

Supporting Information

SiP-heterocycles derived from a bulky phosphanylsilylene

Chenfeng Wang,^{‡a} Ming-Der Su,^{‡cd} Zijie Fang,^a Jiahao Zhou,^a Haoqi Zhang,^a Xiaodi Li,^a Darui Zuo,^a Zheng-Feng Zhang,^c and Yan Li^{*ab}

^a *College of Material, Chemistry and Chemical Engineering, Key Laboratory of Organosilicon Chemistry and Material Technology, Ministry of Education, Hangzhou Normal University, Hangzhou, 311121, China.*

^b *Key Laboratory of Silicone Materials Technology of Zhejiang Province, Hangzhou Normal University, Hangzhou 311121, PR China.*

^c *Department of Applied Chemistry, National Chiayi University, Chiayi, 60004, Taiwan.*

^d *Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 80708, Taiwan.*

Corresponding Author: E-mail: yli@hznu.edu.cn

[‡]C. Wang and M.-D. Su have equal contribution to this work.

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I. Experimental sections

All key manipulations were carried out under dry argon or nitrogen atmosphere by using Schlenk line and glovebox techniques. Toluene, THF and hexane were dried by refluxing with sodium/potassium benzophenone under N₂. LSiCl was synthesized according to the literature^{S1}. ¹H, ¹³C{¹H}, ³¹P{¹H}, ²⁹Si{¹H} and ¹⁹F{¹H} NMR spectra were recorded on a Bruker Avance II 400 or 500 spectrometer. Elemental analysis was performed on a Thermo Quest Italia SPA EA 1110 instrument. Commercial reagents were purchased from TCI and Sigma-Aldrich and were used directly. UV–visible spectra were taken on a Cary 4000 (Agilent Technologies) UV–visible spectrophotometer. The PL spectra were recorded using an Edinburgh Instruments FLS920 spectrophotometer.

1: At 0 °C, *t*BuLi (3.9 mL, 5.1 mmol, 1.3 M in hexane) was added dropwise to a toluene solution (120 mL) of Ad₂PH (1.5 g, 5.0 mmol). The reaction was allowed to warm to room temperature and stirred for 3 hours. Then, the resulted suspension was slowly transferred to a toluene solution (10 mL) of LSiCl (1.5 g, 5.0 mmol) via syringe at room temperature. The reaction mixture was stirred overnight followed by being filtered to obtain a yellow filtrate. The filtrate was dried under vacuum and the residue was washed by hexane (2×10 mL) to obtain compound **1** as grey-yellow powder. Yield: 2.0 g, 70%. X-ray quality single crystals of **1** were grown in its toluene solution at 0 °C. m.p.: 195 °C (dec.). Elemental analysis calcd (%) for C₃₅H₅₃N₂PSi (560.85): C, 74.95; H, 9.53; N, 4.99. Anal. found: C, 74.77; H, 9.29; N, 5.09. ¹H NMR (400 MHz, C₆D₆, 298 K, ppm): δ 7.26 (m, 1H, PhH), 7.07-6.95 (m, 4H, PhH), 2.65-2.45 (m, 12H, AdH), 2.04-1.74 (m, 18H, AdH), 1.35 (s, 18H, NCM₃). ¹³C{¹H} NMR (100 MHz, C₆D₆, 298 K, ppm): δ 155.3 (NCN), 134.9, 130.0, 129.1, 127.2 (PhC), 53.9 (NCMe₃), 45.5, 44.0, 37.2, 31.8, 29.7 (AdC + NCM₃). ²⁹Si{¹H} NMR (95 MHz, C₆D₆, 298 K, ppm): δ 46.6 (d, ¹J_{P,Si} = 199.0 Hz). ³¹P{¹H} NMR (163 MHz, C₆D₆, 298 K, ppm): 28.7.

2: To a mixture of **1** (0.17 g, 0.30 mmol) and PhC≡CPh (0.054 g, 0.30 mmol) was added toluene (30 mL) at room temperature and the suspension was stirred for 4 h. Then, the resulted suspension was filtered and the filtrate was dried under vacuum to obtain **2** as light-yellow powder in quantitative yield. X-ray quality single crystals of **2** were grown in its toluene solution at 0 °C. m.p.: 190 °C (dec.). Elemental analysis calcd (%) for C₄₉H₆₃N₂PSi (739.07): C, 79.63; H, 8.59; N, 3.79. Anal. found: C, 79.51; H, 8.33; N, 3.87. ¹H NMR (400 MHz, C₆D₆, 298 K, ppm): δ 7.79 (m, 3H, PhH), 7.38-7.04 (m, 12H, PhH), 2.71

(m, 12H, AdH), 1.95-1.82 (m, 18H, AdH), 1.39 (s, 18H, NCM_e₃). ¹³C{¹H} NMR (100 MHz, C₆D₆, 298 K, ppm): δ 171.7 (NCN), 139.4, 137.5, 134.8, 131.6, 129.0, 128.3, 128.1, 125.9, 125.3 (PhC + C≡C), 53.9 (NCMe₃), 43.6, 43.8, 37.2, 31.7, 29.6 (AdC + NCM_e₃). ²⁹Si{¹H} NMR (95 MHz, C₆D₆, 298 K, ppm): δ -141.4 (d, ¹J_{P,Si} = 60.6 Hz). ³¹P{¹H} NMR (163 MHz, C₆D₆, 298 K, ppm): 14.9.

3a: In a sealed thick-walled vessel, **2** (0.22 g, 0.30 mmol) was stirred in toluene (30 mL) at 80 °C under microwave (560 W) for 20 min. After workup, the vessel was transferred in the glovebox, where the resulted dark-red solution was filtered and the filtrate was concentrated to 3 mL. Orange crystals of **3** were obtained at room temperature after two days. Yield: 0.16 g, 72%. m.p.: 190 °C (dec.). Elemental analysis calcd (%) for C₄₉H₆₃N₂PSi (739.07): C, 79.63; H, 8.59; N, 3.79. Anal. found: C, 79.34; H, 8.39; N, 3.52. ¹H NMR (400 MHz, C₆D₆, 298 K, ppm): δ 7.42 (d, 1H, PhH), 7.15-6.77 (m, 9H, PhH), 6.11 (m, 1H, CH=C), 5.87 (m, 1H, CH=C), 5.81 (d, 1H, C=C-CH=C), 5.37 (m, 1H, CH=C), 4.84 (m, 1H, C=C-CH), 3.15-1.68 (m, 30H, AdH + NH), 1.56 (s, 9H, NCM_e₃), 1.46 (s, 9H, NCM_e₃). ¹³C{¹H} NMR (100 MHz, C₆D₆, 298 K, ppm): δ 154.0, 145.2, 142.6, 140.1, 138.2, 133.5, 131.8, 131.7, 131.3, 129.7, 127.1, 126.9, 126.7, 125.7, 124.7, 121.7 (PhC + C=C + C=C-CH), 55.0, 52.7, 51.2, 47.9, 45.5, 44.2, 41.6, 41.5, 41.4, 40.2, 40.0, 39.5, 37.3, 37.0, 34.0, 33.4, 32.6, 32.2, 29.9, 29.8, 29.7, 29.1, 28.0 (AdC + NCM_e₃ + NCM_e₃). ²⁹Si{¹H} NMR (95 MHz, C₆D₆, 298 K, ppm): δ -19.2 (d, ¹J_{P,Si} = 19.8 Hz). ³¹P{¹H} NMR (163 MHz, C₆D₆, 298 K, ppm): -20.2. IR (Nujol mull, cm⁻¹): $\tilde{\nu}$ 3381 (N-H). UV-visible absorption band at 465 nm (in toluene). PL emission band at 580 nm (in toluene).

3b: In a sealed thick-walled vessel, **1** (0.17 g, 0.30 mmol) and PhC≡CH (0.031 g, 0.30 mmol) was stirred in toluene (30 mL) at 80 °C under microwave (560 W) for 20 min. After workup, the vessel was transferred in the glovebox, where the resulted dark-red solution was filtered and the filtrate was concentrated to 3 mL to obtain orange crystals of **3b**. Yield: 0.15 g, 75%. m.p.: 185 °C (dec.). Elemental analysis calcd (%) for C₄₃H₅₉N₂PSi (663.02): C, 77.90; H, 8.97; N, 4.23. Anal. found: C, 77.79; H, 8.88; N, 4.18. ¹H NMR (400 MHz, C₆D₆, 298 K, ppm): δ 7.41 (d, 1H, PhH), 7.21 (m, 2H, PhH), 7.06-7.00 (m, 2H, PhH), 6.45 (s, 1H, PhC=CH), 6.17 (m, 1H, CH=C), 6.10 (d, 1H, C=C-CH=C), 5.96 (m, 1H, CH=C), 5.54 (m, 1H, CH=C), 4.75 (m, 1H, C=C-CH), 3.14-1.57 (m, 30H, AdH + NH), 1.39 (s, 9H, NCM_e₃), 1.31 (s, 9H, NCM_e₃). ¹³C{¹H} NMR (100 MHz, C₆D₆, 298 K, ppm): δ 144.4, 143.2, 142.7, 141.1, 130.4, 130.0, 128.8, 128.2, 125.7, 125.3, 124.9, 121.6, 119.6 (PhC + C=C + C=C-CH), 52.9, 52.4, 51.5, 47.8, 45.5, 44.2, 41.9, 41.2, 40.0, 39.8, 37.4, 37.2,

36.9, 33.8, 32.6, 32.2, 31.6, 30.3, 29.6, 28.9, 28.0 (AdC + NCMe₃ + NCMe₃). ²⁹Si{¹H} NMR (95 MHz, C₆D₆, 298 K, ppm): δ -19.7 (d, ¹J_{P,Si} = 17.9 Hz). ³¹P{¹H} NMR (163 MHz, C₆D₆, 298 K, ppm): -24.8. IR (Nujol mull, cm⁻¹): $\tilde{\nu}$ 3385 (N–H). UV-visible absorption bands at 463 nm (in toluene). PL emission bands at 609 nm (in toluene).

3c: The synthetic procedure is similar to that of **3b**, where ArC≡CH (Ar = 4-*i*Pr-C₆H₄; 0.043 g, 0.30 mmol) was employed and orange crystals of **3c** were obtained. Yield: 0.16 g, 78%. m.p.: 205 °C (dec.). Elemental analysis calcd (%) for C₄₆H₆₅N₂PSi (705.06): C, 78.36; H, 9.29; N, 3.97. Anal. found: C, 78.27; H, 9.36; N, 3.89. ¹H NMR (400 MHz, C₆D₆, 298 K, ppm): δ 7.42 (d, 2H, PhH), 7.11 (m, 2H, PhH), 6.43 (s, 1H, 4-*i*Pr-PhC=CH), 6.15 (m, 2H, C=C-CH=C + CH=C), 5.95 (m, 1H, CH=C), 5.55 (m, 1H, CH=C), 4.74 (m, 1H, C=C-CH), 3.11 (m, 1H, AdH), 2.84 (m, 1H, AdH), 2.72 (m, 2H, CHMe₂ + AdH), 2.42-1.63 (m, 30H, AdH + NH), 1.37 (s, 9H, NCMe₃), 1.30 (s, 9H, NCMe₃), 1.15 (m, 6H, CHMe₂). ¹³C{¹H} NMR (100 MHz, C₆D₆, 298 K, ppm): δ 145.3, 144.6, 143.1, 141.0, 140.2, 130.3, 128.9, 125.9, 125.8, 121.5, 119.6 (PhC + C=C + C=C-CH), 52.9, 52.4, 51.4, 47.8, 45.5, 44.2, 41.6, 41.9, 41.3, 40.9, 39.4, 37.2, 36.9, 33.8, 32.6, 32.2, 30.4, 29.5, 28.0 (AdC + CHMe₂ + NCMe₃ + NCMe₃), 24.1, 23.9 (CHMe₂). ²⁹Si{¹H} NMR (95 MHz, C₆D₆, 298 K, ppm): δ -19.7 (d, ¹J_{P,Si} = 18.0 Hz). ³¹P{¹H} NMR (163 MHz, C₆D₆, 298 K, ppm): -24.9. IR (Nujol mull, cm⁻¹): $\tilde{\nu}$ 3373 (N–H). UV-visible absorption bands at 474 nm (in toluene). PL emission band at 596 nm (in toluene).

3d: The synthetic procedure is similar to that of **3b**, where ArC≡CH (Ar = 3-F-C₆H₄; 0.036 g, 0.30 mmol) was employed and orange crystals of **3d** were obtained. Yield: 0.15 g, 71%. m.p.: 200 °C (dec.). Elemental analysis calcd (%) for C₄₃H₅₈FN₂PSi (680.97): C, 75.84; H, 8.58; N, 4.11. Anal. found: C, 75.92; H, 8.65; N, 4.19. ¹H NMR (400 MHz, C₆D₆, 298 K, ppm): δ 7.21-6.95 (m, 3H, PhH), 6.75 (m, 1H, PhH), 6.45 (s, 1H, 3-F-PhC=CH), 6.15 (m, 1H, CH=C), 6.02 (d, 1H, C=C-CH=C), 5.92 (m, 1H, CH=C), 5.58 (m, 1H, CH=C), 4.70 (m, 1H, C=C-CH), 3.12-1.66 (m, 30H, AdH + NH), 1.34 (s, 9H, NCMe₃), 1.29 (s, 9H, NCMe₃). ¹³C{¹H} NMR (100 MHz, C₆D₆, 298 K, ppm): δ 164.1, 162.1, 145.3, 143.8, 143.6, 141.5, 130.6, 129.2, 129.0, 128.6, 128.2, 125.8, 122.1, 114.6, 111.5 (PhC + C=C + C=C-CH), 53.1, 42.4, 51.5, 47.9, 47.7, 45.3, 45.2, 44.3, 41.9, 41.3, 40.0, 39.3, 37.1, 36.8, 33.7, 32.5, 32.2, 30.3, 29.5, 29.0, 27.9 (AdC + NCMe₃ + NCMe₃). ²⁹Si{¹H} NMR (95 MHz, C₆D₆, 298 K, ppm): δ -19.6 (d, ¹J_{P,Si} = 19.0 Hz). ¹⁹F{¹H} NMR (376 MHz, C₆D₆, 298 K, ppm): -113.9. ³¹P{¹H} NMR (163 MHz, C₆D₆, 298 K, ppm): -25.1. IR (Nujol mull, cm⁻¹): $\tilde{\nu}$ 3381 (N–H). UV-visible absorption bands at 467 nm (in toluene). PL emission band at 593 nm (in toluene).

4: To a mixture of **1** (0.17 g, 0.30 mmol) and AdC≡P (0.11 g, 0.60 mmol) was added toluene (20 mL) at room temperature and the reaction was stirred for 8 hours. The resulted orange suspension was filtered and the filtrate was concentrated under vacuum to 2 mL. Red crystals of **4** were grown at room temperature. Yield: 0.16 g, 52%. m.p.: 225 °C (dec.). Elemental analysis calcd (%) for C₆₄H₉₁N₂P₃Si (1009.38): C, 76.15; H, 9.09; N, 2.78. Anal. found: C, 76.28; H, 9.18; N, 2.87. ¹H NMR (400 MHz, C₆D₆, 298 K, ppm): δ 7.25 (m, 1H, PhH), 7.08-6.82 (m, 4H, PhH), 2.68-1.63 (m, 29H, AdH), 1.49-1.16 (m, 39H, NCM₃ + AdH), 0.91 (m, 10H, AdH). ¹³C{¹H} NMR (100 MHz, C₆D₆, 298 K, ppm): δ 174.8 (NCN), 140.6, 137.5, 129.0, 125.3, (PhC), 67.5 (C=Si), 65.6 (C=P), 59.7, 54.6, 43.5, 42.4, 38.2, 37.5, 37.2, 36.7, 32.9, 32.0, 31.3, 31.2, 30.4, 30.2, 29.9, 29.6, 29.5, 28.9, 28.8, 22.8, 22.7, 21.1 (AdC + NCM₃ + NCM₃). ²⁹Si{¹H} NMR (95 MHz, C₆D₆, 298 K, ppm): δ 29.5 (m). ³¹P{¹H} NMR (163 MHz, C₆D₆, 298 K, ppm): δ 343.2 (br, P=C), 29.3 (d, ¹J_{P,P} = 378.1 Hz, PAd₂), -143.5 (dd, ¹J_{P,P} = 378.1 Hz, ²J_{P,P} = 7.0 Hz, SiP).

II. UV-visible, PL emission and IR spectra of 3a-d

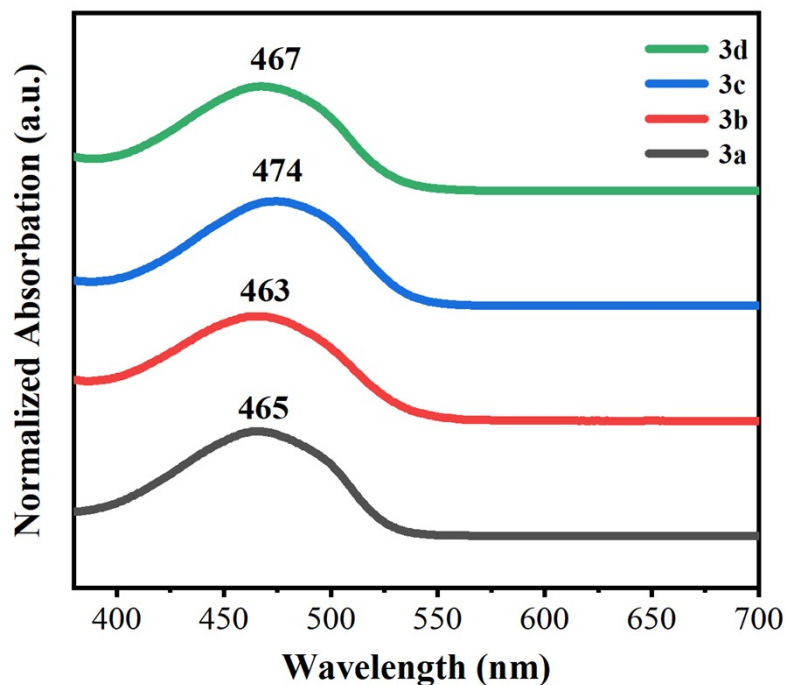


Fig. S1 UV-visible spectra of compounds **3a-d** measured in toluene

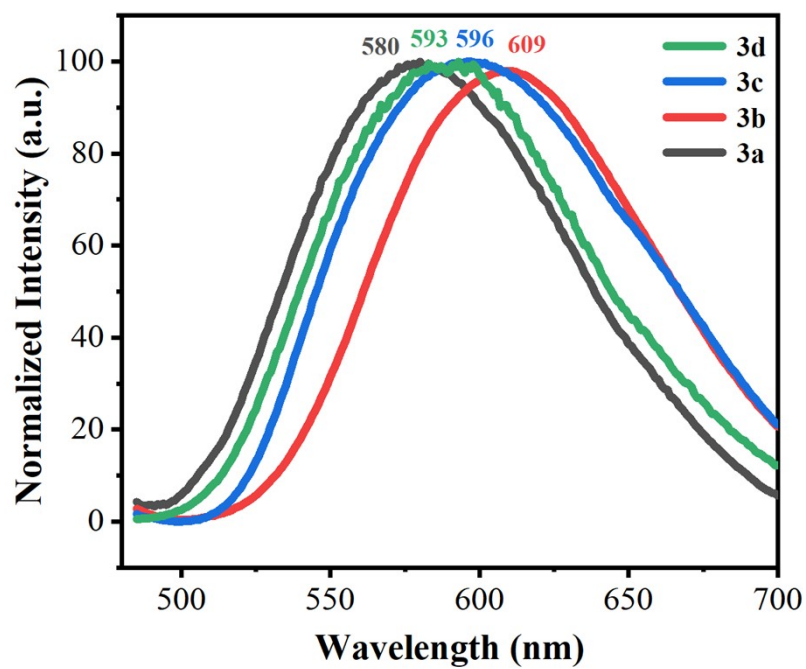
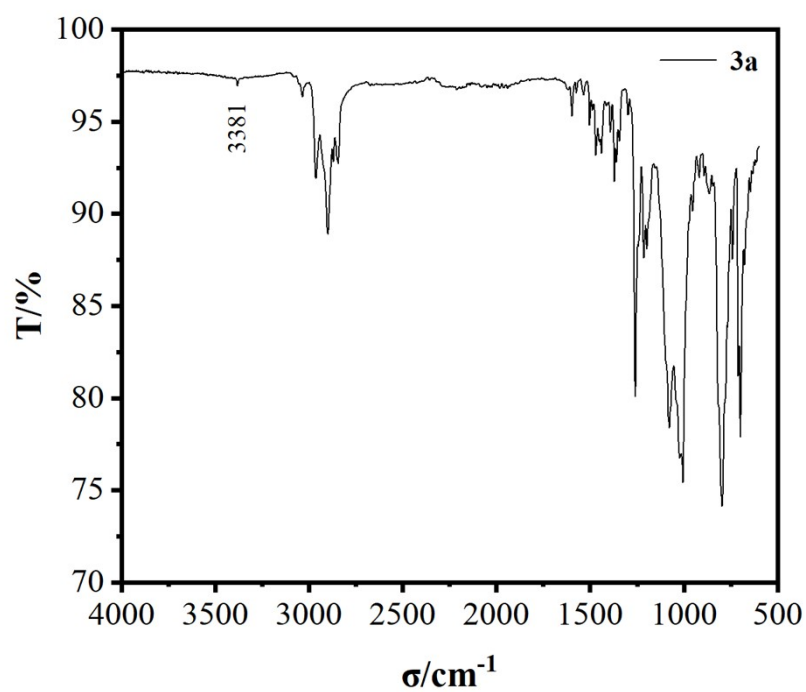
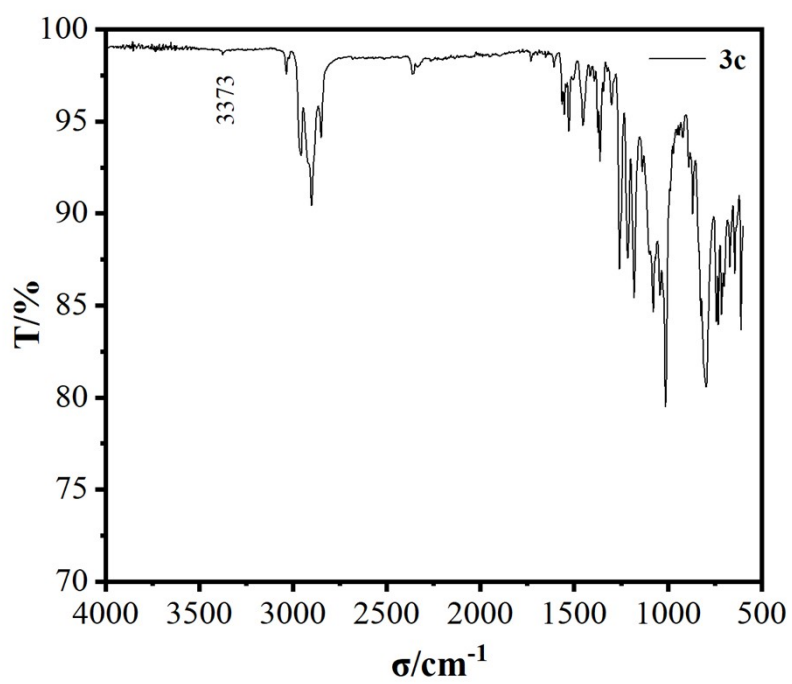
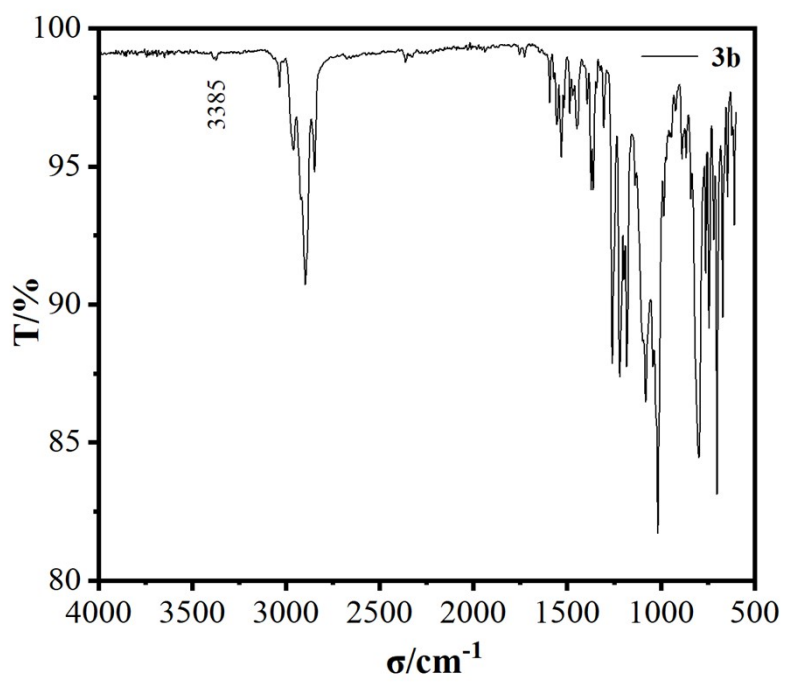


Fig. S2 PL emission spectra of compounds **3a-d** measured in toluene (excitation wavelength: 455 nm)





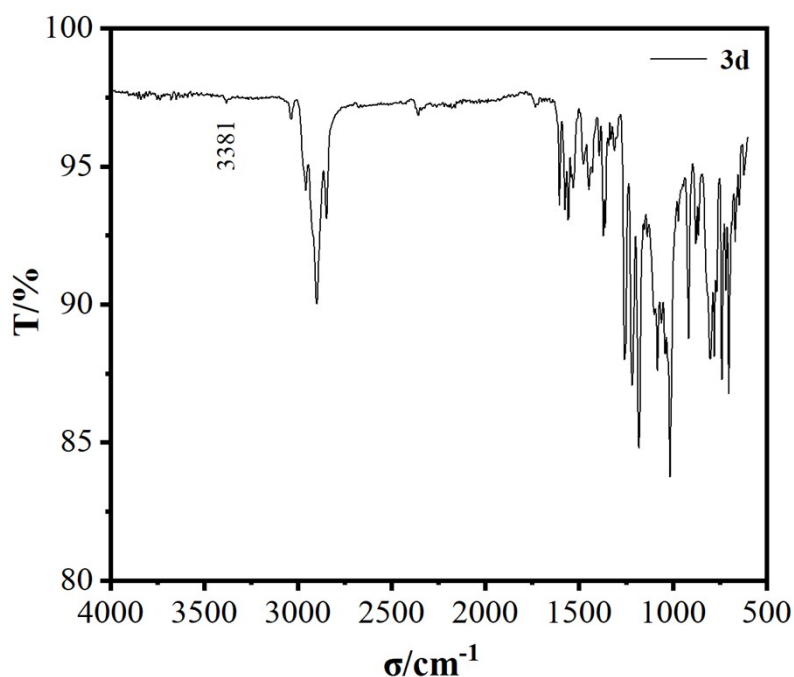


Fig. S3 IR spectra of compounds **3a-d**

III. X-Ray crystallographic details

Crystallographic data were collected on a Smart ApexIIDUO system. During measurements a graphite-monochromatic Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$) was applied. Absorption corrections were all employed using the spherical harmonics program (multi-scan type). All the structures were solved by direct methods (SHELXT)^{S2} and refined against F^2 using SHELXL.^{S3} In general, the non-hydrogen atoms were located by difference Fourier synthesis and refined anisotropically, and hydrogen atoms were included using a riding mode with U_{iso} tied to the U_{iso} of the parent atoms unless otherwise specified. A summary of cell parameters, data collection, and structure solution and refinements is given in Table S1.

Table S1 Crystal data and refinements

	1	2	3a(S)	3a(R)
CCDC No.	2204068	2204070	2277645	2223430
Empirical formula	C ₃₅ H ₅₃ N ₂ PSi	C ₅₆ H ₇₁ N ₂ PSi	C ₄₉ H ₆₃ N ₂ PSi	C ₄₉ H ₆₃ N ₂ PSi
formula weight	560.85	831.20	739.07	739.07
crystal system	Monoclinic	Monoclinic	monoclinic	orthorhombic
space group	$P2_1/c$	$P2_1$	$P2_1$	$P2_12_12_1$
$a/\text{\AA}$	20.8037(13)	11.6045(3)	16.6726(8)	13.281(3)

<i>b</i> /Å	8.7396(5)	18.8105(6)	13.2923(6)	16.693(3)
<i>c</i> /Å	18.1837(10)	11.9676(3)	18.7216(9)	18.753(4)
<i>α</i> /deg	90	90	90	90
<i>β</i> /deg	100.716(2)	115.1440(10)	90.063(2)	90
<i>γ</i> /deg	90	90	90	90
<i>V</i> /Å ³	3248.4(3)	2364.82(12)	4149.0(3)	4157.4(14)
<i>Z</i>	4	2	4	4
ρ_{calcd} /g·cm ⁻³	1.147	1.167	1.183	1.181
μ /mm ⁻¹	0.147	0.122	0.729	0.728
<i>F</i> (000)	1224.0	900.0	1600.0	1600.0
crystal size/mm ³	0.19x0.09x0.04	0.48x0.39x0.3	0.23x0.07x0.06	0.02x0.01x0.01
index ranges	-26 ≤ <i>h</i> ≤ 26 -9 ≤ <i>k</i> ≤ 11 -23 ≤ <i>l</i> ≤ 23	-14 ≤ <i>h</i> ≤ 14 -23 ≤ <i>k</i> ≤ 24 -15 ≤ <i>l</i> ≤ 15	-21 ≤ <i>h</i> ≤ 21 -17 ≤ <i>h</i> ≤ 16 -24 ≤ <i>l</i> ≤ 21	-16 ≤ <i>h</i> ≤ 15 -18 ≤ <i>h</i> ≤ 20 -23 ≤ <i>l</i> ≤ 22
Flack			0.058(18)	0.12(5)
collected data	55442	28644	69132	31628
unique data	7136	9836	18646	8461
	(<i>R</i> _{int} = 0.1099)	(<i>R</i> _{int} = 0.0242)	(<i>R</i> _{int} = 0.1027)	(<i>R</i> _{int} = 0.1479)
data/restraints/parameters	7136/97/413	9836/1/548	18646/1/967	8461/0/484
GOF on <i>F</i> ²	1.038	1.054	1.071	0.972
final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0493 <i>wR</i> ₂ = 0.1012	<i>R</i> ₁ = 0.0383 <i>wR</i> ₂ = 0.1189	<i>R</i> ₁ = 0.0587 <i>wR</i> ₂ = 0.1315	<i>R</i> ₁ = 0.0837 <i>wR</i> ₂ = 0.1914
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0874 <i>wR</i> ₂ = 0.1203	<i>R</i> ₁ = 0.0400 <i>wR</i> ₂ = 0.1213	<i>R</i> ₁ = 0.1024 <i>wR</i> ₂ = 0.1526	<i>R</i> ₁ = 0.1517 <i>wR</i> ₂ = 0.2414
Largest diff peak/hole (e·Å ⁻³)	0.30/-0.24	0.70/-0.28	0.25/-0.41	0.43/-0.53

$$^a R_1 = \sum(|F_o| - |F_c|) / \sum|F_o|, wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)]^{1/2}, \text{GOF} = [\sum w(F_o^2 - F_c^2)^2 / (N_o - N_p)]^{1/2}.$$

	3c	3d	4
CCDC No.	2223427	2223428	2204071
Empirical formula	C ₄₆ H ₆₅ N ₂ PSi	C ₄₃ H ₅₈ FN ₂ PSi	C ₆₄ H ₉₁ N ₂ P ₃ Si
formula weight	705.06	680.97	1009.38
crystal system	triclinic	tetragonal	monoclinic
space group	<i>P</i> -1	<i>P</i> 42/ <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> /Å	11.1312(7)	26.734(2)	12.369(3)
<i>b</i> /Å	11.1624(7)	26.734(2)	23.579(5)
<i>c</i> /Å	18.2271(11)	10.4241(14)	19.827(5)
<i>α</i> /deg	87.154(3)	90	90
<i>β</i> /deg	73.572(2)	90	98.041(9)
<i>γ</i> /deg	67.701(3)	90	90
<i>V</i> /Å ³	2005.6(2)	7449.9(17)	5726(2)
<i>Z</i>	2	8	4
ρ_{calcd} /g·cm ⁻³	1.168	1.214	1.171
μ /mm ⁻¹	0.737	0.809	0.166
<i>F</i> (000)	768	2944.0	2192.0

crystal size/mm ³	0.2x0.15x0.1	0.306x0.074x0.0	0.2x0.09x0.08
		54	
index ranges	-13 ≤ <i>h</i> ≤ 13	-33 ≤ <i>h</i> ≤ 34	-15 ≤ <i>h</i> ≤ 15
	-13 ≤ <i>k</i> ≤ 13	-34 ≤ <i>k</i> ≤ 34	-30 ≤ <i>k</i> ≤ 28
	-21 ≤ <i>l</i> ≤ 21	-13 ≤ <i>l</i> ≤ 13	-25 ≤ <i>l</i> ≤ 25
collected data	21618	75128	104984
unique data	7208	8246	12688
	(<i>R</i> _{int} = 0.0535)	(<i>R</i> _{int} = 0.1354)	(<i>R</i> _{int} = 0.1173)
data/restraints/parameters	7208/0/459	8246/0/439	12688/237/691
GOF on <i>F</i> ²	1.137	1.024	1.056
final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0709	<i>R</i> ₁ = 0.0672	<i>R</i> ₁ = 0.0702
	<i>wR</i> ₂ = 0.1840	<i>wR</i> ₂ = 0.1687	<i>wR</i> ₂ = 0.1728
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0822	<i>R</i> ₁ = 0.1112	<i>R</i> ₁ = 0.0886
	<i>wR</i> ₂ = 0.1899	<i>wR</i> ₂ = 0.1922	<i>wR</i> ₂ = 0.1860
Largest diff peak/hole (e·Å ⁻³)	0.68/-0.41	0.73/-0.54	0.89/-0.63

^a $R_1 = \sum(|F_o| - |F_c|) / \sum |F_o|$, $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)]^{1/2}$, $GOF = [\sum w(F_o^2 - F_c^2)^2 / (N_o - N_p)]^{1/2}$.

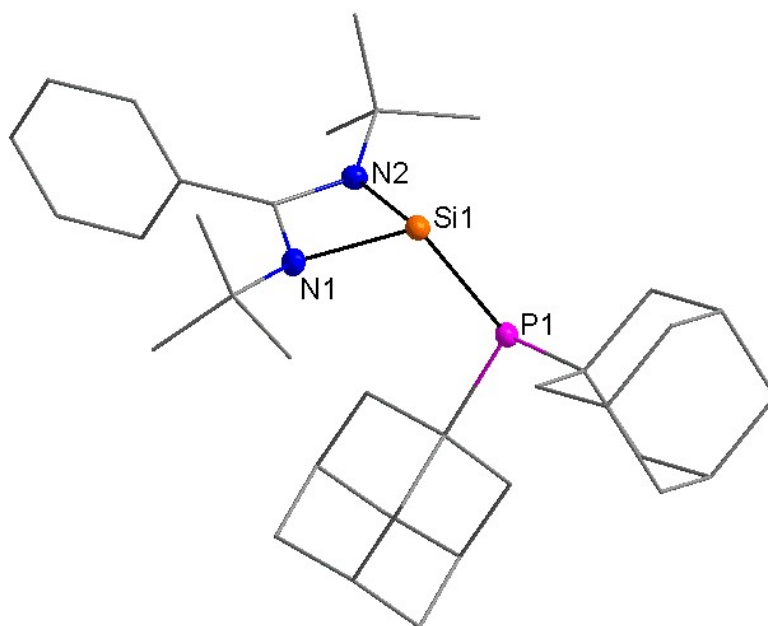


Fig. S4 Molecular structures of **1**. H atoms are omitted for clarity.

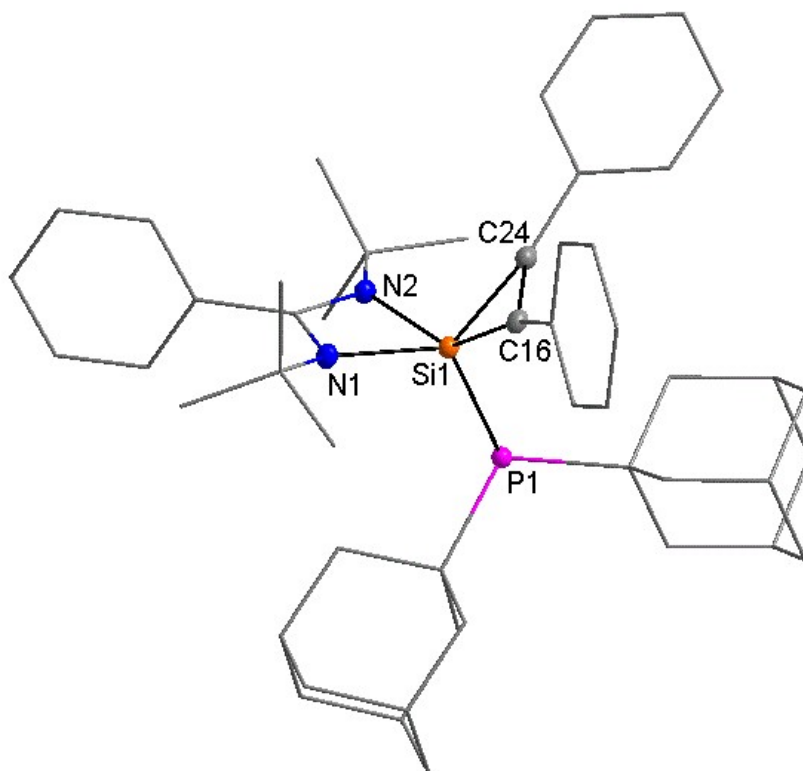


Fig. S5 Molecular structure of **2** (H atoms are omitted for clarity).

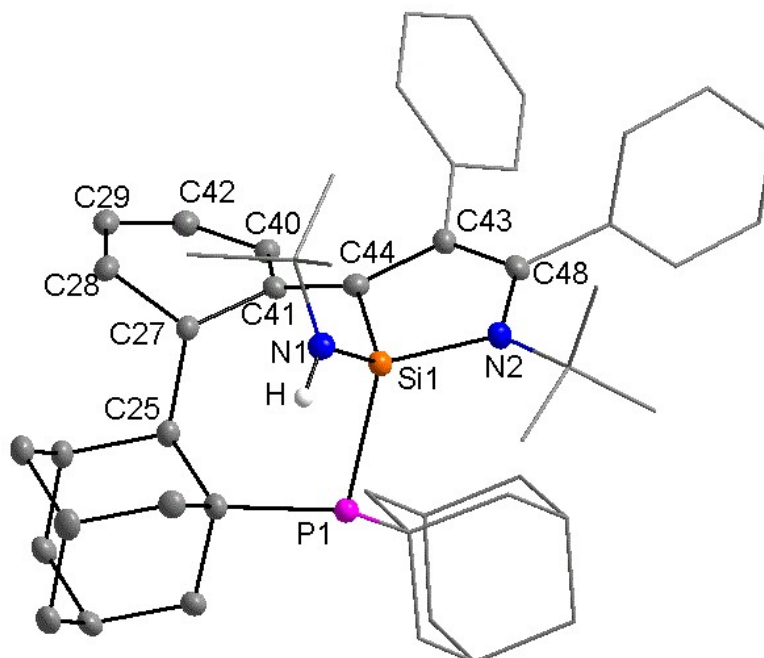


Fig. S6 Molecular structures of **3a(R)**. H atoms are omitted for clarity, except for *NH*.

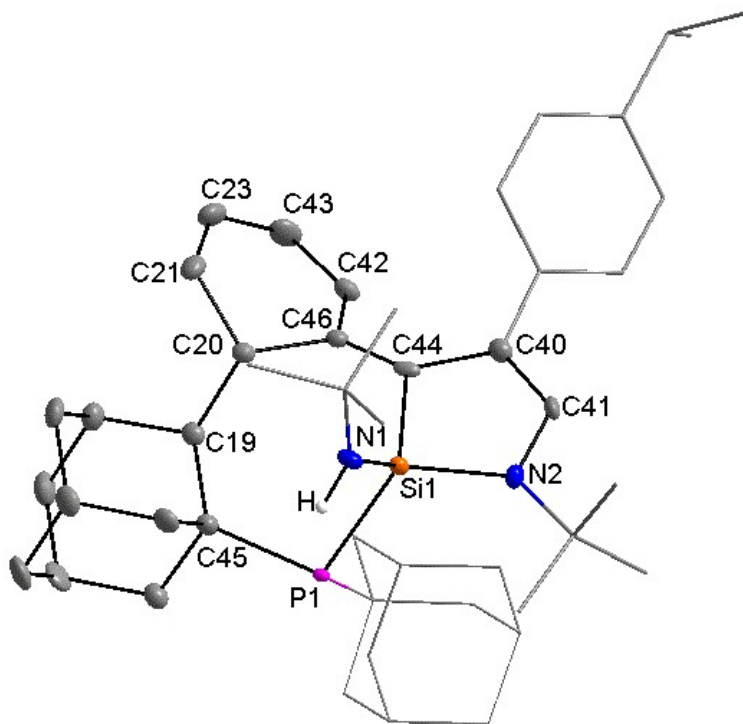


Fig. S7 Molecular structures of **3c**. H atoms are omitted for clarity, except for *NH*.

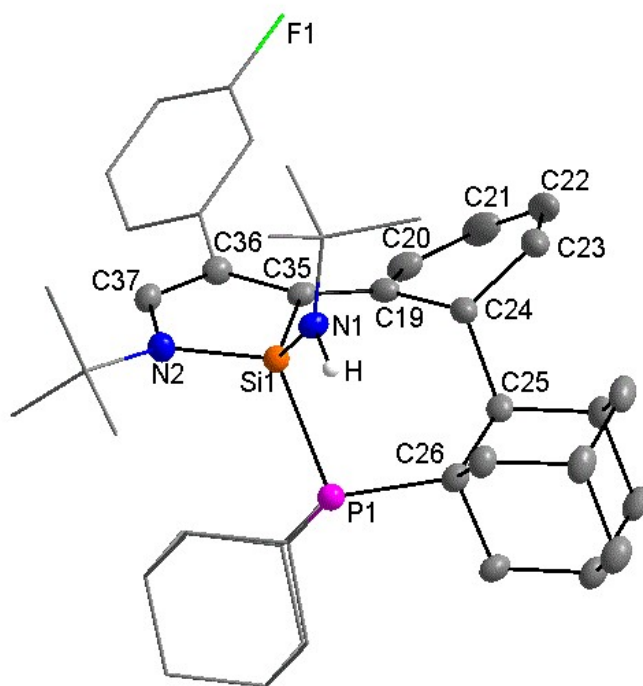


Fig. S8 Molecular structures of **3d**. H atoms are omitted for clarity, except for *NH*.

IV. Theoretical calculations

The theoretical investigations were carried out through the DFT method under B3LYP-D3(BJ)/def2-SVP level of theory using Gaussian 16 B.01 program^{S4-S10}. The maximum forces of all structures were calculated to be less than 0.000450 Hartree/Bohr. The frequency calculations were computed to be zero imaginary frequency and one imaginary frequency for minimum and transition state, respectively.

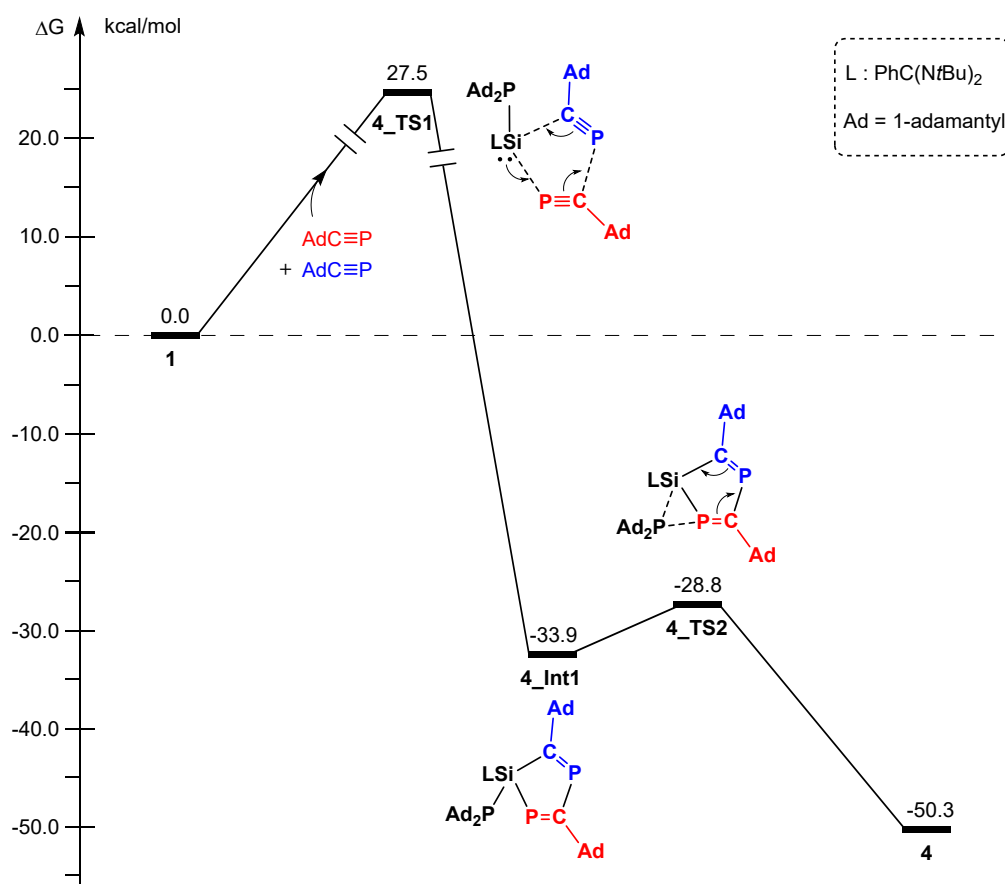


Fig. S9 The free energy profile for the formation of **4** at the B3LYP-D3(BJ)/def2-SVP level of theory.

Table S2 Cartesian coordinates for the formation of compound **3c** and **4**

1 (LSi-PAd₂, L = PhC(NtBu)₂)

P	7.35417900	8.12353000	1.18745800
Si	7.17031300	6.32849200	2.65182200
N	8.89358000	5.96095100	3.49030900
N	8.22400800	5.03496100	1.66918600
C	9.15340500	4.96236300	2.62872600
C	9.36854200	6.15260000	4.87310200
C	8.88953200	4.99634600	5.77075500
H	7.79778700	4.88167600	5.69070500

H	9.14305700	5.19572100	6.82392700
H	9.36421200	4.04752300	5.48617700
C	10.90026900	6.27339100	4.94270400
H	11.39774400	5.32929600	4.68646500
H	11.20338400	6.54600500	5.96540200
H	11.26464200	7.05396500	4.25896800
C	8.73478700	7.45918000	5.37568800
H	9.07236300	8.31820200	4.78224900
H	9.00732200	7.63399900	6.42688600
H	7.63657600	7.40515100	5.31191900
C	10.24663100	3.95684700	2.73608100
C	10.03575700	2.70460200	3.32935300
H	9.05159400	2.45580300	3.72937600
C	11.07959500	1.77978400	3.41212700
H	10.90568400	0.80698400	3.87768900
C	12.34087900	2.09742600	2.90120400
H	13.15583800	1.37275800	2.96530800
C	12.55671900	3.34502600	2.30780200
H	13.53997300	3.59929400	1.90564000
C	11.51546000	4.27009000	2.22668500
H	11.67845700	5.24355900	1.76233700
C	7.94497900	4.14008900	0.53138400
C	7.35469500	2.81172700	1.04051600
H	8.09576600	2.23856600	1.61410300
H	7.02884100	2.18762300	0.19356700
H	6.48389700	3.00587300	1.68479400
C	9.20258300	3.87028700	-0.31116900
H	9.66394500	4.81361000	-0.63620200
H	8.92399300	3.29898200	-1.20993500
H	9.95168900	3.28527100	0.23730700
C	6.89913100	4.84451500	-0.34413300
H	5.98750500	5.06077600	0.23426200
H	6.62370700	4.19917200	-1.19175300
H	7.27726500	5.80183000	-0.72684800
C	6.27124200	9.49440400	1.96264000
C	6.90806500	10.30449600	3.10969400
H	7.81595800	10.81481900	2.75607300
H	7.21555900	9.62427000	3.91953100
C	5.92098300	11.35835900	3.64882600
H	6.40585100	11.92036300	4.46536400
C	4.65811600	10.66060800	4.17893500
H	3.95556600	11.40578300	4.59034200
H	4.92234000	9.97590800	5.00300600
C	3.99259600	9.87621700	3.03569800

H	3.09489900	9.35893900	3.41445500
C	4.98251500	8.82533700	2.50381400
H	4.51248000	8.22428500	1.70679500
H	5.23145300	8.12277400	3.31337600
C	5.83841100	10.47406000	0.83952800
H	6.71456500	10.97520800	0.40689300
H	5.36791000	9.90150900	0.02389500
C	4.86195000	11.53566700	1.37764500
H	4.59336200	12.22411500	0.55839700
C	3.59815500	10.84390500	1.90988300
H	3.09776300	10.29324900	1.09534300
H	2.87894300	11.59287900	2.28439400
C	5.53588800	12.32301900	2.51437900
H	6.43515700	12.83911300	2.13575500
H	4.85322400	13.10262300	2.89400700
C	9.14613900	8.74517600	0.94858200
C	9.83753600	7.64558700	0.10411400
H	9.81848200	6.69666100	0.65603700
H	9.26608100	7.48178000	-0.82425000
C	11.28730600	8.03221900	-0.23391700
H	11.74531900	7.22383000	-0.82975000
C	12.08458500	8.23571100	1.06489700
H	12.11125400	7.29955700	1.64762600
H	13.13109800	8.49874200	0.83337600
C	11.42488700	9.34568300	1.89739400
H	11.98565100	9.48682200	2.83755500
C	9.97653400	8.94137500	2.23243500
H	9.52191900	9.71073100	2.87097400
H	9.97040700	8.00280000	2.79794400
C	9.17994800	10.05796300	0.13336800
H	8.58784300	9.94066800	-0.78914400
H	8.72082100	10.87353400	0.71102800
C	10.63003900	10.45042400	-0.20980200
H	10.61855000	11.38967400	-0.78835400
C	11.28785500	9.33881600	-1.04330100
H	10.73575000	9.19756900	-1.98792900
H	12.32004200	9.62346800	-1.31092000
C	11.42273500	10.65530400	1.09232200
H	12.45683600	10.96578400	0.86383800
H	10.96712600	11.46449800	1.68847800

ArCCH (Ar = 4-*i*Pr-Ph)

C	-10.18735500	1.09092200	-0.08531800
C	-11.37463900	1.21776900	-0.30525100

C	-8.78799100	0.94224100	0.17410100
H	-12.42423300	1.32966100	-0.49977300
C	-8.12492000	-0.26506800	-0.11554700
C	-8.04057700	2.00239400	0.72608000
C	-6.67980800	1.85299400	0.97639400
C	-6.01268500	0.65034000	0.68930100
H	-8.54299200	2.94404000	0.95529400
H	-6.12587700	2.69194300	1.40465000
C	-6.76150900	-0.40033000	0.14051300
H	-8.69065500	-1.09485900	-0.54328000
C	-4.52743200	0.48925800	0.96331000
H	-6.26401900	-1.34603400	-0.09130600
C	-3.68771900	1.46734700	0.12764200
H	-4.25392700	-0.53364800	0.65279000
C	-4.21020200	0.61935900	2.46085500
H	-4.44777900	1.62948400	2.83215000
H	-3.13995500	0.43794200	2.65026200
H	-4.79213500	-0.10121000	3.05575900
H	-3.89549700	1.35352000	-0.94737600
H	-2.61152900	1.29575700	0.29074800
H	-3.90375600	2.51276800	0.40168200

3c_TS1

P	-0.36630200	0.73509900	-0.59402000
Si	0.29701000	-1.27344700	0.31755600
N	1.77108600	-1.86844500	-0.63024700
N	1.81856200	-1.16419300	1.40895700
C	-0.27580600	-3.31798000	1.27449600
C	3.97485800	-2.14198000	0.54904300
C	-1.03916700	-2.47566500	0.51741400
C	2.55355200	-1.72287400	0.44708600
C	4.28881200	-3.46719900	0.87844000
H	3.48331200	-4.17108000	1.09162200
C	-2.37154500	0.49109200	1.40618500
H	-2.81151400	-0.23897000	0.72020800
H	-1.67778200	-0.05869800	2.05799300
C	-1.61369600	1.57496000	0.60495700
C	-1.03482000	2.59001000	1.61341200
H	-0.49820400	3.39581400	1.09621500
C	1.09140700	1.91702900	-0.92953400
C	5.00104600	-1.22325700	0.29731400
H	4.75035600	-0.19453800	0.03790800
C	1.95356100	-2.62489400	-1.88677800
C	2.07131300	-1.03778300	2.86024000

C	-2.15760700	3.21348800	2.46692200
C	-3.49008800	1.10709000	2.26293800
H	-3.99507000	0.29457800	2.81111900
C	2.05095700	2.17973000	0.24862700
H	1.51575300	2.62488800	1.09696100
H	2.45589800	1.22110000	0.60085500
C	0.55009200	3.26283200	-1.47215100
H	-0.11444600	3.06964900	-2.33040000
H	-0.05400200	3.77635900	-0.71266000
C	1.70802200	4.18504300	-1.89533500
H	1.28955400	5.13980800	-2.25574000
C	1.91618500	1.27017500	-2.06892700
H	2.31094700	0.30472500	-1.72777500
H	1.25778000	1.06386300	-2.92823400
C	5.62412900	-3.86936100	0.94431500
H	5.86532400	-4.90295500	1.20219200
C	-3.15819300	3.93604800	1.54894600
H	-3.94999600	4.41149200	2.15272800
H	-2.64835800	4.74249600	0.99387100
C	-2.88409000	2.11179800	3.25359000
H	-3.67272200	2.55272400	3.88725900
H	-2.17664300	1.59874600	3.92751500
C	-3.77284800	2.92604500	0.56613900
H	-4.48571300	3.44145500	-0.09959800
C	6.33483800	-1.62972300	0.36306100
H	7.13088300	-0.90975300	0.16079000
C	-2.65627200	2.29976400	-0.28855600
H	-2.16740100	3.08142900	-0.88952200
H	-3.08452200	1.57463600	-0.99826700
C	3.07625600	2.18178200	-2.50719400
H	3.64132100	1.67979700	-3.31119600
C	3.19969400	3.11238100	-0.18146300
H	3.85784800	3.29555200	0.68501700
C	2.62064700	4.44548900	-0.68427000
H	3.43687900	5.13300600	-0.96460100
H	2.04823700	4.93675800	0.12114900
C	6.64802100	-2.95362600	0.68420800
H	7.69183600	-3.27186000	0.73440800
C	2.51393300	3.51624500	-3.01986500
H	3.33515900	4.17625800	-3.34786600
H	1.86697200	3.34377500	-3.89650400
C	-4.49826200	1.81990200	1.34854500
H	-4.94876700	1.09457900	0.65070700
H	-5.31959700	2.25104700	1.94666900

C	0.76410900	-2.25843000	-2.78656500
H	0.72150600	-1.17771300	-2.97565200
H	-0.18322100	-2.56289100	-2.31878000
H	0.85001600	-2.78116700	-3.75026600
C	4.00316700	2.45019900	-1.31138200
H	4.84278400	3.09744200	-1.61710600
H	4.44465200	1.50446400	-0.95700600
C	3.18441400	-0.01734600	3.14171300
H	4.12829300	-0.30767500	2.66009700
H	3.36552600	0.04007000	4.22615800
H	2.90218300	0.98417000	2.78735700
C	1.90554400	-4.13555500	-1.59283100
H	2.80079200	-4.46204600	-1.04692400
H	1.86231900	-4.70069500	-2.53692200
H	1.02141500	-4.37419200	-0.98574800
C	2.41969200	-2.40749900	3.46939600
H	1.69680600	-3.15140400	3.10196800
H	2.36505000	-2.34831400	4.56760200
H	3.43851700	-2.72039900	3.20527800
C	0.75545600	-0.54653000	3.47288100
H	0.44810700	0.40538100	3.01932600
H	0.87544100	-0.38811200	4.55431300
H	-0.03879000	-1.29003400	3.31290700
C	3.26947700	-2.26372300	-2.59250500
H	3.33505200	-1.18444900	-2.79154600
H	3.31697800	-2.79069900	-3.55751300
H	4.14722000	-2.56340200	-2.00555200
H	-0.30509500	2.09406500	2.26995300
H	-1.70743400	3.93749900	3.16737000
H	-0.79613900	-4.23928400	1.62543300
C	-2.45232600	-2.52627300	0.08064900
C	-5.20419700	-2.50677000	-0.66292200
C	-3.42319000	-3.16345300	0.86997100
C	-2.88473700	-1.90206300	-1.10445100
C	-4.23051200	-1.89276700	-1.46693800
C	-4.76984400	-3.15079100	0.50474900
H	-3.11113700	-3.65043900	1.79723800
H	-2.15628900	-1.37669700	-1.72579100
H	-4.52765700	-1.38321900	-2.38757400
H	-5.50798600	-3.63641300	1.15047000
C	-6.68031500	-2.43800900	-1.01522000
H	-7.21475600	-3.06788700	-0.28305700
C	-6.97560500	-3.00194900	-2.41220400
H	-6.49168700	-2.39932400	-3.19784900

H	-8.05909700	-3.00070900	-2.61466400
H	-6.60800700	-4.03507900	-2.50971600
C	-7.21582700	-1.00423600	-0.86904400
H	-6.71576800	-0.32364300	-1.57757300
H	-7.03762700	-0.61611900	0.14578000
H	-8.29914900	-0.96237300	-1.06958700

3c_Int1

P	6.31653200	5.46617800	15.72728100
Si	7.95233900	7.01906800	15.17902600
N	9.51435700	5.67267300	15.39705000
N	8.97473700	6.78214500	13.60359700
C	7.45020400	8.80475400	15.22830600
C	11.02108800	5.31314700	13.43912900
C	8.27105900	8.46326800	16.25267000
C	9.86739700	5.92123300	14.16054300
C	12.31329800	5.83652700	13.56548900
H	12.48396900	6.71118800	14.19451100
C	5.33026400	7.28907900	17.56098100
H	5.74374100	6.57697000	18.29533500
H	6.14154300	7.96980000	17.28660300
C	4.82813100	6.50490300	16.31808200
C	4.21901400	7.48793100	15.30047100
H	3.81844600	6.93013200	14.43929000
C	5.93131600	4.59868100	14.06432200
C	10.80574500	4.19362500	12.62307300
H	9.79987300	3.78563700	12.52395700
C	10.15857700	4.83254900	16.42205300
C	9.22051400	7.69037100	12.44862500
C	3.08206100	8.29933000	15.95054800
C	4.19144400	8.10287900	18.19723500
H	4.59529800	8.66587700	19.05551100
C	5.86611700	5.50436900	12.82076900
H	5.05217600	6.23727700	12.92106500
H	6.80019400	6.06834400	12.74522000
C	4.62303600	3.78083100	14.13494200
H	4.62531300	3.13520600	15.02920500
H	3.76345800	4.46051100	14.22463400
C	4.43915900	2.93282000	12.86040700
H	3.49948900	2.36164200	12.94723300
C	7.10057300	3.59769100	13.87572200
H	8.05001900	4.14548900	13.83783200
H	7.15686400	2.93187600	14.75250900
C	13.37884200	5.24851100	12.87974300

H	14.38312800	5.66568300	12.98017900
C	1.97813200	7.33846000	16.42348000
H	1.13992500	7.90577200	16.86351100
H	1.57151800	6.77867200	15.56338200
C	3.63058600	9.08478600	17.15395800
H	2.83093600	9.69971700	17.60191100
H	4.42490700	9.77559600	16.82385100
C	2.55767800	6.36292400	17.46268600
H	1.77219100	5.66007500	17.78913200
C	11.87127200	3.60525200	11.94411900
H	11.69423100	2.73206100	11.31253800
C	3.70786200	5.55850000	16.82532800
H	3.29962200	4.95976600	16.00276600
H	4.12985600	4.84991400	17.55721300
C	6.92355400	2.76821800	12.59335600
H	7.78030100	2.07910400	12.48805200
C	5.67100800	4.67125300	11.53946700
H	5.62516400	5.35166500	10.67128900
C	4.36619100	3.86566600	11.63889800
H	4.20810000	3.27691300	10.71852600
H	3.50584300	4.55015900	11.73670800
C	13.16072000	4.13211100	12.06902000
H	13.99460500	3.67215900	11.53436000
C	5.61962100	1.96196000	12.69505000
H	5.47954200	1.34248900	11.79226600
H	5.66826900	1.27372200	13.55644600
C	3.07985200	7.15561800	18.66934100
H	3.47173700	6.46556200	19.43579100
H	2.25832800	7.72628100	19.13619700
C	9.14608600	4.63449300	17.55966800
H	8.28500200	4.04081200	17.22914400
H	8.75076200	5.59791000	17.90884100
H	9.63387800	4.12789600	18.40629100
C	6.85736300	3.70658200	11.37604200
H	6.74988100	3.11911500	10.44774900
H	7.79551900	4.27980700	11.28713500
C	9.79552900	6.95755600	11.22190200
H	10.84140200	6.65589800	11.34724400
H	9.74741600	7.63353300	10.35448900
H	9.19994300	6.06312400	10.98719600
C	11.38819400	5.58077500	16.97262000
H	12.16752700	5.68330900	16.20507000
H	11.82220300	5.02932400	17.82152900
H	11.10426200	6.58555800	17.31830600

C	10.18850200	8.80432100	12.89192400
H	9.76976300	9.36599700	13.73888800
H	10.37961200	9.50558600	12.06410100
H	11.15477900	8.38113300	13.20381600
C	7.89120600	8.32540700	12.00427100
H	7.23279800	7.58430400	11.52832600
H	8.10294300	9.10989300	11.26111100
H	7.35428600	8.77459600	12.84736000
C	10.57067400	3.44417700	15.90045200
H	9.72456600	2.95304300	15.39806300
H	10.87348200	2.81335700	16.75026600
H	11.41456800	3.48830200	15.20150100
H	4.99870900	8.16044500	14.91506500
H	2.66916400	9.00161400	15.20634100
C	8.84787900	9.19510000	17.38074300
C	8.95683700	10.59732000	17.35460600
C	9.29022500	8.52587400	18.53594500
C	9.48386600	11.29561400	18.43975700
H	8.62458500	11.13866300	16.46506200
C	9.80956200	9.22866400	19.62187100
H	9.20647800	7.43975600	18.57989200
C	9.91826700	10.62788800	19.59532600
H	9.56167700	12.38586100	18.39414100
H	10.13601400	8.67486300	20.50603500
H	6.98172100	9.77091000	14.98720100
C	10.49684300	11.39685800	20.77046700
H	10.42371800	12.46989500	20.51990700
C	9.69304500	11.16599400	22.05790900
C	11.98403100	11.07051000	20.97730700
H	10.08742700	11.78455200	22.87966200
H	8.63178500	11.41741700	21.91697000
H	9.74671400	10.11264900	22.37819000
H	12.12275600	10.00668400	21.23055000
H	12.56604100	11.27656300	20.06635200
H	12.40949700	11.66886900	21.79896600

3c_TS2

P	4.65324200	6.87493300	14.45565500
Si	4.94151600	9.06822300	13.96927900
N	3.95035500	10.32911900	14.19816000
N	6.73294100	9.62395600	14.43837500
C	6.12972800	10.64493200	16.68703300
C	7.38461900	8.44629200	16.47440000
C	4.76937600	10.67325700	16.64994200

H	4.29058700	11.52437900	17.16314800
C	6.81877900	9.55413600	15.93561800
C	8.21297100	7.40861400	15.70153800
H	8.52447700	7.81914600	14.73458200
C	7.02083300	11.63574200	17.39194900
C	8.34943900	11.34591000	17.75835300
H	8.75298000	10.36244400	17.55835000
C	6.91069100	6.22737200	12.92743700
H	6.09994600	6.15058600	12.19168600
H	7.29702000	7.25454700	12.86868500
C	6.33602800	5.92881300	14.34830800
C	7.49685000	6.00836300	15.42582200
H	7.09731400	5.68643900	16.39077500
C	3.73926300	6.56759000	16.12451300
C	9.14758100	12.29532600	18.40043300
H	10.16559400	12.03486600	18.67504300
C	8.66307900	13.57136600	18.70658900
C	7.33665500	8.28044000	17.93386700
H	6.51958000	8.76334600	18.45707800
C	2.59887300	10.81307700	13.84326900
C	7.37467800	10.86986800	13.70608200
C	8.59959600	4.96994500	15.00159400
H	9.39552000	5.00773600	15.74930100
C	8.04381800	5.23801000	12.55590300
H	8.43521700	5.50289600	11.56481600
C	4.63394700	6.24297300	17.34227300
H	5.20515000	5.32609600	17.15400000
H	5.34410900	7.05214600	17.51400000
C	2.75933000	5.37094700	15.89830700
H	2.11407000	5.58917800	15.03844300
H	3.32042500	4.45662200	15.67245100
C	1.89208100	5.13914000	17.16430100
H	1.22118400	4.28862600	16.98261000
C	2.88548600	7.82903500	16.43239400
H	3.52622500	8.71197400	16.57258000
H	2.22413100	8.02918500	15.58006400
C	9.49943600	7.15955800	16.49872500
H	10.39506500	6.90672800	15.94210100
C	8.04844200	3.52917600	14.97320400
H	8.86433000	2.83404100	14.73202700
H	7.65621700	3.25981400	15.96291300
C	6.54073400	12.92526500	17.70136600
H	5.52668500	13.18618100	17.42107800
C	9.17314200	5.31550500	13.60691600

H	9.96584300	4.59946000	13.35115600
H	9.62433800	6.31639600	13.60366900
C	6.93112100	3.43752100	13.92215400
H	6.50635100	2.42514000	13.90419700
C	8.33154600	7.64111800	18.58541600
H	8.31670800	7.53629700	19.66384000
C	5.82626200	4.43565900	14.31492600
H	5.43372500	4.16785700	15.30179700
H	4.99900400	4.37313000	13.59770400
C	9.54587500	14.60050300	19.40709200
H	10.52114700	14.12985200	19.58908800
C	2.01731200	7.59874400	17.69261500
H	1.43743100	8.51053100	17.88882800
C	3.76224000	6.02594900	18.60755800
H	4.42429500	5.80966300	19.45681000
C	2.80751600	4.83220900	18.37304500
H	2.19569100	4.65913200	19.26880300
H	3.39008300	3.92064200	18.18026800
C	9.51038800	7.20217400	17.84119500
H	10.41334500	6.96522400	18.39454400
C	1.05989200	6.40750600	17.46348000
H	0.43798400	6.24358500	18.35445400
H	0.39175300	6.62351000	16.61885800
C	7.47974100	3.79874000	12.52420700
H	6.67702000	3.72766200	11.77841500
H	8.27299200	3.09561500	12.23713000
C	1.90065300	11.31994700	15.13079000
H	1.81049600	10.50740800	15.85383900
H	0.90616200	11.70303700	14.87441700
H	2.49356300	12.11845000	15.58227800
C	7.33970400	13.86657000	18.34217000
H	6.92982900	14.84882600	18.55461800
C	2.94067900	7.30329900	18.89740700
H	2.34126900	7.16357300	19.80750100
H	3.61585200	8.15383200	19.05779400
C	8.85237500	10.93227900	14.13312700
H	8.93712500	11.12377500	15.20535700
H	9.33473400	11.75486300	13.59429100
H	9.38091700	10.00365200	13.88417300
C	1.73094100	9.71804700	13.17776100
H	2.21132900	9.37245400	12.25567600
H	0.73755100	10.11374500	12.93566400
H	1.61649100	8.86633000	13.85332700
C	6.64656200	12.17790700	14.04485400

H	5.56978400	12.03436100	13.95251400
H	6.98870200	12.94334000	13.33817900
H	6.87765300	12.50342400	15.05855100
C	7.26780000	10.56289900	12.19794600
H	7.73971000	9.60393900	11.94871100
H	7.78759300	11.35206600	11.64487900
H	6.22205300	10.53738300	11.87949700
C	2.75877200	12.00046800	12.85952500
H	3.36853100	12.78266600	13.32083400
H	1.77691800	12.41423200	12.60182100
H	3.25357200	11.66002900	11.94359300
C	8.94837800	15.01446300	20.77484600
H	7.97395800	15.49532200	20.63435300
H	9.61206200	15.72345500	21.28415300
H	8.80977400	14.13804500	21.41617200
C	9.77183100	15.84592200	18.51386000
H	10.21813700	15.55814700	17.55627800
H	10.43778200	16.55999200	19.01298300
H	8.81858700	16.34728900	18.31257200
H	7.28999800	8.83186500	14.08267400

3c_Int2

P	5.55635700	10.91526700	14.54182900
Si	5.63840800	8.88415100	13.32607200
N	5.93170900	7.30113600	14.33335000
N	7.51418300	9.01537400	12.79549700
C	8.31692000	7.65274400	14.66193400
C	9.92202300	8.40623700	12.95376700
C	7.06650700	7.13327500	15.00283400
C	8.50498300	8.39590100	13.44389100
C	10.35167500	7.48966900	11.98561300
H	9.64032300	6.77948200	11.56180000
C	9.43102400	7.21525500	15.56950800
C	10.57609900	6.51427400	15.14993100
H	10.71908500	6.27964100	14.09833500
C	3.67701000	10.46230400	16.75524100
C	3.80717900	10.99983000	15.31413500
C	3.33185400	12.47775700	15.29148800
H	3.40434200	12.86043200	14.26097000
C	6.85464700	11.36647700	15.86853000
C	11.54323500	6.09136900	16.06166700
H	12.42141600	5.55537300	15.69037700
C	11.41411400	6.32424900	17.43688200
C	10.86009200	9.25581600	13.55360200

C	4.85339000	6.28307800	14.56357800
C	7.69880300	9.71472600	11.44212100
C	1.88674200	12.60515200	15.80748900
H	1.59329600	13.66866300	15.79556400
C	2.22523800	10.58344100	17.25937400
H	2.16908300	10.19202000	18.28966600
C	6.51490200	12.70500200	16.56405200
H	6.32841600	13.48106400	15.80378100
H	5.59493600	12.60688600	17.15743500
C	8.16571200	11.58376900	15.07154200
H	8.43076500	10.65383200	14.55510100
H	7.99632400	12.34360500	14.29148400
C	9.31707600	12.01876900	15.99275200
H	10.23067100	12.15728000	15.38794100
C	7.12137900	10.30079500	16.94709400
H	6.21671400	10.12045400	17.54401700
H	7.36625300	9.35643000	16.44684700
C	11.68861600	7.46014900	11.58326800
H	12.01054900	6.74408100	10.82353200
C	0.94807800	11.79818600	14.89809700
H	-0.09667800	11.89289100	15.24168700
H	0.98817700	12.19311300	13.86882900
C	9.29063600	7.41477000	16.95680300
H	8.41080400	7.93358400	17.33434800
C	1.80403700	12.06268400	17.24442800
H	0.77666500	12.16903200	17.63343000
H	2.46219400	12.64909500	17.90859000
C	1.38055400	10.32447200	14.91367800
H	0.72590600	9.73659400	14.24785000
C	12.19583900	9.22470400	13.15508200
H	12.91585100	9.89698600	13.62702400
C	2.83193900	10.19925300	14.41893300
H	2.91385000	10.53952700	13.37391500
H	3.11634200	9.13793500	14.41949400
C	12.48722400	5.88014100	18.41535000
H	13.26364300	5.36223700	17.82628700
C	8.27239700	10.73610500	17.87637700
H	8.44029500	9.95653800	18.63939200
C	7.66136300	13.14163500	17.49665600
H	7.38178700	14.08990200	17.98654400
C	8.94671200	13.34266800	16.67852800
H	9.76881300	13.67691400	17.33465100
H	8.79346200	14.13150600	15.92256800
C	12.61358000	8.33346800	12.16227900

H	13.66017300	8.31016700	11.85006300
C	9.55776100	10.93682800	17.05730100
H	10.38830700	11.23317600	17.72107600
H	9.85212700	9.98806000	16.58258700
C	1.28832600	9.77597800	16.34702500
H	1.57038200	8.70911600	16.36304100
H	0.24966500	9.83899200	16.71493200
C	3.77232600	6.39637700	13.47993500
H	3.25385800	7.36281300	13.50144500
H	3.02704600	5.60228400	13.64013400
H	4.20290500	6.27492700	12.47552800
C	10.25521700	6.98386200	17.86672600
H	10.09874600	7.18036400	18.93047100
C	7.89400400	12.05840000	18.56418700
H	8.69549400	12.37210900	19.25495400
H	6.98102100	11.92282000	19.16936600
C	6.58384700	10.75870000	11.22933500
H	5.58125900	10.31251000	11.26613100
H	6.71989400	11.19810200	10.23060200
H	6.62317200	11.55623500	11.98187500
C	4.22264500	6.50132100	15.94767700
H	4.97444500	6.43163500	16.74900000
H	3.44762600	5.74476800	16.14515100
H	3.75639500	7.49419900	16.00642900
C	7.56539200	8.65248900	10.33940500
H	8.36664100	7.90572800	10.39033500
H	7.61461800	9.13358200	9.35023900
H	6.59560700	8.13965500	10.42701100
C	9.01559000	10.50521500	11.29901000
H	9.21273700	11.10748000	12.19588400
H	8.89409500	11.19941400	10.45496400
H	9.89215000	9.88920600	11.08608500
C	5.45481500	4.86759400	14.46627800
H	5.96605200	4.73612500	13.50045000
H	4.65472800	4.11581600	14.53981100
H	6.17767400	4.65801500	15.26730100
C	11.94446600	4.88051700	19.44712000
H	11.17250600	5.34371100	20.08286900
H	12.75008100	4.52386400	20.10921200
H	11.49147000	4.00647000	18.95445300
C	13.15195100	7.08327400	19.10169200
H	13.56787600	7.78332600	18.36088700
H	13.96931400	6.75632500	19.76485800
H	12.42522300	7.64008500	19.71534100

H	3.99383800	13.10320400	15.90498300
H	7.06116400	6.44274900	15.85462400
H	4.33418200	11.02401100	17.43351100
H	10.54041400	9.94360300	14.33599200
H	4.00781100	9.41299400	16.79325300

3c_TS3

P	4.49973800	6.90885200	14.49227900
Si	5.15418500	8.80107300	13.35411100
N	4.35804900	10.23420700	14.22132600
N	7.03736100	9.23804700	13.98410700
C	6.23084600	10.74533500	15.74050900
C	7.92193000	8.87945700	16.19972500
C	5.02791800	11.01896000	15.08621600
H	4.55560500	11.96700000	15.34604100
C	7.08463700	9.66241400	15.36324800
C	8.80129300	7.88349800	15.64326300
C	6.57695500	11.64024700	16.87444500
C	7.88552400	12.11459900	17.07335700
H	8.67530100	11.80598100	16.38711200
C	6.12128600	5.77922400	12.52676400
H	5.15615500	5.59642500	12.02675200
H	6.44470300	6.78398700	12.21880200
C	5.93325500	5.71926400	14.06610700
C	7.27672400	5.94623300	14.76575600
C	4.16581600	6.92866400	16.38081900
C	8.19335800	12.95547500	18.14027800
H	9.22159900	13.30634400	18.26621300
C	7.21350400	13.36540100	19.05730500
C	7.81807700	8.93193600	17.62907400
H	7.11822900	9.63052200	18.08033200
C	3.03660400	10.72984100	13.70096600
C	7.87092500	10.04301500	12.96100000
C	8.32828300	4.97253600	14.26947300
H	9.29071500	5.16161800	14.76698000
C	7.16894800	4.75765300	12.05687000
H	7.28274100	4.84245000	10.96251000
C	5.31164500	6.53422300	17.32790600
H	5.65442200	5.51369700	17.10659800
H	6.16529400	7.20271200	17.18337200
C	2.98804300	5.94589300	16.61226400
H	2.15257600	6.20774500	15.94292100
H	3.29532700	4.92230900	16.34397800
C	2.52340700	5.98693400	18.08044400

H	1.69198100	5.27415500	18.21446000
C	3.69018200	8.34473900	16.76281900
H	4.51432400	9.05486000	16.62569500
H	2.87750700	8.65963800	16.08980500
C	9.59508200	7.08811700	16.50669600
H	10.32609700	6.40472400	16.07174700
C	7.87054800	3.53303600	14.63131500
H	8.63287300	2.79966900	14.31047800
H	7.77005100	3.44288800	15.72529700
C	5.59583700	12.04545300	17.79970300
H	4.57878700	11.65922000	17.70108400
C	8.50784300	5.06046900	12.74506200
H	9.27990800	4.34663700	12.41000900
H	8.85761300	6.06823900	12.46508400
C	6.52800300	3.24011800	13.94328100
H	6.18594500	2.22586300	14.21213000
C	8.55125700	8.10111000	18.44046100
H	8.43129100	8.15928200	19.52453800
C	5.47594100	4.26338200	14.40377200
H	5.31574800	4.16588200	15.48797500
H	4.50493800	4.06865700	13.91504000
C	7.56428900	14.26935400	20.22658800
H	8.63683800	14.51202300	20.13300600
C	3.20836900	8.39423800	18.22187300
H	2.87220300	9.42033200	18.45324300
C	4.84929300	6.59138400	18.79686200
H	5.70020600	6.31661000	19.44315100
C	3.69145900	5.60185200	19.00433800
H	3.36223000	5.61144000	20.05781700
H	4.02734700	4.57484700	18.78027600
C	9.45973300	7.16516900	17.87514400
H	10.06547700	6.53006500	18.52586000
C	2.04647900	7.40850400	18.42168700
H	1.68558800	7.45031700	19.46384100
H	1.19750300	7.68723100	17.77389200
C	6.70629000	3.33854300	12.42009400
H	5.75447100	3.11059400	11.91102000
H	7.44555400	2.59548100	12.07423700
C	2.22672500	11.41874500	14.81325900
H	2.16358300	10.77956800	15.70582100
H	1.20527900	11.60520600	14.45036600
H	2.64403100	12.39125900	15.10998300
C	5.90709000	12.89393900	18.86219100
H	5.11647800	13.17622800	19.56223300

C	4.37646800	8.01208900	19.14425400
H	4.06232500	8.06162700	20.20123100
H	5.20361100	8.72901100	19.01845900
C	8.12669400	9.11042400	11.77565600
H	8.69294900	8.21814100	12.08380900
H	8.71645400	9.63742300	11.01183600
H	7.18013600	8.78390000	11.32074600
C	2.22070600	9.52964100	13.19793000
H	2.75417200	8.98143100	12.40508600
H	1.26819500	9.88122300	12.77499400
H	2.00436800	8.82103500	14.00918400
C	9.20027000	10.49993500	13.57037400
H	9.03758400	11.15771900	14.43331500
H	9.75475700	11.07044100	12.81071500
H	9.83203700	9.66177300	13.88928800
C	7.08367900	11.27666800	12.51297300
H	6.12086900	10.99177600	12.06797000
H	7.66430500	11.81682000	11.75092100
H	6.90129800	11.95815400	13.35400500
C	3.28111900	11.71156400	12.54350300
H	3.90797900	12.55474000	12.87233000
H	2.32834200	12.11732500	12.16881200
H	3.79097700	11.20394800	11.71105700
C	7.36830900	13.55273200	21.57154500
H	6.30963200	13.29049500	21.73074700
H	7.68285200	14.19599500	22.40941800
H	7.95297500	12.62094000	21.61411300
C	6.78483400	15.59201400	20.18160400
H	6.94741100	16.11778800	19.22811700
H	7.09748800	16.25953500	21.00091600
H	5.70139900	15.41982000	20.28823100
H	7.38917800	8.25766400	13.98500400
H	7.19851900	5.94887700	15.84910300
H	9.10267400	7.92010200	14.60265700

3c_Int3

P	4.65401400	6.93717700	14.51953400
Si	4.89544000	8.86466800	13.23784700
N	4.17580500	10.24251900	14.27430100
N	6.80653100	9.36952800	13.72646000
C	6.14735100	10.63855600	15.70215700
C	7.55254300	8.52256100	15.85929400
C	4.90839700	10.94878700	15.16677100
H	4.45192900	11.86885600	15.53243900

C	6.89445500	9.50440300	15.16783000
C	8.30098400	7.37912700	15.17972900
H	8.54378700	7.64911600	14.14089500
C	6.66419600	11.45037100	16.82623700
C	8.04463200	11.61526400	17.05606900
H	8.75911500	11.10128100	16.41347400
C	6.60109000	5.96165300	12.75744300
H	5.68729100	5.86678600	12.14902200
H	7.01879300	6.94888700	12.50820300
C	6.22650600	5.85116000	14.25882100
C	7.53354200	5.99485200	15.13583200
H	7.26439500	5.77968800	16.17661200
C	4.09659900	6.95986500	16.37303600
C	8.51943600	12.39649200	18.10754800
H	9.59941900	12.49709600	18.25000000
C	7.64933100	13.05267700	18.98917000
C	7.61428600	8.54818900	17.31107600
H	6.84495300	9.08782800	17.86115800
C	2.82079100	10.75311600	13.87964700
C	7.54981400	10.37121000	12.82877000
C	8.52562000	4.87580800	14.68805400
H	9.43103700	4.95413900	15.30316900
C	7.62577400	4.88754500	12.34775700
H	7.87422500	5.02419000	11.28160700
C	5.04657400	6.30053000	17.39259100
H	5.26416400	5.26243000	17.10526900
H	6.00025800	6.83676000	17.42412800
C	2.76276600	6.16565300	16.38424900
H	2.06441900	6.61084200	15.65694200
H	2.94375600	5.13297600	16.04406500
C	2.13301800	6.15937400	17.78931800
H	1.18961900	5.58800700	17.75820300
C	3.79955800	8.39145900	16.85316300
H	4.72254400	8.98095100	16.86045200
H	3.12035000	8.88425400	16.14649000
C	9.63805700	7.20186500	15.88190900
H	10.48692700	6.84008500	15.29804100
C	7.92983600	3.48012900	14.91145200
H	8.68094800	2.71262500	14.65603400
H	7.67943300	3.34480900	15.97715300
C	5.79267800	12.08754400	17.73542000
H	4.71521600	11.93544200	17.64446700
C	8.89326200	5.03432200	13.20325200
H	9.63232700	4.26633000	12.91842300

H	9.37279900	6.00955700	13.01398700
C	6.67661500	3.31972300	14.04980000
H	6.22290300	2.32802700	14.21606200
C	8.66183900	7.98875000	17.96890000
H	8.72300600	8.03480600	19.05828800
C	5.67308100	4.40337500	14.45466500
H	5.37757700	4.25422000	15.50258400
H	4.75421200	4.31185800	13.85624500
C	8.17829900	13.89338100	20.13818200
H	9.27950100	13.88104900	20.06300500
C	3.16866500	8.39341700	18.25578800
H	2.97489100	9.43772200	18.55700800
C	4.42069200	6.29701500	18.80205700
H	5.13236900	5.82391500	19.49999200
C	3.10572600	5.50209500	18.78194100
H	2.66081800	5.47366900	19.79161900
H	3.29949200	4.45709300	18.48484000
C	9.76597400	7.43054900	17.20445100
H	10.71689300	7.23701400	17.70888100
C	1.84966600	7.60520500	18.22934700
H	1.37652400	7.61544500	19.22643800
H	1.13993100	8.08004800	17.52990000
C	7.03009900	3.48842000	12.56528400
H	6.12688500	3.36073900	11.94537900
H	7.75290700	2.71640500	12.25007100
C	2.14346400	11.52634800	15.02362200
H	2.15319300	10.94626400	15.95845400
H	1.09503400	11.71792300	14.75175100
H	2.60825400	12.50440900	15.21401700
C	6.27336200	12.87618100	18.77912900
H	5.55532500	13.34440500	19.45784300
C	4.14106500	7.74042700	19.24957700
H	3.71423300	7.74832400	20.26738300
H	5.08154500	8.31457800	19.29007100
C	8.89231200	10.73176400	13.46914100
H	8.75219800	11.33873200	14.37163100
H	9.48861900	11.31786000	12.75361500
H	9.46909200	9.83595400	13.74343600
C	1.93435700	9.54141200	13.54395400
H	2.38340000	8.92012400	12.75190800
H	0.95198300	9.87934600	13.18180400
H	1.77972500	8.90633400	14.42784000
C	6.72157100	11.63225900	12.58656600
H	5.74892700	11.38647400	12.14139000

H	7.26383000	12.28389000	11.88507400
H	6.55676200	12.18775600	13.51741300
C	7.77896400	9.63561100	11.50193500
H	8.43312300	8.75872800	11.63883200
H	8.26976000	10.30829100	10.78393200
H	6.82525600	9.29659500	11.07107900
C	2.94501800	11.66496100	12.64747100
H	3.59768900	12.52371800	12.86778600
H	1.95939100	12.05169300	12.34384100
H	3.37430300	11.10994600	11.79973100
C	7.80215400	13.29209900	21.50122200
H	6.70899100	13.28311700	21.64255000
H	8.24060800	13.87799000	22.32563800
H	8.15790400	12.25395000	21.58872600
C	7.72404800	15.35689500	20.03251800
H	8.02019500	15.79635200	19.06750800
H	8.16520300	15.96555600	20.83872800
H	6.62797000	15.43979100	20.11485000
H	7.23845500	8.47435400	13.50343700

3c_TS4

P	4.33740400	6.64840200	14.31000300
Si	4.87762200	8.80726000	14.44560800
N	3.93476900	10.28487000	14.55178100
N	6.47450900	9.33777800	13.70838500
C	5.88556500	10.79366200	15.85789700
C	7.33097100	8.58502700	16.05735600
C	4.65732600	11.15759000	15.37772600
H	4.23817800	12.15055600	15.54530600
C	6.33069500	9.43382800	15.40577600
C	8.04103400	7.47014900	15.30214500
H	8.27820800	7.78079400	14.26662800
C	6.72126700	11.69842400	16.66865200
C	8.12584600	11.64272200	16.59900200
H	8.59879800	10.86245000	16.00191300
C	6.51171800	5.96511500	12.72326600
H	5.64424300	5.80073200	12.06179200
H	6.85405900	6.99205000	12.52623600
C	6.07899500	5.79195600	14.20278900
C	7.31761600	6.03643200	15.16198500
H	7.01509800	5.78254400	16.18422500
C	3.62951200	6.47120600	16.09661900
C	8.91230900	12.53993700	17.32034300
H	10.00122600	12.46659100	17.25101800

C	8.34288600	13.52108700	18.14292500
C	7.45849000	8.64855500	17.45203700
H	6.77969900	9.30148500	18.01104400
C	2.64462100	10.68861700	13.94691900
C	6.97579000	10.28858100	12.65814000
C	8.40034500	4.99323100	14.74380100
H	9.25609400	5.15418000	15.41016600
C	7.63837300	4.98294800	12.35610900
H	7.92950800	5.15736500	11.30603500
C	4.67955600	6.37187100	17.21699700
H	5.31614500	5.49256900	17.05725700
H	5.34839300	7.24372400	17.20830400
C	2.73627600	5.20455600	16.11964400
H	1.97276900	5.27354300	15.32699100
H	3.33548700	4.30850100	15.90561600
C	2.05958700	5.05127200	17.49593400
H	1.44844200	4.13323700	17.48897700
C	2.71755600	7.68408700	16.38941800
H	3.30972600	8.61248000	16.40427500
H	1.95958400	7.78827400	15.59573300
C	9.39320500	7.33325300	15.98088000
H	10.26182200	7.07906600	15.36802900
C	7.91699700	3.54997400	14.90967400
H	8.73701400	2.84956900	14.67328100
H	7.62700100	3.36570400	15.95774200
C	6.14861900	12.67138900	17.51022500
H	5.06282100	12.70943200	17.62793000
C	8.83720200	5.21082700	13.28631800
H	9.64999200	4.51009000	13.02966600
H	9.24430800	6.22519700	13.14748900
C	6.72487300	3.31160100	13.98232100
H	6.33470600	2.28693800	14.10558400
C	8.46407300	7.96986900	18.14169800
H	8.55039000	8.03782000	19.22715000
C	5.62452400	4.30428400	14.36895000
H	5.33655300	4.12551700	15.41427600
H	4.73027000	4.12133500	13.74973200
C	9.21390000	14.47577700	18.94123400
H	10.26080700	14.25353100	18.67211500
C	2.02431200	7.54044500	17.75490700
H	1.38798800	8.42627800	17.92149300
C	3.99059400	6.23113100	18.58641700
H	4.77202600	6.16661500	19.36054600
C	3.13276900	4.95503500	18.59442600

H	2.65287400	4.82093400	19.57878100
H	3.77060800	4.07103800	18.42442300
C	9.51237500	7.43643000	17.34263800
H	10.47402500	7.19421200	17.81051400
C	1.16224500	6.26932100	17.76350600
H	0.65350300	6.16301500	18.73644900
H	0.37509700	6.33828800	16.99301300
C	7.13300700	3.54096500	12.51981400
H	6.27267500	3.36030700	11.85243600
H	7.92361500	2.82894000	12.22914500
C	1.61324600	10.97631200	15.05131600
H	1.44910200	10.08675500	15.67468000
H	0.64964200	11.27513000	14.61139500
H	1.94931800	11.79318600	15.70738800
C	6.94188200	13.56724100	18.22356600
H	6.45813900	14.30399200	18.87033900
C	3.09957800	7.45468900	18.84979900
H	2.62479000	7.37804900	19.84257700
H	3.71213000	8.37187400	18.85185700
C	8.48573000	10.04185500	12.52782900
H	8.99013700	10.21082400	13.49050600
H	8.92006300	10.72172800	11.78006600
H	8.69713100	9.00927100	12.20704700
C	2.15095200	9.54111000	13.05859900
H	2.87827300	9.31562700	12.26205300
H	1.20059200	9.81464400	12.57790200
H	1.98554300	8.61940500	13.63380700
C	6.73212100	11.75577000	13.01153600
H	5.66604000	11.97790500	13.12579500
H	7.12367000	12.37692400	12.19167500
H	7.24965600	12.04179000	13.93543100
C	6.24983300	9.92513600	11.35625900
H	6.42244800	8.87251600	11.08407600
H	6.60484300	10.55564100	10.52689200
H	5.16478500	10.07921900	11.46168400
C	2.83596800	11.94065800	13.07209800
H	3.21586100	12.79197400	13.65580300
H	1.87733400	12.24435200	12.62487300
H	3.54645500	11.74118400	12.25654900
C	9.06648500	14.24231000	20.45275200
H	8.03875900	14.45742400	20.78844700
H	9.74799100	14.89669100	21.02067400
H	9.29154400	13.19751900	20.71588000
C	8.94349300	15.94263200	18.57524700

H	9.07687100	16.11472300	17.49594500
H	9.62719200	16.61530500	19.11839400
H	7.91325700	16.23555000	18.83582800
H	7.06527700	8.50596900	13.65868700
3c			
P	4.69825600	6.98472200	14.51998800
Si	5.54550000	9.07049000	14.18521600
N	4.43601500	10.44948400	14.52075200
N	6.15284200	9.02502100	12.56735600
H	5.78881900	8.27646100	11.98516900
C	6.04834600	10.69515300	16.26540600
C	7.67479400	8.71410000	16.02190700
C	4.91495500	11.13548900	15.61672300
H	4.39258100	12.03785000	15.94071100
C	6.65750300	9.53641100	15.61746600
C	8.21530300	7.63604600	15.07806600
H	7.96945800	7.92783800	14.05041900
C	6.59339400	11.46001700	17.40936600
C	7.93963400	11.86665100	17.44378300
H	8.60177800	11.58357100	16.62367800
C	6.63801700	5.72019600	12.99366700
H	5.71783000	5.50645000	12.42491000
H	7.03750600	6.66769600	12.60985600
C	6.27957500	5.86423300	14.49670600
C	7.58312700	6.20192700	15.31123200
H	7.34172900	6.14645400	16.38080600
C	3.94887100	6.98516600	16.29043300
C	8.43451400	12.61774700	18.50791500
H	9.48604300	12.91940000	18.50765400
C	7.61376600	13.00165200	19.57966900
C	8.31951600	8.80094500	17.32536200
H	7.76640800	9.23746000	18.15680800
C	3.28169000	10.97493000	13.75567700
C	7.09408900	9.89506200	11.84021500
C	8.61191800	5.06302500	15.03803200
H	9.52625700	5.29256600	15.60134500
C	7.67042200	4.60623700	12.75959300
H	7.89513800	4.55067800	11.68083800
C	4.94993700	6.97479200	17.46234800
H	5.58716600	6.08060100	17.41504800
H	5.61449900	7.84495000	17.39477900
C	3.00777400	5.75639000	16.41300700
H	2.27900300	5.77404900	15.58600800

H	3.57083300	4.82011300	16.31575100
C	2.27441400	5.76051800	17.76759400
H	1.63585000	4.86300400	17.82789700
C	3.06185500	8.24159300	16.42768400
H	3.67724700	9.14282300	16.36564500
H	2.34180500	8.27651300	15.59349100
C	9.73137600	7.62092600	15.19046000
H	10.31032800	7.29312500	14.32485600
C	8.06642800	3.71324900	15.52570000
H	8.83251300	2.93061200	15.38911500
H	7.84491200	3.76262800	16.60526800
C	5.77032600	11.84454600	18.48298000
H	4.72540900	11.52453300	18.49080900
C	8.94433300	4.94742800	13.54049400
H	9.70843400	4.16549600	13.39038600
H	9.37209300	5.88465800	13.15389700
C	6.79703300	3.36486300	14.74239200
H	6.37744700	2.41098500	15.10439800
C	9.60147600	8.39109500	17.49433300
H	10.09010400	8.46831800	18.46873900
C	5.76861400	4.47802800	14.97521200
H	5.53318500	4.51883300	16.04686600
H	4.83150100	4.24015500	14.44565800
C	8.16966100	13.80992700	20.74009000
H	9.23141600	14.00775500	20.51252200
C	2.31267500	8.25751300	17.77062700
H	1.70310200	9.17599200	17.82244600
C	4.20361300	6.98434600	18.81021400
H	4.94627200	6.97395100	19.62563500
C	3.30540700	5.74051100	18.90924900
H	2.79035500	5.71793000	19.88491600
H	3.91959200	4.82549700	18.84844800
C	10.36165100	7.93436300	16.33871400
H	11.45067500	7.86349700	16.41041100
C	1.40760300	7.02300500	17.88072700
H	0.86337100	7.03052300	18.84074500
H	0.65002500	7.03495100	17.07854300
C	7.11237300	3.26114900	13.24425000
H	6.19869800	3.00295500	12.68218400
H	7.84461900	2.45633100	13.06089600
C	2.08588500	11.24390400	14.68883000
H	1.77229200	10.32534000	15.20175700
H	1.23311000	11.62117900	14.10424300
H	2.32001400	12.00002300	15.45247400

C	6.26979400	12.60312400	19.54293800
H	5.59860200	12.87569700	20.36173500
C	3.34171100	8.25270600	18.91303000
H	2.82849500	8.28848100	19.88929600
H	3.98309400	9.14764100	18.84913600
C	8.32198900	9.07254400	11.40719700
H	8.85724100	8.67941900	12.28368500
H	9.02543100	9.68709500	10.82342900
H	8.01923100	8.21849100	10.77980100
C	2.86414800	9.93062100	12.71226100
H	3.67189000	9.74693300	11.99172800
H	1.98148200	10.28336900	12.15877400
H	2.61241900	8.97188000	13.19007600
C	7.54709500	11.04872700	12.74402800
H	6.68915800	11.63360900	13.10585400
H	8.21089000	11.72503500	12.18504300
H	8.09428000	10.67674200	13.62140600
C	6.39829300	10.45407900	10.58726000
H	6.04172700	9.63374100	9.94264400
H	7.08650100	11.07516000	9.99234400
H	5.52923800	11.06810300	10.86316200
C	3.67733500	12.28422700	13.04934000
H	3.99445400	13.04662000	13.77733400
H	2.83036000	12.69379700	12.47696100
H	4.51187100	12.11200200	12.35579300
C	8.11924700	13.01876800	22.05616500
H	7.07909500	12.79628500	22.34533800
H	8.57948000	13.59111800	22.87817200
H	8.65179700	12.05966400	21.96356500
C	7.46642100	15.16818300	20.88067700
H	7.52747300	15.74614800	19.94565000
H	7.92326300	15.76603700	21.68617800
H	6.39932000	15.04047600	21.12548800

AdC≡P

P	19.09563900	12.83541800	3.69801600
C	17.74336400	12.33835700	3.12506700
C	16.46917700	11.87038900	2.58530800
C	16.49999200	11.89239800	1.03080100
H	17.32631500	11.25525000	0.67713700
H	16.71153100	12.91803200	0.68851000
C	15.15668600	11.39958000	0.46873500

H	15.20017400	11.42341300	-0.63286200
C	14.89669500	9.96023000	0.94593100
H	15.69368000	9.29030600	0.58119400
H	13.94641700	9.58867300	0.52681000
C	14.84281100	9.92923100	2.48323700
H	14.66104300	8.89754600	2.82758700
C	16.18453300	10.41550700	3.05475700
H	16.17058700	10.38782700	4.15606400
H	17.00746300	9.76192800	2.72393000
C	15.30830100	12.78378000	3.07110000
H	15.50603400	13.81947300	2.75160800
H	15.28489600	12.78264100	4.17258800
C	13.97052100	12.28645100	2.49988200
H	13.16259100	12.94703000	2.85607000
C	13.71077600	10.84691500	2.97651700
H	13.65145000	10.81717100	4.07772000
H	12.74033900	10.49056900	2.59177200
C	14.02466100	12.31703500	0.96256400
H	13.05957100	11.98563500	0.54360400
H	14.19195200	13.34881400	0.60974900

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P	8.89639900	8.88826100	4.75621700
P	8.00881500	8.19756500	1.37432400
P	6.89568700	7.49582800	7.20129100
Si	8.02667100	6.91163200	3.35143400
N	9.58904900	5.75652500	3.40831600
N	7.77298400	5.24927300	2.32743300
C	8.95326400	4.78830100	2.71558600
C	10.68353300	5.59260900	4.40928400
C	11.58086600	4.36610800	4.16635800
H	11.07178800	3.41395400	4.34742200
H	12.42627600	4.42701100	4.86755400
H	11.98968700	4.35400700	3.14709800
C	11.60848100	6.81516100	4.33598000
H	12.08864500	6.87613500	3.34996600
H	12.39615600	6.73071700	5.09911800
H	11.06990700	7.75178100	4.51561400
C	10.05271100	5.47739000	5.80694400
H	9.45339100	6.36369700	6.05252900
H	10.83378700	5.36174000	6.57469600
H	9.38698400	4.60222400	5.85644400
C	9.44846900	3.41406600	2.43180200
C	9.02577200	2.33761700	3.22374800

H	8.35112000	2.52036800	4.06135500
C	9.46911300	1.04589400	2.94182800
H	9.14039600	0.21099800	3.56482400
C	10.32926900	0.81995900	1.86173700
H	10.67291300	-0.19280100	1.63896200
C	10.74842400	1.89125100	1.06820500
H	11.42024500	1.71850700	0.22439700
C	10.31202100	3.18706600	1.35396200
H	10.64328900	4.03008400	0.74410400
C	6.85015000	4.73516400	1.28854100
C	6.51036400	3.24343100	1.46895600
H	7.33573600	2.59019800	1.16214500
H	5.64177900	2.99816100	0.83924400
H	6.25257500	3.00824000	2.50787600
C	7.45396400	4.93993000	-0.11216600
H	7.64361700	6.00689600	-0.28860900
H	6.75140300	4.57215700	-0.87656800
H	8.39406600	4.38037100	-0.22150400
C	5.56172800	5.56246700	1.39956400
H	5.12001200	5.47442000	2.40040600
H	4.82462600	5.21210300	0.66231100
H	5.77263000	6.62125200	1.20037500
C	6.29225400	6.36332500	6.29632400
C	5.43874700	5.19022500	6.04060000
C	4.96810400	4.60983600	7.40941000
H	5.85600200	4.32117000	7.99437900
H	4.45615100	5.40604100	7.97211400
C	4.03655900	3.40674500	7.20443400
H	3.72446300	3.02034400	8.18941000
C	4.78562000	2.30817600	6.43158200
H	5.66451000	1.97375100	7.00895300
H	4.13537700	1.42775100	6.29246700
C	5.22736900	2.85924200	5.06578700
H	5.76538900	2.07341100	4.50759400
C	6.16424000	4.06337000	5.26775900
H	6.51102100	4.45949000	4.30422200
H	7.06053700	3.76025800	5.83487300
C	4.17654300	5.60808400	5.23949200
H	3.65743300	6.41213200	5.78507900
H	4.49038900	6.03058300	4.27287600
C	3.24282400	4.40158600	5.04036300
H	2.35919400	4.72406200	4.46431400
C	2.79930200	3.85491000	6.40785200
H	2.10728800	3.00683900	6.26893400

H	2.25146900	4.63110300	6.96848100
C	3.98297900	3.29466100	4.27180600
H	3.31508900	2.43017000	4.11705500
H	4.27197700	3.65563700	3.27418100
C	8.16294700	9.36971400	6.08413100
C	7.99006400	10.49665400	7.04344000
C	8.71020500	10.19937700	8.38727400
H	9.77236700	9.98795500	8.18253700
H	8.28262400	9.29402900	8.84366100
C	8.57091900	11.39391600	9.34621600
H	9.08356400	11.15197100	10.29238600
C	7.08129700	11.66395800	9.62007500
H	6.97303600	12.50036100	10.33144600
H	6.61605700	10.77956900	10.08732200
C	6.36791400	11.99720600	8.29845100
H	5.29854900	12.18555400	8.49193200
C	6.49653800	10.80526400	7.33691400
H	6.01253100	9.91886000	7.77316200
H	5.97798900	11.01543500	6.38894200
C	8.63030700	11.77935300	6.43453800
H	8.14230400	12.00053400	5.47243300
H	9.69037000	11.57402900	6.21653700
C	8.49513600	12.97041000	7.39464800
H	8.95845900	13.85775900	6.93098800
C	9.20956500	12.64325800	8.71651700
H	9.13577900	13.49780400	9.41064700
H	10.28315600	12.46791200	8.53260700
C	7.00688000	13.24445300	7.66612400
H	6.49074900	13.49702100	6.72432000
H	6.89602600	14.11197000	8.33896000
C	6.96267500	9.76562100	1.71485800
C	7.68948700	11.04132500	2.18773300
H	8.44472800	11.34312600	1.44707900
H	8.22172300	10.84575700	3.12943200
C	6.69088200	12.19828400	2.38313600
H	7.24181100	13.08859300	2.73205600
C	5.64030100	11.79895900	3.43085500
H	4.93727600	12.63205900	3.60398400
H	6.13284300	11.58611000	4.39203600
C	4.88082600	10.55364500	2.94642500
H	4.13383700	10.25770100	3.70230400
C	5.87611300	9.39540200	2.75600400
H	5.33362000	8.49400000	2.42582000
H	6.33532600	9.15279800	3.72485500

C	6.23063700	10.09528800	0.38400100
H	6.96142300	10.35425000	-0.39680900
H	5.69879700	9.19767800	0.02975800
C	5.23838100	11.25784900	0.56951600
H	4.74749100	11.46712800	-0.39616900
C	4.18170000	10.86408400	1.61394200
H	3.61848800	9.98084800	1.26720200
H	3.45220700	11.68164000	1.74682500
C	5.99460700	12.50799000	1.04838200
H	6.74057600	12.81158100	0.29374500
H	5.29536400	13.35322800	1.16954100
C	9.75192600	8.65743200	0.75753400
C	10.43449300	7.31262500	0.39648500
H	10.55168200	6.70690800	1.30745800
H	9.78997800	6.74278700	-0.29055900
C	11.80713900	7.55096200	-0.25847200
H	12.26357600	6.57521300	-0.49981300
C	12.71683900	8.32302500	0.71017200
H	12.88636200	7.73205400	1.62469900
H	13.70596600	8.49132600	0.25044100
C	12.05896600	9.66672500	1.06249500
H	12.69905200	10.21827600	1.77182800
C	10.68563000	9.41836700	1.71905300
H	10.24098000	10.37776900	2.01242500
H	10.81553000	8.83869100	2.64056300
C	9.60313000	9.47858000	-0.54683500
H	8.93778100	8.94485100	-1.24525100
H	9.13099300	10.44869500	-0.33191400
C	10.97598600	9.72013300	-1.20021900
H	10.83484100	10.31092600	-2.12115600
C	11.62452000	8.36992200	-1.54629100
H	10.98883100	7.81811900	-2.25970900
H	12.59954800	8.52995400	-2.03781400
C	11.87550000	10.49286000	-0.22104400
H	12.85528100	10.69864500	-0.68535700
H	11.42060400	11.46927500	0.01862800

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P	9.34183600	8.69047100	4.90485000
P	7.49827200	7.97720400	1.93450600
P	6.67075100	8.14804100	6.43837200
Si	8.08391000	7.00711200	4.00792300
N	9.09138400	5.48865400	3.87785400
N	7.59984600	4.80460900	2.27836400

C	8.76349100	4.64828200	2.80378000
C	10.14187900	5.16454100	4.92758000
C	10.40481600	3.65438300	5.09978500
H	9.46480500	3.08575600	5.13424200
H	10.91397400	3.51051500	6.06415600
H	11.05064600	3.22853200	4.32784400
C	11.46952000	5.86675000	4.59638400
H	11.85400700	5.54719700	3.61986500
H	12.22676600	5.61920900	5.35661100
H	11.35491000	6.95997400	4.58711800
C	9.65854300	5.62644500	6.31595600
H	9.40889200	6.69106500	6.35875700
H	10.46617600	5.46074700	7.04378200
H	8.78433800	5.05170800	6.63883100
C	9.79079400	3.66730600	2.30259400
C	9.57172300	2.28961500	2.44874100
H	8.67601900	1.94545900	2.96574900
C	10.50419100	1.36298400	1.98381100
H	10.32112200	0.29462000	2.12051000
C	11.67135200	1.79983700	1.34974600
H	12.40168900	1.07543500	0.98181800
C	11.89773100	3.16929100	1.19307500
H	12.80445300	3.52340200	0.69700200
C	10.96753100	4.09443000	1.67243500
H	11.15608700	5.15783100	1.54571200
C	7.10664100	4.29015600	0.97877600
C	6.88239000	2.76400300	0.95675800
H	7.81557900	2.20299200	0.83608000
H	6.22835700	2.50554500	0.10939900
H	6.38412200	2.42943500	1.87864600
C	8.03718300	4.69137900	-0.17991500
H	8.15200700	5.78288000	-0.20383100
H	7.59963900	4.37293000	-1.13885600
H	9.02997200	4.23218500	-0.09464500
C	5.73744100	4.95309600	0.73124400
H	4.98484000	4.58232500	1.44012800
H	5.38449600	4.72049200	-0.28530800
H	5.82041000	6.04241600	0.84027400
C	6.67373400	6.90956100	5.27389300
C	5.61950400	5.80355400	5.37458800
C	4.57659700	6.04019500	6.49445100
H	5.08442800	6.14544100	7.46745100
H	4.04914100	6.99120600	6.31139400
C	3.56439100	4.88275200	6.56400600

H	2.83851500	5.09427100	7.36702700
C	4.30468500	3.57033900	6.86927400
H	4.81847900	3.64240100	7.84318500
H	3.58594000	2.73636300	6.94333700
C	5.32518700	3.29665800	5.75417300
H	5.87418300	2.36423800	5.97181100
C	6.33102700	4.45506400	5.68188600
H	7.08286500	4.25366200	4.90835900
H	6.85748700	4.54778700	6.64463000
C	4.84540800	5.64792300	4.04543000
H	4.29045800	6.57240900	3.84243900
H	5.56815900	5.50511000	3.23498900
C	3.85277100	4.47789500	4.10990200
H	3.33603500	4.39751200	3.13822200
C	2.82705600	4.74966500	5.22135400
H	2.08843500	3.93137400	5.27386200
H	2.26944700	5.67602000	5.00157800
C	4.60179000	3.17000000	4.40543000
H	3.89767300	2.32057900	4.42589000
H	5.33402600	2.97079300	3.60753500
C	8.19590500	9.11519600	6.09264600
C	8.39116000	10.32686800	7.00782900
C	8.52995600	9.84094700	8.47816200
H	9.40003500	9.16697400	8.54859000
H	7.64333300	9.25109200	8.76169800
C	8.69242600	11.03332100	9.43508700
H	8.78457500	10.65451500	10.46692400
C	7.45922400	11.94662400	9.32732600
H	7.55122700	12.79208400	10.03016000
H	6.55000800	11.38916900	9.60955900
C	7.33124500	12.46841700	7.88621500
H	6.44456400	13.11935300	7.80443400
C	7.16861500	11.28195100	6.92282300
H	6.24453600	10.73045700	7.15935500
H	7.06883400	11.64689700	5.88959000
C	9.65266500	11.14698200	6.65922300
H	9.58237200	11.50038900	5.61720700
H	10.54158600	10.49677800	6.70974500
C	9.82009300	12.33961000	7.61495200
H	10.72857400	12.89838200	7.33437800
C	9.95427400	11.82609000	9.05817600
H	10.09313600	12.67280600	9.75195000
H	10.84644700	11.18351200	9.14992400
C	8.59354100	13.26058700	7.51025800

H	8.50133900	13.65319400	6.48321900
H	8.71201500	14.12990300	8.17940800
C	6.31390200	9.45412900	2.23393800
C	6.70649400	10.54610100	3.24698200
H	7.65780100	11.01672400	2.97091800
H	6.85753700	10.09383500	4.23127700
C	5.60581500	11.62008600	3.34350700
H	5.92423900	12.38999200	4.06675600
C	4.29970200	10.96984600	3.82454100
H	3.50775400	11.73133200	3.92853100
H	4.44952700	10.51719100	4.81925300
C	3.87367000	9.89216500	2.81429600
H	2.94655000	9.40347900	3.15851900
C	4.98111300	8.83135500	2.70807100
H	4.67423300	8.03154500	2.01561700
H	5.13342800	8.37064200	3.69099600
C	6.06066600	10.11863600	0.85767700
H	6.97906400	10.59997000	0.49282100
H	5.78046200	9.35044100	0.11772200
C	4.95368900	11.18425100	0.96235500
H	4.80454100	11.63778800	-0.03212700
C	3.64560100	10.53278200	1.43711100
H	3.31976300	9.76694900	0.71277700
H	2.84307400	11.28814800	1.49295900
C	5.38580800	12.26555100	1.96664100
H	6.31555600	12.75098800	1.62308300
H	4.61579500	13.05324500	2.03206100
C	9.13485000	8.64504100	1.18131100
C	10.22239600	7.59584800	1.49172400
H	10.40262400	7.53944900	2.57249900
H	9.86145400	6.60927800	1.17131100
C	11.54557500	7.92915900	0.78634400
H	12.29496800	7.16151400	1.04768500
C	12.03158600	9.30699600	1.26306900
H	12.19940200	9.29064900	2.35298100
H	12.99563800	9.55689600	0.78803400
C	10.97481700	10.36633500	0.90955500
H	11.31726400	11.35778600	1.25063000
C	9.64578900	10.03284900	1.61542100
H	8.90627800	10.80603400	1.36330100
H	9.78498400	10.05969300	2.70614900
C	8.94430500	8.66376600	-0.36184800
H	8.58048900	7.68349300	-0.70373200
H	8.17731300	9.39746900	-0.64465400

C	10.26627600	9.00659100	-1.07420200
H	10.08913700	9.01852500	-2.16283900
C	11.32495600	7.94616000	-0.73342800
H	10.99099600	6.95245600	-1.07771900
H	12.27132700	8.16936700	-1.25502100
C	10.75636800	10.38817400	-0.61188500
H	11.69488000	10.65192800	-1.12900600
H	10.01430600	11.16086400	-0.87624600

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Si	0.52186800	0.21973700	-0.43303700
P	-1.27784000	-0.53499800	-1.59989500
P	-0.51334600	-1.26886500	1.29966200
P	-1.43090500	2.45919700	-1.00191400
N	1.91631500	-0.11019400	-1.71268400
N	2.32770900	-0.26457100	0.40762200
C	2.83817600	-0.43772400	-0.80563200
C	1.95982500	-0.10225800	-3.19299100
C	3.36057800	0.17370100	-3.76540300
H	3.80517500	1.07345800	-3.31629900
H	3.25954800	0.35290100	-4.84635700
H	4.05347100	-0.66484300	-3.63326200
C	1.45693400	-1.45425000	-3.72971500
H	2.09274300	-2.27504100	-3.36499400
H	1.48265800	-1.46311200	-4.83053100
H	0.42273500	-1.64464600	-3.40996300
C	1.04528200	1.03823600	-3.67025700
H	0.01502600	0.91375600	-3.31554800
H	1.02459800	1.06074200	-4.77013200
H	1.41527400	2.00749900	-3.30687500
C	4.18480600	-0.98249800	-1.13226000
C	5.30014100	-0.14735800	-1.27759500
H	5.19233900	0.92707800	-1.12179500
C	6.53732000	-0.68745200	-1.62417600
H	7.40261200	-0.03071500	-1.73824000
C	6.67106300	-2.06550700	-1.82733600
H	7.64151700	-2.48658200	-2.09964300
C	5.56124900	-2.90118100	-1.68188100
H	5.65911700	-3.97751000	-1.83978800
C	4.31915100	-2.36174500	-1.33693800
H	3.44709600	-3.00977200	-1.23182300
C	3.00355600	-0.48202200	1.71779600
C	4.44477900	0.06750600	1.75270500
H	5.15536400	-0.56524900	1.21035800

H	4.77600400	0.10870800	2.80133000
H	4.49788300	1.08794800	1.34661300
C	3.03334000	-1.97938500	2.06245800
H	2.01047200	-2.36049000	2.15852000
H	3.55314700	-2.13609500	3.02038200
H	3.56322800	-2.55621300	1.29120000
C	2.21297800	0.26540000	2.79918800
H	2.28786400	1.35014300	2.66164000
H	2.62819600	0.02069600	3.78798600
H	1.15861900	-0.03230100	2.78394500
C	0.09912700	2.04213900	-0.35237900
C	0.96478200	3.20765300	0.15517900
C	0.69738900	4.53007200	-0.61782100
H	0.89574100	4.36619300	-1.69050700
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4

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H	3.48320100	9.89233300	3.37737000
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C	6.14535200	9.84732000	0.48187100
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C	10.97346200	10.29019500	-0.49909500
H	10.84728300	10.69522200	-1.51733800
C	11.89311300	9.05915200	-0.54287300
H	11.46470600	8.29029900	-1.20872700
H	12.87719300	9.33511100	-0.95882500
C	11.59436900	11.36229300	0.41225000
H	12.57310700	11.67904400	0.01290200
H	10.95043600	12.25812800	0.43459300

V. Collected ^1H , ^{13}C , ^{29}Si , ^{31}P and ^{19}F NMR spectra of compounds 1, 2, 3a-d and 4

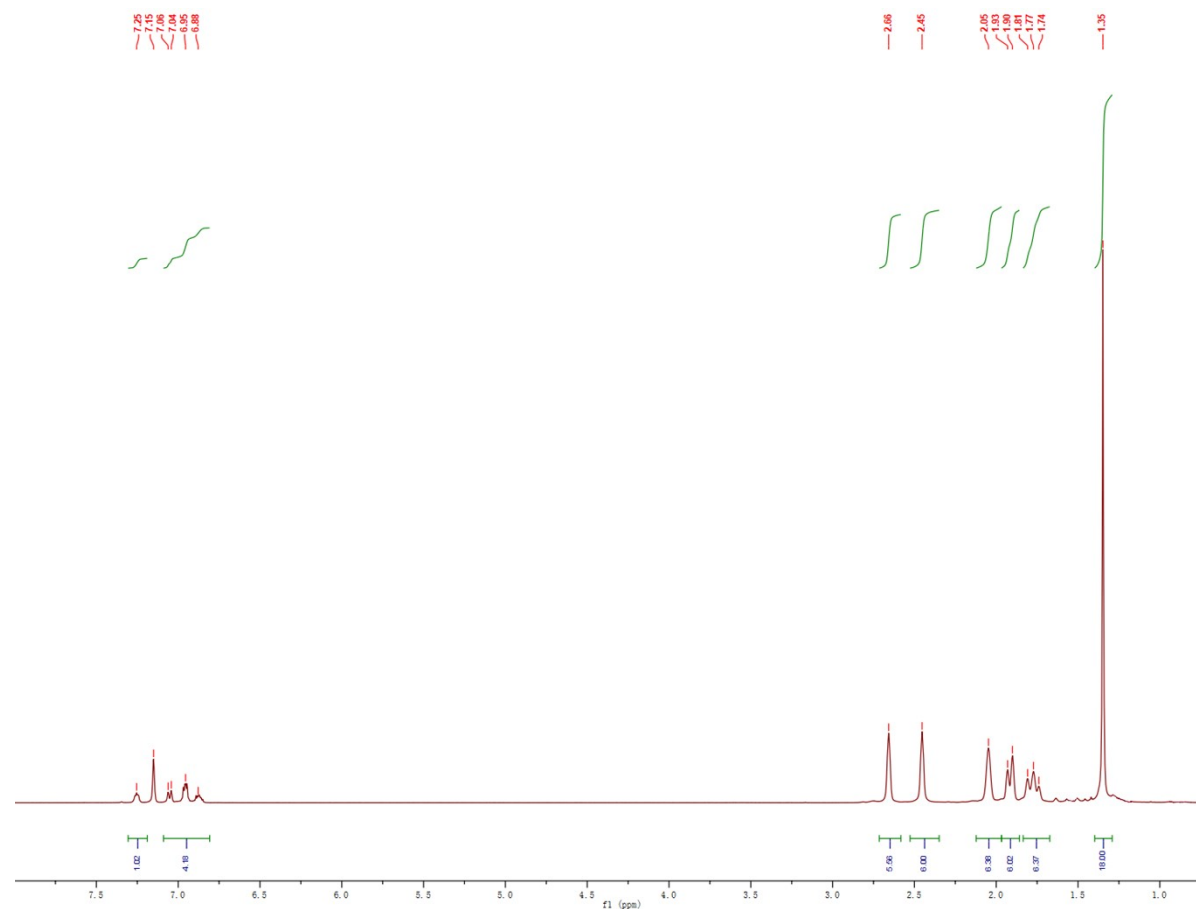


Fig. S10 ^1H NMR spectrum of 1 in C_6D_6

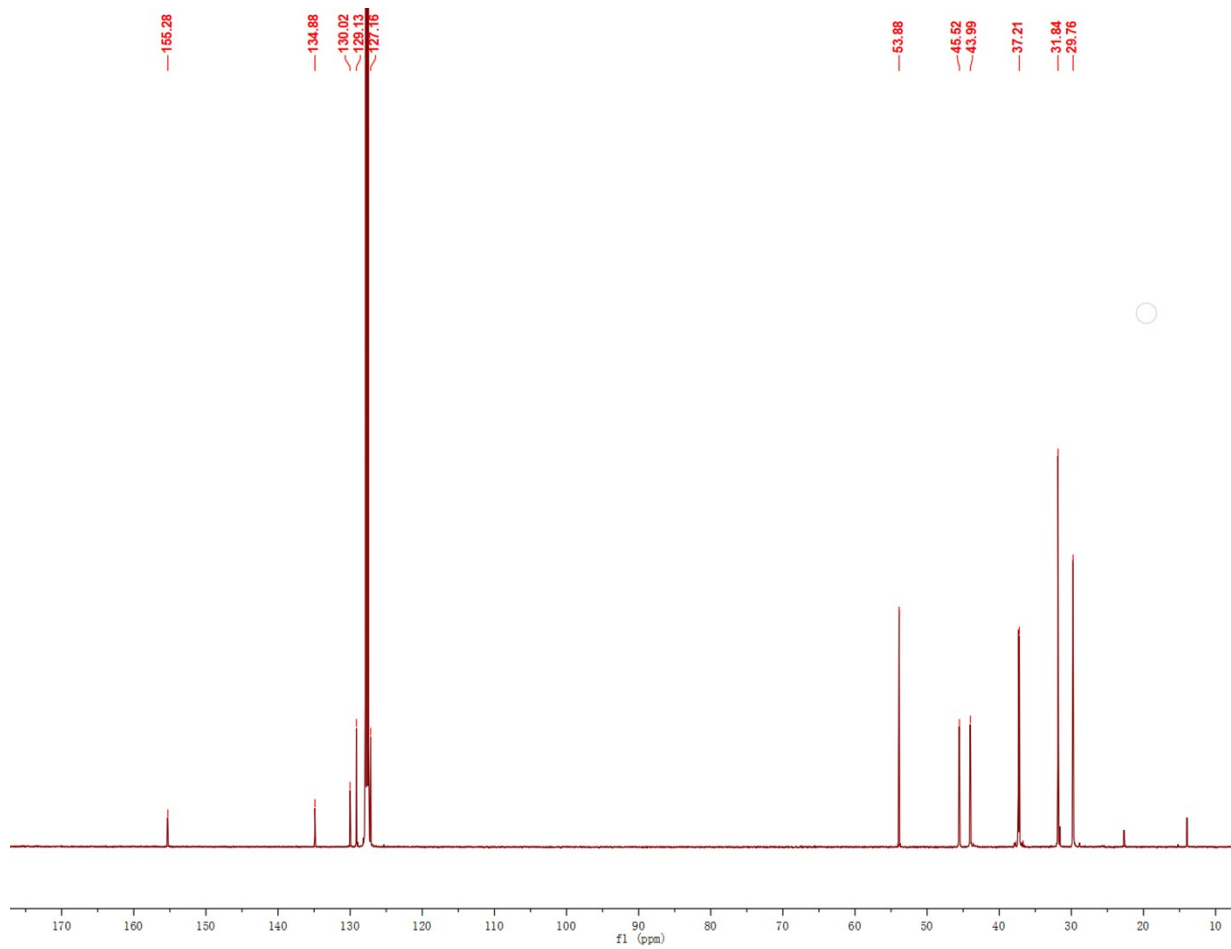


Fig. S11 ^{13}C NMR spectrum of **1** in C_6D_6

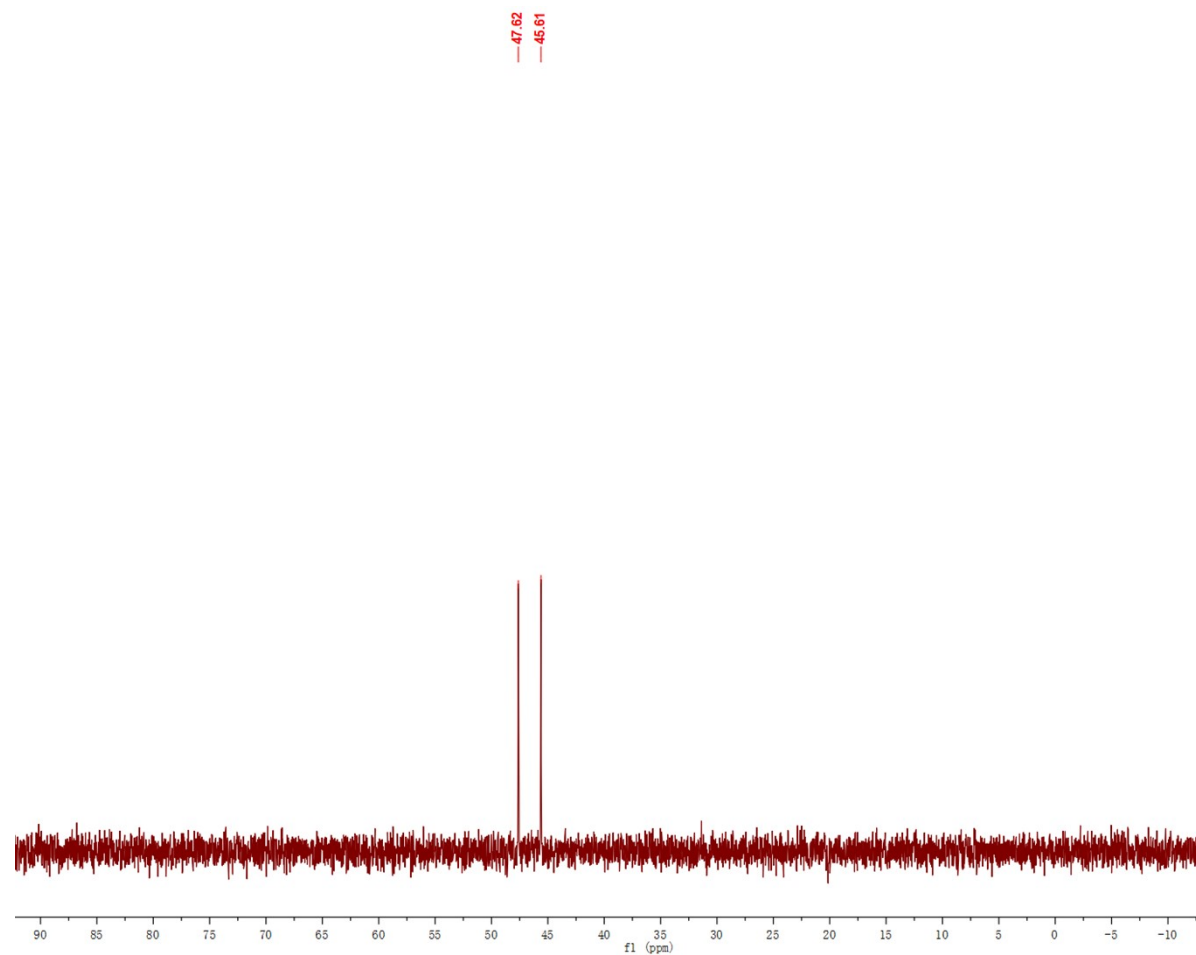


Fig. S12 ^{29}Si NMR spectrum of **1** in C_6D_6

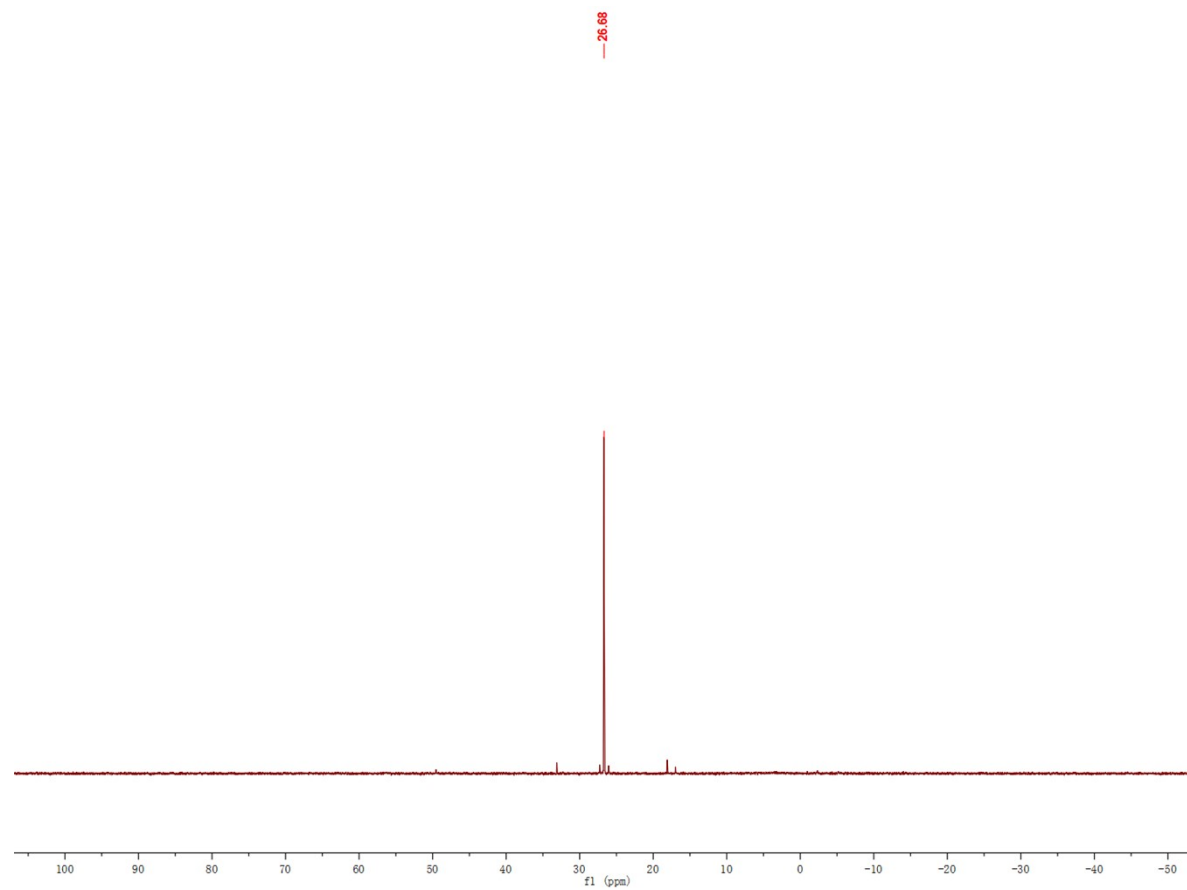


Fig. S13 ^{31}P NMR spectrum of **1** in C_6D_6

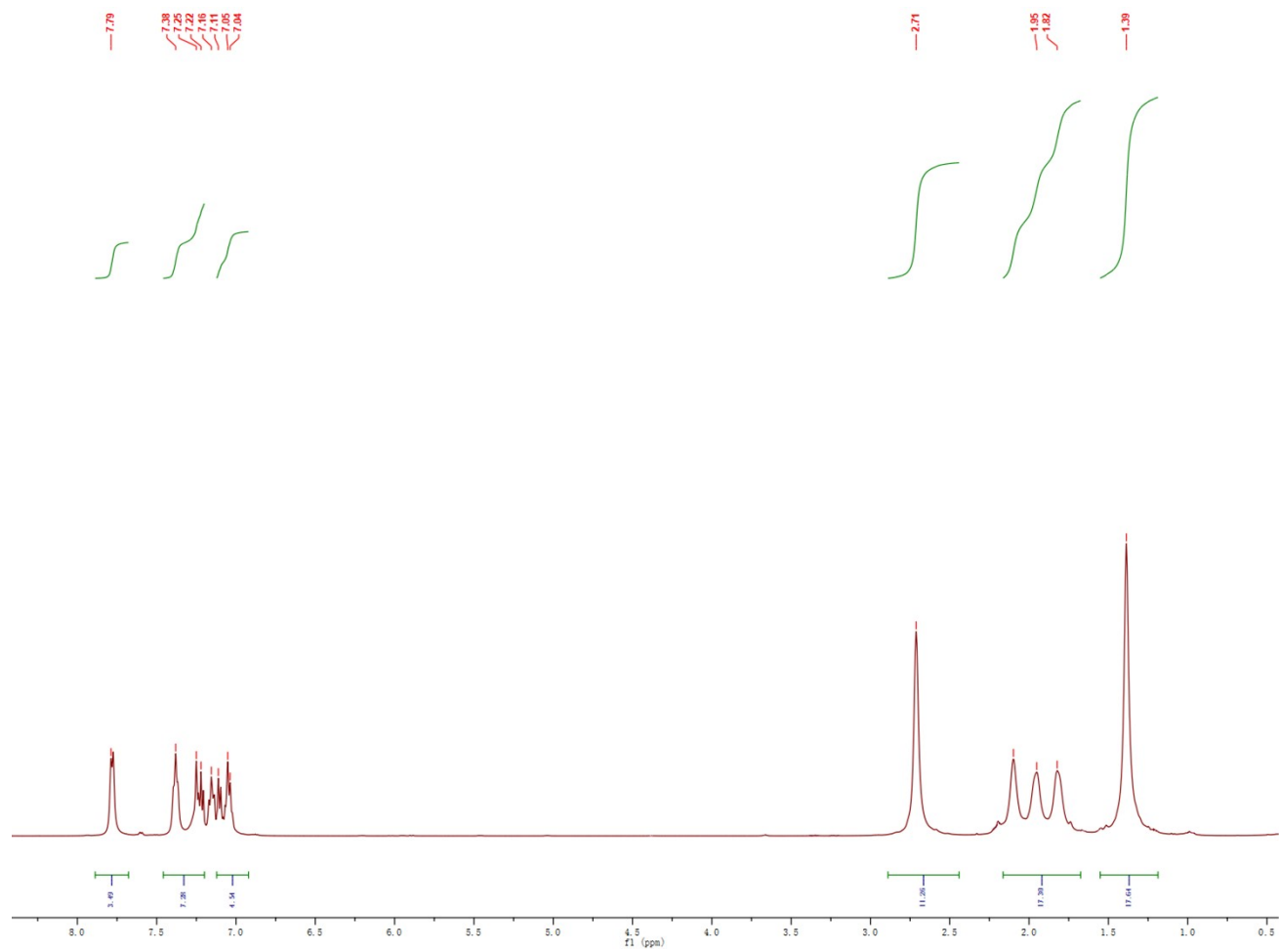


Fig. S14 ^1H NMR spectrum of **2** in C_6D_6

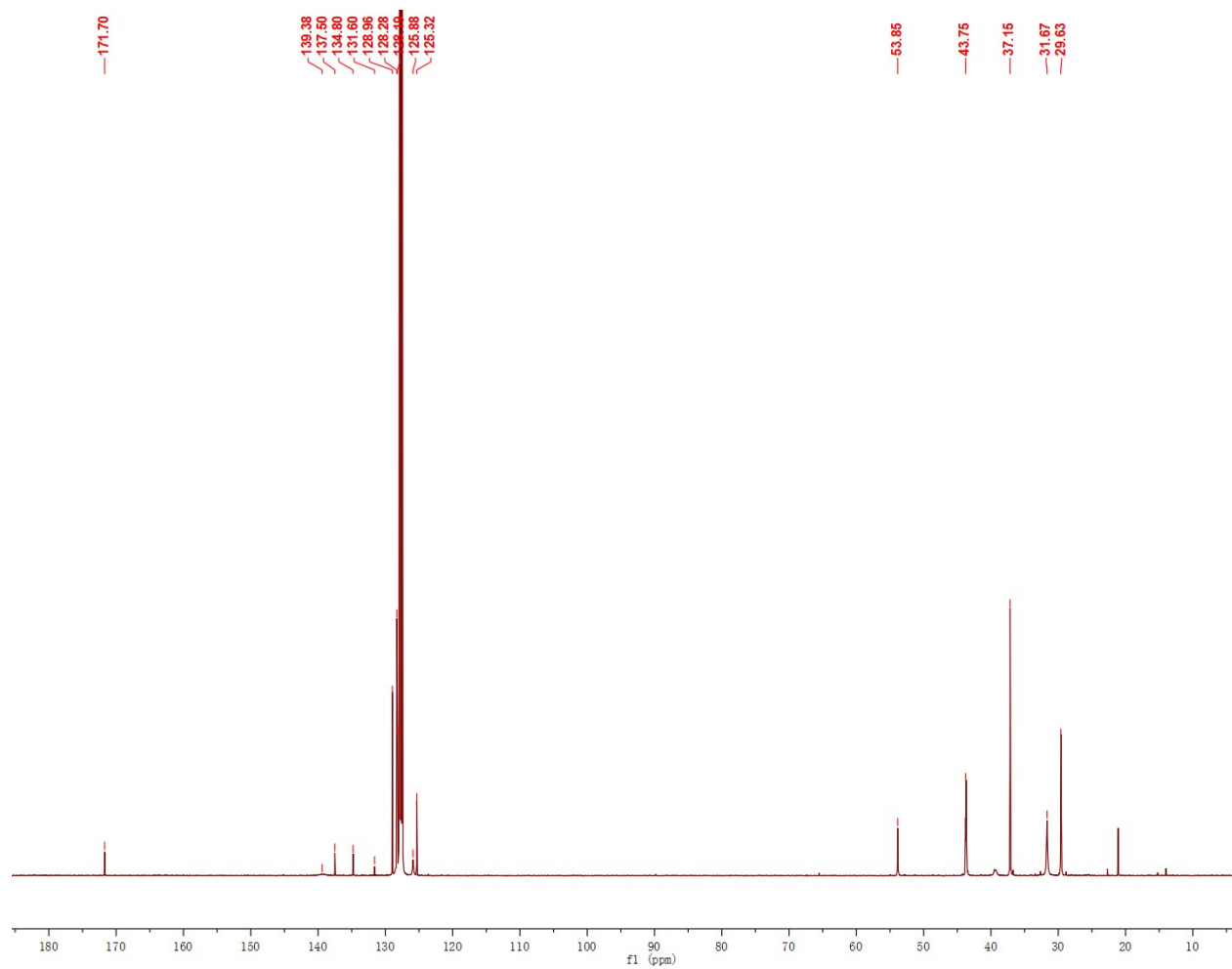


Fig. S15 ^{13}C NMR spectrum of **2** in C_6D_6

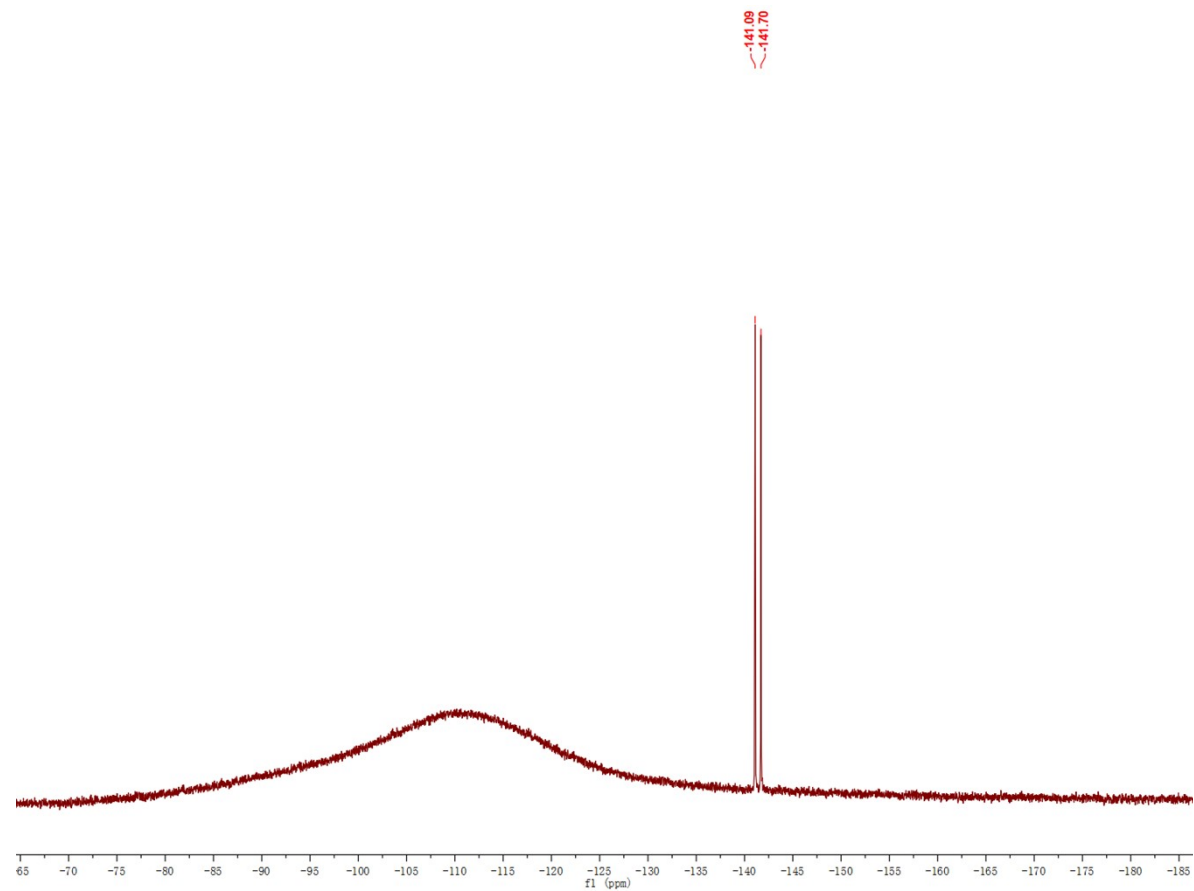


Fig. S16 ^{29}Si NMR spectrum of **2** in C_6D_6

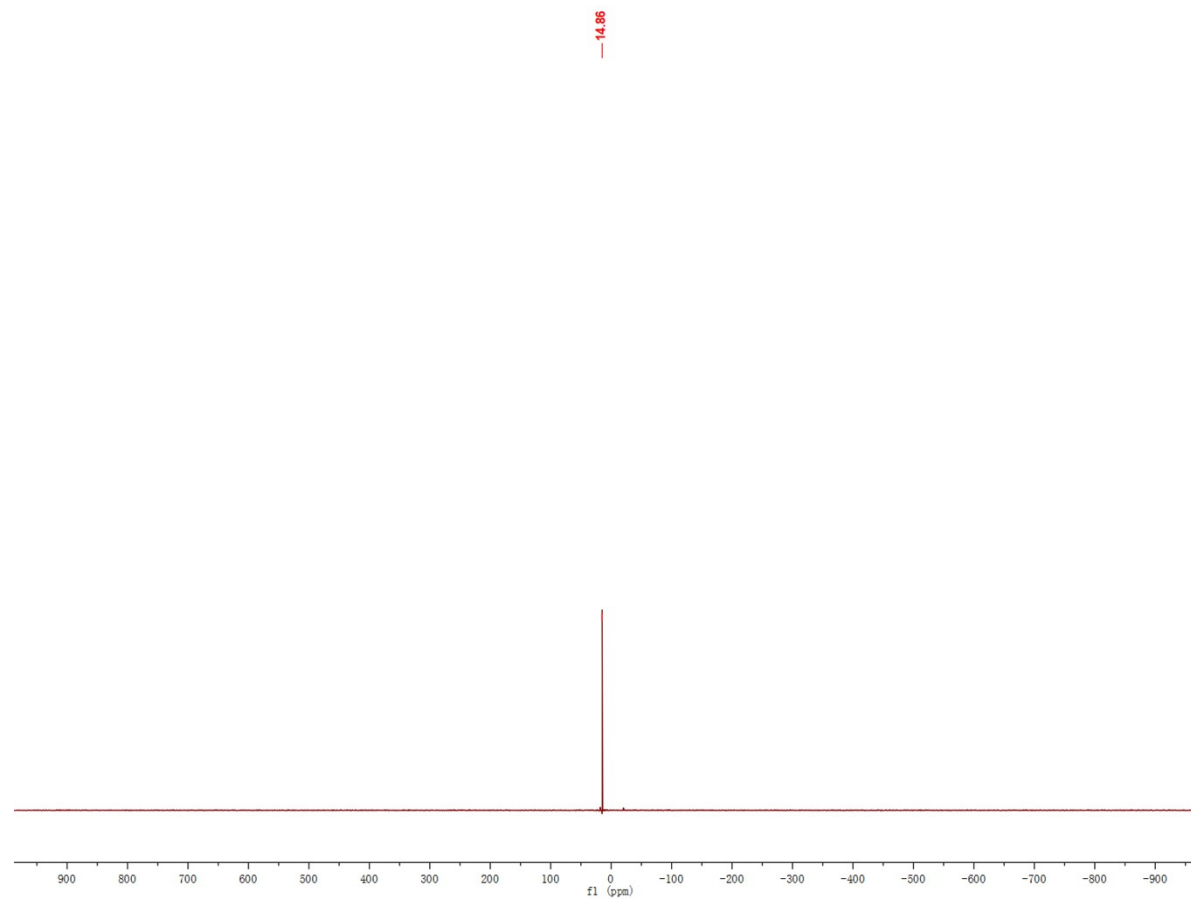


Fig. S17 ^{31}P NMR spectrum of **2** in C_6D_6

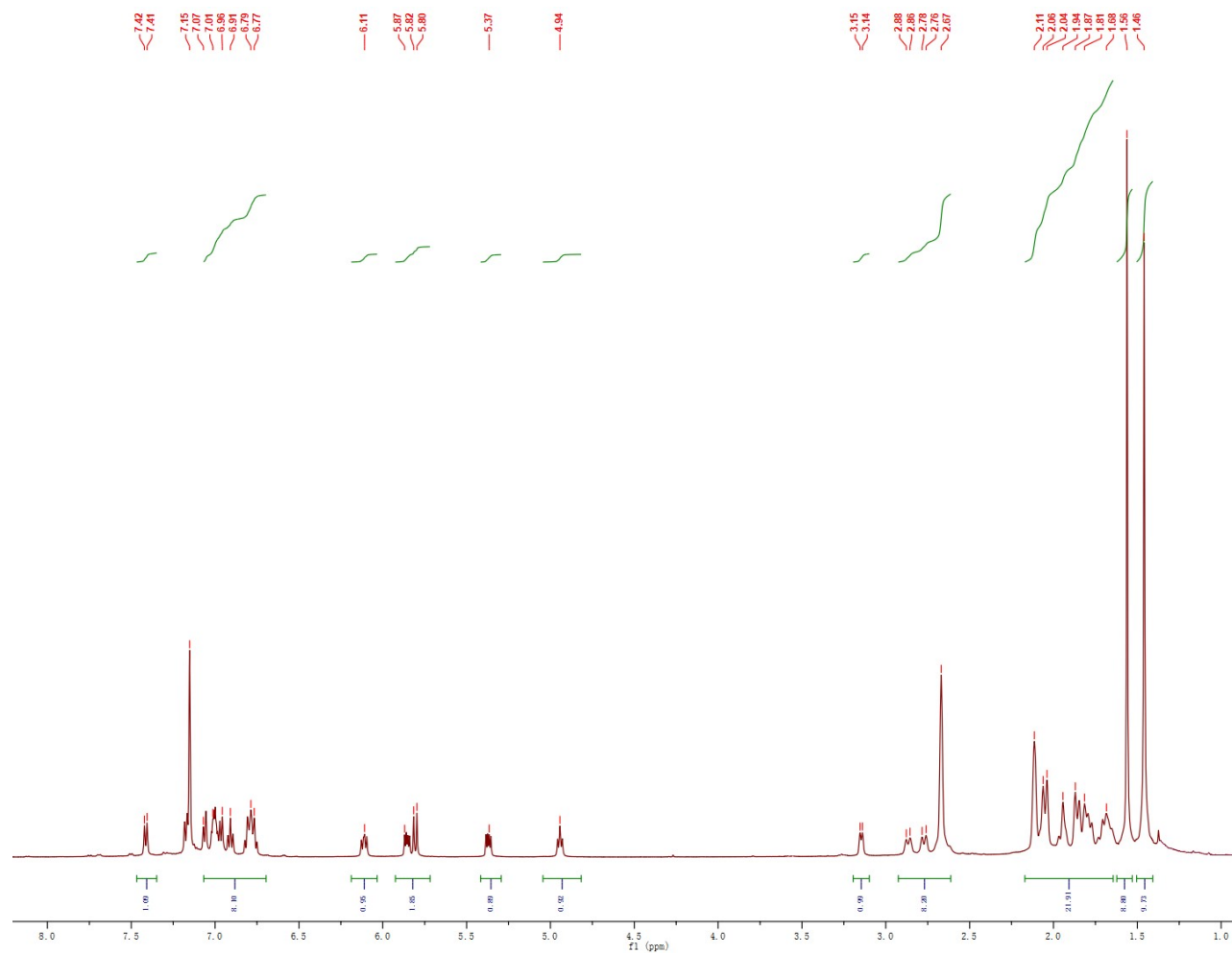


Fig. S18 ^1H NMR spectrum of **3a** in C_6D_6

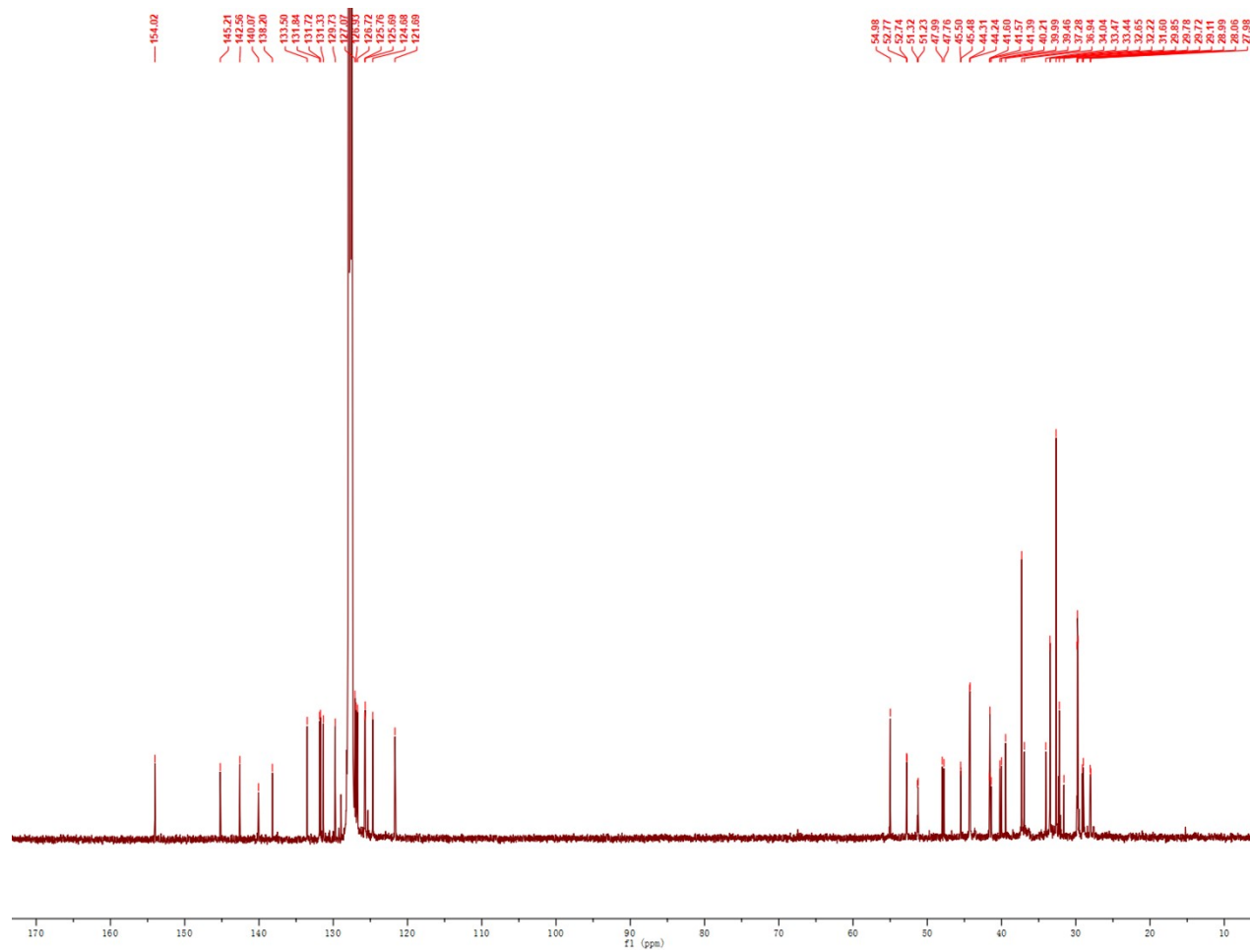


Fig. S19 ^{13}C NMR spectrum of **3a** in C_6D_6

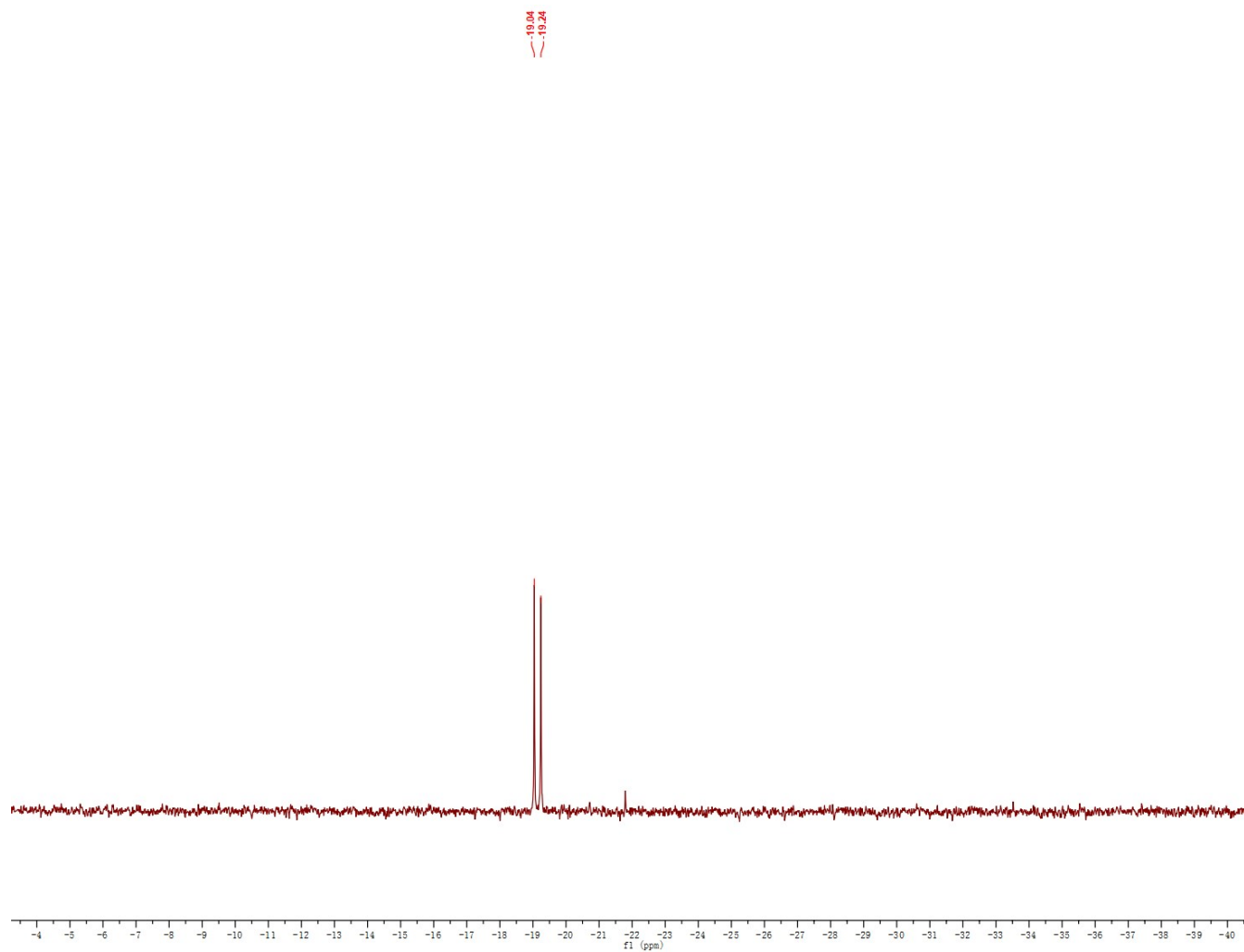


Fig. S20 ^{29}Si NMR spectrum of **3a** in C_6D_6

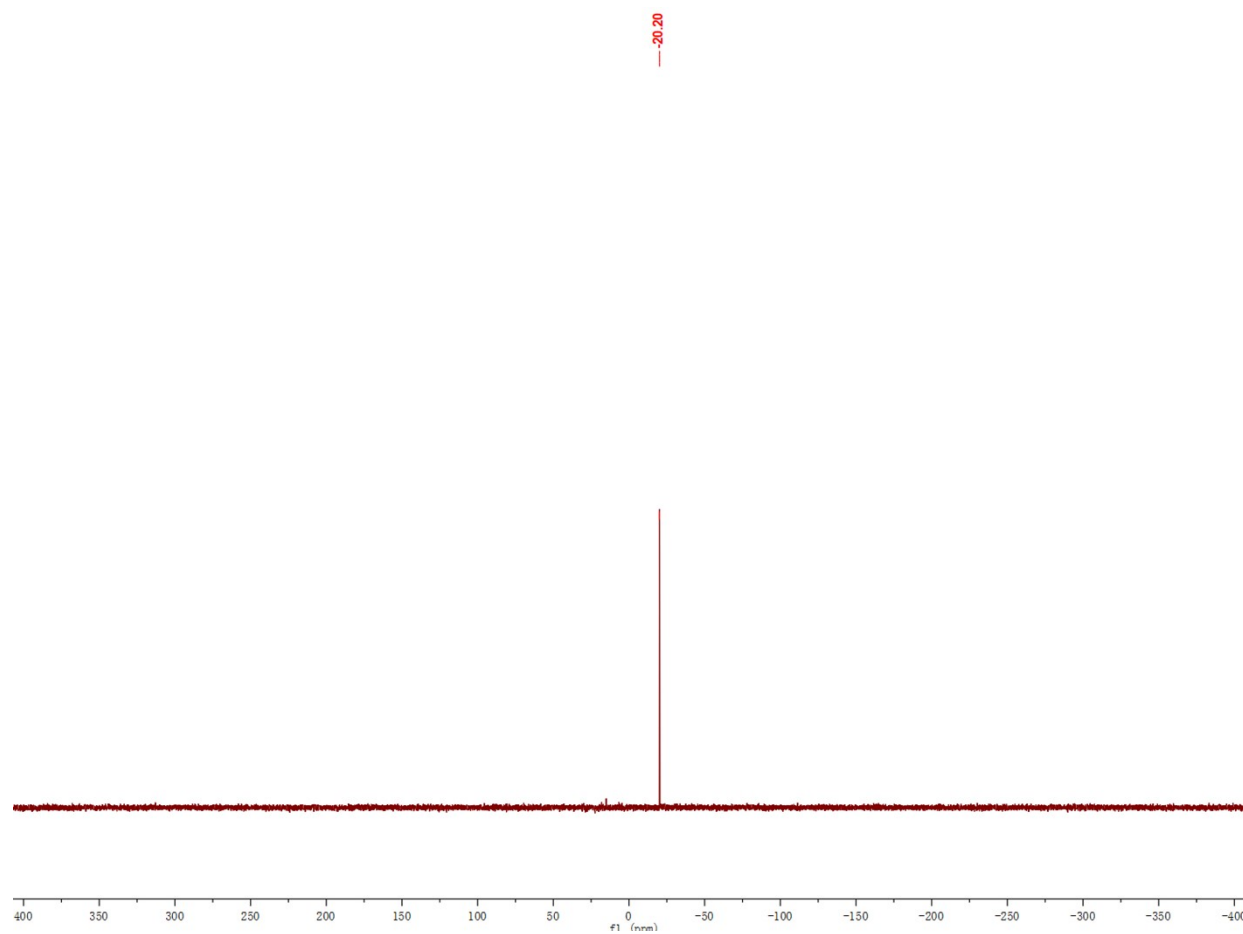


Fig. S21 ^{31}P NMR spectrum of **3a** in C_6D_6

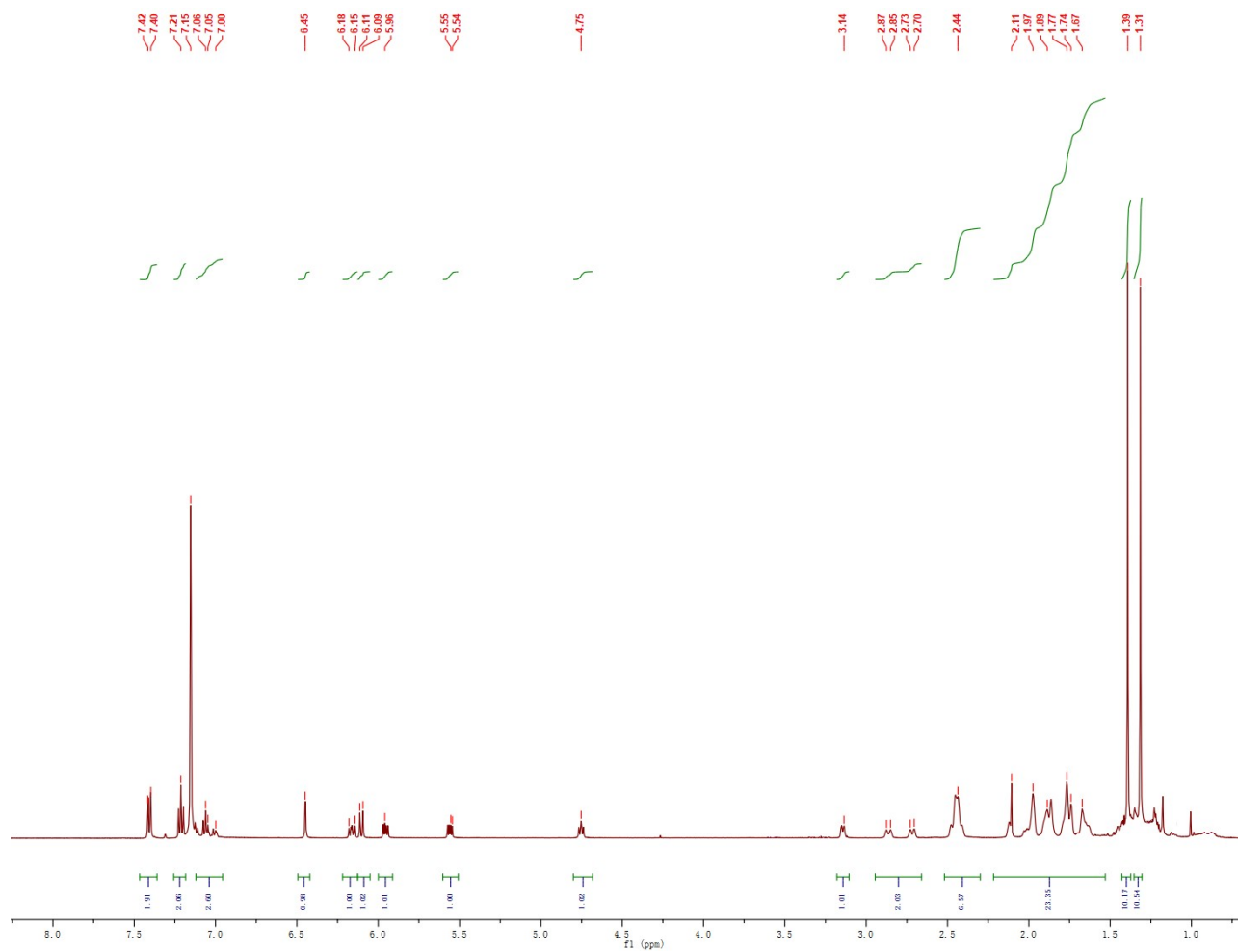


Fig. S22 ^1H NMR spectrum of **3b** in C_6D_6

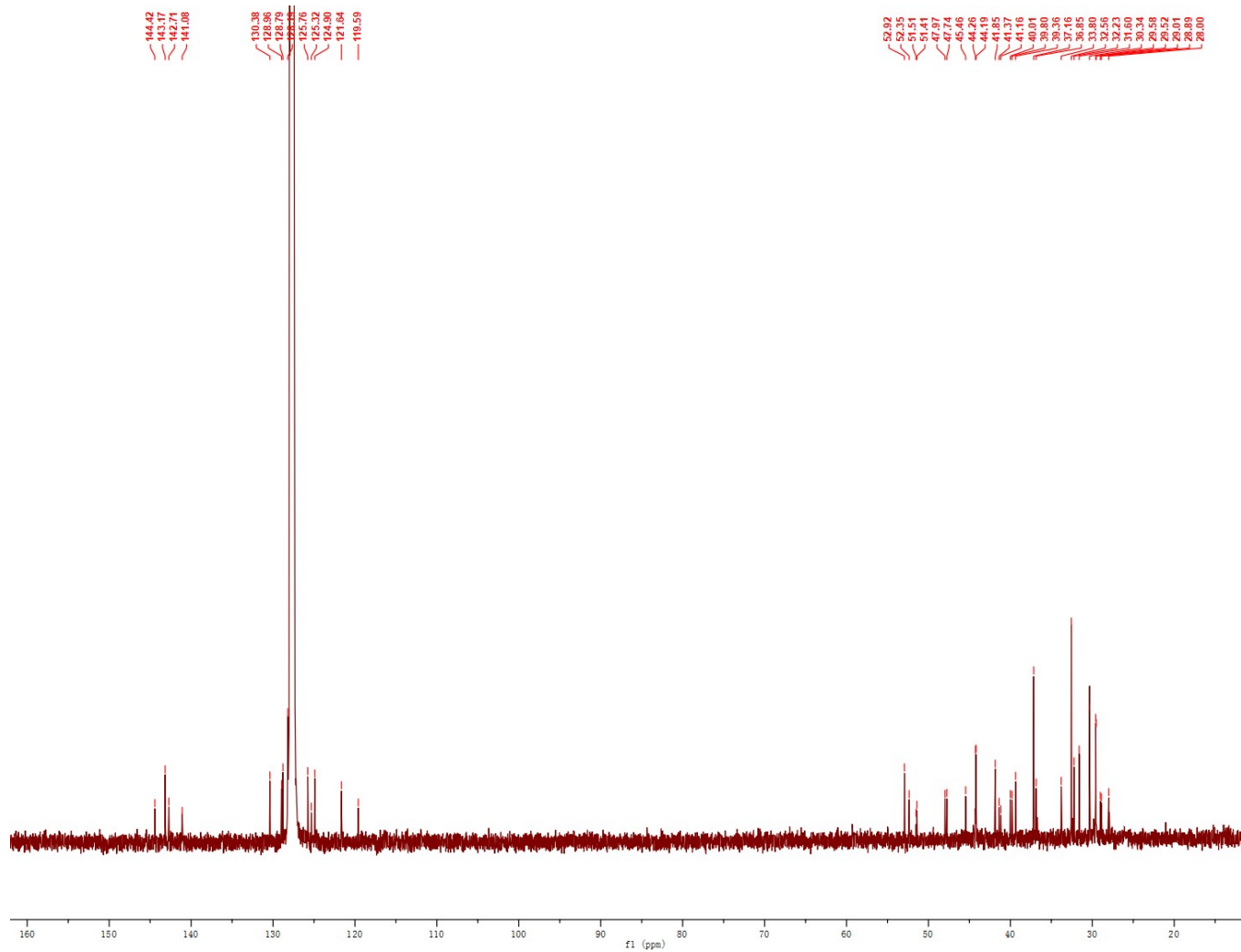


Fig. S23 ^{13}C NMR spectrum of **3b** in C_6D_6

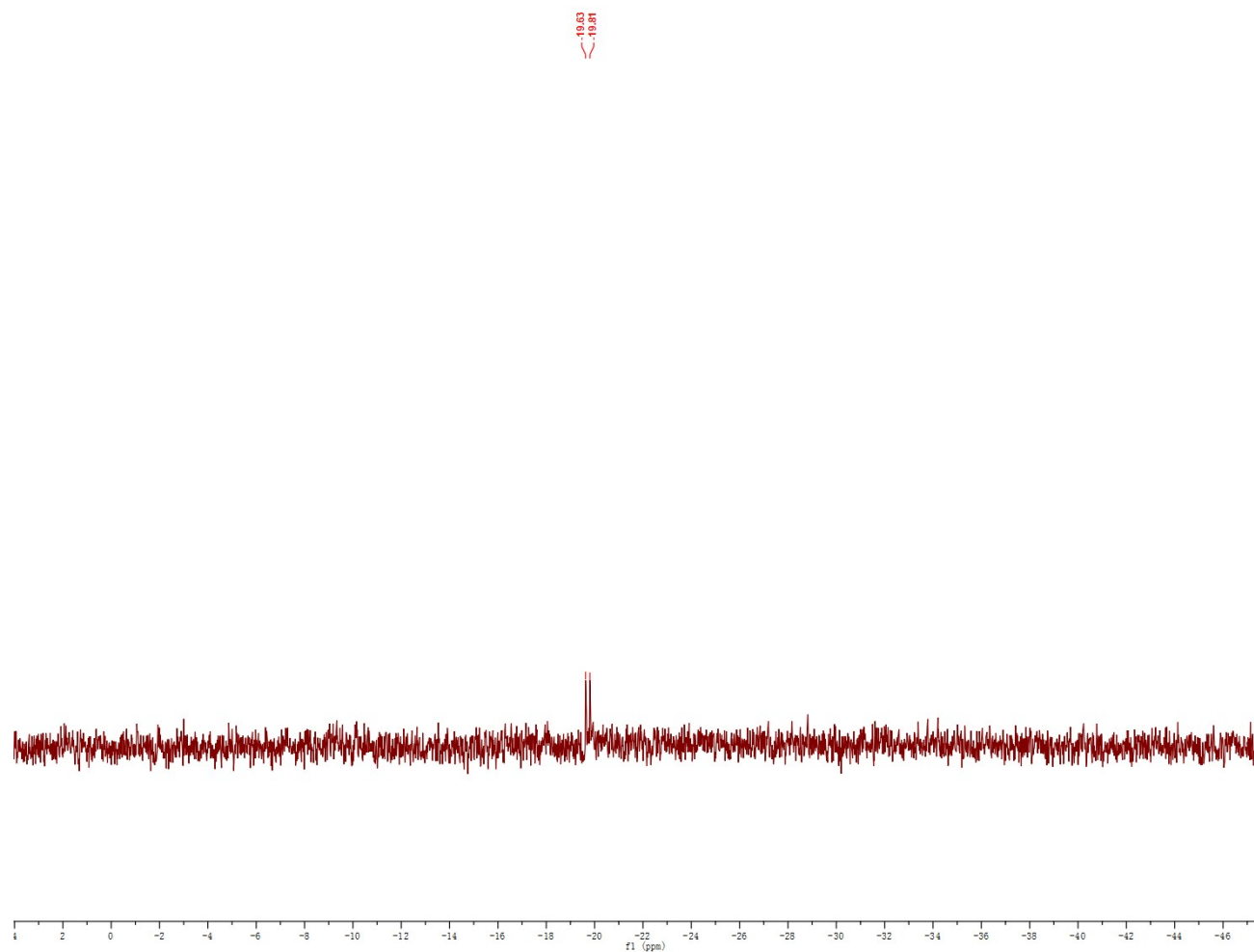


Fig. S24 ^{29}Si NMR spectrum of **3b** in C_6D_6

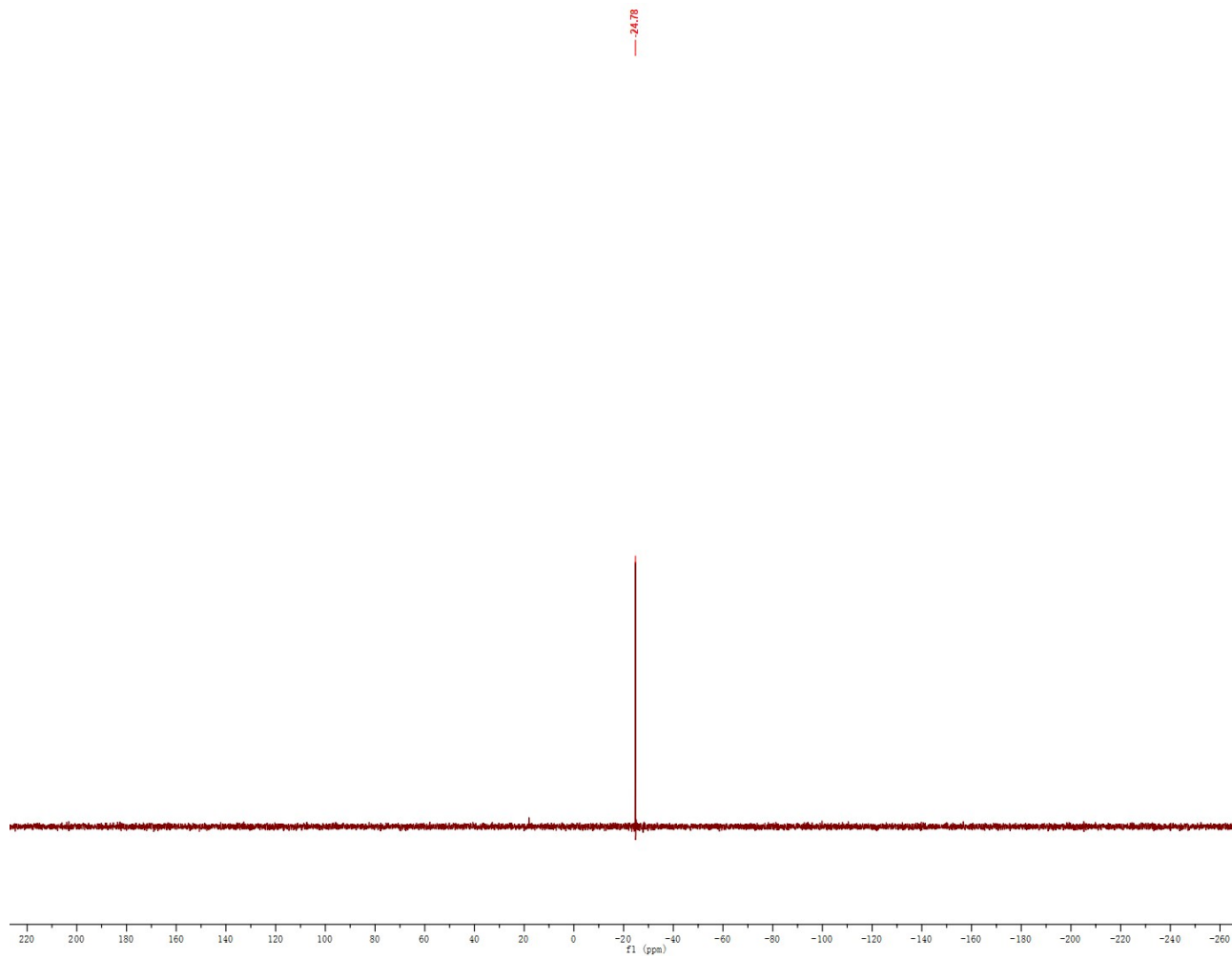


Fig. S25 ^{31}P NMR spectrum of **3b** in C_6D_6

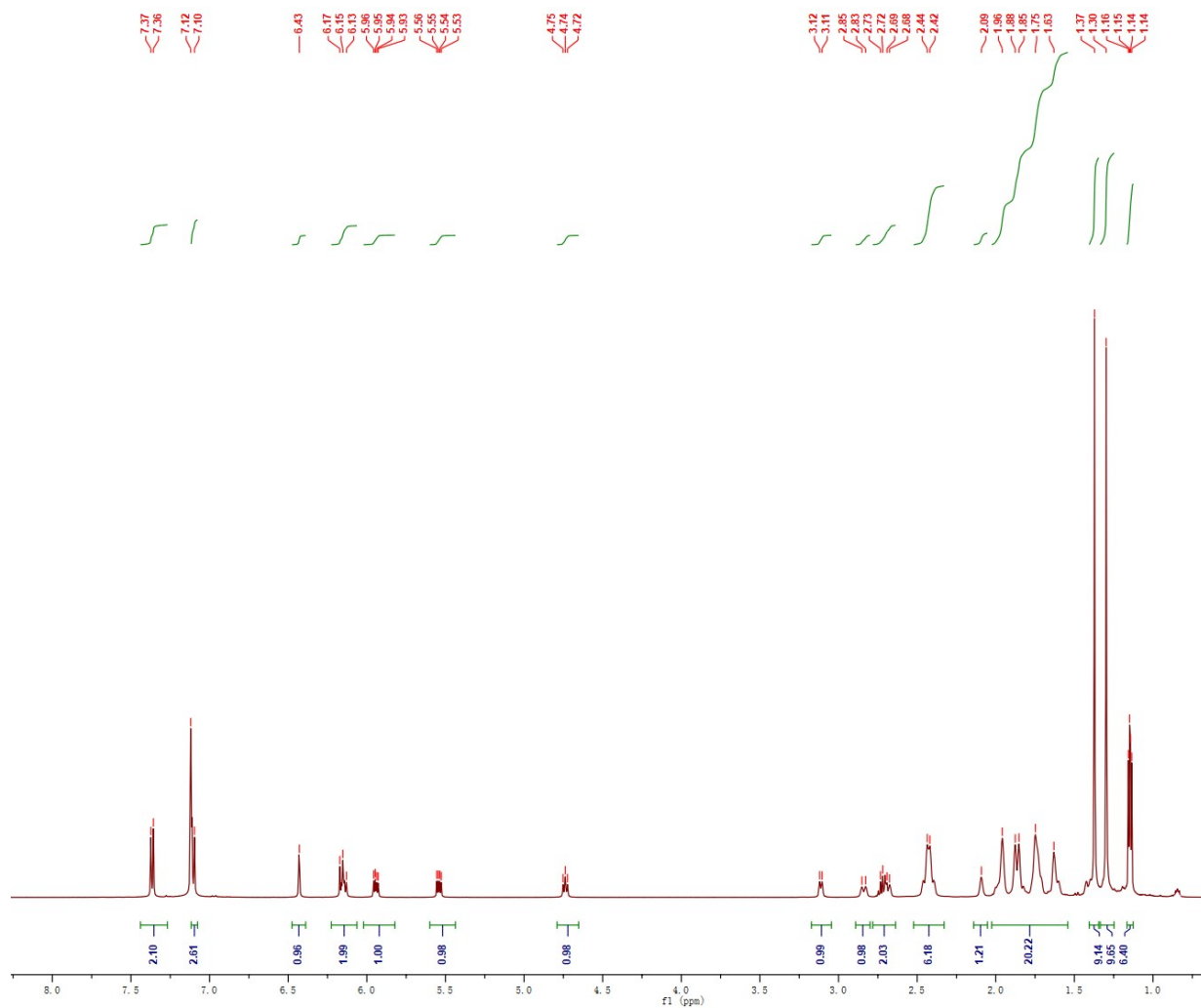


Fig. S26 ¹H NMR spectrum of **3c** in C₆D₆

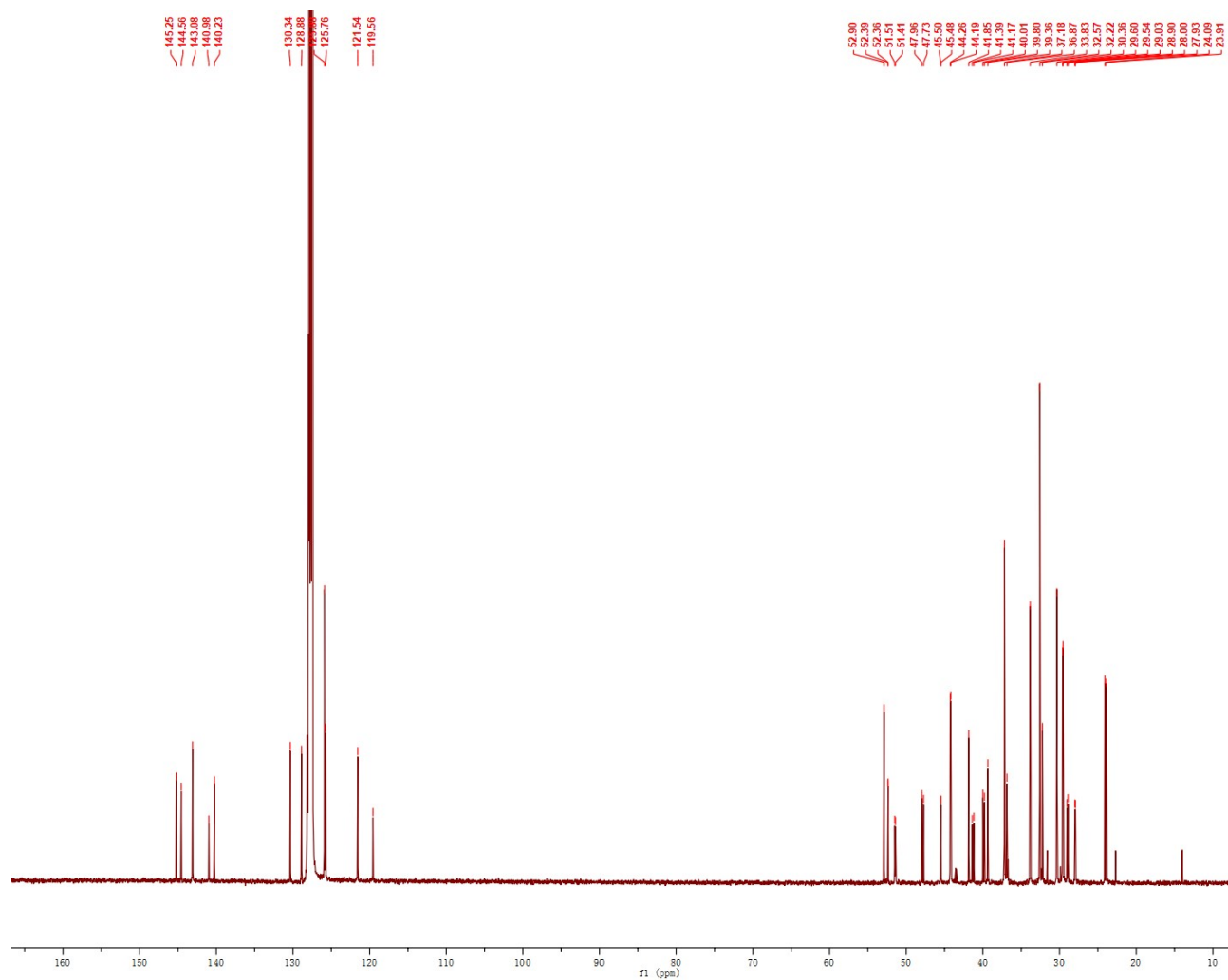


Fig. S27 ^{13}C NMR spectrum of **3c** in C_6D_6

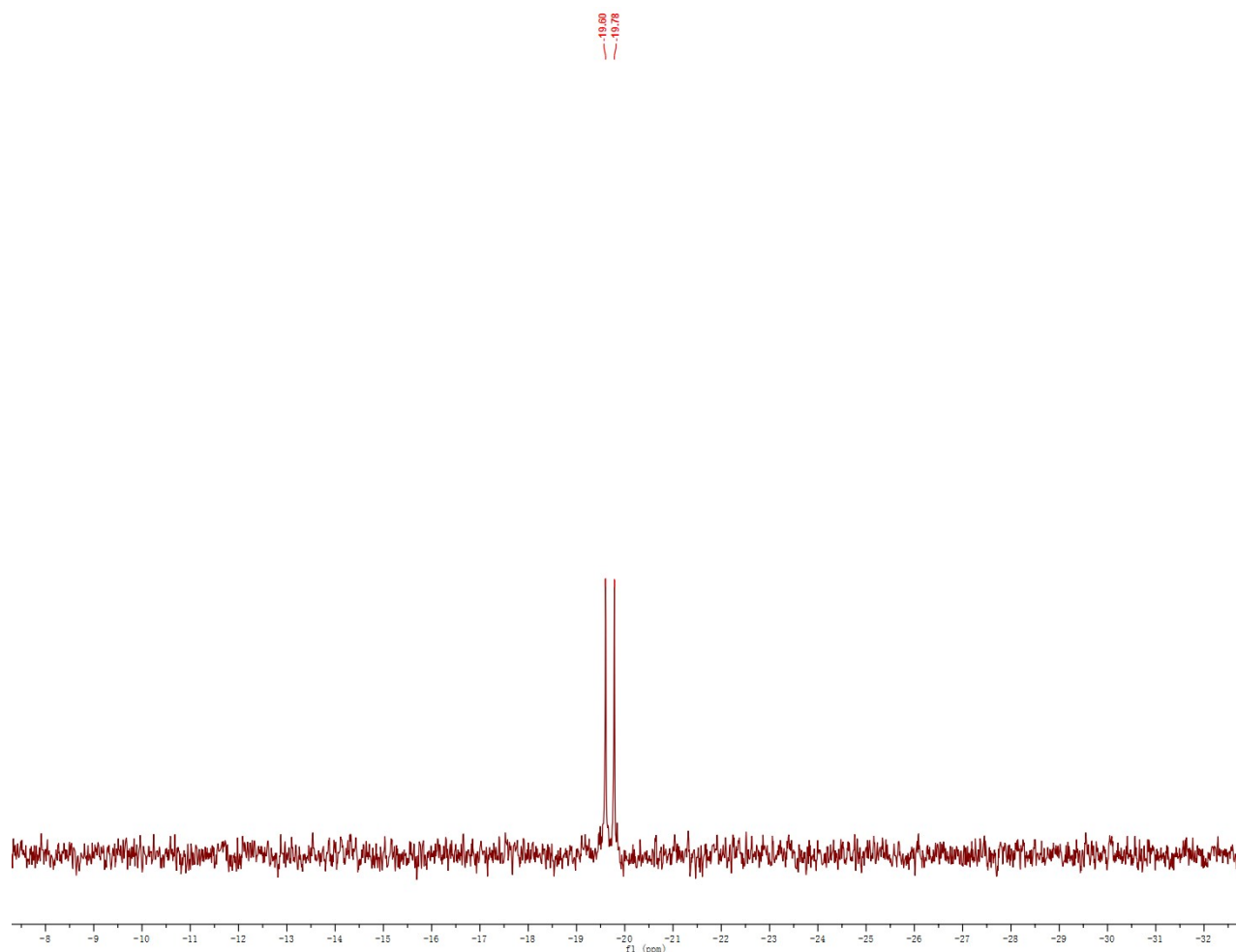


Fig. S28 ^{29}Si NMR spectrum of **3c** in C_6D_6

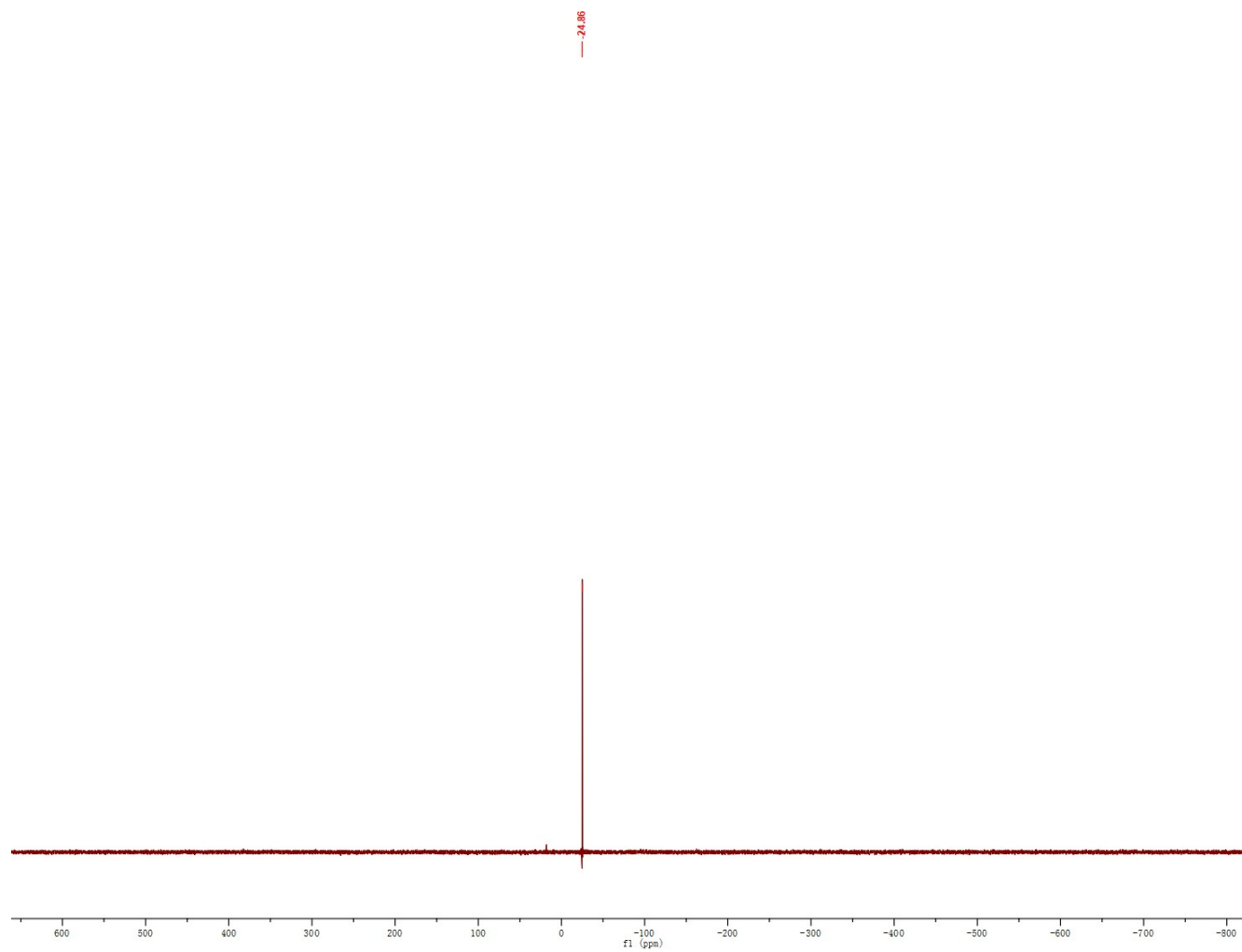


Fig. S29 ^{31}P NMR spectrum of **3c** in C_6D_6

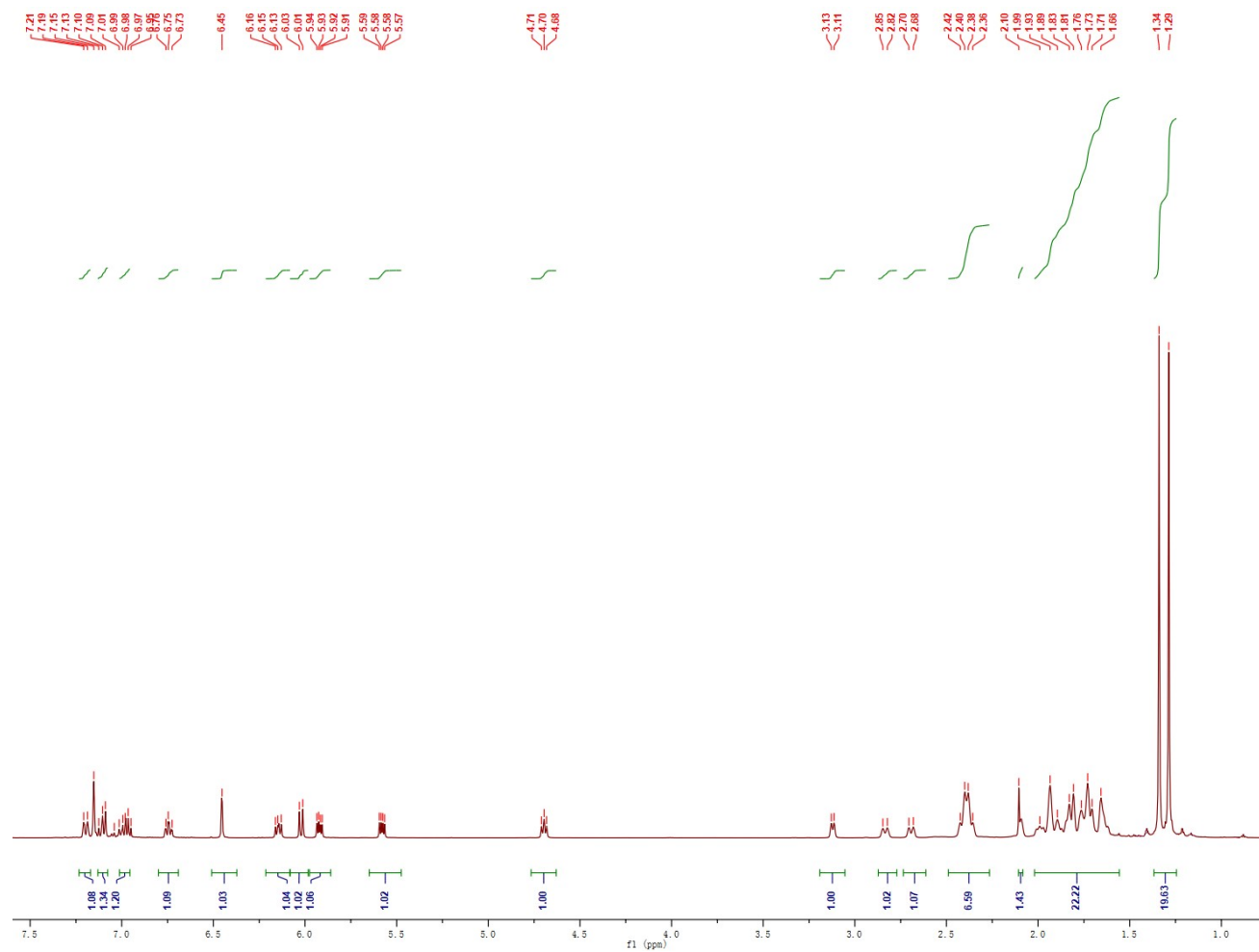


Fig. S30 ^1H NMR spectrum of **3d** in C_6D_6

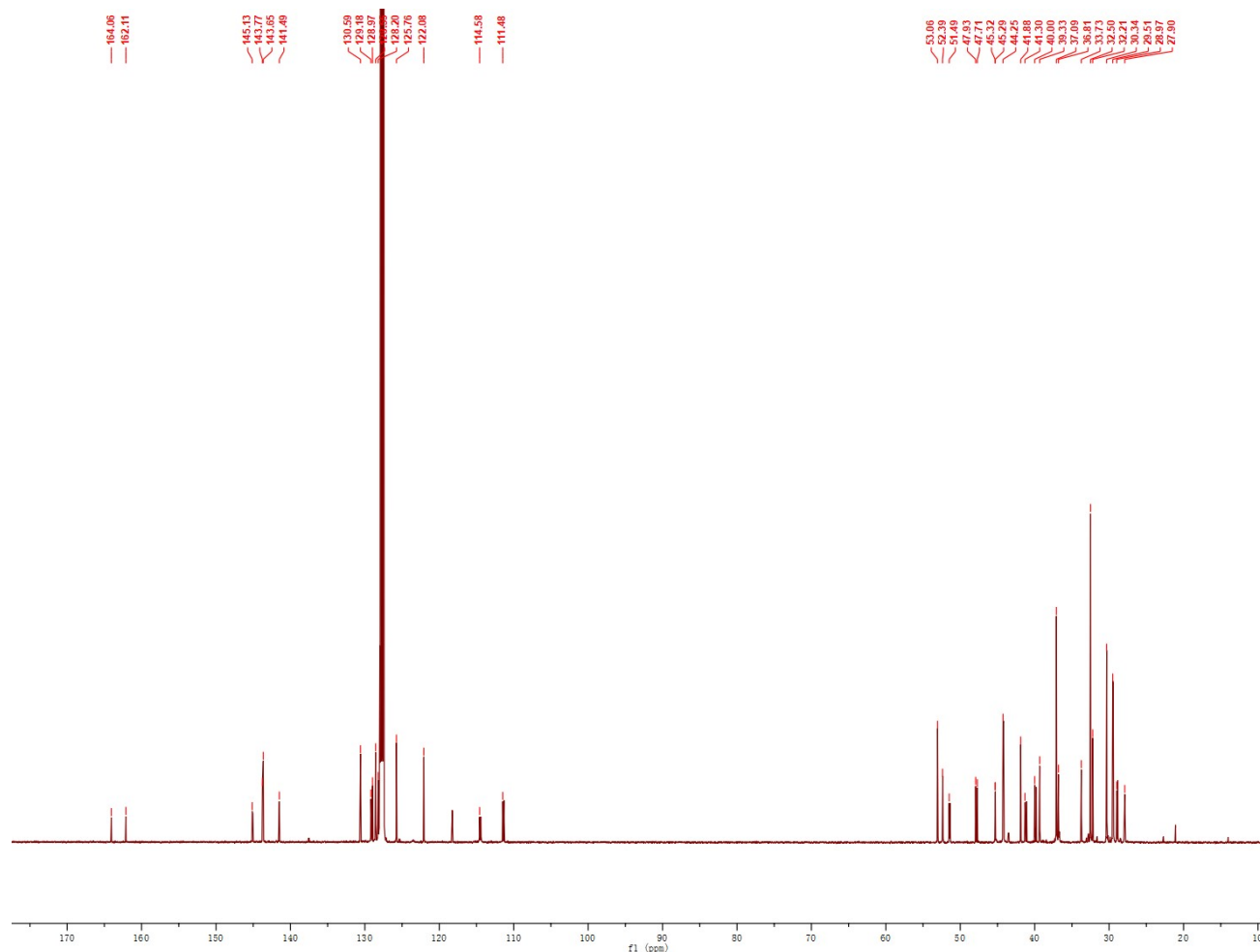


Fig. S31 ^{13}C NMR spectrum of **3d** in C_6D_6

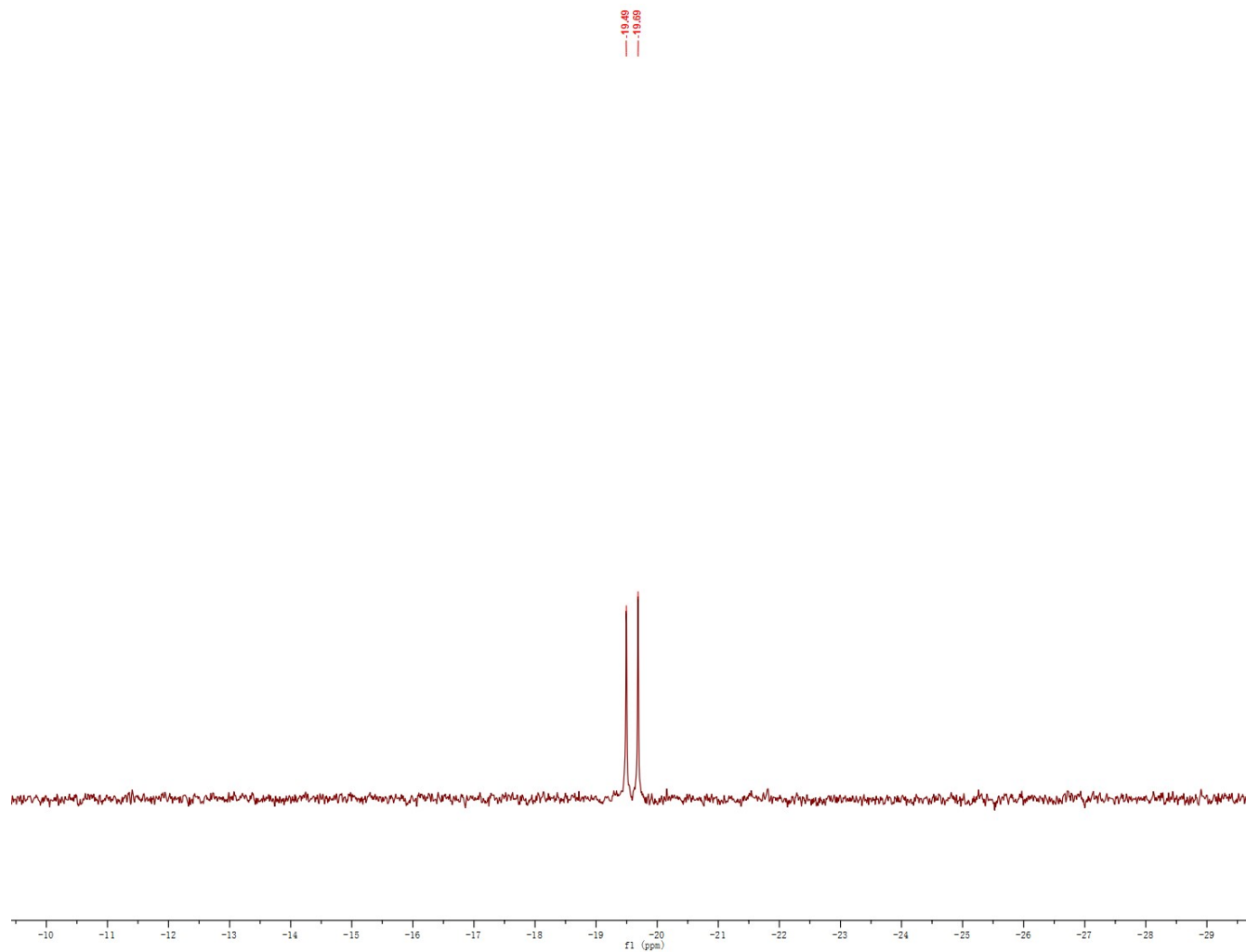


Fig. S32 ^{29}Si NMR spectrum of **3d** in C_6D_6

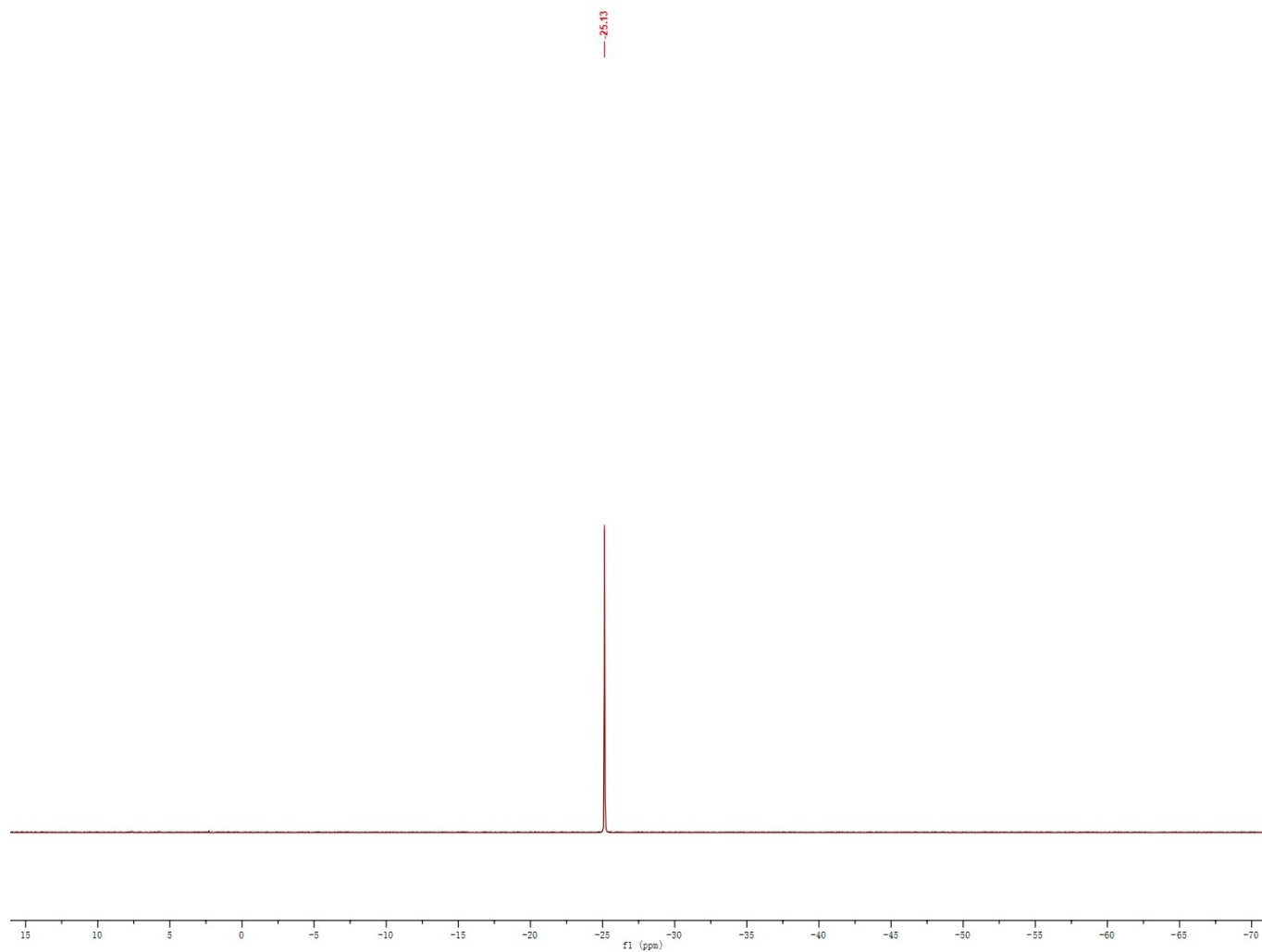


Fig. S33 ^{31}P NMR spectrum of **3d** in C_6D_6

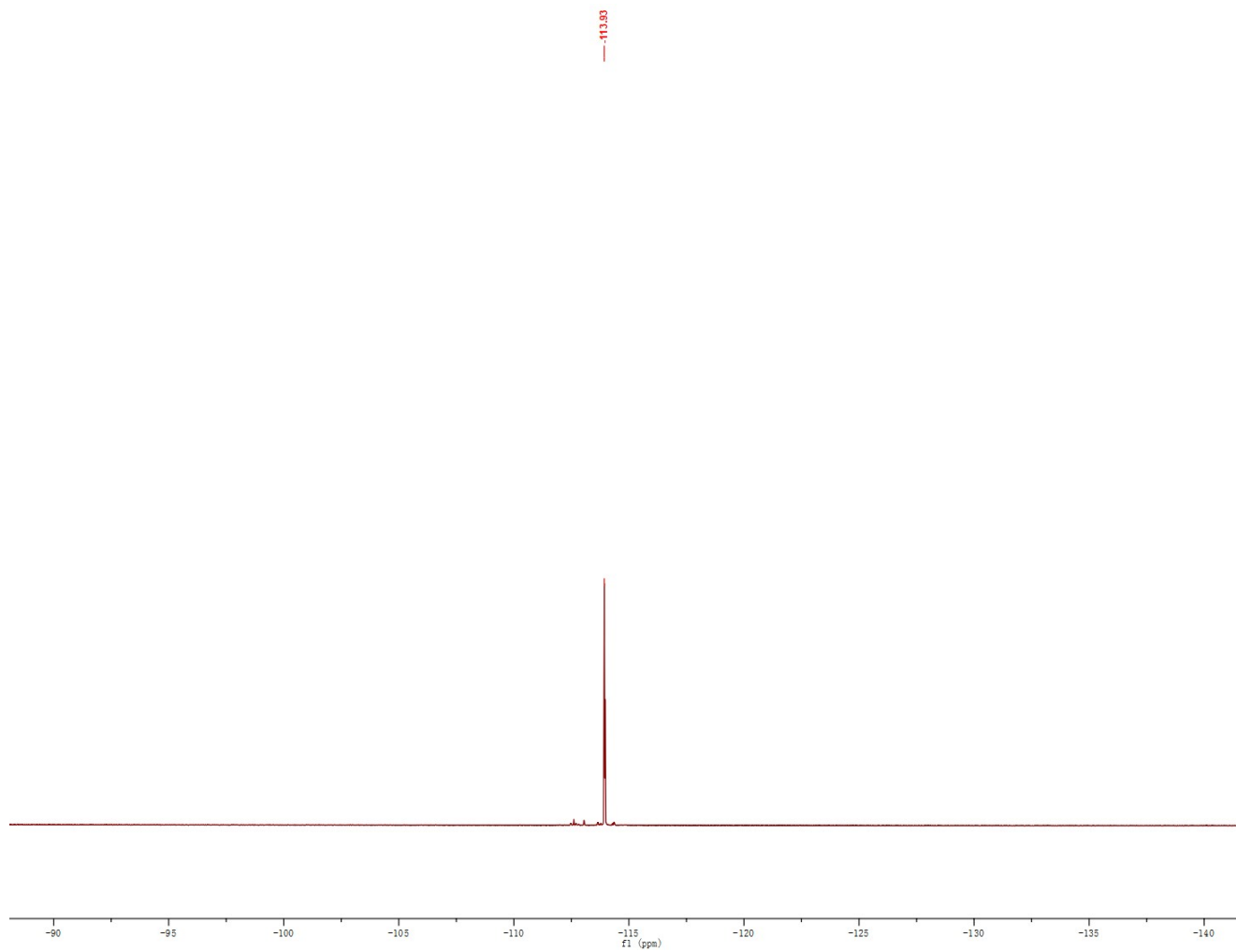


Fig. S34 ^{19}F NMR spectrum of **3d** in C_6D_6

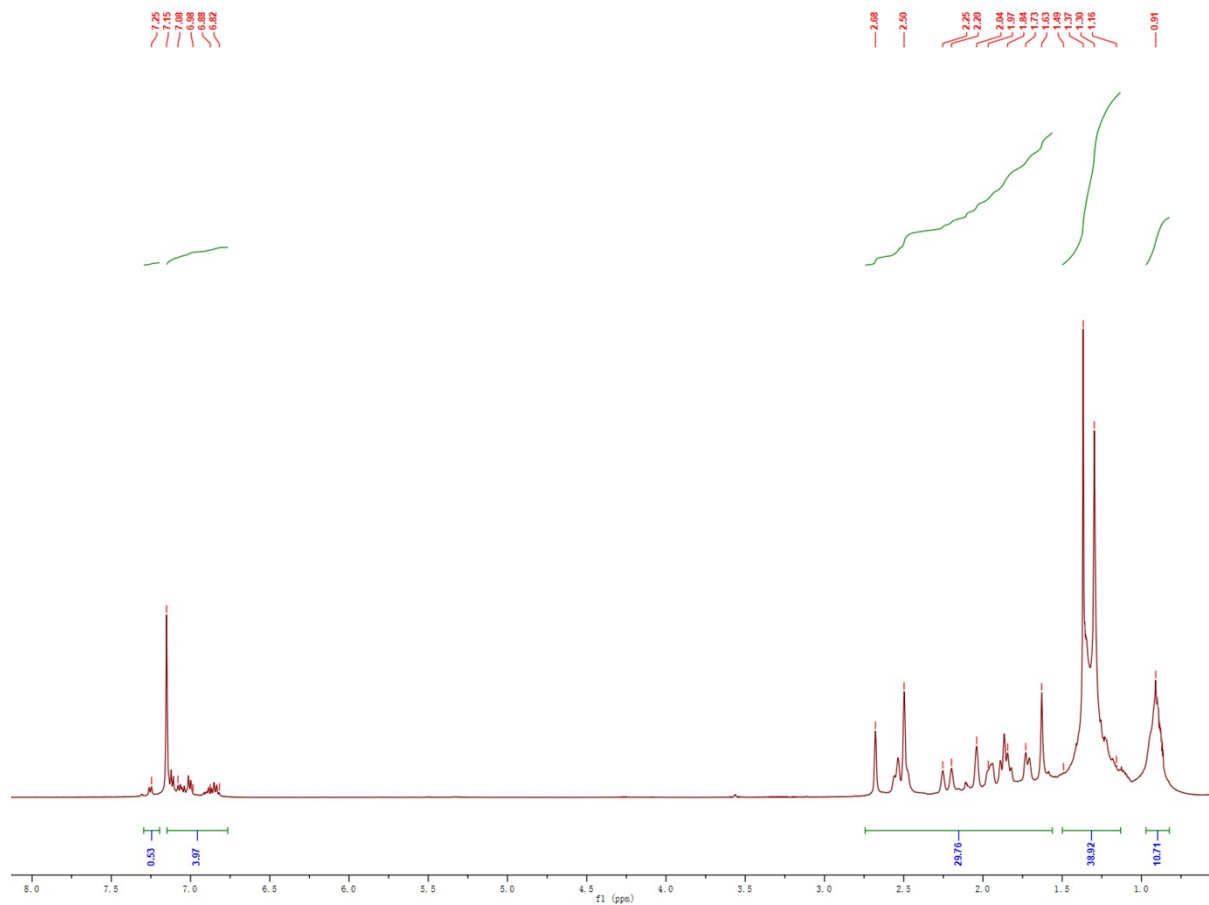


Fig. S35 ^1H NMR spectrum of **4** in C_6D_6

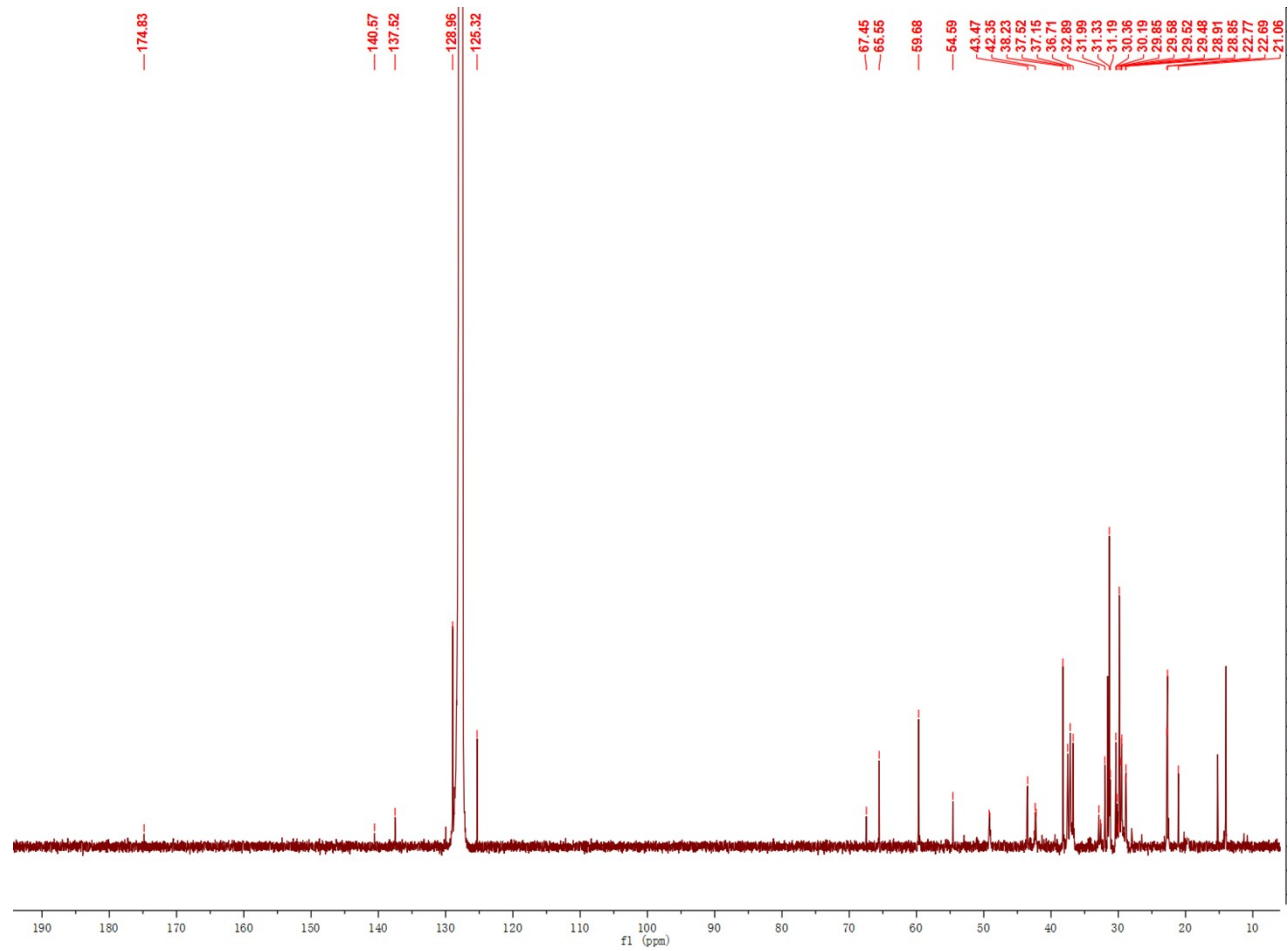


Fig. S36 ^{13}C NMR spectrum of **4** in C_6D_6

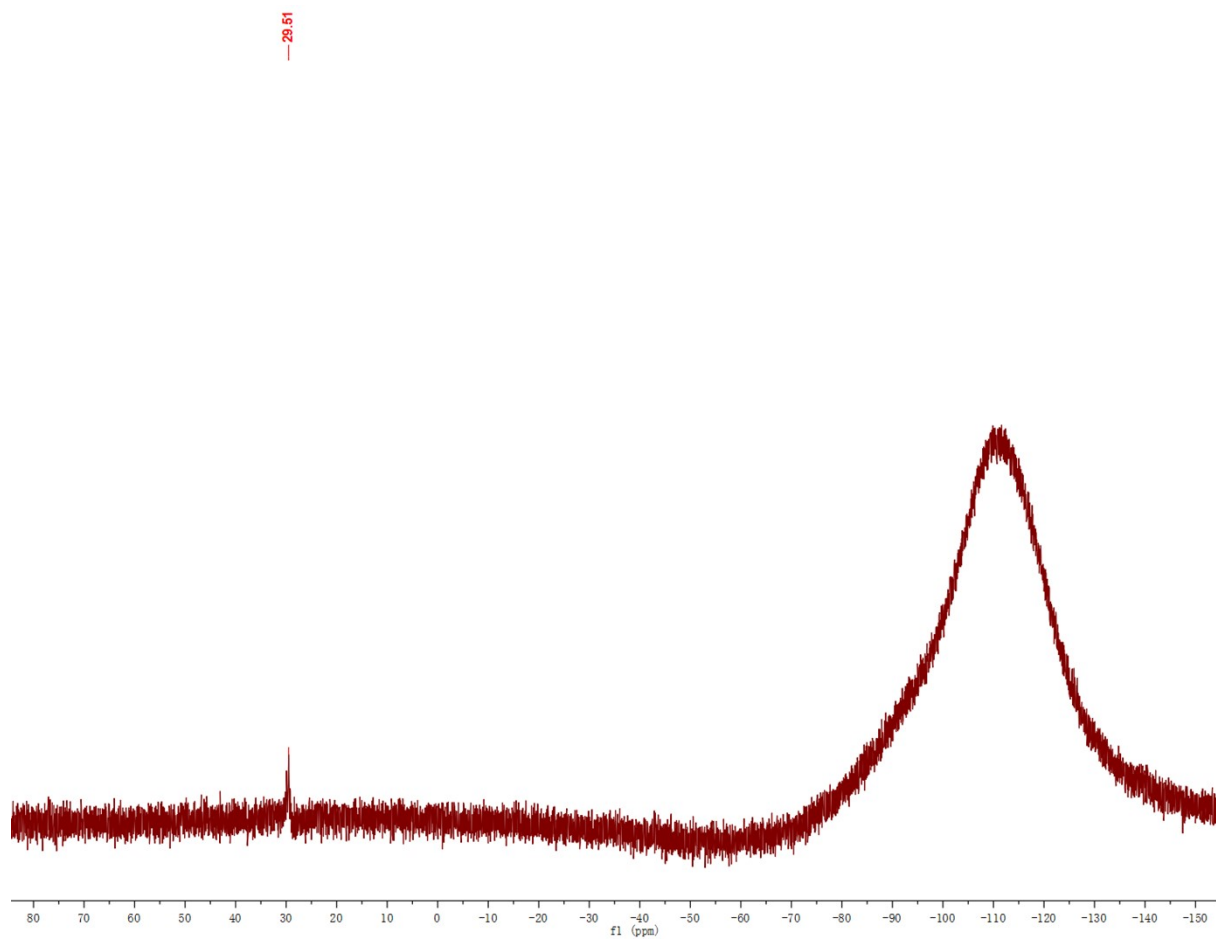


Fig. S37 ^{29}Si NMR spectrum of **4** in C_6D_6

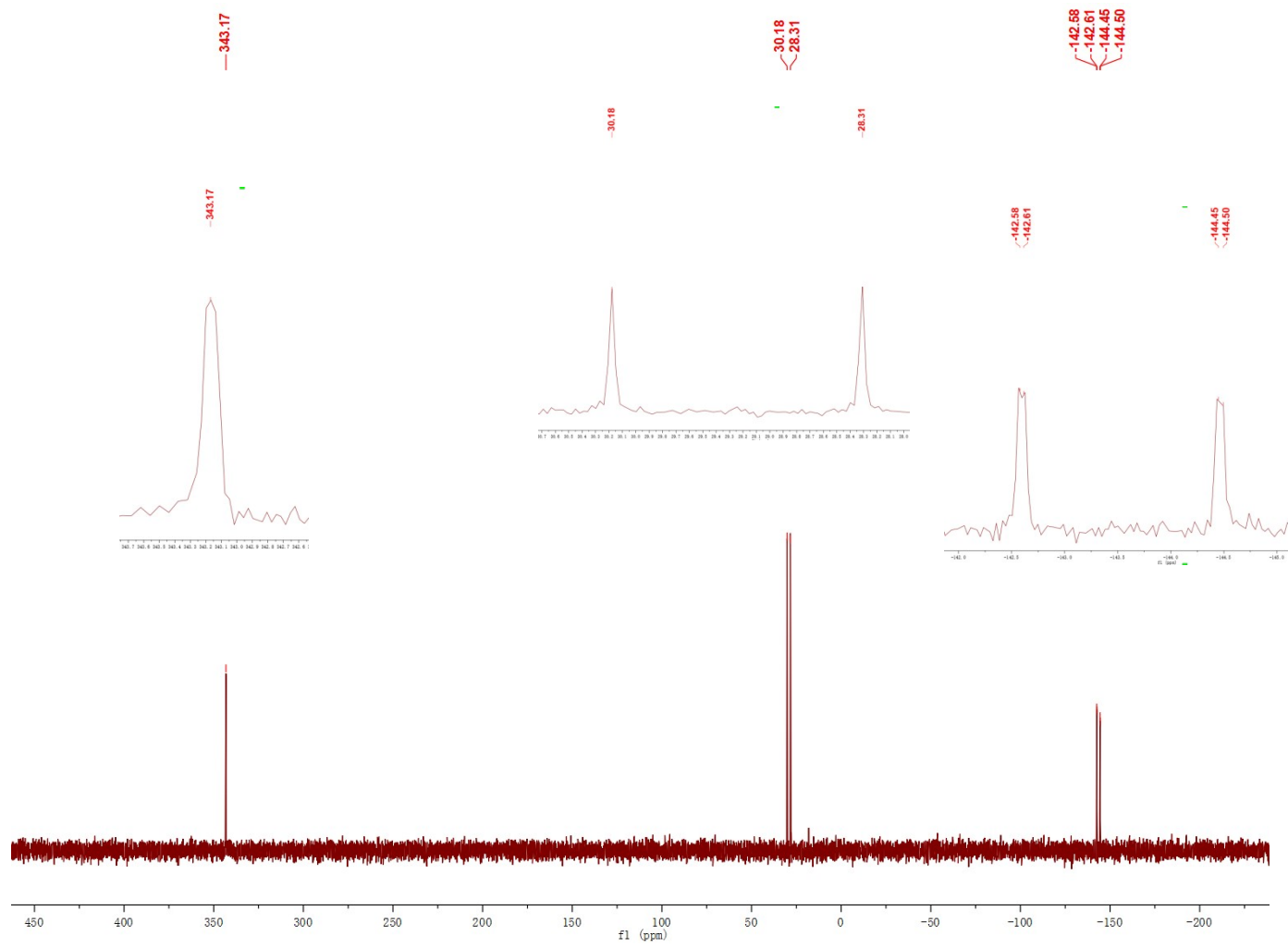


Fig. S38 ^{31}P NMR spectrum of **4** in C_6D_6

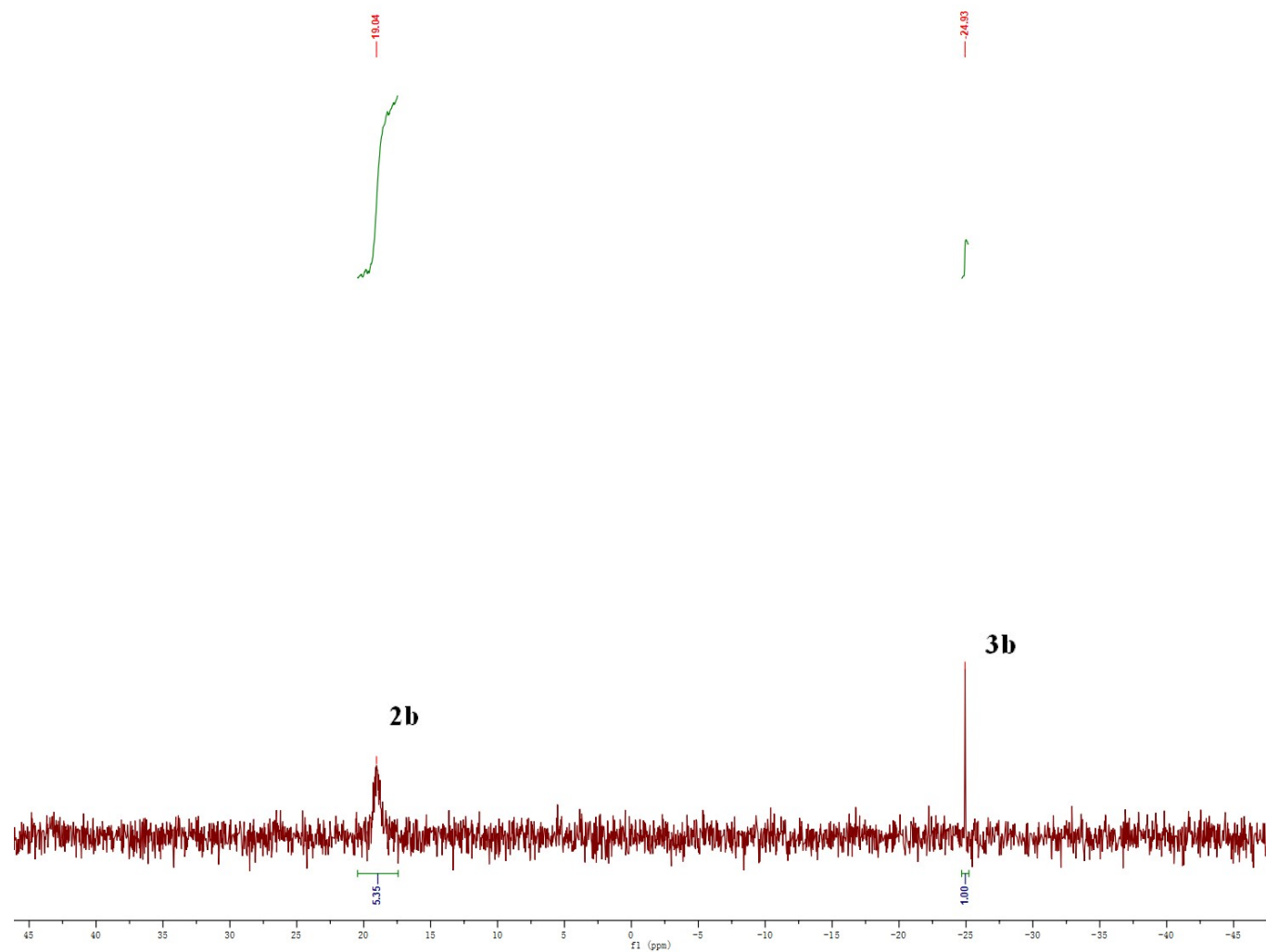


Fig. S39 ^{31}P NMR spectrum recorded after a slow conversion of silirene intermediate **2b** to **3b** at r.t. (in C_6D_6)

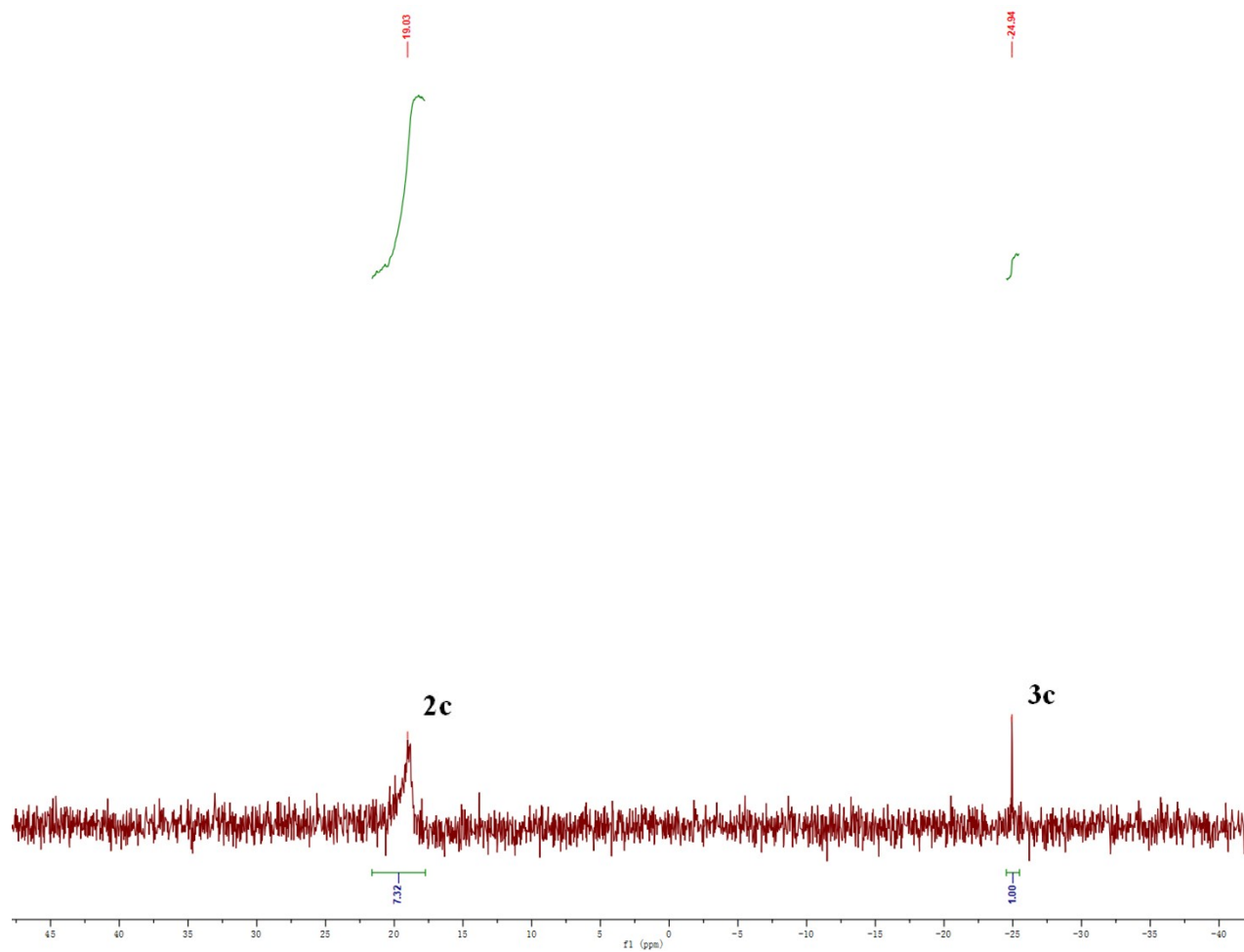


Fig. S40 ^{31}P NMR spectrum recorded after a slow conversion of silirene intermediate **2c** to **3c** at r.t. (in C_6D_6)

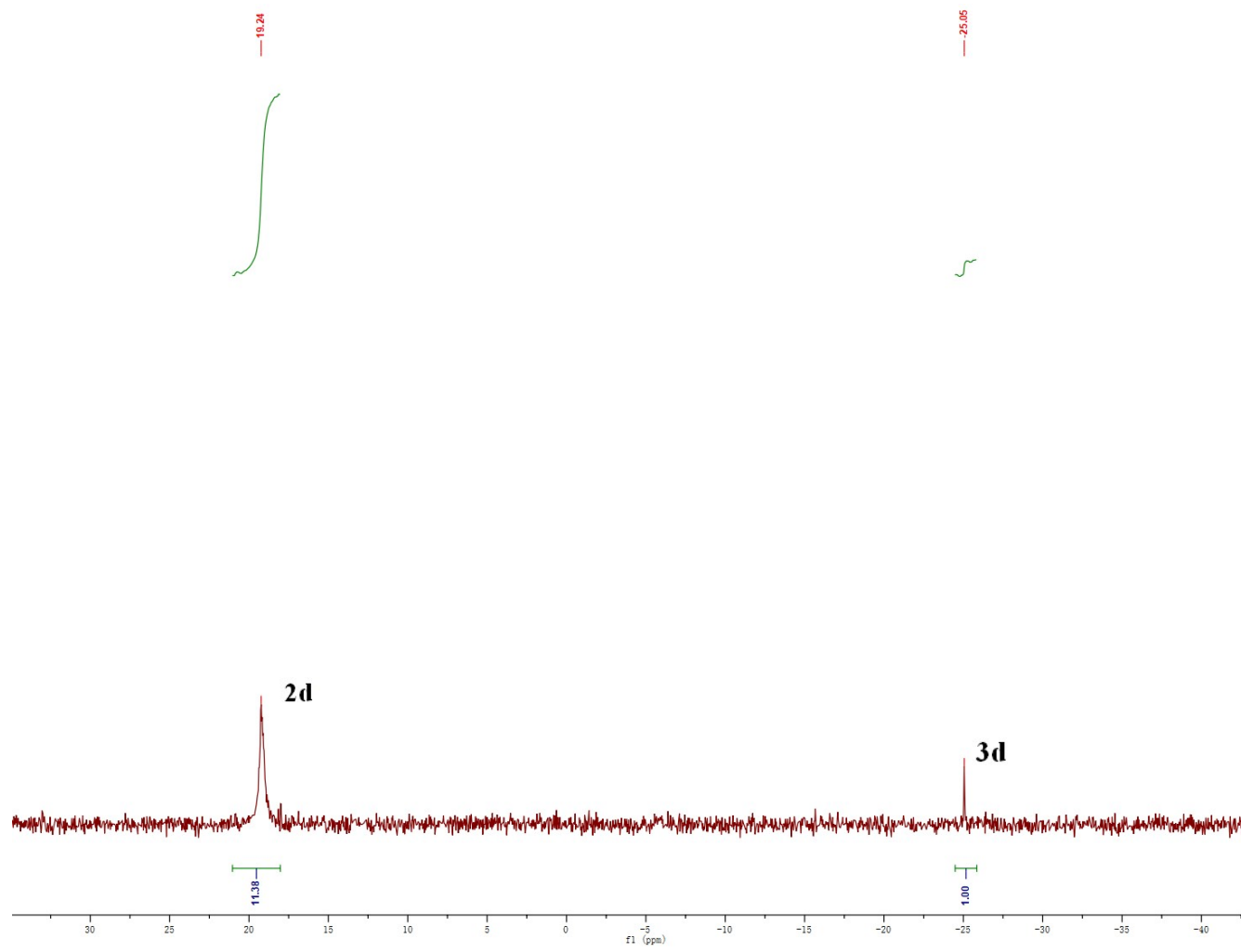


Fig. S41 ^{31}P NMR spectrum recorded after a slow conversion of silirene intermediate **2d** to **3d** at r.t. (in C_6D_6)

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