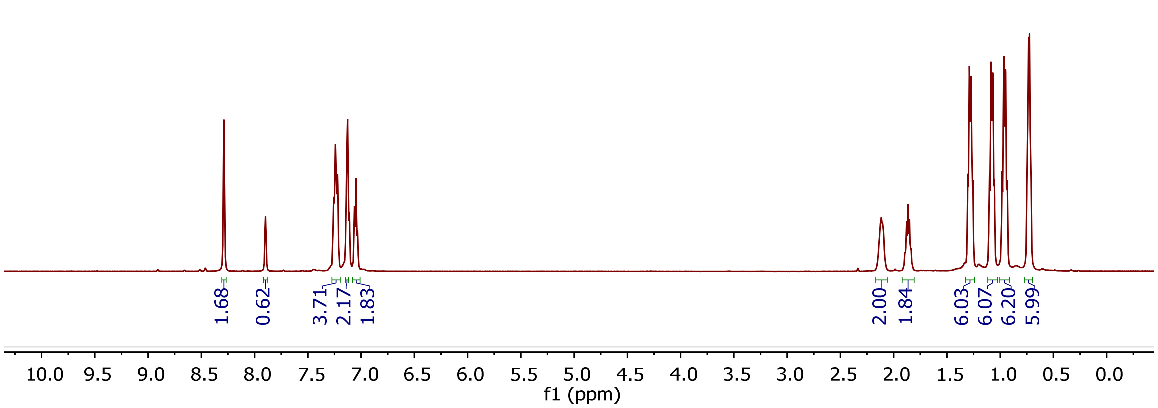

Figure S13. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **2Pd**

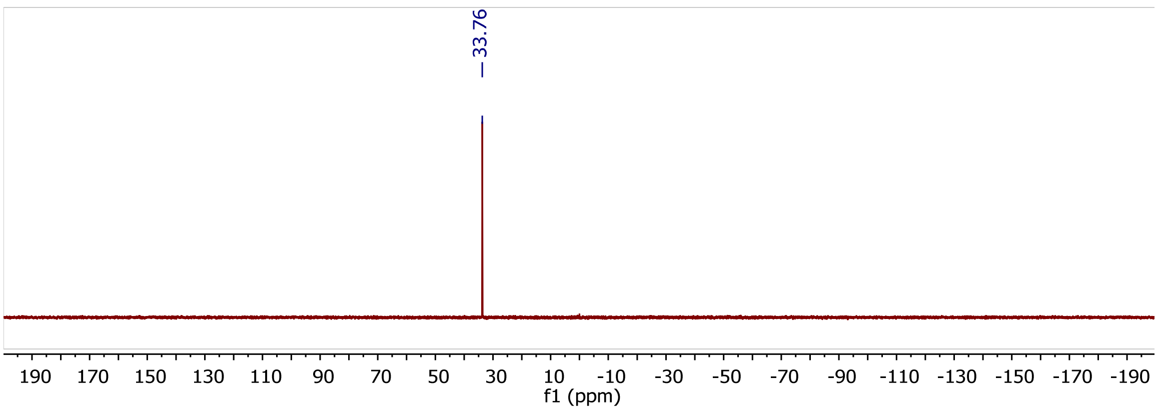

Figure S14. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **2Pd**

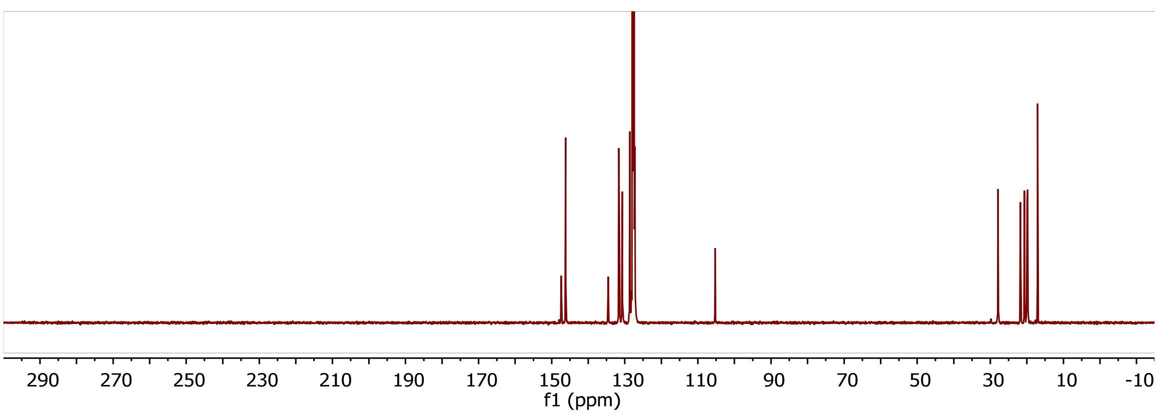

Figure S15. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **2Pd**

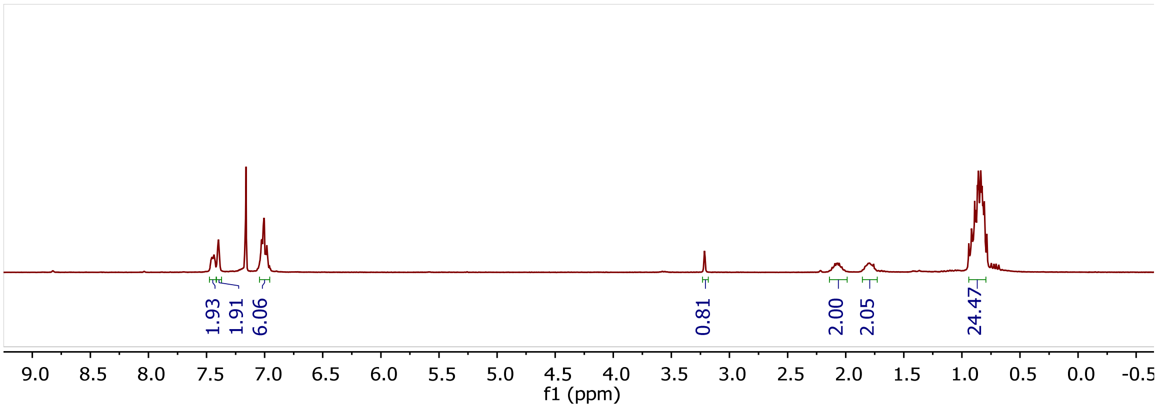

Figure S16. ^{1}H NMR (300 MHz, C_6D_6) spectrum of **2Ni-B(C_6F_5)$_3$**

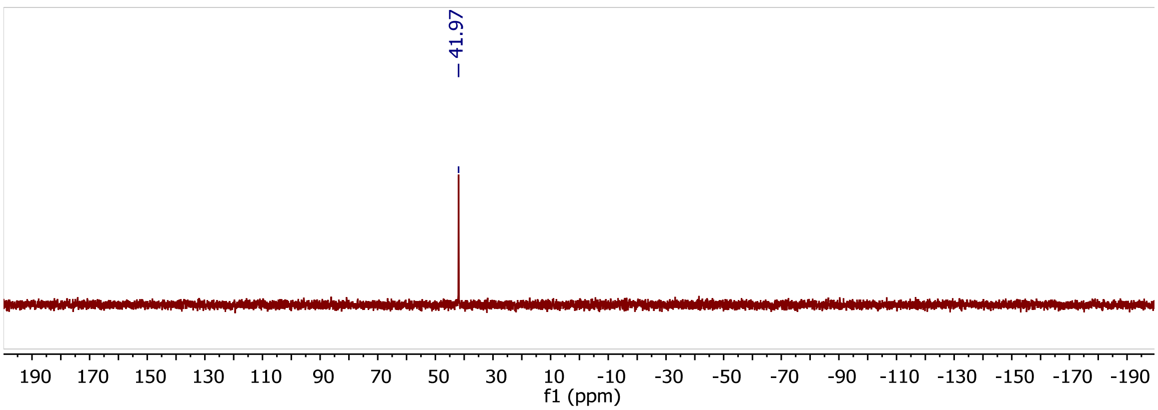

Figure S17. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **2Ni-B(C_6F_5)$_3$**

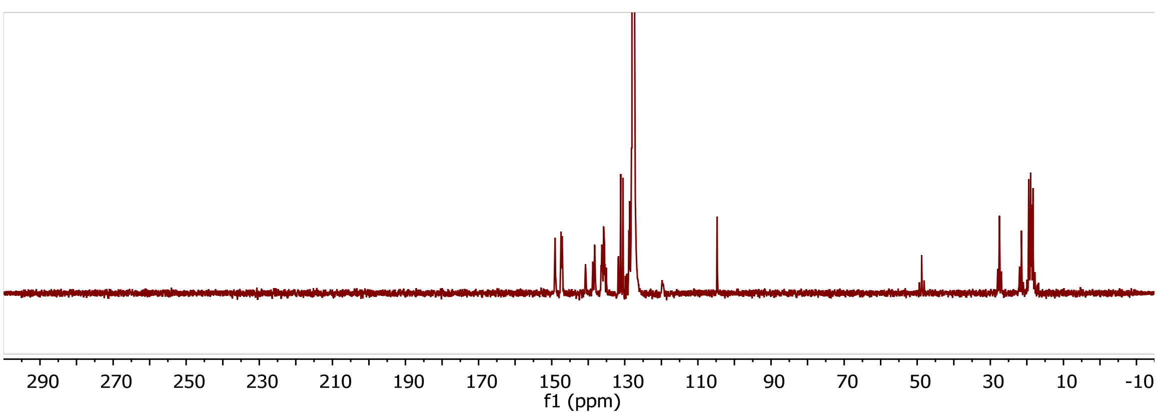

Figure S18. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **2Ni-B(C_6F_5)$_3$**

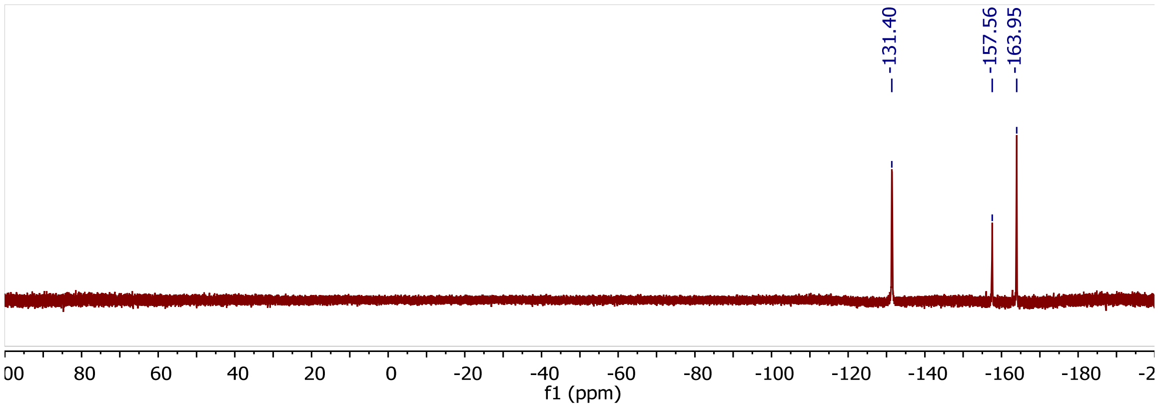

Figure S19. $^{19}F\{^{1}H\}$ NMR (282 MHz, C_6D_6) spectrum of **2Ni-B(C$_6$F$_5$)$_3$**

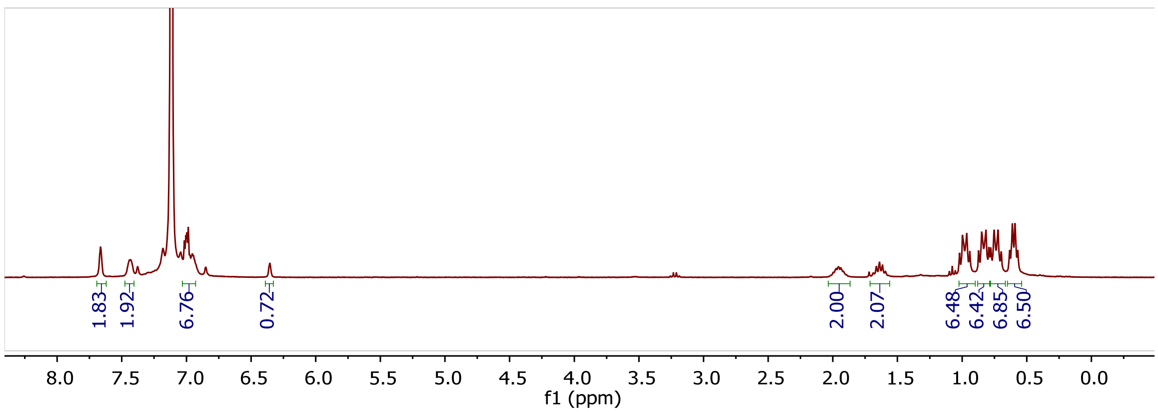

Figure S20. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **2Pd-B(C$_6$F$_5$)$_3$**

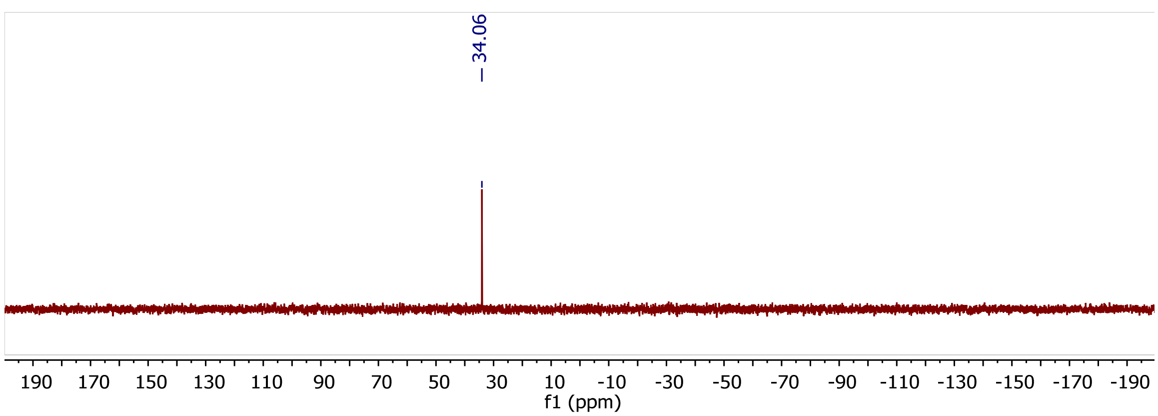

Figure S21. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **2Pd-B(C$_6$F$_5$)$_3$**

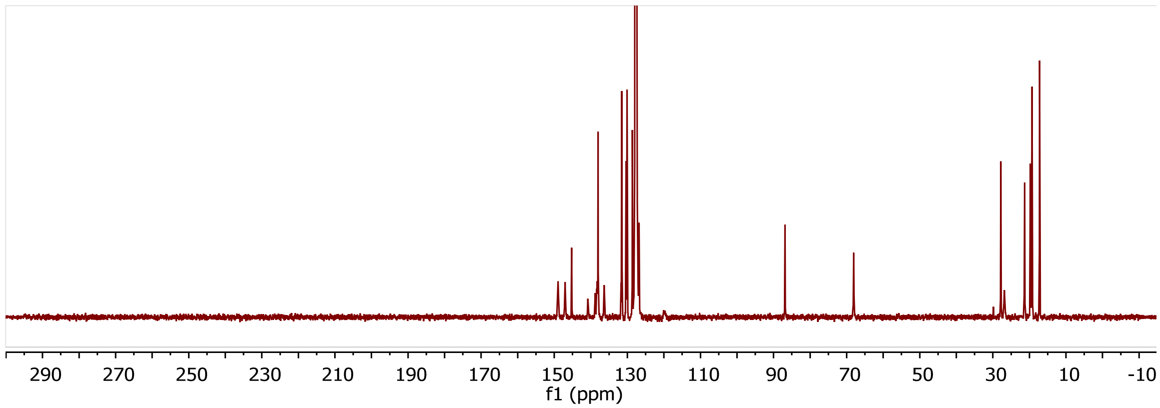

Figure S22. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **2Pd-B(C_6F_5)$_3$**

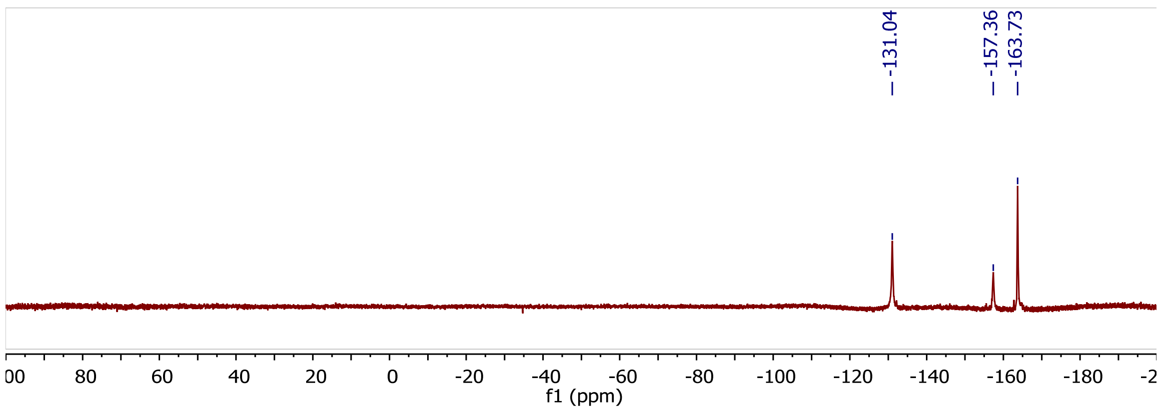

Figure S23. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **2Pd-B(C_6F_5)$_3$**

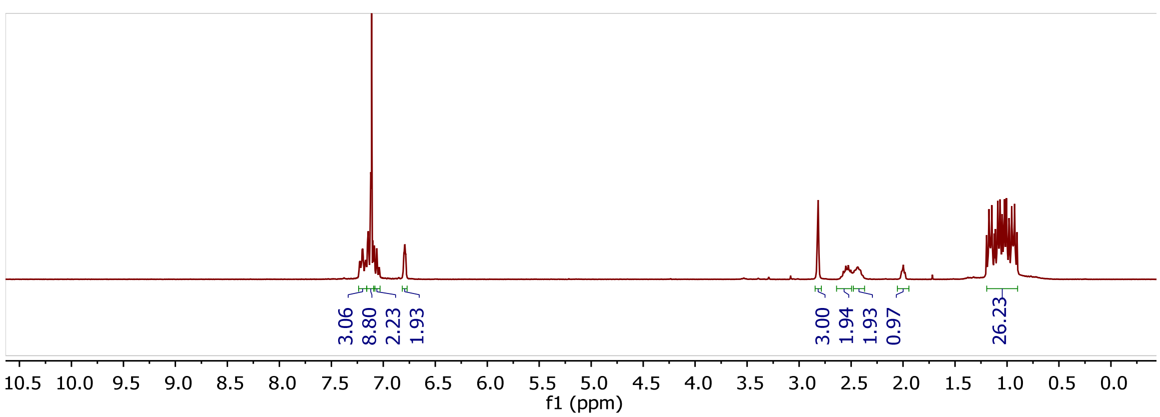

Figure S24. ^{1}H NMR (300 MHz, C_6D_6) spectrum of **2Ni-Me**

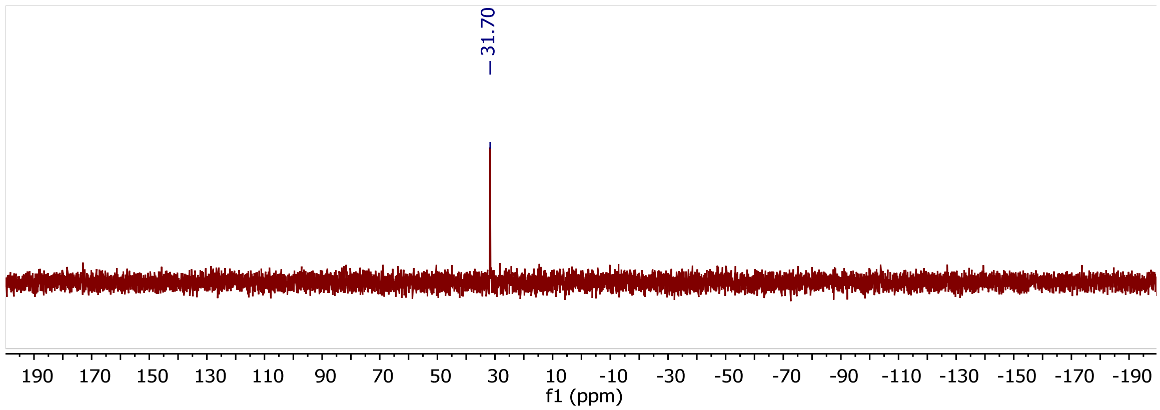

Figure S25. $^{31}P\{^1H\}$ NMR (121 MHz, C_6D_6) spectrum of **2Ni-Me**

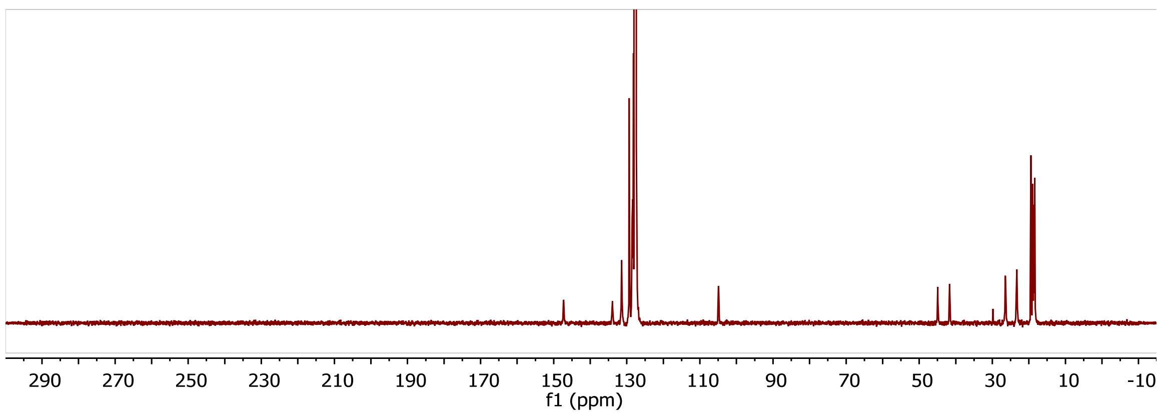

Figure S26. $^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6) spectrum of **2Ni-Me**

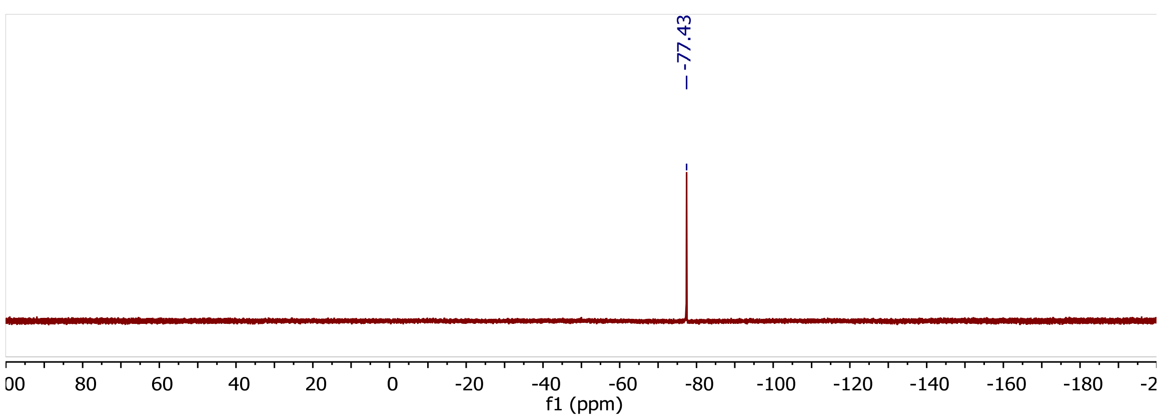

Figure S27. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **2Ni-Me**

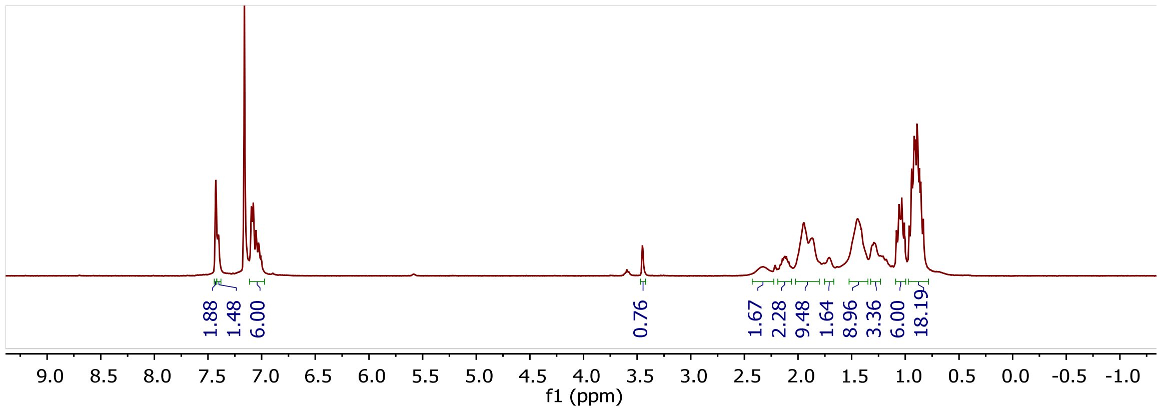

Figure S28. ^{1}H NMR (300 MHz, C_6D_6) spectrum of **2Ni-BCy$_2$OTf**

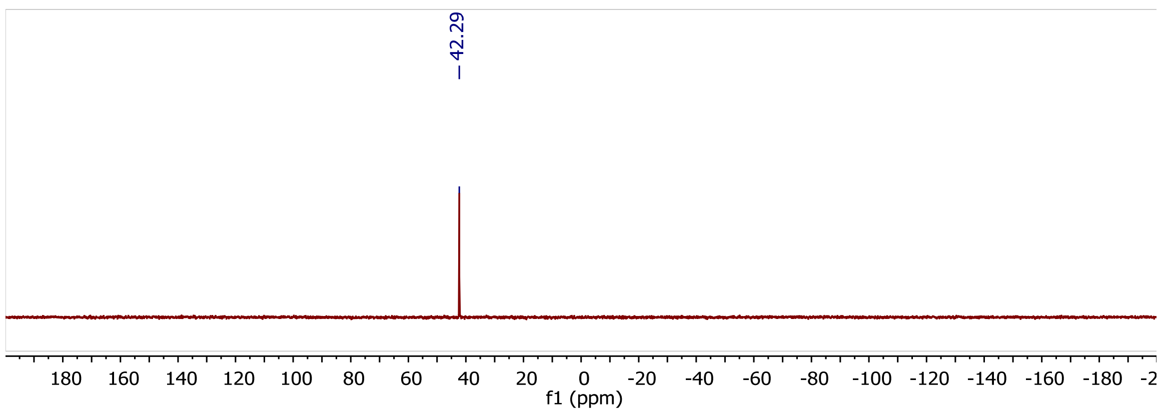

Figure S29. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **2Ni-BCy$_2$OTf**

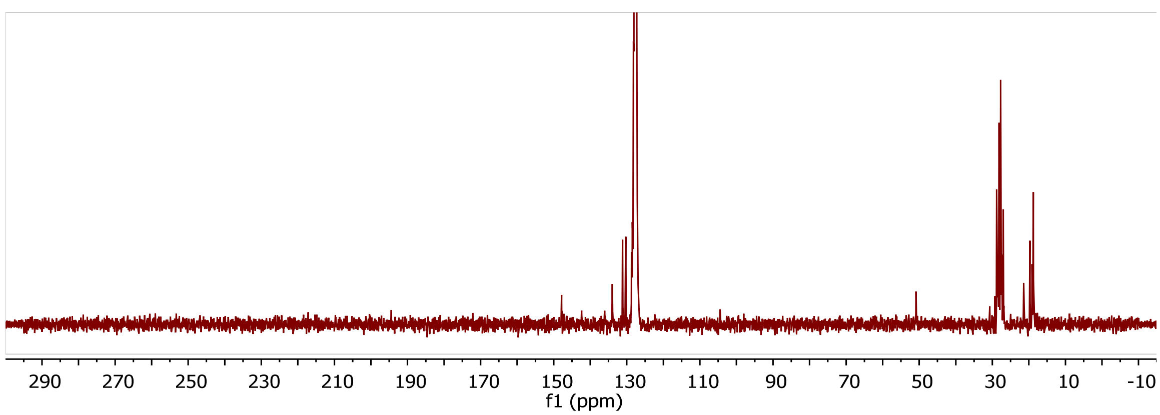

Figure S30. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **2Ni-BCy$_2$OTf**

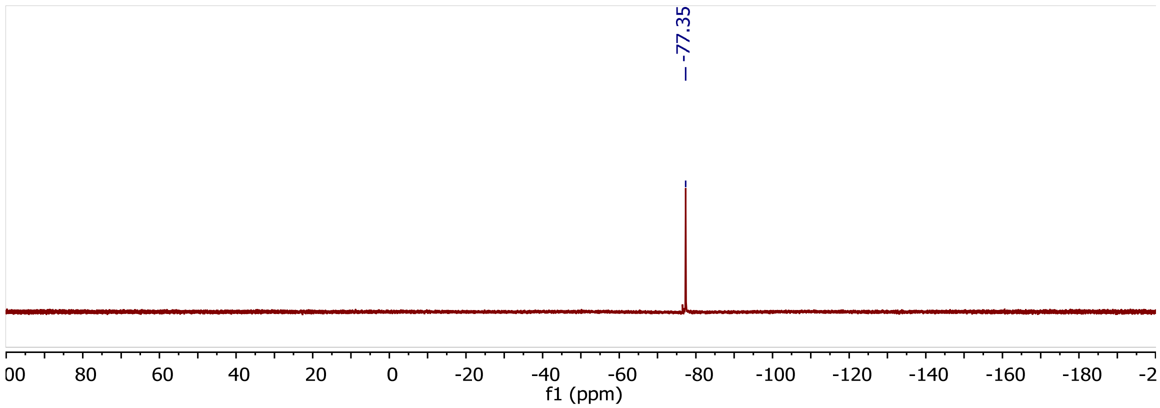

Figure S31. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **2Ni-BCy$_2$OTf**

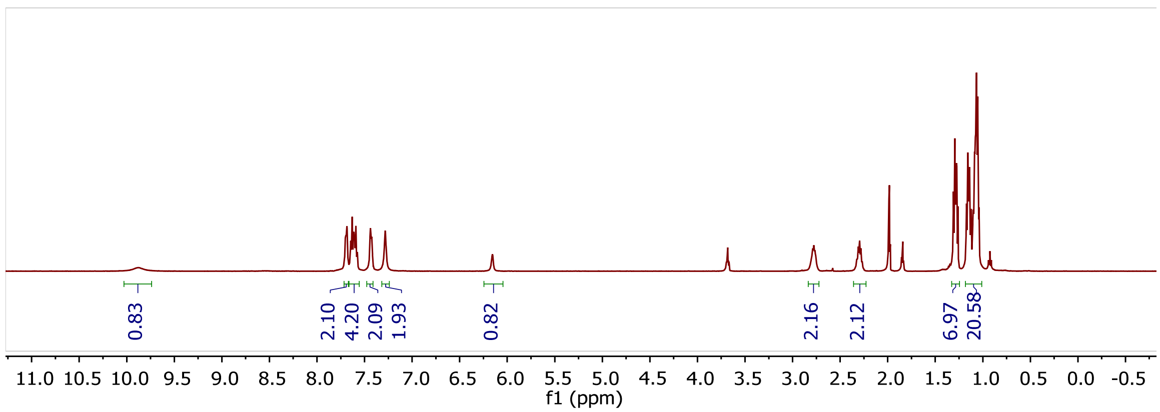

Figure S32. ^{1}H NMR (500 MHz, CD_3CN) spectrum of **2Pd-H**

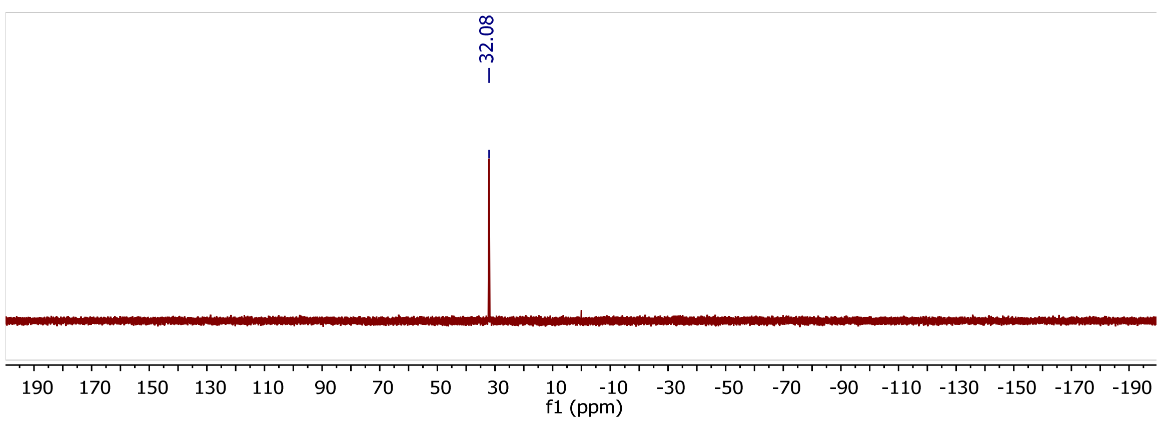

Figure S33. $^{31}P\{^{1}H\}$ NMR (121 MHz, CD_3CN) spectrum of **2Pd-H**

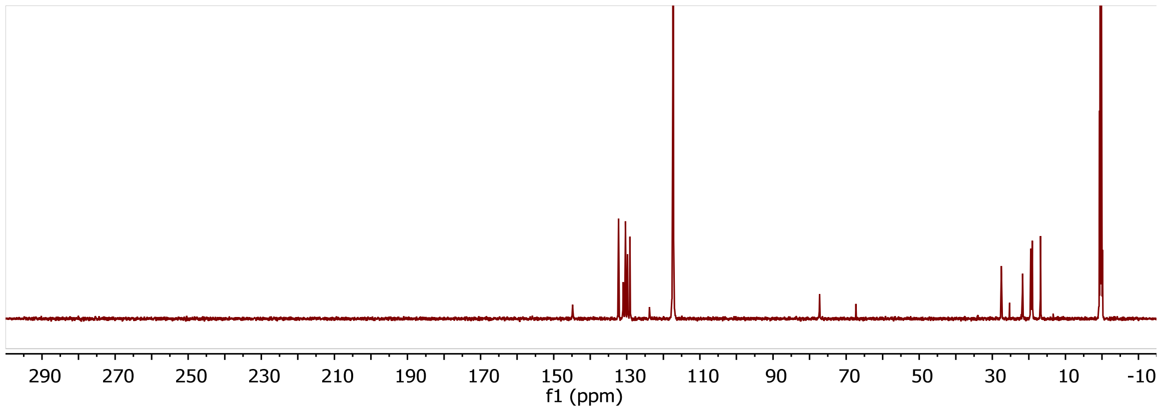

Figure S34. $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_3CN) spectrum of **2Pd-H**

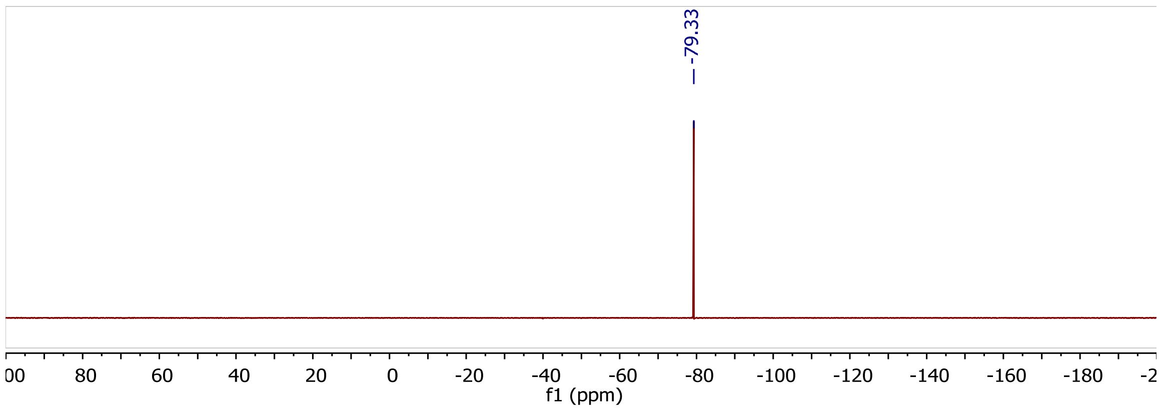

Figure S35. ^{19}F NMR (282 MHz, CD_3CN) spectrum of **2Pd-H**

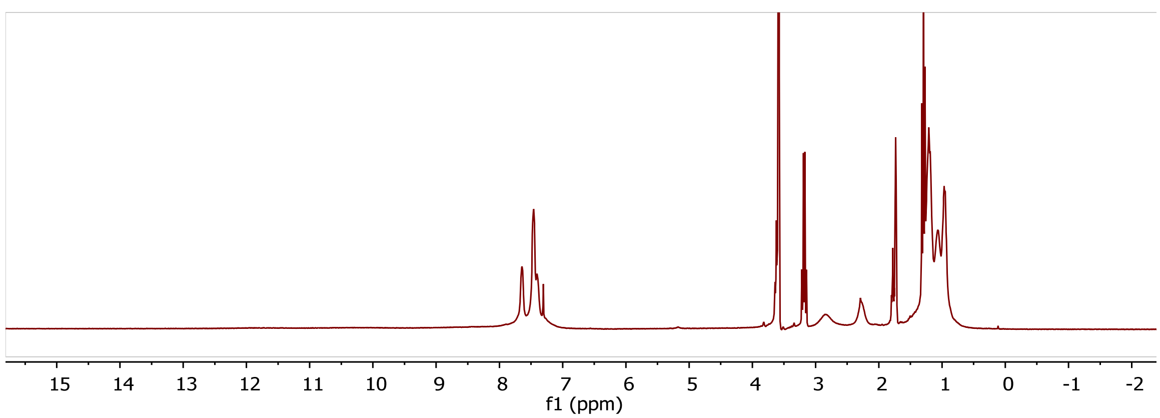

Figure S36. ^{1}H NMR (300 MHz, d_8-THF) spectrum of **3Ni**

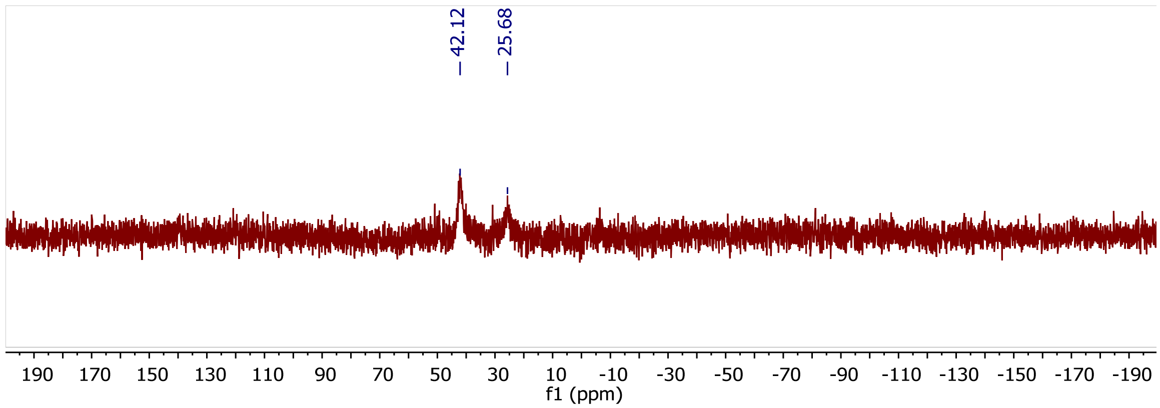

Figure S37. $^{31}P\{^{1}H\}$ NMR (121 MHz, *d₈*-THF) spectrum of **3Ni**

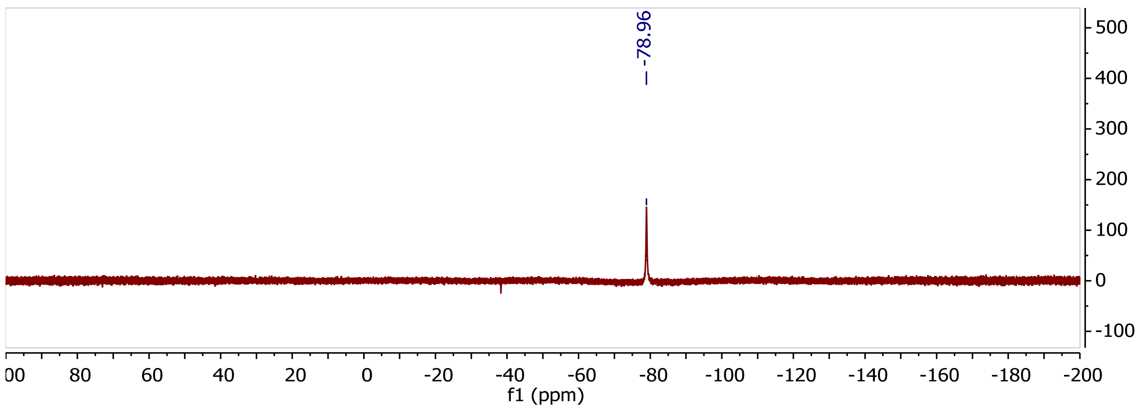

Figure S38. ^{19}F NMR (282 MHz, *d₈*-THF) spectrum of **3Ni**

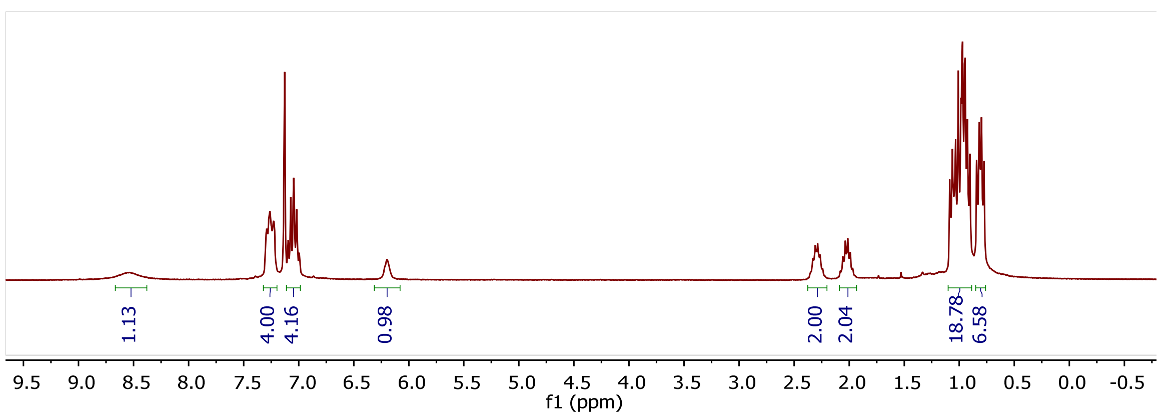

Figure S39. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **4Ni**

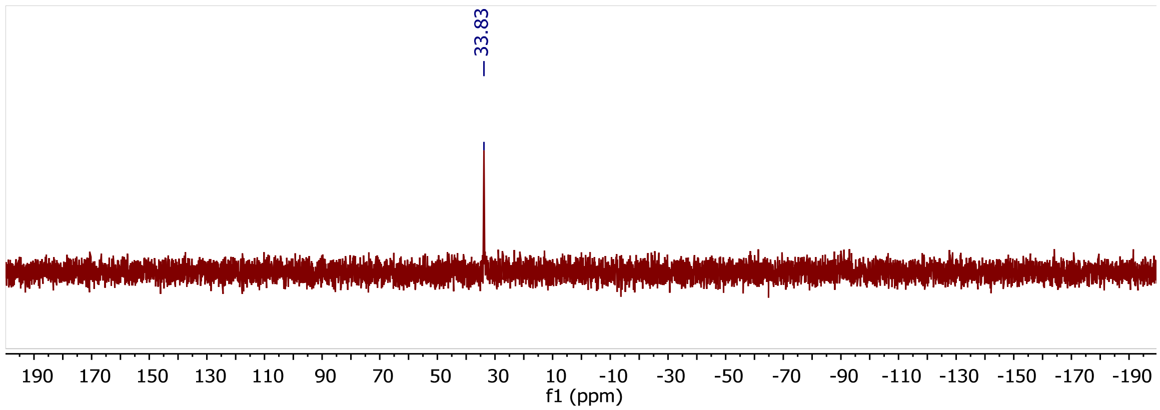

Figure S40. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **4Ni**

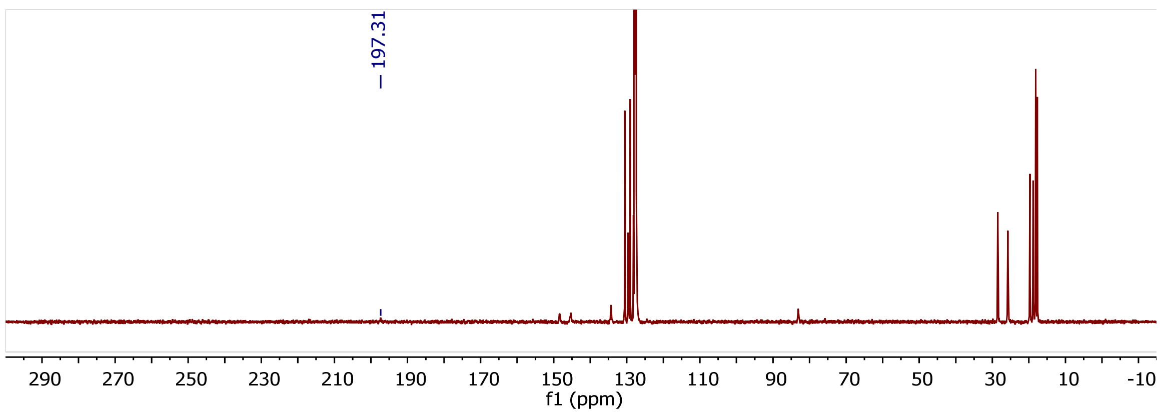

Figure S41. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **4Ni**

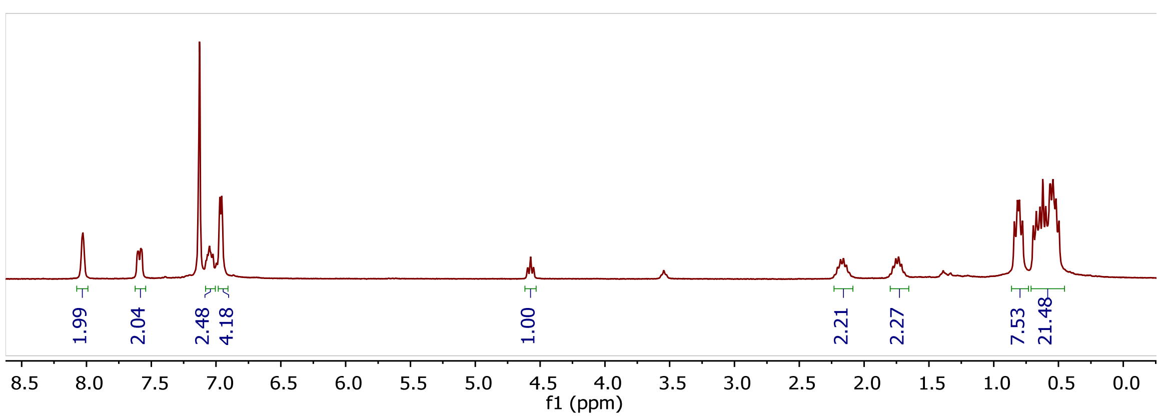

Figure S42. ^{1}H NMR (300 MHz, C_6D_6) spectrum of **4Ni-B(C_6F_5)$_3$**

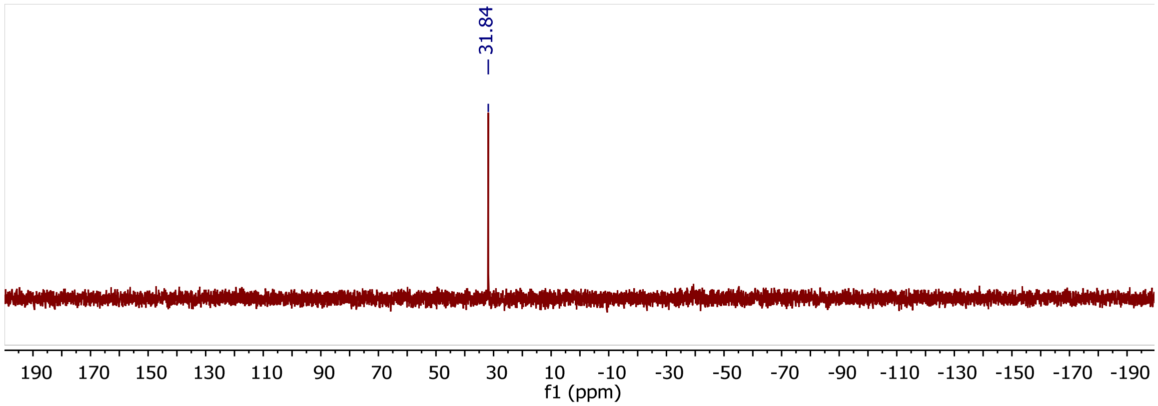

Figure S43. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **4Ni-B(C$_6$F$_5$)$_3$**

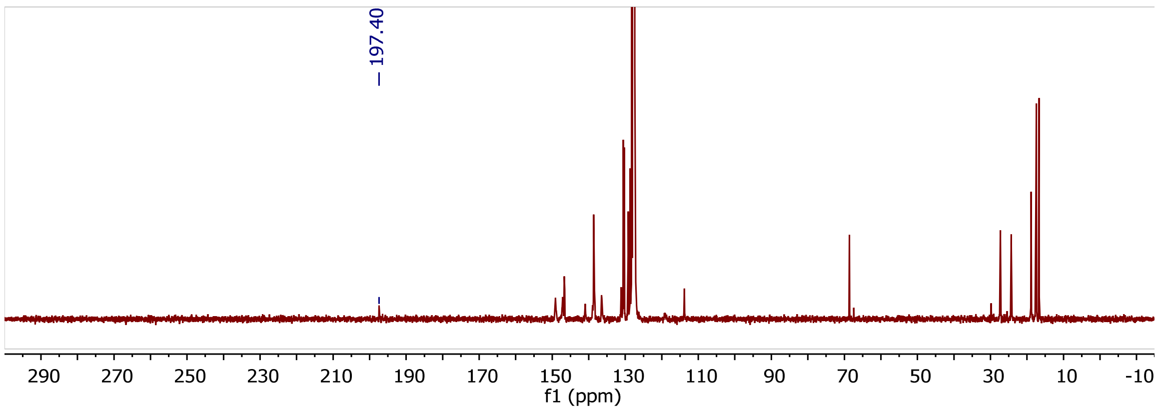

Figure S44. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **4Ni-B(C$_6$F$_5$)$_3$**

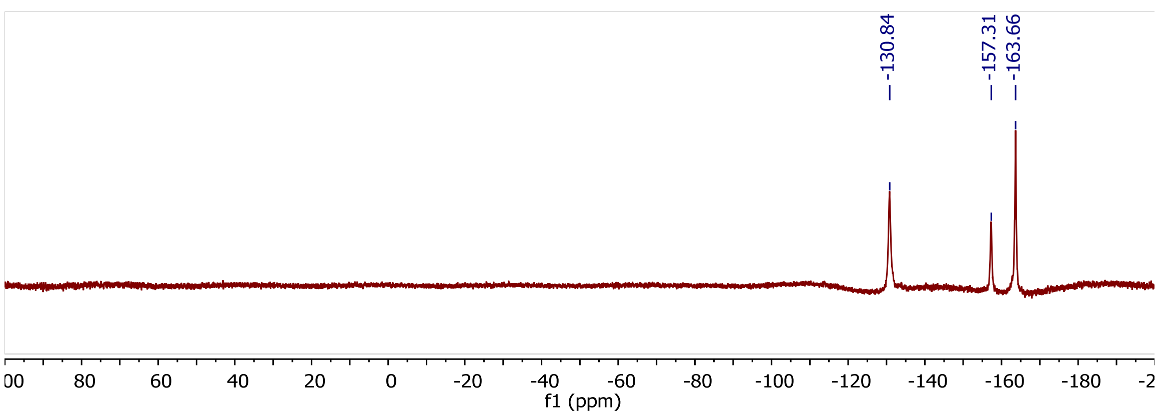

Figure S45. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **4Ni-B(C$_6$F$_5$)$_3$**

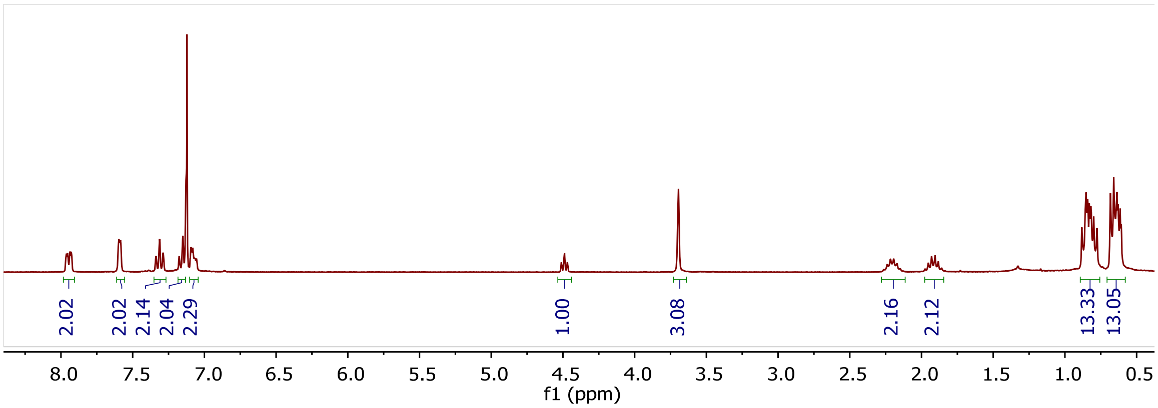

Figure S46. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **4Ni-Me**

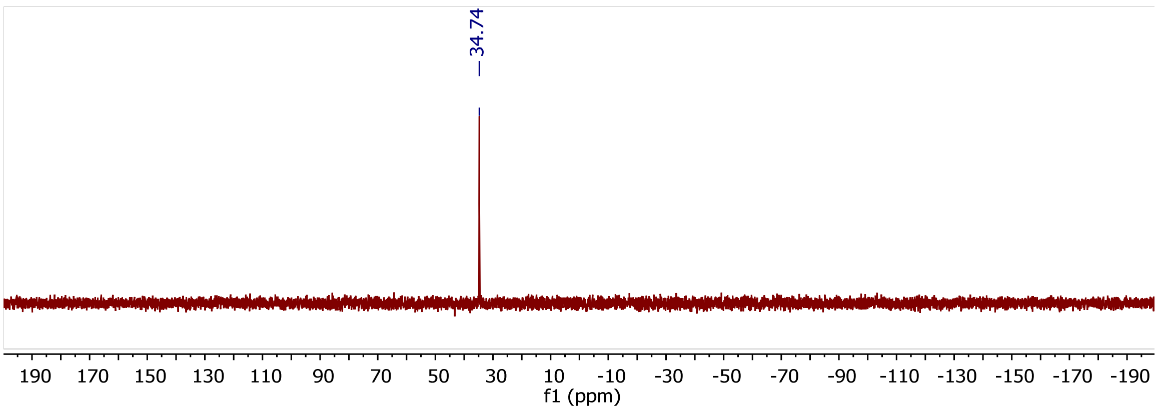

Figure S47. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **4Ni-Me**

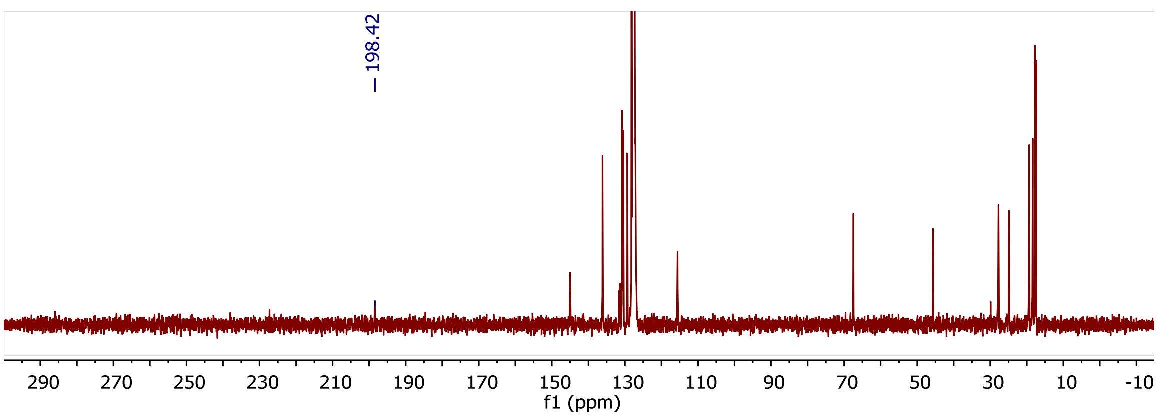

Figure S48. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **4Ni-Me**

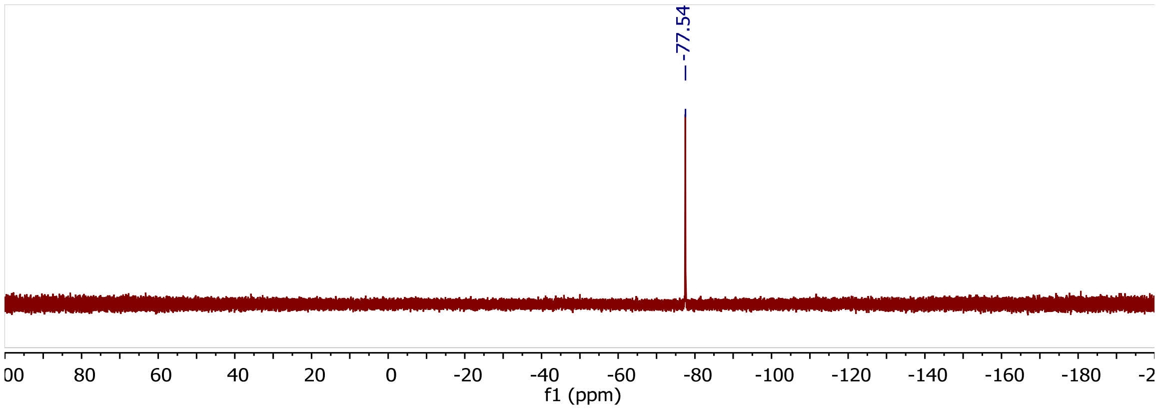

Figure S49. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **4Ni-Me**

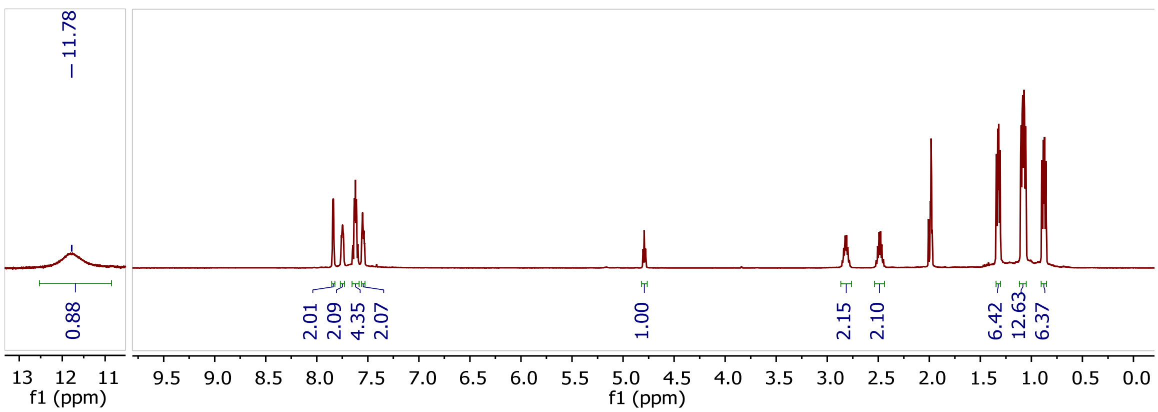

Figure S50. ^{1}H NMR (500 MHz, CD_3CN) spectrum of **4Ni-H**

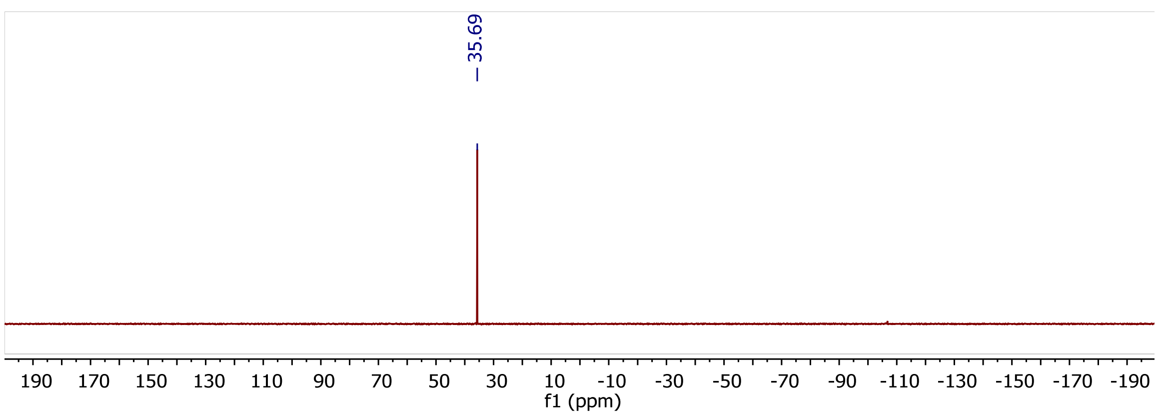

Figure S51. ^{31}P{^{1}H} NMR (121 MHz, CD_3CN) spectrum of **4Ni-H**

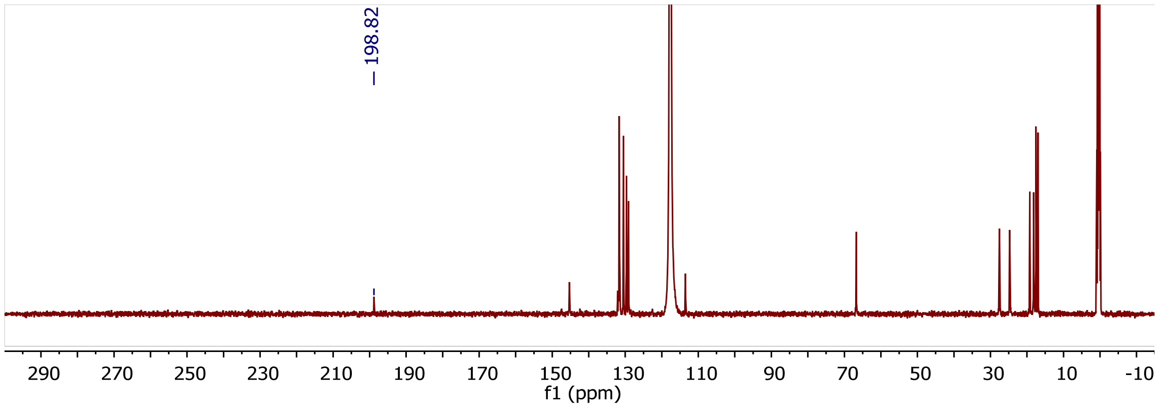

Figure S52. $^{13}C\{^1H\}$ NMR (126 MHz, CD_3CN) spectrum of **4Ni-H**

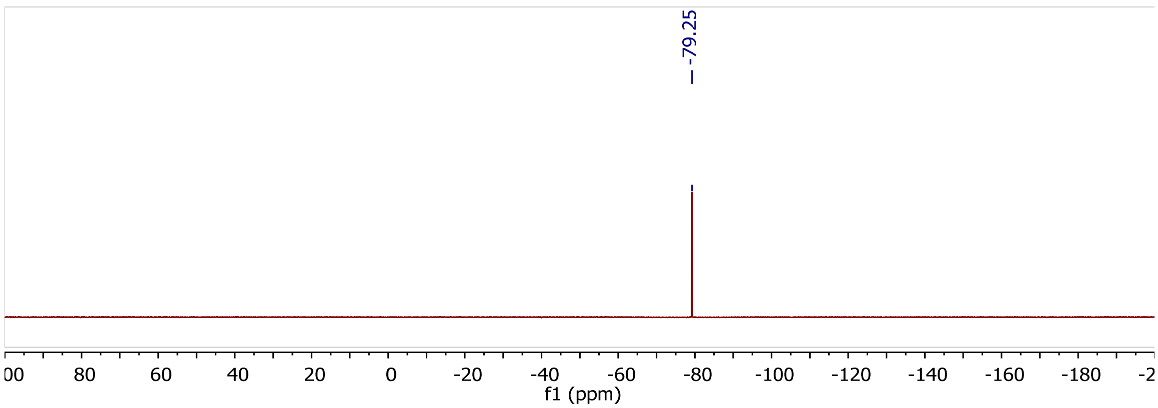

Figure S53. ^{19}F NMR (282 MHz, CD_3CN) spectrum of **4Ni-H**

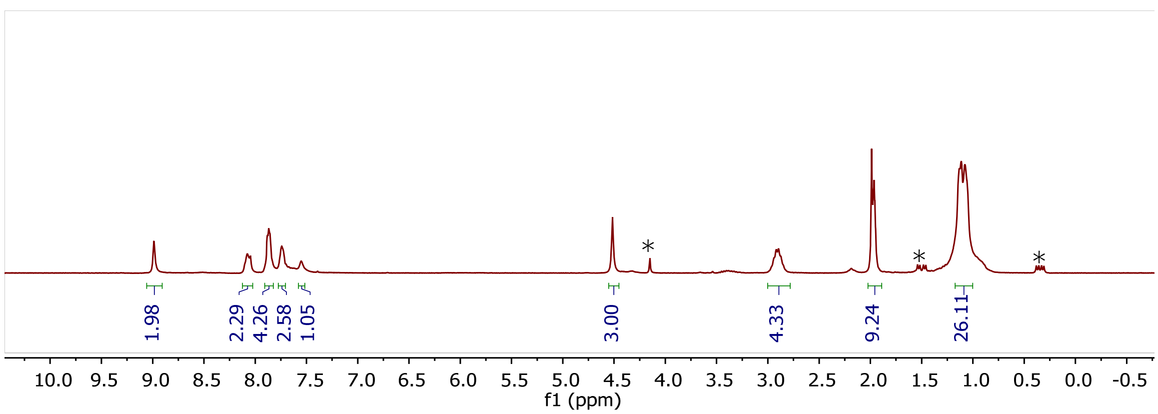

Figure S54. ^1H NMR (500 MHz, C_6D_6) spectrum of **5Ni**. Peaks marked with an asterisk are from the gradual decomposition of **5Ni** in solution.

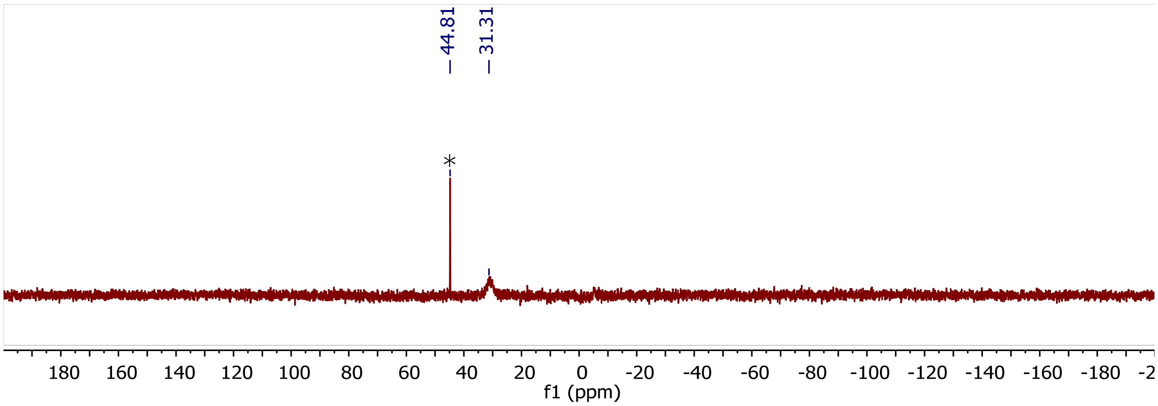

Figure S55. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **5Ni**. Peaks marked with an asterisk are from the gradual decomposition of **5Ni** in solution.

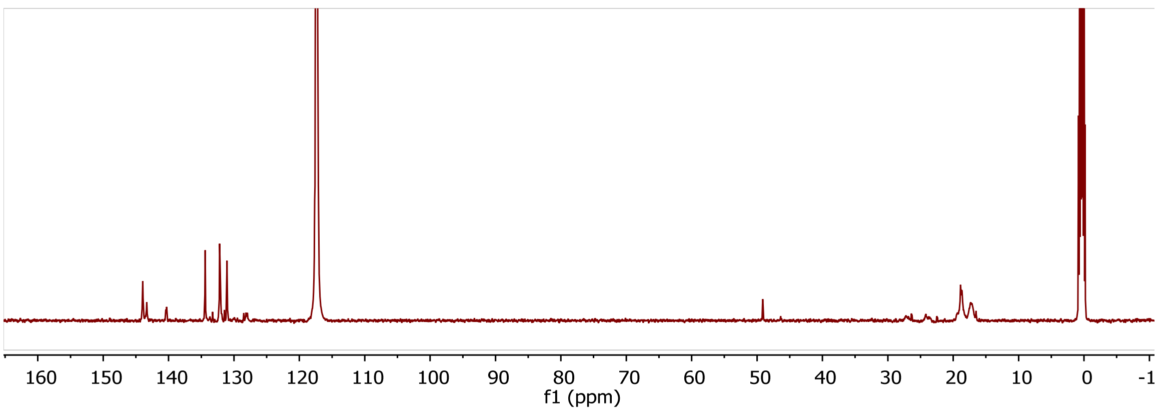

Figure S56. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **5Ni**

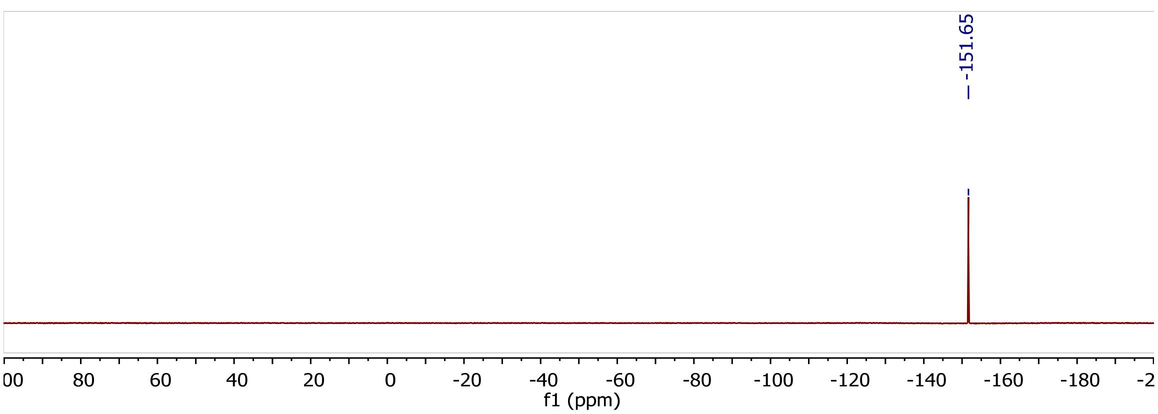

Figure S57. ^{19}F NMR (282 MHz, C_6D_6) spectrum of **5Ni**

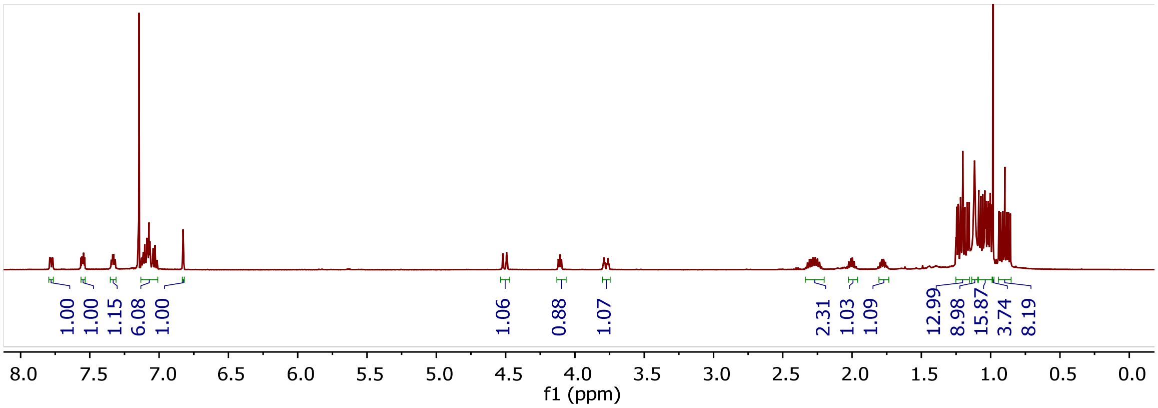

Figure S58. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **6Ni**

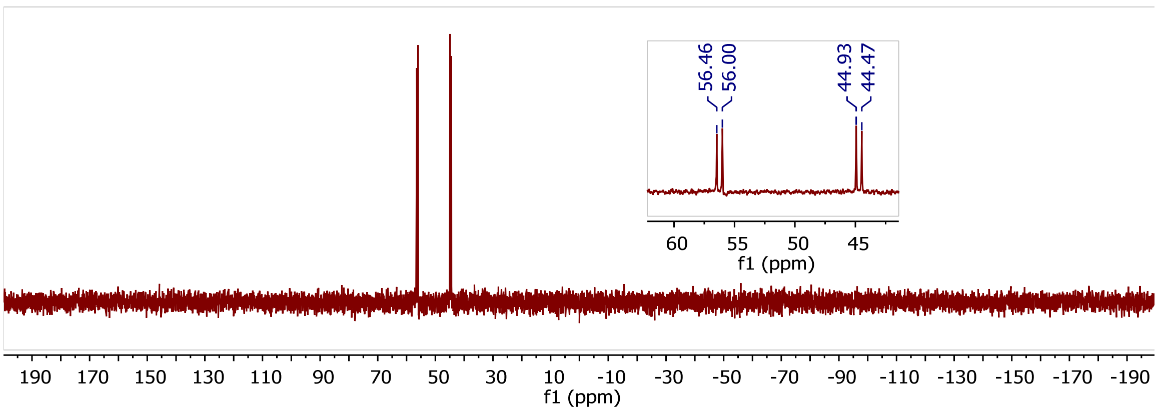

Figure S59. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **6Ni**

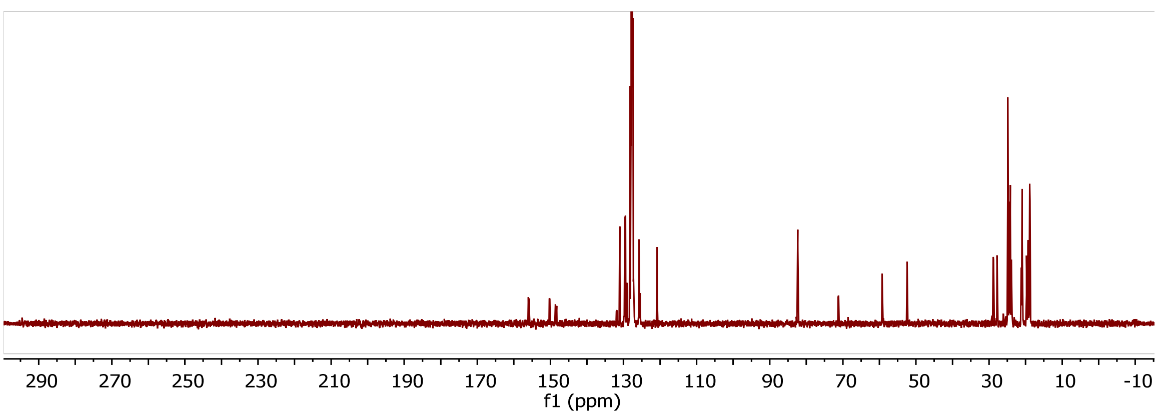

Figure S60. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **6Ni**

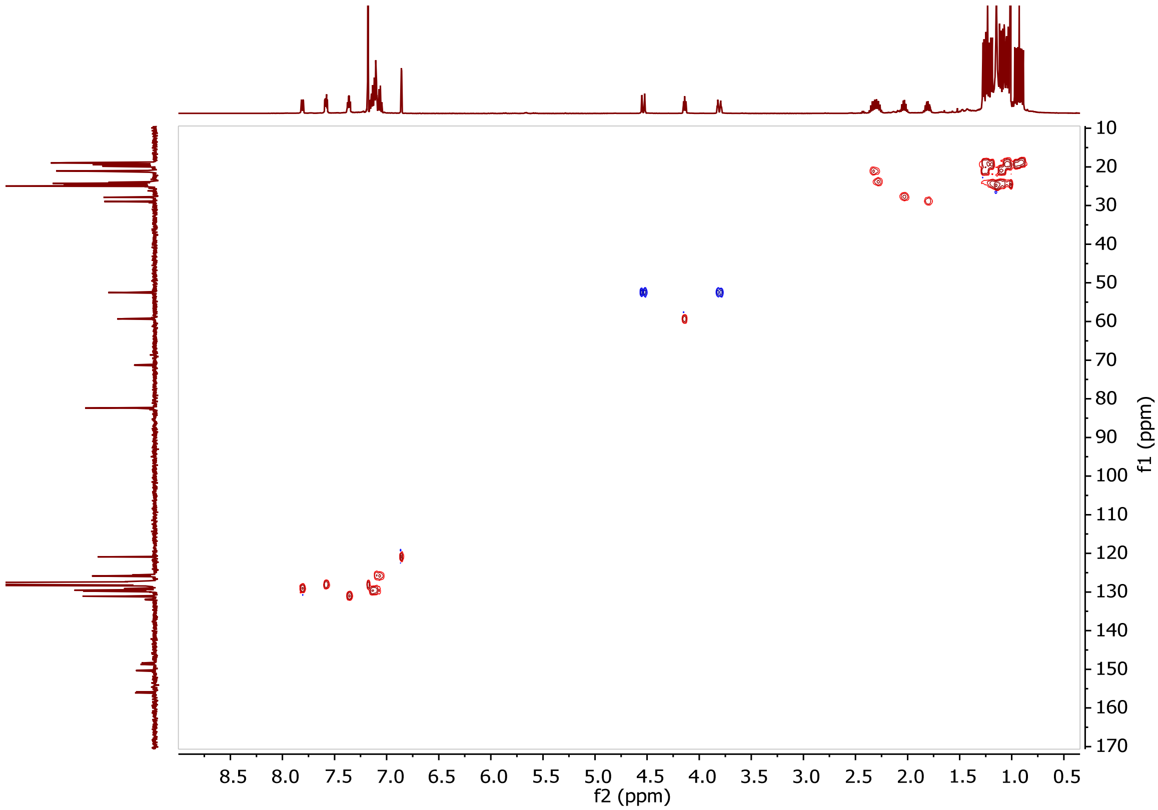

Figure S61. gHSQCAD NMR (500 MHz ^{1}H, C_6D_6) spectrum of **6Ni**

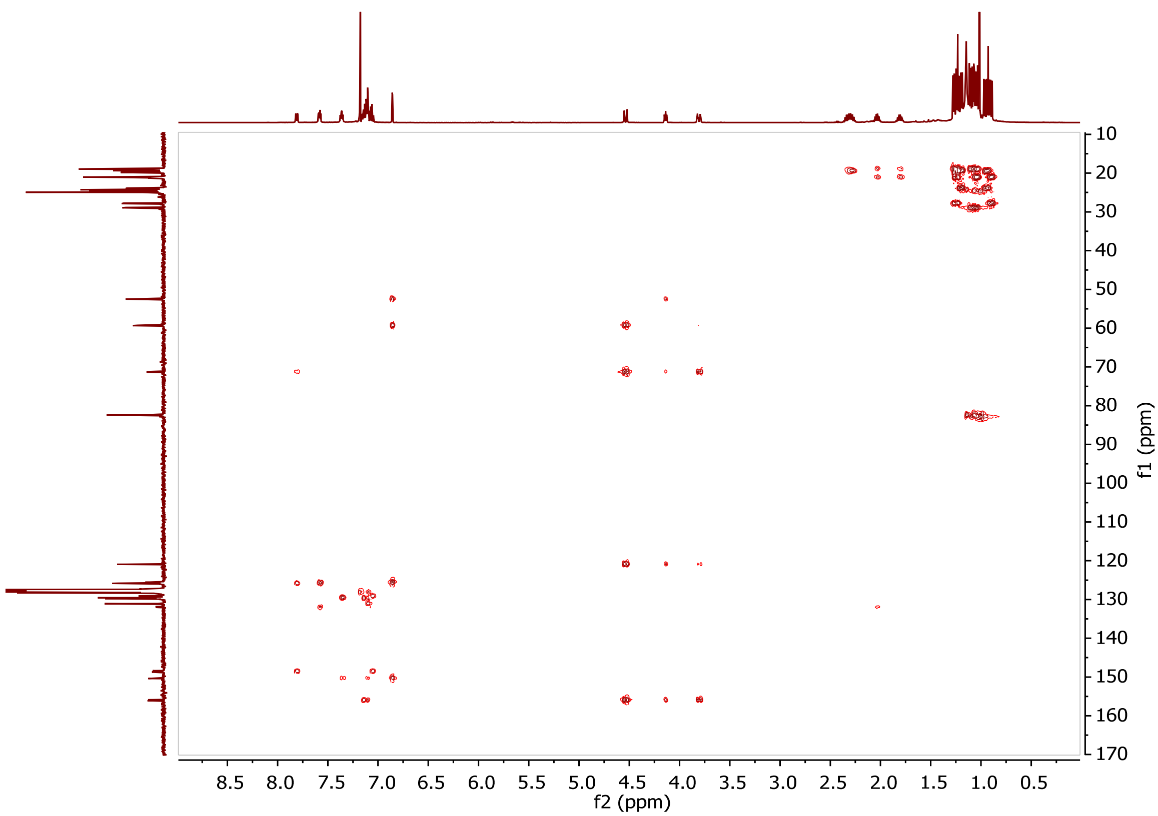

Figure S62. gHMBCAD NMR (500 MHz ^{1}H, C_6D_6) spectrum of **6Ni**

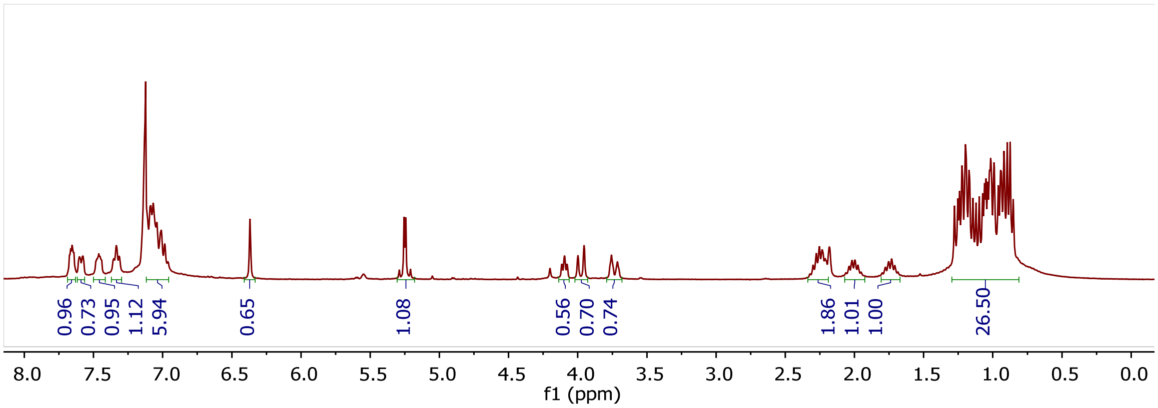

Figure S63. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **7Ni**

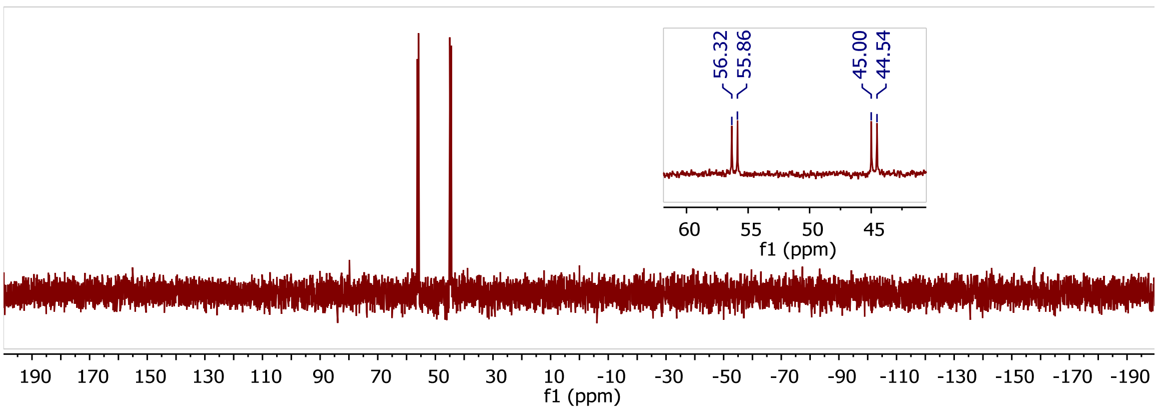

Figure S64. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **7Ni**

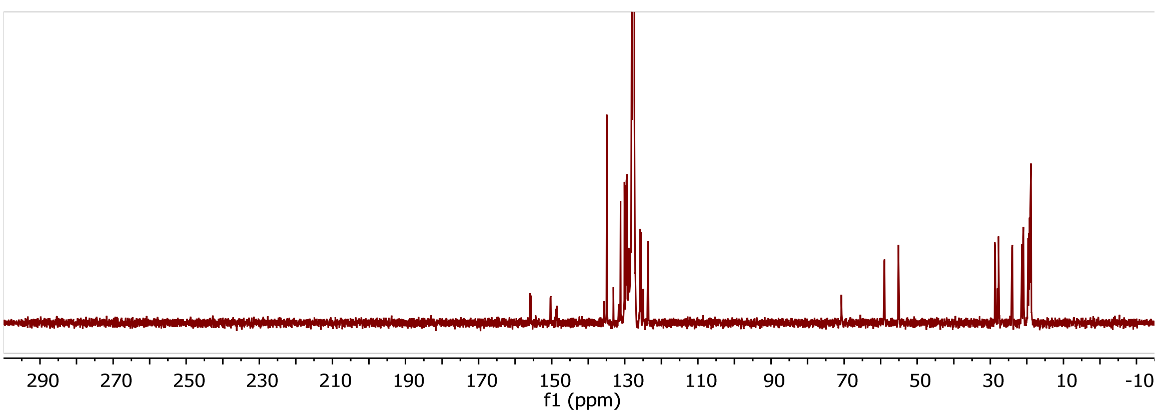

Figure S65. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **7Ni**

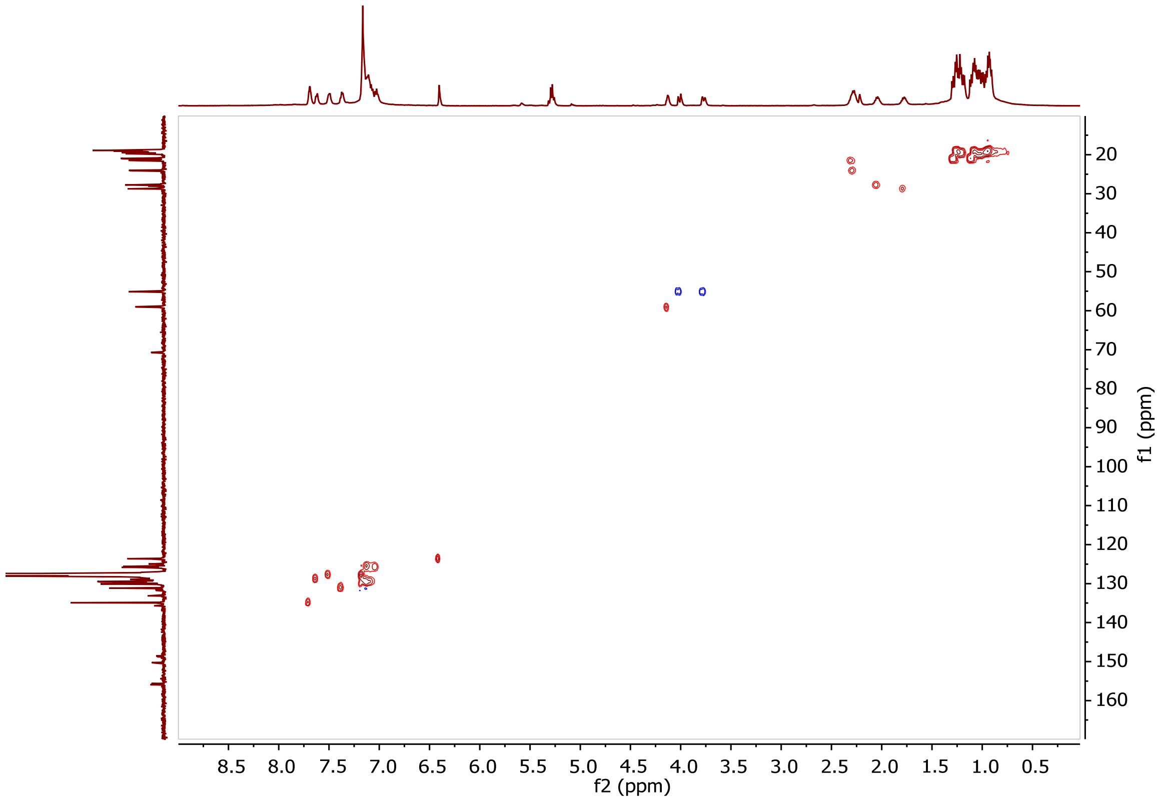

Figure S66. gHSQCAD NMR (500 MHz ^{1}H, C_6D_6) spectrum of **7Ni**

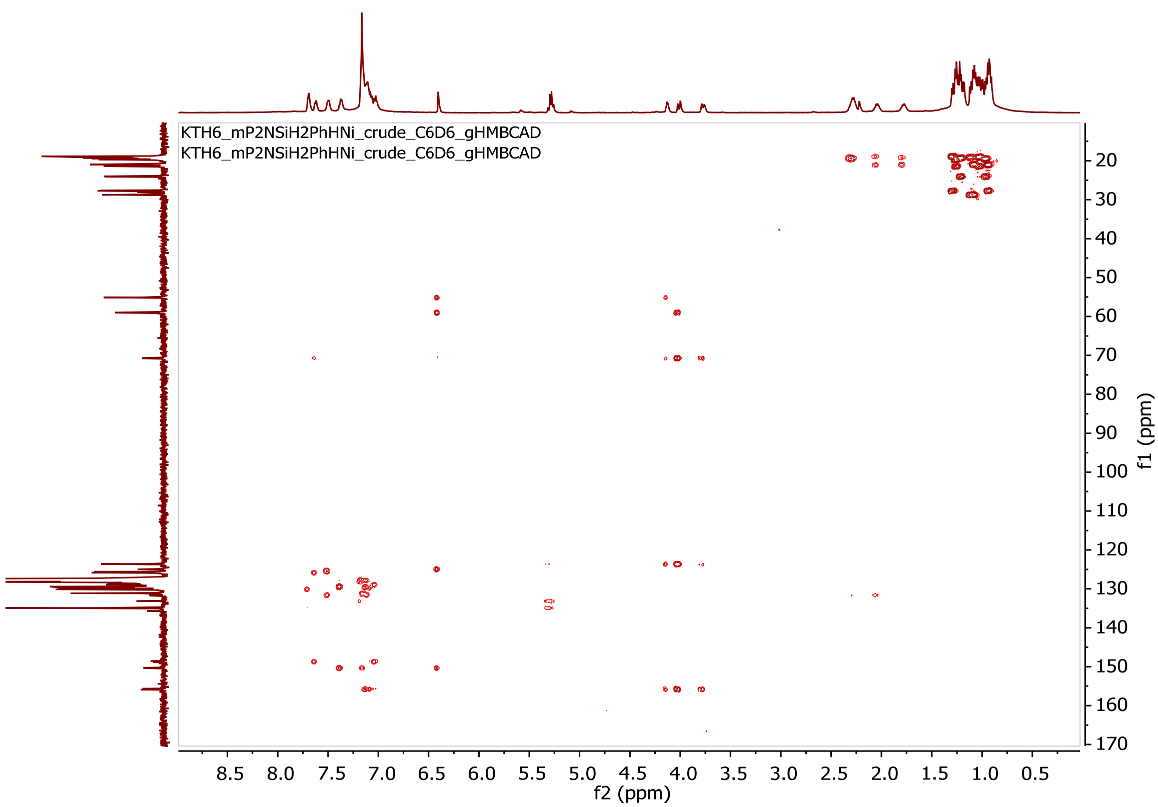

Figure S67. gHMCAD NMR (500 MHz ^{1}H, C_6D_6) spectrum of **7Ni**

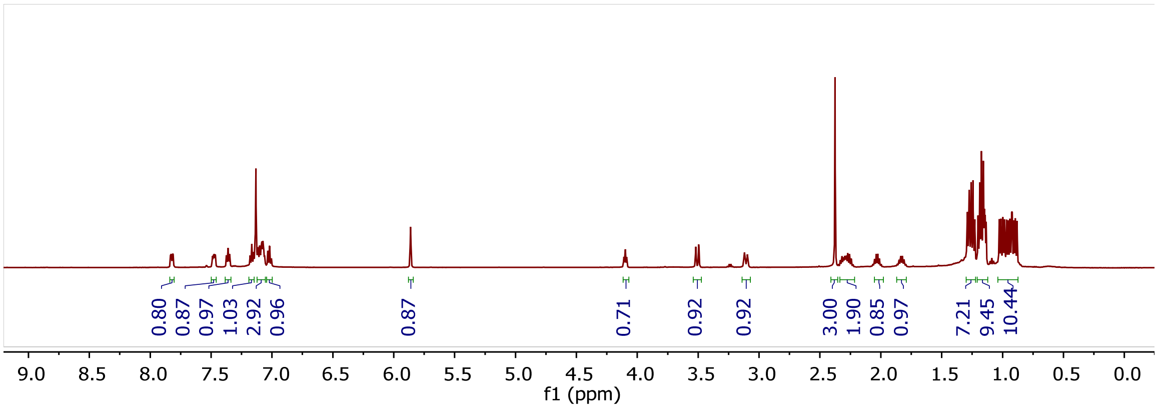

Figure S68. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **8Ni**

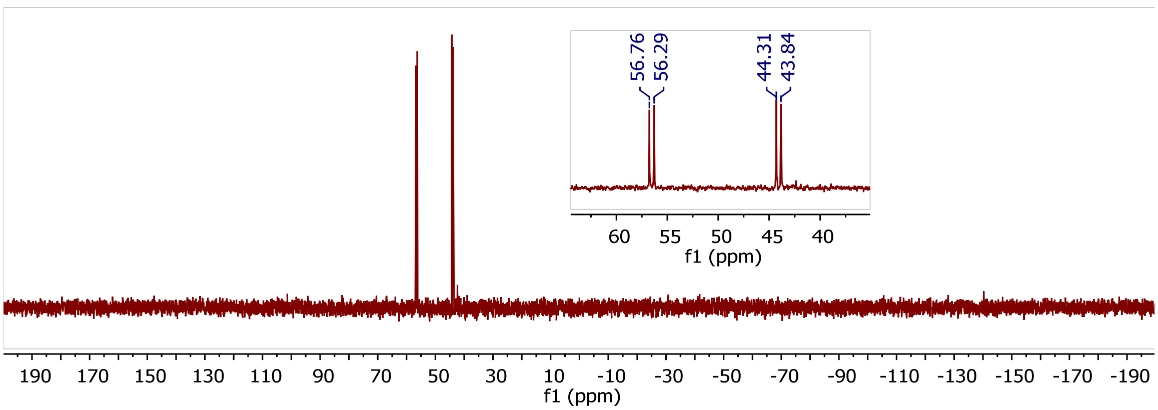

Figure S69. $^{31}P\{^{1}H\}$ NMR (121 MHz, C_6D_6) spectrum of **8Ni**

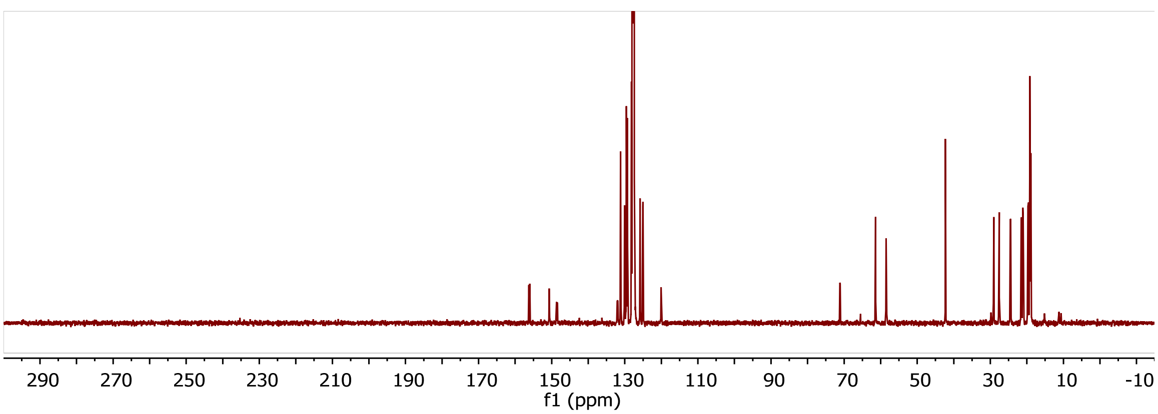

Figure S70. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **8Ni**

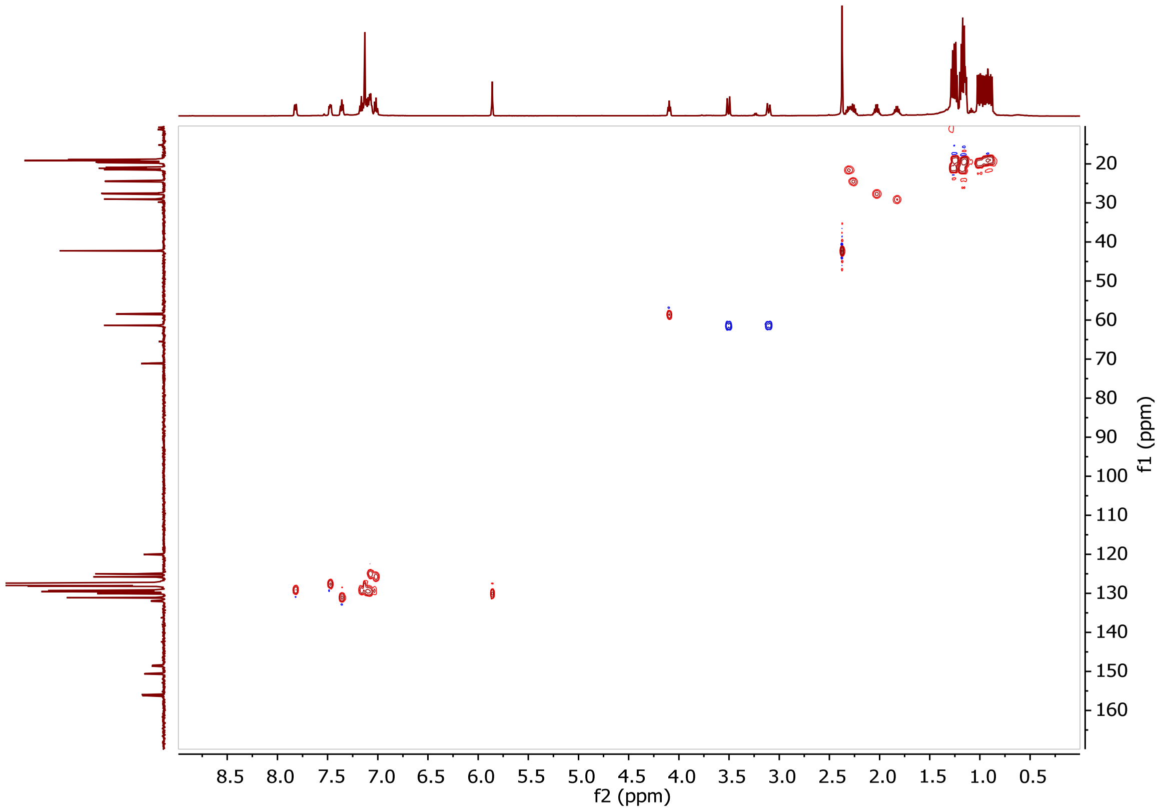

Figure S71. gHSQCAD NMR (500 MHz [1]H, C_6D_6) spectrum of **8Ni**

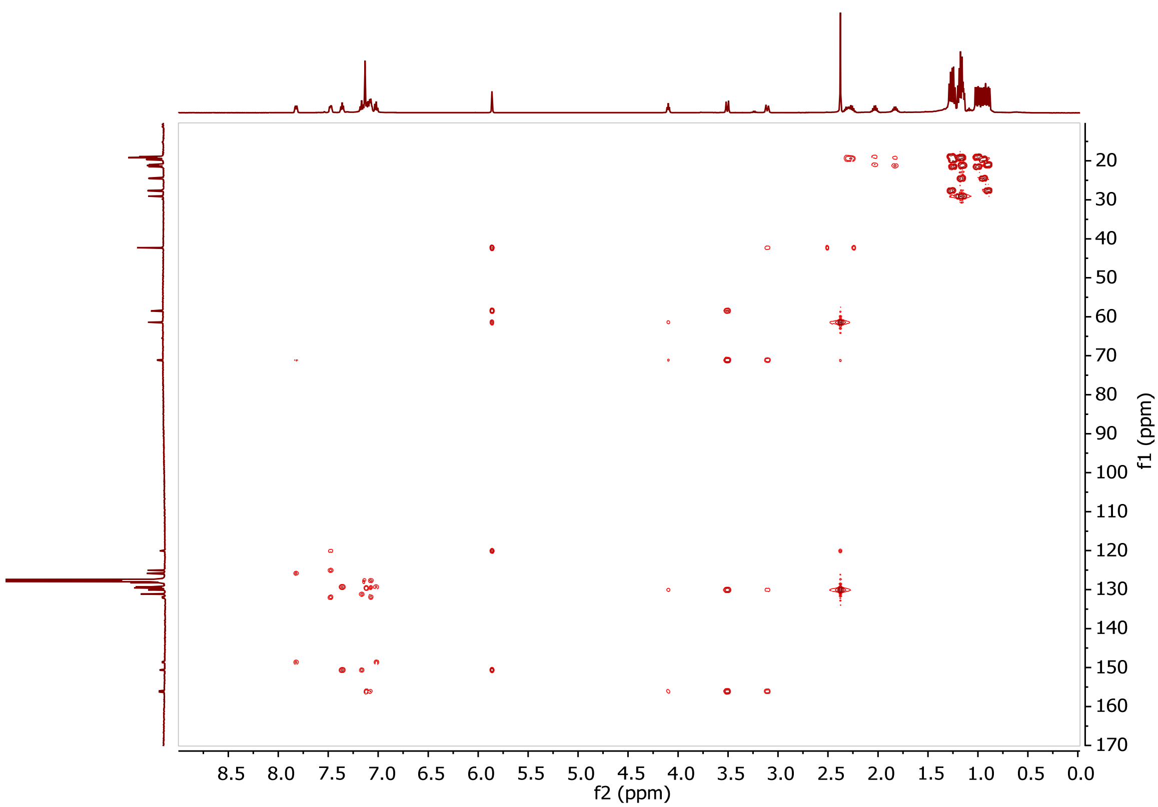

Figure S72. gHMCAD NMR (500 MHz [1]H, C_6D_6) spectrum of **8Ni**

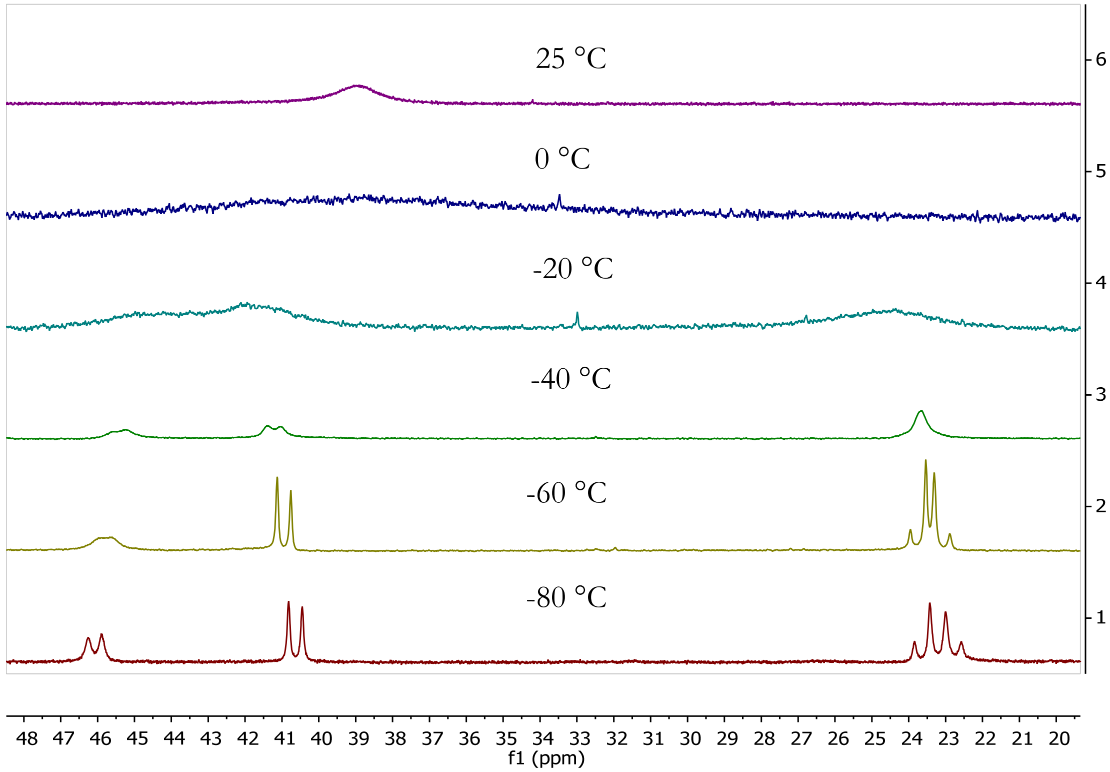

Figure S73. Variable temperature NMR (202 MHz ^{31}P, d_8-toluene) data for **2Ni**

Crystallographic Information

CCDC 1400900-1400909 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal and refinement data for reported complexes.

Complex	**2Ni**	**2Pd**	**2Ni-B(C$_6$F$_5$)$_3$**	**2Pd-B(C$_6$F$_5$)$_3$**	**3Ni**
empirical formula	$C_{63}H_{90}N_2Ni_2P_4$	$C_{29}H_{39}NP_2Pd$	$C_{46}H_{43}B_5F_{15}NNiP_2$	$C_{47}H_{39}BF_{15}NP_2Pd$	$C_{65}H_{85}F_3N_2Ni_2$ O_3P_4S
formula wt	1116.66	569.95	1069.51	1081.94	1272.71
T (K)	100	100(2)	99.99	100.03	100.01
a, Å	18.7148(7)	8.6112(7)	40.5679(17)	13.4502(7)	20.003(3)
b, Å	13.0646(5)	17.8635(16)	12.1876(4)	14.6571(7)	13.924(2)
c, Å	25.9359(9)	8.8154(11)	20.6773(7)	22.5392(11)	22.832(4)
α, deg	90	90	90	90	90
β, deg	109.324(2)	99.464(4)	114.405(2)	91.080(2)	22.832(4)
γ, deg	90	90	90	90	90
V, Å^3	5984.1(4)	1337.6(2)	9309.9(6)	4442.6(4)	6267.1(18)
Z	4	4	4	4	4
cryst syst	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	P 1 21/n 1	P 21	C 1 2/c 1	P 1 21/c 1	P 1 21/n 1
d_{calcd}, g/cm^3	1.239	1.415	1.526	1.618	1.349
θ range, deg	1.630-30.557	2.342 to 45.810	1.759 to 30.538	2.280 to 36.326	1.720-28.677
μ, mm^{-1}	1.058	0.831	0.582	0.589	0.792
abs cor	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
GOF[c]	0.775	0.885	1.017	1.014	1.003
R1,[a] wR2[b] (I > 2σ(I))	0.0364, 0.0843	0.0639, 0.1107	0.0361, 0.0867	0.0414, 0.0897	0.0437, 0.0840

[a] $R1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$ [b] $wR2 = \{ \Sigma [w(F_o^2-F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$ [c] $GOF = S = \{ \Sigma [w(F_o^2-F_c^2)^2] / (n-p) \}^{1/2}$

Table S2. Crystal and refinement data for reported complexes.

Complex	**2Ni-BCy$_2$OTf**	**2Pd-H**	**4Ni**	**4Ni-H**	**5Ni**
empirical formula	$C_{42}H_{61}BF_3NNiO_3P_2S$	$C_{30}H_{40}F_3NO_3P_2PdS$	$C_{30}H_{39}NNiOP_2$	$C_{31}H_{40}F_3NNiO_4P_2S$	$C_{64}H_{90}B_4F_{16}N_6Ni_2O_2P_4$
formula wt	848.43	720.03	550.27	700.35	1563.95
T (K)	100.01	100.01	100.0	99.98	100.11
a, Å	15.7224(11)	12.2515(8)	11.5436(5)	12.7394(14)	11.4094(4)
b, Å	12.6201(9)	11.1901(7)	15.7065(6)	15.2760(17)	11.4298(4)
c, Å	22.1023(15)	24.2291(15)	15.3374(5)	16.7217(19)	30.3230(12)
α, deg	90	90	90	90	92.4620(10)
β, deg	109.324(2)	102.437(3)	90.135(2)	101.186(2)	100.545(2)
γ, deg	90	90	90	90	107.826(2)
V, Å^3	4170.8(5)	3243.8(4)	2780.81(18)	3192.3(6)	3680.2(2)
Z	4	4	4	4	2
cryst syst	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
space group	P 1 21/c 1	P 1 21/c 1	P 1 21/c 1	P 1 21/c 1	P -1
d_{calcd}, g/cm^3	1.351	1.474	1.314	1.457	1.411
θ range, deg	2.522 to 30.530	1.702 to 30.570	1.764 to 30.552	1.822 to 30.519	2.981 to 78.736
μ, mm^{-1}	0.645	0.783	0.836	0.828	2.208
abs cor	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
GOF^c	1.041	1.076	1.005	1.050	1.078
R1,^{a} wR2^b (I > 2σ(I))	0.0417, 0.1143	0.0211, 0.0508	0.0321, 0.0724	0.0248, 0.0634	0.0810, 0.2035

^{a} $R1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$ ^{b} $wR2 = \{ \Sigma [w(F_o^2-F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$ ^{c} $GOF = S = \{ \Sigma [w(F_o^2-F_c^2)^2] / (n-p) \}^{1/2}$

References

1. Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J., *Organometallics* **1996,** *15* (5), 1518-1520.
2. Fulmer, G. R.; Miller, A. J. M.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I., *Organometallics* **2010,** *29* (9), 2176-2179.
3. APEX2, Version 2 User Manual, M86-E01078, Bruker Analytical X-ray Systems, Madison, WI, June 2006.
4. Sheldrick, G.M. "SADABS (version 2008/1): Program for Absorption Correction for Data from Area Detector Frames", University of Göttingen, 2008.
5. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
6. Dolomanov, O.V. (2009). OLEX2. J. Appl. Cryst. 42, 339-341.
7. Brandenburg, K. (1999). DIAMOND. Crystal Impact GbR, Bonn, Germany.