Phosphine-substituted Fe-Te clusters related to the active site of [FeFe]-H_2ases

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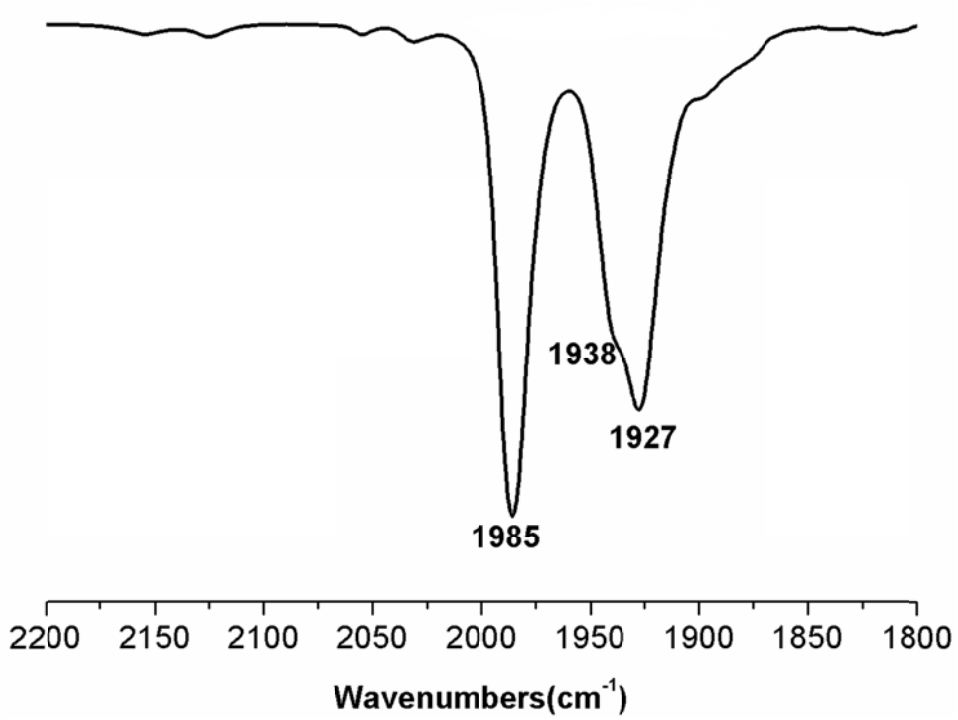

Figure S1. FT-IR (in CH_2Cl_2, 25°C) spectrum of **1-*anti***. *Assignments:* ν_{CO} = 1985, 1938, 1927 cm^{-1}.

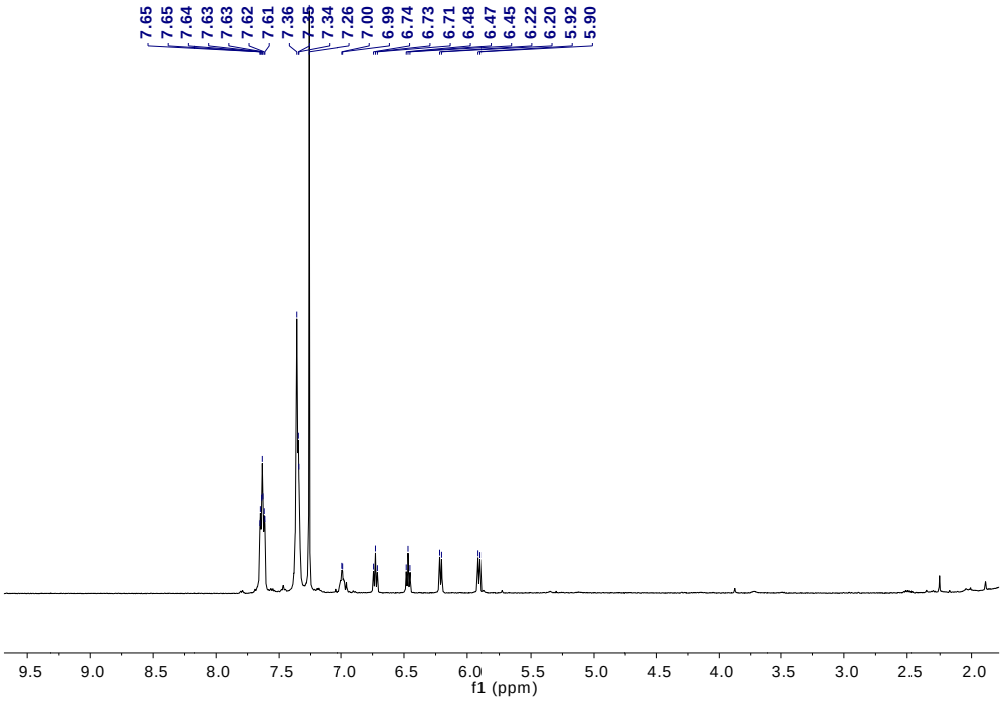

Figure S2. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) spectrum of **1-*anti***. *Assignments:* δ = 7.65-5.90 (m, 40H, $8C_6H_5$) ppm.

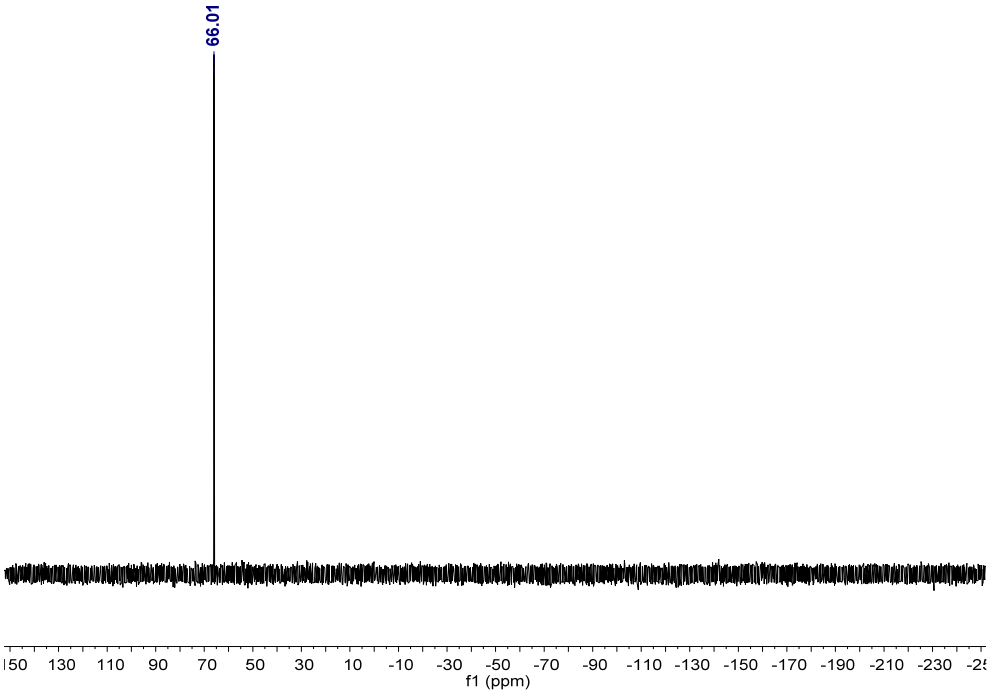

Figure S3. ^{31}P NMR (202 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **1-*anti***. *Assignments:* δ = 66.01 ppm.

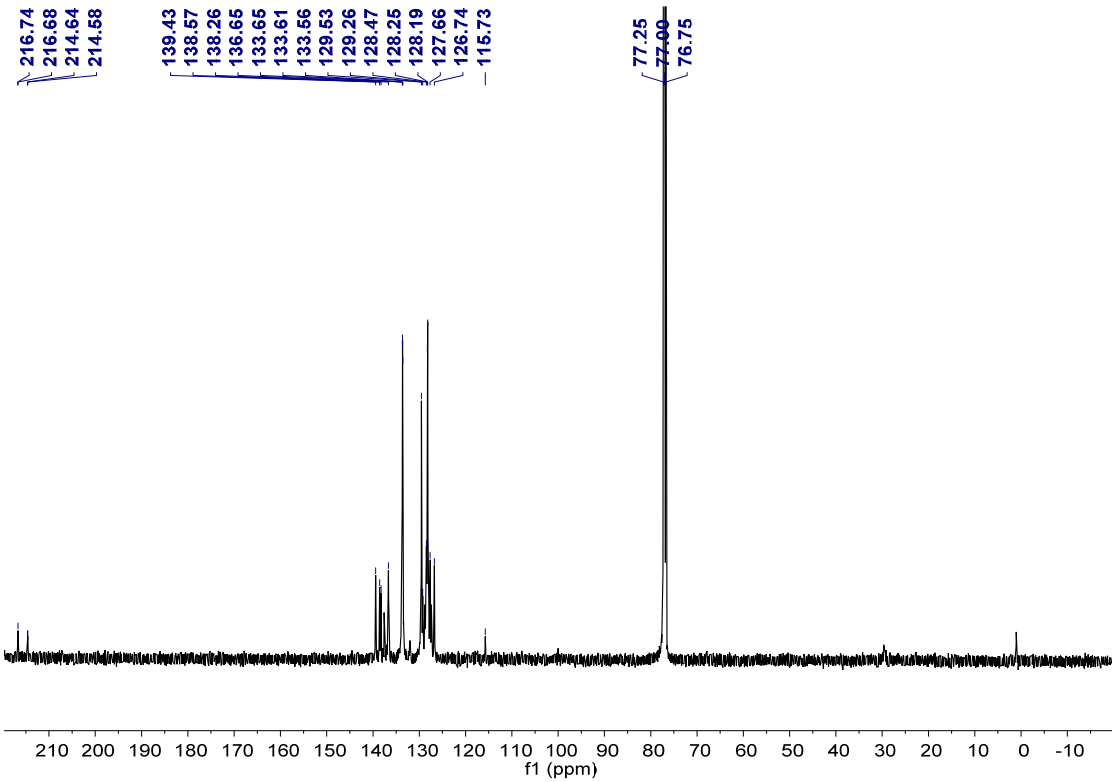

Figure S4. ^{13}C NMR (126 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **1-*anti***. *Assignments:* δ = 216.7, 214.6 (2d, $^{2}J_{P\text{-}C}$ = 7.6 Hz, $PFe(CO)_2$), 115.7-139.4 (m, C_6H_5) ppm.

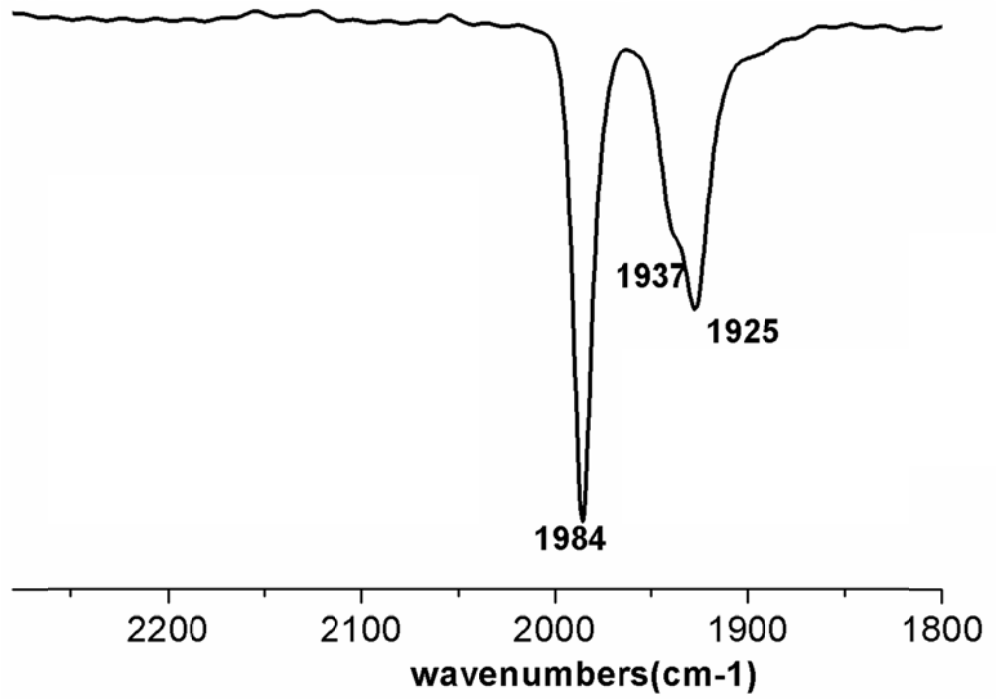

Figure S5. FT-IR (in CH_2Cl_2, 25°C) spectrum of **1-*syn***. *Assignments:* ν_{CO} = 1984, 1937, 1925 cm^{-1}.

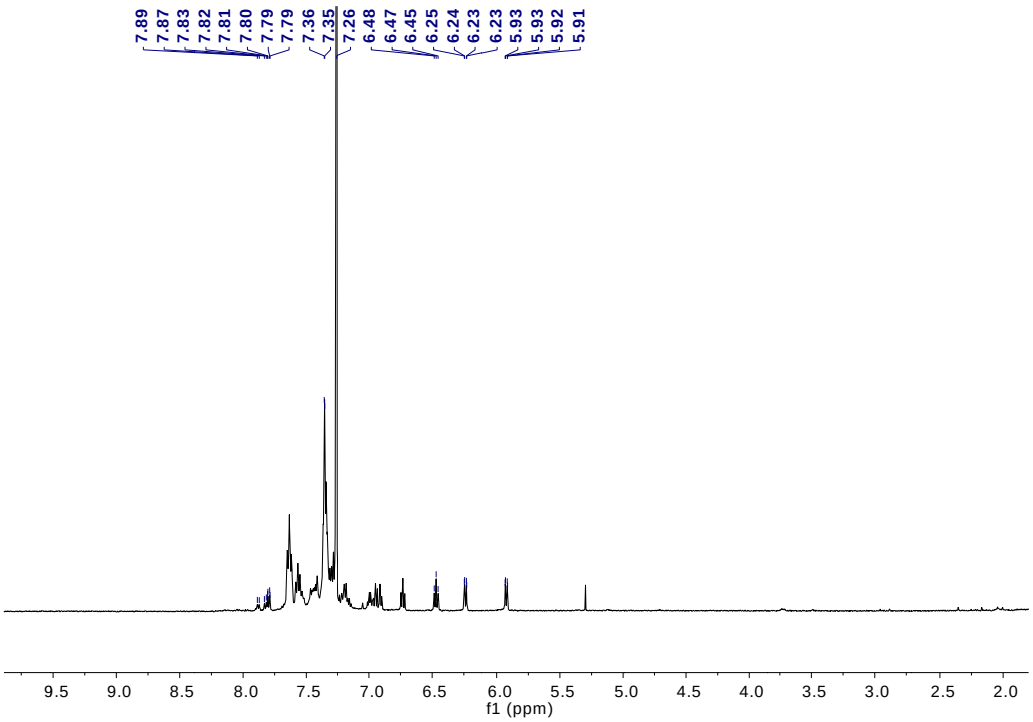

Figure S6. ^1H NMR (500 MHz, $CDCl_3$, 25 °C) spectrum of **1-*syn***. *Assignments:* δ = 7.89-5.91 (m, 40H, $8C_6H_5$) ppm.

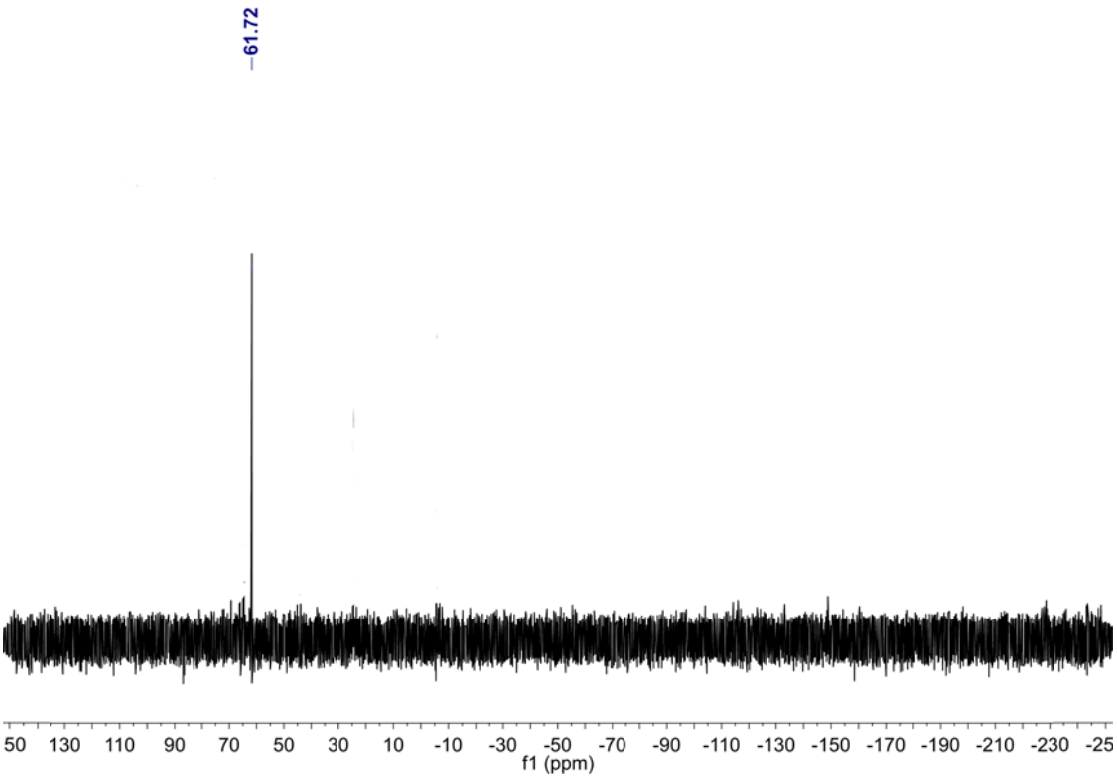

Figure S7. ^{31}P NMR (202 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **1-*syn***. *Assignments:* δ = 61.72 ppm.

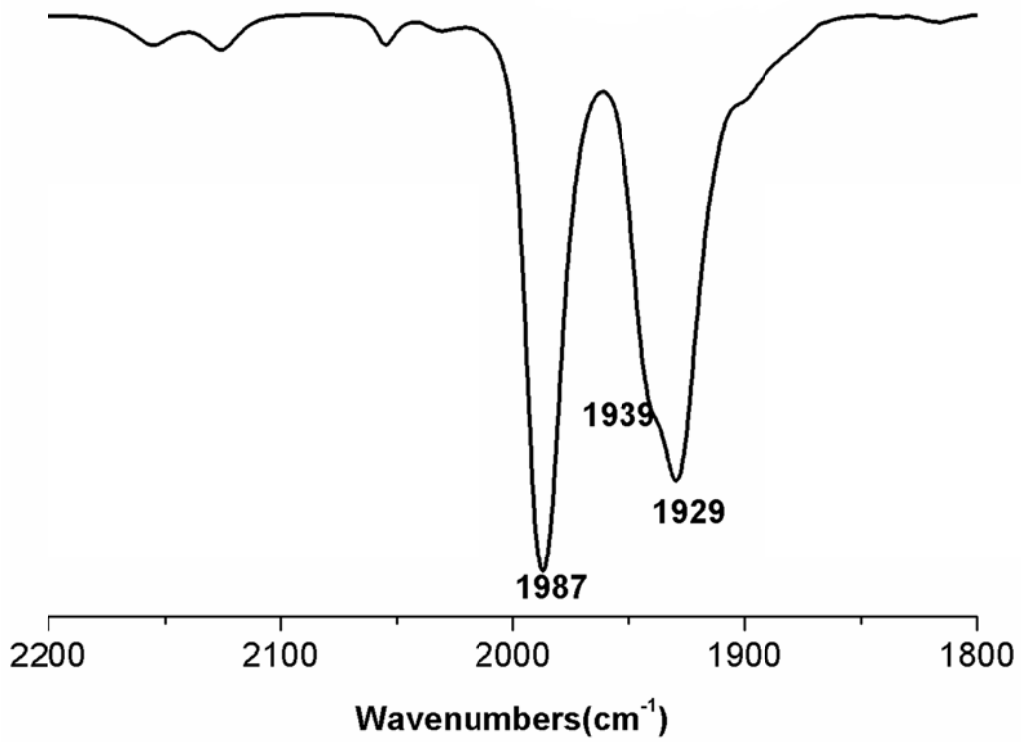

Figure S8. FT-IR (in CH_2Cl_2, 25°C) spectrum of **2-*anti***. *Assignments:* ν_{CO} = 1987, 1939, 1929 cm^{-1}.

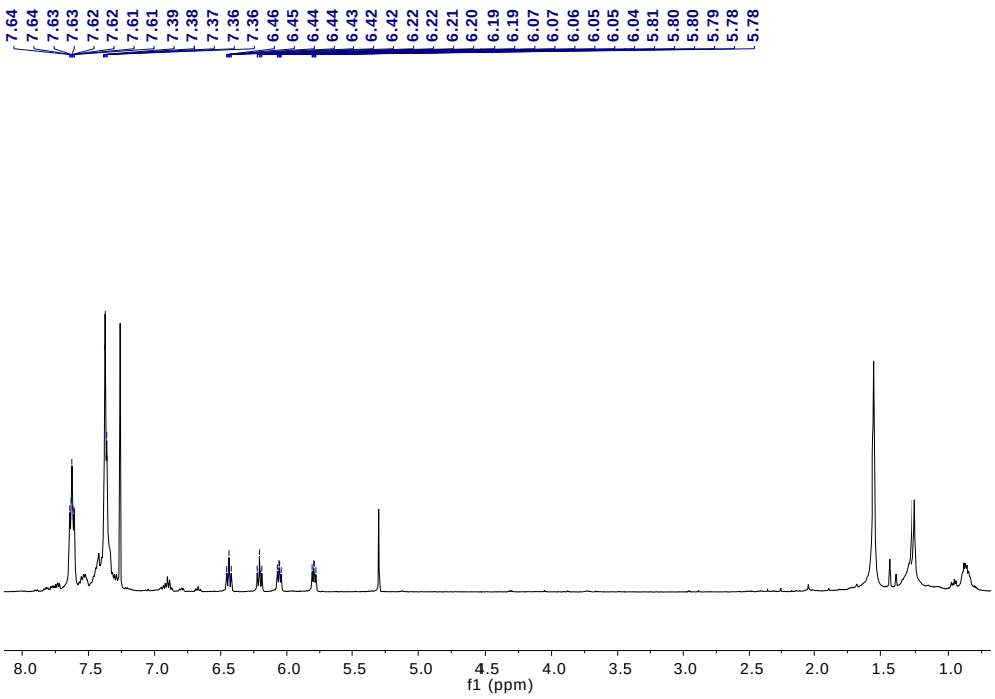

Figure S9. ^{1}H NMR (500 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **2-*anti***. *Assignments:* δ = 7.64-5.78 (m, 38H, $6C_6H_5 + 2C_6H_4$) ppm.

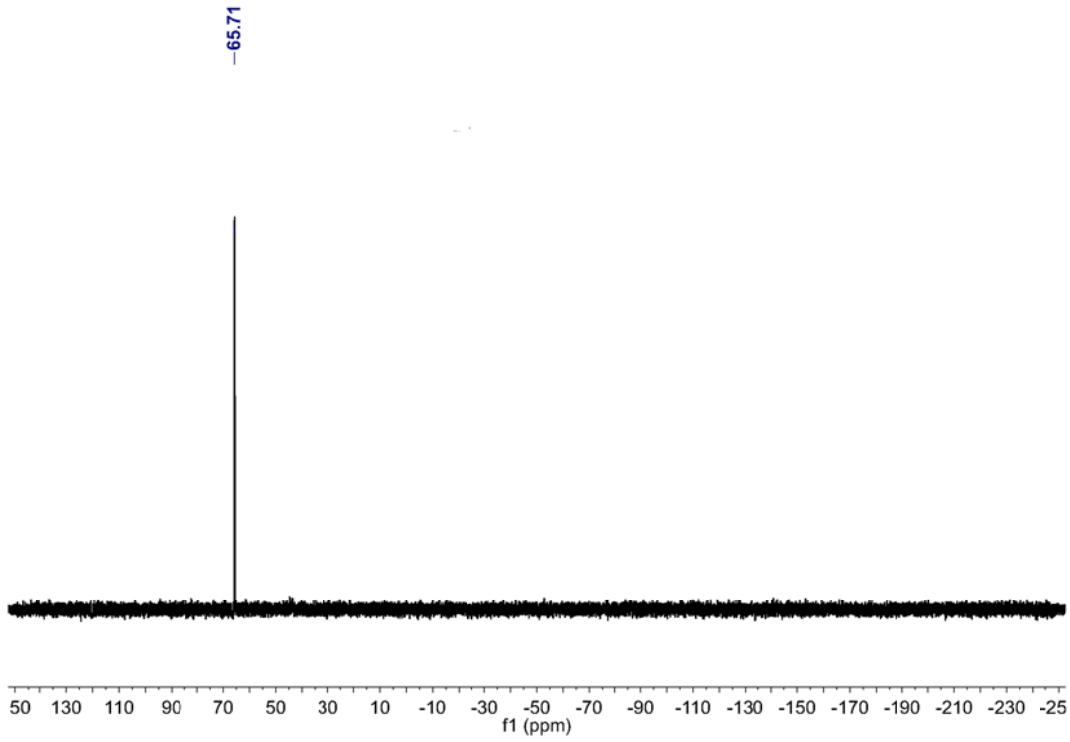

Figure S10. ^{31}P NMR (202 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **2-*anti***. *Assignments:* δ = 65.71 ppm.

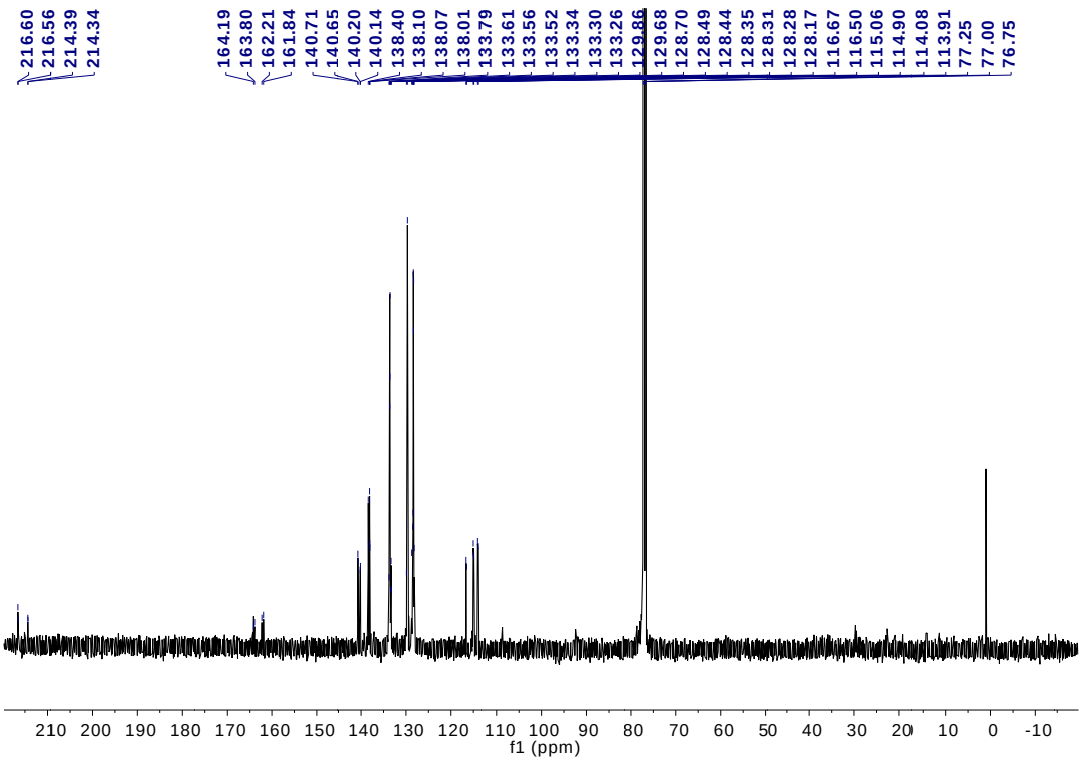

Figure S11. ^{13}C NMR (126 MHz, $CDCl_3$, 25 ^oC) spectrum of **2-*anti***. *Assignments:* δ = 216.6, 214.4 (2d, $^2J_{P-C}$ = 6.8 Hz, $PFe(CO)_2$), 113.9-164.2 (m, C_6H_5 + C_6H_4) ppm.

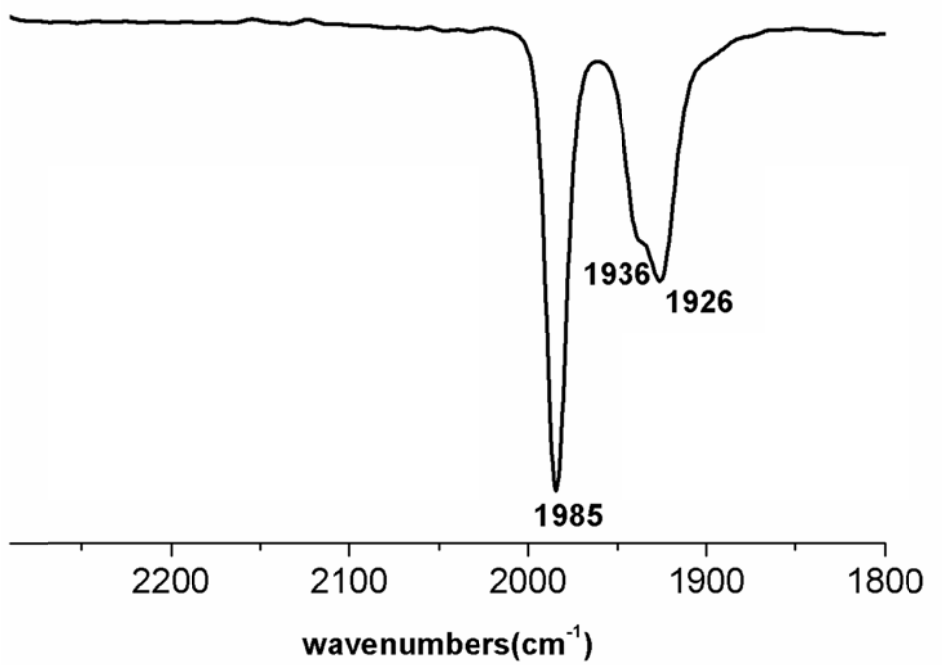

Figure S12. FT-IR (in CH_2Cl_2, 25^oC) spectrum of **2-*syn***. *Assignments:* ν_{CO} = 1985, 1936, 1926 cm^{-1}.

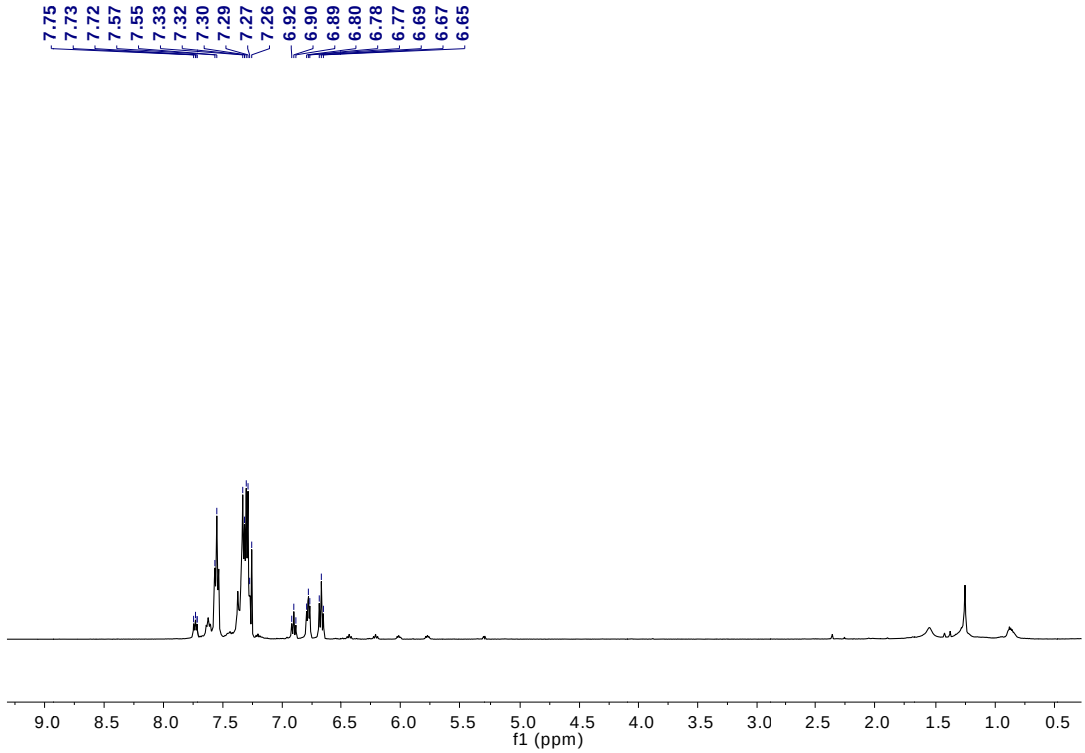

Figure S13. ^{1}H NMR (500 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **2-*syn*** in $CDCl_3$. *Assignments:* δ = 7.75-6.65 (m, 38H, $6C_6H_5 + 2C_6H_4$) ppm.

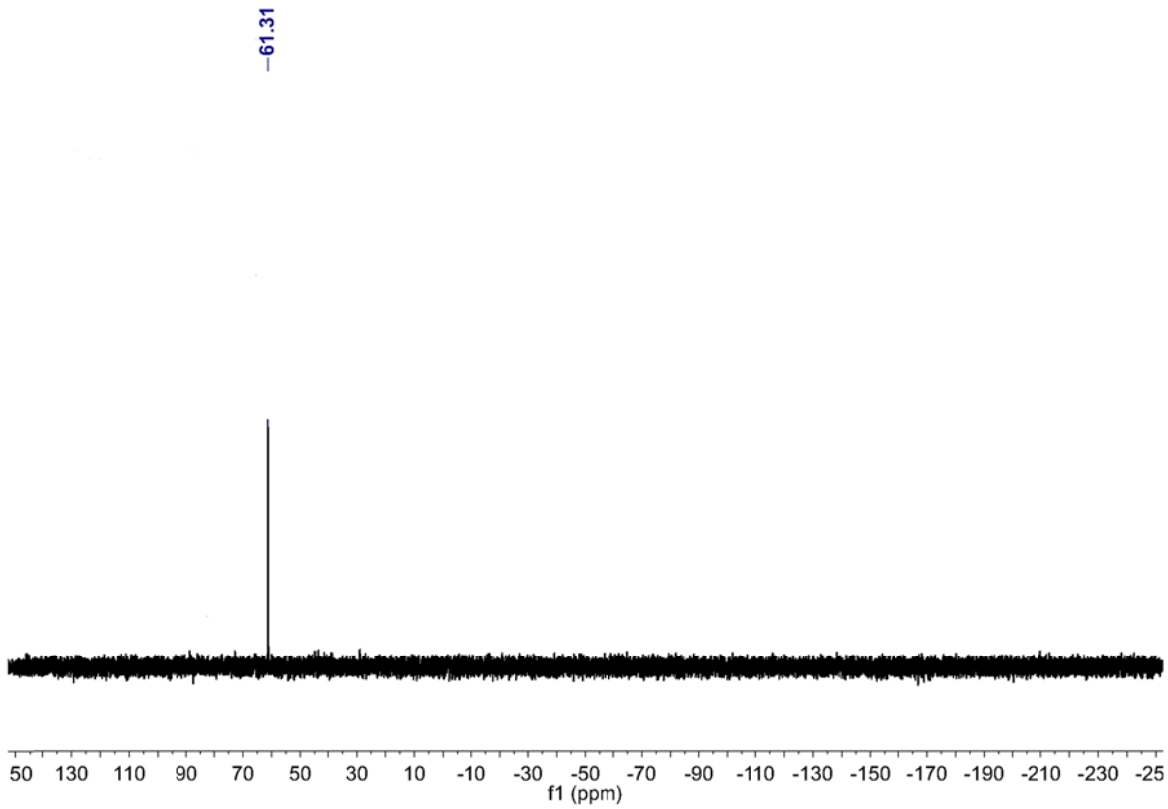

Figure S14. ^{31}P NMR (202 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **2-*syn***. *Assignments:* δ = 61.31 ppm.

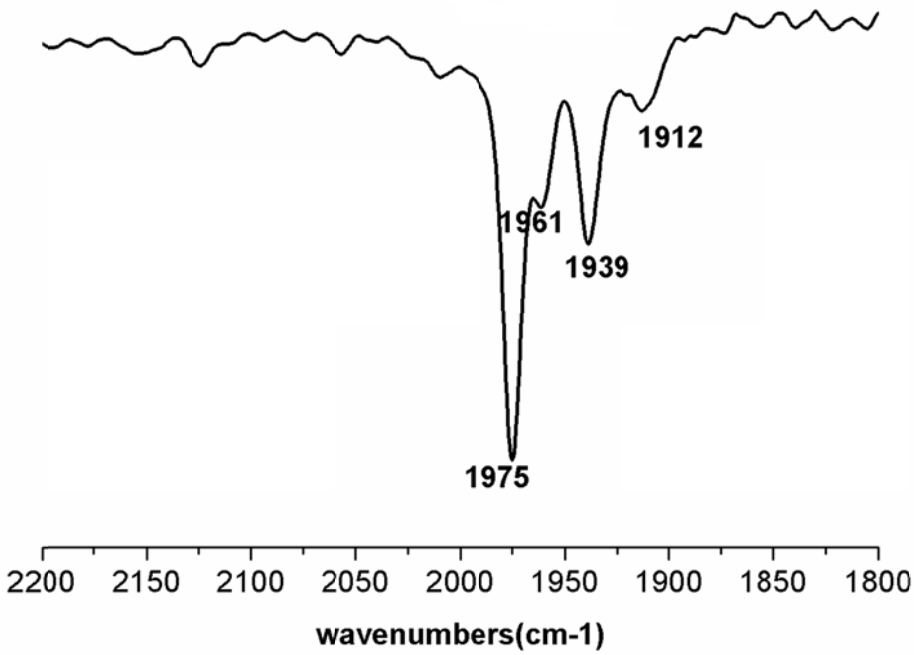

Figure S15. FT-IR (in CH_2Cl_2, 25°C) spectrum of **3** ppm.
Assignments: ν_{CO} = 1975, 1961, 1939, 1912 cm^{-1}.

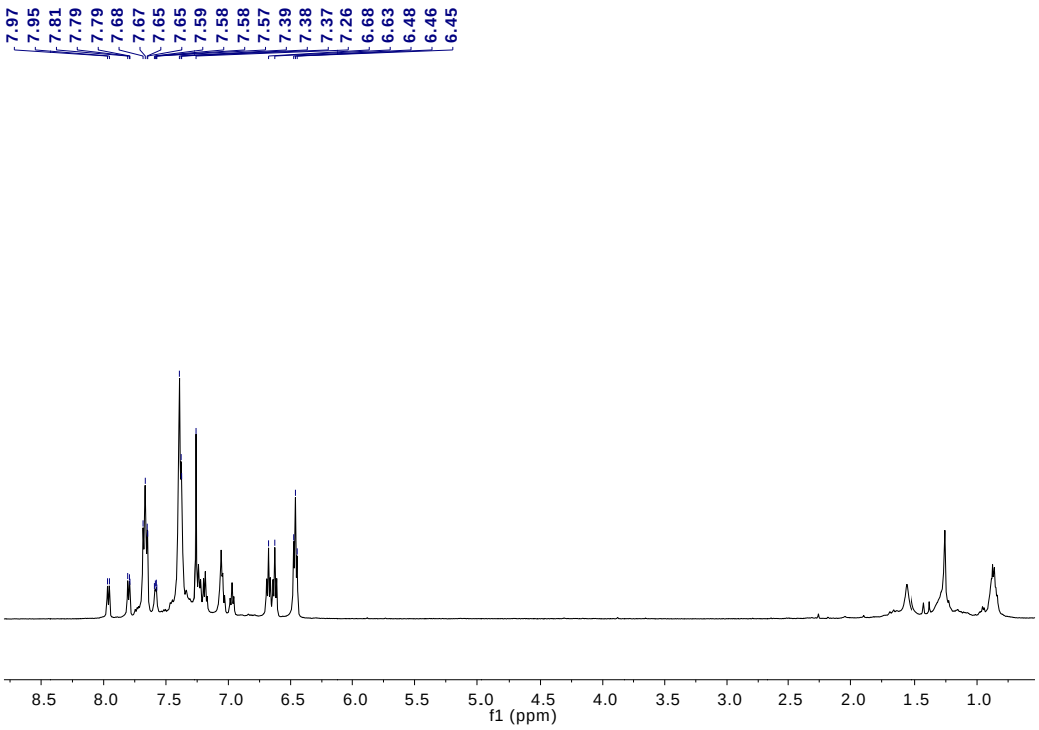

Figure S16. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) spectrum of **3**. *Assignments:* δ = 7.97-6.45 (m, 40H, $8C_6H_5$) ppm.

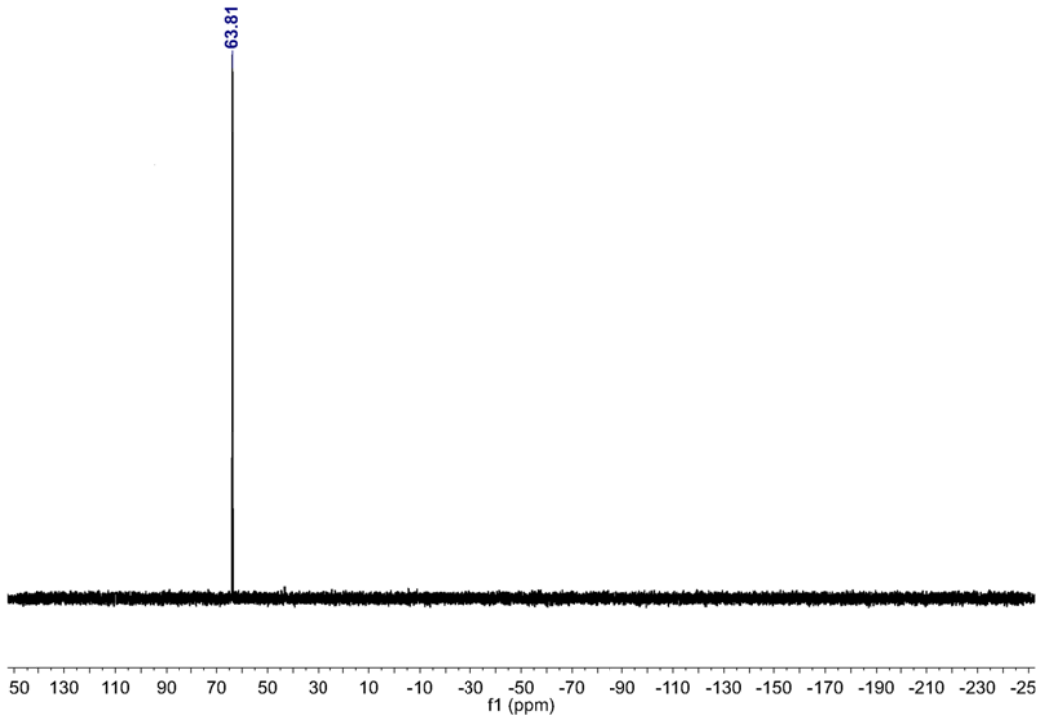

Figure S17. ^{31}P NMR (202 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **3**. *Assignments:* δ = 63.81 ppm.

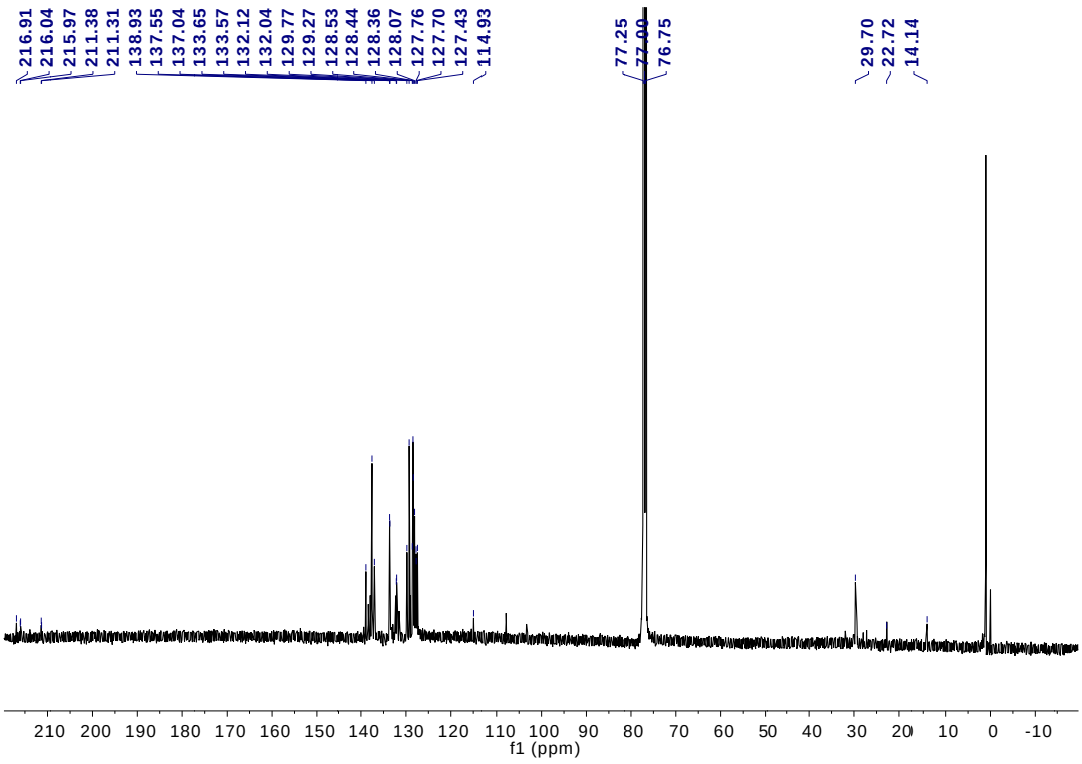

Figure S18. ^{13}C NMR (126 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **3**. *Assignments:* δ = 216.9, 216.0 (2d, $^{2}J_{P\text{-}C}$ = 7.6 Hz, $PFe(CO)_2$), 115.7-139.4 (m, C_6H_5) ppm.

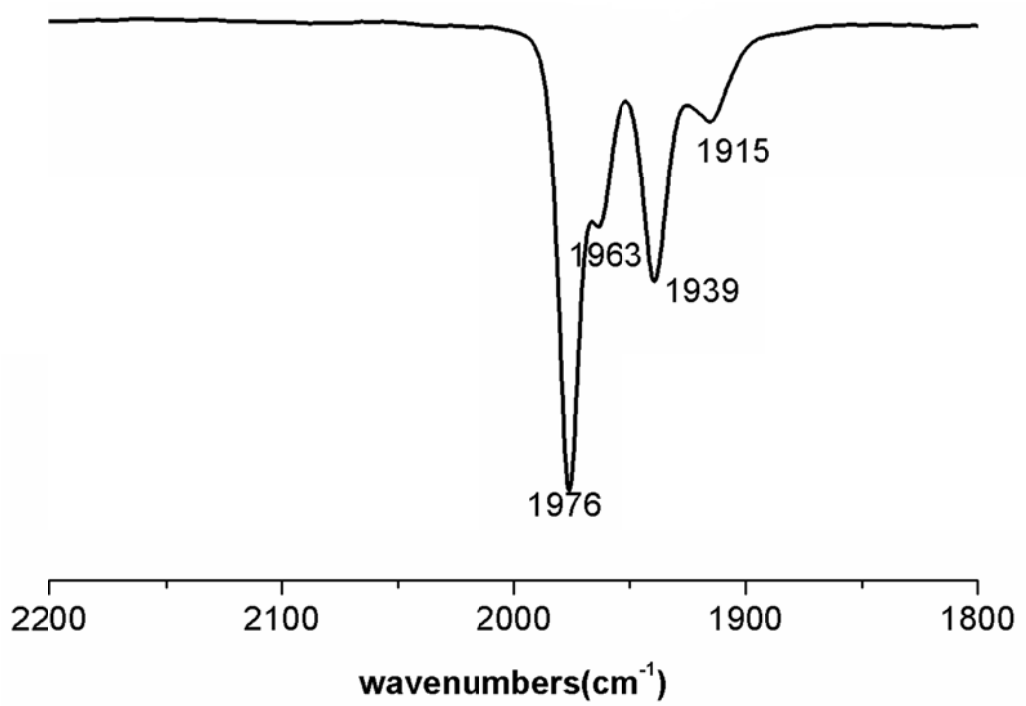

Figure S19. FT-IR (in CH_2Cl_2, 25°C) spectrum of **4**. *Assignments:* ν_{CO} = 1976, 1963, 1939, 1915 cm^{-1}.

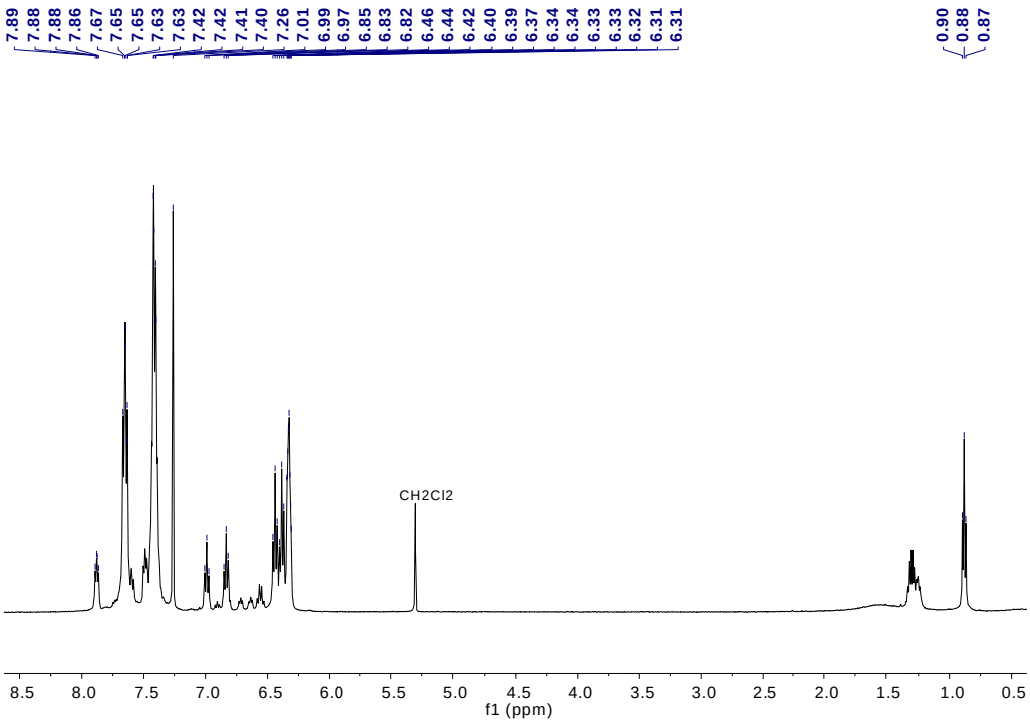

Figure S20. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) spectrum of **4**. *Assignments:* δ = 7.89-6.31 (m, 38H, $6C_6H_5 + 6C_6H_4$) ppm.

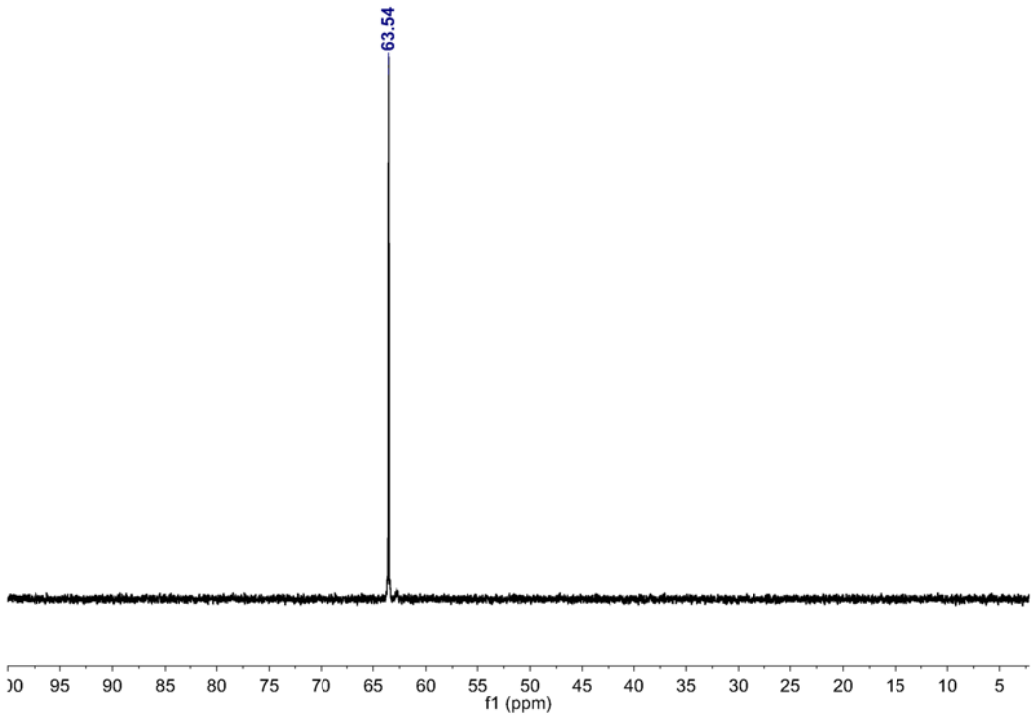

Figure S21. ^{31}P NMR (202 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **4**. *Assignments:* δ = 63.54 ppm.

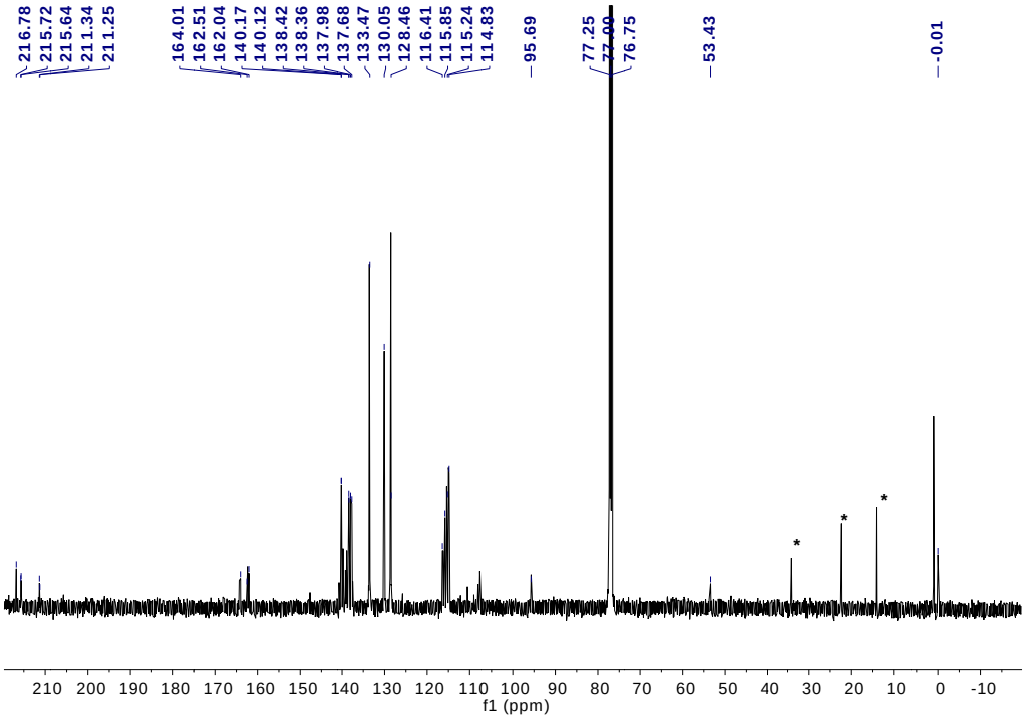

Figure S22. ^{13}C NMR (126 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **4** (* Traces of hexane). *Assignments:* δ = 216.8 (s, FeCO), 215.6, 211.3(2d, $^{2}J_{P\text{-}C}$ = 10.1 Hz, $PFe(CO)_2$) ppm, 114.8-164.0 (m, C_6H_5 + C_6H_4).

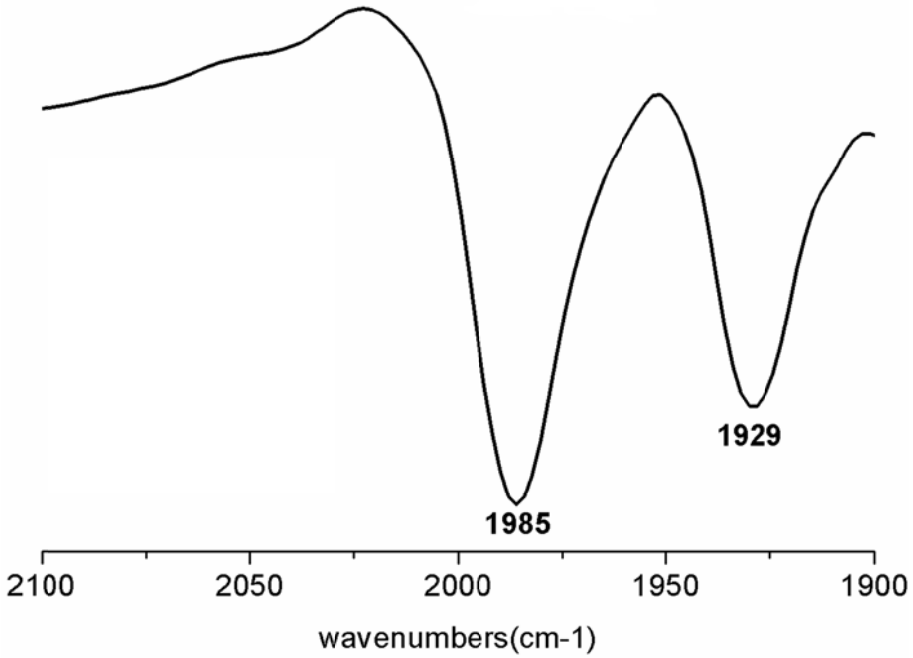

Figure S23. FT-IR (in CH_2Cl_2, 25°C) spectrum of **5**. *Assignments:* ν_{CO} = 1985, 1929 cm^{-1}.

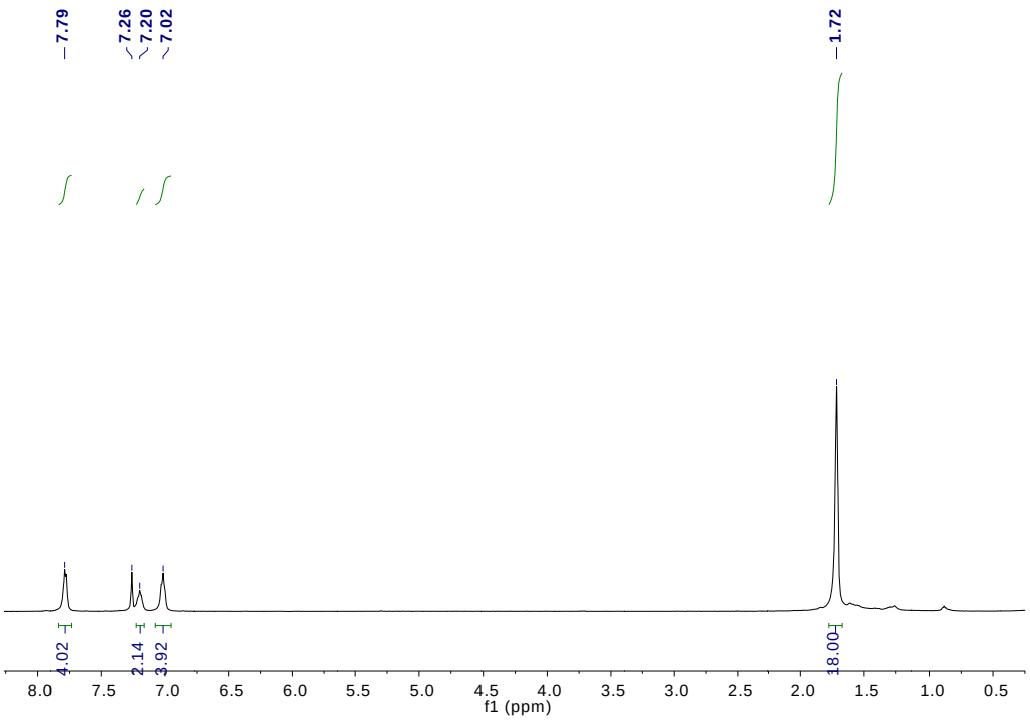

Figure S24. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) spectrum of **5**. *Assignments:* δ = 7.79, 7.20, 7.02 (3s, 10H, $2C_6H_5$), 1.72 (s, 18H, $6CH_3$) ppm.

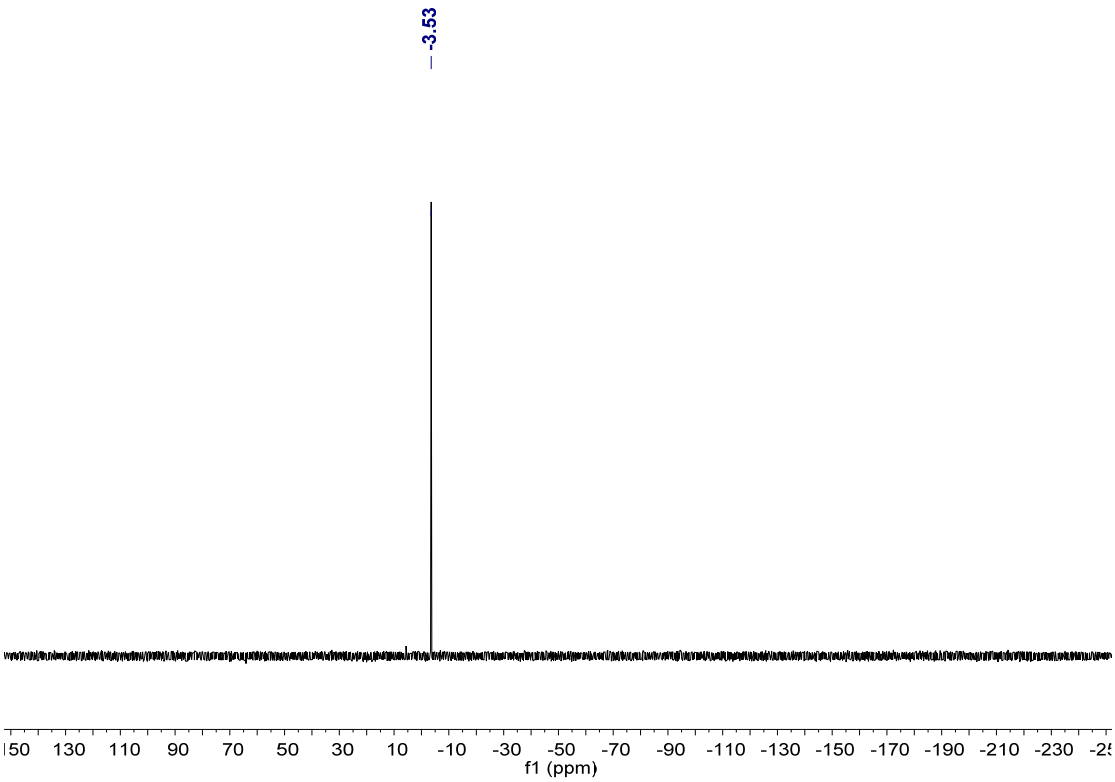

Figure S25. ^{31}P NMR (202 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **5**. *Assignments:* δ = -3.53 ppm.

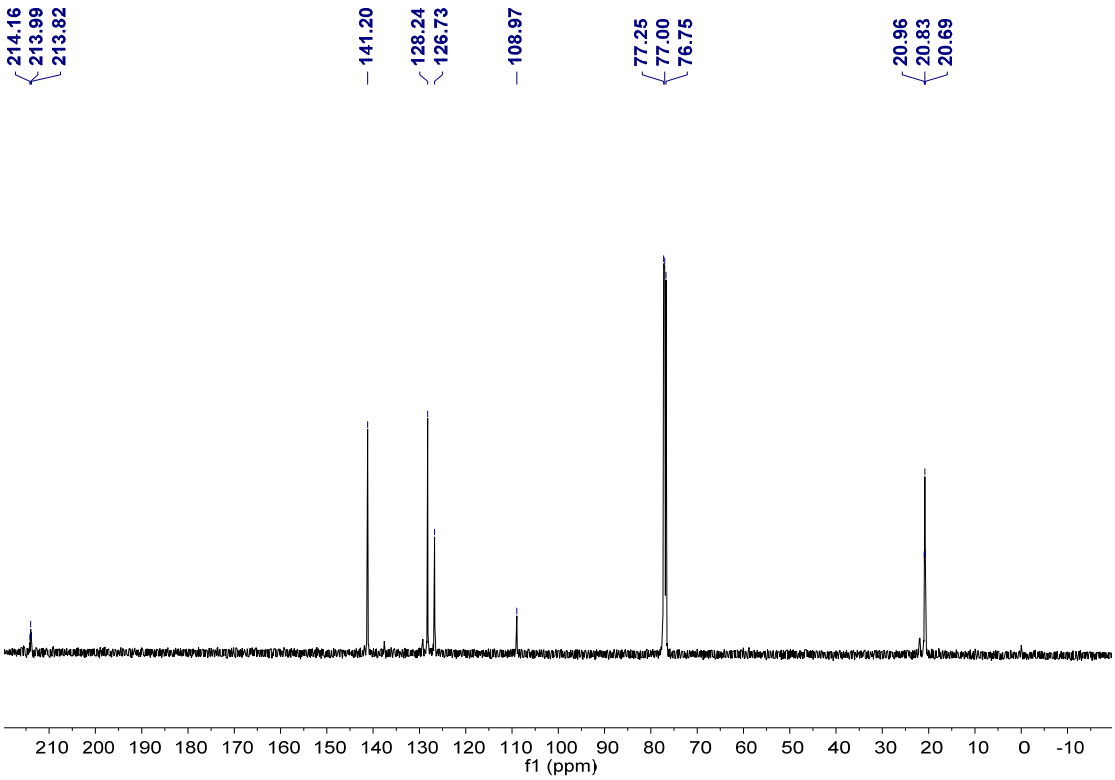

Figure S26. ^{13}C NMR (126 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **5**. *Assignments:* δ = 214.0 (t, J = 21.4, $Fe(CO)_2$), 141.2, 128.2, 126.7, 109.0 (C_6H_5), 20.8 (t, $J_{P\text{-}C}$ = 17.6Hz, PCH_3) ppm.

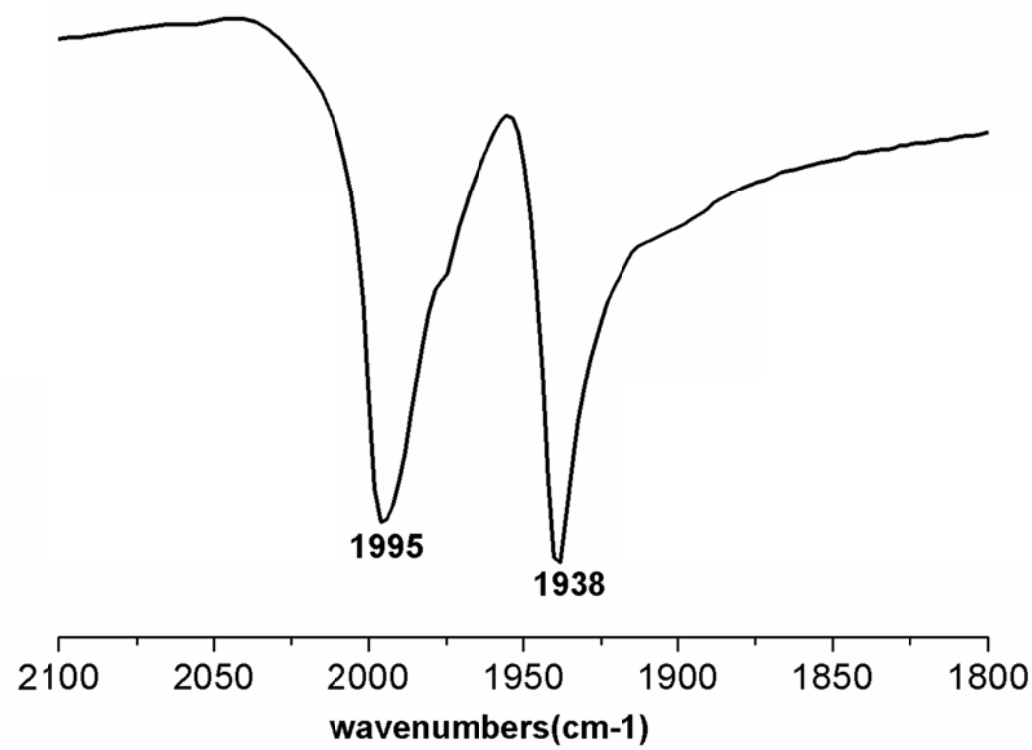

Figure S27. FT-IR (in CH_2Cl_2, 25°C) spectrum of **6**. *Assignments:* ν_{CO} = 1995, 1938 cm^{-1}.

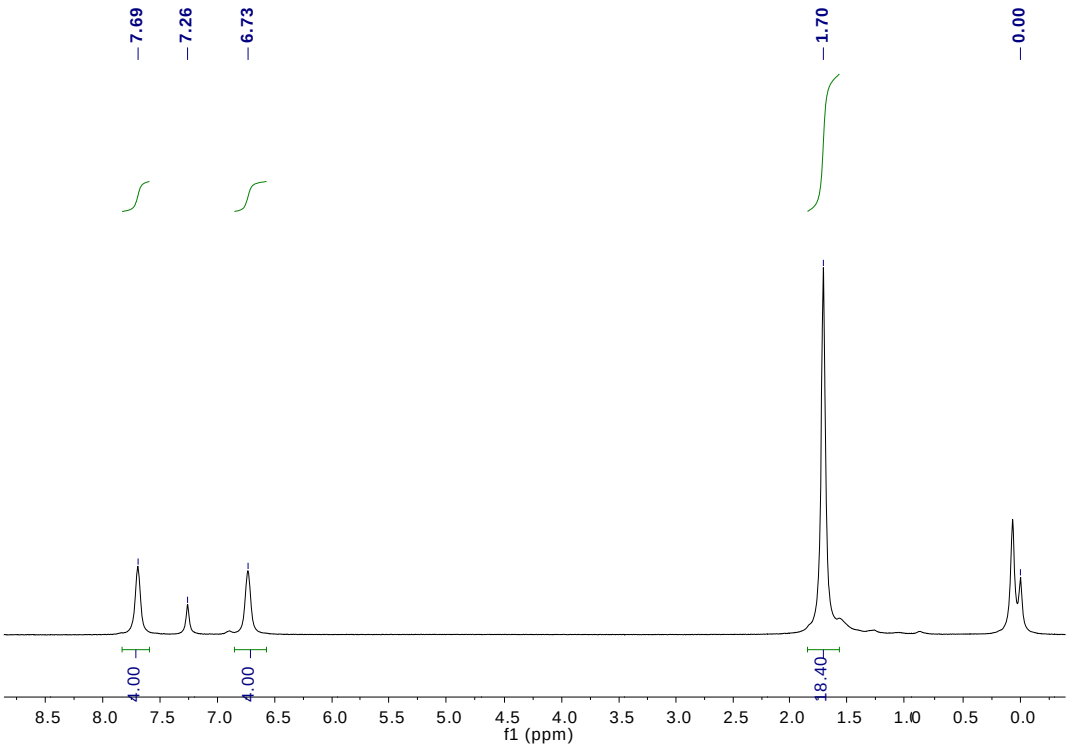

Figure S28. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) spectrum of **6**. *Assignments:* δ = 7.69, 6.73 (2s, 8H, $2C_6H_4$), 1.70 (s, 18H, $6CH_3$) ppm.

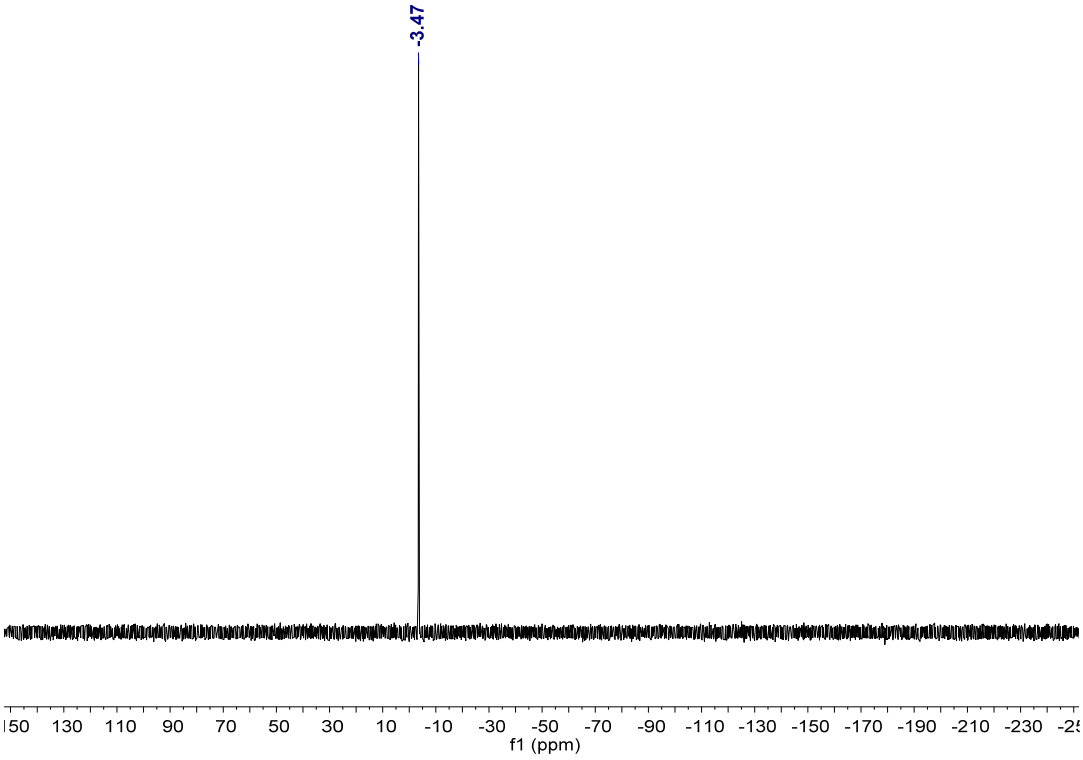

Figure S29. ^{31}P NMR (202 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **6**. *Assignments:* δ = -3.47 ppm.

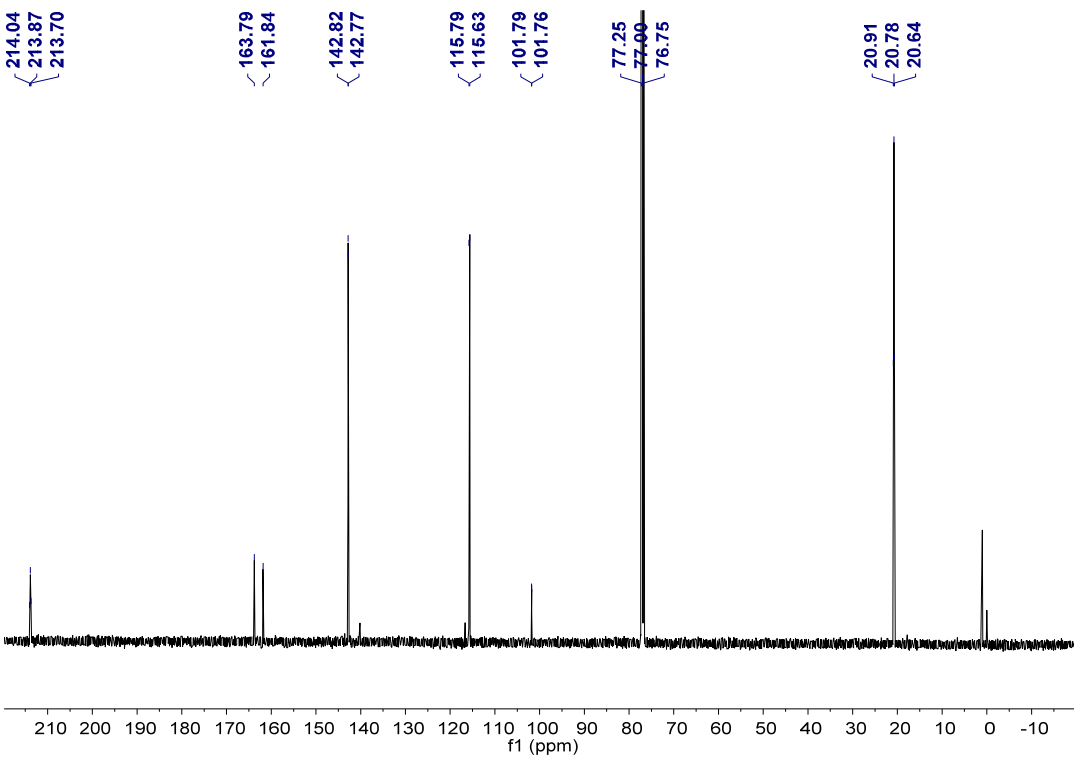

Figure S30. ^{13}C NMR (126 MHz, $CDCl_3$, 25 ^{o}C) spectrum of **6**. *Assignments:* δ = 213.9 (t, J = 21.4, $Fe(CO)_2$), 162.8 (d, $^{1}J_{F\text{-}C}$ = 246 Hz, *p*-C of C_6H_4Te), 142.8 (d, $^{3}J_{F\text{-}C}$ = 6.3 Hz, *o*-C of C_6H_4Te), 115.7 (d, $^{2}J_{F\text{-}C}$ = 20.2 Hz, *m*-C of C_6H_4Te), 101.8 (d, $^{4}J_{F\text{-}C}$ =

3.8 Hz, *ipso*-C of C_6H_4Te), 20.8 (t, $J_{P\text{-}C}$ = 17.6Hz, PCH_3) ppm.

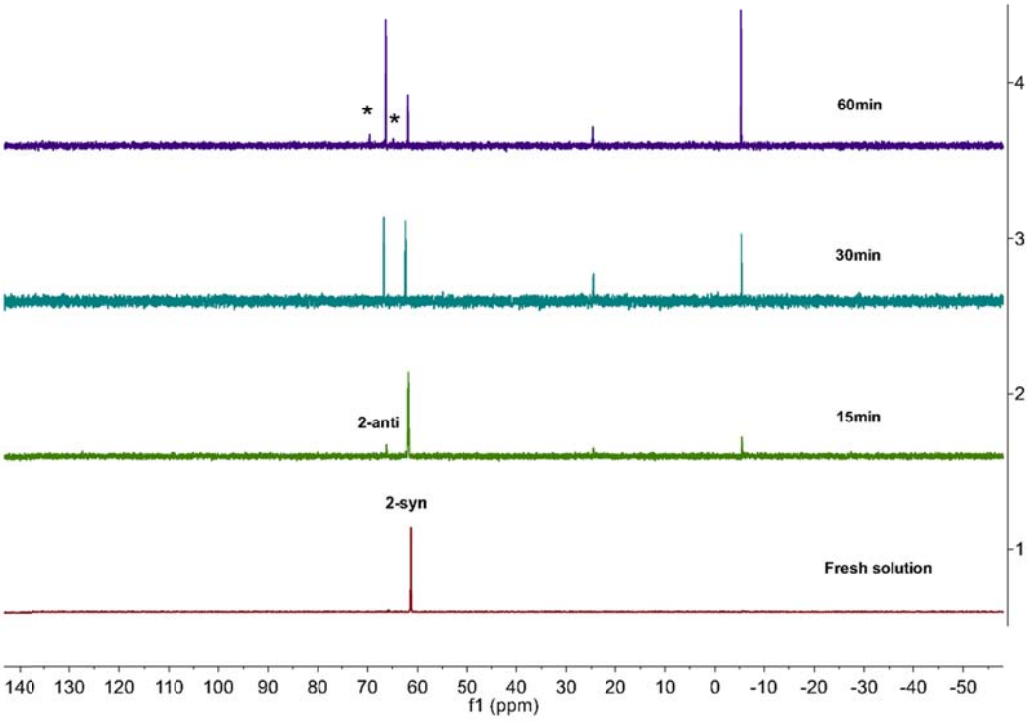

Figure S31. Slide of ^{31}P NMR of **2-syn** in toluene (100 ^{o}C).
(* *anti*-/*syn*-$Fe_2(\mu\text{-TeC6H4-F-4})_2(CO)_5(Ph_3P)$).

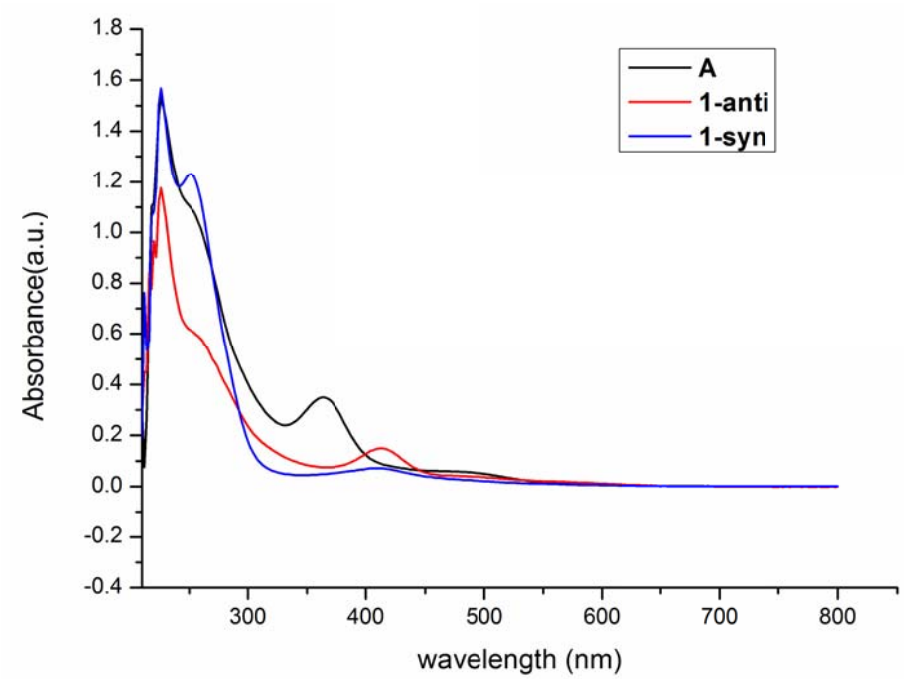

Figure S32 UV-visible spectra of **A** (black), **1-anti** (red) and **1-syn** (b**l**ue) recorded in CH_2Cl_2 at 25 ^oC.

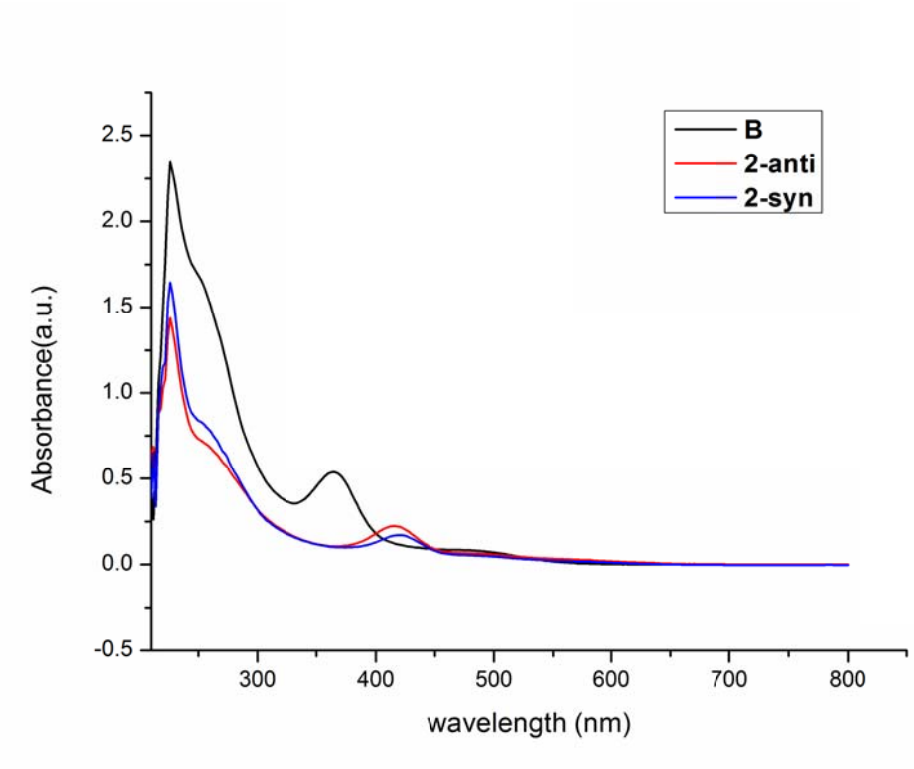

Figure S33 UV-visible spectra of **B** (black), **2-anti** (red) and **2-syn** (b**l**ue) recorded in CH_2Cl_2 at 25 ^oC.

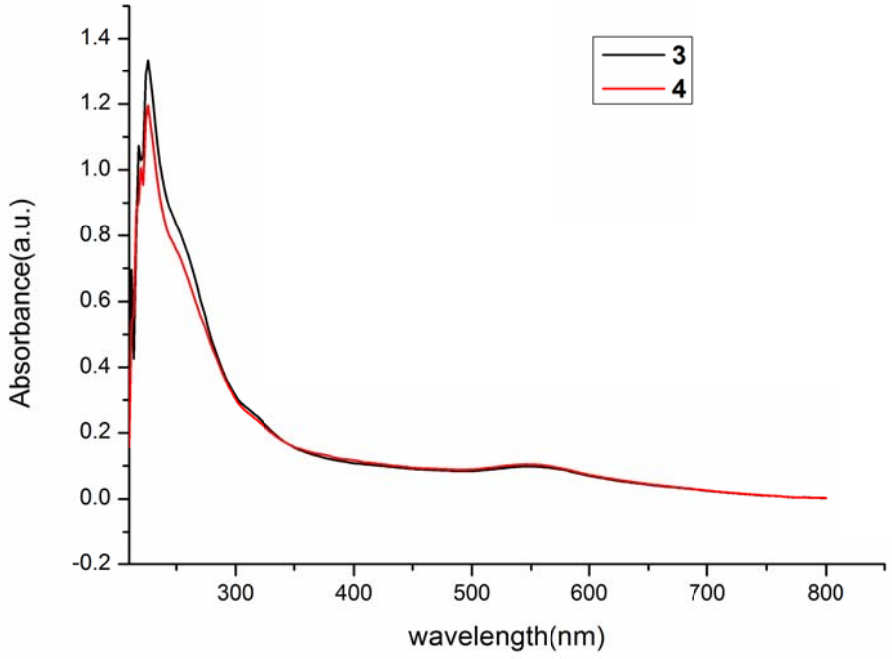

Figure S34 UV-visible spectra of **3** (black) and **4** (red) recorded in CH_2Cl_2 at 25 ^oC.

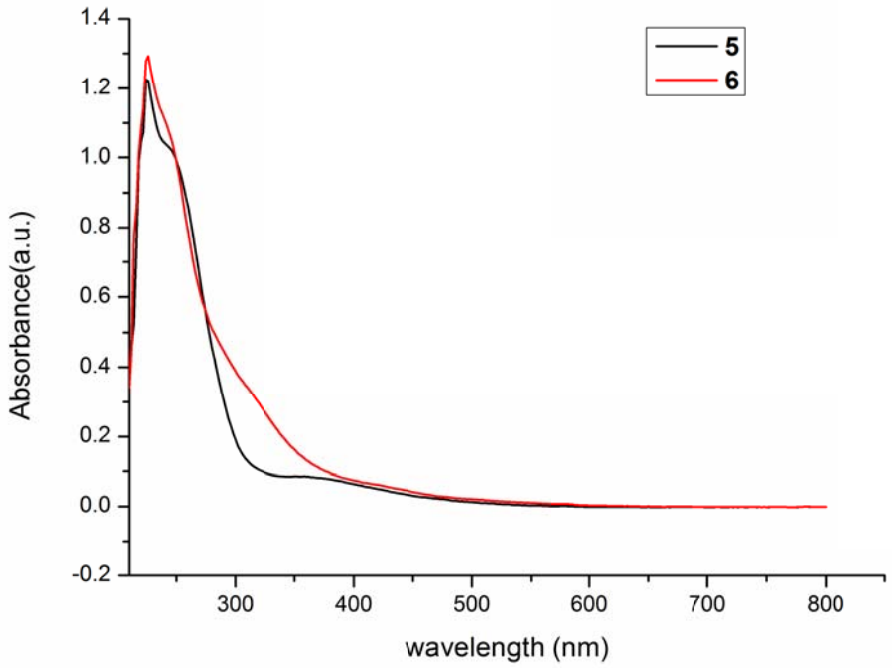

Figure S35 UV-visible spectra of **5** (black) and **6** (red) recorded in CH_2Cl_2 at 25 ^oC.

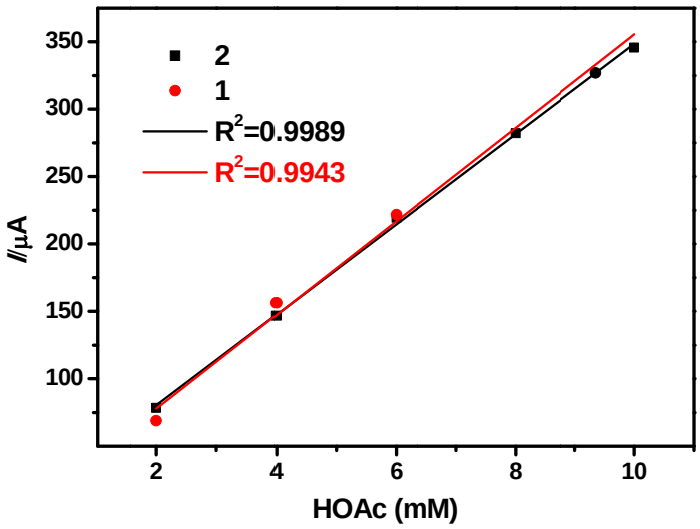

Figure S36 Dependence of current heights of the reduction events for **1** and **2** on the concentration of HOAc in CH_3CN

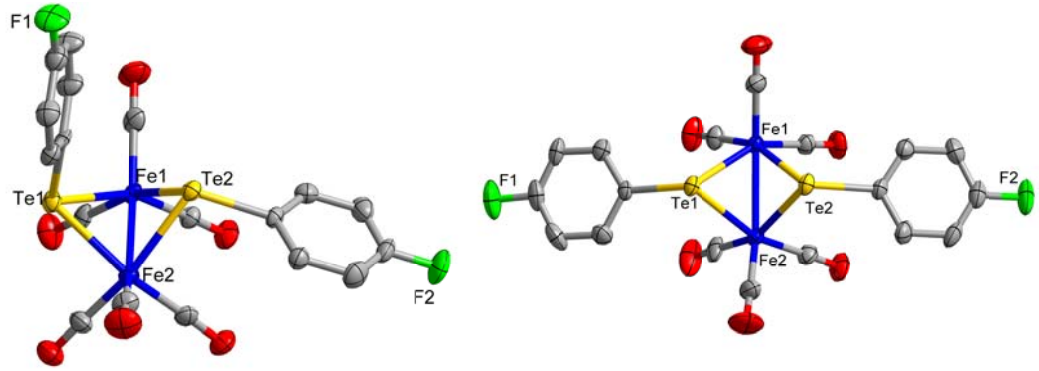

Figure S37. Molecular structures of compounds **B-*anti***: (left) and **B-*syn*** (right) with thermal ellipsoids at 30% probability. Selected distance (Å) and angles (º) for **B-*anti***: Fe(1)-Fe(2) 2.6268(17) Te(1)-Fe(1) 2.5443(14) Te(1)-Fe(2) 2.5466(14) Fe(1)-Te(1)-Fe(2) 62.13(4) Fe(2)-Te(2)-Fe(1) 61.87(4).
For **B-*syn***: Fe(1)-Fe(2) 2.5897(12) Te(1)-Fe(1) 2.5542(9) Te(1)-Fe(2) 2.5554(9) Fe(1)-Te(1)-Fe(2) 60.91(3) Fe(1)-Te(2)-Fe(2) 60.98(3)

Table S1. Crystal data and structure refinement parameters for **1-*anti***, **2-*anti***, **2-*syn*** **and 4-6**.

compound	**1-*anti***	**2-*anti***	**2-*syn***	**4·CH_2Cl_2**	**5**	**6**
Mol formula	$C_{52}H_{40}Fe_2O_4P_2Te_2$	$C_{52}H_{38}F_2Fe_2O_4P_2Te_2$	$C_{52}H_{38}F_2Fe_2O_4P_2Te_2$	$C_{79}H_{56}Cl_2F_6Fe_4O_6P_2Te_6$	$C_{20}H_{28}FeO_2P_2Te_2$	$C_{20}H_{26}F_2FeO_2P_2Te_2$
Mol wt	1157.68	1193.66	1193.66	2337.08	673.41	709.40
Wavelength (Å)	0.71073	1.54178	0.71073	0.71073	0.71073	0.71073
Cryst syst	Trigonal	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	P3(1)	P2(1)	P2(1)/n	P2(1)/c	P2(1)/c	P-1
a /Å	11.0760(11)	14.4916(10)	15.7523(13)	10.5984(9)	16.7672(15)	10.5443(8)
b /Å	11.0760(11)	21.8071(11)	18.9568(16)	28.117(3)	16.7707(15)	11.4210(9)
c /Å	34.329(3)	17.8631(12)	17.0727(14)	27.262(3)	9.2532(8)	12.3027(11)
α /deg	90	90	90	90	90	73.951(2)
β /deg	90	112.899(4)	108.237(3)	100.664(3)	104.480(4)	76.513(2)
γ/deg	120	90	90	90	90	66.4360(10)
V/Å^3	3647.2(6)	5200.2(6)	4842.1(7)	7983.7(13)	2171.1(10)	1292.38(18)
Z	3	4	4	4	4	2
D_c/gcm^{-3}	1.581	1.525	1.637	1.944	1.775	1.823
abs coeff/mm^{-1}	1.881	14.128	1.898	3.033	3.008	2.947
F(000)	1710	2344	2344	4448	1296	680
index ranges	-13≤ h ≤ 13 -13≤ k ≤13 -40≤ l ≤34	-17 ≤ h ≤ 14 -25 ≤ k ≤ 22 -21 ≤ l ≤ 21	-18≤ h ≤18 -22≤ k ≤17 -20≤ l ≤ 19	-12 ≤ h ≤ 11 -33 ≤ k ≤ 27 -31 ≤ l ≤ 32	-19 ≤ h ≤19 -16 ≤ k ≤19 -10≤ l ≤11	-12 ≤ h ≤12 -7 ≤ k ≤13 -13 ≤ l ≤14
no. of reflns	18484	34095	24398	14068	12345	6503
no. of indepreflns	6887	13943	8538	40681	4431	4471
Goodness of fit	1.037	1.034	1.018	1.041	1.062	1.064
R	0.0731	0.0579,	0.0565,	0.0522	0.0309	0.0391
R_w	0.1625	0.1351	0.1164	0.1413	0.0741	0.0796

Table S2 Selected distances (Å) and angles (º) for **1-*anti***.

1-*anti*			
Te(1)-Fe(1)	2.559(3)	Fe(1)-C(1)	1.77(2)
Te(1)-Fe(2)	2.574(3)	Fe(1)-P(1)	2.269(6)
Te(2)-C(47)	2.146(10)	Fe(1)-Fe(2)	2.653(4)
Te(2)-Fe(2)	2.580(3)	Fe(2)-C(3)	1.760(19)
Te(2)-Fe(1)	2.597(3)	Fe(2)-C(4)	1.77(3)
Fe(1)-C(2)	1.733(18)	Fe(2)-P(2)	2.253(6)
C(2)-Fe(1)-C(1)	86.1(11)	C(3)-Fe(2)-C(4)	91.5(11)
C(2)-Fe(1)-P(1)	98.7(8)	C(3)-Fe(2)-P(2)	99.0(7)
C(1)-Fe(1)-P(1)	96.5(7)	C(4)-Fe(2)-P(2)	94.9(7)
C(2)-Fe(1)-Te(1)	91.9(9)	C(3)-Fe(2)-Te(1)	92.6(7)
C(1)-Fe(1)-Te(1)	159.5(7)	C(4)-Fe(2)-Te(1)	153.8(7)
P(1)-Fe(1)-Te(1)	103.96(18)	P(2)-Fe(2)-Te(1)	109.99(17)
C(2)-Fe(1)-Te(2)	153.3(8)	C(3)-Fe(2)-Te(2)	155.3(7)

C(1)-Fe(1)-Te(2)	90.8(7)	C(4)-Fe(2)-Te(2)	83.8(7)
P(1)-Fe(1)-Te(2)	107.92(17)	P(2)-Fe(2)-Te(2)	105.53(16)
Te(1)-Fe(1)-Te(2)	81.83(9)	Te(1)-Fe(2)-Te(2)	81.90(9)
C(2)-Fe(1)-Fe(2)	95.7(8)	C(3)-Fe(2)-Fe(1)	97.1(7)
C(1)-Fe(1)-Fe(2)	100.7(7)	C(4)-Fe(2)-Fe(1)	95.3(7)
P(1)-Fe(1)-Fe(2)	158.2(2)	P(2)-Fe(2)-Fe(1)	160.74(18)
Te(1)-Fe(1)-Fe(2)	59.14(9)	Te(1)-Fe(2)-Fe(1)	58.59(9)
Te(2)-Fe(1)-Fe(2)	58.83(9)	Te(2)-Fe(2)-Fe(1)	59.49(9)

Table S3 Selected distances (Å) and angles (º) for **2-*anti***.

2-*anti*			
Te(1)-Fe(1)	2.569(3)	Fe(1)-C(1)	1.765(18)
Te(1)-Fe(2)	2.560(3)	Fe(1)-C(2)	1.77(2)
Te(2)-Fe(2)	2.561(3)	Fe(1)-P(1)	2.244(5)
Te(2)-Fe(1)	2.582(3)	Fe(1)-Fe(2)	2.631(4)
Fe(2)-P(2)	2.224(5)	Fe(2)-C(3)	1.76(2)
Te(2)-Fe(2)	2.561(3)	Fe(2)-C(4)	1.80(2)
C(1)-Fe(1)-C(2)	95.7(9)	C(3)-Fe(2)-C(4)	94.8(9)
C(1)-Fe(1)-P(1)	94.8(5)	C(3)-Fe(2)-P(2)	95.6(6)
C(2)-Fe(1)-P(1)	92.8(7)	C(4)-Fe(2)-P(2)	95.6(8)
C(1)-Fe(1)-Te(1)	84.7(6)	C(3)-Fe(2)-Te(2)	156.3(6)
C(2)-Fe(1)-Te(1)	153.1(7)	C(4)-Fe(2)-Te(2)	90.0(6)
P(1)-Fe(1)-Te(1)	114.02(16)	P(2)-Fe(2)-Te(2)	107.00(15)
C(1)-Fe(1)-Te(2)	156.3(5)	C(3)-Fe(2)-Te(1)	84.9(6)
C(2)-Fe(1)-Te(2)	89.3(6)	C(4)-Fe(2)-Te(1)	153.0(8)
P(1)-Fe(1)-Te(2)	108.14(15)	P(2)-Fe(2)-Te(1)	111.37(18)
Te(1)-Fe(1)-Te(2)	80.58(8)	Te(2)-Fe(2)-Te(1)	80.44(8)
C(1)-Fe(1)-Fe(2)	97.4(5)	C(3)-Fe(2)-Fe(1)	97.4(6)
C(2)-Fe(1)-Fe(2)	94.1(7)	C(4)-Fe(2)-Fe(1)	94.3(7)
P(1)-Fe(1)-Fe(2)	165.40(18)	P(2)-Fe(2)-Fe(1)	162.95(18)
Te(1)-Fe(1)-Fe(2)	59.38(8)	Te(2)-Fe(2)-Fe(1)	59.07(8)
Te(2)-Fe(1)-Fe(2)	59.11(8)	Te(1)-Fe(2)-Fe(1)	59.13(8)

Table S4 Selected distances (Å) and angles (º) for **2-*syn***.

2-*syn*			
Te(1)-Fe(1)	2.5759(9)	Fe(1)-C(2)	1.759(8)
Te(1)-Fe(2)	2.5856(10)	Fe(1)-C(1)	1.768(7)
Te(2)-C(11)	2.144(6)	Fe(1)-P(1)	2.2818(18)
Te(2)-Fe(1)	2.5882(9)	Fe(1)-Fe(2)	2.6516(12)
Te(2)-Fe(2)	2.5957(9)	Fe(2)-C(4)	1.749(7)
F(1)-C(14)	1.379(8)	Fe(2)-C(3)	1.764(8)
F(2)-C(8)	1.373(7)	Fe(2)-P(2)	2.2735(18)
C(2)-Fe(1)-C(1)	88.7(3)	C(4)-Fe(2)-C(3)	88.8(3)
C(2)-Fe(1)-P(1)	100.3(2)	C(4)-Fe(2)-P(2)	101.3(2)

C(1)-Fe(1)-P(1)	101.9(2)	C(3)-Fe(2)-P(2)	100.2(2)
C(2)-Fe(1)-Te(1)	90.5(2)	C(4)-Fe(2)-Te(1)	93.5(2)
C(1)-Fe(1)-Te(1)	154.0(2)	C(3)-Fe(2)-Te(1)	157.0(2)
P(1)-Fe(1)-Te(1)	103.80(5)	P(2)-Fe(2)-Te(1)	101.68(5)
C(2)-Fe(1)-Te(2)	157.3(2)	C(4)-Fe(2)-Te(2)	154.4(2)
C(1)-Fe(1)-Te(2)	90.9(2)	C(3)-Fe(2)-Te(2)	88.4(2)
P(1)-Fe(1)-Te(2)	102.06(5)	P(2)-Fe(2)-Te(2)	104.19(5)
Te(1)-Fe(1)-Te(2)	80.00(3)	Te(1)-Fe(2)-Te(2)	79.68(3)
C(2)-Fe(1)-Fe(2)	98.0(2)	C(4)-Fe(2)-Fe(1)	96.2(2)
C(1)-Fe(1)-Fe(2)	95.1(2)	C(3)-Fe(2)-Fe(1)	98.1(2)
P(1)-Fe(1)-Fe(2)	155.20(6)	P(2)-Fe(2)-Fe(1)	154.75(6)
Te(1)-Fe(1)-Fe(2)	59.27(3)	Te(1)-Fe(2)-Fe(1)	58.91(3)
Te(2)-Fe(1)-Fe(2)	59.37(3)	Te(2)-Fe(2)-Fe(1)	59.10(3)

Table S5 Selected distances (Å) and angles (º) for **4**.

4			
Fe(1)-C(1)	1.735(10)	Fe(3)-C(4)	1.755(10)
Fe(1)-C(2)	1.748(11)	Fe(3)-Te(3)	2.5018(14)
Fe(1)-P(1)	2.244(3)	Fe(3)-Te(4)	2.5099(14)
Fe(1)-Te(1)	2.5230(14)	Fe(3)-Te(5)	2.5417(14)
Fe(1)-Te(2)	2.5731(13)	Fe(3)-Te(6)	2.5874(14)
Fe(1)-Fe(2)	2.6731(17)	Fe(3)-Fe(4)	2.6822(18)
Fe(2)-C(3)	1.765(10)	Fe(4)-C(5)	1.747(12)
Fe(2)-Te(4)	2.5007(13)	Fe(4)-C(6)	1.760(13)
Fe(2)-Te(3)	2.5174(14)	Fe(4)-P(2)	2.253(3)
Fe(2)-Te(1)	2.5537(13)	Fe(4)-Te(5)	2.5122(15)
Fe(2)-Te(2)	2.6009(13)	Fe(4)-Te(6)	2.5667(15)
Fe(2)-Fe(3)	2.9273(17)		
C(1)-Fe(1)-C(2)	94.2(4)	C(4)-Fe(3)-Te(3)	96.1(3)
C(1)-Fe(1)-P(1)	99.4(3)	C(4)-Fe(3)-Te(4)	95.7(4)
C(2)-Fe(1)-P(1)	92.8(3)	Te(3)-Fe(3)-Te(4)	108.04(5)
C(1)-Fe(1)-Te(1)	88.9(3)	C(4)-Fe(3)-Te(5)	91.7(3)
C(2)-Fe(1)-Te(1)	161.5(3)	Te(3)-Fe(3)-Te(5)	153.27(6)
P(1)-Fe(1)-Te(1)	104.74(8)	Te(4)-Fe(3)-Te(5)	96.52(5)
C(1)-Fe(1)-Te(2)	149.0(3)	C(4)-Fe(3)-Te(6)	160.2(4)
C(2)-Fe(1)-Te(2)	86.8(3)	Te(3)-Fe(3)-Te(6)	83.74(4)
P(1)-Fe(1)-Te(2)	111.49(8)	Te(4)-Fe(3)-Te(6)	103.24(5)
Te(1)-Fe(1)-Te(2)	81.25(4)	Te(5)-Fe(3)-Te(6)	80.44(4)
C(1)-Fe(1)-Fe(2)	90.4(3)	C(4)-Fe(3)-Fe(4)	102.2(3)
C(2)-Fe(1)-Fe(2)	102.9(3)	Te(3)-Fe(3)-Fe(4)	95.90(5)
P(1)-Fe(1)-Fe(2)	160.91(9)	Te(4)-Fe(3)-Fe(4)	148.34(6)
Te(1)-Fe(1)-Fe(2)	58.79(4)	Te(5)-Fe(3)-Fe(4)	57.41(4)
Te(2)-Fe(1)-Fe(2)	59.40(4)	Te(6)-Fe(3)-Fe(4)	58.26(4)
C(3)-Fe(2)-Te(4)	97.9(3)	C(4)-Fe(3)-Fe(2)	93.0(3)

C(3)-Fe(2)-Te(3)	96.4(3)	Te(3)-Fe(3)-Fe(2)	54.57(4)
Te(4)-Fe(2)-Te(3)	107.84(5)	Te(4)-Fe(3)-Fe(2)	54.11(4)
C(3)-Fe(2)-Te(1)	90.2(3)	Te(5)-Fe(3)-Fe(2)	150.57(6)
Te(4)-Fe(2)-Te(1)	151.96(6)	Te(6)-Fe(3)-Fe(2)	102.84(5)
Te(3)-Fe(2)-Te(1)	97.76(5)	Fe(4)-Fe(3)-Fe(2)	148.39(6)
C(3)-Fe(2)-Te(2)	161.0(3)	C(5)-Fe(4)-C(6)	92.3(5)
Te(4)-Fe(2)-Te(2)	83.84(4)	C(5)-Fe(4)-P(2)	98.7(3)
Te(3)-Fe(2)-Te(2)	101.02(5)	C(6)-Fe(4)-P(2)	91.3(3)
Te(1)-Fe(2)-Te(2)	80.14(4)	C(5)-Fe(4)-Te(5)	90.2(3)
C(3)-Fe(2)-Fe(1)	102.6(3)	C(6)-Fe(4)-Te(5)	163.0(3)
Te(4)-Fe(2)-Fe(1)	94.31(5)	P(2)-Fe(4)-Te(5)	104.97(9)
Te(3)-Fe(2)-Fe(1)	148.40(6)	C(5)-Fe(4)-Te(6)	147.3(3)
Te(1)-Fe(2)-Fe(1)	57.67(4)	C(6)-Fe(4)-Te(6)	87.4(3)
Te(2)-Fe(2)-Fe(1)	58.38(4)	P(2)-Fe(4)-Te(6)	114.01(9)
C(3)-Fe(2)-Fe(3)	95.2(3)	Te(5)-Fe(4)-Te(6)	81.40(4)
Te(4)-Fe(2)-Fe(3)	54.40(4)	C(5)-Fe(4)-Fe(3)	89.6(3)
Te(3)-Fe(2)-Fe(3)	54.07(4)	C(6)-Fe(4)-Fe(3)	104.7(3)
Te(1)-Fe(2)-Fe(3)	151.71(6)	P(2)-Fe(4)-Fe(3)	161.71(10)
Te(2)-Fe(2)-Fe(3)	101.05(5)	Te(5)-Fe(4)-Fe(3)	58.48(4)
Fe(1)-Fe(2)-Fe(3)	146.09(6)	Te(6)-Fe(4)-Fe(3)	59.02(4)

Table S6 Selected distances (Å) and angles (º) for **5**.

5			
Te(1)-Fe(1)	2.6456(6)	Fe(1)-C(2)	1.741(5)
Te(2)-Fe(1)	2.6440(7)	Fe(1)-C(1)	1.749(5)
Fe(1)-P(2)	2.2785(14)	Fe(1)-P(1)	2.2784(14)
C(2)-Fe(1)-C(1)	94.7(2)	C(2)-Fe(1)-Te(2)	176.64(16)
C(2)-Fe(1)-P(1)	88.89(18)	C(1)-Fe(1)-Te(2)	88.16(16)
C(1)-Fe(1)-P(1)	93.38(16)	P(1)-Fe(1)-Te(2)	92.79(4)
C(2)-Fe(1)-P(2)	90.50(18)	P(2)-Fe(1)-Te(2)	87.61(4)
C(1)-Fe(1)-P(2)	90.79(16)	C(2)-Fe(1)-Te(1)	93.96(15)
P(1)-Fe(1)-P(2)	175.82(5)	C(1)-Fe(1)-Te(1)	171.30(16)
Te(2)-Fe(1)-Te(1)	83.268(19)	P(1)-Fe(1)-Te(1)	85.62(4)
P(2)-Fe(1)-Te(1)	90.29(4)		

Table S7 Selected distances (Å) and angles (º) for **6**.

6			
Fe(1)-C(1)	1.757(6)	Fe(1)-P(1)	2.2841(17)
Fe(1)-C(2)	1.762(7)	Fe(1)-Te(2)	2.6378(9)
Fe(1)-P(2)	2.2824(17)	Fe(1)-Te(1)	2.6489(8)
C(1)-Fe(1)-C(2)	94.5(3)	P(2)-Fe(1)-Te(2)	90.59(5)
C(1)-Fe(1)-P(2)	91.17(19)	P(1)-Fe(1)-Te(2)	87.57(5)

C(2)-Fe(1)-P(2)	89.57(19)	C(1)-Fe(1)-Te(1)	175.3(2)
C(1)-Fe(1)-P(1)	89.96(19)	C(2)-Fe(1)-Te(1)	90.12(19)
C(2)-Fe(1)-P(1)	92.13(19)	P(2)-Fe(1)-Te(1)	87.92(5)
P(2)-Fe(1)-P(1)	177.88(7)	P(1)-Fe(1)-Te(1)	90.81(5)
C(1)-Fe(1)-Te(2)	92.0(2)	Te(2)-Fe(1)-Te(1)	83.36(3)
C(2)-Fe(1)-Te(2)	173.46(19)	C(3)-Te(1)-Fe(1)	105.08(15)
C(9)-Te(2)-Fe(1)	107.02(16)		