Supporting information

Tandem Hydrogenation and Condensation of Fluorinated α,β-Unsaturated Ketones With Primary Amines, Catalyzed by Nickel

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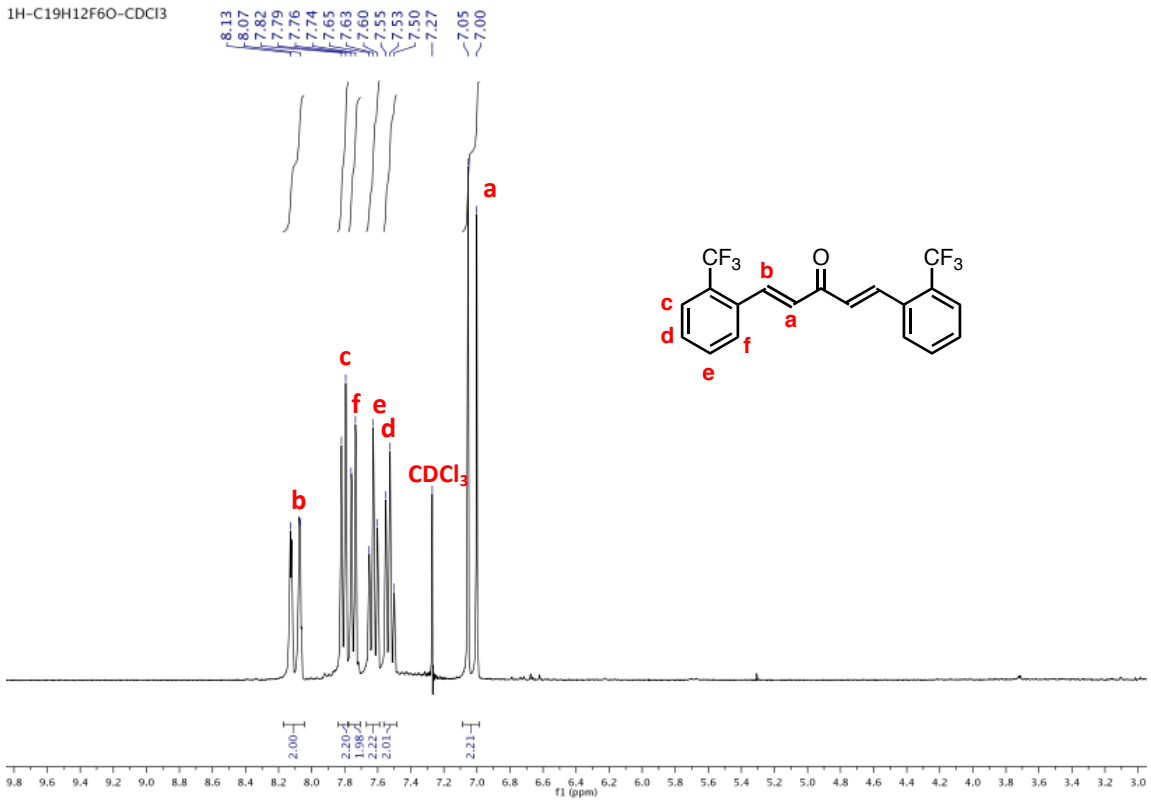


Figure S1. ^{1}H spectrum of $C_{19}H_{12}F_6O$: 1,5-bis(2-(trifluoromethyl)phenyl)penta-1,4-dien-3-one, **1a**, in $CDCl_3$.

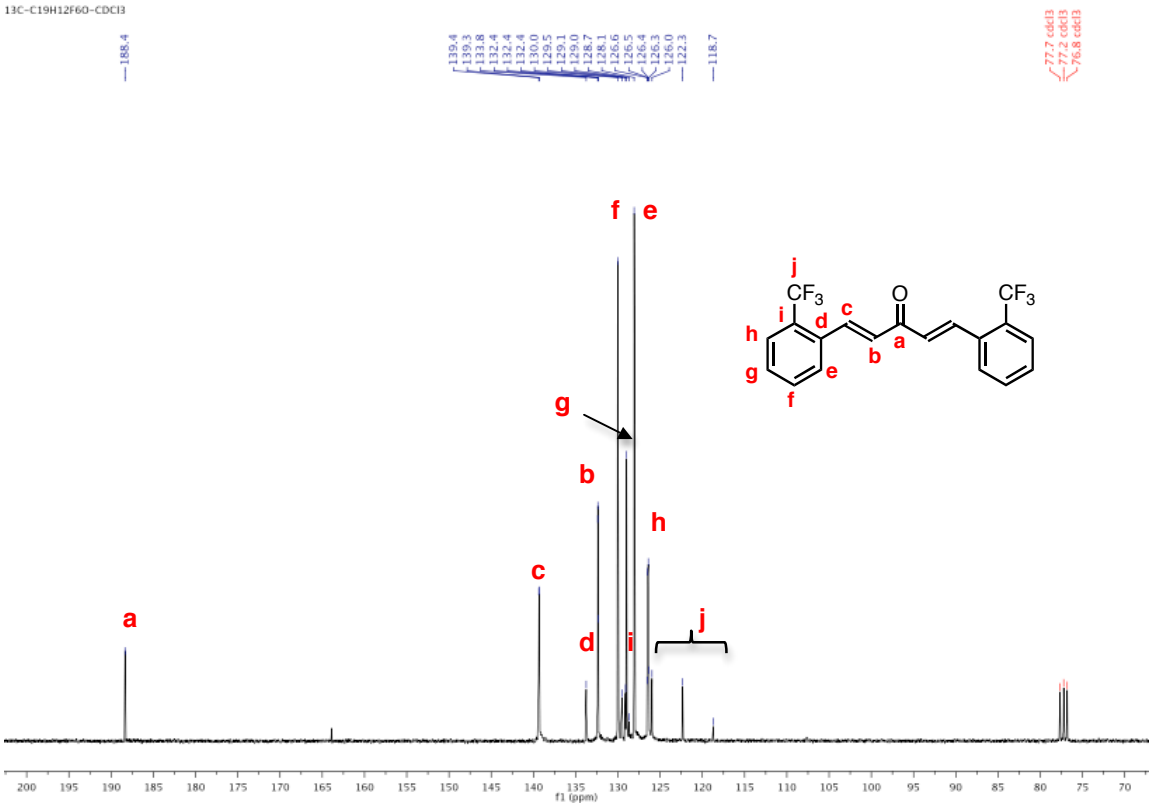


Figure S2. $^{13}C\{^{1}H\}$ spectrum of $C_{19}H_{12}F_6O$ **1a**, in $CDCl_3$.

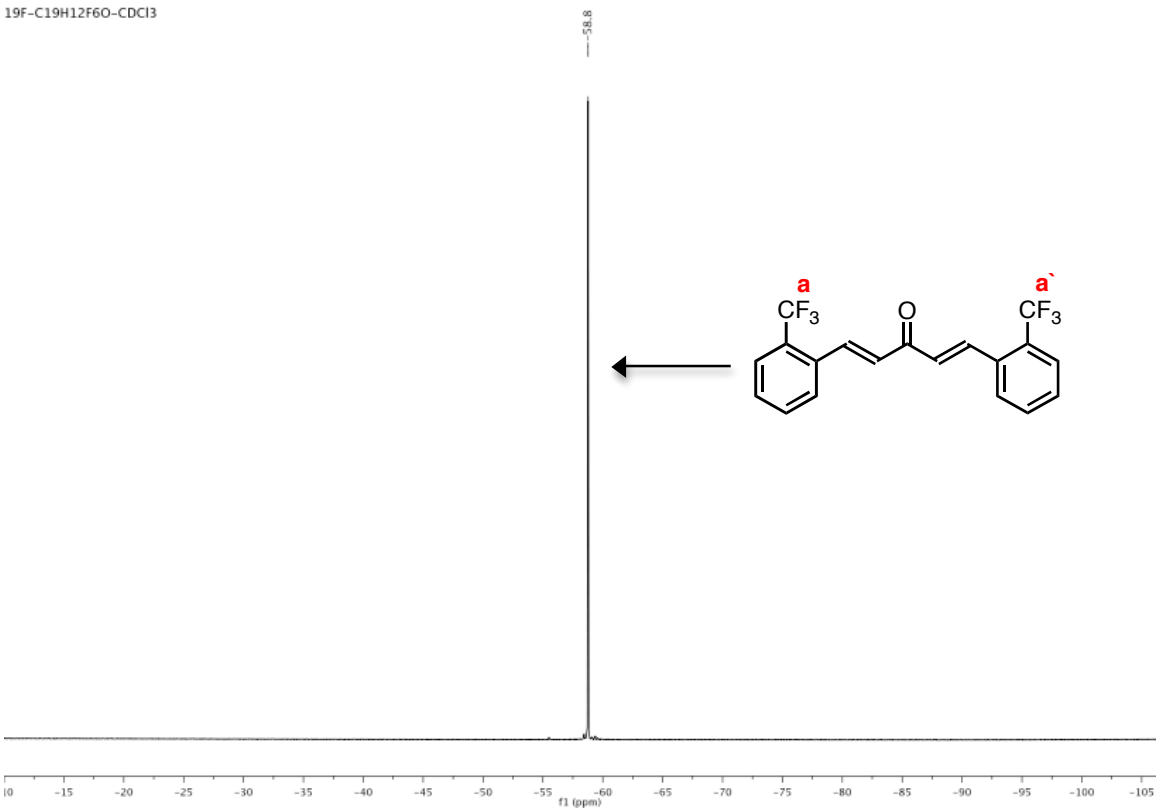


Figure S3. ^{19}F spectrum of $C_{19}H_{12}F_6O$ **1a**, in $CDCl_3$.

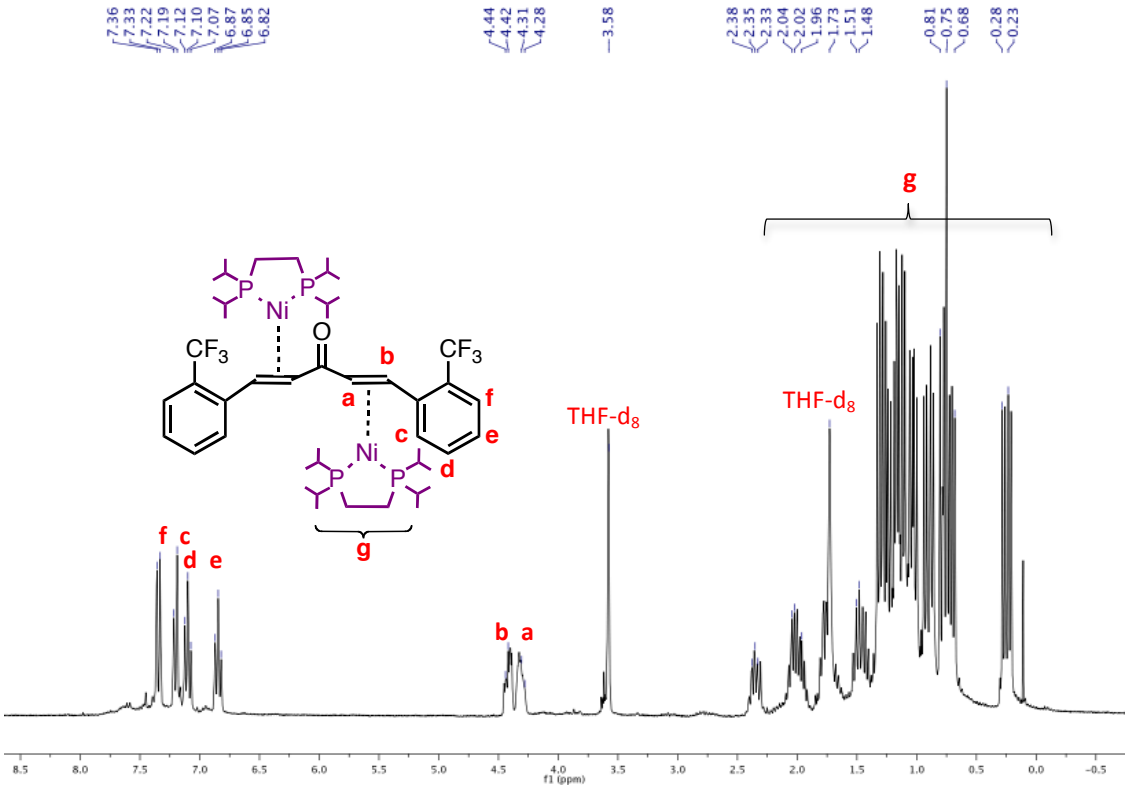


Figure S4. ^{1}H spectrum of [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)], ($C_{19}H_{12}F_6O$: 1,5-bis(2-(trifluoromethyl)phenyl)penta-1,4-dien-3-one), **2a**, in THF-d_8.

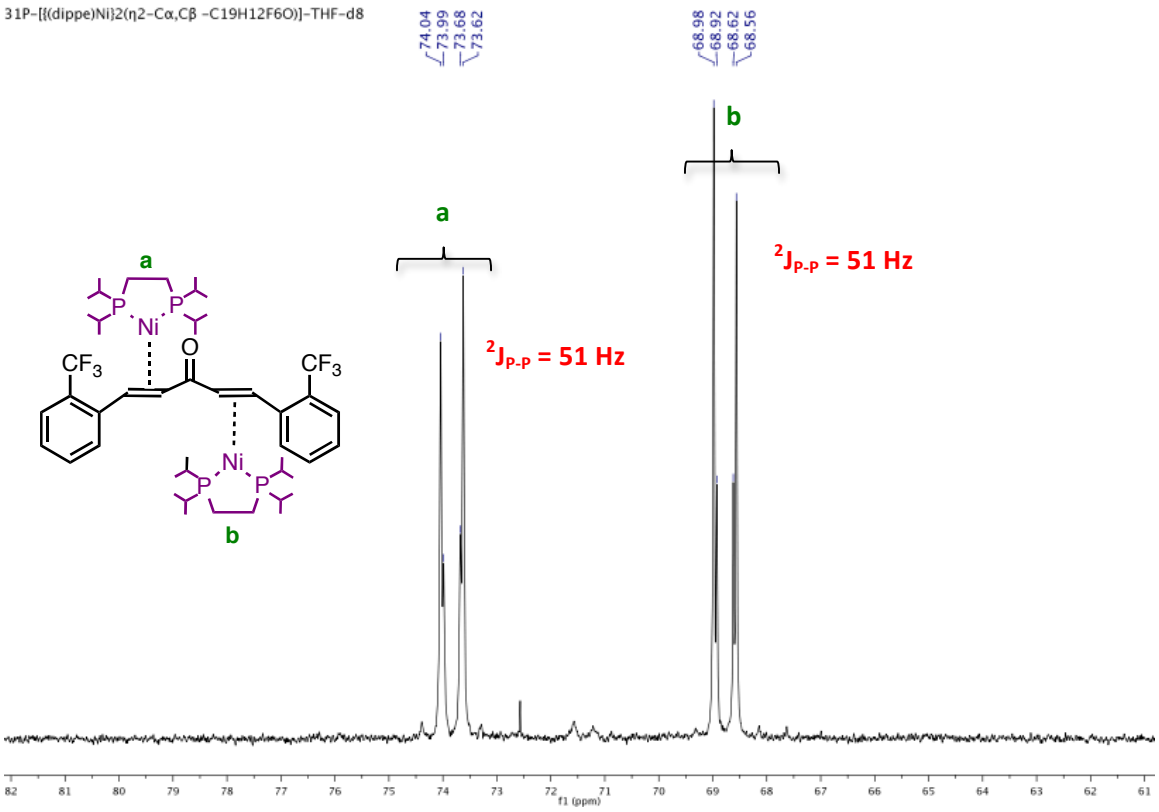


Figure S5. $^{31}P\{^1H\}$ spectrum of [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)] **2a**, in THF-d_8.

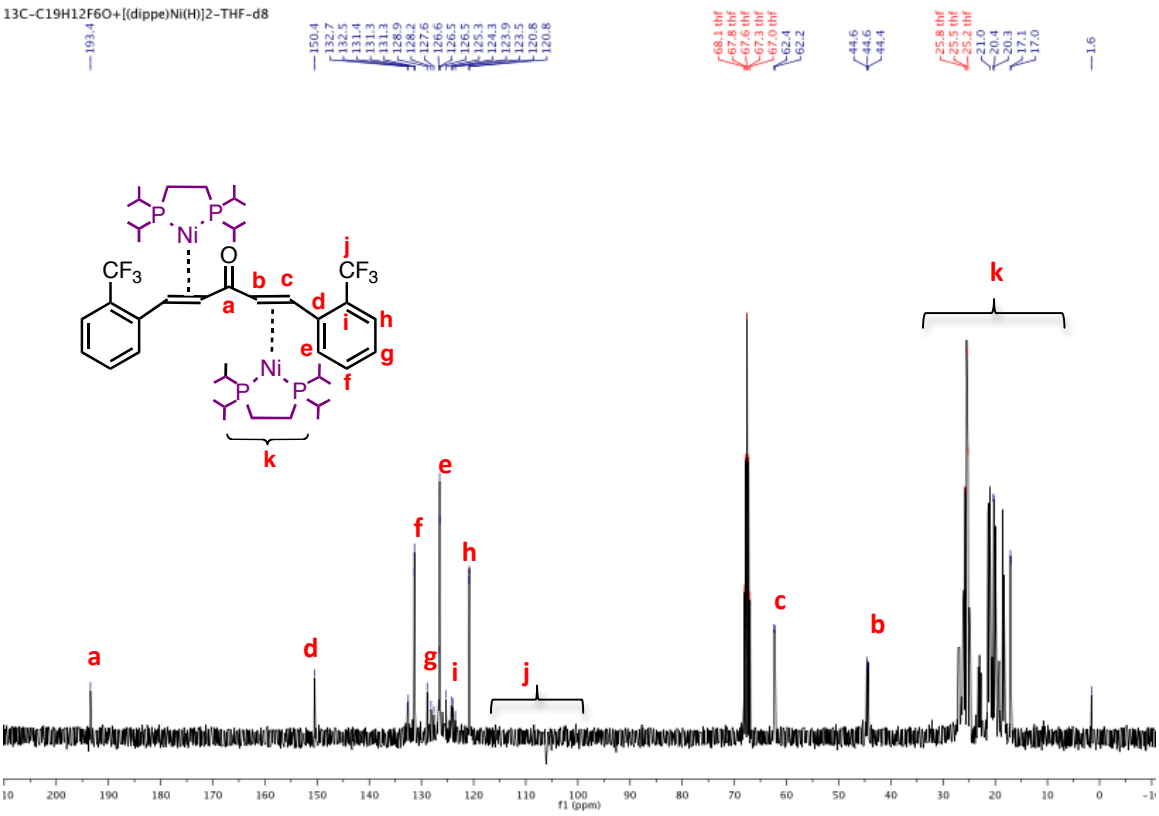


Figure S6. $^{13}C\{^1H\}$ spectrum of [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)] **2a**, in THF-d_8.

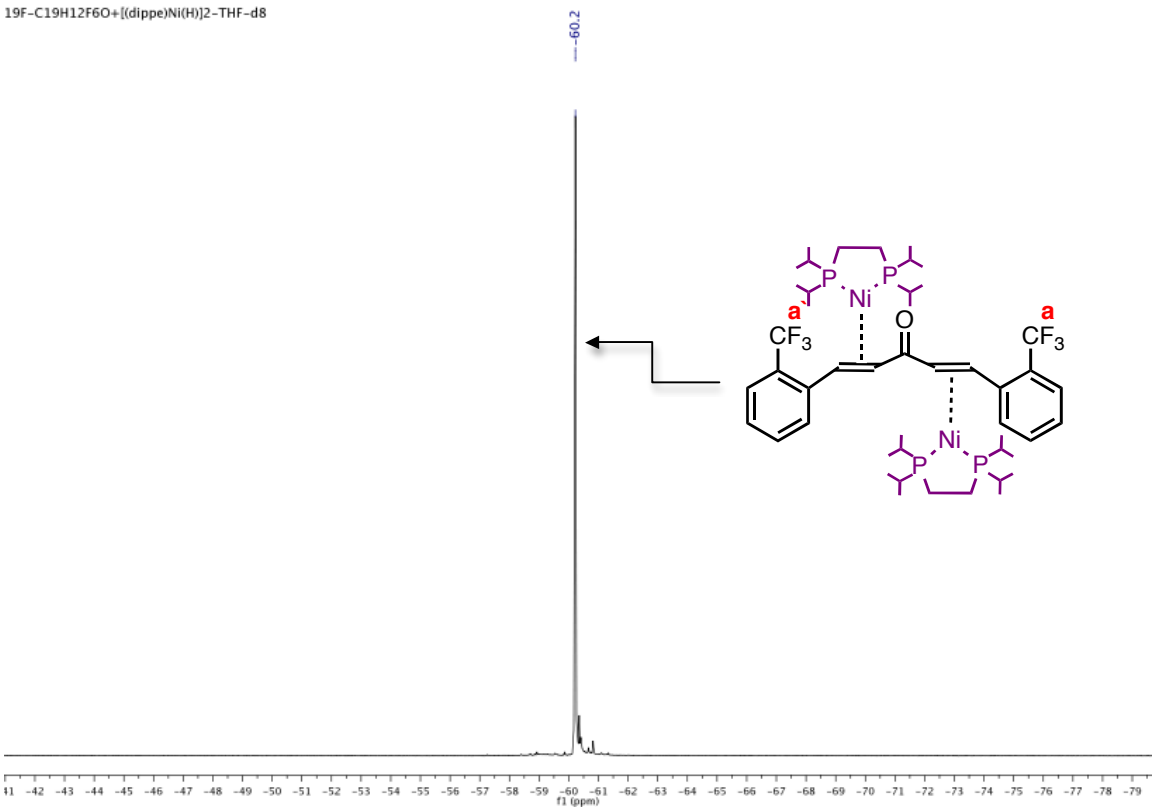


Figure S7. ^{19}F spectrum of [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)] **2a**, in THF-d_8.

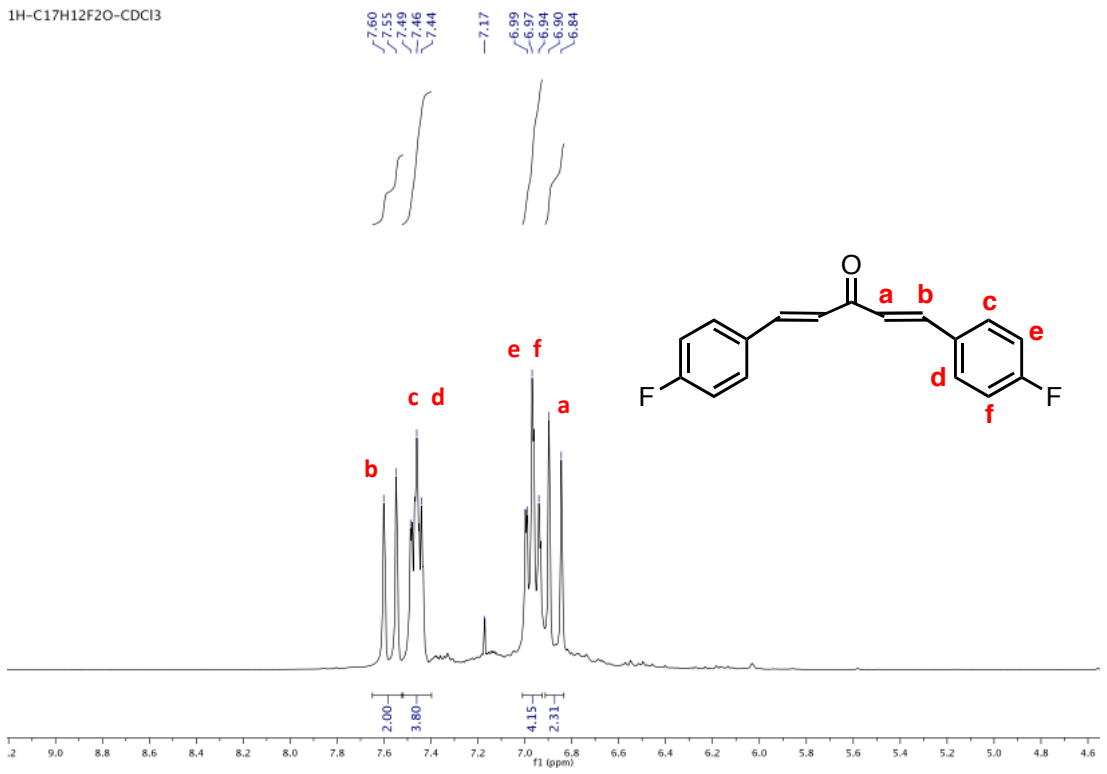


Figure S8. ^1H spectrum of $C_{17}H_{12}F_2O$: 1,5-bis(4-fluorophenyl)penta-1,4-dien-3-one, **1b**, in $CDCl_3$.

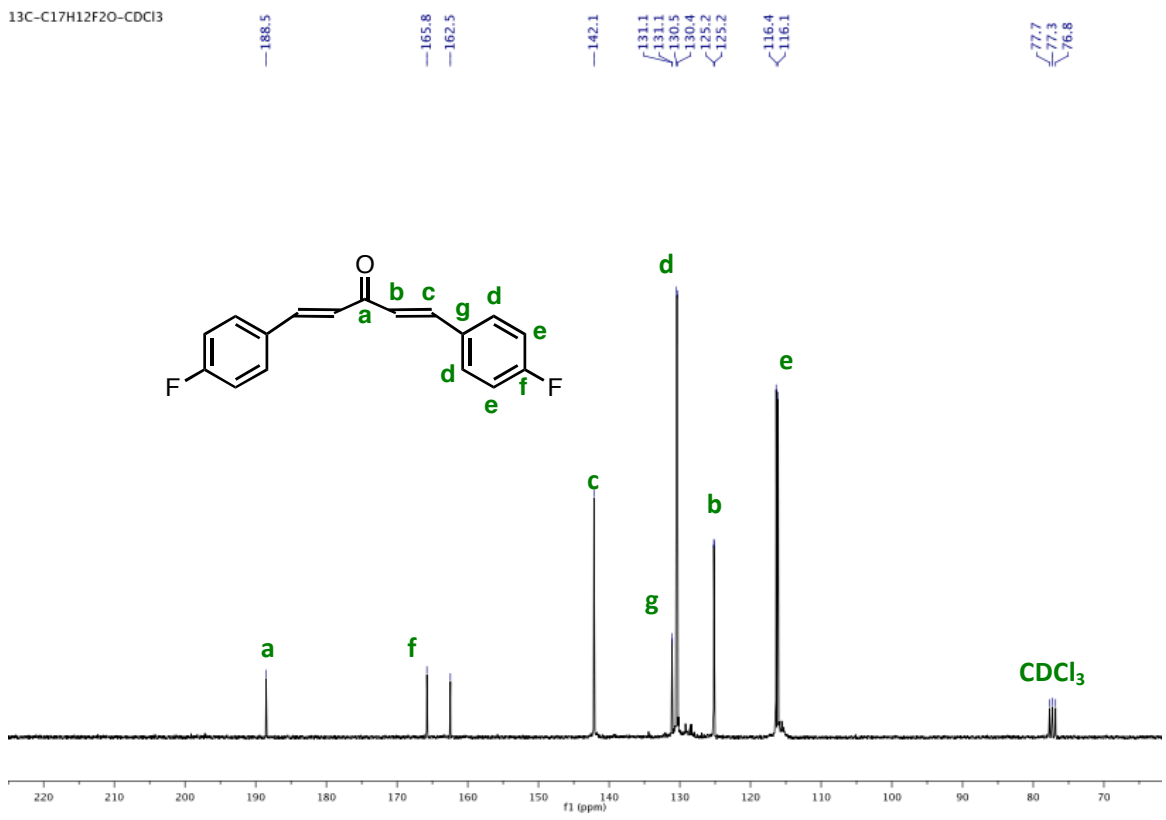


Figure S9. $^{13}C\{^{1}H\}$ spectrum of $C_{17}H_{12}F_2O$ **1b**, in $CDCl_3$.

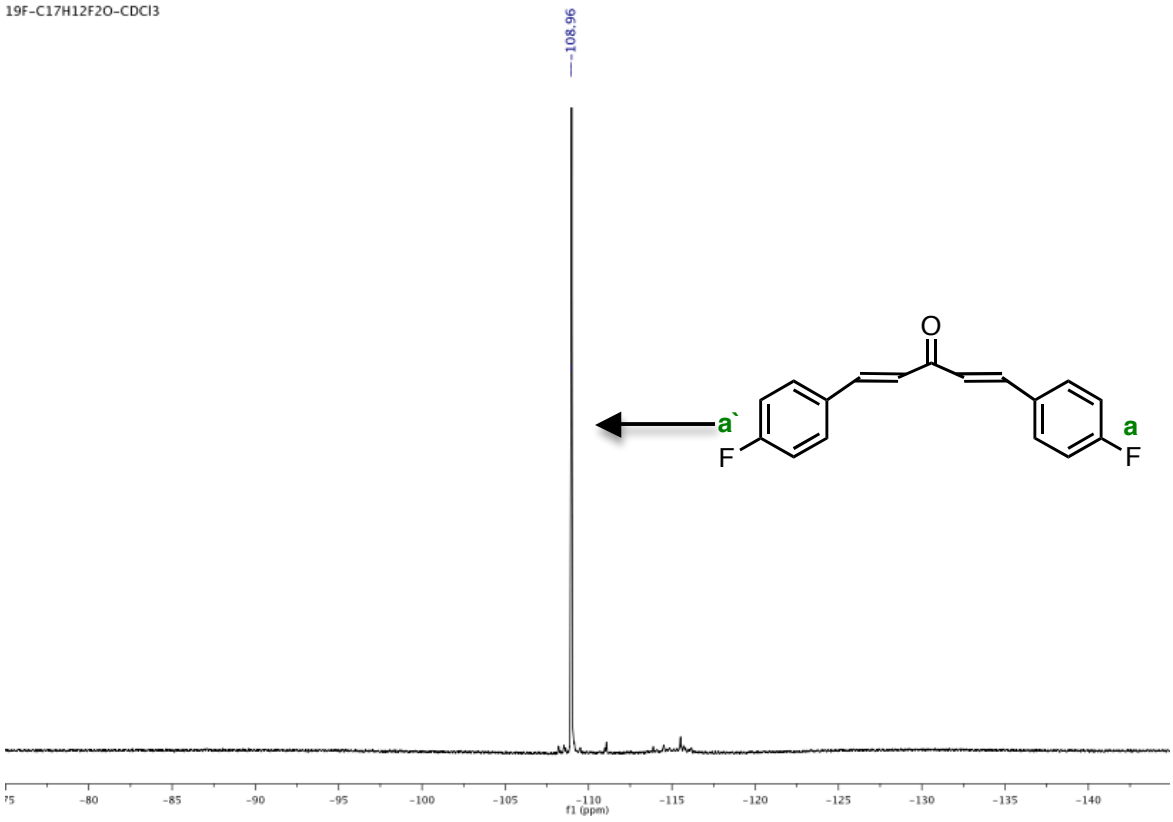


Figure S10. ^{19}F spectrum of $C_{17}H_{12}F_2O$ **1b**, in $CDCl_3$.

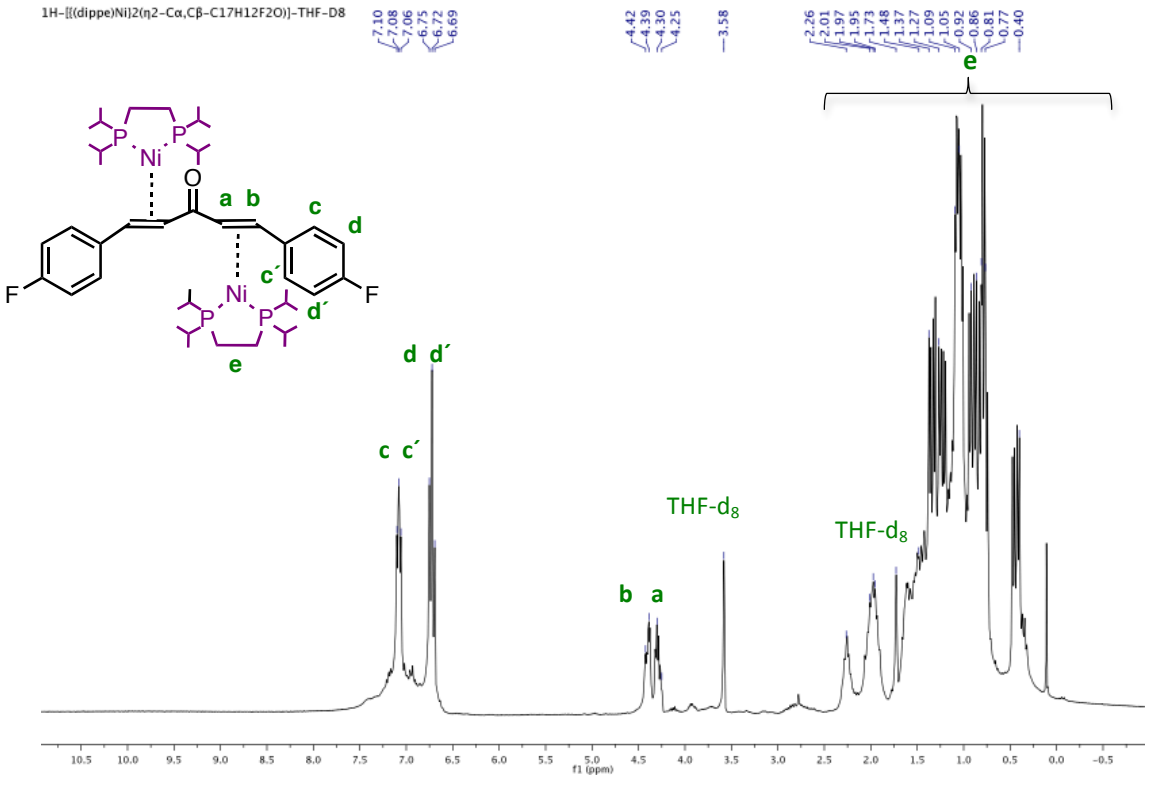


Figure S11. ^{1}H spectrum of [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{17}H_{12}F_2O$)], ($C_{17}H_{12}F_2O$: 1,5-bis(4-fluorophenyl)penta-1,4-dien-3-one), **2b**, in THF-d_8.

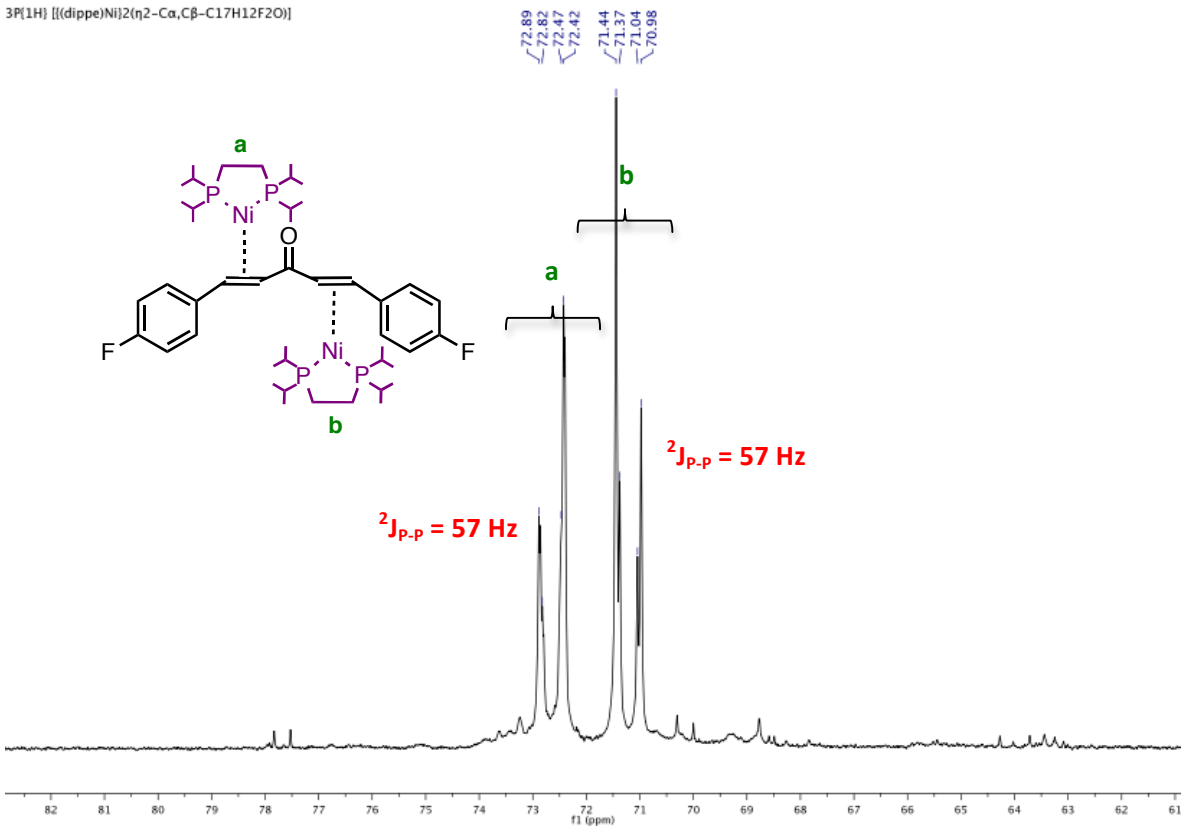


Figure S12. ^{3}P{^{1}H} spectrum of [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{17}H_{12}F_2O$)], **2b**, in THF-d_8.

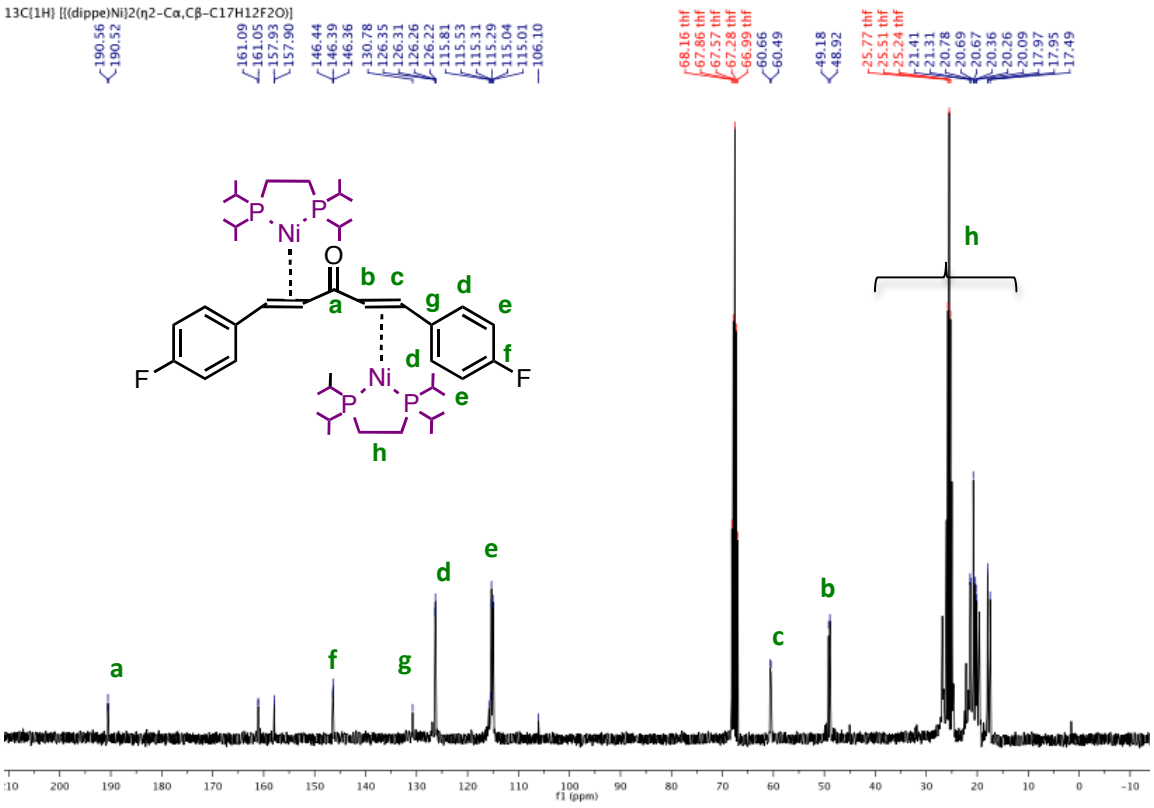


Figure S13. $^{13}C\{^{1}H\}$ spectrum of $[\{(dippe)Ni\}_2(\eta^2\text{-}C\alpha,C\beta\text{-}C_{17}H_{12}F_2O)]$, **2b**, in THF-$d_8$.

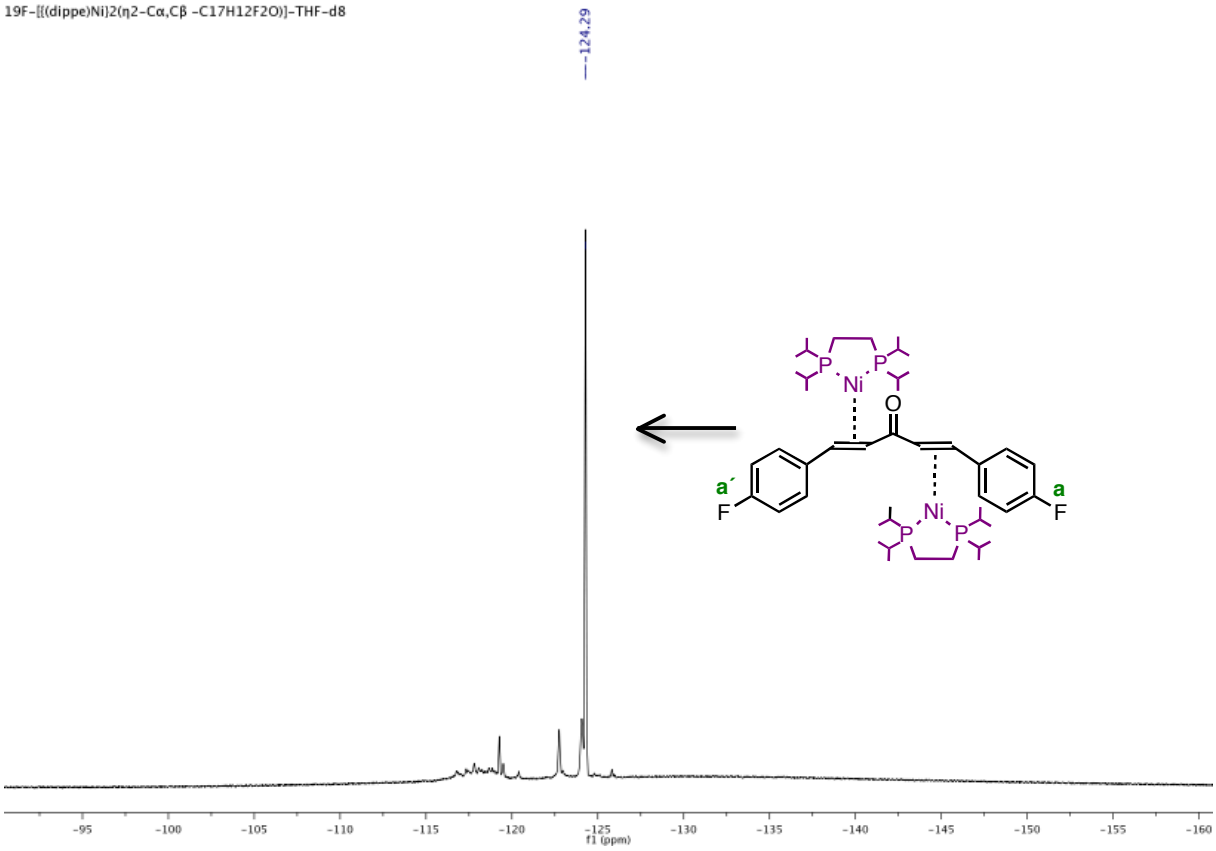


Figure S14. ^{19}F spectrum of $[\{(dippe)Ni\}_2(\eta^2\text{-}C\alpha,C\beta\text{-}C_{17}H_{12}F_2O)]$, **2b**, in THF-$d_8$.

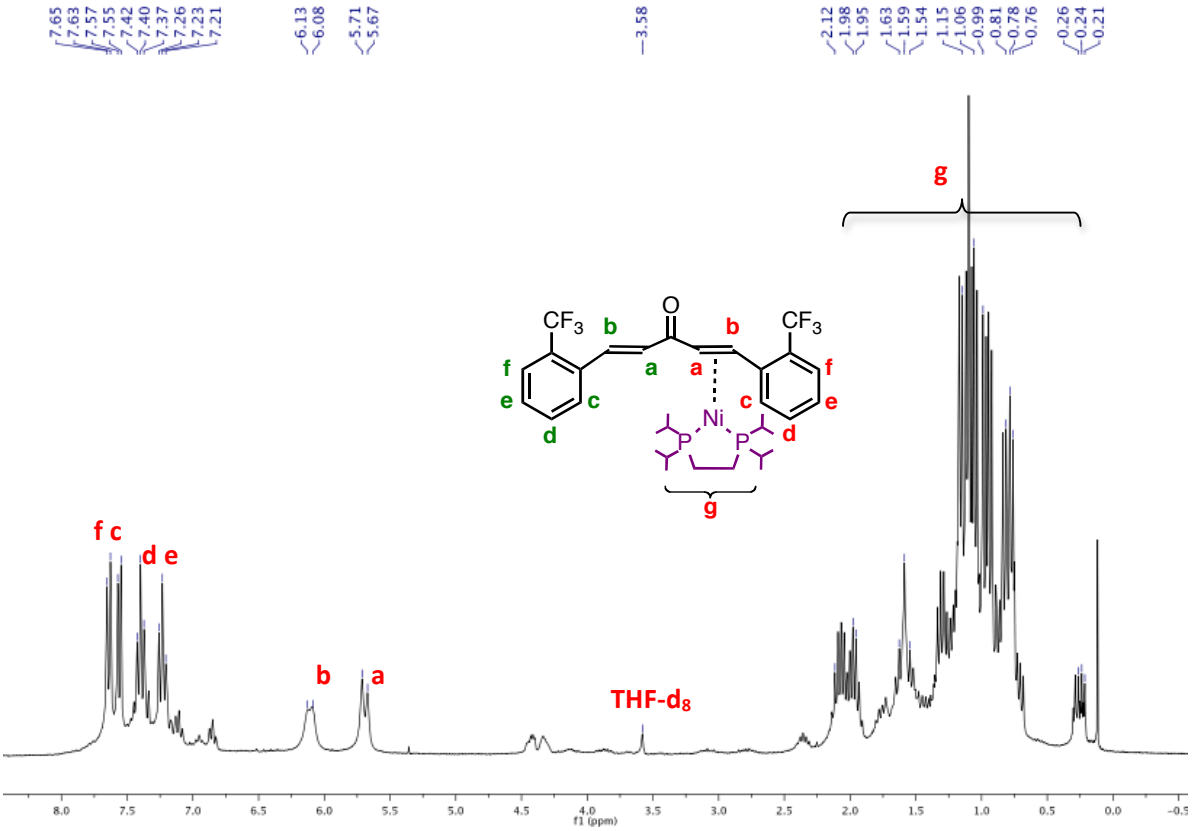


Figure S15. ^{1}H spectrum of [{(dippe)Ni}(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)] **3a**, in THF-d_8.

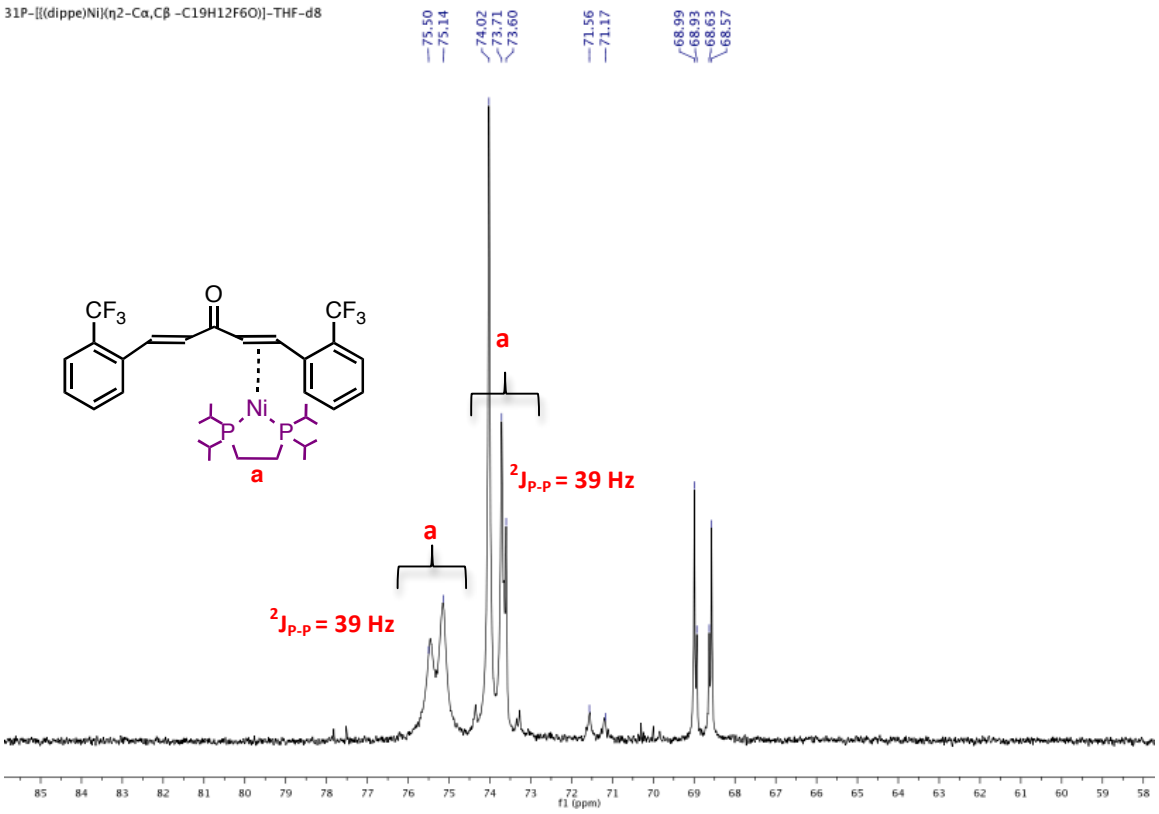


Figure S16. $^{31}P\{^{1}H\}$ spectrum of [{(dippe)Ni}(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)] **3a**, in THF-d_8.

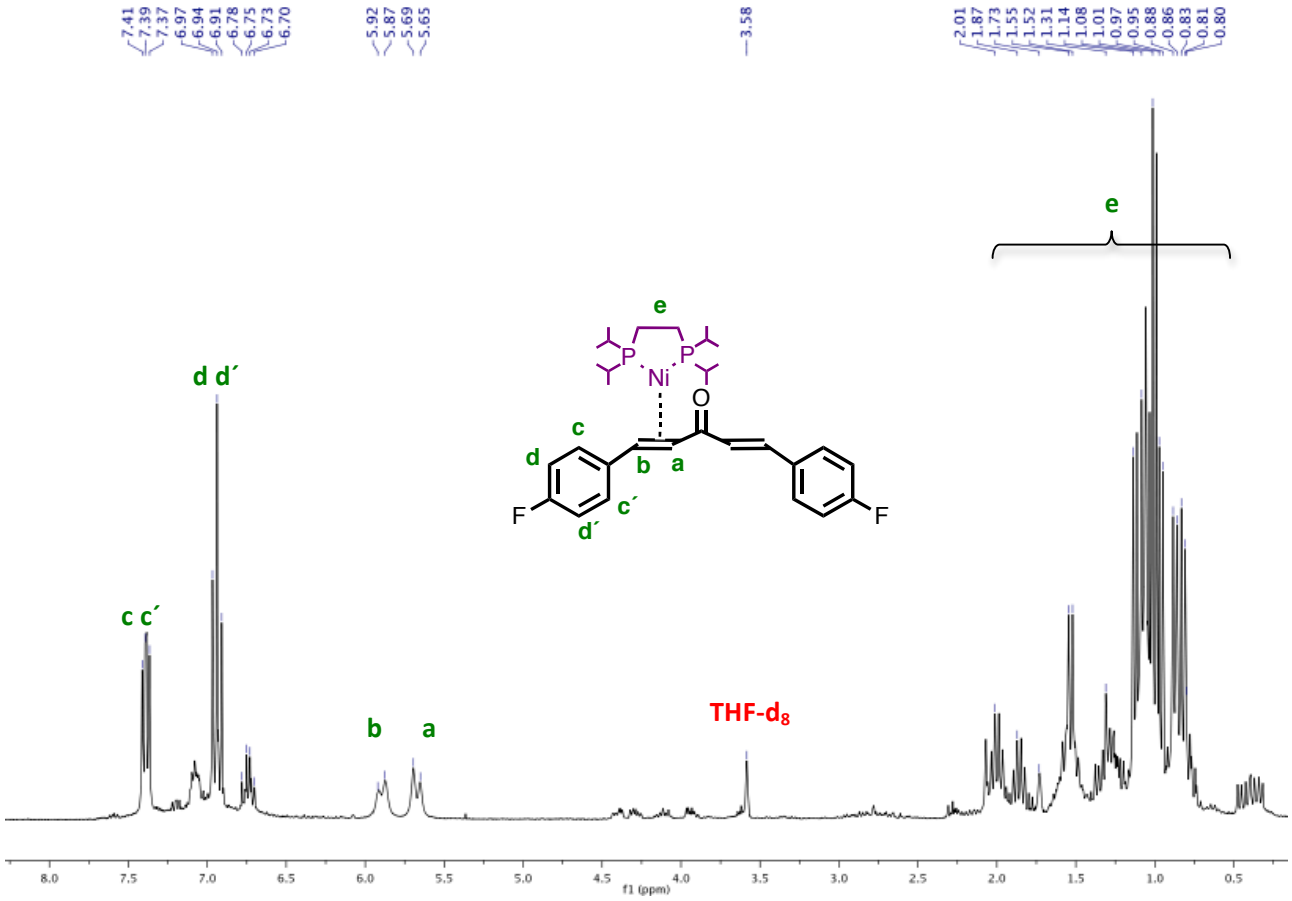


Figure S17. ^{1}H spectrum of [(dippe)Ni(η^2-Cα,Cβ - $C_{17}H_{12}F_2O$)] **3b**, in THF-d_8.

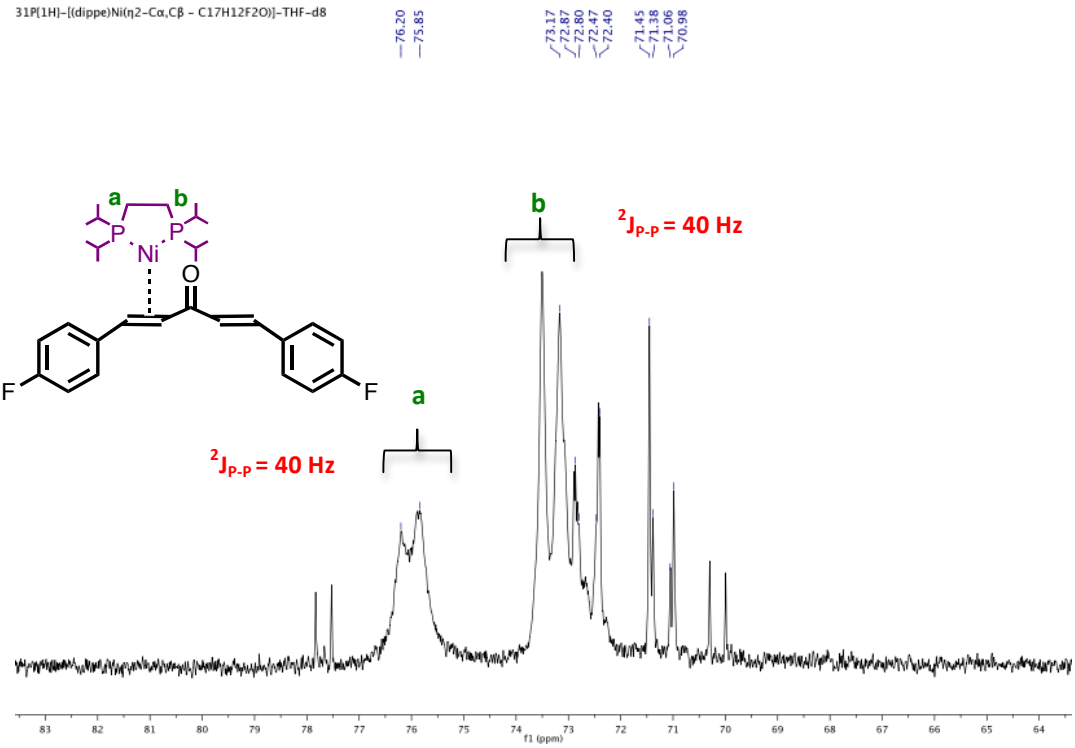


Figure S18. $^{31}P\{^{1}H\}$ spectrum of [(dippe)Ni(η^2-Cα,Cβ - $C_{17}H_{12}F_2O$)] **3b**, in THF-d_8.

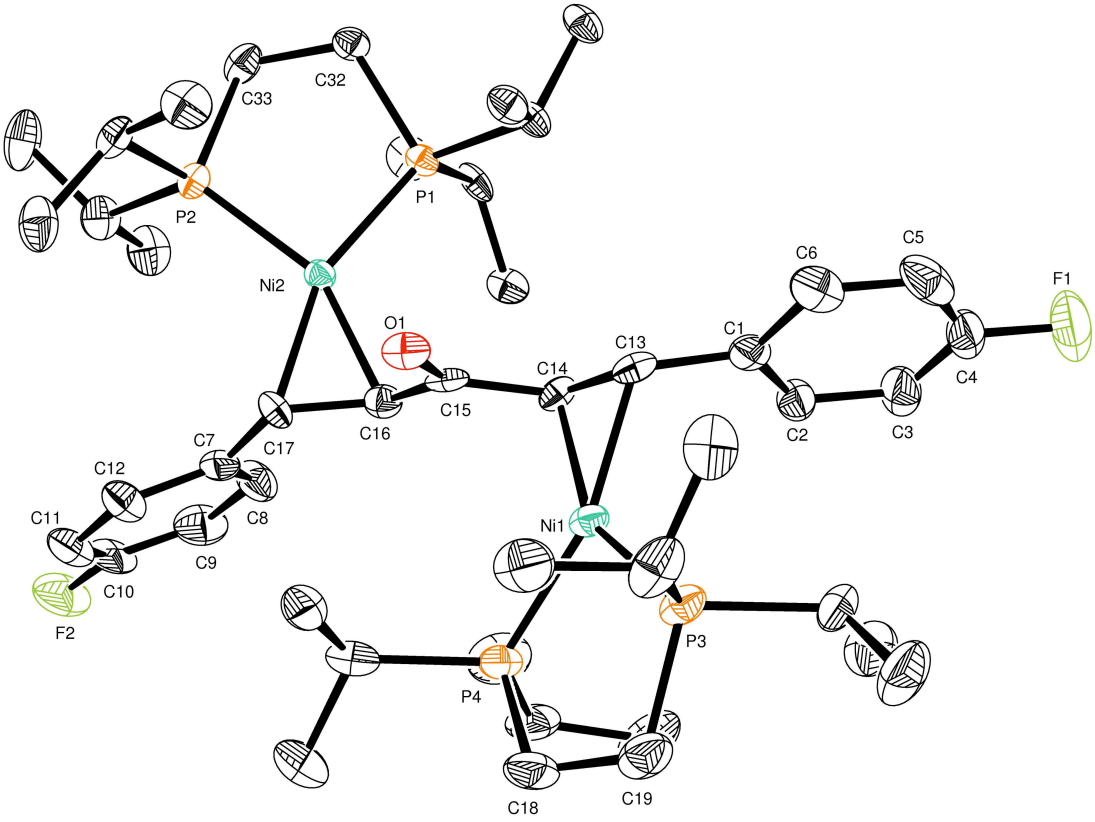


Figure S19. ORTEP drawing of [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{17}H_{12}F_2O$)] **2b**.

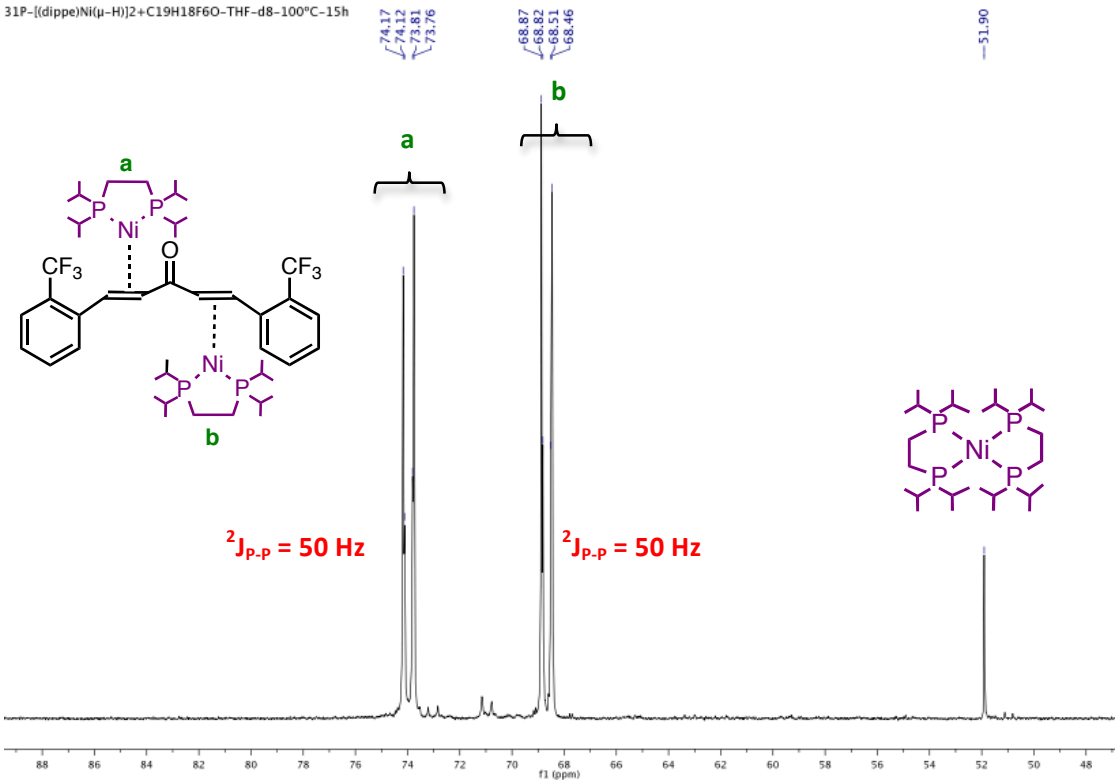


Figure S20. $^{31}P\{^1H\}$ spectrum equimolar mixture of [(dippe)Ni(μ-H)]$_2$ **2** with $C_{19}H_{12}F_6O$ **1a** at 100 ºC for 7 days in THF-d_8.

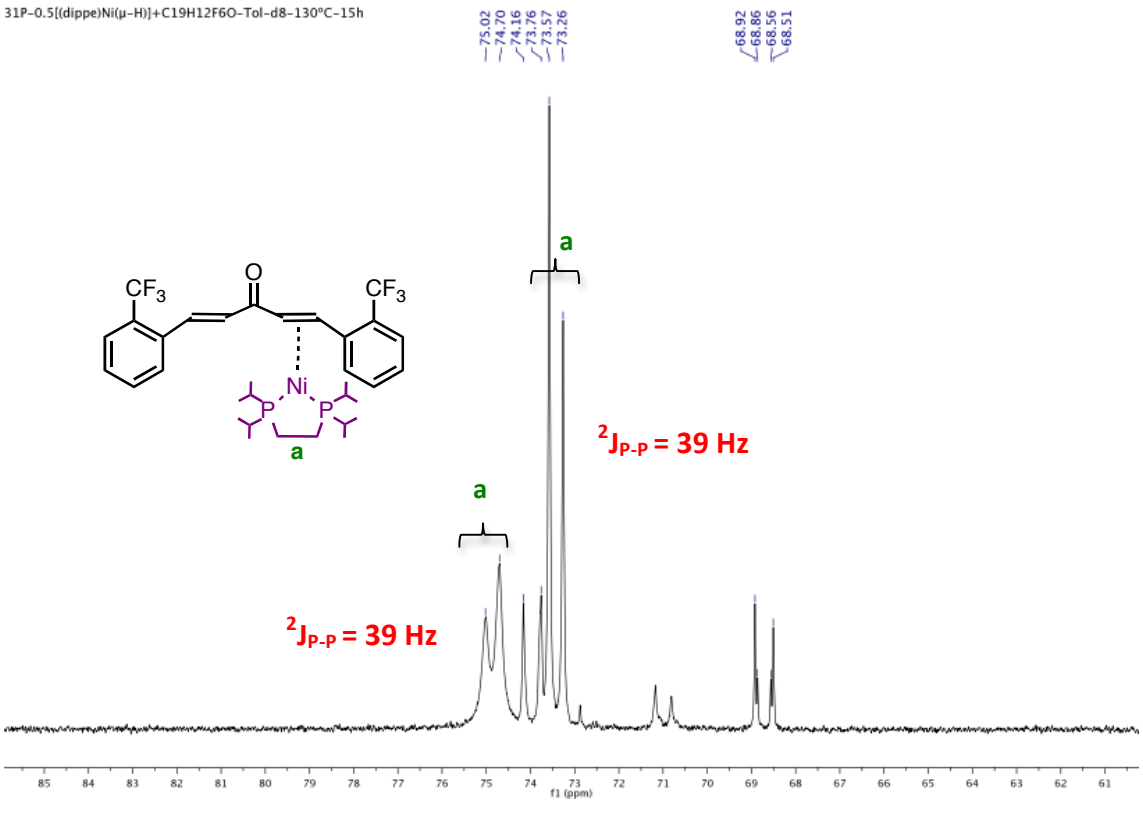


Figure S21. $^{31}P\{^{1}H\}$ spectrum of reaction between $[(dippe)Ni(\mu\text{-}H)]_2$ **2** (1 equiv.) and $C_{19}H_{12}F_6O$ **1a** (2 equiv.) at 130 ºC for 15 hours in Tol-d_8.

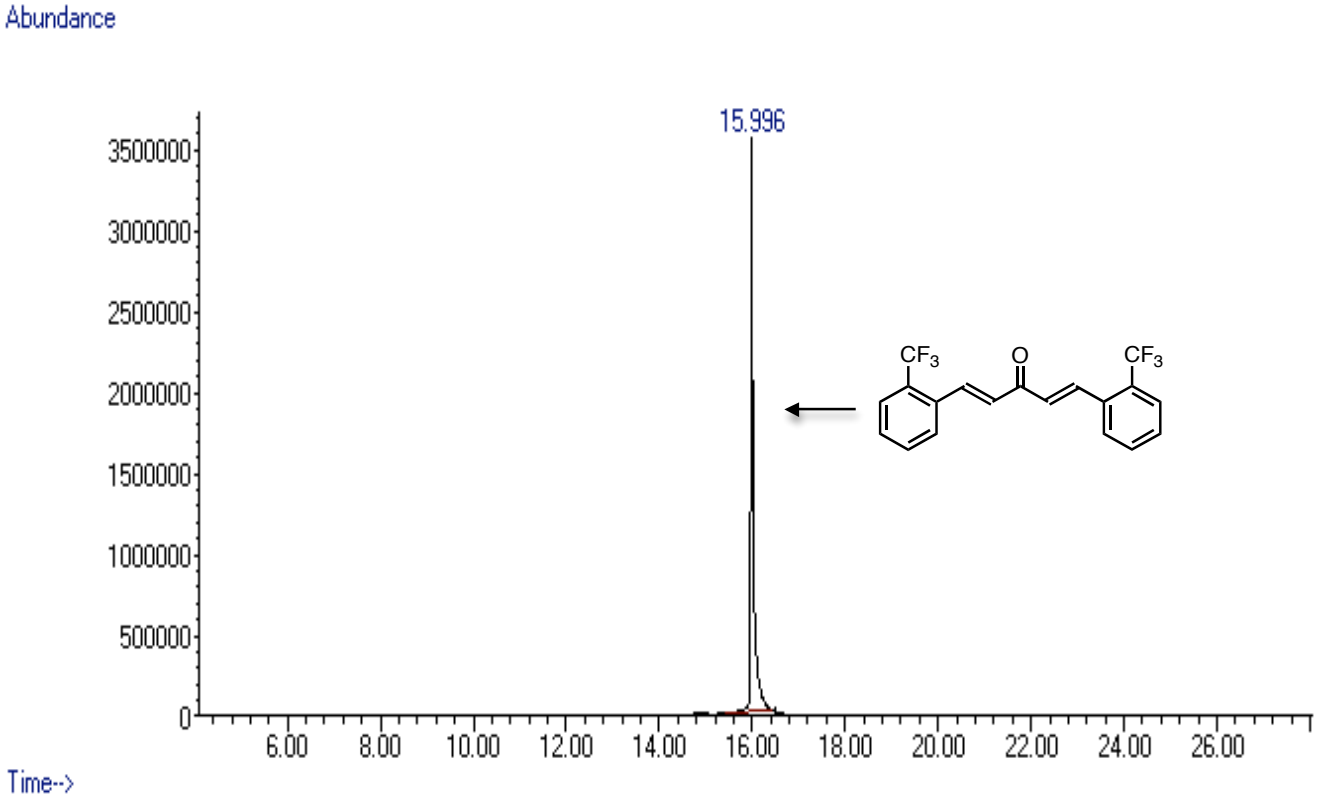


Figure S22. Chromatogram of $C_{19}H_{12}F_6O$: 1,5-bis(2-(trifluoromethyl)phenyl)penta-1,4-dien-3-one **1a**.

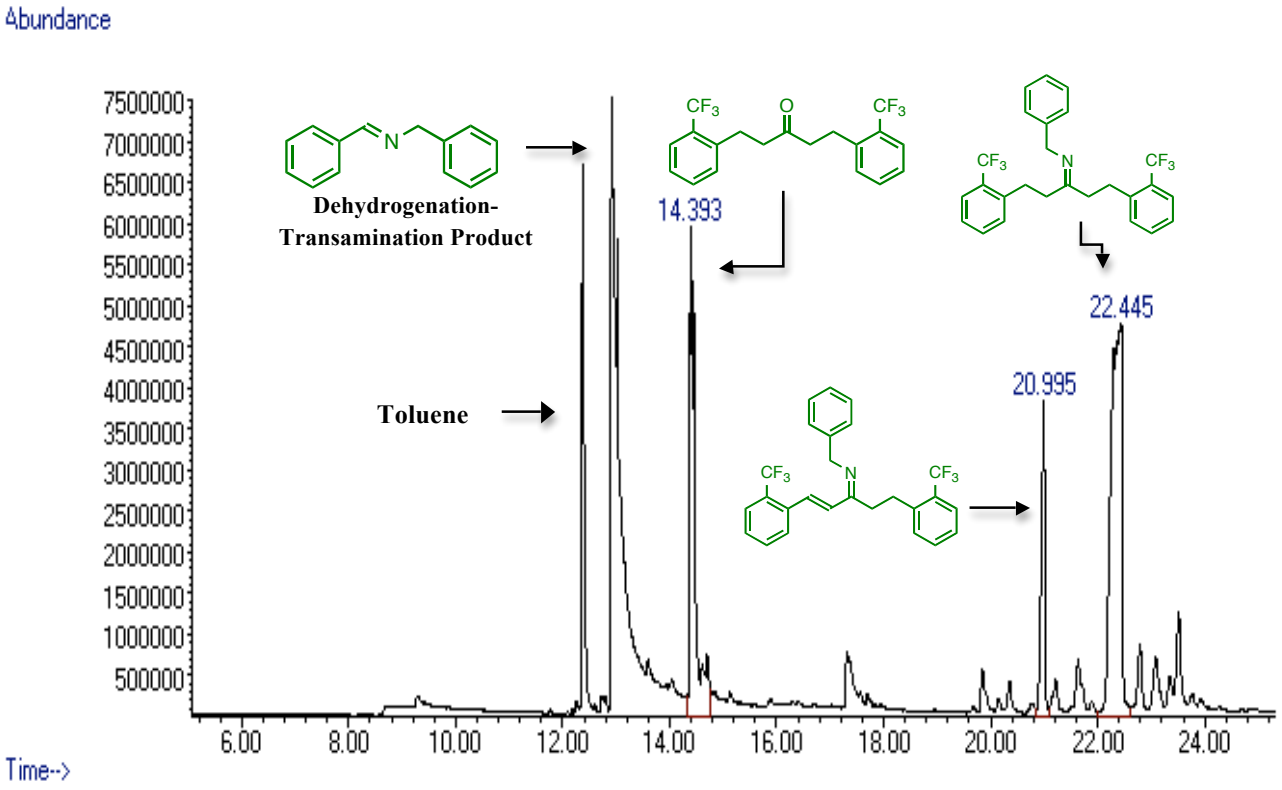


Figure S23. Chromatogram reduction and condensation products from **1a**, table 1, entry 4.

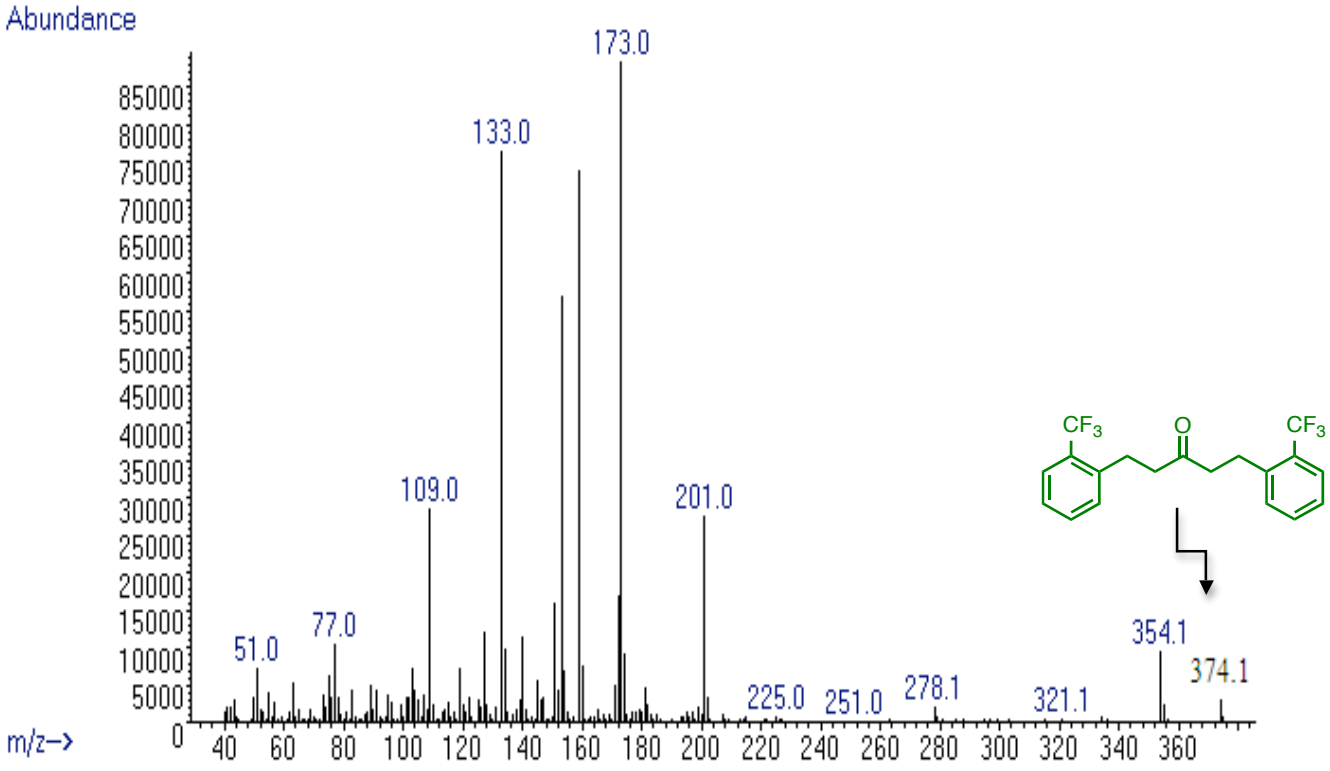


Figure S24. Mass spectrum product **4**, table 1, entry 4.

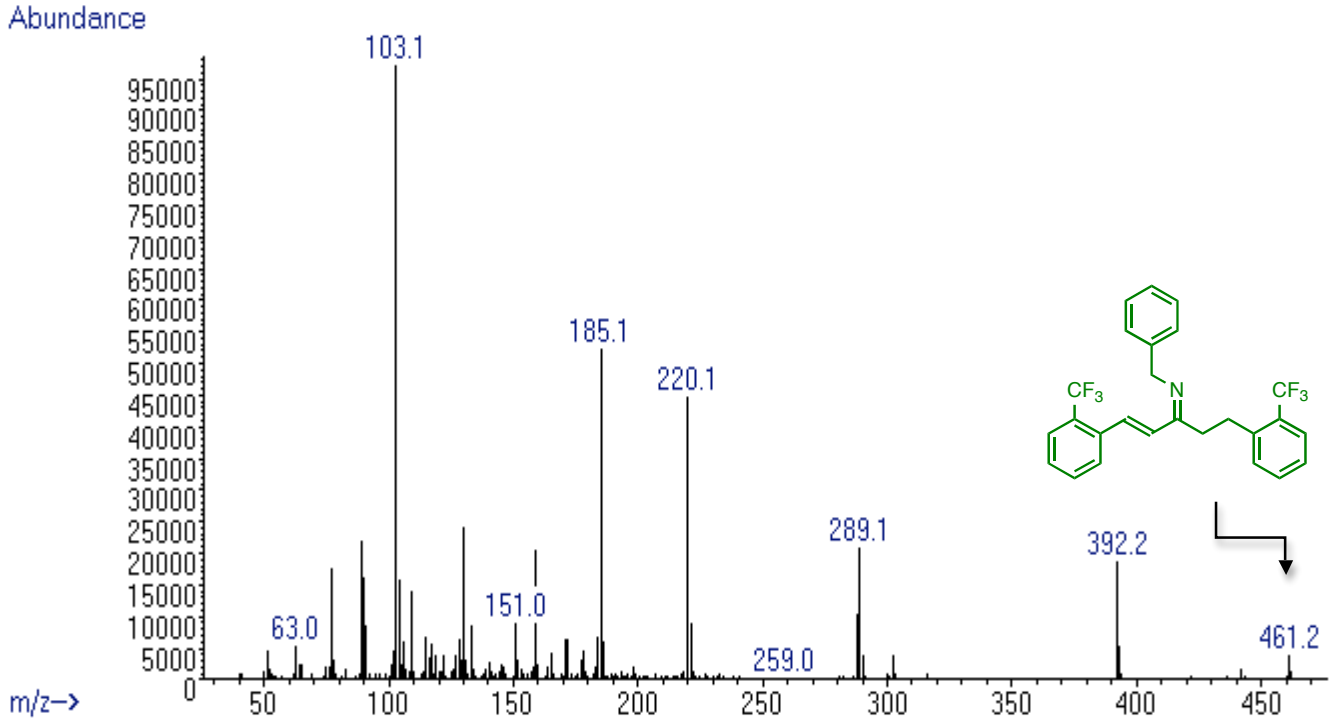


Figure S25. Mass spectrum product **6**, table 1, entry 4.

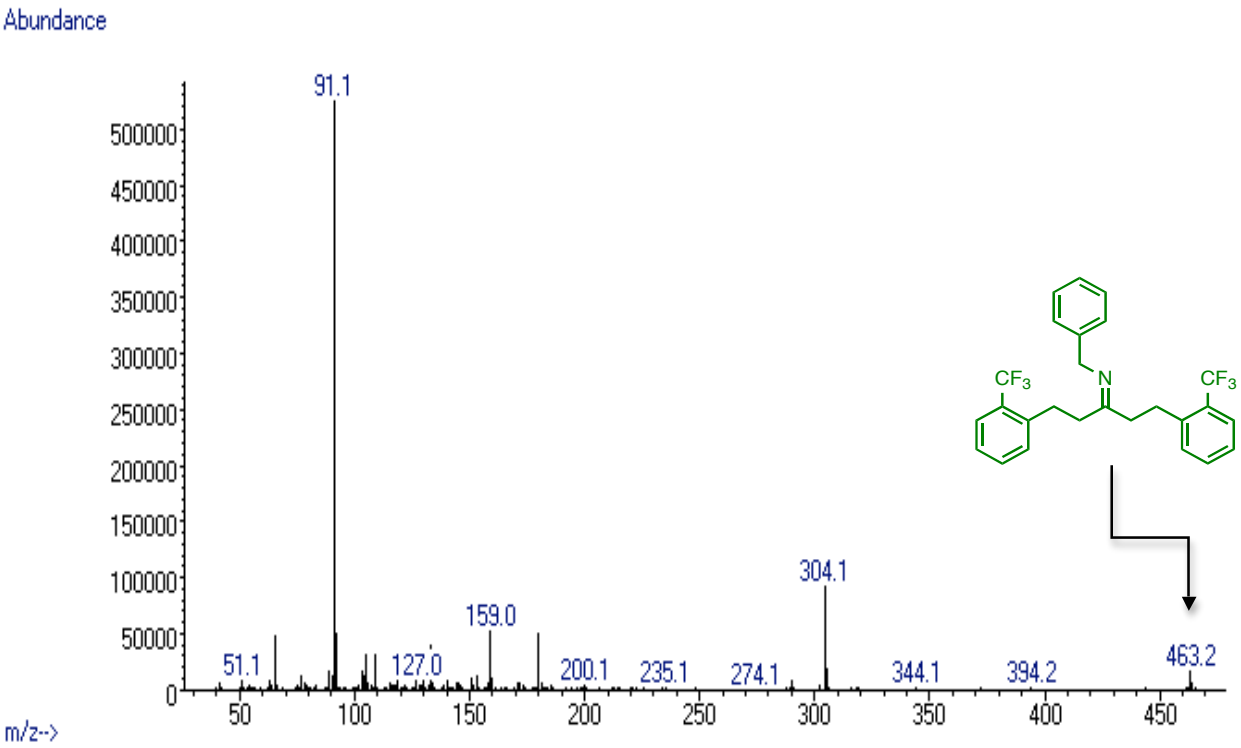


Figure S26. Mass spectrum product **7**, table 1, entry 4.

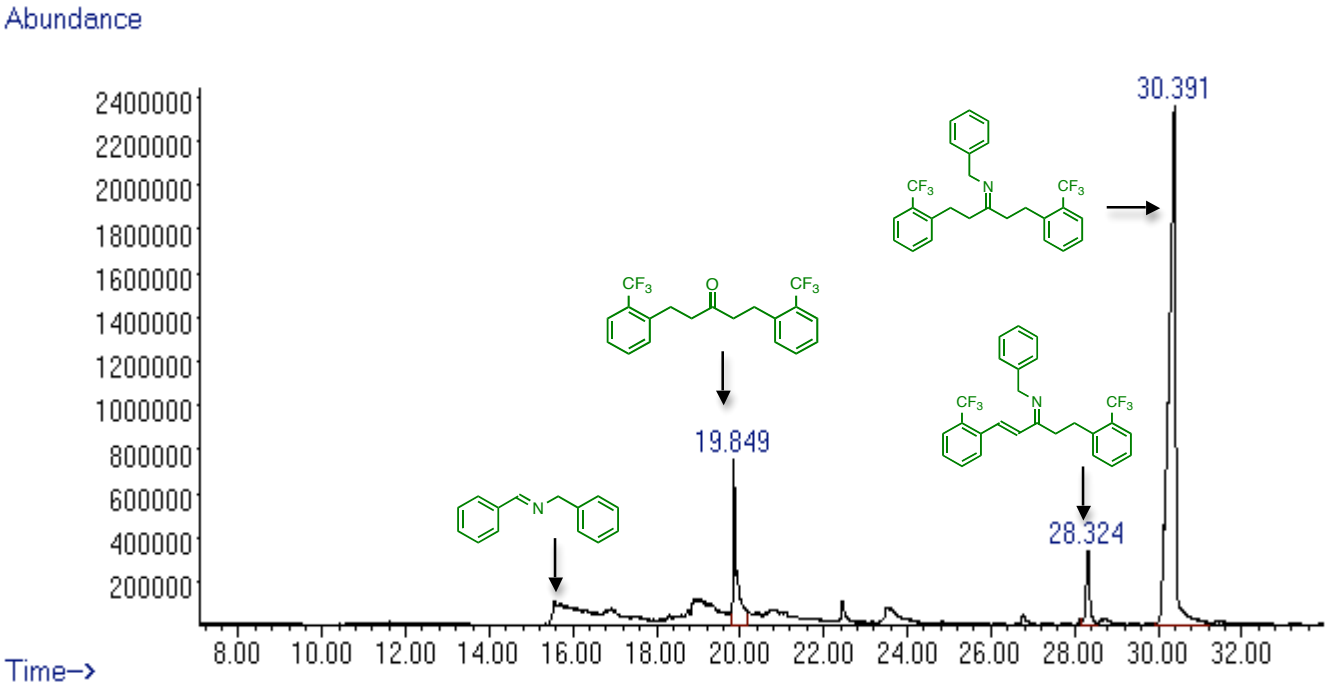


Figure S27. Chromatogram reduction and condensation products from **1a**, table 2, entry 5.

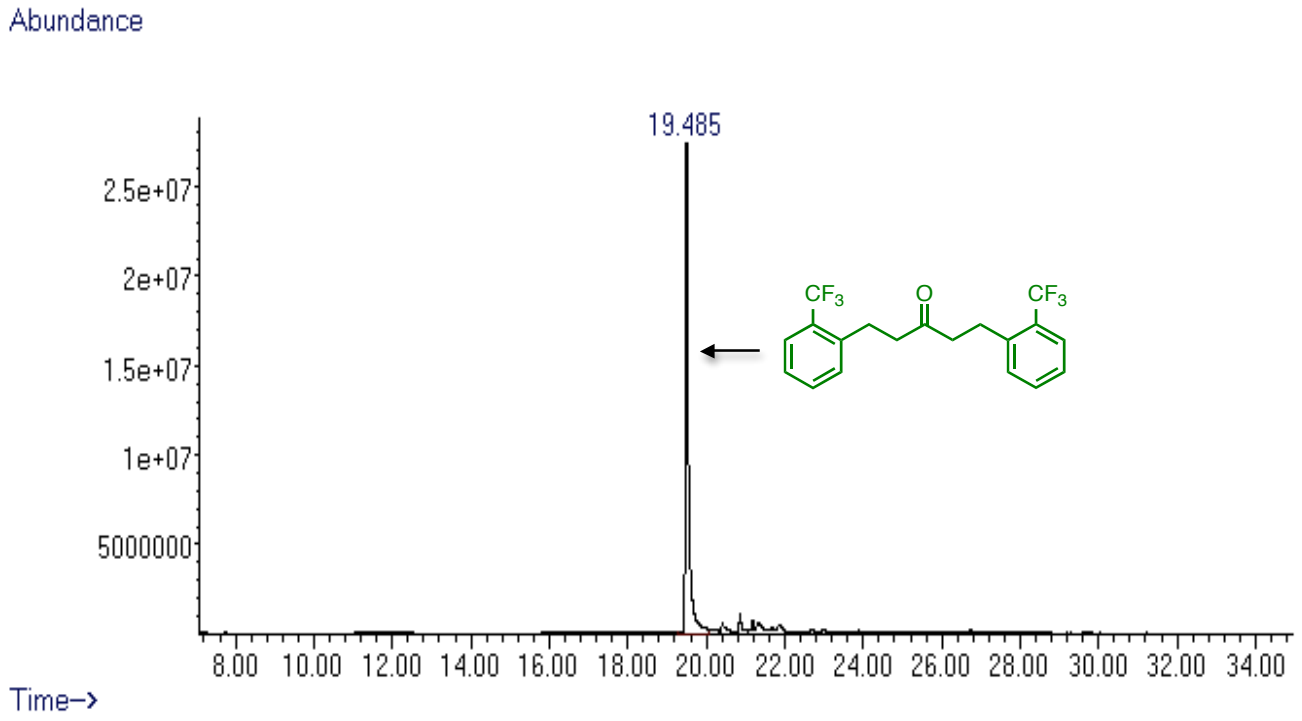


Figure S28. Chromatogram reduction product $C_{19}H_{16}F_6O$ **4**, table 2, entry 5.

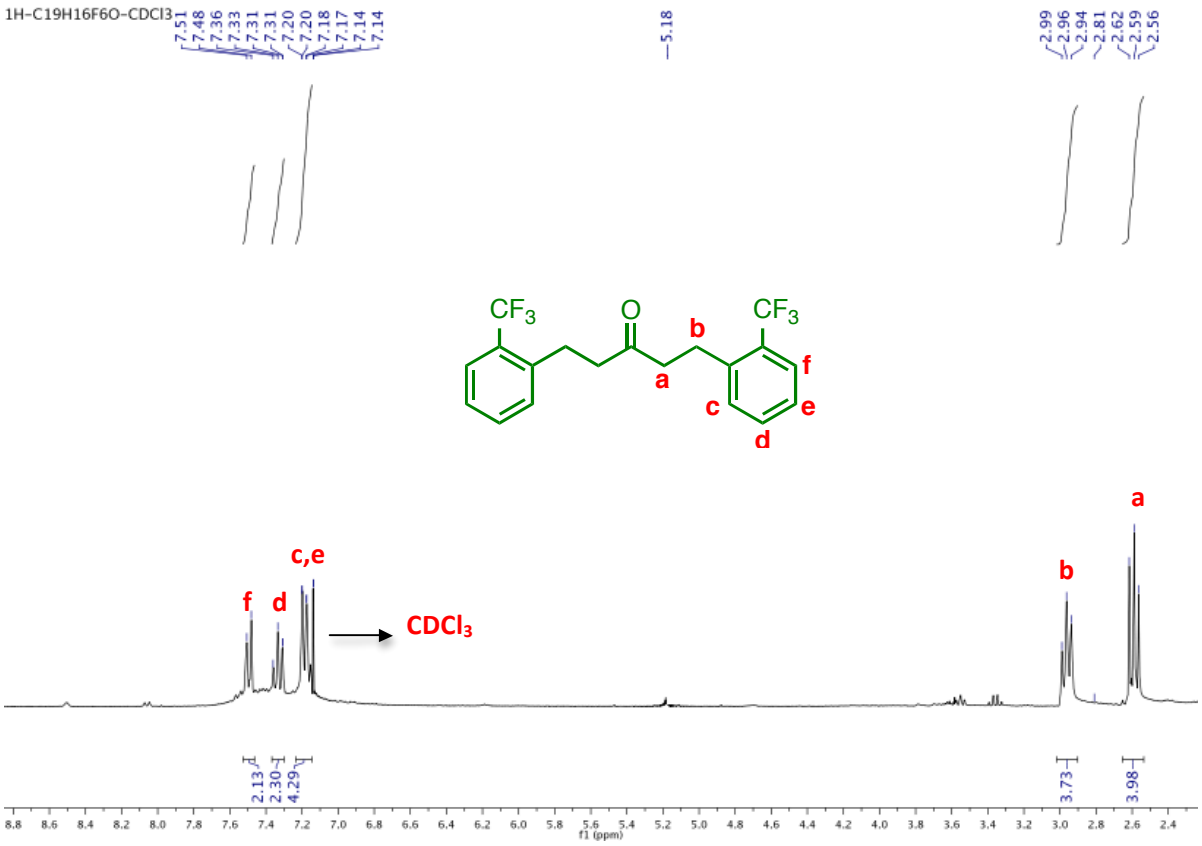


Figure S29. ^{1}H spectrum of reduction product $C_{19}H_{16}F_6O$ **4** in $CDCl_3$. (300 MHz).

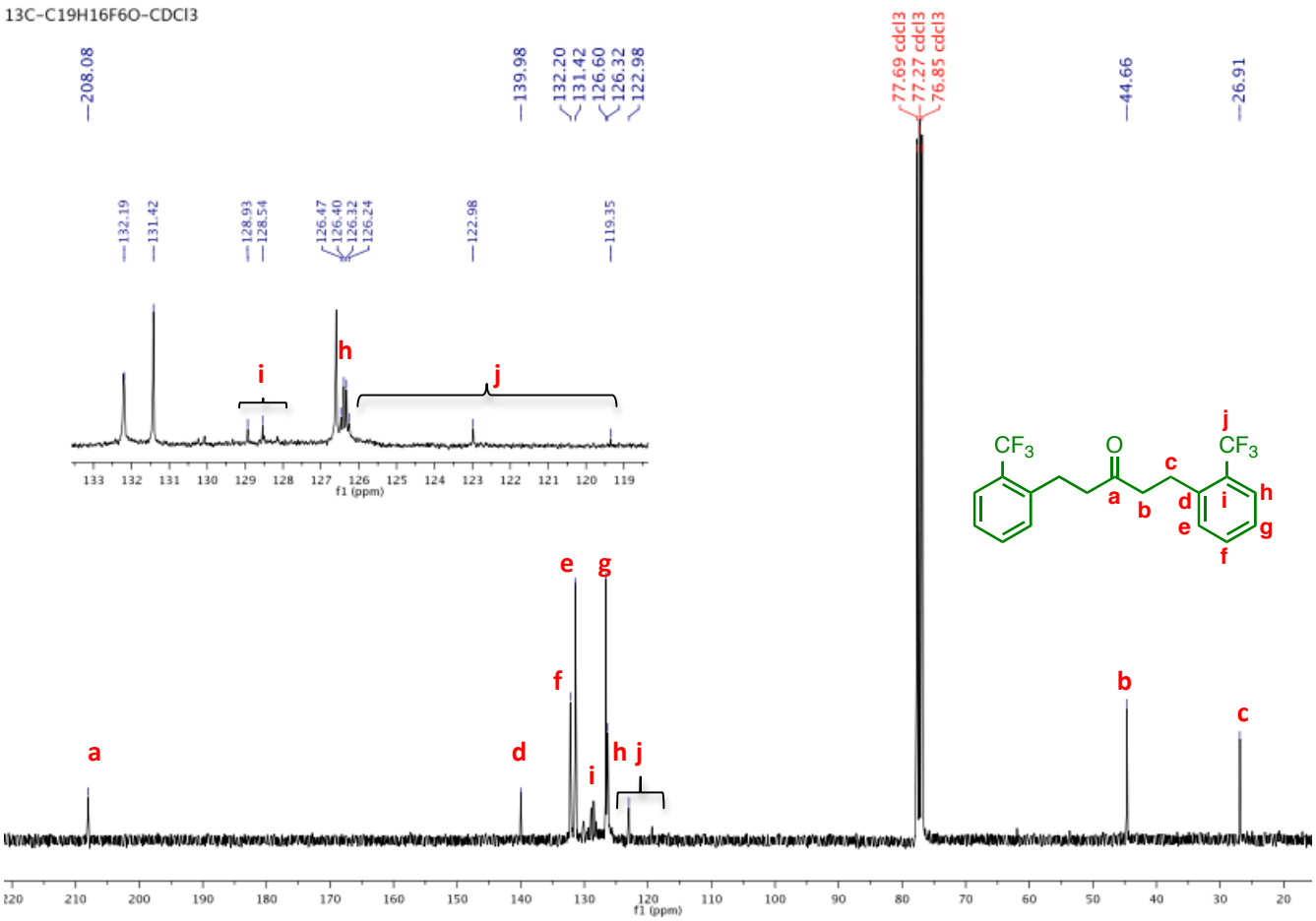


Figure S30. $^{13}C\{^{1}H\}$ spectrum of reduction product $C_{19}H_{16}F_6O$ **4** in $CDCl_3$. (300 MHz).

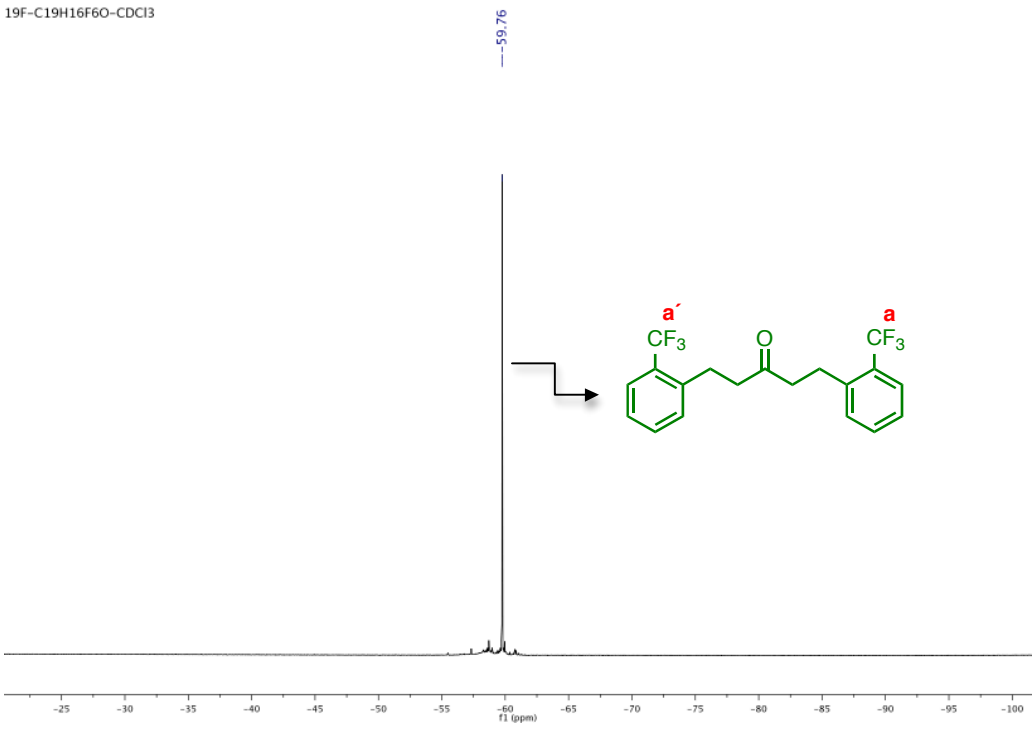
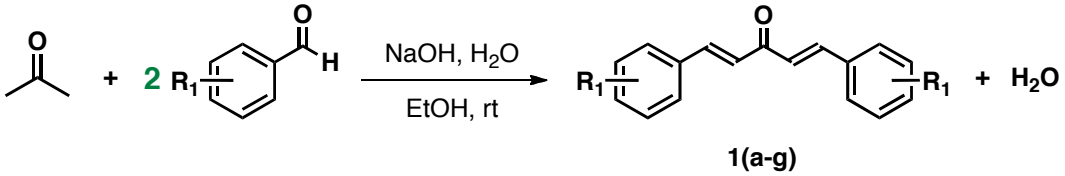


Figure S31. ^{19}F spectrum of reduction product $C_{19}H_{16}F_6O$ **4** in $CDCl_3$. (300 MHz)

Table S1. Synthesis of Dibenzalacetone Derivatives 1(a-g) [a]



1(a-g)

Entry	R_1	Yield (%) [b] 1(a-g)
1	*o*-CF_3	**1a** 84
2	*p*-F	**1b** 93
3	*o*-F	**1c** 42
4	*p*-CF_3	**1d** 85
5	*o*-CH_3	**1e** 80
6	*o*-OCH_3	**1f** 82
7	*o*-Br	**1g** 91

[a] All reactions were carried out in 95 % EtOH, (1.25 M) NaOH, **Acetone** (3.5 mmol) and **Benzaldehydes** (7 mmol) at room temperature. [b] Yields refer to isolated pure products. All products were characterized by ^{1}H, $^{13}C\{^{1}H\}$ NMR spectra and GC-MS.

Table S2. Crystal data and structure refinement for [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)], **2a**.

Identification code	shelx	
Empirical formula	C47 H76 F6 Ni2 O P4	
Formula weight	1012.38	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21 /c	
Unit cell dimensions	a = 14.9031(5) Å	α= 90°.
	b = 22.0459(6) Å	β= 98.964(3)°.
	c = 15.6218(7) Å	γ = 90°.
Volume	5069.9(3) Å^3	
Z	4	
Density (calculated)	1.326 Mg/m^3	
Absorption coefficient	0.924 mm^{-1}	
F(000)	2144	
Theta range for data collection	3.38 to 26.37°.	
Index ranges	-18<=h<=18, -21<=k<=27, -18<=l<=19	
Reflections collected	41452	
Independent reflections	10339 [R(int) = 0.0513]	
Completeness to theta = 26.37°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10339 / 0 / 557	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0345, wR2 = 0.0707	
R indices (all data)	R1 = 0.0494, wR2 = 0.0794	
Largest diff. peak and hole	0.489 and -0.510 e.Å^{-3}	

Table S3. Atomic coordinates for [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)], **2a** (x 10^4) and U(eq) (Å^2 x 10^3).

	x	y	z	U(eq)
C(1)	4989(1)	7083(1)	1340(2)	21(1)
C(2)	4918(2)	6811(1)	521(2)	28(1)
C(3)	4228(2)	6959(1)	-150(2)	39(1)
C(4)	3578(2)	7382(1)	-17(2)	47(1)
C(5)	3621(2)	7656(1)	771(2)	39(1)
C(6)	4317(1)	7515(1)	1450(2)	27(1)
C(7)	9766(1)	6024(1)	2419(2)	20(1)
C(8)	9795(1)	5917(1)	1540(2)	25(1)
C(9)	10407(2)	5520(1)	1256(2)	32(1)
C(10)	11033(2)	5217(1)	1850(2)	34(1)
C(11)	11031(2)	5314(1)	2721(2)	31(1)
C(12)	10414(1)	5708(1)	3014(2)	24(1)
C(13)	4328(2)	7838(1)	2283(2)	34(1)
C(14)	10456(2)	5784(1)	3962(2)	34(1)
C(15)	5726(1)	6907(1)	2041(2)	17(1)
C(16)	6558(1)	6648(1)	1852(2)	16(1)
C(17)	7400(1)	6689(1)	2488(2)	15(1)
C(18)	8240(1)	6557(1)	2133(2)	16(1)
C(19)	9087(1)	6438(1)	2696(2)	17(1)
C(20)	7216(1)	8265(1)	1881(2)	23(1)
C(21)	7329(2)	8334(1)	2863(2)	29(1)
C(22)	6801(2)	8834(1)	1420(2)	35(1)
C(23)	8018(1)	7961(1)	347(2)	23(1)
C(24)	7285(2)	7488(1)	63(2)	30(1)
C(25)	8879(2)	7816(1)	-28(2)	37(1)
C(26)	11321(2)	7596(1)	2261(2)	32(1)
C(27)	11205(2)	7370(1)	1327(2)	42(1)
C(28)	11754(2)	7103(1)	2879(2)	39(1)
C(29)	10532(2)	8110(1)	3692(2)	32(1)
C(30)	9749(2)	8471(1)	3966(2)	40(1)
C(31)	11410(2)	8482(1)	3884(2)	45(1)
C(32)	10016(2)	8554(1)	1923(2)	28(1)
C(33)	9006(1)	8709(1)	1710(2)	26(1)

C(34)	3586(1)	5491(1)	2202(2)	25(1)
C(35)	3205(2)	6037(1)	1665(2)	36(1)
C(36)	3691(2)	4958(1)	1608(2)	35(1)
C(37)	4305(1)	6153(1)	3771(2)	23(1)
C(38)	3662(2)	5827(1)	4295(2)	38(1)
C(39)	5139(2)	6393(1)	4370(2)	32(1)
C(40)	6775(2)	4732(1)	1548(2)	24(1)
C(41)	5952(2)	4675(1)	841(2)	36(1)
C(42)	7551(2)	5040(1)	1179(2)	31(1)
C(43)	7555(1)	5160(1)	3278(2)	20(1)
C(44)	7390(2)	5427(1)	4141(2)	24(1)
C(45)	8024(2)	4540(1)	3412(2)	33(1)
C(46)	5731(2)	4639(1)	2972(2)	24(1)
C(47)	5078(2)	4991(1)	3457(2)	23(1)
O(7)	7397(1)	6822(1)	3254(1)	20(1)
Ni(1)	9022(1)	7282(1)	2233(1)	16(1)
Ni(2)	5801(1)	6025(1)	2301(1)	15(1)
P(1)	8288(1)	8019(1)	1535(1)	18(1)
P(2)	10221(1)	7841(1)	2558(1)	22(1)
P(3)	4675(1)	5700(1)	2888(1)	19(1)
P(4)	6487(1)	5162(1)	2488(1)	18(1)
F(1)	4318(1)	7464(1)	2963(1)	41(1)
F(2)	5062(1)	8195(1)	2500(1)	39(1)
F(3)	3606(1)	8207(1)	2291(1)	49(1)
F(4)	11133(1)	5461(1)	4422(1)	57(1)
F(5)	10600(1)	6361(1)	4236(1)	40(1)
F(6)	9696(1)	5609(1)	4259(1)	45(1)

Table S4. Bond lengths [Å] and angles [º] for [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)], **2a**.

C(1)-C(2)	1.401(3)	C(16)-H(16)	1.0000
C(1)-C(6)	1.412(3)	C(17)-O(7)	1.234(3)
C(1)-C(15)	1.477(3)	C(17)-C(18)	1.475(3)
C(2)-C(3)	1.386(3)	C(18)-C(19)	1.445(3)
C(2)-H(2)	0.9500	C(18)-Ni(1)	1.9703(18)
C(3)-C(4)	1.383(4)	C(18)-H(18)	1.0000
C(3)-H(3)	0.9500	C(19)-Ni(1)	1.9933(19)
C(4)-C(5)	1.364(4)	C(19)-H(19)	1.0000
C(4)-H(4)	0.9500	C(20)-C(21)	1.525(4)
C(5)-C(6)	1.398(3)	C(20)-C(22)	1.529(3)
C(5)-H(5)	0.9500	C(20)-P(1)	1.846(2)
C(6)-C(13)	1.482(4)	C(20)-H(20)	1.0000
C(7)-C(8)	1.400(3)	C(21)-H(21A)	0.9800
C(7)-C(12)	1.415(3)	C(21)-H(21B)	0.9800
C(7)-C(19)	1.477(3)	C(21)-H(21C)	0.9800
C(8)-C(9)	1.386(3)	C(22)-H(22A)	0.9800
C(8)-H(8)	0.9500	C(22)-H(22B)	0.9800
C(9)-C(10)	1.381(4)	C(22)-H(22C)	0.9800
C(9)-H(9)	0.9500	C(23)-C(24)	1.525(3)
C(10)-C(11)	1.378(4)	C(23)-C(25)	1.525(3)
C(10)-H(10)	0.9500	C(23)-P(1)	1.841(2)
C(11)-C(12)	1.393(3)	C(23)-H(23)	1.0000
C(11)-H(11)	0.9500	C(24)-H(24A)	0.9800
C(12)-C(14)	1.483(4)	C(24)-H(24B)	0.9800
C(13)-F(1)	1.346(3)	C(24)-H(24C)	0.9800
C(13)-F(2)	1.348(3)	C(25)-H(25A)	0.9800
C(13)-F(3)	1.351(3)	C(25)-H(25B)	0.9800
C(14)-F(6)	1.345(3)	C(25)-H(25C)	0.9800
C(14)-F(4)	1.347(3)	C(26)-C(27)	1.526(4)
C(14)-F(5)	1.350(3)	C(26)-C(28)	1.529(3)
C(15)-C(16)	1.437(3)	C(26)-P(2)	1.852(2)
C(15)-Ni(2)	1.9860(19)	C(26)-H(26)	1.0000
C(15)-H(15)	1.0000	C(27)-H(27A)	0.9800
C(16)-C(17)	1.477(3)	C(27)-H(27B)	0.9800
C(16)-Ni(2)	1.9760(19)	C(27)-H(27C)	0.9800

C(28)-H(28A)	0.9800	C(38)-H(38B)	0.9800
C(28)-H(28B)	0.9800	C(38)-H(38C)	0.9800
C(28)-H(28C)	0.9800	C(39)-H(39A)	0.9800
C(29)-C(30)	1.527(4)	C(39)-H(39B)	0.9800
C(29)-C(31)	1.533(3)	C(39)-H(39C)	0.9800
C(29)-P(2)	1.858(3)	C(40)-C(41)	1.523(3)
C(29)-H(29)	1.0000	C(40)-C(42)	1.529(3)
C(30)-H(30A)	0.9800	C(40)-P(4)	1.853(2)
C(30)-H(30B)	0.9800	C(40)-H(40)	1.0000
C(30)-H(30C)	0.9800	C(41)-H(41A)	0.9800
C(31)-H(31A)	0.9800	C(41)-H(41B)	0.9800
C(31)-H(31B)	0.9800	C(41)-H(41C)	0.9800
C(31)-H(31C)	0.9800	C(42)-H(42A)	0.9800
C(32)-C(33)	1.528(3)	C(42)-H(42B)	0.9800
C(32)-P(2)	1.858(2)	C(42)-H(42C)	0.9800
C(32)-H(32A)	0.9900	C(43)-C(44)	1.526(3)
C(32)-H(32B)	0.9900	C(43)-C(45)	1.534(3)
C(33)-P(1)	1.854(2)	C(43)-P(4)	1.856(2)
C(33)-H(33A)	0.9900	C(43)-H(43)	1.0000
C(33)-H(33B)	0.9900	C(44)-H(44A)	0.9800
C(34)-C(36)	1.521(3)	C(44)-H(44B)	0.9800
C(34)-C(35)	1.525(3)	C(44)-H(44C)	0.9800
C(34)-P(3)	1.858(2)	C(45)-H(45A)	0.9800
C(34)-H(34)	1.0000	C(45)-H(45B)	0.9800
C(35)-H(35A)	0.9800	C(45)-H(45C)	0.9800
C(35)-H(35B)	0.9800	C(46)-C(47)	1.535(3)
C(35)-H(35C)	0.9800	C(46)-P(4)	1.854(2)
C(36)-H(36A)	0.9800	C(46)-H(46A)	0.9900
C(36)-H(36B)	0.9800	C(46)-H(46B)	0.9900
C(36)-H(36C)	0.9800	C(47)-P(3)	1.851(2)
C(37)-C(39)	1.529(3)	C(47)-H(47A)	0.9900
C(37)-C(38)	1.533(3)	C(47)-H(47B)	0.9900
C(37)-P(3)	1.855(2)	Ni(1)-P(1)	2.1572(6)
C(37)-H(37)	1.0000	Ni(1)-P(2)	2.1644(6)
C(38)-H(38A)	0.9800	Ni(2)-P(3)	2.1554(6)

Ni(2)-P(4)	2.1572(6)	F(1)-C(13)-F(2)	105.6(2)
C(2)-C(1)-C(6)	116.4(2)	F(1)-C(13)-F(3)	104.8(2)
C(2)-C(1)-C(15)	120.5(2)	F(2)-C(13)-F(3)	105.21(17)
C(6)-C(1)-C(15)	123.1(2)	F(1)-C(13)-C(6)	113.54(19)
C(3)-C(2)-C(1)	122.1(2)	F(2)-C(13)-C(6)	113.5(2)
C(3)-C(2)-H(2)	118.9	F(3)-C(13)-C(6)	113.4(2)
C(1)-C(2)-H(2)	118.9	F(6)-C(14)-F(4)	105.5(2)
C(4)-C(3)-C(2)	119.9(3)	F(6)-C(14)-F(5)	105.1(2)
C(4)-C(3)-H(3)	120.0	F(4)-C(14)-F(5)	105.0(2)
C(2)-C(3)-H(3)	120.0	F(6)-C(14)-C(12)	113.9(2)
C(5)-C(4)-C(3)	119.9(2)	F(4)-C(14)-C(12)	112.7(2)
C(5)-C(4)-H(4)	120.1	F(5)-C(14)-C(12)	113.8(2)
C(3)-C(4)-H(4)	120.1	C(16)-C(15)-C(1)	121.2(2)
C(4)-C(5)-C(6)	120.7(3)	C(16)-C(15)-Ni(2)	68.36(10)
C(4)-C(5)-H(5)	119.6	C(1)-C(15)-Ni(2)	114.85(14)
C(6)-C(5)-H(5)	119.6	C(16)-C(15)-H(15)	114.8
C(5)-C(6)-C(1)	120.9(3)	C(1)-C(15)-H(15)	114.8
C(5)-C(6)-C(13)	117.7(2)	Ni(2)-C(15)-H(15)	114.8
C(1)-C(6)-C(13)	121.4(2)	C(15)-C(16)-C(17)	120.5(2)
C(8)-C(7)-C(12)	116.0(2)	C(15)-C(16)-Ni(2)	69.10(11)
C(8)-C(7)-C(19)	121.24(19)	C(17)-C(16)-Ni(2)	106.00(14)
C(12)-C(7)-C(19)	122.7(2)	C(15)-C(16)-H(16)	116.9
C(9)-C(8)-C(7)	122.9(2)	C(17)-C(16)-H(16)	116.9
C(9)-C(8)-H(8)	118.6	Ni(2)-C(16)-H(16)	116.9
C(7)-C(8)-H(8)	118.6	O(7)-C(17)-C(18)	122.92(18)
C(10)-C(9)-C(8)	119.9(3)	O(7)-C(17)-C(16)	122.41(19)
C(10)-C(9)-H(9)	120.0	C(18)-C(17)-C(16)	114.67(19)
C(8)-C(9)-H(9)	120.0	C(19)-C(18)-C(17)	121.3(2)
C(11)-C(10)-C(9)	119.0(2)	C(19)-C(18)-Ni(1)	69.47(11)
C(11)-C(10)-H(10)	120.5	C(17)-C(18)-Ni(1)	109.65(13)
C(9)-C(10)-H(10)	120.5	C(19)-C(18)-H(18)	115.8
C(10)-C(11)-C(12)	121.6(2)	C(17)-C(18)-H(18)	115.8
C(10)-C(11)-H(11)	119.2	Ni(1)-C(18)-H(18)	115.8
C(12)-C(11)-H(11)	119.2	C(18)-C(19)-C(7)	120.5(2)
C(11)-C(12)-C(7)	120.6(2)	C(18)-C(19)-Ni(1)	67.78(10)
C(11)-C(12)-C(14)	118.1(2)	C(7)-C(19)-Ni(1)	117.87(15)
C(7)-C(12)-C(14)	121.3(2)		

C(23)-C(25)-H(25C)	109.5	C(29)-C(31)-H(31C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(31A)-C(31)-H(31C)	109.5
H(25B)-C(25)-H(25C)	109.5	H(31B)-C(31)-H(31C)	109.5
C(27)-C(26)-C(28)	110.2(2)	C(33)-C(32)-P(2)	112.34(15)
C(27)-C(26)-P(2)	111.24(16)	C(33)-C(32)-H(32A)	109.1
C(28)-C(26)-P(2)	110.58(18)	P(2)-C(32)-H(32A)	109.1
C(27)-C(26)-H(26)	108.2	C(33)-C(32)-H(32B)	109.1
C(28)-C(26)-H(26)	108.2	P(2)-C(32)-H(32B)	109.1
P(2)-C(26)-H(26)	108.2	H(32A)-C(32)-H(32B)	107.9
C(26)-C(27)-H(27A)	109.5	C(32)-C(33)-P(1)	111.99(14)
C(26)-C(27)-H(27B)	109.5	C(32)-C(33)-H(33A)	109.2
H(27A)-C(27)-H(27B)	109.5	P(1)-C(33)-H(33A)	109.2
C(26)-C(27)-H(27C)	109.5	C(32)-C(33)-H(33B)	109.2
H(27A)-C(27)-H(27C)	109.5	P(1)-C(33)-H(33B)	109.2
H(27B)-C(27)-H(27C)	109.5	H(33A)-C(33)-H(33B)	107.9
C(26)-C(28)-H(28A)	109.5	C(36)-C(34)-C(35)	109.8(2)
C(26)-C(28)-H(28B)	109.5	C(36)-C(34)-P(3)	112.33(16)
H(28A)-C(28)-H(28B)	109.5	C(35)-C(34)-P(3)	109.85(15)
C(26)-C(28)-H(28C)	109.5	C(36)-C(34)-H(34)	108.2
H(28A)-C(28)-H(28C)	109.5	C(35)-C(34)-H(34)	108.2
H(28B)-C(28)-H(28C)	109.5	P(3)-C(34)-H(34)	108.2
C(30)-C(29)-C(31)	109.4(2)	C(34)-C(35)-H(35A)	109.5
C(30)-C(29)-P(2)	110.30(17)	C(34)-C(35)-H(35B)	109.5
C(31)-C(29)-P(2)	115.8(2)	H(35A)-C(35)-H(35B)	109.5
C(30)-C(29)-H(29)	107.0	C(34)-C(35)-H(35C)	109.5
C(31)-C(29)-H(29)	107.0	H(35A)-C(35)-H(35C)	109.5
P(2)-C(29)-H(29)	107.0	H(35B)-C(35)-H(35C)	109.5
C(29)-C(30)-H(30A)	109.5	C(34)-C(36)-H(36A)	109.5
C(29)-C(30)-H(30B)	109.5	C(34)-C(36)-H(36B)	109.5
H(30A)-C(30)-H(30B)	109.5	H(36A)-C(36)-H(36B)	109.5
C(29)-C(30)-H(30C)	109.5	C(34)-C(36)-H(36C)	109.5
H(30A)-C(30)-H(30C)	109.5	H(36A)-C(36)-H(36C)	109.5
H(30B)-C(30)-H(30C)	109.5	H(36B)-C(36)-H(36C)	109.5
C(29)-C(31)-H(31A)	109.5	C(39)-C(37)-C(38)	110.7(2)
C(29)-C(31)-H(31B)	109.5	C(39)-C(37)-P(3)	109.44(15)
H(31A)-C(31)-H(31B)	109.5	C(38)-C(37)-P(3)	115.31(16)

C(39)-C(37)-H(37)	107.0	C(44)-C(43)-H(43)	106.8
C(38)-C(37)-H(37)	107.0	C(45)-C(43)-H(43)	106.8
P(3)-C(37)-H(37)	107.0	P(4)-C(43)-H(43)	106.8
C(37)-C(38)-H(38A)	109.5	C(43)-C(44)-H(44A)	109.5
C(37)-C(38)-H(38B)	109.5	C(43)-C(44)-H(44B)	109.5
H(38A)-C(38)-H(38B)	109.5	H(44A)-C(44)-H(44B)	109.5
C(37)-C(38)-H(38C)	109.5	C(43)-C(44)-H(44C)	109.5
H(38A)-C(38)-H(38C)	109.5	H(44A)-C(44)-H(44C)	109.5
H(38B)-C(38)-H(38C)	109.5	H(44B)-C(44)-H(44C)	109.5
C(37)-C(39)-H(39A)	109.5	C(43)-C(45)-H(45A)	109.5
C(37)-C(39)-H(39B)	109.5	C(43)-C(45)-H(45B)	109.5
H(39A)-C(39)-H(39B)	109.5	H(45A)-C(45)-H(45B)	109.5
C(37)-C(39)-H(39C)	109.5	C(43)-C(45)-H(45C)	109.5
H(39A)-C(39)-H(39C)	109.5	H(45A)-C(45)-H(45C)	109.5
H(39B)-C(39)-H(39C)	109.5	H(45B)-C(45)-H(45C)	109.5
C(41)-C(40)-C(42)	109.6(2)	C(47)-C(46)-P(4)	111.06(14)
C(41)-C(40)-P(4)	110.91(16)	C(47)-C(46)-H(46A)	109.4
C(42)-C(40)-P(4)	110.69(15)	P(4)-C(46)-H(46A)	109.4
C(41)-C(40)-H(40)	108.5	C(47)-C(46)-H(46B)	109.4
C(42)-C(40)-H(40)	108.5	P(4)-C(46)-H(46B)	109.4
P(4)-C(40)-H(40)	108.5	H(46A)-C(46)-H(46B)	108.0
C(40)-C(41)-H(41A)	109.5	C(46)-C(47)-P(3)	111.92(16)
C(40)-C(41)-H(41B)	109.5	C(46)-C(47)-H(47A)	109.2
H(41A)-C(41)-H(41B)	109.5	P(3)-C(47)-H(47A)	109.2
C(40)-C(41)-H(41C)	109.5	C(46)-C(47)-H(47B)	109.2
H(41A)-C(41)-H(41C)	109.5	P(3)-C(47)-H(47B)	109.2
H(41B)-C(41)-H(41C)	109.5	H(47A)-C(47)-H(47B)	107.9
C(40)-C(42)-H(42A)	109.5	C(18)-Ni(1)-C(19)	42.75(8)
C(40)-C(42)-H(42B)	109.5	C(18)-Ni(1)-P(1)	108.93(6)
H(42A)-C(42)-H(42B)	109.5	C(19)-Ni(1)-P(1)	151.48(6)
C(40)-C(42)-H(42C)	109.5	C(18)-Ni(1)-P(2)	159.50(6)
H(42A)-C(42)-H(42C)	109.5	C(19)-Ni(1)-P(2)	117.02(6)
H(42B)-C(42)-H(42C)	109.5	P(1)-Ni(1)-P(2)	91.44(2)
C(44)-C(43)-C(45)	110.90(19)	C(16)-Ni(2)-C(15)	42.54(8)
C(44)-C(43)-P(4)	110.26(14)	C(16)-Ni(2)-P(3)	155.18(6)
C(45)-C(43)-P(4)	114.73(15)		

C(15)-Ni(2)-P(3)	112.91(6)
C(16)-Ni(2)-P(4)	112.08(6)
C(15)-Ni(2)-P(4)	154.27(6)
P(3)-Ni(2)-P(4)	91.96(2)
C(23)-P(1)-C(20)	104.63(11)
C(23)-P(1)-C(33)	103.68(11)
C(20)-P(1)-C(33)	102.85(10)
C(23)-P(1)-Ni(1)	118.08(7)
C(20)-P(1)-Ni(1)	117.79(8)
C(33)-P(1)-Ni(1)	107.91(7)
C(26)-P(2)-C(29)	103.52(12)
C(26)-P(2)-C(32)	100.99(11)
C(29)-P(2)-C(32)	103.56(11)
C(26)-P(2)-Ni(1)	120.40(8)
C(29)-P(2)-Ni(1)	118.68(8)
C(32)-P(2)-Ni(1)	107.12(7)
C(47)-P(3)-C(37)	102.09(11)
C(47)-P(3)-C(34)	104.87(10)
C(37)-P(3)-C(34)	103.16(10)
C(47)-P(3)-Ni(2)	105.61(7)
C(37)-P(3)-Ni(2)	118.65(7)
C(34)-P(3)-Ni(2)	120.27(8)
C(40)-P(4)-C(46)	103.58(10)
C(40)-P(4)-C(43)	104.18(10)
C(46)-P(4)-C(43)	103.83(10)
C(40)-P(4)-Ni(2)	120.52(8)
C(46)-P(4)-Ni(2)	107.32(7)
C(43)-P(4)-Ni(2)	115.61(7)

Table S5. Anisotropic displacement parameters ($Å^2$ x 10^3) for [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)], **2a**.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	13(1)	17(1)	32(2)	10(1)	1(1)	-4(1)
C(2)	21(1)	28(1)	32(2)	7(1)	-1(1)	-3(1)
C(3)	35(2)	42(2)	37(2)	13(1)	-9(1)	-14(1)
C(4)	25(1)	44(2)	65(2)	29(2)	-19(1)	-7(1)
C(5)	16(1)	32(1)	67(2)	21(1)	-2(1)	0(1)
C(6)	13(1)	19(1)	49(2)	13(1)	3(1)	-3(1)
C(7)	15(1)	14(1)	30(1)	3(1)	3(1)	-2(1)
C(8)	17(1)	23(1)	35(2)	1(1)	3(1)	2(1)
C(9)	22(1)	30(1)	47(2)	-9(1)	12(1)	-2(1)
C(10)	20(1)	20(1)	65(2)	-3(1)	15(1)	4(1)
C(11)	18(1)	18(1)	57(2)	7(1)	3(1)	3(1)
C(12)	15(1)	18(1)	37(2)	7(1)	1(1)	-1(1)
C(13)	19(1)	18(1)	68(2)	9(1)	16(1)	4(1)
C(14)	20(1)	37(1)	43(2)	16(1)	-4(1)	7(1)
C(15)	15(1)	12(1)	25(1)	2(1)	2(1)	-1(1)
C(16)	16(1)	14(1)	18(1)	2(1)	2(1)	-2(1)
C(17)	17(1)	7(1)	20(1)	3(1)	1(1)	-2(1)
C(18)	14(1)	12(1)	22(1)	3(1)	2(1)	-2(1)
C(19)	14(1)	15(1)	23(1)	5(1)	4(1)	0(1)
C(20)	18(1)	16(1)	35(2)	2(1)	3(1)	2(1)
C(21)	27(1)	25(1)	37(2)	-2(1)	9(1)	4(1)
C(22)	28(1)	27(1)	50(2)	6(1)	2(1)	11(1)
C(23)	22(1)	23(1)	25(1)	10(1)	1(1)	0(1)
C(24)	33(1)	35(1)	22(2)	5(1)	1(1)	-6(1)
C(25)	30(1)	52(2)	29(2)	5(1)	6(1)	2(1)
C(26)	12(1)	31(1)	53(2)	5(1)	5(1)	-4(1)
C(27)	26(1)	44(2)	58(2)	2(1)	16(1)	2(1)
C(28)	16(1)	35(1)	64(2)	2(1)	-1(1)	0(1)
C(29)	30(1)	27(1)	35(2)	2(1)	-4(1)	-6(1)
C(30)	44(2)	39(2)	37(2)	-5(1)	2(1)	-2(1)
C(31)	38(2)	38(2)	53(2)	-4(1)	-13(1)	-13(1)
C(32)	22(1)	21(1)	39(2)	6(1)	3(1)	-7(1)
C(33)	24(1)	15(1)	36(2)	7(1)	1(1)	-2(1)
C(34)	15(1)	29(1)	30(2)	4(1)	2(1)	-5(1)

C(35)	21(1)	35(1)	47(2)	8(1)	-6(1)	-2(1)
C(36)	26(1)	34(1)	42(2)	-3(1)	-6(1)	-6(1)
C(37)	18(1)	24(1)	29(2)	2(1)	6(1)	1(1)
C(38)	36(1)	40(1)	41(2)	4(1)	21(1)	-1(1)
C(39)	30(1)	34(1)	32(2)	-6(1)	4(1)	3(1)
C(40)	27(1)	16(1)	28(2)	-3(1)	2(1)	2(1)
C(41)	38(2)	36(1)	32(2)	-14(1)	1(1)	1(1)
C(42)	36(1)	28(1)	31(2)	-5(1)	11(1)	2(1)
C(43)	20(1)	15(1)	24(1)	1(1)	0(1)	2(1)
C(44)	23(1)	24(1)	25(1)	-1(1)	0(1)	1(1)
C(45)	31(1)	27(1)	38(2)	-1(1)	-4(1)	12(1)
C(46)	25(1)	13(1)	32(2)	4(1)	0(1)	-1(1)
C(47)	22(1)	19(1)	29(2)	9(1)	5(1)	-3(1)
O(7)	19(1)	21(1)	20(1)	-2(1)	1(1)	1(1)
Ni(1)	12(1)	14(1)	22(1)	2(1)	1(1)	0(1)
Ni(2)	13(1)	12(1)	19(1)	2(1)	2(1)	0(1)
P(1)	15(1)	14(1)	24(1)	4(1)	2(1)	0(1)
P(2)	14(1)	20(1)	32(1)	3(1)	0(1)	-3(1)
P(3)	14(1)	17(1)	24(1)	4(1)	3(1)	-2(1)
P(4)	18(1)	12(1)	22(1)	0(1)	1(1)	1(1)
F(1)	48(1)	24(1)	55(1)	4(1)	26(1)	7(1)
F(2)	22(1)	26(1)	71(1)	-6(1)	12(1)	-2(1)
F(3)	24(1)	27(1)	99(2)	5(1)	20(1)	12(1)
F(4)	41(1)	75(1)	51(1)	23(1)	-7(1)	30(1)
F(5)	30(1)	49(1)	38(1)	-3(1)	-1(1)	-2(1)
F(6)	31(1)	57(1)	46(1)	25(1)	9(1)	1(1)

Table S6. Crystal data and structure refinement for [(dippe)Ni(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)], **3a**.

Identification code	shelx	
Empirical formula	C33 H44 F6 Ni O P2	
Formula weight	691.33	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 14.9903(5) Å	α= 90°.
	b = 17.0446(8) Å	β= 90°.
	c = 26.6128(15) Å	γ = 90°.
Volume	6799.6(5) $Å^3$	
Z	8	
Density (calculated)	1.351 Mg/m^3	
Absorption coefficient	0.722 mm^{-1}	
F(000)	2896	
Crystal size	0.3707 0.2217 0.0944 mm^3	
Theta range for data collection	3.35 to 25.68°.	
Index ranges	-15<=h<=18, -20<=k<=20, -32<=l<=18	
Reflections collected	30385	
Independent reflections	6446 [R(int) = 0.0711]	
Completeness to theta = 25.68°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6446 / 60 / 396	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0595, wR2 = 0.1374	
R indices (all data)	R1 = 0.0993, wR2 = 0.1651	
Largest diff. peak and hole	1.045 and -0.697 e.$Å^{-3}$	

Table S7. Atomic coordinates for [(dippe)Ni(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)], **3a** (x 10^4) and U(eq) ($Å^2$ x 10^3).

	x	y	z	U(eq)
C(1)	7760(4)	6681(3)	985(3)	76(2)
C(2)	6773(3)	6676(3)	1153(3)	72(2)
C(3)	6544(11)	6493(10)	2155(6)	78(2)
C(4)	6123(8)	6099(8)	2553(5)	78(2)
C(5)	7470(8)	6839(9)	2269(5)	78(2)
C(3A)	6724(13)	6252(12)	2294(7)	78(2)
C(4A)	6534(10)	5764(10)	2711(6)	78(2)
C(5A)	7734(10)	6415(11)	2366(7)	78(2)
C(6)	5334(3)	5689(3)	1524(2)	59(2)
C(7)	5164(3)	5244(4)	1040(3)	86(2)
C(8)	4731(4)	6417(3)	1552(3)	101(3)
C(9)	8047(3)	5499(3)	208(2)	50(1)
C(10)	7056(3)	5418(3)	63(2)	71(2)
C(11)	8514(4)	6097(3)	-130(2)	71(2)
C(12)	9382(3)	5798(4)	979(2)	64(2)
C(13)	9594(4)	5955(6)	1532(3)	119(3)
C(14)	9899(3)	5083(4)	798(3)	82(2)
C(15)	6584(3)	3827(3)	2743(2)	46(1)
C(16)	6765(3)	3852(4)	3254(2)	73(2)
C(17)	7588(3)	4082(5)	3426(2)	101(3)
C(18)	8243(3)	4270(5)	3082(2)	99(3)
C(19)	8072(3)	4243(4)	2580(2)	68(2)
C(20)	7236(2)	4019(3)	2388(2)	44(1)
C(21)	7087(2)	4001(3)	1839(2)	39(1)
C(22)	7781(2)	3823(3)	1494(2)	38(1)
C(23)	7554(2)	3701(3)	974(2)	36(1)
C(24)	8287(3)	3459(3)	626(2)	42(1)
C(25)	8108(3)	3220(3)	162(2)	41(1)
C(26)	8724(3)	2849(3)	-192(2)	45(1)
C(27)	9515(3)	2501(3)	-27(2)	51(1)
C(28)	10079(3)	2114(3)	-356(2)	60(1)
C(29)	9869(3)	2059(4)	-859(2)	71(2)
C(30)	9100(3)	2403(3)	-1034(2)	66(2)
C(31)	8524(3)	2791(3)	-707(2)	53(1)

C(32)	7701(3)	3154(4)	-915(2)	59(1)
C(33)	5673(3)	3572(3)	2582(2)	49(1)
O(1)	6771(2)	3740(2)	811(1)	48(1)
Ni(1)	7432(1)	4938(1)	1411(1)	39(1)
P(1)	8168(1)	5675(1)	889(1)	48(1)
P(2)	6544(1)	5886(1)	1602(1)	55(1)
F(1)	7636(2)	3923(2)	-815(1)	75(1)
F(2)	6946(2)	2835(2)	-739(1)	66(1)
F(3)	7637(2)	3092(3)	-1417(1)	99(1)
F(4)	5249(1)	4119(2)	2307(1)	55(1)
F(5)	5664(2)	2920(2)	2296(1)	70(1)
F(6)	5126(2)	3417(2)	2972(1)	67(1)

Table S8. Bond lengths [Å] and angles [º] for [(dippe)Ni(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)], **3a**.

C(1)-C(2)	1.544(7)	C(8)-H(8B)	0.9800
C(1)-P(1)	1.838(6)	C(8)-H(8C)	0.9800
C(1)-H(1A)	0.9900	C(9)-C(11)	1.529(7)
C(1)-H(1B)	0.9900	C(9)-C(10)	1.541(7)
C(2)-P(2)	1.832(6)	C(9)-P(1)	1.847(5)
C(2)-H(2A)	0.9900	C(9)-H(9)	1.0000
C(2)-H(2B)	0.9900	C(10)-H(10A)	0.9800
C(3)-C(4)	1.403(17)	C(10)-H(10B)	0.9800
C(3)-C(5)	1.539(17)	C(10)-H(10C)	0.9800
C(3)-P(2)	1.799(17)	C(11)-H(11A)	0.9800
C(3)-H(3)	1.0000	C(11)-H(11B)	0.9800
C(4)-H(4A)	0.9800	C(11)-H(11C)	0.9800
C(4)-H(4B)	0.9800	C(12)-C(14)	1.522(8)
C(4)-H(4C)	0.9800	C(12)-C(13)	1.530(8)
C(5)-H(5A)	0.9800	C(12)-P(1)	1.847(4)
C(5)-H(5B)	0.9800	C(12)-H(12)	1.0000
C(5)-H(5C)	0.9800	C(13)-H(13A)	0.9800
C(3A)-C(4A)	1.42(2)	C(13)-H(13B)	0.9800
C(3A)-C(5A)	1.55(2)	C(13)-H(13C)	0.9800
C(3A)-P(2)	1.96(2)	C(14)-H(14A)	0.9800
C(3A)-H(3A)	1.0000	C(14)-H(14B)	0.9800
C(4A)-H(4A1)	0.9800	C(14)-H(14C)	0.9800
C(4A)-H(4A2)	0.9800	C(15)-C(16)	1.388(7)
C(4A)-H(4A3)	0.9800	C(15)-C(20)	1.397(6)
C(5A)-H(5A1)	0.9800	C(15)-C(33)	1.495(6)
C(5A)-H(5A2)	0.9800	C(16)-C(17)	1.374(8)
C(5A)-H(5A3)	0.9800	C(16)-H(16)	0.9500
C(6)-C(7)	1.517(8)	C(17)-C(18)	1.382(8)
C(6)-C(8)	1.537(7)	C(17)-H(17)	0.9500
C(6)-P(2)	1.857(5)	C(18)-C(19)	1.360(7)
C(6)-H(6)	1.0000	C(18)-H(18)	0.9500
C(7)-H(7A)	0.9800	C(19)-C(20)	1.406(6)
C(7)-H(7B)	0.9800	C(19)-H(19)	0.9500
C(7)-H(7C)	0.9800	C(20)-C(21)	1.480(6)
C(8)-H(8A)	0.9800	C(21)-C(22)	1.421(5)

C(21)-Ni(1)	2.027(4)	P(1)-C(1)-H(1B)	109.5
C(21)-H(21)	0.9500	H(1A)-C(1)-H(1B)	108.1
C(22)-C(23)	1.439(6)	C(1)-C(2)-P(2)	111.9(4)
C(22)-Ni(1)	1.984(4)	C(1)-C(2)-H(2A)	109.2
C(22)-H(22)	0.9500	P(2)-C(2)-H(2A)	109.2
C(23)-O(1)	1.253(4)	C(1)-C(2)-H(2B)	109.2
C(23)-C(24)	1.495(5)	P(2)-C(2)-H(2B)	109.2
C(23)-Ni(1)	2.414(4)	H(2A)-C(2)-H(2B)	107.9
C(24)-C(25)	1.330(6)	C(4)-C(3)-C(5)	116.1(12)
C(24)-H(24)	0.9500	C(4)-C(3)-P(2)	110.0(10)
C(25)-C(26)	1.463(6)	C(5)-C(3)-P(2)	112.4(10)
C(25)-H(25)	0.9500	C(4)-C(3)-H(3)	105.8
C(26)-C(27)	1.396(6)	C(5)-C(3)-H(3)	105.8
C(26)-C(31)	1.406(6)	P(2)-C(3)-H(3)	105.8
C(27)-C(28)	1.384(6)	C(4A)-C(3A)-C(5A)	101.8(13)
C(27)-H(27)	0.9500	C(4A)-C(3A)-P(2)	121.4(13)
C(28)-C(29)	1.378(8)	C(5A)-C(3A)-P(2)	107.9(11)
C(28)-H(28)	0.9500	C(4A)-C(3A)-H(3A)	108.4
C(29)-C(30)	1.374(8)	C(5A)-C(3A)-H(3A)	108.4
C(29)-H(29)	0.9500	P(2)-C(3A)-H(3A)	108.4
C(30)-C(31)	1.393(6)	C(3A)-C(4A)-H(4A1)	109.5
C(30)-H(30)	0.9500	C(3A)-C(4A)-H(4A2)	109.5
C(31)-C(32)	1.487(7)	H(4A1)-C(4A)-H(4A2)	109.5
C(32)-F(1)	1.341(6)	C(3A)-C(4A)-H(4A3)	109.5
C(32)-F(2)	1.341(6)	H(4A1)-C(4A)-H(4A3)	109.5
C(32)-F(3)	1.342(6)	H(4A2)-C(4A)-H(4A3)	109.5
C(33)-F(4)	1.343(5)	C(3A)-C(5A)-H(5A1)	109.5
C(33)-F(5)	1.348(5)	C(3A)-C(5A)-H(5A2)	109.5
C(33)-F(6)	1.350(5)	H(5A1)-C(5A)-H(5A2)	109.5
Ni(1)-P(2)	2.1548(13)	C(3A)-C(5A)-H(5A3)	109.5
Ni(1)-P(1)	2.1743(14)	H(5A1)-C(5A)-H(5A3)	109.5
C(2)-C(1)-P(1)	110.7(3)	H(5A2)-C(5A)-H(5A3)	109.5
C(2)-C(1)-H(1A)	109.5	C(7)-C(6)-C(8)	110.3(5)
P(1)-C(1)-H(1A)	109.5	C(7)-C(6)-P(2)	110.4(3)
C(2)-C(1)-H(1B)	109.5	C(8)-C(6)-P(2)	115.0(4)
		C(7)-C(6)-H(6)	106.9

C(8)-C(6)-H(6)	106.9	C(13)-C(12)-H(12)	108.3
P(2)-C(6)-H(6)	106.9	P(1)-C(12)-H(12)	108.3
C(6)-C(7)-H(7A)	109.5	C(12)-C(13)-H(13A)	109.5
C(6)-C(7)-H(7B)	109.5	C(12)-C(13)-H(13B)	109.5
H(7A)-C(7)-H(7B)	109.5	H(13A)-C(13)-H(13B)	109.5
C(6)-C(7)-H(7C)	109.5	C(12)-C(13)-H(13C)	109.5
H(7A)-C(7)-H(7C)	109.5	H(13A)-C(13)-H(13C)	109.5
H(7B)-C(7)-H(7C)	109.5	H(13B)-C(13)-H(13C)	109.5
C(6)-C(8)-H(8A)	109.5	C(12)-C(14)-H(14A)	109.5
C(6)-C(8)-H(8B)	109.5	C(12)-C(14)-H(14B)	109.5
H(8A)-C(8)-H(8B)	109.5	H(14A)-C(14)-H(14B)	109.5
C(6)-C(8)-H(8C)	109.5	C(12)-C(14)-H(14C)	109.5
H(8A)-C(8)-H(8C)	109.5	H(14A)-C(14)-H(14C)	109.5
H(8B)-C(8)-H(8C)	109.5	H(14B)-C(14)-H(14C)	109.5
C(11)-C(9)-C(10)	110.7(4)	C(16)-C(15)-C(20)	121.1(4)
C(11)-C(9)-P(1)	115.1(4)	C(16)-C(15)-C(33)	117.9(4)
C(10)-C(9)-P(1)	110.8(3)	C(20)-C(15)-C(33)	121.0(4)
C(11)-C(9)-H(9)	106.6	C(17)-C(16)-C(15)	120.9(5)
C(10)-C(9)-H(9)	106.6	C(17)-C(16)-H(16)	119.6
P(1)-C(9)-H(9)	106.6	C(15)-C(16)-H(16)	119.6
C(9)-C(10)-H(10A)	109.5	C(16)-C(17)-C(18)	118.8(5)
C(9)-C(10)-H(10B)	109.5	C(16)-C(17)-H(17)	120.6
H(10A)-C(10)-H(10B)	109.5	C(18)-C(17)-H(17)	120.6
C(9)-C(10)-H(10C)	109.5	C(19)-C(18)-C(17)	120.7(5)
H(10A)-C(10)-H(10C)	109.5	C(19)-C(18)-H(18)	119.6
H(10B)-C(10)-H(10C)	109.5	C(17)-C(18)-H(18)	119.6
C(9)-C(11)-H(11A)	109.5	C(18)-C(19)-C(20)	122.2(4)
C(9)-C(11)-H(11B)	109.5	C(18)-C(19)-H(19)	118.9
H(11A)-C(11)-H(11B)	109.5	C(20)-C(19)-H(19)	118.9
C(9)-C(11)-H(11C)	109.5	C(15)-C(20)-C(19)	116.3(4)
H(11A)-C(11)-H(11C)	109.5	C(15)-C(20)-C(21)	123.8(4)
H(11B)-C(11)-H(11C)	109.5	C(19)-C(20)-C(21)	119.9(4)
C(14)-C(12)-C(13)	109.8(5)	C(22)-C(21)-C(20)	122.2(3)
C(14)-C(12)-P(1)	111.8(4)	C(22)-C(21)-Ni(1)	67.6(2)
C(13)-C(12)-P(1)	110.4(3)	C(20)-C(21)-Ni(1)	120.1(3)
C(14)-C(12)-H(12)	108.3	C(22)-C(21)-H(21)	118.9

C(20)-C(21)-H(21)	118.9	C(30)-C(31)-C(32)	118.6(5)
Ni(1)-C(21)-H(21)	82.8	C(26)-C(31)-C(32)	120.8(4)
C(21)-C(22)-C(23)	118.6(3)	F(1)-C(32)-F(2)	105.3(4)
C(21)-C(22)-Ni(1)	70.9(2)	F(1)-C(32)-F(3)	105.6(5)
C(23)-C(22)-Ni(1)	88.2(3)	F(2)-C(32)-F(3)	104.9(4)
C(21)-C(22)-H(22)	120.7	F(1)-C(32)-C(31)	113.1(4)
C(23)-C(22)-H(22)	120.7	F(2)-C(32)-C(31)	113.7(5)
Ni(1)-C(22)-H(22)	110.6	F(3)-C(32)-C(31)	113.5(4)
O(1)-C(23)-C(22)	123.1(4)	F(4)-C(33)-F(5)	105.1(4)
O(1)-C(23)-C(24)	119.3(4)	F(4)-C(33)-F(6)	105.5(3)
C(22)-C(23)-C(24)	117.4(3)	F(5)-C(33)-F(6)	105.4(4)
O(1)-C(23)-Ni(1)	92.8(3)	F(4)-C(33)-C(15)	112.7(4)
C(22)-C(23)-Ni(1)	55.2(2)	F(5)-C(33)-C(15)	114.3(4)
C(24)-C(23)-Ni(1)	126.5(3)	F(6)-C(33)-C(15)	113.0(4)
C(25)-C(24)-C(23)	120.8(4)	C(22)-Ni(1)-C(21)	41.48(16)
C(25)-C(24)-H(24)	119.6	C(22)-Ni(1)-P(2)	148.87(12)
C(23)-C(24)-H(24)	119.6	C(21)-Ni(1)-P(2)	107.52(12)
C(24)-C(25)-C(26)	127.1(4)	C(22)-Ni(1)-P(1)	119.39(12)
C(24)-C(25)-H(25)	116.5	C(21)-Ni(1)-P(1)	160.60(12)
C(26)-C(25)-H(25)	116.5	P(2)-Ni(1)-P(1)	91.72(5)
C(27)-C(26)-C(31)	117.3(4)	C(22)-Ni(1)-C(23)	36.57(15)
C(27)-C(26)-C(25)	121.2(4)	C(21)-Ni(1)-C(23)	66.57(16)
C(31)-C(26)-C(25)	121.5(4)	P(2)-Ni(1)-C(23)	144.66(10)
C(28)-C(27)-C(26)	121.4(5)	P(1)-Ni(1)-C(23)	99.14(11)
C(28)-C(27)-H(27)	119.3	C(1)-P(1)-C(9)	104.8(3)
C(26)-C(27)-H(27)	119.3	C(1)-P(1)-C(12)	101.8(3)
C(29)-C(28)-C(27)	120.5(5)	C(9)-P(1)-C(12)	104.0(2)
C(29)-C(28)-H(28)	119.8	C(1)-P(1)-Ni(1)	106.36(18)
C(27)-C(28)-H(28)	119.8	C(9)-P(1)-Ni(1)	118.91(16)
C(30)-C(29)-C(28)	119.5(5)	C(12)-P(1)-Ni(1)	118.89(19)
C(30)-C(29)-H(29)	120.3	C(3)-P(2)-C(2)	96.4(6)
C(28)-C(29)-H(29)	120.3	C(3)-P(2)-C(6)	101.2(5)
C(29)-C(30)-C(31)	120.7(5)	C(2)-P(2)-C(6)	104.1(3)
C(29)-C(30)-H(30)	119.7	C(3)-P(2)-C(3A)	18.1(8)
C(31)-C(30)-H(30)	119.7	C(2)-P(2)-C(3A)	110.7(6)
C(30)-C(31)-C(26)	120.7(4)	C(6)-P(2)-C(3A)	107.2(6)
		C(3)-P(2)-Ni(1)	128.6(6)

Table S9. Anisotropic displacement parameters ($Å^2$ x 10^3) for [(dippe)Ni(η^2-Cα,Cβ -$C_{19}H_{12}F_6O$)], **3a**.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	64(3)	59(3)	103(5)	-10(3)	43(3)	-11(3)
C(2)	60(3)	46(3)	109(5)	-2(3)	40(3)	2(3)
C(3)	66(4)	97(6)	72(5)	-19(4)	22(3)	-20(4)
C(4)	66(4)	97(6)	72(5)	-19(4)	22(3)	-20(4)
C(5)	66(4)	97(6)	72(5)	-19(4)	22(3)	-20(4)
C(3A)	66(4)	97(6)	72(5)	-19(4)	22(3)	-20(4)
C(4A)	66(4)	97(6)	72(5)	-19(4)	22(3)	-20(4)
C(5A)	66(4)	97(6)	72(5)	-19(4)	22(3)	-20(4)
C(6)	32(2)	49(3)	95(4)	12(3)	19(2)	9(2)
C(7)	35(3)	116(5)	106(6)	-11(4)	-4(3)	11(3)
C(8)	55(3)	73(4)	174(8)	31(4)	28(4)	27(3)
C(9)	49(3)	57(3)	43(3)	15(2)	3(2)	18(2)
C(10)	56(3)	85(4)	72(4)	9(3)	-14(3)	15(3)
C(11)	77(4)	75(4)	60(4)	24(3)	8(3)	14(3)
C(12)	31(2)	109(4)	52(3)	11(3)	8(2)	-11(3)
C(13)	65(4)	227(9)	65(5)	6(5)	-2(3)	-74(5)
C(14)	28(2)	121(5)	98(5)	39(4)	8(3)	8(3)
C(15)	26(2)	68(3)	43(3)	2(2)	4(2)	12(2)
C(16)	39(2)	147(6)	35(3)	9(3)	11(2)	17(3)
C(17)	42(3)	234(9)	26(3)	6(4)	0(2)	15(4)
C(18)	31(2)	232(9)	33(3)	-16(4)	-2(2)	-9(4)
C(19)	25(2)	146(5)	32(3)	-8(3)	1(2)	-1(3)
C(20)	24(2)	73(3)	36(3)	1(2)	3(2)	6(2)
C(21)	22(2)	57(3)	37(2)	-4(2)	0(2)	2(2)
C(22)	24(2)	60(3)	31(2)	-11(2)	-3(2)	1(2)
C(23)	27(2)	46(2)	37(2)	-10(2)	3(2)	-1(2)
C(24)	26(2)	59(3)	41(3)	-5(2)	1(2)	1(2)
C(25)	26(2)	61(3)	34(3)	-9(2)	1(2)	-2(2)
C(26)	29(2)	63(3)	44(3)	-13(2)	6(2)	-6(2)
C(27)	30(2)	73(3)	49(3)	-17(2)	3(2)	-3(2)
C(28)	30(2)	81(4)	69(4)	-25(3)	6(2)	-1(2)
C(29)	42(3)	100(4)	72(4)	-41(3)	15(3)	3(3)
C(30)	48(3)	106(4)	43(3)	-28(3)	7(2)	-6(3)
C(31)	37(2)	79(3)	42(3)	-15(2)	7(2)	-3(2)

C(32)	47(3)	94(4)	37(3)	-14(3)	5(2)	2(3)
C(33)	32(2)	54(3)	60(3)	6(2)	16(2)	6(2)
O(1)	25(1)	77(2)	41(2)	-19(2)	-3(1)	4(1)
Ni(1)	22(1)	58(1)	37(1)	-4(1)	3(1)	4(1)
P(1)	29(1)	65(1)	51(1)	-1(1)	9(1)	2(1)
P(2)	36(1)	56(1)	73(1)	-14(1)	21(1)	-2(1)
F(1)	68(2)	86(2)	69(2)	10(2)	-1(2)	6(2)
F(2)	37(1)	103(2)	59(2)	-7(2)	-6(1)	-2(2)
F(3)	72(2)	187(4)	37(2)	-19(2)	-3(2)	30(2)
F(4)	24(1)	68(2)	72(2)	16(2)	-1(1)	2(1)
F(5)	54(2)	67(2)	90(2)	-10(2)	13(2)	-4(2)
F(6)	42(1)	84(2)	75(2)	18(2)	24(1)	-4(1)

Table S10. Crystal data and structure refinement for [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{17}H_{12}F_2O$)], **2b**.

Identification code	shelx	
Empirical formula	C45 H76 F2 Ni2 O P4	
Formula weight	912.36	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 14.4964(8) Å	α= 90°.
	b = 15.4616(9) Å	β= 90°.
	c = 21.4898(11) Å	γ = 90°.
Volume	4816.7(5) Å^3	
Z	4	
Density (calculated)	1.258 Mg/m^3	
Absorption coefficient	0.953 mm^{-1}	
F(000)	1952	
Crystal size	0.333 x 0.0371 x 0.0303 mm^3	
Theta range for data collection	3.39 to 25.29°.	
Index ranges	-17<=h<=16, -15<=k<=18, -25<=l<=25	
Reflections collected	37408	
Independent reflections	8745 [R(int) = 0.1483]	
Completeness to theta = 25.29°	99.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8745 / 0 / 504	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0660, wR2 = 0.0879	
R indices (all data)	R1 = 0.1203, wR2 = 0.1011	
Absolute structure parameter	0.518(17)	
Largest diff. peak and hole	0.669 and -0.402 e.Å^{-3}	

Table S11. Atomic coordinates for [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{17}H_{12}F_2O$)], **2b** (x 10^4) and U(eq) (Å^2 x 10^3).

	x	y	z	U(eq)
C(1)	8659(4)	-273(4)	9234(3)	33(2)
C(2)	9477(4)	-377(4)	8913(3)	39(2)
C(3)	10062(5)	-1061(5)	9029(4)	50(2)
C(4)	9848(6)	-1645(5)	9469(4)	52(2)
C(5)	9058(6)	-1561(5)	9812(3)	57(2)
C(6)	8453(5)	-885(4)	9698(3)	47(2)
C(7)	7579(5)	4152(4)	7964(3)	34(2)
C(8)	8478(5)	4342(5)	7765(3)	46(2)
C(9)	8646(6)	5018(5)	7350(3)	57(2)
C(10)	7929(6)	5477(4)	7129(3)	50(2)
C(11)	7058(5)	5312(4)	7294(3)	46(2)
C(12)	6884(5)	4653(4)	7712(3)	41(2)
C(13)	7975(4)	418(4)	9085(3)	29(1)
C(14)	8202(4)	1224(4)	8803(3)	28(2)
C(15)	7595(4)	1955(4)	8818(2)	28(1)
C(16)	7943(4)	2770(4)	8548(3)	29(2)
C(17)	7363(4)	3490(3)	8429(2)	30(2)
C(18)	6594(5)	168(5)	6871(3)	57(2)
C(19)	6690(4)	-766(4)	7124(3)	52(2)
C(20)	5856(4)	-1058(4)	8334(4)	52(2)
C(21)	5211(4)	-285(5)	8276(3)	57(2)
C(22)	5978(4)	-1312(4)	9016(3)	52(2)
C(23)	7644(5)	-1791(4)	8053(3)	47(2)
C(24)	8562(5)	-1740(5)	7709(4)	62(2)
C(25)	7127(5)	-2618(4)	7885(4)	67(2)
C(26)	8312(5)	1122(4)	6767(3)	54(2)
C(27)	8871(5)	280(5)	6747(4)	76(3)
C(28)	8925(5)	1862(5)	6970(4)	72(2)
C(29)	6646(5)	1988(5)	7202(3)	55(2)
C(30)	5782(5)	1975(5)	7600(3)	60(2)
C(31)	6432(6)	2243(5)	6537(4)	87(3)
C(32)	8720(4)	3998(4)	10615(3)	29(2)
C(33)	8355(4)	4885(4)	10399(3)	35(2)

C(34)	10228(4)	3435(4)	9768(3)	32(2)
C(35)	10419(4)	3071(4)	9122(3)	35(2)
C(36)	10540(4)	4373(4)	9817(3)	45(2)
C(37)	8970(4)	2207(4)	10331(3)	26(2)
C(38)	7980(4)	1911(4)	10462(3)	33(2)
C(39)	9540(4)	2145(4)	10926(3)	34(2)
C(40)	6443(4)	4809(4)	9969(3)	37(2)
C(41)	6208(4)	3937(4)	10261(3)	45(2)
C(42)	5757(4)	5009(4)	9440(3)	48(2)
C(43)	7773(4)	5867(4)	9313(3)	40(2)
C(44)	8747(4)	5998(4)	9050(3)	51(2)
C(45)	7494(5)	6623(4)	9733(3)	60(2)
O(1)	6798(3)	1910(3)	9043(2)	34(1)
Ni(1)	7569(1)	445(1)	8201(1)	28(1)
Ni(2)	8038(1)	3621(1)	9221(1)	23(1)
P(1)	8987(1)	3283(1)	9956(1)	24(1)
P(2)	7642(1)	4792(1)	9680(1)	27(1)
P(3)	6971(1)	-782(1)	7965(1)	37(1)
P(4)	7317(1)	965(1)	7286(1)	39(1)
F(1)	10416(3)	-2327(3)	9581(2)	86(2)
F(2)	8127(3)	6159(2)	6736(2)	71(1)

Table S12. Bond lengths [Å] and angles [º] for [{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{17}H_{12}F_2O$)], **2b**.

C(1)-C(2)	1.381(8)	C(17)-Ni(2)	1.974(5)
C(1)-C(6)	1.406(8)	C(17)-H(17)	1.0000
C(1)-C(13)	1.492(8)	C(18)-C(19)	1.550(9)
C(2)-C(3)	1.379(8)	C(18)-P(4)	1.847(7)
C(2)-H(2)	0.9500	C(18)-H(18A)	0.9900
C(3)-C(4)	1.343(10)	C(18)-H(18B)	0.9900
C(3)-H(3)	0.9500	C(19)-P(3)	1.853(7)
C(4)-F(1)	1.360(8)	C(19)-H(19A)	0.9900
C(4)-C(5)	1.368(10)	C(19)-H(19B)	0.9900
C(5)-C(6)	1.387(9)	C(20)-C(21)	1.523(9)
C(5)-H(5)	0.9500	C(20)-C(22)	1.528(9)
C(6)-H(6)	0.9500	C(20)-P(3)	1.850(7)
C(7)-C(12)	1.382(8)	C(20)-H(20)	1.0000
C(7)-C(8)	1.403(8)	C(21)-H(21A)	0.9800
C(7)-C(17)	1.464(7)	C(21)-H(21B)	0.9800
C(8)-C(9)	1.396(9)	C(21)-H(21C)	0.9800
C(8)-H(8)	0.9500	C(22)-H(22A)	0.9800
C(9)-C(10)	1.344(9)	C(22)-H(22B)	0.9800
C(9)-H(9)	0.9500	C(22)-H(22C)	0.9800
C(10)-C(11)	1.336(9)	C(23)-C(24)	1.524(9)
C(10)-F(2)	1.382(7)	C(23)-C(25)	1.526(8)
C(11)-C(12)	1.381(8)	C(23)-P(3)	1.850(6)
C(11)-H(11)	0.9500	C(23)-H(23)	1.0000
C(12)-H(12)	0.9500	C(24)-H(24A)	0.9800
C(13)-C(14)	1.424(7)	C(24)-H(24B)	0.9800
C(13)-Ni(1)	1.988(5)	C(24)-H(24C)	0.9800
C(13)-H(13)	1.0000	C(25)-H(25A)	0.9800
C(14)-C(15)	1.434(7)	C(25)-H(25B)	0.9800
C(14)-Ni(1)	1.990(6)	C(25)-H(25C)	0.9800
C(14)-H(14)	1.0000	C(26)-C(28)	1.512(9)
C(15)-O(1)	1.255(6)	C(26)-C(27)	1.535(9)
C(15)-C(16)	1.475(7)	C(26)-P(4)	1.840(7)
C(16)-C(17)	1.419(7)	C(26)-H(26)	1.0000
C(16)-Ni(2)	1.958(6)	C(27)-H(27A)	0.9800
C(16)-H(16)	1.0000	C(27)-H(27B)	0.9800

C(27)-H(27C)	0.9800	C(38)-H(38B)	0.9800
C(28)-H(28A)	0.9800	C(38)-H(38C)	0.9800
C(28)-H(28B)	0.9800	C(39)-H(39A)	0.9800
C(28)-H(28C)	0.9800	C(39)-H(39B)	0.9800
C(29)-C(30)	1.516(9)	C(39)-H(39C)	0.9800
C(29)-C(31)	1.517(9)	C(40)-C(41)	1.526(8)
C(29)-P(4)	1.866(7)	C(40)-C(42)	1.543(8)
C(29)-H(29)	1.0000	C(40)-P(2)	1.846(6)
C(30)-H(30A)	0.9800	C(40)-H(40)	1.0000
C(30)-H(30B)	0.9800	C(41)-H(41A)	0.9800
C(30)-H(30C)	0.9800	C(41)-H(41B)	0.9800
C(31)-H(31A)	0.9800	C(41)-H(41C)	0.9800
C(31)-H(31B)	0.9800	C(42)-H(42A)	0.9800
C(31)-H(31C)	0.9800	C(42)-H(42B)	0.9800
C(32)-C(33)	1.542(7)	C(42)-H(42C)	0.9800
C(32)-P(1)	1.838(6)	C(43)-C(45)	1.532(8)
C(32)-H(32A)	0.9900	C(43)-C(44)	1.535(8)
C(32)-H(32B)	0.9900	C(43)-P(2)	1.849(6)
C(33)-P(2)	1.865(6)	C(43)-H(43)	1.0000
C(33)-H(33A)	0.9900	C(44)-H(44A)	0.9800
C(33)-H(33B)	0.9900	C(44)-H(44B)	0.9800
C(34)-C(36)	1.523(8)	C(44)-H(44C)	0.9800
C(34)-C(35)	1.525(8)	C(45)-H(45A)	0.9800
C(34)-P(1)	1.860(6)	C(45)-H(45B)	0.9800
C(34)-H(34)	1.0000	C(45)-H(45C)	0.9800
C(35)-H(35A)	0.9800	Ni(1)-P(3)	2.1461(17)
C(35)-H(35B)	0.9800	Ni(1)-P(4)	2.1558(18)
C(35)-H(35C)	0.9800	Ni(2)-P(2)	2.1417(16)
C(36)-H(36A)	0.9800	Ni(2)-P(1)	2.1582(17)
C(36)-H(36B)	0.9800	C(2)-C(1)-C(6)	117.2(6)
C(36)-H(36C)	0.9800	C(2)-C(1)-C(13)	123.1(6)
C(37)-C(39)	1.526(7)	C(6)-C(1)-C(13)	119.6(6)
C(37)-C(38)	1.532(8)	C(3)-C(2)-C(1)	121.8(7)
C(37)-P(1)	1.849(5)	C(3)-C(2)-H(2)	119.1
C(37)-H(37)	1.0000	C(1)-C(2)-H(2)	119.1
C(38)-H(38A)	0.9800	C(4)-C(3)-C(2)	120.0(7)

C(4)-C(3)-H(3)	120.0	C(13)-C(14)-Ni(1)	68.9(3)
C(2)-C(3)-H(3)	120.0	C(15)-C(14)-Ni(1)	102.1(4)
C(3)-C(4)-F(1)	120.4(8)	C(13)-C(14)-H(14)	117.0
C(3)-C(4)-C(5)	120.6(7)	C(15)-C(14)-H(14)	117.0
F(1)-C(4)-C(5)	119.0(8)	Ni(1)-C(14)-H(14)	117.0
C(4)-C(5)-C(6)	120.3(7)	O(1)-C(15)-C(14)	122.0(5)
C(4)-C(5)-H(5)	119.8	O(1)-C(15)-C(16)	121.0(6)
C(6)-C(5)-H(5)	119.8	C(14)-C(15)-C(16)	117.1(5)
C(5)-C(6)-C(1)	119.9(7)	C(17)-C(16)-C(15)	122.6(5)
C(5)-C(6)-H(6)	120.0	C(17)-C(16)-Ni(2)	69.4(3)
C(1)-C(6)-H(6)	120.0	C(15)-C(16)-Ni(2)	107.9(4)
C(12)-C(7)-C(8)	116.1(6)	C(17)-C(16)-H(16)	115.8
C(12)-C(7)-C(17)	120.2(6)	C(15)-C(16)-H(16)	115.8
C(8)-C(7)-C(17)	123.6(6)	Ni(2)-C(16)-H(16)	115.8
C(9)-C(8)-C(7)	120.9(6)	C(16)-C(17)-C(7)	123.1(5)
C(9)-C(8)-H(8)	119.5	C(16)-C(17)-Ni(2)	68.3(3)
C(7)-C(8)-H(8)	119.5	C(7)-C(17)-Ni(2)	114.2(4)
C(10)-C(9)-C(8)	119.0(7)	C(16)-C(17)-H(17)	114.4
C(10)-C(9)-H(9)	120.5	C(7)-C(17)-H(17)	114.4
C(8)-C(9)-H(9)	120.5	Ni(2)-C(17)-H(17)	114.4
C(11)-C(10)-C(9)	122.5(7)	C(19)-C(18)-P(4)	113.7(5)
C(11)-C(10)-F(2)	120.2(7)	C(19)-C(18)-H(18A)	108.8
C(9)-C(10)-F(2)	117.2(7)	P(4)-C(18)-H(18A)	108.8
C(10)-C(11)-C(12)	119.0(7)	C(19)-C(18)-H(18B)	108.8
C(10)-C(11)-H(11)	120.5	P(4)-C(18)-H(18B)	108.8
C(12)-C(11)-H(11)	120.5	H(18A)-C(18)-H(18B)	107.7
C(11)-C(12)-C(7)	122.4(6)	C(18)-C(19)-P(3)	112.0(4)
C(11)-C(12)-H(12)	118.8	C(18)-C(19)-H(19A)	109.2
C(7)-C(12)-H(12)	118.8	P(3)-C(19)-H(19A)	109.2
C(14)-C(13)-C(1)	124.4(5)	C(18)-C(19)-H(19B)	109.2
C(14)-C(13)-Ni(1)	69.1(3)	P(3)-C(19)-H(19B)	109.2
C(1)-C(13)-Ni(1)	114.7(4)	H(19A)-C(19)-H(19B)	107.9
C(14)-C(13)-H(13)	113.6	C(21)-C(20)-C(22)	110.6(6)
C(1)-C(13)-H(13)	113.6	C(21)-C(20)-P(3)	108.7(5)
Ni(1)-C(13)-H(13)	113.6	C(22)-C(20)-P(3)	111.6(5)
C(13)-C(14)-C(15)	122.6(5)	C(21)-C(20)-H(20)	108.6

C(22)-C(20)-H(20)	108.6	C(27)-C(26)-H(26)	108.5
P(3)-C(20)-H(20)	108.6	P(4)-C(26)-H(26)	108.5
C(20)-C(21)-H(21A)	109.5	C(26)-C(27)-H(27A)	109.5
C(20)-C(21)-H(21B)	109.5	C(26)-C(27)-H(27B)	109.5
H(21A)-C(21)-H(21B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(20)-C(21)-H(21C)	109.5	C(26)-C(27)-H(27C)	109.5
H(21A)-C(21)-H(21C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(21B)-C(21)-H(21C)	109.5	H(27B)-C(27)-H(27C)	109.5
C(20)-C(22)-H(22A)	109.5	C(26)-C(28)-H(28A)	109.5
C(20)-C(22)-H(22B)	109.5	C(26)-C(28)-H(28B)	109.5
H(22A)-C(22)-H(22B)	109.5	H(28A)-C(28)-H(28B)	109.5
C(20)-C(22)-H(22C)	109.5	C(26)-C(28)-H(28C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(28A)-C(28)-H(28C)	109.5
H(22B)-C(22)-H(22C)	109.5	H(28B)-C(28)-H(28C)	109.5
C(24)-C(23)-C(25)	110.9(6)	C(30)-C(29)-C(31)	111.5(6)
C(24)-C(23)-P(3)	111.5(5)	C(30)-C(29)-P(4)	111.4(5)
C(25)-C(23)-P(3)	115.0(5)	C(31)-C(29)-P(4)	114.7(5)
C(24)-C(23)-H(23)	106.3	C(30)-C(29)-H(29)	106.2
C(25)-C(23)-H(23)	106.3	C(31)-C(29)-H(29)	106.2
P(3)-C(23)-H(23)	106.3	P(4)-C(29)-H(29)	106.2
C(23)-C(24)-H(24A)	109.5	C(29)-C(30)-H(30A)	109.5
C(23)-C(24)-H(24B)	109.5	C(29)-C(30)-H(30B)	109.5
H(24A)-C(24)-H(24B)	109.5	H(30A)-C(30)-H(30B)	109.5
C(23)-C(24)-H(24C)	109.5	C(29)-C(30)-H(30C)	109.5
H(24A)-C(24)-H(24C)	109.5	H(30A)-C(30)-H(30C)	109.5
H(24B)-C(24)-H(24C)	109.5	H(30B)-C(30)-H(30C)	109.5
C(23)-C(25)-H(25A)	109.5	C(29)-C(31)-H(31A)	109.5
C(23)-C(25)-H(25B)	109.5	C(29)-C(31)-H(31B)	109.5
H(25A)-C(25)-H(25B)	109.5	H(31A)-C(31)-H(31B)	109.5
C(23)-C(25)-H(25C)	109.5	C(29)-C(31)-H(31C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(31A)-C(31)-H(31C)	109.5
H(25B)-C(25)-H(25C)	109.5	H(31B)-C(31)-H(31C)	109.5
C(28)-C(26)-C(27)	109.9(6)	C(33)-C(32)-P(1)	112.0(4)
C(28)-C(26)-P(4)	112.7(5)	C(33)-C(32)-H(32A)	109.2
C(27)-C(26)-P(4)	108.6(5)	P(1)-C(32)-H(32A)	109.2
C(28)-C(26)-H(26)	108.5	C(33)-C(32)-H(32B)	109.2

P(1)-C(32)-H(32B)	109.2	H(38A)-C(38)-H(38C)	109.5
H(32A)-C(32)-H(32B)	107.9	H(38B)-C(38)-H(38C)	109.5
C(32)-C(33)-P(2)	111.8(4)	C(37)-C(39)-H(39A)	109.5
C(32)-C(33)-H(33A)	109.3	C(37)-C(39)-H(39B)	109.5
P(2)-C(33)-H(33A)	109.3	H(39A)-C(39)-H(39B)	109.5
C(32)-C(33)-H(33B)	109.3	C(37)-C(39)-H(39C)	109.5
P(2)-C(33)-H(33B)	109.3	H(39A)-C(39)-H(39C)	109.5
H(33A)-C(33)-H(33B)	107.9	H(39B)-C(39)-H(39C)	109.5
C(36)-C(34)-C(35)	111.1(5)	C(41)-C(40)-C(42)	109.6(5)
C(36)-C(34)-P(1)	113.1(4)	C(41)-C(40)-P(2)	109.6(4)
C(35)-C(34)-P(1)	109.0(4)	C(42)-C(40)-P(2)	111.2(4)
C(36)-C(34)-H(34)	107.8	C(41)-C(40)-H(40)	108.8
C(35)-C(34)-H(34)	107.8	C(42)-C(40)-H(40)	108.8
P(1)-C(34)-H(34)	107.8	P(2)-C(40)-H(40)	108.8
C(34)-C(35)-H(35A)	109.5	C(40)-C(41)-H(41A)	109.5
C(34)-C(35)-H(35B)	109.5	C(40)-C(41)-H(41B)	109.5
H(35A)-C(35)-H(35B)	109.5	H(41A)-C(41)-H(41B)	109.5
C(34)-C(35)-H(35C)	109.5	C(40)-C(41)-H(41C)	109.5
H(35A)-C(35)-H(35C)	109.5	H(41A)-C(41)-H(41C)	109.5
H(35B)-C(35)-H(35C)	109.5	H(41B)-C(41)-H(41C)	109.5
C(34)-C(36)-H(36A)	109.5	C(40)-C(42)-H(42A)	109.5
C(34)-C(36)-H(36B)	109.5	C(40)-C(42)-H(42B)	109.5
H(36A)-C(36)-H(36B)	109.5	H(42A)-C(42)-H(42B)	109.5
C(34)-C(36)-H(36C)	109.5	C(40)-C(42)-H(42C)	109.5
H(36A)-C(36)-H(36C)	109.5	H(42A)-C(42)-H(42C)	109.5
H(36B)-C(36)-H(36C)	109.5	H(42B)-C(42)-H(42C)	109.5
C(39)-C(37)-C(38)	109.6(5)	C(45)-C(43)-C(44)	111.0(5)
C(39)-C(37)-P(1)	114.5(4)	C(45)-C(43)-P(2)	114.1(4)
C(38)-C(37)-P(1)	111.2(4)	C(44)-C(43)-P(2)	111.7(4)
C(39)-C(37)-H(37)	107.1	C(45)-C(43)-H(43)	106.5
C(38)-C(37)-H(37)	107.1	C(44)-C(43)-H(43)	106.5
P(1)-C(37)-H(37)	107.1	P(2)-C(43)-H(43)	106.5
C(37)-C(38)-H(38A)	109.5	C(43)-C(44)-H(44A)	109.5
C(37)-C(38)-H(38B)	109.5	C(43)-C(44)-H(44B)	109.5
H(38A)-C(38)-H(38B)	109.5	H(44A)-C(44)-H(44B)	109.5
C(37)-C(38)-H(38C)	109.5	C(43)-C(44)-H(44C)	109.5

H(44A)-C(44)-H(44C)	109.5	C(20)-P(3)-Ni(1)	117.1(2)
H(44B)-C(44)-H(44C)	109.5	C(19)-P(3)-Ni(1)	107.9(2)
C(43)-C(45)-H(45A)	109.5	C(26)-P(4)-C(18)	103.9(3)
C(43)-C(45)-H(45B)	109.5	C(26)-P(4)-C(29)	103.8(3)
H(45A)-C(45)-H(45B)	109.5	C(18)-P(4)-C(29)	102.9(3)
C(43)-C(45)-H(45C)	109.5	C(26)-P(4)-Ni(1)	118.0(2)
H(45A)-C(45)-H(45C)	109.5	C(18)-P(4)-Ni(1)	106.7(2)
H(45B)-C(45)-H(45C)	109.5	C(29)-P(4)-Ni(1)	119.5(2)
C(13)-Ni(1)-C(14)	41.9(2)		
C(13)-Ni(1)-P(3)	109.08(17)		
C(14)-Ni(1)-P(3)	150.96(17)		
C(13)-Ni(1)-P(4)	158.29(17)		
C(14)-Ni(1)-P(4)	116.40(17)		
P(3)-Ni(1)-P(4)	92.61(7)		
C(16)-Ni(2)-C(17)	42.3(2)		
C(16)-Ni(2)-P(2)	152.78(18)		
C(17)-Ni(2)-P(2)	110.53(17)		
C(16)-Ni(2)-P(1)	114.99(18)		
C(17)-Ni(2)-P(1)	157.30(17)		
P(2)-Ni(2)-P(1)	92.17(6)		
C(32)-P(1)-C(37)	101.6(3)		
C(32)-P(1)-C(34)	107.1(3)		
C(37)-P(1)-C(34)	102.8(3)		
C(32)-P(1)-Ni(2)	106.58(19)		
C(37)-P(1)-Ni(2)	121.90(19)		
C(34)-P(1)-Ni(2)	115.3(2)		
C(40)-P(2)-C(43)	103.2(3)		
C(40)-P(2)-C(33)	104.0(3)		
C(43)-P(2)-C(33)	103.1(3)		
C(40)-P(2)-Ni(2)	114.8(2)		
C(43)-P(2)-Ni(2)	122.4(2)		
C(33)-P(2)-Ni(2)	107.36(19)		
C(23)-P(3)-C(20)	102.9(3)		
C(23)-P(3)-C(19)	103.1(3)		
C(20)-P(3)-C(19)	103.2(3)		
C(23)-P(3)-Ni(1)	120.6(2)		

Table S13. Anisotropic displacement parameters ($Å^2$ x 10^3) for[{(dippe)Ni}$_2$(η^2-Cα,Cβ -$C_{17}H_{12}F_2O$)], **2b**.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	43(4)	25(4)	30(4)	-5(3)	-8(4)	-10(3)
C(2)	41(4)	34(4)	40(4)	-1(3)	-8(4)	3(4)
C(3)	45(5)	41(5)	63(6)	-6(4)	-26(4)	6(4)
C(4)	68(6)	29(5)	59(6)	-6(4)	-34(5)	4(4)
C(5)	81(6)	41(5)	49(5)	18(4)	-25(5)	-25(5)
C(6)	55(5)	42(5)	43(5)	5(4)	-8(4)	-20(4)
C(7)	41(4)	36(4)	26(3)	-7(3)	-8(4)	-1(4)
C(8)	45(4)	58(5)	34(4)	16(4)	3(4)	7(4)
C(9)	68(6)	67(6)	36(5)	7(4)	13(4)	-11(5)
C(10)	87(6)	41(4)	23(4)	18(3)	-5(4)	-9(5)
C(11)	60(5)	42(4)	37(4)	9(4)	-18(4)	-8(4)
C(12)	45(4)	40(4)	39(4)	9(4)	-10(4)	-7(4)
C(13)	32(3)	31(4)	24(3)	-11(3)	5(3)	-9(3)
C(14)	28(4)	28(4)	27(4)	-7(3)	8(3)	1(3)
C(15)	27(4)	42(4)	14(3)	-10(3)	1(3)	-5(4)
C(16)	28(3)	35(4)	26(4)	-1(3)	1(3)	-1(3)
C(17)	25(3)	34(4)	29(3)	7(3)	-8(3)	2(3)
C(18)	57(5)	74(5)	39(5)	-16(4)	-21(4)	7(4)
C(19)	44(4)	56(5)	56(5)	-23(4)	-10(4)	0(4)
C(20)	34(4)	41(4)	80(6)	-23(4)	-4(4)	-12(3)
C(21)	36(4)	80(6)	55(5)	-14(5)	-4(4)	6(4)
C(22)	38(4)	48(5)	70(6)	6(5)	10(4)	-6(4)
C(23)	56(5)	34(4)	50(5)	-15(3)	-6(4)	12(4)
C(24)	47(5)	74(6)	65(6)	-13(5)	4(4)	19(4)
C(25)	74(6)	37(4)	90(6)	-21(4)	-4(5)	-1(4)
C(26)	78(5)	60(5)	25(4)	-4(4)	10(4)	-5(4)
C(27)	67(5)	85(6)	74(6)	-30(5)	40(5)	2(5)
C(28)	80(6)	79(6)	57(6)	-2(5)	24(5)	-20(5)
C(29)	72(6)	67(5)	26(4)	-4(4)	-8(4)	5(4)
C(30)	55(5)	78(6)	48(5)	-12(5)	-19(4)	29(4)
C(31)	126(8)	93(7)	42(5)	11(5)	-23(5)	37(6)
C(32)	30(4)	30(4)	27(4)	-2(3)	-6(3)	-5(3)
C(33)	30(4)	32(4)	44(4)	-12(3)	2(3)	-1(3)

C(34)	18(3)	42(4)	35(4)	16(3)	-9(3)	0(3)
C(35)	23(3)	53(4)	30(4)	5(4)	5(3)	-4(3)
C(36)	28(4)	54(5)	55(5)	4(4)	0(3)	-13(3)
C(37)	20(3)	31(4)	27(4)	10(3)	-2(3)	-3(3)
C(38)	34(4)	33(4)	31(4)	6(3)	-2(3)	-5(3)
C(39)	27(3)	46(4)	30(4)	17(3)	6(3)	1(3)
C(40)	34(4)	36(4)	42(4)	-10(4)	7(4)	7(3)
C(41)	30(4)	58(5)	46(5)	7(4)	10(4)	-8(4)
C(42)	32(4)	47(5)	64(5)	8(4)	7(4)	8(3)
C(43)	42(4)	28(4)	48(4)	3(3)	1(4)	-7(3)
C(44)	49(5)	40(4)	64(6)	12(4)	4(4)	-8(4)
C(45)	63(5)	23(4)	95(6)	-1(4)	5(5)	6(4)
O(1)	25(2)	48(3)	29(3)	-4(2)	1(2)	-8(2)
Ni(1)	25(1)	33(1)	26(1)	-8(1)	-1(1)	-1(1)
Ni(2)	21(1)	26(1)	21(1)	1(1)	-1(1)	1(1)
P(1)	19(1)	31(1)	23(1)	4(1)	-1(1)	-2(1)
P(2)	26(1)	24(1)	31(1)	-3(1)	3(1)	0(1)
P(3)	31(1)	40(1)	39(1)	-15(1)	-2(1)	0(1)
P(4)	44(1)	48(1)	26(1)	-7(1)	-5(1)	7(1)
F(1)	100(3)	42(3)	114(4)	7(3)	-52(3)	13(3)
F(2)	102(3)	71(3)	41(2)	20(2)	-6(3)	-11(3)