

Supporting Information

Synthesis of Aryl Cobalt and Iron Complexes and their Catalytic Activity on Hydrosilylation of Alkenes

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S1. Crystallographic Data for Complexes 1-7

complex	1	2	4	6	7
formula	C ₁₄ H ₂₇ ClCoF ₄ NP ₃	C ₁₇ H ₃₆ F ₄ FeNP ₄	C ₁₅ H ₂₇ ClF ₅ FeP ₃	C ₂₂ H ₃₂ CoF ₄ NP ₃	C ₂₅ H ₃₇ CoP ₃
<i>M</i> _z	472.65	510.20	486.57	538.32	489.38
crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
space group	Cc	P2 ₁ /c	C2/c	P2 ₁ /c	P2 ₁
a [Å]	9.2381(2)	8.9999(2)	15.0248(3)	18.3827(5)	8.8303(2)
b [Å]	15.2301(4)	10.1154(2)	9.0984(2)	8.7737(2)	16.4996(4)
c [Å]	15.7220(4)	26.2786(5)	31.9118(6)	16.3807(4)	9.2364(2)
α [$^{\circ}$]	90	90	90	90	90
β [$^{\circ}$]	106.586(3)	98.2920(18)	95.403(2)	102.742(3)	96.734(2)
γ [$^{\circ}$]	90	90	90	90	90
V [Å ³]	2119.99(9)	2367.33(9)	4343.01(15)	2576.89(11)	1336.43(5)
T [K]	173.00(10)	172.99(10)	173	173.0	173
Z	4	4	8	4	2
μ [mm ⁻¹]	9.947	7.981	9.162	7.327	6.781
total reflns	6948	15188	12589	14681	18004
unique reflns	2431	4177	3806	4564	5375
R _{int}	0.0528	0.0527	0.0547	0.0703	0.0723
R ₁ [I>2σ(I)]	0.0308	0.0442	0.0433	0.0594	0.0450
wR(F ²)[I>2σ(I)]	0.0753	0.1082	0.1049	0.1361	0.1170
R ₁ (all data)	0.0322	0.0492	0.0489	0.0761	0.0511
wR(F ²)(all data)	0.0760	0.1108	0.1079	0.1456	0.1200
GOF on F ²	1.029	1.055	1.025	1.075	1.212

S2 IR spectra of complexes 1-7

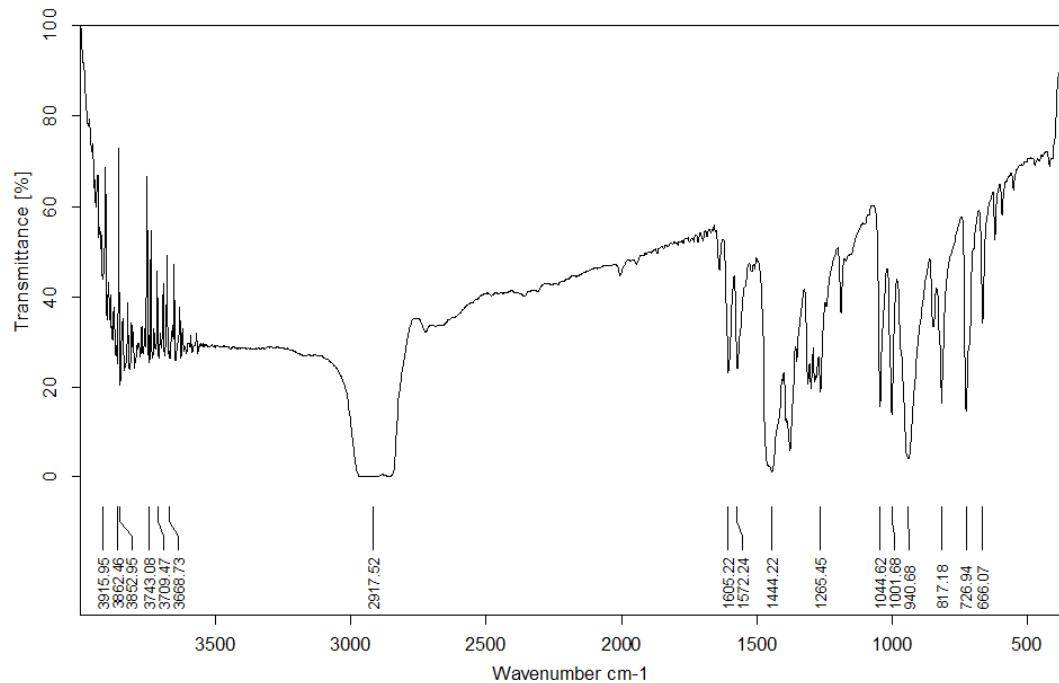


Fig.S1 IRspectrum of complex 1

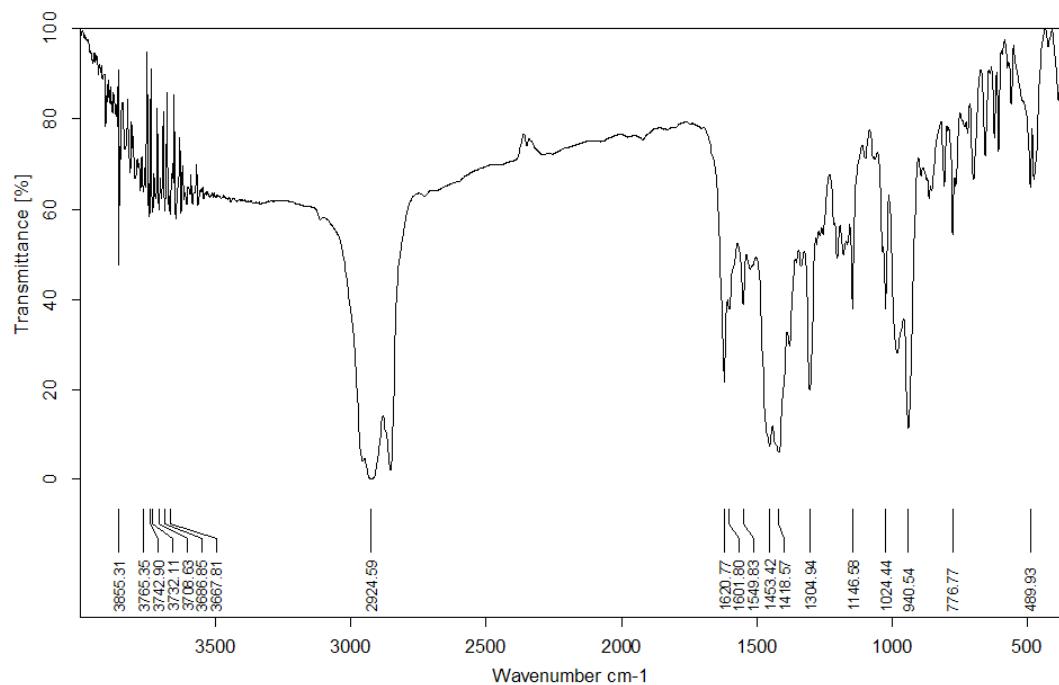


Fig.S2 IR spectrum of complex 2

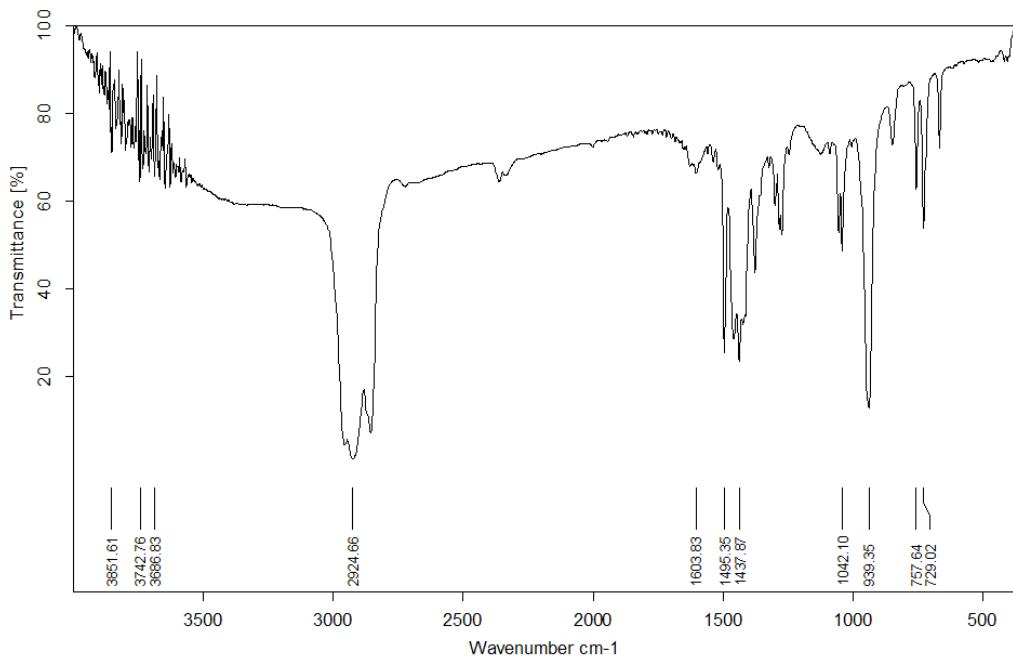


Fig.S3 IR spectrum of complex 4

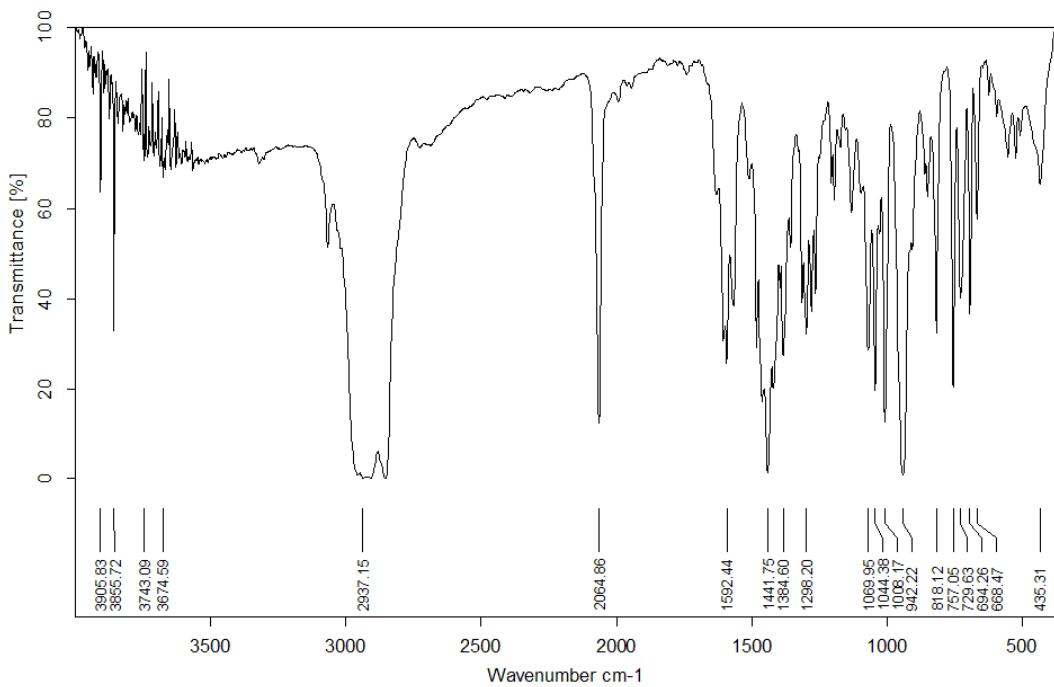


Fig.S4 IR spectrum of complex 6

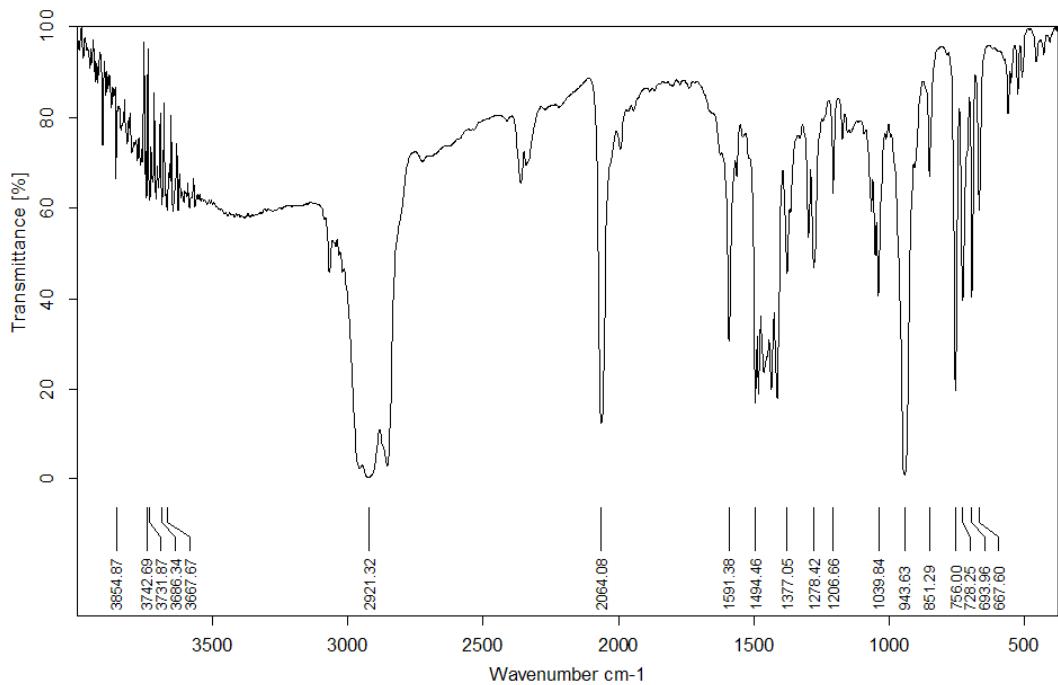


Fig.S5 IR spectrum of complex 7

S3 Mass spectrum of complex 5

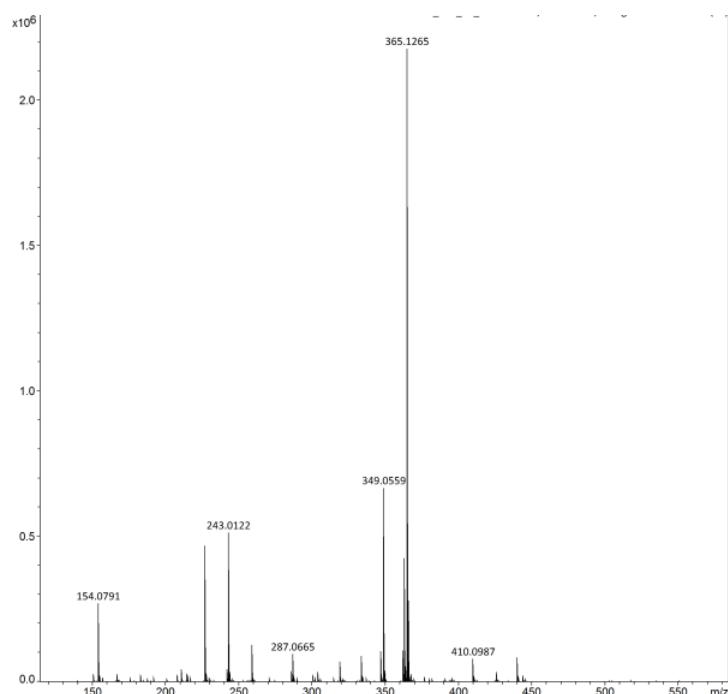


Fig.S6 Mass spectrum of complex 5

S4 ^1H NMR and ^{13}C NMR Spectra of Hydrosilylation Products

Diphenyl(1-phenylethyl)silane (2a**)¹**

^1H NMR (300 MHz, CDCl_3): δ (ppm) 7.45-7.43 (m, 2H), 7.42-7.35 (m, 2H), 7.31-7.21 (m, 5H), 7.18-7.15 (m, 2H), 7.00-6.98 (m, 3H), 6.88-6.78 (m, 1H), 4.74 (d, $J = 6.0$ Hz, 1H), 2.72 (qd, $J = 9.0, 3.0$ Hz, 1H), 1.36 (d, $J = 6.0$ Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3): δ (ppm) 146.62, 135.67, 135.52, 133.97, 132.47, 129.93, 129.30, 128.04, 127.70, 125.90, 125.05, 27.02, 16.24.

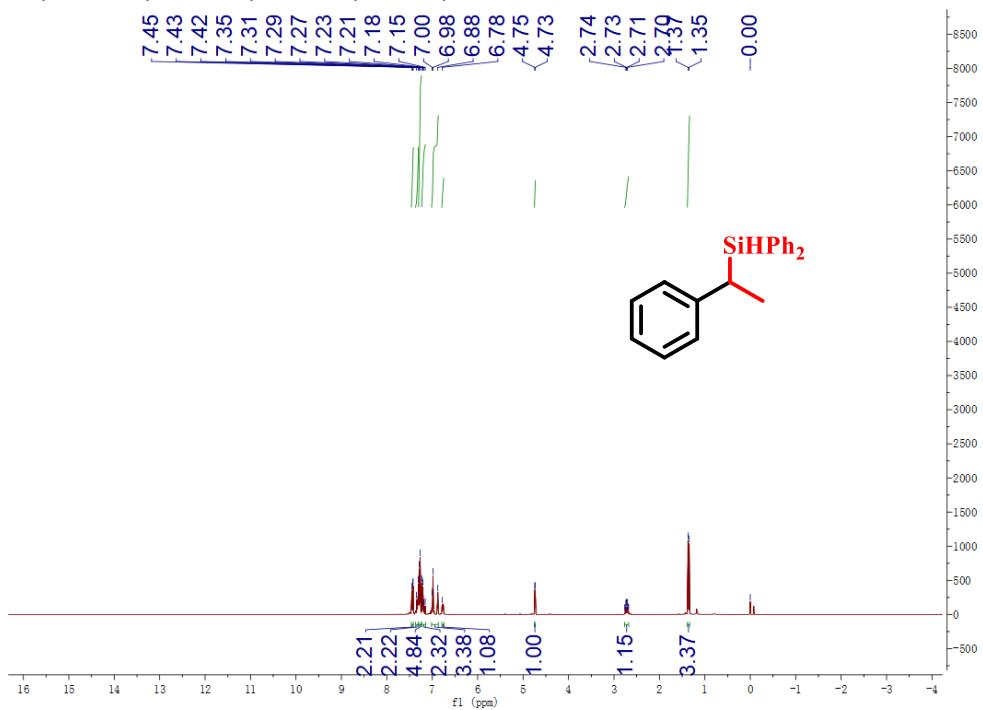


Fig.S7 ^1H NMR spectrum of **2a**

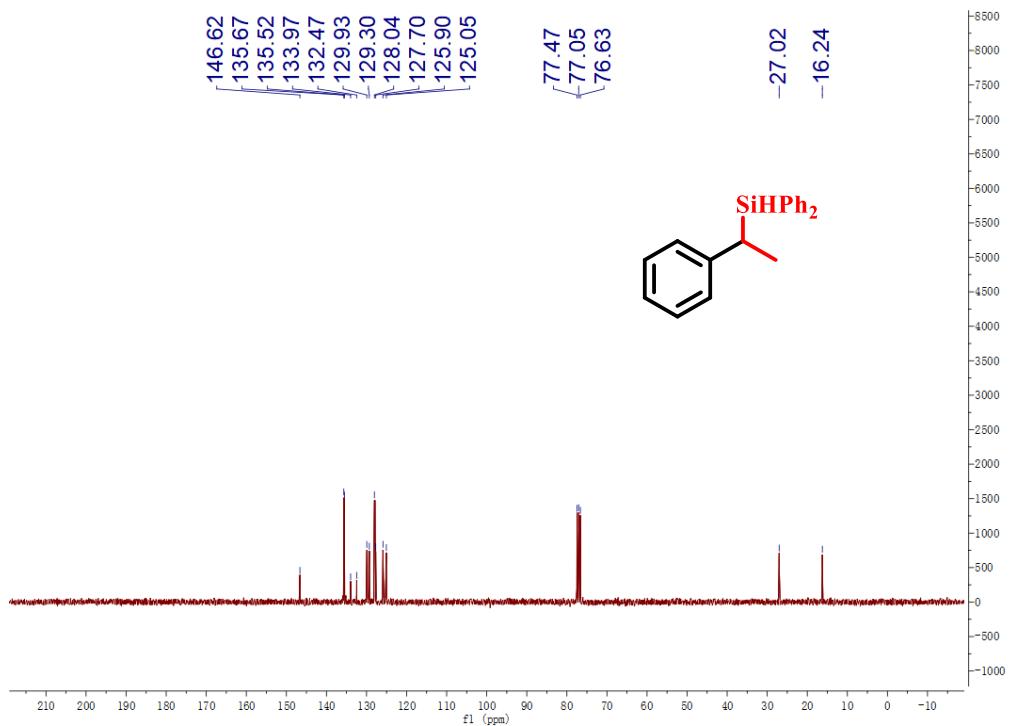


Fig.S8 ^{13}C NMR spectrum of **2a**

Diphenyl(1-(p-tolyl)ethyl)silane (2b**)¹**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.44-7.42 (m, 2H) 7.29-7.23 (m, 4H), 7.21-7.18 (m, 2H), 7.16-7.13 (m, 2H), 6.91-6.88 (m, 2H), 6.82-6.80 (m, 2H), 4.74 (d, J = 3.0 Hz, 1H), 2.69 (qd, J = 6.0, 3.0 Hz, 1H), 2.18 (s, 3H), 1.35 (d, J = 9.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 141.29, 135.83, 135.69, 134.35, 133.30, 129.76, 129.64, 129.00, 128.00, 127.83, 127.70, 26.47, 21.08, 16.83.

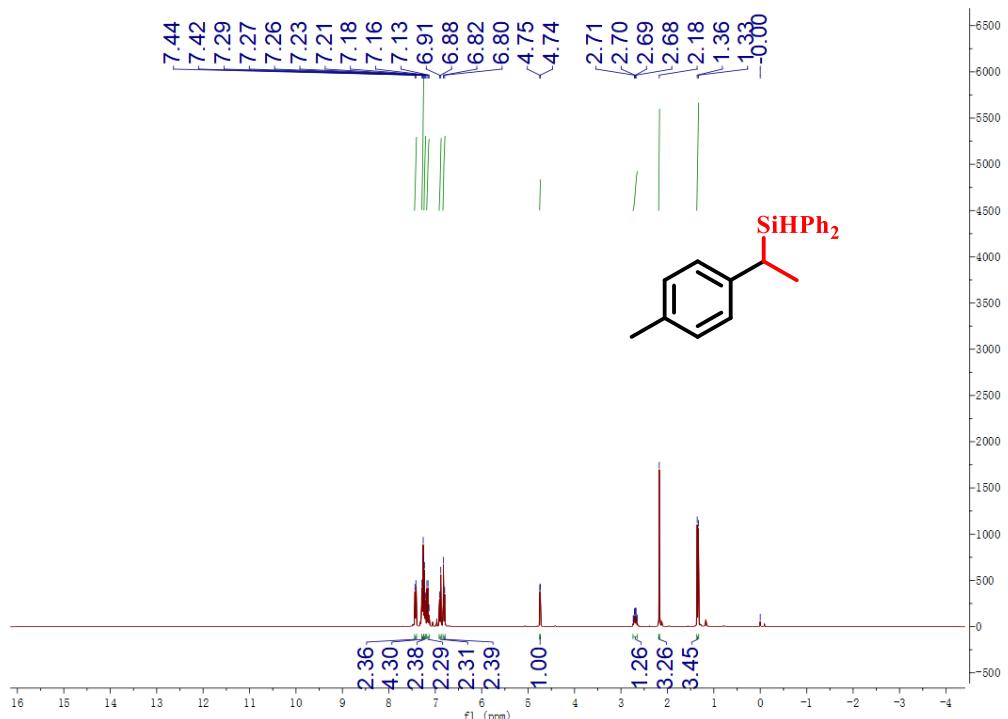


Fig.S9 ¹H NMR spectrum of **2b**

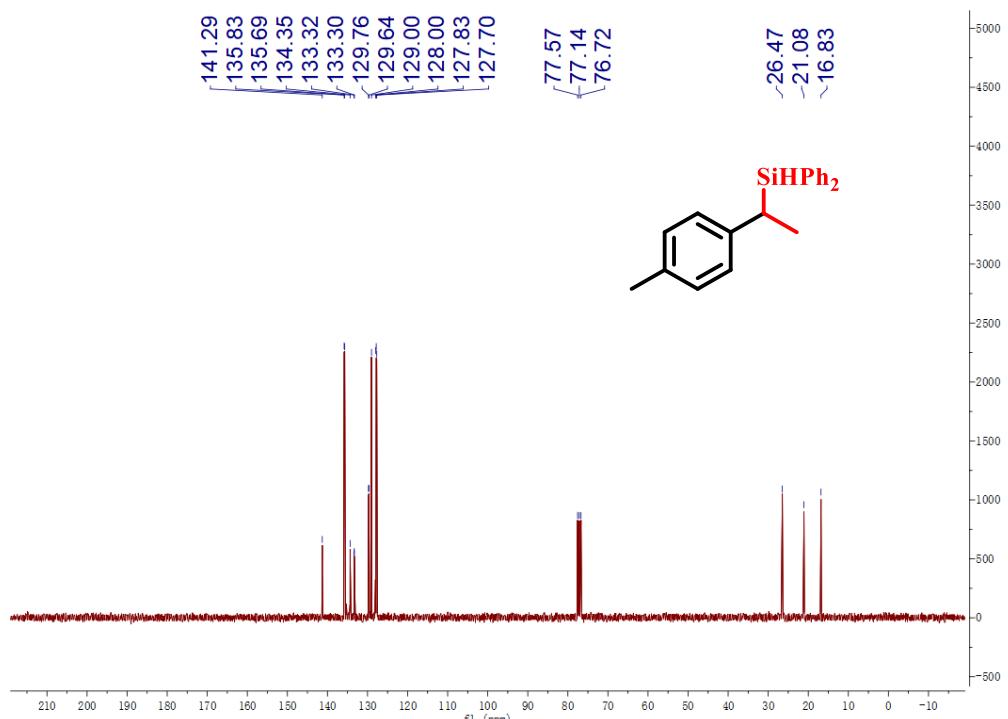


Fig.S10 ¹³C NMR spectrum of **2b**

Diphenyl(1-(m-tolyl)ethyl)silane (2c**)¹**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.41-7.38 (m, 1H), 7.24-7.08 (m, 7H), 7.13-7.10 (m, 2H), 7.08-7.6.94 (m, 1H), 6.91-6.75 (m, 1H), 6.71-6.66 (m, 2H), 4.73 (d, J = 3.0 Hz, 1H), 2.66 (qd, J = 6.0, 3.0 Hz, 1H), 2.08 (s, 3H), 1.33 (d, J = 6.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 144.37, 137.72, 135.95, 135.82, 135.38, 133.36, 129.89, 129.76, 128.87, 128.27, 127.90, 125.91, 124.94, 77.68, 77.26, 76.84, 27.06, 21.63, 16.72.

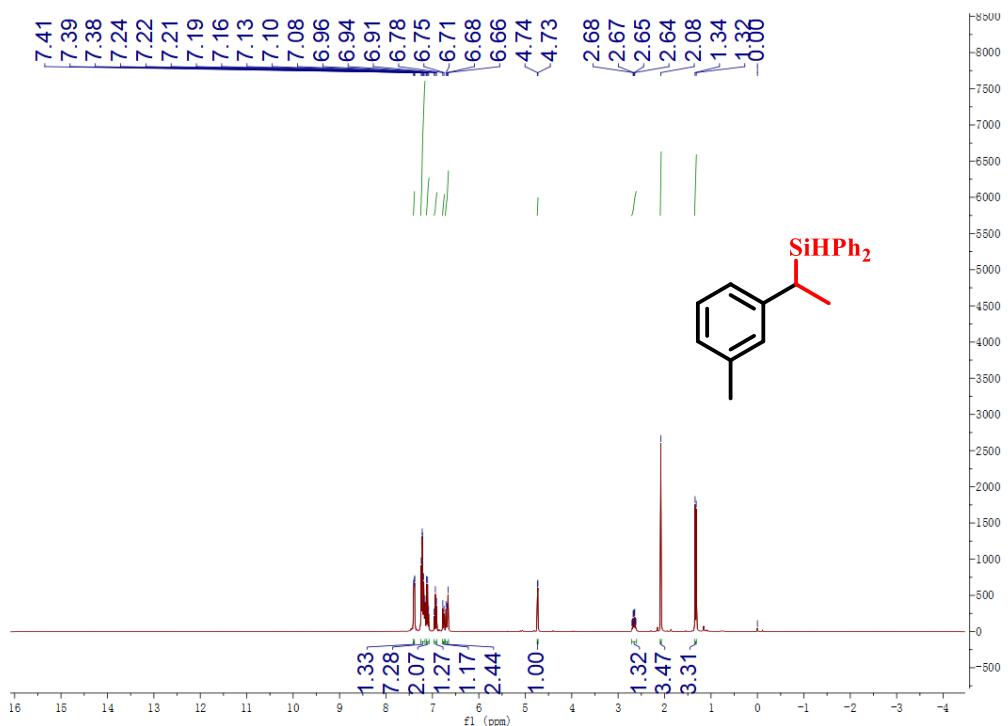


Fig.S11 ¹H NMR spectrum of **2c**

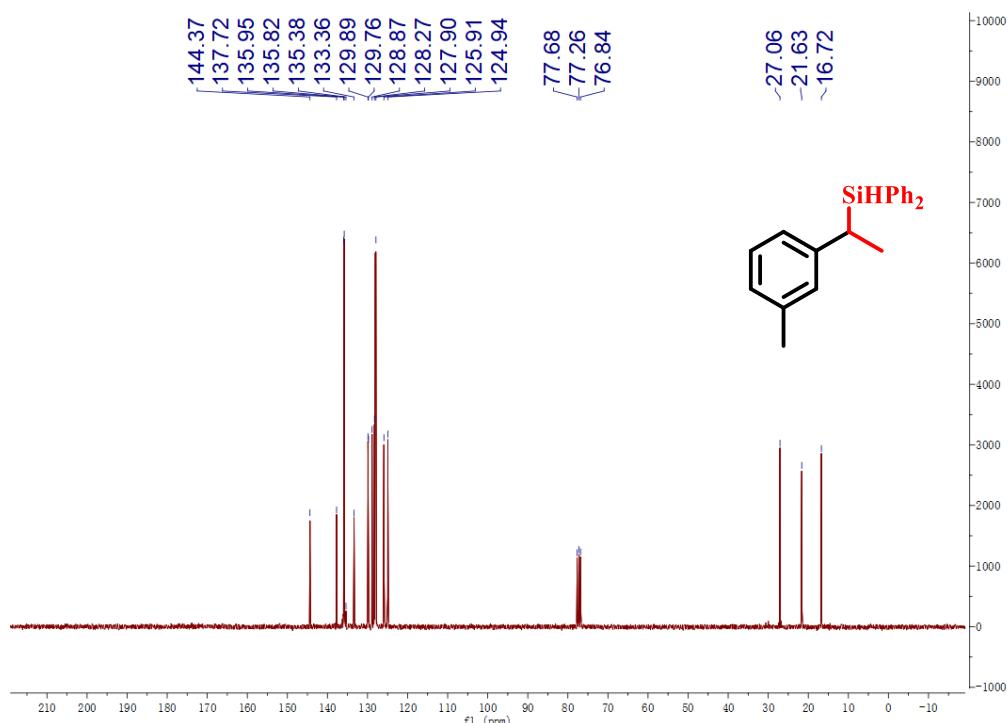


Fig.S12 ¹³C NMR spectrum of **2c**

Diphenyl(1-(o-tolyl)ethyl)silane (2d**)²**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.46-7.44 (m, 2H), 7.35-7.32 (m, 2H), 7.31-7.28 (m, 2H), 7.25-7.20 (m, 3H), 7.17 (m, 1H), 7.15 (m, 1H), 7.01-6.94 (m, 3H), 4.72 (d, J = 6.0 Hz, 1H), 2.92 (qd, J = 9.0, 3.0 Hz, 1H), 1.99 (s, 3H), 1.36 (d, J = 6.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 142.87, 135.86, 135.33, 133.38, 132.86, 130.10, 129.80, 129.57, 127.97, 127.73, 126.81, 126.08, 124.77, 77.49, 77.07, 76.64, -29.76, -20.13, -16.62.

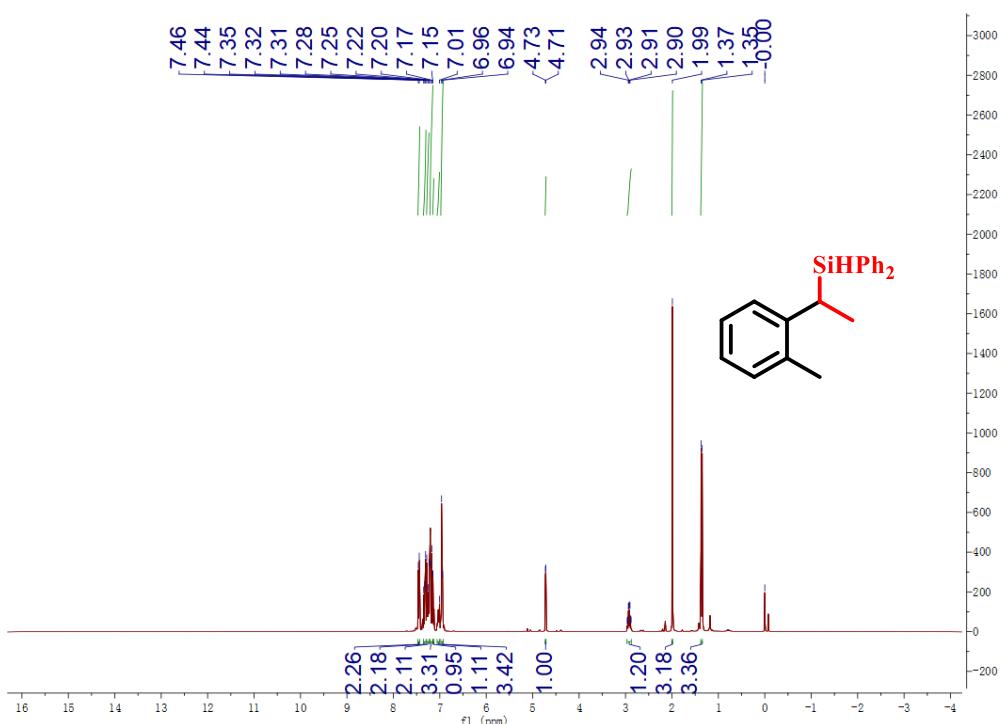


Fig.S13 ¹H NMR spectrum of **2d**

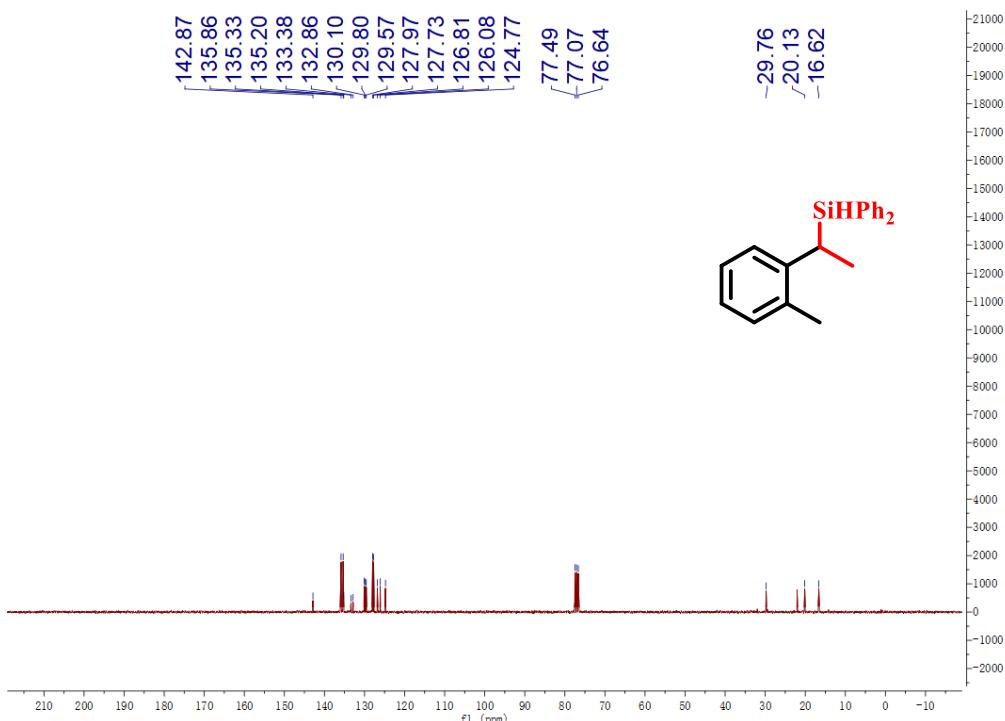


Fig.S14 ¹³C NMR spectrum of **2d**

(1-(4-methoxyphenyl)ethyl)diphenylsilane (2e**)¹**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.45-7.43 (m, 2H), 7.43-7.17 (m, 8H), 6.86-6.83 (m, 2H), 6.68-6.65 (m, 2H), 4.75 (d, J = 3.0 Hz, 1H), 3.69 (s, 3H), 2.70 (qd, J = 6.0, 3.0 Hz, 1H), 1.36 (d, J = 9.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 157.13, 136.32, 135.71, 135.59, 133.24, 129.66, 129.53, 128.55, 127.91, 127.73, 113.66, 55.24, 25.82, 16.87.

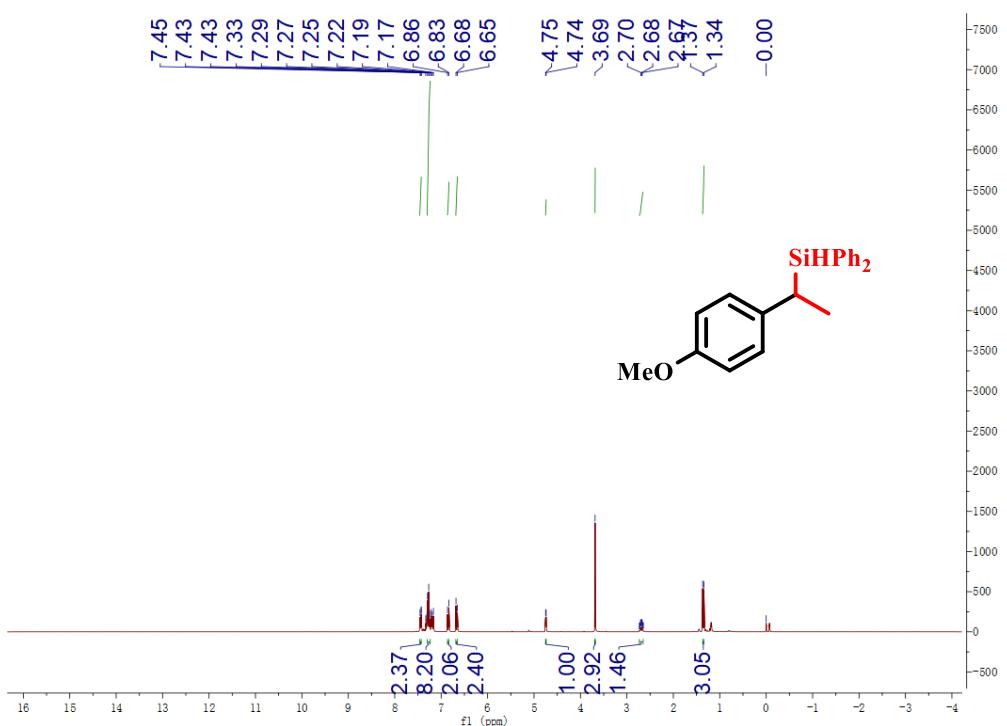


Fig.S15 ¹H NMR spectrum of **2e**

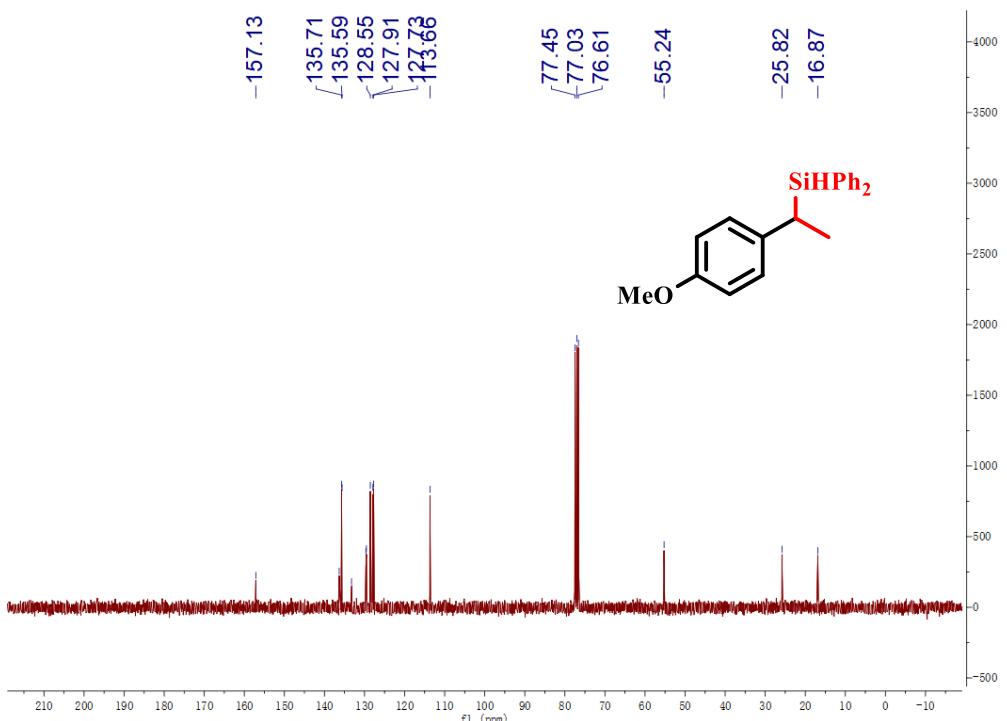


Fig.S16 ¹³C NMR spectrum of **2e**

(1-(4-(tert-butyl)phenyl)ethyl)diphenylsilane (2f**)¹**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.42-7.39 (m, 2H), 7.27-7.25 (m, 2H), 7.23-7.21 (m, 2H), 7.19-7.18 (m, 2H), 7.13-7.08 (m, 4H), 6.86-6.83 (m, 2H), 4.74 (d, J = 6.0 Hz, 1H), 2.69 (qd, J = 6.0, 3.0 Hz, 1H), 1.34 (d, J = 6.0 Hz, 3H), 1.22 (s, 9H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 147.84, 141.25, 135.90, 135.74, 133.41, 133.36, 129.81, 129.64, 128.05, 127.82, 127.47, 127.19, 125.19, 34.42, 31.62, 26.41, 16.68.

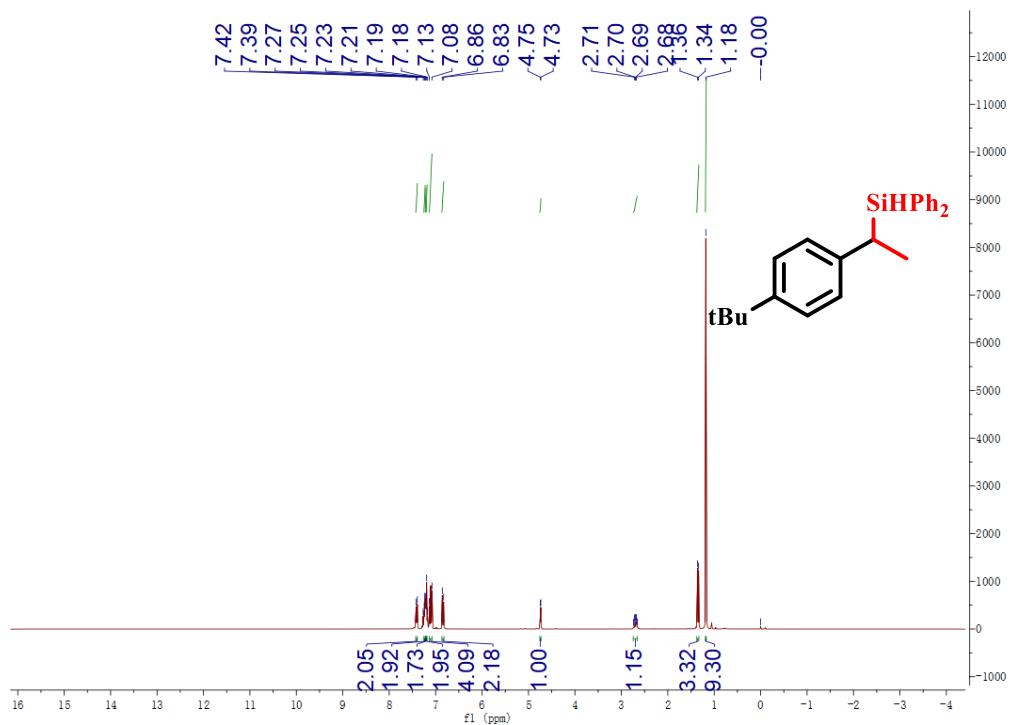


Fig.S17 ¹H NMR spectrum of **2f**

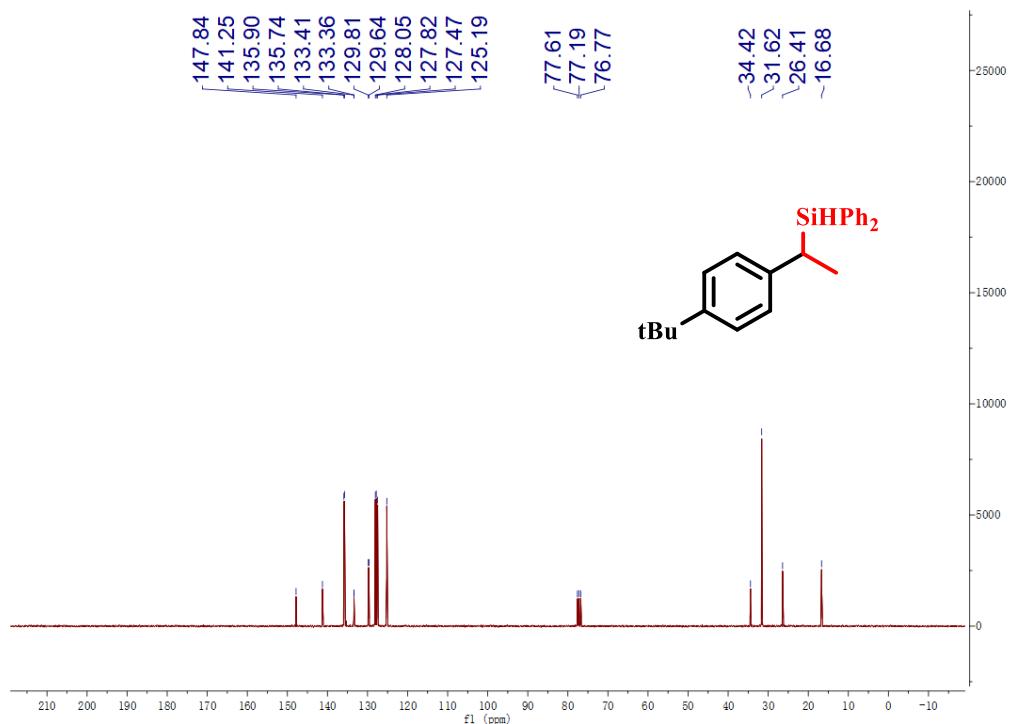


Fig.S18 ¹³C NMR spectrum of **2f**

(1-(naphthalen-1-yl)ethyl)diphenylsilane (2i)¹

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.53-7.50 (m, 1H), 7.46-7.42 (m, 2H), 7.40-7.31 (m, 2H), 7.27-7.18 (m, 6H), 7.18-7.11 (m, 3H), 7.09-7.05 (m, 2H), 7.02 (m, 1H), 4.80 (d, J = 3.0 Hz, 1H), 2.87 (qd, J = 6.0, 3.0 Hz, 1H), 1.44 (d, J = 6.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 141.01, 135.97, 135.38, 133.90, 133.23, 132.80, 131.45, 129.76, 129.62, 128.83, 127.87, 127.81, 125.55, 125.53, 125.34, 125.25, 124.09, 123.59, 21.19, 17.14.

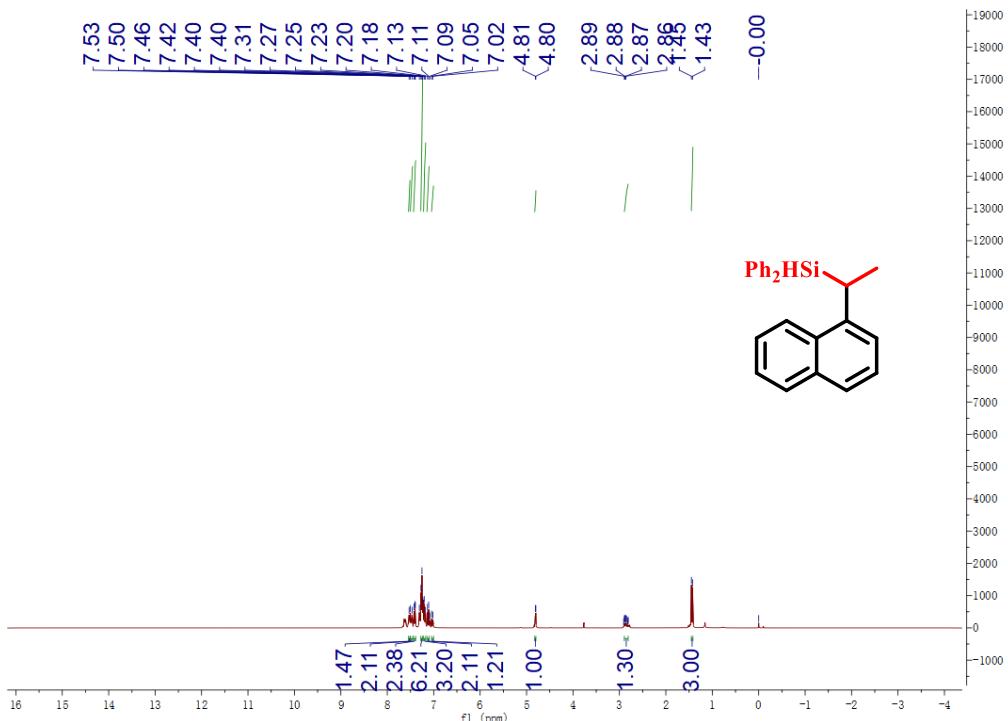


Fig.S19 ¹H NMR spectrum of 2i

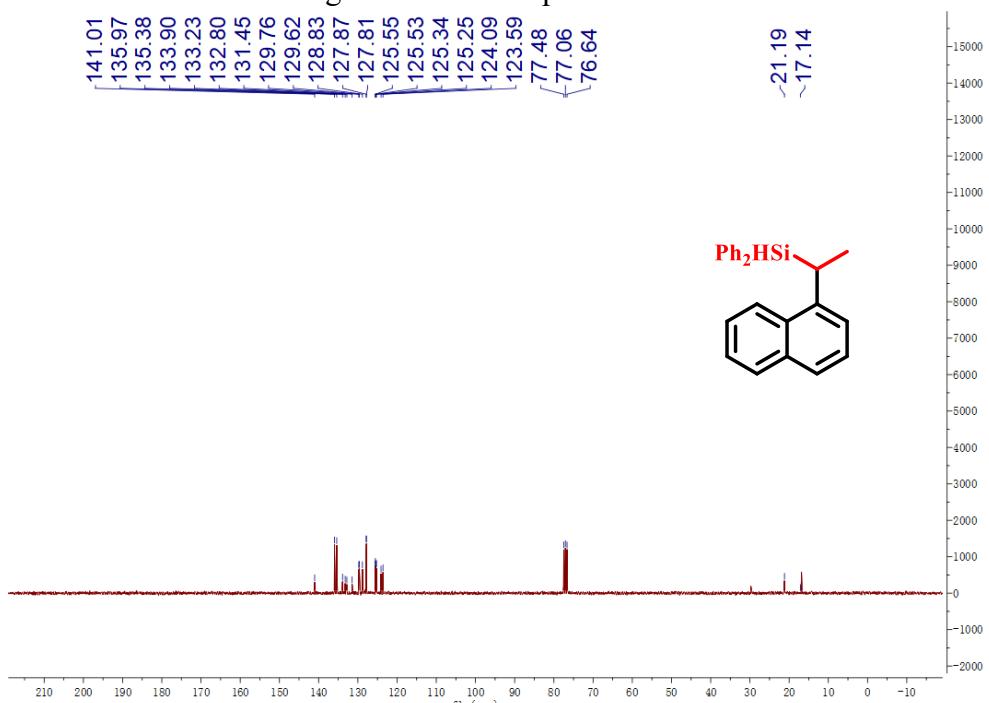


Fig.S20 ¹³C NMR spectrum of 2i

(1-(naphthalen-2-yl)ethyl)diphenylsilane (2j)¹

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.59-7.52 (m, 1H), 7.49-7.45 (m, 2H), 7.41-7.38 (m, 2H), 7.30-7.26 (m, 2H), 7.24-7.19 (m, 4H), 7.16-7.12 (m, 3H), 7.10-7.07 (m, 2H), 7.03-7.01 (m, 1H), 4.79 (d, J = 3.0 Hz, 1H), 2.86 (qd, J = 6.0, 3.0 Hz, 1H), 1.42 (d, J = 9.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 142.38, 136.07, 135.93, 135.52, 134.02, 133.23, 131.89, 130.09, 129.98, 128.42, 128.27, 128.11, 127.88, 127.67, 127.59, 126.08, 125.61, 125.09, 77.79, 77.37, 76.95, -27.55, -16.92.

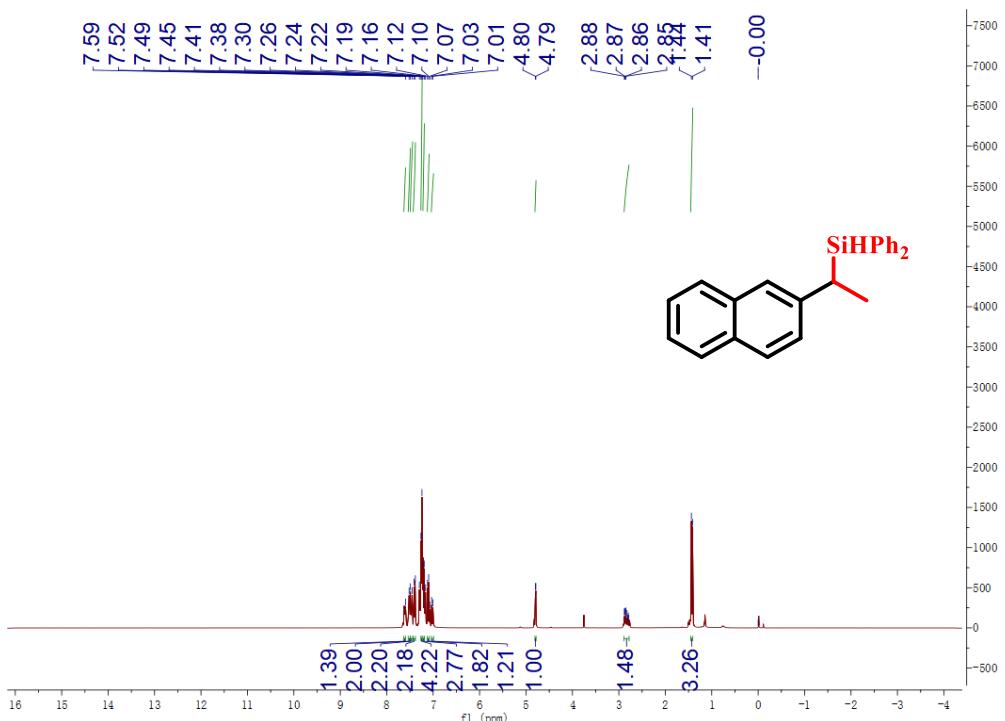


Fig.S21 ¹H NMR spectrum of 2j

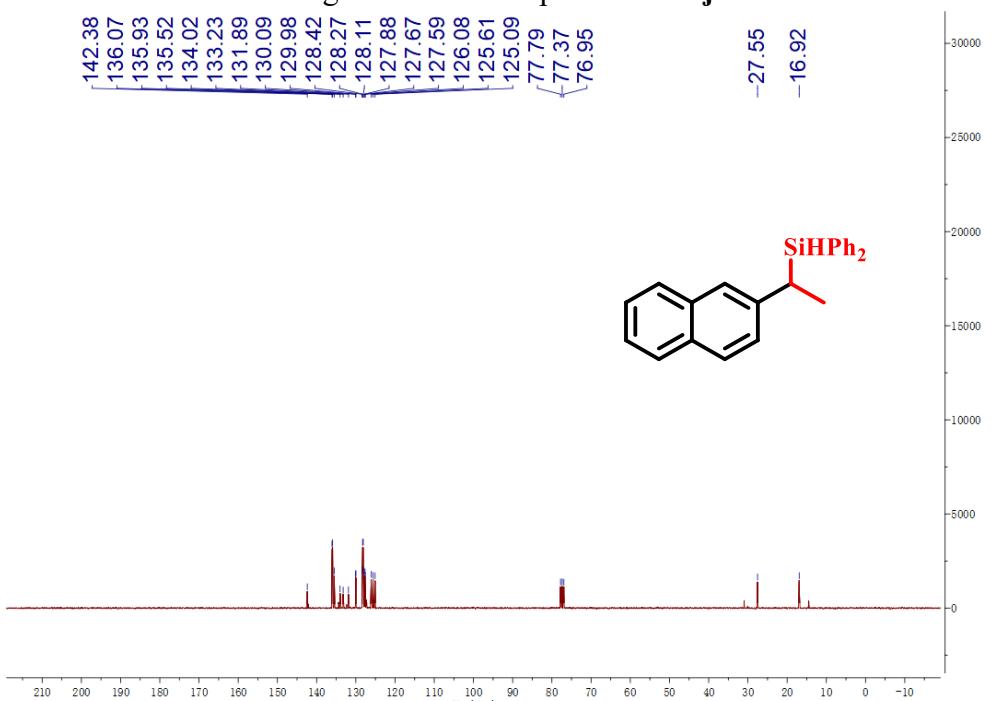


Fig.S22 ¹³C NMR spectrum of 2j

(1-(thiophen-2-yl) ethyl)diphenylsilane (2k**)¹**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.47-7.45 (m, 2H), 7.35-7.30 (m, 3H), 7.27-7.22 (m, 3H), 6.78-6.77 (m, 2H), 6.75 (m, 1H), 6.51 (m, 1H), 6.49 (m, 1H), 4.83 (d, J = 6.0 Hz, 1H), 3.04 (qd, J = 6.0, 3.0 Hz, 1H), 1.42 (d, J = 6.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 148.17, 135.70, 135.60, 132.63, 132.74, 132.63, 129.89, 129.82, 128.02, 127.88, 126.75, 122.84, 121.83, 77.49, 77.06, 76.64, -22.29, -18.09.

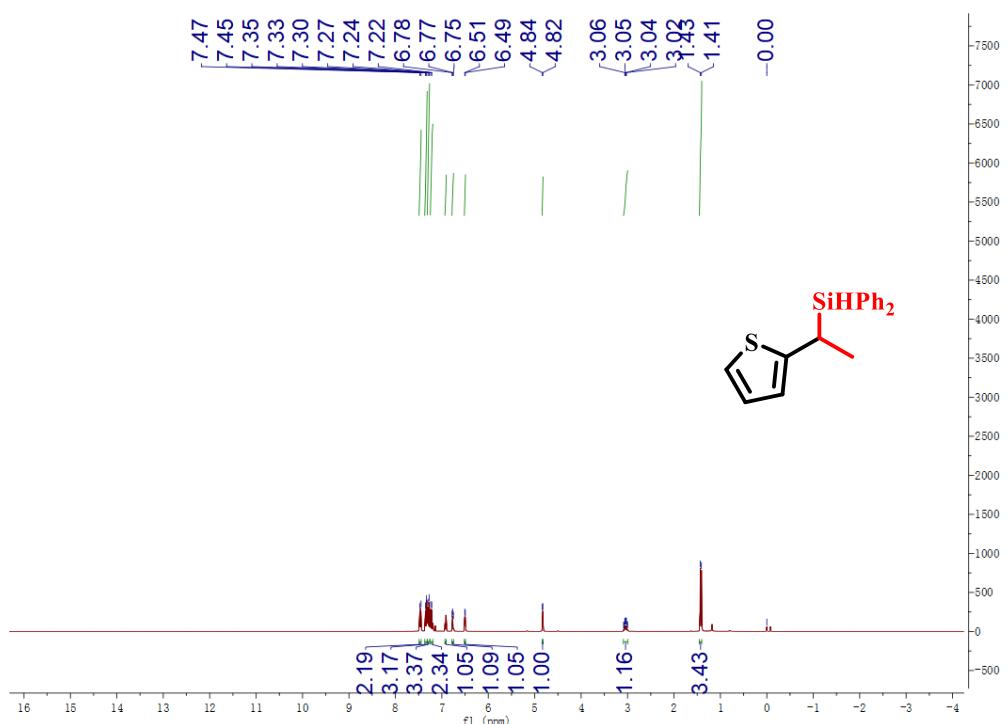


Fig.S23 ¹H NMR spectrum of **2k**

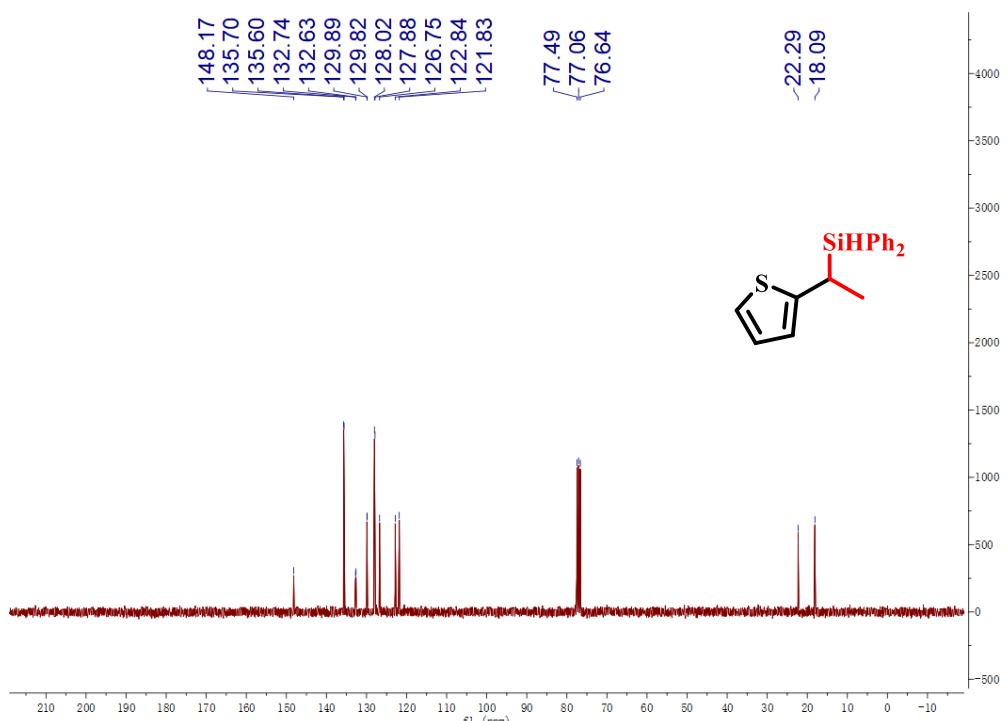


Fig.S24 ¹³C NMR spectrum of **2k**

(1-([1,1'-biphenyl]-4-yl)ethyl)diphenylsilane(2l)¹

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.45-7.43 (m, 4H), 7.41 (m, 1H), 7.32-7.29(m, 3H), 7.28-7.24 (m, 5H), 7.21 (m, 1H), 7.18 (m, 1H), 7.15-6.13 (m, 2H), 6.96-6.93 (m, 2H), 6.93 (m, 1H), 4.75 (d, J = 3.0 Hz, 1H), 2.75 (qd, J = 9.0, 3.0 Hz, 1H), 1.37 (d, J = 9.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 143.75, 141.25, 137.89, 135.93, 135.79, 133.14, 129.96, 129.84, 128.89, 128.30, 128.15, 127.98, 127.03, 127.00, 77.67, 77.24, 76.82, -26.91, -16.68.

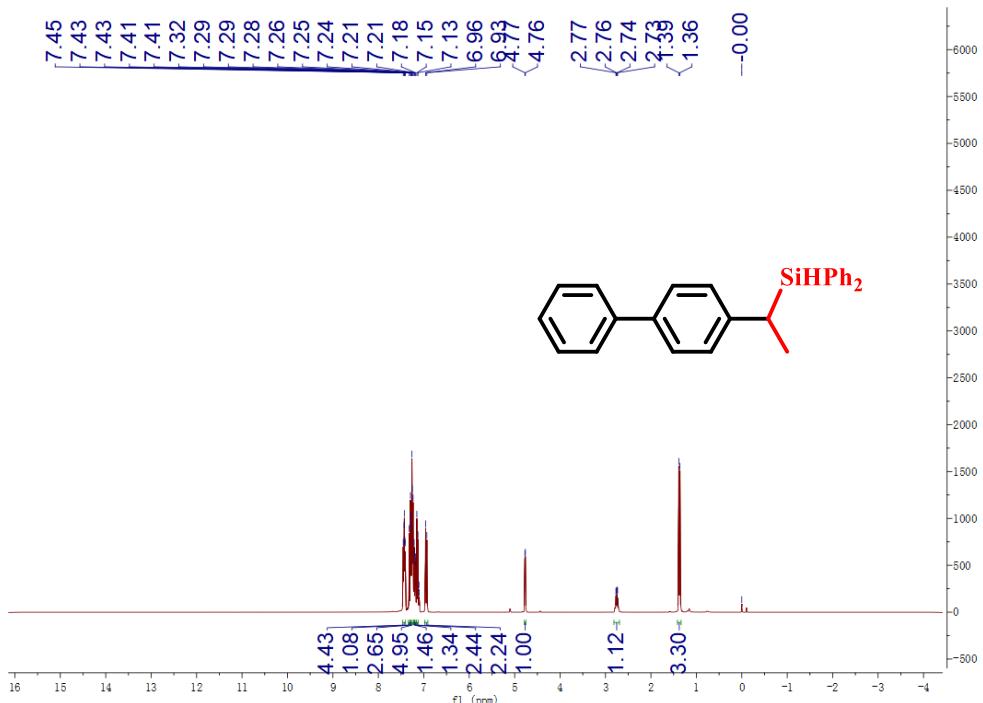


Fig.S25 ¹H NMR spectrum of 2l

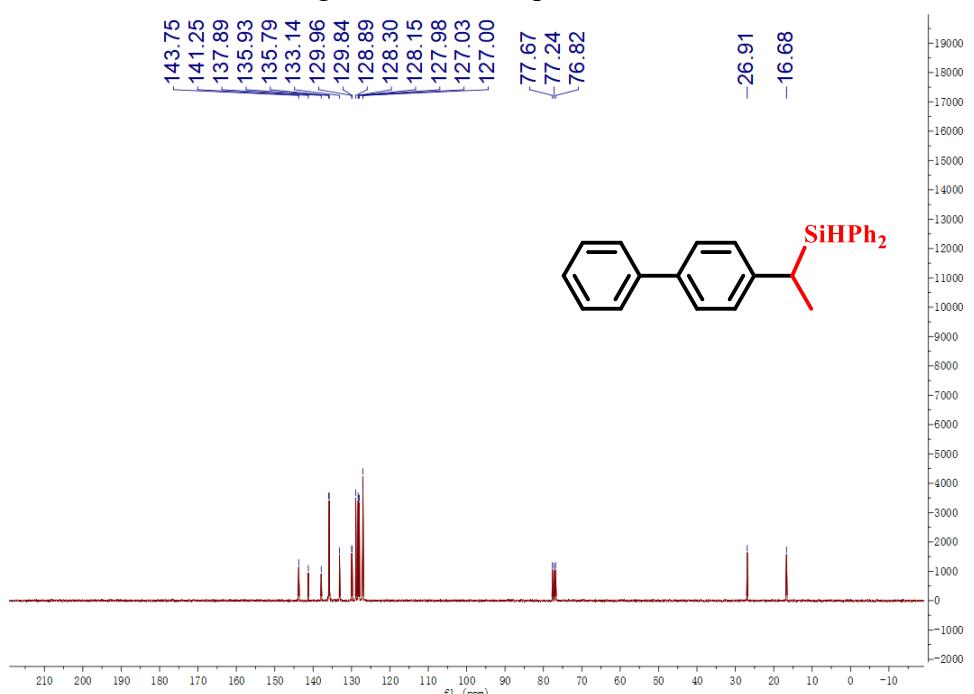


Fig.S26 ¹³C NMR spectrum of 2l

(1-(3-chlorophenyl)ethyl)diphenylsilane (2m**)³**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.45-7.43 (m, 2H), 7.35 (m, 1H), 7.32-7.21 (m, 6H), 7.18-7.15 (m, 2H), 7.00-6.98 (m, 2H), 6.88 (m, 1H), 4.74 (d, J = 6.0 Hz, 1H), 2.72 (qd, J = 9.0, 3.0 Hz, 1H), 1.36 (d, J = 6.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 146.62, 135.67, 135.52, 133.97, 132.47, 129.93, 129.82, 129.30, 128.04, 127.87, 127.70, 125.90, 125.05, 27.02, 16.24.

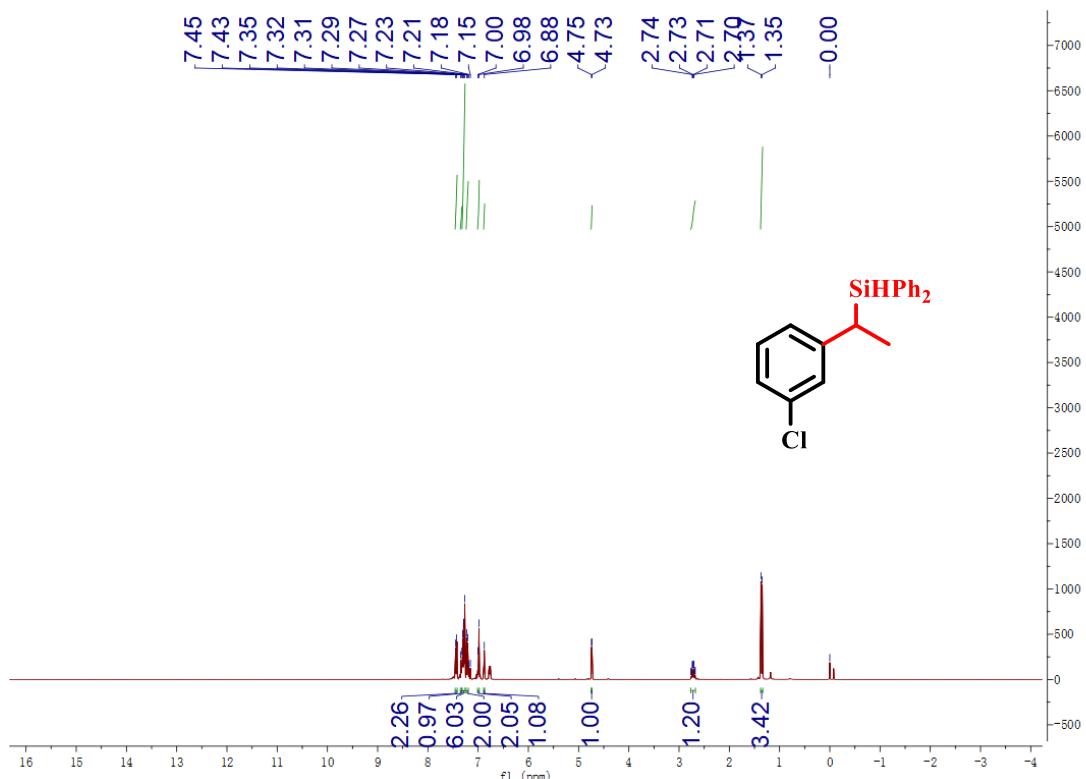


Fig.S27 ¹H NMR spectrum of **2m**

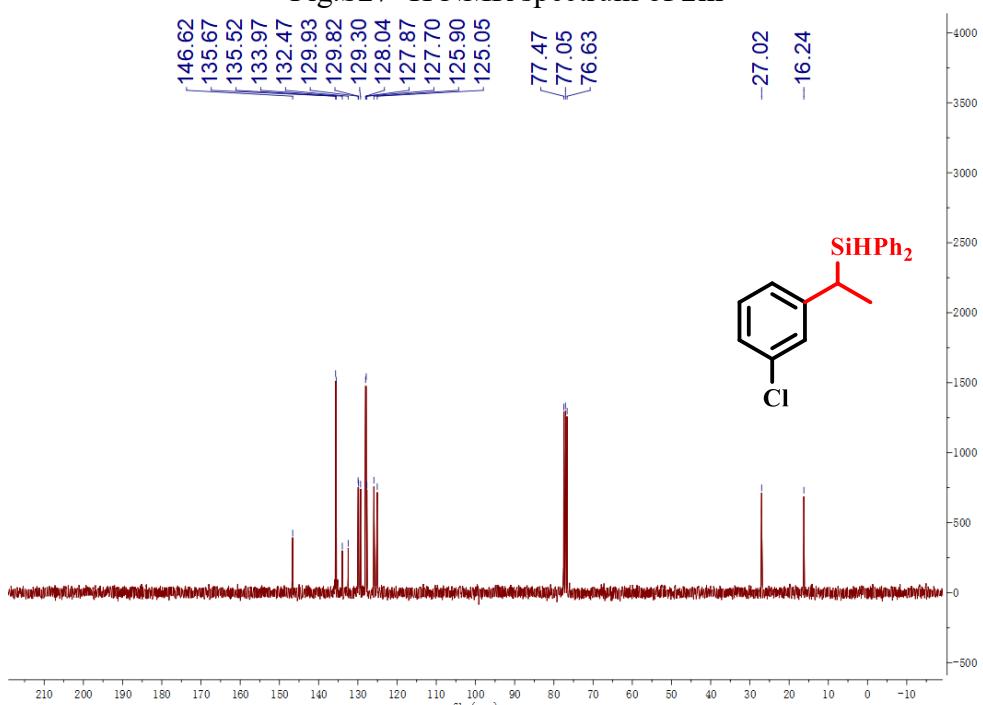


Fig.S28 ¹³C NMR spectrum of **2m**

(1-(2-chlorophenyl)ethyl)diphenylsilane (2n**)³**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.55-7.53 (m, 2H), 7.42-7.29 (m, 7H), 7.26-7.13 (m, 3H), 7.10-7.05 (m, 2H), 4.83 (d, J = 3.0 Hz, 1H), 3.45 (qd, J = 6.0, 3.0 Hz, 1H), 1.43 (d, J = 9.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 142.39, 135.88, 135.32, 135.18, 132.43, 129.87, 129.65, 129.32, 128.24, 128.07, 127.96, 127.77, 126.75, 125.97, 77.46, 77.04, 76.61, -22.79, -16.07.

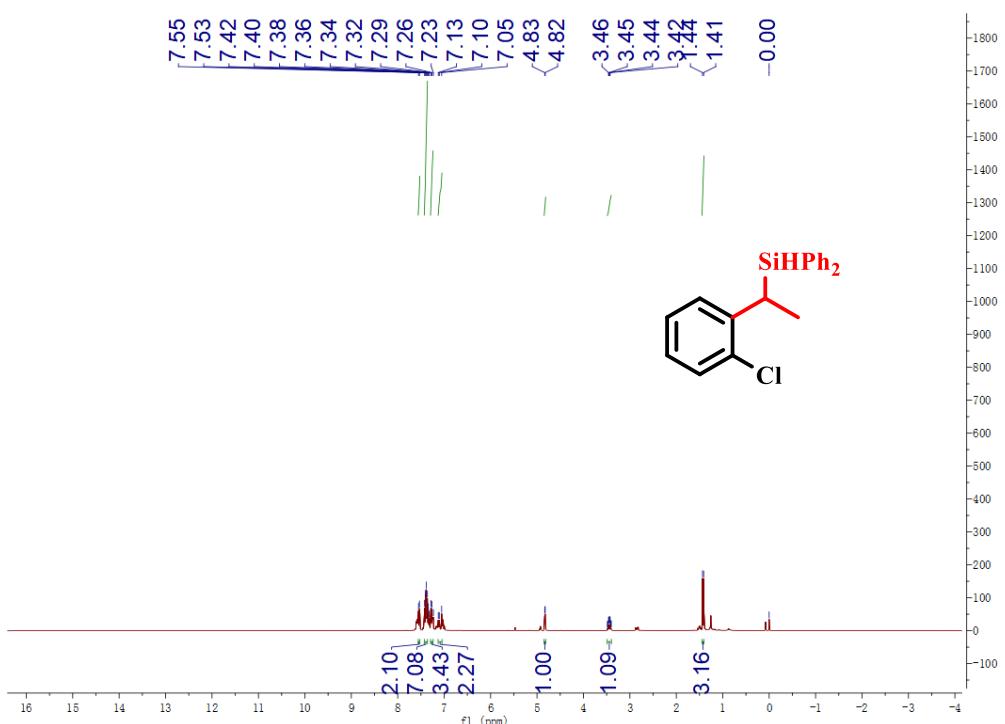


Fig.S29 ¹H NMR spectrum of **2n**

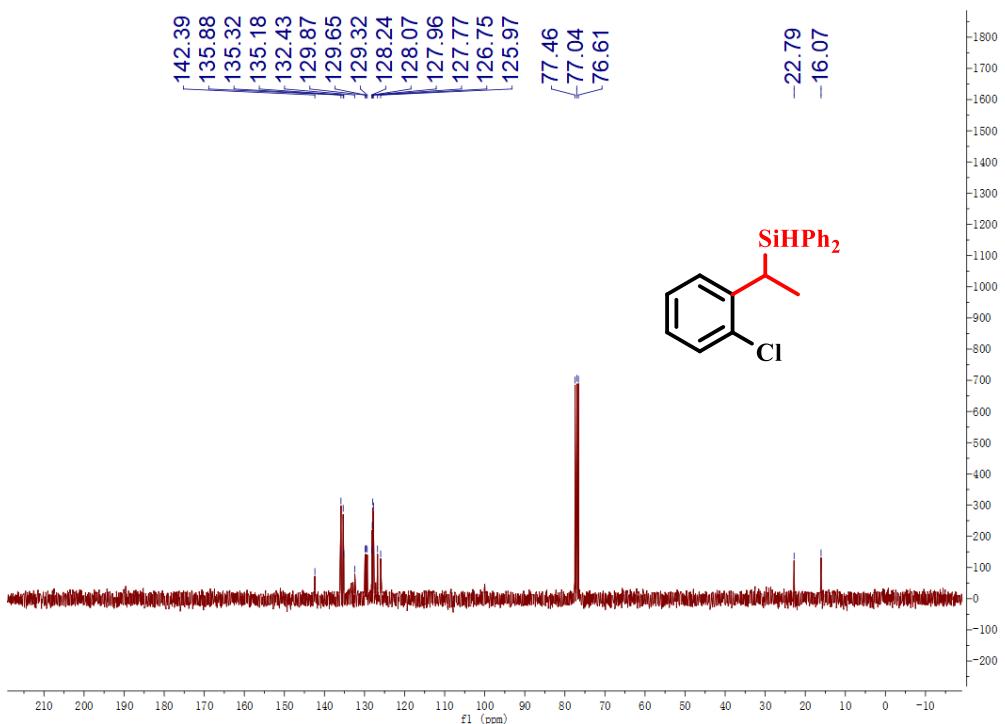


Fig.S30 ¹³C NMR spectrum of **2n**

(1-(4-chlorophenyl)ethyl)diphenylsilane (2o**)³**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.42-7.40 (m, 2H), 7.31-7.20 (m, 6H), 7.17-7.15 (m, 2H), 7.09-7.02 (m, 2H), 6.99-6.79 (m, 2H), 4.72 (d, J = 6.0 Hz, 1H), 2.70 (qd, J = 9.0, 3.0 Hz, 1H), 1.33 (d, J = 9.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 135.68, 135.55, 135.16, 129.89, 129.79, 128.96, 128.23, 128.13, 128.03, 127.88, 26.58, 16.43.

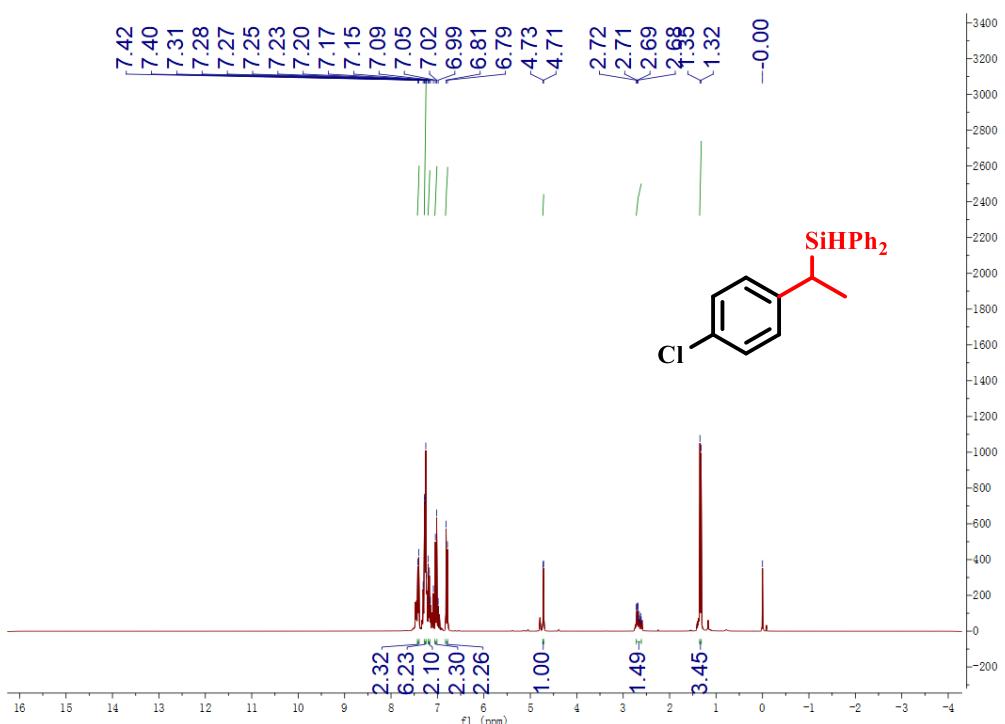


Fig.S31 ¹H NMR spectrum of **2o**

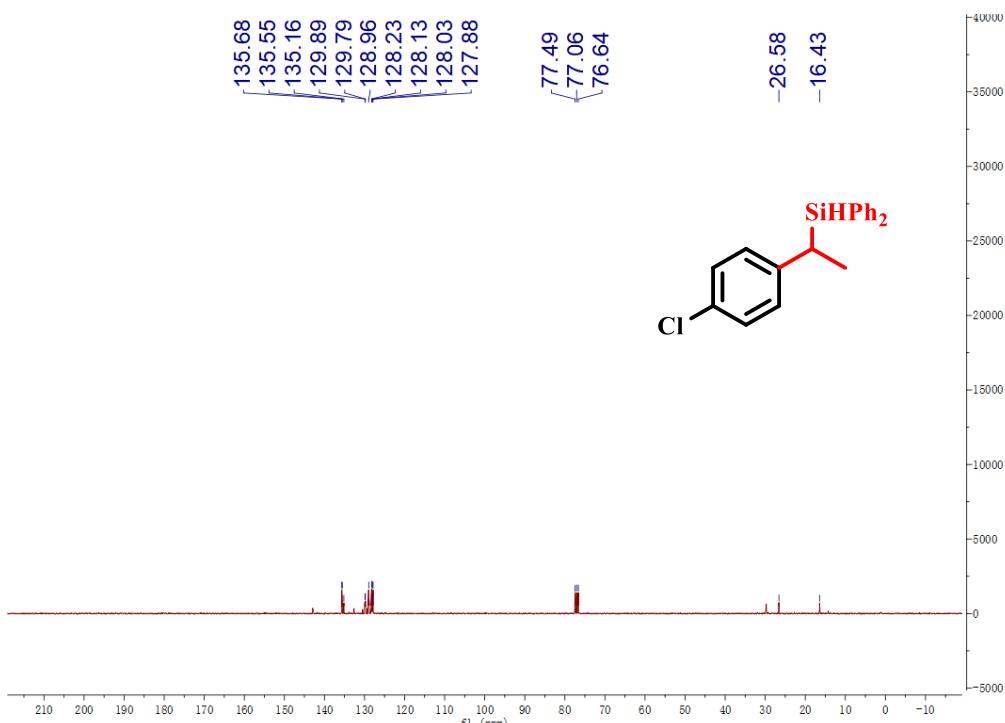


Fig.S32 ¹³C NMR spectrum of **2o**

(1-(4-Bromophenyl)ethyl)diphenylsilane (2p**)³**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.68 (m, 1H), 7.68-7.66 (m, 2H), 7.65 (m, 1H), 7.53-7.47 (m, 6H), 7.46-7.44 (m, 2H), 7.13-7.11 (m, 2H), 5.00 (d, J = 3.0 Hz, 1H), 2.80 (qd, J = 9.0, 3.0 Hz, 1H), 1.58 (d, J = 6.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 143.29, 135.62, 135.22, 133.93, 131.44, 129.83, 129.75, 128.23, 128.20, 128.23, 128.20, 119.51, 30.03, 14.29.

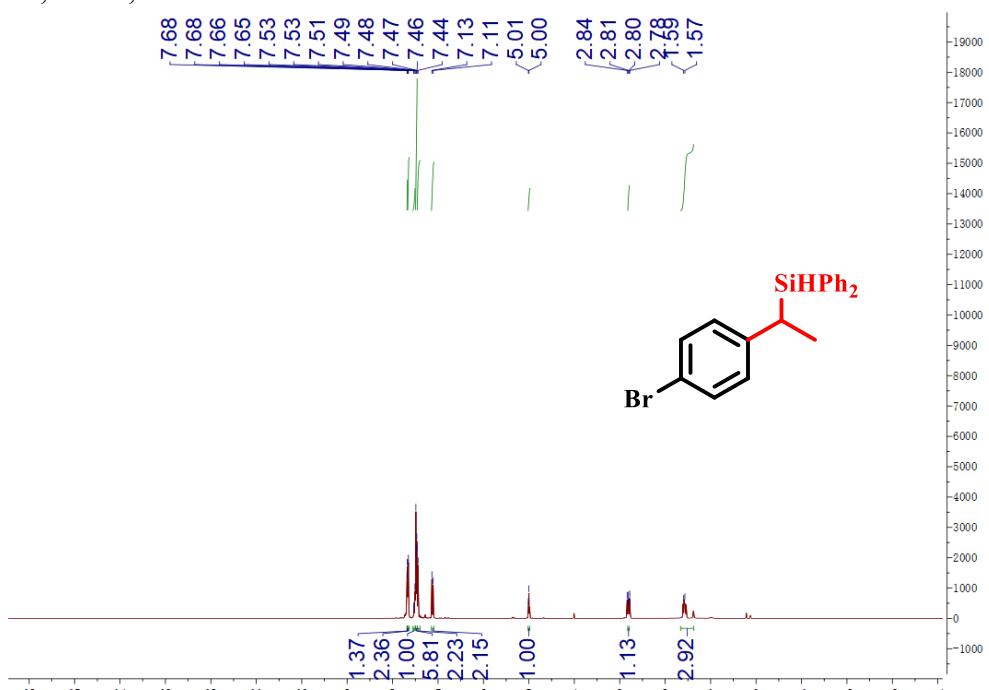


Fig.S33 ¹H NMR spectrum of **2p**

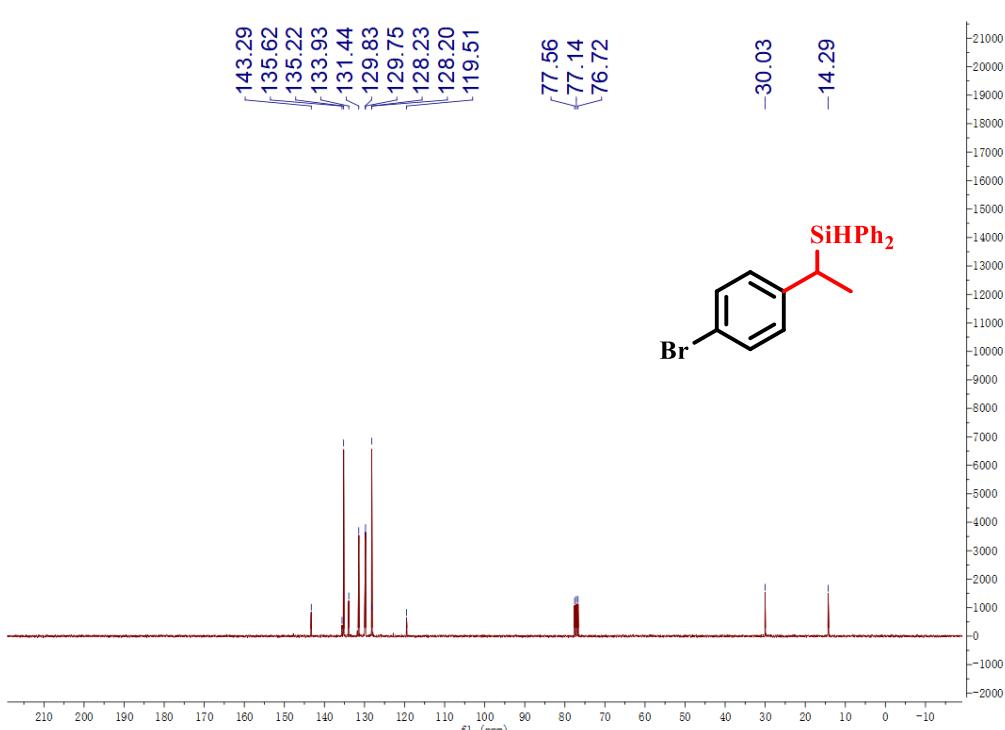


Fig.S34 ¹³C NMR spectrum of **2p**

(1-(3-fluorophenyl)ethyl)diphenylsilane (2q)¹

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.39-7.37(m, 2H), 7.24-7.13 (m, 4H), 7.13-7.08 (m, 2H), 6.97-6.95 (m, 2H), 6.92-6.89 (m, 1H), 6.63-6.58(m, 3H), 4.71 (d, J = 3.0 Hz, 1H), 2.68 (qd, J = 6.0, 3.0 Hz, 1H), 1.30 (d, J = 6.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 164.60, 161.36, 135.75, 135.59, 132.64, 129.99, 129.87, 129.57, 129.45, 128.12, 127.94, 123.47, 111.66, 77.13, 76.71, -27.18, -16.38.

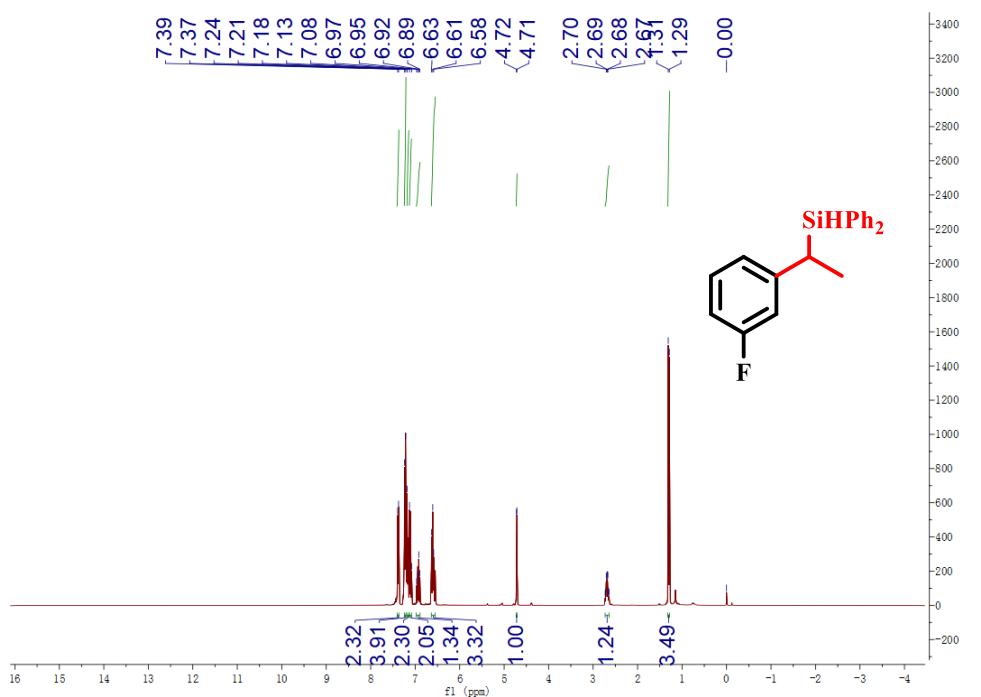


Fig.S35 ¹H NMR spectrum of 2q

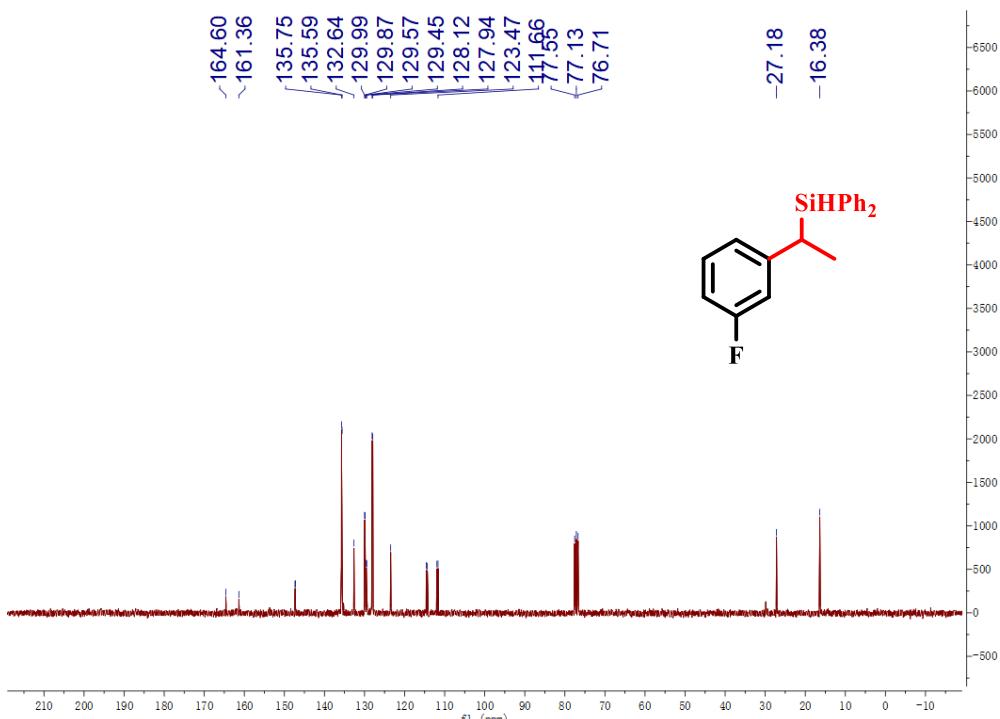


Fig.S36 ¹³C NMR spectrum of 2q

(1-(4-fluorophenyl)ethyl)diphenylsilane (2r)¹

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.44-7.41 (m, 2H), 7.29-7.25 (m, 3H), 7.23-7.17(m, 3H), 6.85-6.82 (m, 2H) 6.81-6.76 (m, 3H), 6.73 (m, 1H), 4.72 (d, J = 3.0 Hz, 1H), 2.70 (qd, J = 6.0, 3.0 Hz , 1H), 1.34 (d, J = 6.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 139.98, 135.67, 135.53, 132.79, 129.83, 129.70, 128.90, 128.80, 128.00, 127.82, 127.80, 115.03, 114.75, 26.22, 16.70.

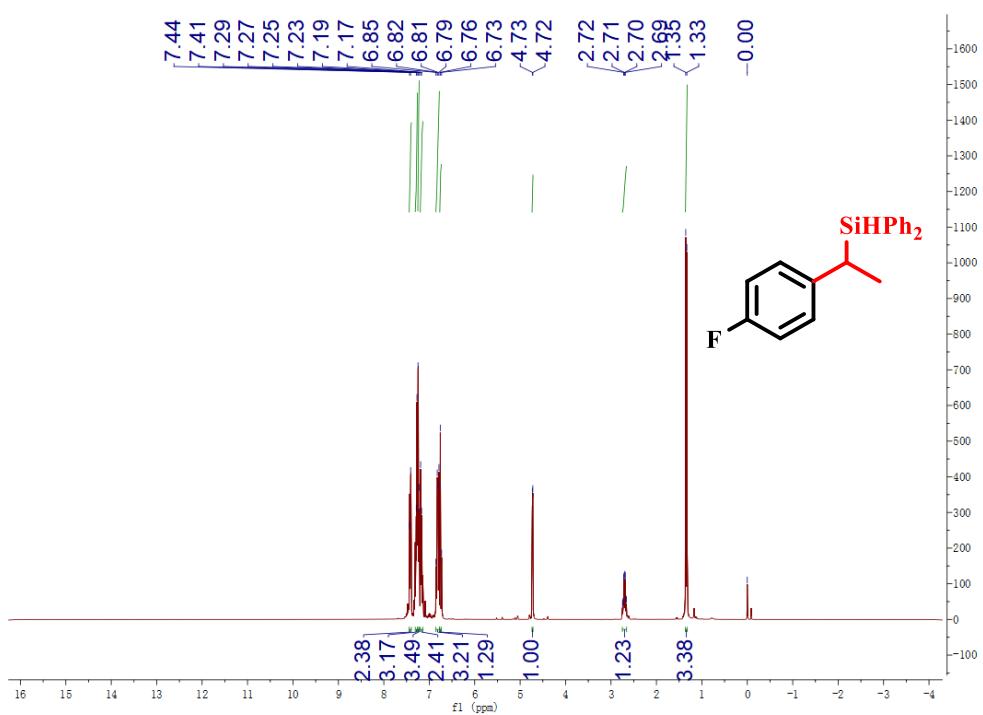


Fig.S37 ¹H NMR spectrum of 2r

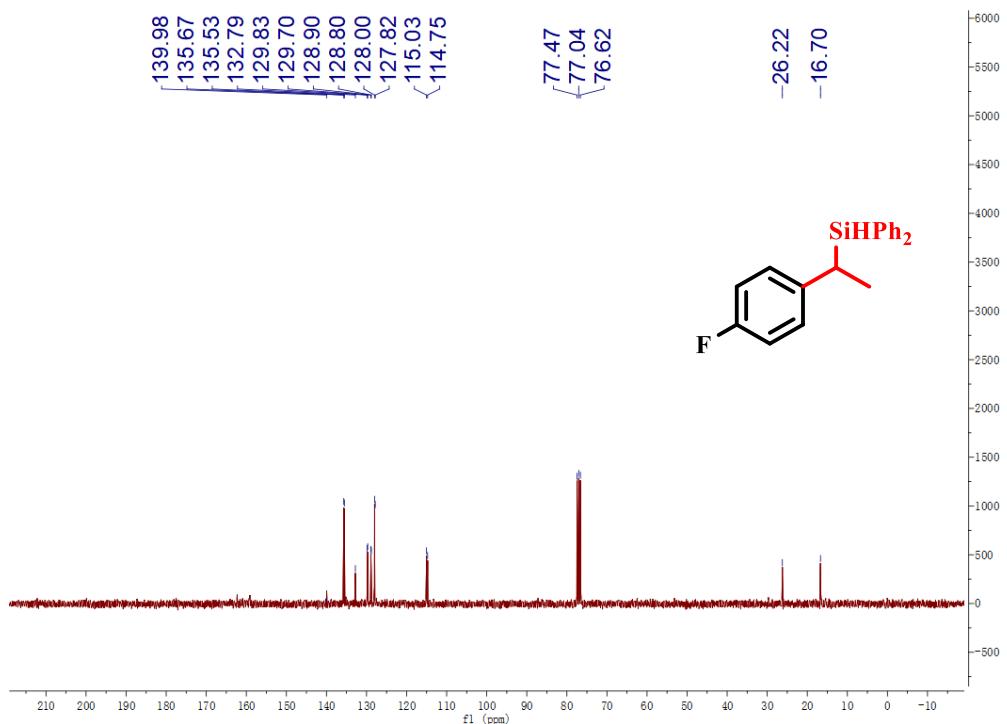


Fig.S38 ¹³C NMR spectrum of 2r

Diphenyl(1-(3-(trifluoromethyl)phenyl)ethyl)silane (2s**)³**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.36-7.38 (m, 2H), 7.25-7.17 (m, 7H), 7.13-7.04 (m, 3H), 7.00-6.98 (m, 2H), 4.70 (d, J = 3.0 Hz, 1H), 2.74 (qd, J = 6.0, 3.0 Hz, 1H), 1.33 (d, J = 9.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 145.63, 135.86, 135.72, 132.44, 131.11, 130.24, 130.12, 128.69, 128.31, 128.15, 124.61, 121.94.

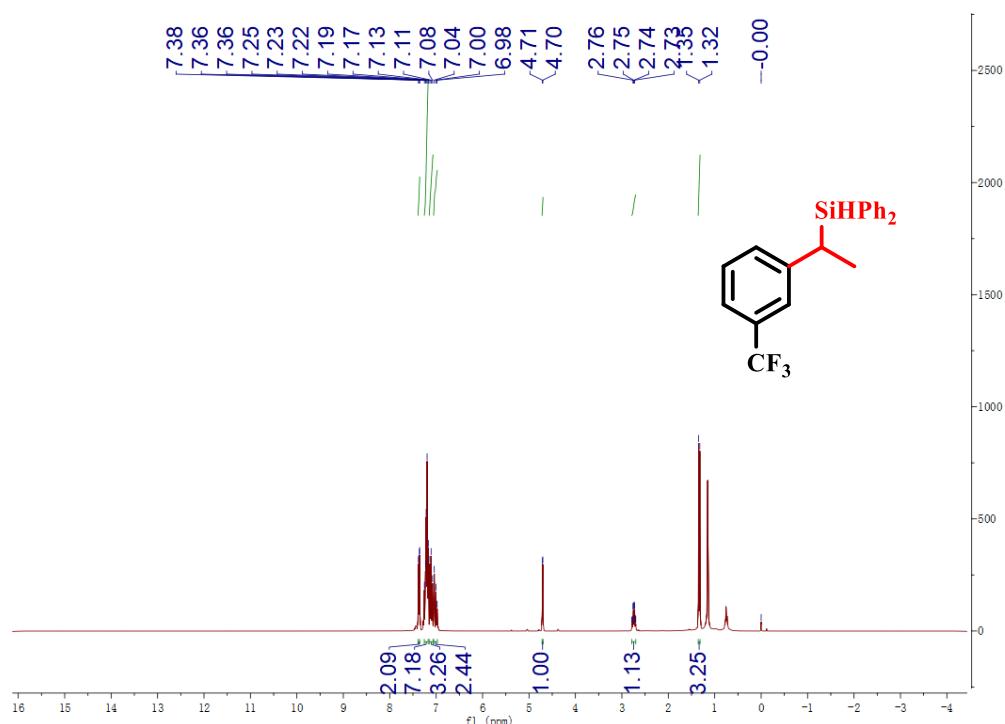


Fig.S39 ¹H NMR spectrum of **2s**

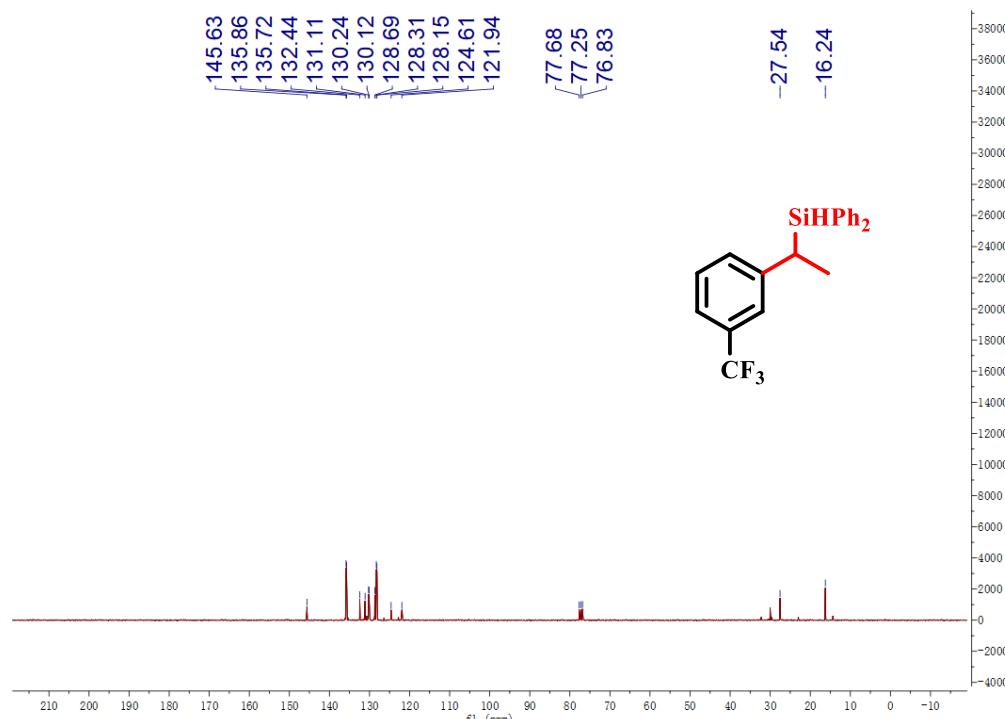


Fig.S40 ¹³C NMR spectrum of **2s**

Diphenyl(1-(4-(trifluoromethyl)phenyl)ethyl)silane (2t**)³**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.45-7.42 (m, 3H), 7.35-7.32 (m, 1H), 7.31-7.23 (m, 5H), 7.21-7.18 (m, 2H), 7.17 (m, 1H), 7.00-6.97 (m, 2H), 4.74 (d, J = 3.0 Hz, 1H), 2.83 (qd, J = 9.0, 3.0 Hz, 1H), 1.40 (d, J = 6.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 135.64, 135.46, 132.24, 129.98, 129.87, 128.06, 127.90, 127.78, 125.03, 27.42, 16.11.

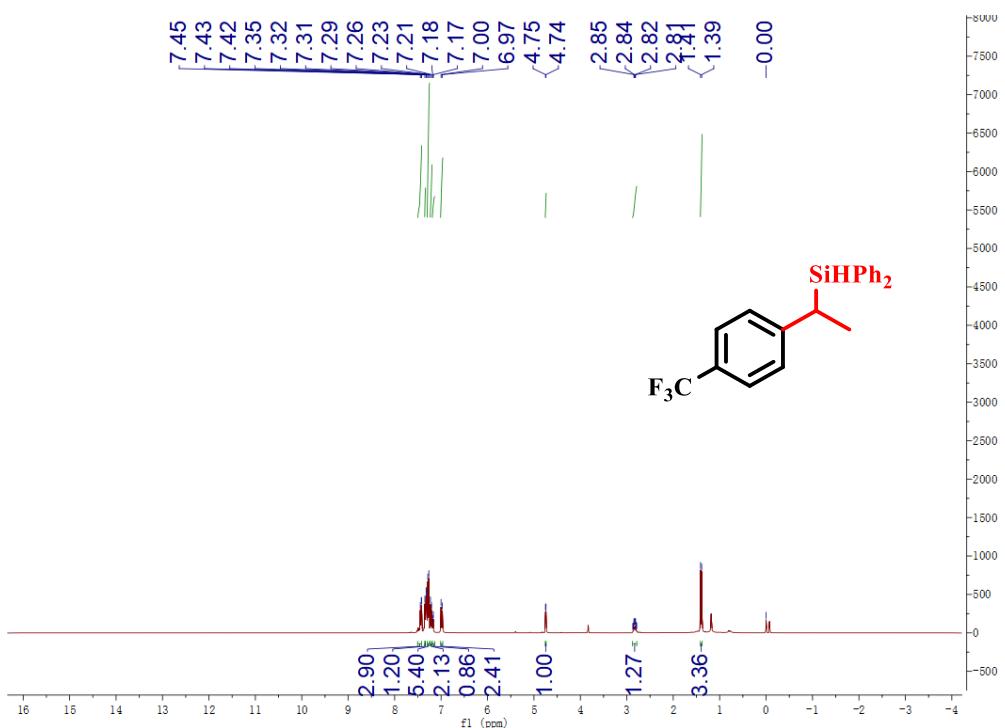


Fig.S41 ¹H NMR spectrum of **2t**

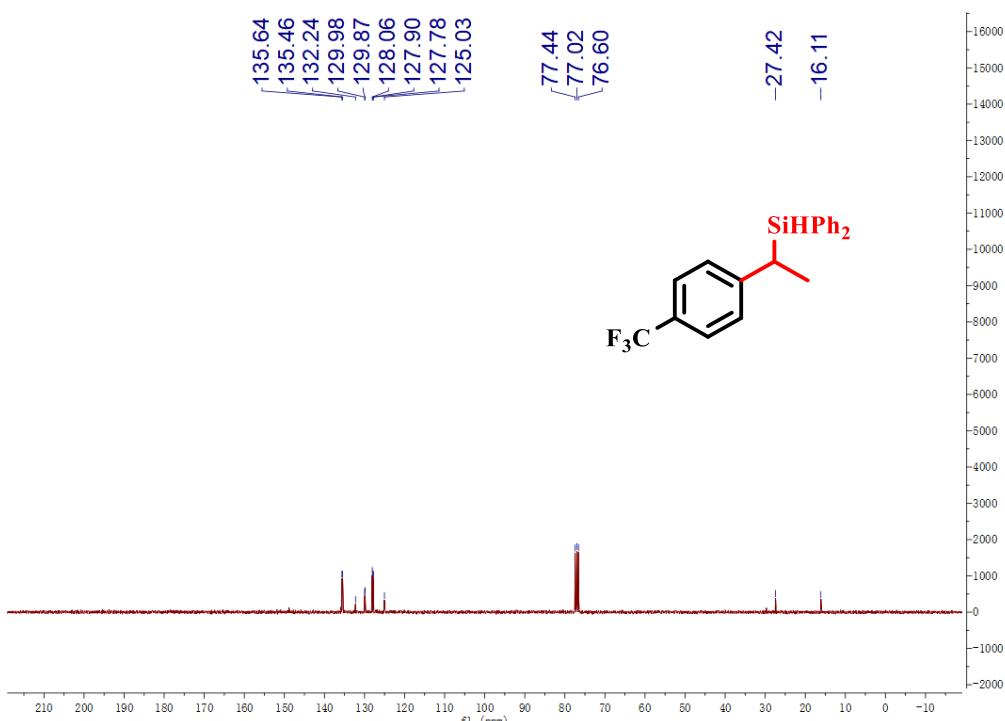


Fig.S42 ¹³C NMR spectrum of **2t**

(n-heptyl)diphenylsilane (3a**)³**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.57-7.54 (m, 4H), 7.54-7.35 (m, 5H), 7.33-7.26(m, 1H), 4.84 (t, J = 3.0 Hz, 1H), 1.54-1.46 (m, 2H), 1.43-1.10 (m, 10H), 0.86 (t, J = 6.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 135.12, 134.74, 129.43, 127.92, 33.11, 31.75, 29.69, 28.87, 24.39, 22.63, 14.05.

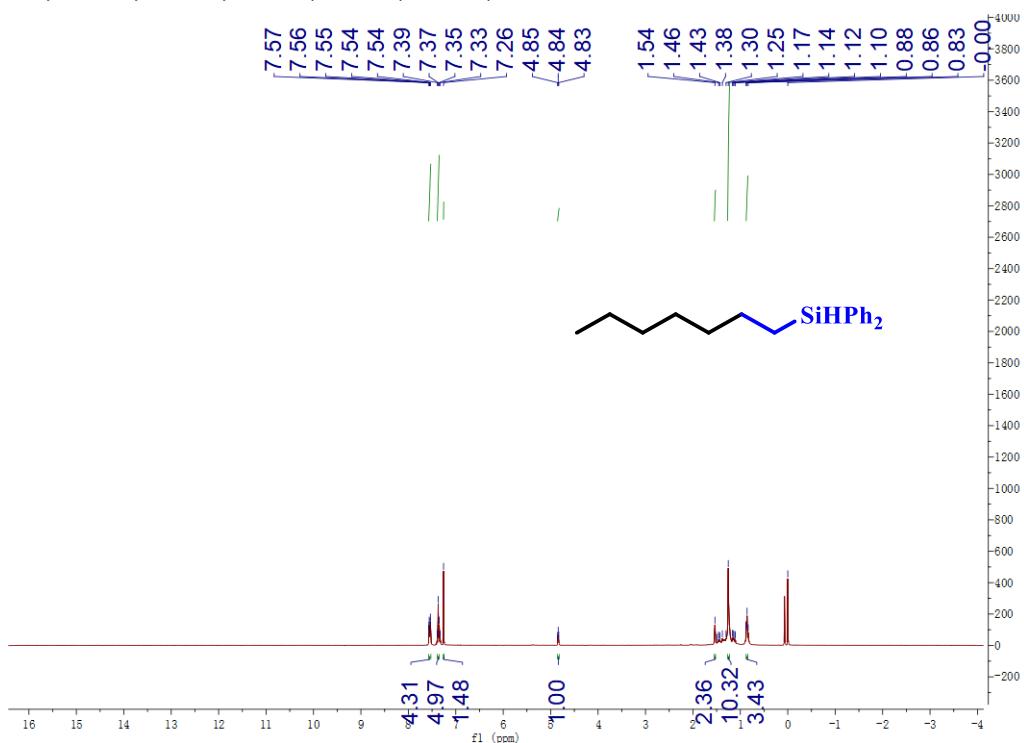


Fig.S43 ¹H NMR spectrum of **3a**

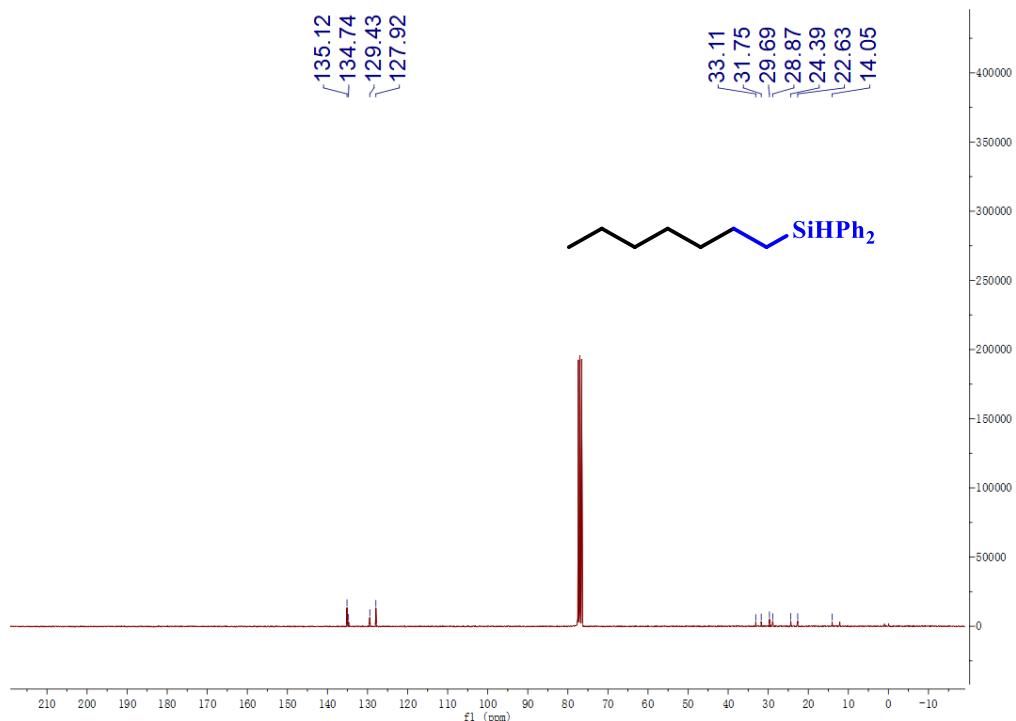


Fig.S44 ¹³C NMR spectrum of **3a**

(n-octyl)diphenylsilane (3b)¹

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.57-7.53 (m, 4H), 7.39-7.33 (m, 5H), 7.32-7.26(m, 1H), 4.84 (t, J = 3.0 Hz, 1H), 1.46-1.10 (m, 14H), 0.86 (t, J = 9.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 135.12, 134.74, 129.44, 127.92, 33.15, 31.87, 29.69, 29.18, 24.38, 22.64, 14.08, 12.14.

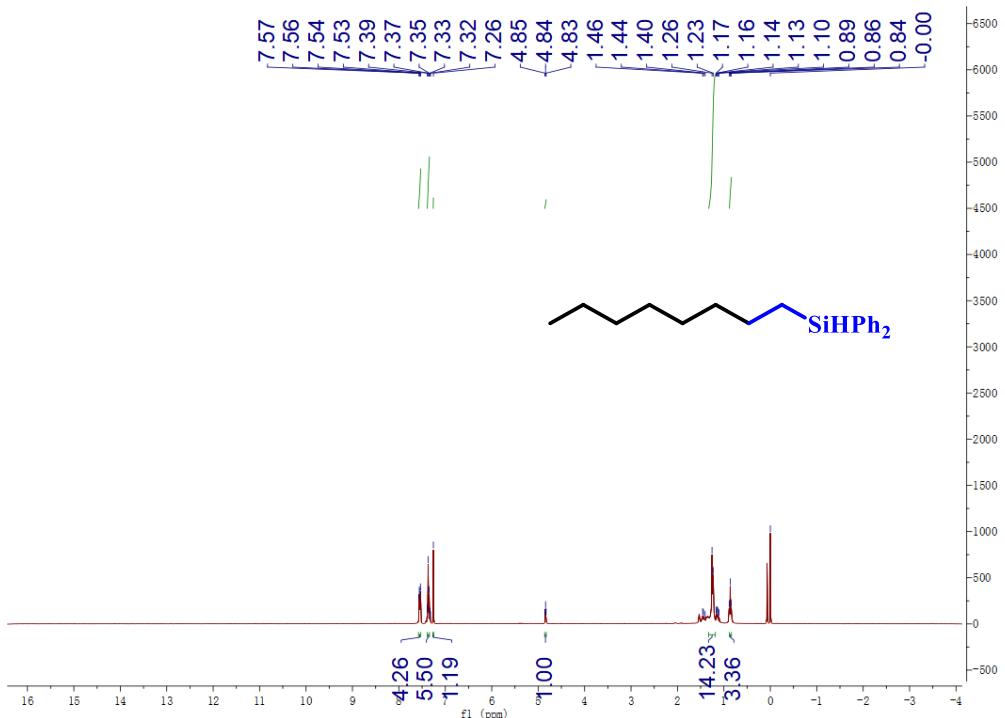


Fig.S45 ¹H NMR spectrum of **3b**

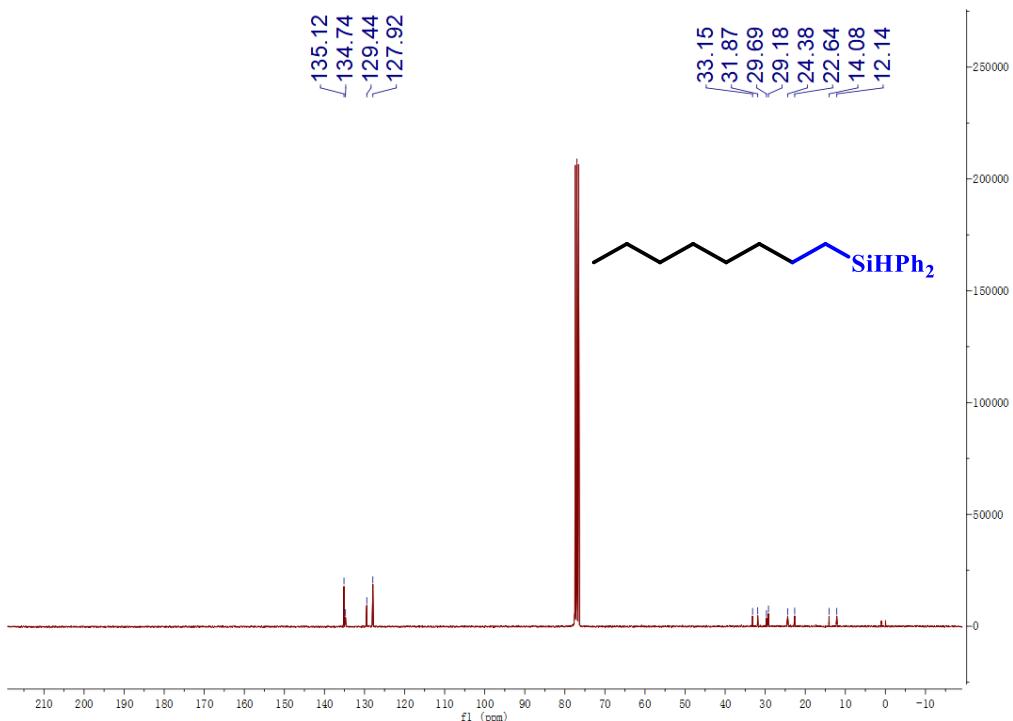


Fig.S46 ¹³C NMR spectrum of **3b**

(6-chlorohexyl)diphenylsilane(3c)⁴

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.56-7.54 (m, 4H), 7.53-7.34 (m, 4H), 7.32-7.31(m, 2H), 4.85 (t, J = 3.0 Hz, 1H), 3.46 (t, J = 6.0 Hz, 2H), 1.73-1.68(m, 2H), 1.48-1.37 (m, 6H), 1.17-1.12(m, 2H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 135.16, 134.57, 129.58, 128.03, 45.13, 32.54, 32.35, 26.50, 24.30, 12.12.

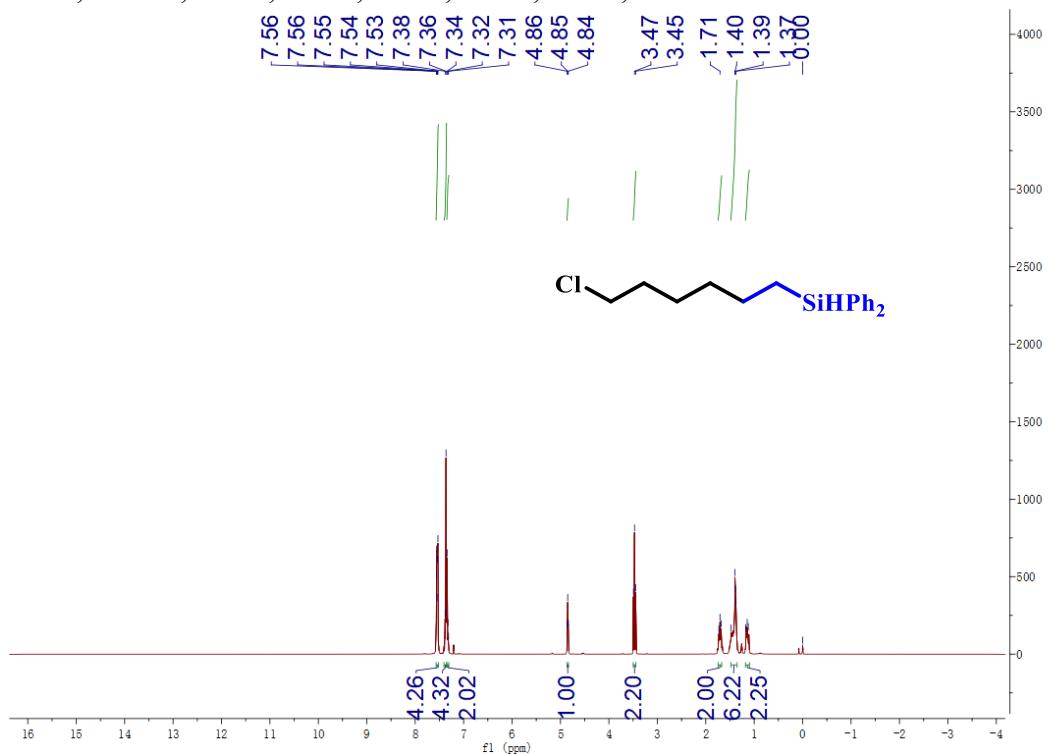


Fig.S47 ¹H NMR spectrum of 3c

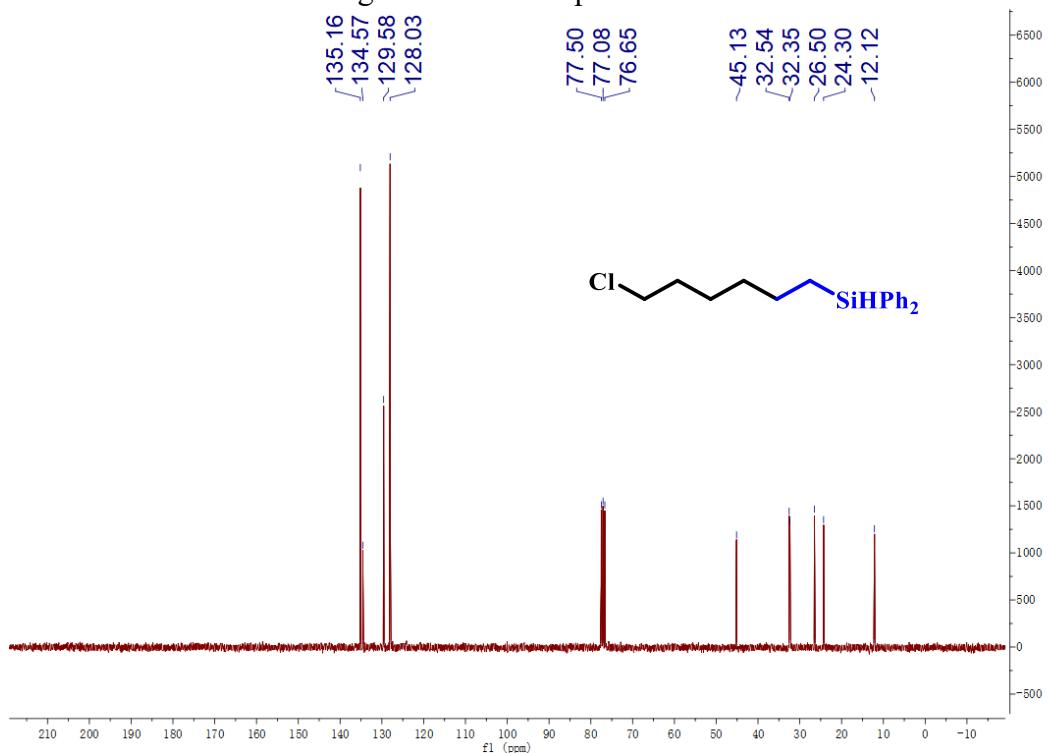


Fig.S48 ¹³C NMR spectrum of 3c

Diphenyl(4-phenylbutyl)silane (3d**)⁵**

¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.56-7.39 (m, 4H), 7.37-7.25 (m, 6H), 7.23-7.18 (m, 2H), 7.16-7.11 (m, 3H), 4.85 (t, J = 3.0 Hz, 1H), 2.59 (t, J = 6.0 Hz, 2H), 1.74-1.64 (m, 2H), 1.57-1.47 (m, 2H), 1.25-1.15 (m, 2H). ¹³C NMR (75 MHz, CDCl₃): δ (ppm) 142.63, 135.14, 134.54, 129.83, 129.53, 128.38, 128.24, 127.98, 125.59, 35.52, 34.87, 24.12, 12.02.

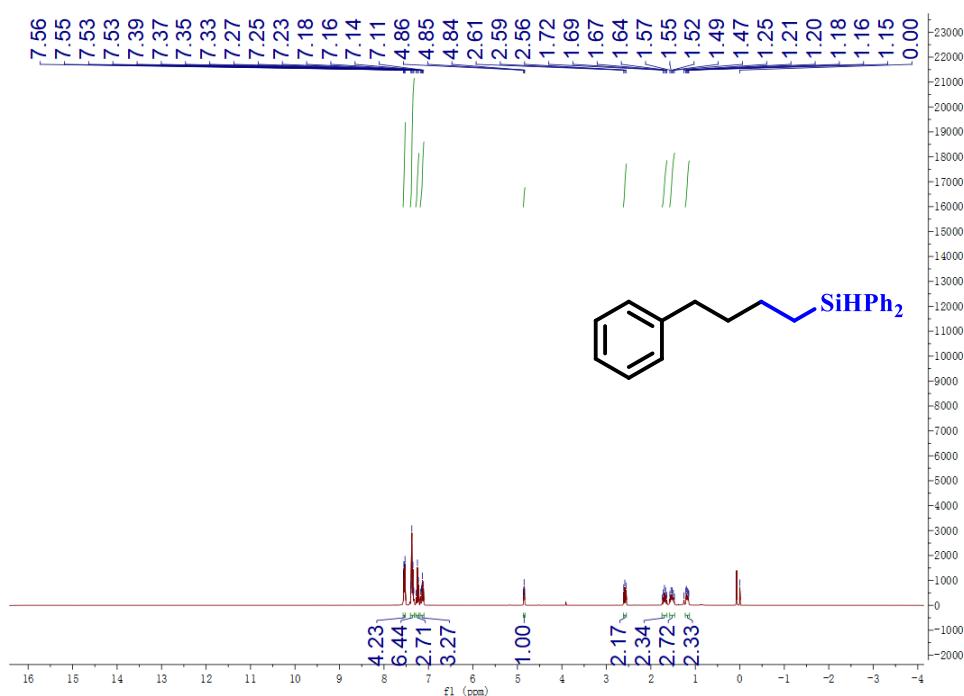


Fig.S49 ¹H NMR spectrum of **3d**

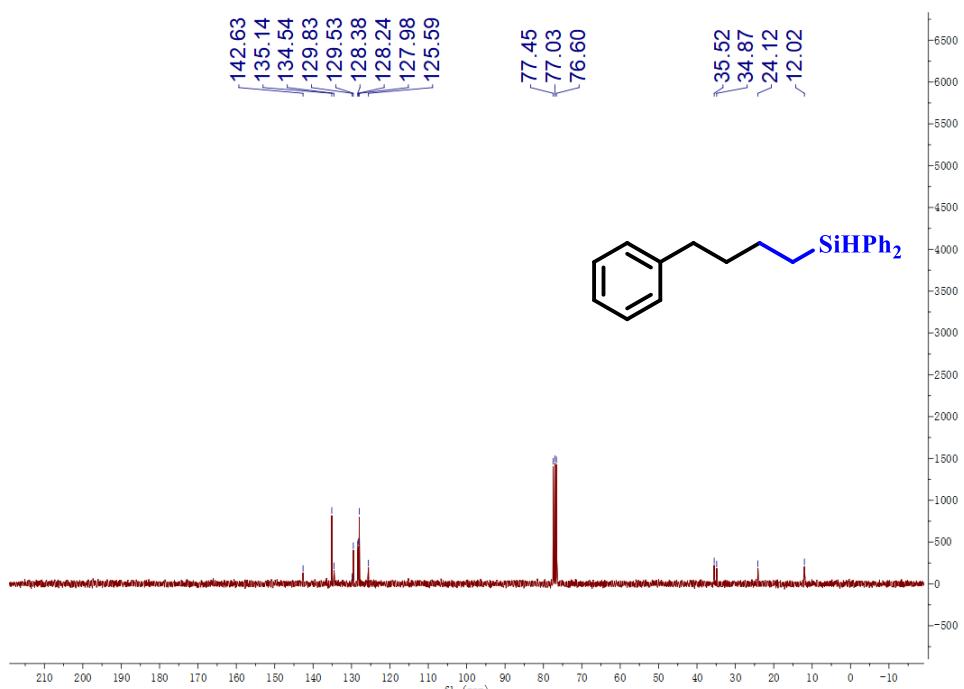


Fig.S50 ¹³C NMR spectrum of **3d**

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