Supporting Information

Development of Unique Dianionic Ir(III) CCC Pincer Complexes with a Favourable Spirocyclic NHC Framework

Zhi-Bo Yan, Kun-Long Dai, Bin-Miao Yang, Zi-Hao Li, Yong-Qiang Tu*, Fu-Min Zhang, Xiao-Ming Zhang, Meng Peng, Qi-Long Chen & Ze-Ran Jing

State Key Laboratory of Applied Organic Chemistry & College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, China

School of Chemistry and Chemical Engineering, Frontiers Science Center for Transformative Molecules, Shanghai Jiao Tong University, Shanghai 200240, China

Contents

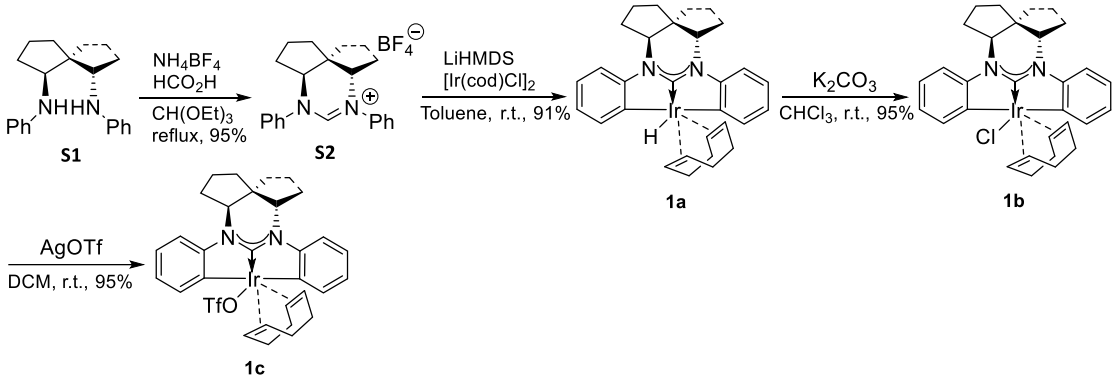
1. General information

All reactions were carried out using oven-dried glassware (150 °C) equipped with a magnetic stir bar under argon atmosphere unless otherwise indicated. The reactions for preparing the Ir(III) complexes from **S2** to **1a-1c** and **1b**-catalyzed reactions were conducted in a glove box (H_2O < 0.5 ppm, O_2 < 0.5 ppm). All reagents were used as received unless otherwise noted. In addition to commercially available extra dry solvents including 1,4-dioxane, hexane, *N,N*-Dimethylformamide (DMF), dimethyl sulfoxide (DMSO), etc., all solvents were purified by standard operating method. Dichloromethane (DCM), 1,2-dichloroethane (DCE) and chloroform ($CHCl_3$) were distilled from calcium hydride. Toluene, benzene, tetrahydrofuran (THF) and diethyl ether (Et_2O) were dried over sodium. Analytical thin-layer chromatography (TLC) was performed on silica gel plates with F-254 indicator and visualized by ultraviolet light (254 nm). Products purifications were performed via column chromatography on silica gel (200-300 mesh) or neutral alumina (200-300 mesh) unless specially stated.

^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on Bruker AM-400 MHz or Varian Mercury-600 MHz. Chemical shifts (δ) were quoted in ppm relative to tetramethylsilane or the residual solvent peak as internal standard ($CDCl_3$: δ_H 7.26 ppm and δ_C 77.00 ppm, CD_2Cl_2: δ_H 5.32 ppm and δ_C 53.84 ppm, C_6D_6: δ_H 7.16 ppm and δ_C 128.00 ppm, acetone-*d*$_6$: δ_H 2.05 ppm and δ_C 29.70 ppm), multiplicities are as indicated: s = singlet, d = doublet, t = triplet, m =multiplet, br = broad. Infrared (IR) spectra were performed on Nicolet FT-170SX spectrometer. Gas Chromatography-Mass Spectrometry (GC-MS) data were collected with Shimadzu GC-MS QP2010SE by means of EI (70 eV) technique. High-resolution mass spectral analysis (HRMS) data were obtained on the Bruker ApexII with ESI resource and SolariX-70FT-MS with MALDI resource. X-ray diffraction data were collected on Agilent SuperNova Eos diffractometer.

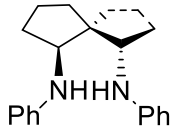
2. Synthesis of dianionic Ir(III) CCC pincer complexes 1a, 1b and 1c

Scheme S1. Synthesis of the dianionic SNHC-Ir complexes 1a, 1b, 1c



2.1. Preparation of the *cis,cis-N,N*-diphenyl spiro[4,4]nonane-1,6-diamine carbene BF_4^- salt S2

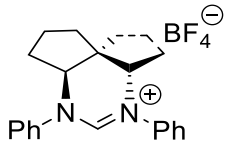
cis,cis-N,N-diphenyl spiro[4,4]nonane-1,6-diamine (**S1**):



S1

The mixture of *cis,cis-* and *cis,trans-N,N*-diphenyl spiro[4,4]nonane-1,6-diamine was prepared according to literature procedures[1] and further purified by more refined column chromatography on silica gel (eluting with PE) to provide >99.5% purity *cis,cis-N,N*-diphenyl spiro[4,4]nonane-1,6-diamine (**S1**) as a light yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.13 (t, *J* = 7.9 Hz, 4H), 6.67 (t, *J* = 7.3 Hz, 2H), 6.56 (d, *J* = 7.8 Hz, 4H), 4.14 (s, 2H), 3.66 (d, *J* = 2.8 Hz, 2H), 2.01-1.86 (m, 2H), 1.86-1.63 (m, 8H), 1.63-1.41 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.6, 129.0, 117.3, 113.7, 60.3, 56.4, 35.6, 31.1, 20.1; **IR** (KBr): 3384, 2957, 2868, 1601, 1500, 1256, 748, 693 cm^{-1}; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{21}H_{27}N_2$, m/z: 307.2169, found: 307.2175, Error 2.1 ppm.

cis,cis-N,N-diphenyl spiro[4,4]nonane-1,6-diamine carbene BF_4^- salt (**S2**):



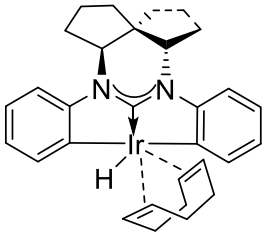
S2

cis,cis-N,N-diphenyl spiro[4,4]nonane-1,6-diamine carbene BF_4^- salt (**S2**) was prepared

according to literature procedures.[1] To a solution of **S1** (3.06 g, 0.01 mol, 1.0 equiv.) in triethoxymethane (15.0 mL), ammonium fluoroborate (4.20 g, 0.04 mol, 4.0 equiv.) was added, followed by addition of formic acid (37.7 μL, 10.0 mol%) at room temperature. The reaction mixture was stirred for 4 h at 120 °C. After the reaction was completed, the mixture was concentrated under reduced pressure to give the crude product, which was purified by column chromatography on silica gel (eluting with DCM:MeOH = 50:1 to 30:1) to provide the desired carbene BF_4^- salt **S2** (3.84 g, 95% yield). m.p. 174.8-176.2 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.56-7.49 (m, 4H), 7.48-7.36 (m, 6H), 4.14 (t, *J* = 5.9 Hz, 2H), 2.16-1.98 (m, 4H), 1.98-1.64 (m, 8H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.4, 140.0, 130.1, 129.4, 124.9, 62.8, 50.0, 35.3, 29.6, 19.9; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -151.79, -151.81, -151.82, -151.86; **IR** (KBr): 2958, 2926, 1661, 1592, 1494, 1058, 734, 698 cm^{-1}; **HRMS (ESI)** calcd for $[M\text{-}BF_4]^+$ $C_{22}H_{25}N_2$, m/z: 317.2012, found: 317.2012, Error 0 ppm.

2.2. Synthesis of the dianionic SNHC-Ir complexes 1a, 1b, 1c

CCC cyclometalated pincer Ir(III) hydride complex SNHC-Ir **(1a)**

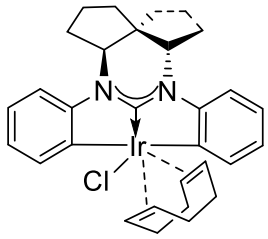


1a

In glove box, the carbene BF_4^- salt **S2** (40.4 mg, 0.1 mmol, 1.0 equiv.) was dissolved in dry toluene (1.0 mL) and then LiHMDS (1.0 mol/L in THF/ethylbenzene, 0.15 mL, 0.15 mmol, 1.5 equiv.) was added to the solution. After the resulting mixture was stirred at room temperature for 30 min, solid $[Ir(cod)Cl]_2$ (33.6 mg, 0.05 mmol, 0.5 equiv.) was added and the reaction system was stirred for 18 h, then that the mixture was taken out from the glove box and purified by flash column chromatography on neutral alumina (eluting with PE:EA = 30:1) to give SNHC-Ir **1a** as white powder (56.1 mg, 91% yield). Colorless and transparent crystals of the complex **1a** was obtained by evaporation of a solution of **1a** in benzene:Et_2O (30:1) in glove box at room temperature. **^{1}H NMR** (600 MHz, C_6D_6) δ 8.33-8.23 (m, 2H), 7.27-7.23 (m, 2H), 7.23-7.19 (m, 2H), 6.75-6.64 (m, 2H), 4.82 (t, *J* = 7.3 Hz, 1H), 4.74 (td, *J* = 8.7, 3.6 Hz, 1H), 3.65 (t, *J* = 9.3 Hz, 1H), 3.40 (d, *J* = 5.0 Hz, 1H), 3.32 (t, *J* = 7.7 Hz, 1H), 3.25 (td, *J* = 8.5, 3.7 Hz, 1H), 3.06-2.98 (m, 1H), 2.82-2.72 (m,

1H), 2.45-2.36 (m, 1H), 2.10-2.01 (m, 1H), 1.99-1.87 (m, 3H), 1.87-1.75 (m, 3H), 1.55-1.48 (m, 1H), 1.49-1.41 (m, 1H), 1.34-1.26 (m, 3H), 1.26-1.19 (m, 2H), 1.19-1.13 (m, 1H), 1.10-1.01 (m, 1H), 0.86-0.76 (m, 1H), -10.58 (s, 1H); **^{13}C NMR** (100 MHz, C_6D_6) δ 199.3, 156.6, 156.5, 139.6, 139.3, 136.0, 135.0, 123.1, 122.7, 122.6, 122.2, 112.9, 110.8, 87.6, 86.4, 78.8, 78.0, 57.9, 57.8, 51.3, 37.0, 35.8, 33.6, 32.5, 31.8, 31.0, 29.5, 29.1, 23.0, 19.7; **IR** (KBr): 2947, 2876, 2085, 1504, 1445, 1018, 750, 724 cm^{-1}; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{30}H_{35}IrN_2Na$, m/z: 639.2323, found: 639.2327, Error 0.6 ppm.

CCC cyclometalated pincer Ir(III) chloride complex SNHC-Ir **(1b)**

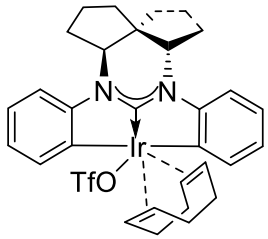


1b

In glove box, compound **1a** (200 mg, 0.324 mmol, 1.0 equiv.) was dissolved in dry $CHCl_3$ (1.0 mL) and K_2CO_3 (53.8 mg, 0.390 mmol, 1.2 equiv.) was added to the solution, the reaction mixture was stirred at room temperature for 3 days. The reaction system was monitored by TLC until the **1a** disappeared completely. Then the mixture was moved out from the glove box, then extracted with CH_2Cl_2 (3 × 20.0 mL). The combined organic layer was washed with brine (20.0 mL), dried over anhydrous Na_2SO_4, concentrated and purified by column chromatography (eluting with petroleum PE:EA = 20:1 to 5:1) to give SNHC-Ir **1b** as white powder (200.7 mg, 95% yield). Pale yellow transparent crystal of the complex **1b** was obtained by evaporation of a solution of **1b** in $CHCl_3$ in glove box at room temperature. m.p. 208.7-209.9 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.18-8.12 (m, 2H), 7.21-7.11 (m, 4H), 6.89-6.83 (m, 1H), 6.83-6.80 (m, 1H), 4.85 (t, *J* = 7.4 Hz, 1H), 4.82-4.76 (m, 1H), 4.11 (t, *J* = 9.3 Hz, 1H), 3.91 (d, *J* = 4.9 Hz, 1H), 3.20-3.10 (m, 2H), 3.06 (td, *J* = 8.3, 2.8 Hz, 1H), 2.95-2.85 (m, 1H), 2.47-2.35 (m, 2H), 2.33-2.20 (m, 3H), 2.17-2.09 (m, 2H), 2.01-1.93 (m, 1H), 1.91-1.82 (m, 3H), 1.82-1.76 (m, 1H), 1.76-1.68 (m, 2H), 1.68-1.64 (m, 1H), 1.64-1.53 (m, 2H), 1.52-1.43 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.3, 154.8, 154.4, 142.3, 141.1, 137.0, 136.4, 124.9, 124.5, 123.8, 123.4, 113.4, 111.2, 95.3, 93.3, 72.8, 72.4, 57.8, 57.7, 51.2, 37.1, 35.6, 34.7, 32.4, 32.3, 30.0, 28.5, 26.9, 22.9, 19.6; **IR** (KBr): 2955, 2870, 1522, 1450, 1308, 1018, 751,

729 cm^{-1}; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{30}H_{34}ClIrN_2Na$, m/z: 673.1925, found: 673.1908, Error 2.5 ppm.

CCC cyclometalated pincer Ir(III) triflate complex SNHC-Ir **(1c)**



1c

In glove box, compound **1b** (130.0 mg, 0.20 mmol, 1.0 equiv.) was dissolved in dry DCM (2.0 mL) and AgOTf (56.5 mg, 0.22 mmol, 1.1 equiv.) was added to the solution, the reaction mixture was stirred at room temperature for 3 h. The system was monitored by TLC until the substrate **1b** disappeared completely. The mixture was taken out from the glove box, purified by a pad of column chromatography (eluting with EA), then the product was concentrated and dissolved in DCM followed by precipitation from pentane to afford SNHC-Ir **1c** as light yellow powder (144.7 mg, 95% yield). Pale yellow transparent crystal of the complex **1c** was obtained by evaporation of a solution of **1c** in $CHCl_3$:Et_2O (30:1) in glove box at room temperature. The NMR data was obtained by *in-situ* NMR experiments conducted in CD_2Cl_2 without any other purification. m.p. 230-231 °C; **^{1}H NMR** (600 MHz, CD_2Cl_2) δ 8.22 (d, *J* = 6.8 Hz, 2H), 7.31-7.23 (m, 2H), 7.23-7.17 (m, 2H), 6.94 (d, *J* = 7.7 Hz, 1H), 6.87 (d, *J* = 7.5 Hz, 1H), 4.92 (s, 2H), 4.11 (t, *J* = 9.1 Hz, 1H), 3.94 (d, *J* = 5.0 Hz, 1H), 3.23-3.16 (m, 1H), 3.14-3.07 (m, 2H), 2.90-2.79 (m, 1H), 2.49-2.39 (m, 1H), 2.39-2.30 (m, 1H), 2.29-2.17 (m, 3H), 2.14-2.05 (m, 1H), 2.02-1.93 (m, 2H), 1.93-1.81 (m, 3H), 1.78-1.71 (m, 2H), 1.71-1.62 (m, 3H), 1.62-1.51 (m, 2H); **^{13}C NMR** (100 MHz, CD_2Cl_2) δ 190.1, 156.6, 156.3, 140.9, 139.8, 137.1, 137.0, 126.5, 126.0, 125.9, 125.7, 114.9, 112.7, 96.2, 94.5, 70.2, 70.2, 58.5, 58.4, 51.8, 37.0, 35.7, 35.3, 33.0, 32.3, 30.3, 27.7, 26.3, 23.1, 19.9; **^{19}F NMR** (376 MHz, CD_2Cl_2) δ -79.01; **IR** (KBr): 3056, 2925, 1529, 1451, 1230, 1030, 753, 636 cm^{-1}; **HRMS (ESI)** calcd for $[M-OTf]^+$ $C_{30}H_{34}IrN_2$, m/z: 615.2347, found: 615.2337, Error 1.4 ppm.

3. X-Ray Structural Characterization of 1a, 1b and 1c

3.1. X-Ray ellipsoid plots of 1a (CCDC 1983096)

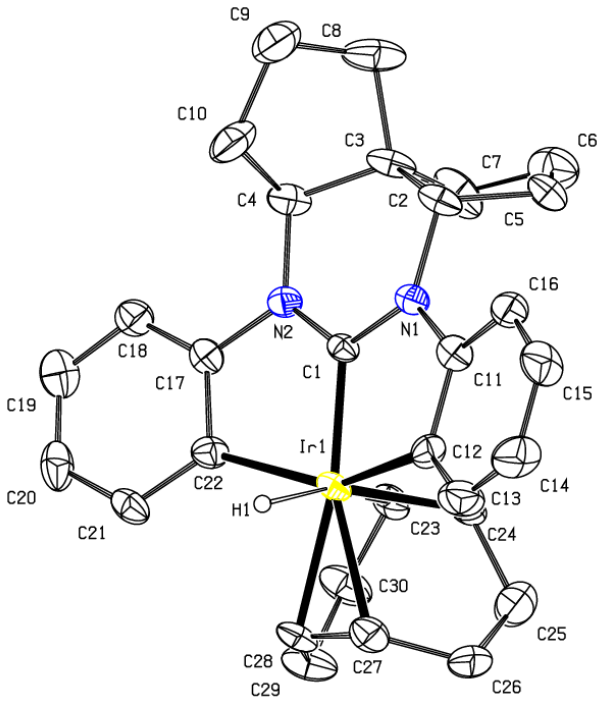


Table S1. Crystal data and structure refinement for **1a** + C_6H_6.

Identification code	**1a** + C_6H_6
Empirical formula	$C_{36}H_{41}IrN_2$
Formula weight	693.91
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.8183(6)
b/Å	19.4005(8)
c/Å	14.7021(7)
α/°	90
β/°	109.184(6)
γ/°	90
Volume/Å^3	2914.3(3)
Z	4
ρ_{calc}g/cm^3	1.582
μ/mm^{-1}	4.609
F(000)	1392.0
Crystal size/mm^3	0.18 × 0.15 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.95 to 52.042
Index ranges	-13 ≤ h ≤ 12, -23 ≤ k ≤ 22, -18 ≤ l ≤ 12

Reflections collected	10587
Independent reflections	5721 [R_{int} = 0.0622, R_{sigma} = 0.1054]
Data/restraints/parameters	5721/12/353
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0559, wR_2 = 0.1063
Final R indexes [all data]	R_1 = 0.0869, wR_2 = 0.1282
Largest diff. peak/hole / e Å^{-3}	1.55/-2.21

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **1a + C_6H_6**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ir1	2425.3(3)	1206.0(2)	2045.8(2)	35.13(14)
N1	3715(7)	1964(3)	3795(5)	36.7(17)
N2	5117(7)	1568(3)	3012(5)	39.1(17)
C1	3907(8)	1635(4)	3044(6)	30.1(19)
C2	4755(10)	2178(4)	4690(6)	45(2)
C3	6067(10)	1879(4)	4725(7)	50(3)
C4	6252(9)	1867(4)	3736(7)	48(2)
C5	4515(11)	1876(5)	5591(7)	58(3)
C6	5550(20)	1343(10)	5982(16)	75(6)
C7	6098(13)	1161(5)	5186(8)	70(4)
C8	7198(11)	2364(5)	5283(9)	80(4)
C9	7406(15)	2871(8)	4544(11)	120(6)
C9B	4980(30)	1089(15)	5620(30)	74(9)
C10	6529(12)	2620(5)	3551(9)	74(4)
C11	2383(9)	2120(4)	3632(7)	40(2)
C12	1455(9)	1831(4)	2781(7)	40(2)
C13	206(11)	2050(5)	2581(8)	63(3)
C14	-196(11)	2529(5)	3133(9)	69(3)
C15	699(11)	2794(5)	3946(8)	63(3)
C16	2005(10)	2605(4)	4196(7)	48(2)
C17	5197(9)	1301(4)	2128(6)	38(2)
C18	6360(10)	1258(4)	1935(7)	48(2)
C19	6360(12)	1014(5)	1058(9)	60(3)
C20	5203(12)	837(5)	388(8)	59(3)
C21	4014(10)	875(4)	575(6)	46(2)
C22	3983(9)	1092(4)	1480(7)	40(2)
C23	3178(10)	171(4)	2652(6)	45(2)
C24	2256(10)	363(4)	3070(7)	46(2)

C25	878(12)	56(6)	2773(9)	80(4)
C26	-111(11)	377(6)	1909(8)	69(3)
C27	460(10)	795(5)	1284(7)	51(3)
C28	1305(10)	521(5)	846(7)	52(3)
C29	1798(11)	-214(4)	960(8)	61(3)
C30	2937(12)	-365(5)	1860(7)	67(3)
C31	2524(13)	215(5)	6509(13)	115(6)
C32	2748(12)	664(10)	7284(8)	152(8)
C33	2147(18)	1307(8)	7152(13)	161(10)
C34	1320(15)	1500(5)	6246(17)	138(9)
C35	1096(11)	1051(9)	5472(11)	143(7)
C36	1697(14)	409(7)	5603(9)	115(6)

Table S3. Anisotropic Displacement Parameters ($Å^2×10^3$) for **1a + C_6H_6**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Ir1	37.1(2)	37.7(2)	23.8(2)	-0.76(15)	0.77(15)	2.57(16)
N1	39(5)	36(4)	32(4)	-3(3)	7(4)	-2(3)
N2	30(4)	48(4)	36(4)	-1(4)	6(3)	-2(3)
C1	39(5)	21(4)	28(5)	-3(3)	8(4)	0(4)
C2	53(7)	38(5)	33(6)	-10(4)	-3(5)	6(4)
C3	46(6)	43(5)	41(6)	-13(5)	-12(5)	7(4)
C4	32(6)	55(6)	51(7)	-21(5)	7(5)	6(4)
C5	61(8)	76(7)	28(6)	0(5)	2(5)	-5(6)
C6	79(10)	66(9)	69(10)	3(8)	8(8)	-1(8)
C7	98(10)	61(7)	36(6)	18(5)	0(6)	36(6)
C8	37(7)	83(8)	96(11)	-40(7)	-10(6)	7(6)
C9	116(14)	147(12)	129(15)	-82(11)	86(12)	-86(11)
C9B	68(12)	72(12)	73(13)	5(9)	13(9)	-5(9)
C10	66(8)	59(7)	110(11)	-22(7)	49(8)	-27(6)
C11	41(6)	35(5)	39(6)	4(4)	9(5)	9(4)
C12	26(5)	49(5)	46(6)	1(4)	12(4)	2(4)
C13	45(7)	82(7)	54(7)	-10(6)	3(5)	-4(6)
C14	34(6)	85(8)	90(10)	-21(7)	24(6)	6(6)
C15	62(8)	74(7)	61(8)	-20(6)	31(6)	13(6)
C16	55(7)	43(5)	51(7)	-13(5)	23(5)	-7(5)
C17	41(6)	35(5)	34(5)	7(4)	8(4)	9(4)
C18	43(6)	52(6)	43(6)	7(5)	6(5)	3(5)
C19	71(9)	55(6)	61(8)	5(6)	31(7)	16(6)

C20	87(9)	47(6)	61(8)	-1(5)	50(7)	7(6)
C21	59(7)	44(5)	28(5)	3(4)	3(5)	4(5)
C22	41(6)	34(5)	44(6)	-10(4)	13(5)	0(4)
C23	53(7)	44(5)	27(5)	12(4)	-2(5)	5(5)
C24	54(7)	45(5)	28(5)	3(4)	0(5)	-7(5)
C25	65(9)	102(9)	72(9)	16(7)	19(7)	-21(7)
C26	46(7)	95(8)	55(8)	-4(6)	1(6)	-26(6)
C27	45(6)	61(6)	36(6)	8(5)	-1(5)	3(5)
C28	52(7)	67(6)	26(5)	-10(5)	-4(5)	-8(5)
C29	65(8)	36(5)	61(7)	-15(5)	-7(6)	13(5)
C30	95(10)	39(6)	47(7)	-7(5)	-1(6)	10(6)
C31	167(19)	81(10)	112(14)	28(11)	66(14)	8(10)
C32	190(20)	160(18)	109(17)	9(15)	60(15)	-54(18)
C33	230(30)	134(18)	160(30)	-56(15)	120(20)	-56(17)
C34	160(20)	83(11)	200(30)	-17(15)	110(20)	-4(12)
C35	107(16)	159(17)	160(20)	57(17)	38(14)	-1(14)
C36	170(19)	93(11)	91(14)	14(9)	55(13)	-3(11)

Table S4. Bond Lengths for **1a** + C_6H_6.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ir1	C1	1.967(8)	C12	C13	1.353(13)
Ir1	C12	2.118(8)	C13	C14	1.395(13)
Ir1	C22	2.123(9)	C14	C15	1.368(14)
Ir1	C23	2.239(8)	C15	C16	1.388(14)
Ir1	C24	2.271(8)	C16	C11	1.400(11)
Ir1	C27	2.201(10)	C17	C18	1.381(12)
Ir1	C28	2.223(9)	C17	C22	1.405(12)
N1	C1	1.349(10)	C18	C19	1.374(13)
N1	C2	1.482(11)	C19	C20	1.358(15)
N1	C11	1.414(11)	C20	C21	1.403(13)
N2	C1	1.333(10)	C21	C22	1.405(12)
N2	C4	1.456(11)	C23	C24	1.384(12)
N2	C17	1.427(11)	C23	C30	1.518(12)
C2	C3	1.519(13)	C24	C25	1.530(14)
C2	C5	1.546(12)	C25	C26	1.501(14)
C3	C4	1.532(12)	C26	C27	1.503(13)
C3	C8	1.548(13)	C27	C28	1.385(13)
C5	C6	1.49(2)	C28	C29	1.513(12)
C5	C9B	1.60(3)	C29	C30	1.511(13)

C7	C3	1.543(12)	C31	C36	1.3900
C7	C6	1.52(2)	C32	C31	1.3900
C8	C9	1.537(17)	C33	C32	1.3900
C9	C10	1.536(17)	C34	C33	1.3900
C9B	C7	1.55(3)	C34	C35	1.3900
C10	C4	1.533(12)	C36	C35	1.3900
C12	C11	1.436(12)			

Table S5. Bond Angles for **1a** + C_6H_6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	Ir1	C12	78.2(3)	C9	C8	C3	106.8(10)
C1	Ir1	C22	77.3(3)	C10	C9	C8	106.3(10)
C1	Ir1	C23	89.0(3)	C7	C9B	C5	100.7(17)
C1	Ir1	C24	91.9(3)	C4	C10	C9	103.3(10)
C1	Ir1	C27	161.2(4)	N1	C11	C12	116.5(7)
C1	Ir1	C28	160.6(4)	C16	C11	N1	121.5(8)
C12	Ir1	C22	148.3(3)	C16	C11	C12	121.5(9)
C12	Ir1	C23	119.1(3)	C11	C12	Ir1	110.3(6)
C12	Ir1	C24	85.0(3)	C13	C12	Ir1	134.0(8)
C12	Ir1	C27	84.8(4)	C13	C12	C11	115.4(8)
C12	Ir1	C28	121.0(4)	C12	C13	C14	124.2(10)
C22	Ir1	C23	80.2(3)	C15	C14	C13	119.5(10)
C22	Ir1	C24	115.6(3)	C14	C15	C16	119.9(9)
C22	Ir1	C27	121.4(4)	C15	C16	C11	119.4(9)
C22	Ir1	C28	85.6(4)	C18	C17	N2	122.7(9)
C23	Ir1	C24	35.7(3)	C18	C17	C22	123.7(9)
C27	Ir1	C23	92.4(4)	C22	C17	N2	113.6(8)
C27	Ir1	C24	78.6(3)	C19	C18	C17	119.7(10)
C27	Ir1	C28	36.5(3)	C20	C19	C18	118.9(11)
C28	Ir1	C23	79.1(3)	C19	C20	C21	122.0(10)
C28	Ir1	C24	87.3(3)	C20	C21	C22	120.7(10)
C1	N1	C2	125.7(8)	C17	C22	Ir1	112.9(6)
C1	N1	C11	112.6(7)	C21	C22	Ir1	132.1(7)
C11	N1	C2	121.6(7)	C21	C22	C17	114.9(8)
C1	N2	C4	122.5(7)	C24	C23	Ir1	73.4(5)
C1	N2	C17	115.0(7)	C24	C23	C30	123.9(9)
C17	N2	C4	121.4(7)	C30	C23	Ir1	111.1(6)
N1	C1	Ir1	120.3(6)	C23	C24	Ir1	70.9(5)
N2	C1	Ir1	120.1(6)	C23	C24	C25	123.1(9)

N2	C1	N1	119.5(8)	C25	C24	Ir1	112.0(7)
N1	C2	C3	110.6(7)	C26	C25	C24	115.9(8)
N1	C2	C5	111.3(8)	C25	C26	C27	114.8(9)
C3	C2	C5	104.1(8)	C26	C27	Ir1	114.0(6)
C2	C3	C4	112.7(8)	C28	C27	Ir1	72.6(6)
C2	C3	C7	104.2(9)	C28	C27	C26	123.0(9)
C2	C3	C8	110.7(7)	C27	C28	Ir1	70.9(5)
C4	C3	C7	114.4(8)	C27	C28	C29	125.0(9)
C4	C3	C8	100.6(9)	C29	C28	Ir1	113.3(6)
C7	C3	C8	114.6(9)	C30	C29	C28	115.8(8)
N2	C4	C3	111.0(8)	C29	C30	C23	115.1(8)
N2	C4	C10	114.7(8)	C36	C31	C32	120.0
C3	C4	C10	104.4(7)	C33	C32	C31	120.0
C2	C5	C9B	104.0(14)	C32	C33	C34	120.0
C6	C5	C2	106.2(11)	C33	C34	C35	120.0
C5	C6	C7	107.3(14)	C36	C35	C34	120.0
C3	C7	C9B	110.7(13)	C31	C36	C35	120.0
C6	C7	C3	99.8(10)				

Table S6. Torsion Angles for **1a** + C_6H_6.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ir1	C12	C11	N1	2.3(9)	C7	C3	C8	C9	153.8(10)
Ir1	C12	C11	C16	173.8(7)	C8	C3	C4	N2	-166.9(7)
Ir1	C12	C13	C14	-172.6(8)	C8	C3	C4	C10	-42.9(9)
Ir1	C23	C24	C25	104.3(9)	C8	C9	C10	C4	-19.1(13)
Ir1	C23	C30	C29	-25.8(12)	C9	C10	C4	N2	160.8(9)
Ir1	C24	C25	C26	-2.6(13)	C9	C10	C4	C3	39.1(11)
Ir1	C27	C28	C29	105.6(9)	C9B	C7	C3	C2	-11.8(18)
Ir1	C28	C29	C30	0.9(13)	C9B	C7	C3	C4	-135.3(17)
N1	C2	C3	C4	37.6(10)	C9B	C7	C3	C8	109.3(18)
N1	C2	C3	C7	-87.0(9)	C11	N1	C1	Ir1	-16.2(9)
N1	C2	C3	C8	149.4(8)	C11	N1	C1	N2	167.6(7)
N1	C2	C5	C6	109.7(12)	C11	N1	C2	C3	173.8(7)
N1	C2	C5	C9B	77.6(15)	C11	N1	C2	C5	58.6(10)
N2	C17	C18	C19	-178.2(8)	C11	C12	C13	C14	0.9(15)
N2	C17	C22	Ir1	-2.1(9)	C12	C13	C14	C15	-1.6(18)
N2	C17	C22	C21	175.5(7)	C13	C12	C11	N1	-172.7(8)
C1	N1	C2	C3	-8.8(12)	C13	C12	C11	C16	-1.2(13)
C1	N1	C2	C5	-124.0(9)	C13	C14	C15	C16	2.4(17)

C1	N1	C11	C12	8.0(10)	C14	C15	C16	C11	-2.7(16)
C1	N1	C11	C16	-163.5(8)	C15	C16	C11	N1	173.2(8)
C1	N2	C4	C3	32.4(11)	C15	C16	C11	C12	2.1(14)
C1	N2	C4	C10	-85.6(10)	C17	N2	C1	Ir1	12.4(9)
C1	N2	C17	C18	173.8(7)	C17	N2	C1	N1	-171.4(7)
C1	N2	C17	C22	-6.0(10)	C17	N2	C4	C3	-160.0(7)
C2	N1	C1	Ir1	166.3(6)	C17	N2	C4	C10	82.0(10)
C2	N1	C1	N2	-9.9(12)	C17	C18	C19	C20	1.8(14)
C2	N1	C11	C12	-174.3(7)	C18	C17	C22	Ir1	178.1(6)
C2	N1	C11	C16	14.2(12)	C18	C17	C22	C21	-4.3(12)
C2	C3	C4	N2	-49.1(10)	C18	C19	C20	C21	-2.1(15)
C2	C3	C4	C10	75.0(10)	C19	C20	C21	C22	-0.8(14)
C2	C3	C8	C9	-88.8(11)	C20	C21	C22	Ir1	-179.2(6)
C2	C5	C6	C7	-17.8(17)	C20	C21	C22	C17	3.9(12)
C2	C5	C9B	C7	33(2)	C22	C17	C18	C19	1.6(13)
C3	C2	C5	C6	-9.5(12)	C23	C24	C25	C26	-83.5(14)
C3	C2	C5	C9B	-41.5(15)	C24	C23	C30	C29	57.9(13)
C3	C7	C6	C5	37.0(16)	C24	C25	C26	C27	17.9(16)
C3	C8	C9	C10	-7.3(13)	C25	C26	C27	Ir1	-25.0(13)
C4	N2	C1	Ir1	-179.3(6)	C25	C26	C27	C28	59.2(14)
C4	N2	C1	N1	-3.1(12)	C26	C27	C28	Ir1	-107.8(9)
C4	N2	C17	C18	5.4(12)	C26	C27	C28	C29	-2.2(15)
C4	N2	C17	C22	-174.4(7)	C27	C28	C29	C30	-81.4(14)
C4	C3	C8	C9	30.5(11)	C28	C29	C30	C23	16.8(15)
C5	C2	C3	C4	157.2(7)	C30	C23	C24	Ir1	-104.7(8)
C5	C2	C3	C7	32.6(9)	C30	C23	C24	C25	-0.4(14)
C5	C2	C3	C8	-91.0(10)	C31	C36	C35	C34	0.0
C5	C9B	C7	C3	-13(2)	C32	C31	C36	C35	0.0
C6	C7	C3	C2	-42.6(13)	C33	C32	C31	C36	0.0
C6	C7	C3	C4	-166.0(12)	C33	C34	C35	C36	0.0
C6	C7	C3	C8	78.5(14)	C34	C33	C32	C31	0.0
C7	C3	C4	N2	69.7(11)	C35	C34	C33	C32	0.0
C7	C3	C4	C10	-166.3(9)					

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **1a** + C_6H_6.

Atom	***x***	***y***	***z***	**U(eq)**
H1	1750(70)	1890(30)	1200(50)	30(20)
H7	4806.47	2682	4732.35	54

H15	7025.24	1588.83	3778.08	57
H8AA	4581.82	2234.3	6065.06	69
H8AB	3651.53	1670.42	5418.58	69
H8BC	3596.98	1903.88	5532.32	69
H8BD	5027.89	2118.65	6168.76	69
H9A	5174.34	937.45	6177.84	90
H9B	6233.23	1521.89	6538.07	90
H10A	5547.41	833.25	4734.26	84
H10B	6981.67	981.13	5441.68	84
H10C	6932.8	1095.79	5690.02	84
H10D	6009.76	807.53	4702.35	84
H12A	6971.91	2610.6	5780.2	96
H12B	7989.97	2100.68	5584.97	96
H13A	7160.91	3334.28	4666.04	143
H13B	8316.53	2874.21	4577.33	143
H9BA	5292.23	910.12	6267.9	88
H9BB	4280.36	796.1	5221.41	88
H14A	5725.88	2884.72	3325.18	88
H14B	6979.66	2650.98	3080.04	88
H2	-424.32	1868.52	2039.73	76
H3	-1066.74	2667.75	2948.86	82
H4	432.72	3100.82	4331.71	75
H5	2624.25	2797.73	4732.94	58
H18	7140.22	1393.09	2397.07	57
H19	7139.9	969.87	925.27	72
H20	5198.43	686.63	-213.71	70
H21	3238.85	756.14	96.37	56
H23	4079.99	178.25	3096.36	54
H24	2622.2	484.01	3753.46	55
H25A	936.75	-431.31	2644.73	97
H25B	556.58	94.55	3314.17	97
H26A	-681.4	671.68	2127.87	83
H26B	-647.1	13.58	1521.02	83
H27	-144.65	1138.71	889.43	61
H28	1183.63	714.36	206.85	63
H29A	1078.88	-515.57	950.99	73
H29B	2055.12	-330.28	405.32	73
H30A	3723.14	-407.23	1684.12	80
H30B	2786.76	-806.71	2114.31	80
H31	2926.19	-214.67	6597.45	138

H32	3301.38	534.65	7890	182
H33	2297.22	1607.05	7670.32	193
H34	917.86	1930.13	6158.08	165
H35	542.66	1180.8	4865.5	172
H36	1546.83	108.4	5085.2	139

Table S8. Atomic Occupancy for **1a** + C_6H_6.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
H8AA	0.6	H8AB	0.6	H8BC	0.4
H8BD	0.4	C6	0.6	H9A	0.6
H9B	0.6	H10A	0.6	H10B	0.6
H10C	0.4	H10D	0.4	C9B	0.4
H9BA	0.4	H9BB	0.4		

3.2. X-Ray ellipsoid plots of 1b (CCDC 1983099)

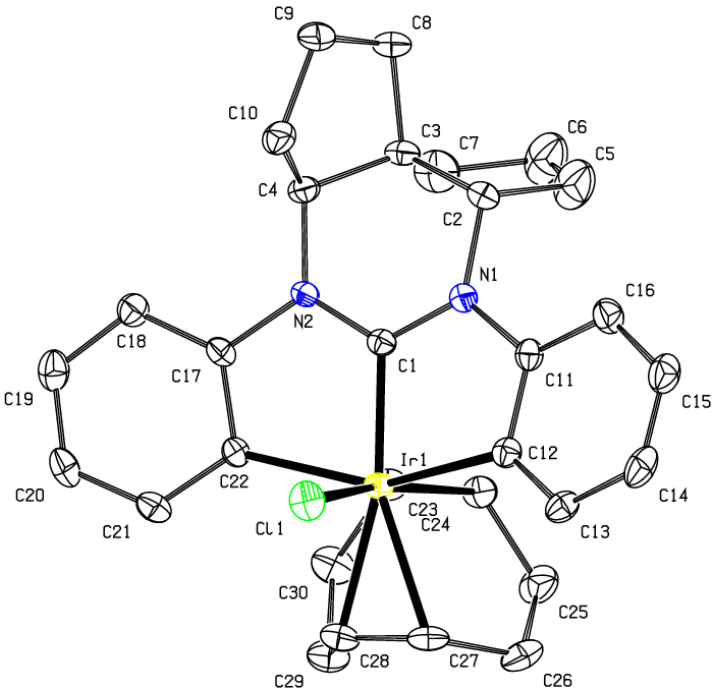


Table S9. Crystal data and structure refinement for **1b + $CHCl_3$**.

Identification code	**1b + $CHCl_3$**
Empirical formula	$C_{31}H_{34}Cl_4IrN_2$
Formula weight	768.60
Temperature/K	296(2)
Crystal system	monoclinic
Space group	Cc
a/Å	18.647(4)
b/Å	15.011(3)
c/Å	10.569(2)
α/°	90
β/°	98.716(3)
γ/°	90
Volume/$Å^3$	2924.1(11)
Z	4
$\rho_{calc}g/cm^3$	1.746
μ/mm^{-1}	4.956
F(000)	1516.0
Crystal size/mm^3	0.300 × 0.200 × 0.200
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.5 to 49.998
Index ranges	$-22 \le h \le 21$, $-9 \le k \le 17$, $-12 \le l \le 12$
Reflections collected	7110
Independent reflections	4786 [R_{int} = 0.0177, R_{sigma} = 0.0568]

Data/restraints/parameters	4786/15/344
Goodness-of-fit on F^2	0.909
Final R indexes [I>=2σ (I)]	$R_1 = 0.0213$, $wR_2 = 0.0514$
Final R indexes [all data]	$R_1 = 0.0225$, $wR_2 = 0.0521$
Largest diff. peak/hole / e $Å^{-3}$	0.85/-1.17
Flack parameter	0.014(10)

Table S10. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **1b + $CHCl_3$**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Ir1	59.3(3)	2657.1(2)	5920.6(3)	23.96(8)
C1	536(3)	2164(5)	7600(7)	25.3(15)
C2	1317(5)	2477(5)	9683(8)	34.7(18)
C3	854(4)	1748(5)	10203(6)	32.2(16)
C4	629(4)	1013(5)	9245(6)	33.2(16)
C5	-460(3)	1405(5)	5971(6)	26.1(14)
C6	-205(3)	926(5)	7108(6)	28.7(15)
C7	-920(4)	-354(6)	6417(8)	42.9(19)
C8	-1173(4)	83(6)	5304(8)	41.3(18)
C9	-954(4)	941(5)	5092(7)	35.1(17)
C10	1340(4)	4044(5)	5633(7)	34.4(16)
C11	993(3)	3483(5)	6381(7)	28.7(15)
C12	1350(4)	3324(5)	7625(7)	28.9(16)
C13	1990(4)	4477(5)	6129(9)	45(2)
C14	-609(5)	4565(6)	6097(8)	52(2)
C15	-871(4)	2995(6)	6835(7)	33.7(16)
C16	-1583(4)	2900(7)	5944(8)	46(2)
C17	-1522(4)	3091(7)	4541(8)	44(2)
C19	-761(4)	2941(7)	4203(8)	37.5(18)
C20	-248(4)	3611(6)	4291(7)	38.2(18)
C21	-380(4)	4545(6)	4754(8)	45(2)
C22	2303(4)	4350(6)	7355(8)	45(2)
C23	1990(4)	3766(5)	8119(8)	40.3(18)
C24	-408(4)	66(5)	7340(7)	35.2(17)
C25	-414(4)	3723(5)	6896(7)	35.0(17)
C26	251(6)	2273(6)	10693(12)	60(3)
C27	637(7)	3129(7)	11223(11)	79(2)
C28	1220(7)	3302(7)	10504(10)	75(2)
C29	1338(4)	1225(6)	11278(7)	44.3(19)

C30	1650(5)	434(6)	10641(8)	52(2)
C31	1314(4)	461(5)	9228(7)	40.7(18)
C34	7649(5)	3003(9)	-257(10)	64(3)
Cl1	780.7(9)	1855.2(13)	4604.5(17)	39.7(4)
Cl2	7883.1(17)	3974(2)	-1047(3)	81.1(8)
Cl3	7814(2)	2059(3)	-1129(4)	98.8(11)
Cl5	8141(4)	2971(5)	1272(4)	180(3)
N1	1040(3)	2652(4)	8314(7)	29.0(14)
N2	317(3)	1394(4)	8013(5)	28.0(12)

Table S11. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **1b + $CHCl_3$**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Ir1	22.18(11)	28.34(13)	21.63(12)	1.5(3)	4.22(7)	1.4(3)
C1	24(3)	27(4)	24(4)	-1(3)	3(3)	4(3)
C2	37(4)	38(4)	27(4)	0(3)	-4(3)	-2(3)
C3	35(4)	39(4)	22(3)	4(3)	1(3)	7(3)
C4	34(4)	33(4)	31(4)	9(3)	-1(3)	-3(3)
C5	18(3)	30(4)	30(4)	-1(3)	3(3)	-3(3)
C6	25(3)	35(4)	25(3)	-3(3)	2(3)	-4(3)
C7	45(5)	38(5)	48(5)	-6(4)	16(4)	-11(4)
C8	35(4)	47(5)	41(4)	-13(4)	4(3)	-13(4)
C9	33(4)	47(5)	25(4)	-3(3)	3(3)	-2(3)
C10	33(4)	33(4)	39(4)	9(3)	10(3)	0(3)
C11	26(3)	27(4)	33(4)	0(3)	5(3)	3(3)
C12	28(4)	26(4)	33(4)	-3(3)	7(3)	0(3)
C13	36(4)	32(4)	70(6)	12(4)	17(4)	-7(3)
C14	65(5)	36(5)	55(5)	1(4)	11(4)	16(4)
C15	29(4)	44(4)	30(4)	1(3)	13(3)	10(3)
C16	26(4)	66(6)	47(5)	-2(4)	8(3)	6(4)
C17	32(4)	59(6)	39(5)	6(4)	4(4)	7(4)
C19	37(4)	51(5)	23(4)	2(4)	2(3)	6(4)
C20	39(4)	53(5)	23(4)	12(3)	4(3)	9(4)
C21	41(4)	43(5)	53(5)	22(4)	8(4)	11(4)
C22	36(4)	35(4)	64(6)	3(4)	4(4)	-7(3)
C23	36(4)	37(4)	45(5)	-4(3)	-2(3)	-5(3)
C24	35(4)	37(4)	35(4)	2(3)	8(3)	-7(3)
C25	46(4)	33(4)	28(4)	-5(3)	10(3)	13(3)
C26	67(8)	63(6)	51(7)	-8(5)	16(5)	17(5)

C27	128(7)	50(4)	67(5)	-11(4)	39(4)	5(5)
C28	124(7)	46(4)	60(5)	-11(4)	34(4)	5(5)
C29	54(5)	48(5)	27(4)	11(3)	-5(3)	2(4)
C30	55(5)	43(5)	48(5)	6(4)	-21(4)	9(4)
C31	51(5)	30(4)	40(4)	0(3)	5(3)	8(3)
C34	39(5)	104(9)	51(6)	2(6)	10(4)	-1(5)
Cl1	36.1(9)	43.6(12)	42.8(10)	-8.7(8)	16.5(8)	3.3(8)
Cl2	99.1(19)	75.5(19)	67.8(17)	-8.0(14)	10.1(14)	-1.2(16)
Cl3	129(3)	73.0(19)	105(3)	10(2)	51(2)	-3(2)
Cl5	248(7)	223(6)	52(2)	30(3)	-31(3)	-11(6)
N1	30(3)	28(3)	28(4)	0(3)	2(3)	-3(2)
N2	30(3)	30(3)	22(3)	2(2)	-2(2)	-5(2)

Table S12. Bond Lengths for **1b + $CHCl_3$**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ir1	C1	2.003(7)	C8	C9	1.380(12)
Ir1	C5	2.119(7)	C10	C11	1.381(10)
Ir1	C11	2.132(7)	C10	C13	1.406(10)
Ir1	C15	2.169(7)	C11	C12	1.401(10)
Ir1	C19	2.230(8)	C12	C23	1.395(10)
Ir1	C20	2.247(7)	C12	N1	1.418(10)
Ir1	C25	2.163(7)	C13	C22	1.351(11)
Ir1	Cl1	2.4000(18)	C14	C21	1.544(12)
C1	N1	1.333(9)	C14	C25	1.532(11)
C1	N2	1.322(9)	C15	C16	1.513(10)
C2	C3	1.546(11)	C15	C25	1.382(11)
C2	C28	1.538(12)	C16	C17	1.532(12)
C2	N1	1.484(11)	C17	C19	1.532(11)
C3	C4	1.513(10)	C19	C20	1.381(12)
C3	C26	1.527(12)	C20	C21	1.516(12)
C3	C29	1.552(9)	C22	C23	1.380(11)
C4	C31	1.525(10)	C26	C27	1.537(16)
C4	N2	1.459(8)	C27	C28	1.441(17)
C5	C6	1.419(9)	C29	C30	1.524(12)
C5	C9	1.393(9)	C30	C31	1.530(10)
C6	C24	1.378(10)	C34	Cl2	1.767(12)
C6	N2	1.439(8)	C34	Cl3	1.742(13)
C7	C8	1.367(11)	C34	Cl5	1.733(10)
C7	C24	1.406(10)			

Table S13. Bond Angles for **1b + $CHCl_3$**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	Ir1	C5	78.0(3)	C24	C6	C5	124.0(6)
C1	Ir1	C11	77.0(3)	C24	C6	N2	121.0(6)
C1	Ir1	C15	88.2(3)	C8	C7	C24	119.5(7)
C1	Ir1	C19	161.7(3)	C7	C8	C9	121.0(7)
C1	Ir1	C20	160.5(3)	C8	C9	C5	122.7(7)
C1	Ir1	C25	90.5(3)	C11	C10	C13	121.4(7)
C1	Ir1	Cl1	96.7(2)	C10	C11	Ir1	131.4(5)
C5	Ir1	C11	150.5(3)	C10	C11	C12	116.3(6)
C5	Ir1	C15	78.3(3)	C12	C11	Ir1	111.8(5)
C5	Ir1	C19	86.0(3)	C11	C12	N1	115.5(6)
C5	Ir1	C20	121.4(3)	C23	C12	C11	121.9(7)
C5	Ir1	C25	115.1(3)	C23	C12	N1	122.5(7)
C5	Ir1	Cl1	82.43(19)	C22	C13	C10	121.0(7)
C11	Ir1	C15	116.3(3)	C25	C14	C21	114.5(7)
C11	Ir1	C19	120.7(3)	C16	C15	Ir1	112.7(5)
C11	Ir1	C20	84.8(3)	C25	C15	Ir1	71.1(4)
C11	Ir1	C25	80.7(3)	C25	C15	C16	125.4(7)
C11	Ir1	Cl1	85.07(19)	C15	C16	C17	113.4(7)
C15	Ir1	C19	79.8(3)	C16	C17	C19	114.0(6)
C15	Ir1	C20	93.7(3)	C17	C19	Ir1	112.5(5)
C15	Ir1	Cl1	158.7(2)	C20	C19	Ir1	72.7(4)
C19	Ir1	C20	35.9(3)	C20	C19	C17	122.2(9)
C19	Ir1	Cl1	90.0(2)	C19	C20	Ir1	71.4(5)
C20	Ir1	Cl1	88.6(2)	C19	C20	C21	123.5(7)
C25	Ir1	C15	37.2(3)	C21	C20	Ir1	112.1(5)
C25	Ir1	C19	88.2(3)	C20	C21	C14	113.3(7)
C25	Ir1	C20	79.5(3)	C13	C22	C23	119.5(7)
C25	Ir1	Cl1	162.2(2)	C22	C23	C12	119.7(7)
N1	C1	Ir1	118.6(5)	C6	C24	C7	118.2(7)
N2	C1	Ir1	119.9(5)	C14	C25	Ir1	115.3(5)
N2	C1	N1	121.4(6)	C15	C25	Ir1	71.7(4)
C28	C2	C3	104.5(7)	C15	C25	C14	122.3(7)
N1	C2	C3	110.0(6)	C3	C26	C27	103.1(9)
N1	C2	C28	110.8(7)	C28	C27	C26	107.9(9)
C2	C3	C29	109.0(6)	C27	C28	C2	108.4(9)
C4	C3	C2	113.0(6)	C30	C29	C3	106.8(6)

C4	C3	C26	117.3(7)	C29	C30	C31	106.4(6)
C4	C3	C29	101.1(6)	C4	C31	C30	102.9(6)
C26	C3	C2	103.6(7)	Cl3	C34	Cl2	110.2(6)
C26	C3	C29	112.9(7)	Cl5	C34	Cl2	109.2(6)
C3	C4	C31	104.8(5)	Cl5	C34	Cl3	111.1(7)
N2	C4	C3	110.2(6)	C1	N1	C2	124.5(6)
N2	C4	C31	115.1(6)	C1	N1	C12	114.1(7)
C6	C5	Ir1	112.1(4)	C12	N1	C2	121.2(6)
C9	C5	Ir1	133.3(5)	C1	N2	C4	122.3(5)
C9	C5	C6	114.5(6)	C1	N2	C6	114.8(5)
C5	C6	N2	114.9(6)	C6	N2	C4	122.7(6)

Table S14. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **1b + CHCl$_3$**.

Atom	***x***	***y***	***z***	**U(eq)**
H2	1828	2299	9790	42
H4	263	642	9562	40
H7	-1085	-924	6562	52
H8	-1499	-202	4680	50
H9	-1144	1221	4329	42
H10	1139	4137	4783	41
H13	2209	4857	5606	54
H14A	-380	5073	6562	62
H14B	-1129	4653	6002	62
H16A	-1934	3307	6218	56
H16B	-1764	2299	6012	56
H17A	-1662	3704	4350	52
H17B	-1861	2712	4002	52
H19	-745	2529	3488	45
H20	68	3586	3631	46
H21A	-756	4825	4149	54
H21B	61	4891	4770	54
H22	2726	4653	7681	54
H23	2204	3667	8961	48
H24	-212	-229	8086	42
H25	-156	3844	7758	42
H26A	58	1948	11360	72
H26B	-141	2405	10005	72
H27A	299	3624	11136	95

H27B	828	3056	12123	95
H28A	1665	3422	11082	90
H28B	1106	3819	9959	90
H29A	1725	1602	11696	53
H29B	1051	1021	11915	53
H30A	1528	-120	11030	62
H30B	2175	480	10728	62
H31A	1638	745	8713	49
H31B	1198	-133	8899	49
H34	7131	3026	-190	77

3.3. X-Ray ellipsoid plots of 1c (CCDC 1983097)

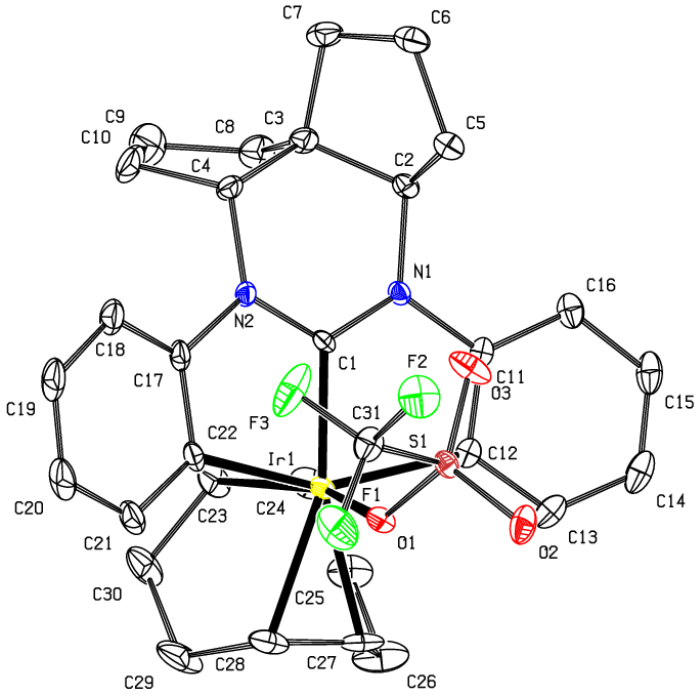


Table S15. Crystal data and structure refinement for **1c**.

Identification code	**1c**
Empirical formula	$C_{31}H_{34}F_3IrN_2O_3S$
Formula weight	763.86
Temperature/K	173.20(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.7644(2)
b/Å	10.27886(12)
c/Å	19.8174(3)
α/°	90
β/°	110.7333(17)
γ/°	90
Volume/Å^3	2812.74(7)
Z	4
ρ_{calc}g/cm^3	1.804
μ/mm^{-1}	10.372
F(000)	1512.0
Crystal size/mm^3	0.07 × 0.05 × 0.04
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.424 to 141.36
Index ranges	-15 ≤ h ≤ 18, -8 ≤ k ≤ 12, -24 ≤ l ≤ 16
Reflections collected	9997
Independent reflections	5316 [R_{int} = 0.0231, R_{sigma} = 0.0305]

Data/restraints/parameters	5316/0/370
Goodness-of-fit on F^2	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0278, wR_2 = 0.0711
Final R indexes [all data]	R_1 = 0.0296, wR_2 = 0.0729
Largest diff. peak/hole / e Å^{-3}	1.10/-1.60

Table S16. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **1c**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ir1	3137.0(2)	6362.8(2)	2797.9(2)	17.54(7)
S1	2380.1(6)	9410.7(8)	2407.6(4)	20.20(17)
F1	3770(2)	10989(3)	3149.7(16)	52.8(7)
F2	2342(2)	11562(2)	3085.7(15)	44.9(6)
F3	3069(3)	10004(3)	3781.2(12)	59.9(9)
O1	3133.0(17)	8395(2)	2549.4(13)	20.8(5)
O2	2307(2)	10158(3)	1783.3(14)	36.0(7)
O3	1509(2)	9013(3)	2506.2(19)	38.5(7)
N1	1217(2)	6072(3)	2858.8(14)	17.8(6)
N2	2398(2)	6556(3)	3969.9(14)	19.3(6)
C1	2125(3)	6348(3)	3254.4(19)	16.6(7)
C2	442(2)	6084(4)	3161.0(18)	21.9(7)
C3	834(3)	5651(4)	3951.4(18)	24.9(8)
C4	1774(3)	6371(4)	4398.2(18)	25.1(8)
C5	-10(3)	7420(4)	3163(2)	29.4(8)
C6	-476(3)	7278(4)	3740(2)	33.0(9)
C7	3(3)	6080(4)	4203(2)	33.3(9)
C8	1105(3)	4209(4)	4054(2)	36.4(9)
C9	1849(4)	4097(5)	4811(3)	51.0(12)
C10	2243(3)	5444(5)	5039(2)	46.7(12)
C11	1015(3)	6047(3)	2099.9(17)	20.7(7)
C12	1815(3)	6215(3)	1890.4(18)	20.9(7)
C13	1625(4)	6331(4)	1154(2)	31.4(9)
C14	692(4)	6222(4)	656(2)	37.9(10)
C15	-78(3)	6007(4)	879(2)	35.4(9)
C16	69(3)	5931(4)	1610.8(19)	27.9(8)
C17	3352(2)	7083(4)	4289.3(17)	23.6(7)
C18	3652(3)	7692(4)	4957.7(19)	33.9(9)
C19	4562(3)	8243(5)	5226(2)	41.8(11)
C20	5163(3)	8162(5)	4832(2)	43.2(11)

C21	4856(3)	7578(4)	4159(2)	35.5(9)
C22	3930(2)	7027(4)	3861.3(18)	23.0(7)
C23	3871(3)	6093(4)	1994(2)	33.7(9)
C24	4574(3)	6322(4)	2663(3)	35(1)
C25	5215(3)	5223(5)	3086(3)	57.8(15)
C26	4770(3)	4403(4)	3515(3)	42.0(11)
C27	3695(3)	4557(4)	3333(2)	31.4(9)
C28	2991(3)	4295(4)	2643(2)	29.9(8)
C29	3239(4)	3784(4)	2009(3)	42.2(11)
C30	3693(4)	4761(4)	1652(3)	53.9(14)
C31	2931(3)	10543(4)	3149(2)	30.4(8)

Table S17. Anisotropic Displacement Parameters ($Å^2×10^3$) for **1c**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir1	15.15(10)	13.9(1)	25.41(9)	4.40(5)	9.45(7)	2.25(5)
S1	16.8(4)	16.1(4)	25.3(4)	2.5(3)	4.5(3)	2.1(3)
F1	35.1(15)	50.8(17)	61.9(17)	-18.3(14)	4.3(13)	-17.5(13)
F2	57.2(17)	20.9(12)	56.5(15)	-7.5(11)	19.9(14)	8.0(12)
F3	111(3)	41.5(16)	23.8(11)	2.4(11)	19.2(14)	15.1(17)
O1	19.5(12)	11.8(11)	32.3(13)	4.9(10)	10.7(10)	1.6(10)
O2	44.4(17)	32.2(16)	25.6(12)	9.4(12)	5.3(12)	10.2(13)
O3	22.5(14)	22.7(14)	73(2)	0.6(14)	20.6(14)	1.2(12)
N1	13.9(14)	20.7(14)	17.1(12)	-2.5(11)	3.6(11)	-1.3(12)
N2	15.8(14)	25.0(15)	14.7(12)	2.8(11)	2.4(11)	-3.8(12)
C1	10.9(16)	16.1(17)	22.3(16)	3.2(12)	5.1(13)	1.4(12)
C2	14.7(16)	26.1(18)	24.0(16)	-3.4(14)	5.6(13)	-8.7(14)
C3	24.3(18)	25.6(19)	26.3(16)	1.6(14)	10.9(14)	-7.1(15)
C4	23.3(19)	35(2)	17.9(15)	1.5(14)	8.2(14)	-8.5(15)
C5	22.6(19)	34(2)	32.8(18)	0.8(16)	10.9(15)	2.2(16)
C6	25(2)	40(2)	38(2)	-11.1(18)	16.0(17)	-4.2(18)
C7	32(2)	42(2)	33.0(19)	-6.9(18)	19.5(17)	-13.7(19)
C8	42(2)	29(2)	41(2)	7.2(18)	18.6(19)	-5.1(19)
C9	55(3)	41(3)	54(3)	17(2)	16(2)	9(2)
C10	47(3)	65(3)	23.9(18)	19(2)	6.6(18)	-15(2)
C11	26.1(18)	14.9(16)	17.8(15)	-0.6(13)	3.7(13)	-0.1(14)
C12	27.9(19)	14.0(16)	19.2(16)	-1.8(12)	6.5(14)	-0.7(14)
C13	48(3)	26(2)	22.5(18)	-1.3(14)	15.3(18)	-2.3(17)
C14	61(3)	28(2)	19.4(17)	-1.6(14)	6.8(18)	0.3(19)

C15	41(2)	28(2)	24.1(17)	-8.2(16)	-4.1(17)	4.2(19)
C16	28(2)	22.8(18)	26.6(17)	-6.2(15)	1.8(15)	1.5(16)
C17	17.9(17)	26.1(18)	19.7(15)	5.7(14)	-2.2(13)	-6.5(15)
C18	30(2)	43(2)	20.8(16)	4.8(16)	-1.3(15)	-8.7(18)
C19	37(2)	49(3)	23.7(18)	5.0(18)	-8.9(17)	-13(2)
C20	24(2)	48(3)	41(2)	13(2)	-8.6(17)	-21(2)
C21	16.8(18)	44(3)	38(2)	14.6(18)	0.0(15)	-5.6(17)
C22	14.8(16)	23.9(18)	24.3(15)	7.1(14)	-0.2(13)	0.4(14)
C23	41(2)	26(2)	53(2)	-1.6(18)	40(2)	-2.0(18)
C24	30(2)	29(2)	59(3)	11.1(18)	30(2)	6.6(16)
C25	31(2)	53(3)	100(4)	34(3)	36(3)	22(2)
C26	25(2)	26(2)	70(3)	15(2)	10(2)	8.8(17)
C27	27(2)	16.3(18)	50(2)	14.7(17)	12.7(17)	8.6(15)
C28	32(2)	8.0(16)	54(2)	3.8(16)	20.0(18)	1.8(15)
C29	53(3)	23(2)	61(3)	-6.2(19)	33(2)	0.7(19)
C30	77(4)	28(2)	82(3)	-16(2)	60(3)	-4(2)
C31	40(2)	20.2(19)	29.0(17)	2.5(15)	10.2(16)	4.8(17)

Table S18. Bond Lengths for **1c**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ir1	O1	2.145(2)	C6	C7	1.548(6)
Ir1	C1	2.002(3)	C7	C3	1.543(5)
Ir1	C12	2.140(4)	C8	C9	1.518(6)
Ir1	C22	2.129(3)	C9	C10	1.508(7)
Ir1	C23	2.238(4)	C10	C4	1.542(5)
Ir1	C24	2.231(4)	C12	C11	1.394(5)
Ir1	C27	2.152(4)	C12	C13	1.391(5)
Ir1	C28	2.147(4)	C13	C14	1.386(7)
S1	O1	1.478(2)	C14	C15	1.376(7)
S1	O2	1.428(3)	C15	C16	1.390(5)
S1	O3	1.427(3)	C16	C11	1.395(5)
S1	C31	1.824(4)	C17	C18	1.389(5)
F1	C31	1.322(5)	C17	C22	1.401(5)
F2	C31	1.339(5)	C18	C19	1.379(6)
F3	C31	1.318(4)	C19	C20	1.376(7)
N1	C1	1.322(5)	C20	C21	1.384(6)
N1	C2	1.467(4)	C21	C22	1.402(5)
N1	C11	1.426(4)	C23	C24	1.383(7)
N2	C1	1.347(4)	C23	C30	1.509(6)

N2	C4	1.470(4)	C24	C25	1.520(6)
N2	C17	1.431(4)	C25	C26	1.503(6)
C2	C3	1.531(5)	C26	C27	1.507(5)
C2	C5	1.527(5)	C27	C28	1.419(6)
C3	C4	1.544(5)	C28	C29	1.521(6)
C3	C8	1.530(5)	C29	C30	1.515(6)
C5	C6	1.536(5)			

Table S19. Bond Angles for **1c**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ir1	C23	85.41(13)	C8	C3	C7	115.7(3)
O1	Ir1	C24	85.20(12)	N2	C4	C3	110.5(3)
O1	Ir1	C27	157.29(13)	N2	C4	C10	111.4(3)
O1	Ir1	C28	159.86(14)	C10	C4	C3	103.1(3)
C1	Ir1	O1	99.75(11)	C2	C5	C6	103.2(3)
C1	Ir1	C12	76.98(14)	C5	C6	C7	106.5(3)
C1	Ir1	C22	78.01(14)	C3	C7	C6	106.6(3)
C1	Ir1	C23	161.33(16)	C9	C8	C3	105.6(4)
C1	Ir1	C24	161.39(17)	C10	C9	C8	107.1(4)
C1	Ir1	C27	89.28(14)	C9	C10	C4	107.9(3)
C1	Ir1	C28	90.22(14)	C12	C11	N1	115.4(3)
C12	Ir1	O1	87.07(11)	C12	C11	C16	123.3(3)
C12	Ir1	C23	85.45(16)	C16	C11	N1	121.2(3)
C12	Ir1	C24	121.38(16)	C11	C12	Ir1	112.0(2)
C12	Ir1	C27	115.38(14)	C13	C12	Ir1	131.4(3)
C12	Ir1	C28	78.12(15)	C13	C12	C11	116.5(4)
C22	Ir1	O1	82.59(12)	C14	C13	C12	121.4(4)
C22	Ir1	C12	150.82(13)	C15	C14	C13	120.7(4)
C22	Ir1	C23	120.58(16)	C14	C15	C16	120.2(4)
C22	Ir1	C24	84.93(16)	C15	C16	C11	117.9(4)
C22	Ir1	C27	78.95(15)	C18	C17	N2	121.6(3)
C22	Ir1	C28	116.79(15)	C18	C17	C22	122.6(3)
C24	Ir1	C23	36.05(17)	C22	C17	N2	115.6(3)
C27	Ir1	C23	92.66(16)	C19	C18	C17	119.4(4)
C27	Ir1	C24	80.12(15)	C20	C19	C18	119.5(4)
C28	Ir1	C23	79.93(15)	C19	C20	C21	121.0(4)
C28	Ir1	C24	90.89(15)	C20	C21	C22	121.3(4)
C28	Ir1	C27	38.55(15)	C17	C22	Ir1	111.9(2)
O1	S1	C31	101.95(17)	C17	C22	C21	116.2(3)

O2	S1	O1	111.49(16)	C21	C22	Ir1	131.2(3)
O2	S1	C31	103.30(18)	C24	C23	Ir1	71.7(2)
O3	S1	O1	115.17(16)	C24	C23	C30	122.5(4)
O3	S1	O2	118.48(19)	C30	C23	Ir1	112.4(3)
O3	S1	C31	103.80(19)	C23	C24	Ir1	72.3(2)
S1	O1	Ir1	132.25(15)	C23	C24	C25	120.7(4)
C1	N1	C2	122.0(3)	C25	C24	Ir1	112.4(3)
C1	N1	C11	114.8(3)	C26	C25	C24	114.7(3)
C11	N1	C2	121.9(3)	C25	C26	C27	116.1(4)
C1	N2	C4	124.9(3)	C26	C27	Ir1	113.3(3)
C1	N2	C17	114.0(3)	C28	C27	Ir1	70.6(2)
C17	N2	C4	120.9(3)	C28	C27	C26	124.1(4)
N1	C1	Ir1	119.7(2)	C27	C28	Ir1	70.9(2)
N1	C1	N2	121.4(3)	C27	C28	C29	123.6(4)
N2	C1	Ir1	118.8(3)	C29	C28	Ir1	114.7(3)
N1	C2	C3	110.4(3)	C30	C29	C28	115.6(4)
N1	C2	C5	114.5(3)	C23	C30	C29	115.3(4)
C5	C2	C3	105.4(3)	F1	C31	S1	111.9(3)
C2	C3	C4	112.6(3)	F1	C31	F2	107.8(3)
C2	C3	C7	101.0(3)	F2	C31	S1	109.6(3)
C7	C3	C4	109.5(3)	F3	C31	S1	111.9(3)
C8	C3	C2	113.8(3)	F3	C31	F1	108.4(4)
C8	C3	C4	104.4(3)	F3	C31	F2	107.1(3)

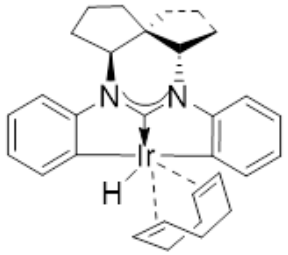
Table S20. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **1c**.

Atom	***x***	***y***	***z***	**U(eq)**
H7	-66.86	5478.51	2885.63	26
H15	1622.21	7209.65	4568.28	30
H8A	-492.97	7618.22	2695.71	35
H8B	478.59	8097.3	3292.13	35
H9A	-1169.43	7147.22	3515.61	40
H9B	-363.19	8052.55	4038.27	40
H10A	253.71	6307.54	4710.51	40
H10B	-464.59	5382.94	4131.62	40
H12A	539.57	3682.96	4005.48	44
H12B	1376.52	3923.84	3699.42	44
H13A	1550.42	3758.65	5138.98	61
H13B	2367.16	3513.26	4814.44	61

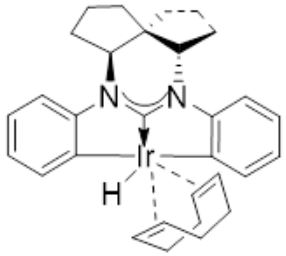
H14A	2941.34	5447.78	5170.79	56
H14B	2089.3	5722.77	5453.96	56
H2	2134.47	6484.44	991.79	38
H3	585.04	6294.56	166.04	45
H4	-698.89	5911.79	539.95	43
H5	-447.11	5807.78	1769.4	33
H18	3243.77	7729	5222.42	41
H19	4768.48	8665.63	5669.11	50
H20	5785.72	8504.8	5020.3	52
H21	5270.87	7551.07	3898.82	43
H23	3774.47	6811.66	1650.98	40
H24	4896.2	7168.32	2712.08	42
H25A	5377.61	4664.18	2750.77	69
H25B	5813.43	5593.01	3412.95	69
H26A	5091.6	4606.26	4021.67	50
H26B	4901.56	3496.69	3448.53	50
H27	3477.35	4355.97	3734.62	38
H28	2382.39	3949.91	2662.82	36
H29A	3679.3	3055.46	2174.8	51
H29B	2650.02	3456.18	1647.94	51
H30A	4306.12	4412.63	1657.12	65
H30B	3275.09	4854.03	1151.41	65

4. NMR and UV–Visible spectra of 1a, 1b and 1c

4.1. NMR spectroscopy of 1a, 1b and 1c



1a

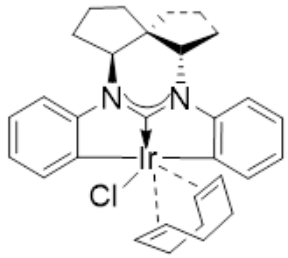


1a

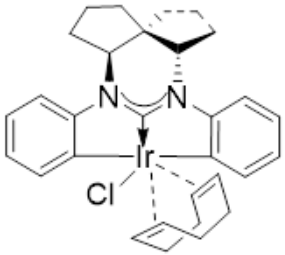
199.34
156.59
156.53
139.55
139.30
136.01
135.01
128.24
128.00
127.76
123.06
122.71
122.63
122.24
112.86
110.80
87.60
86.44
78.80
78.04
57.88
57.75
51.27
37.02
35.77
33.56
32.45
31.83
31.03
29.47
29.12
23.02
19.74

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

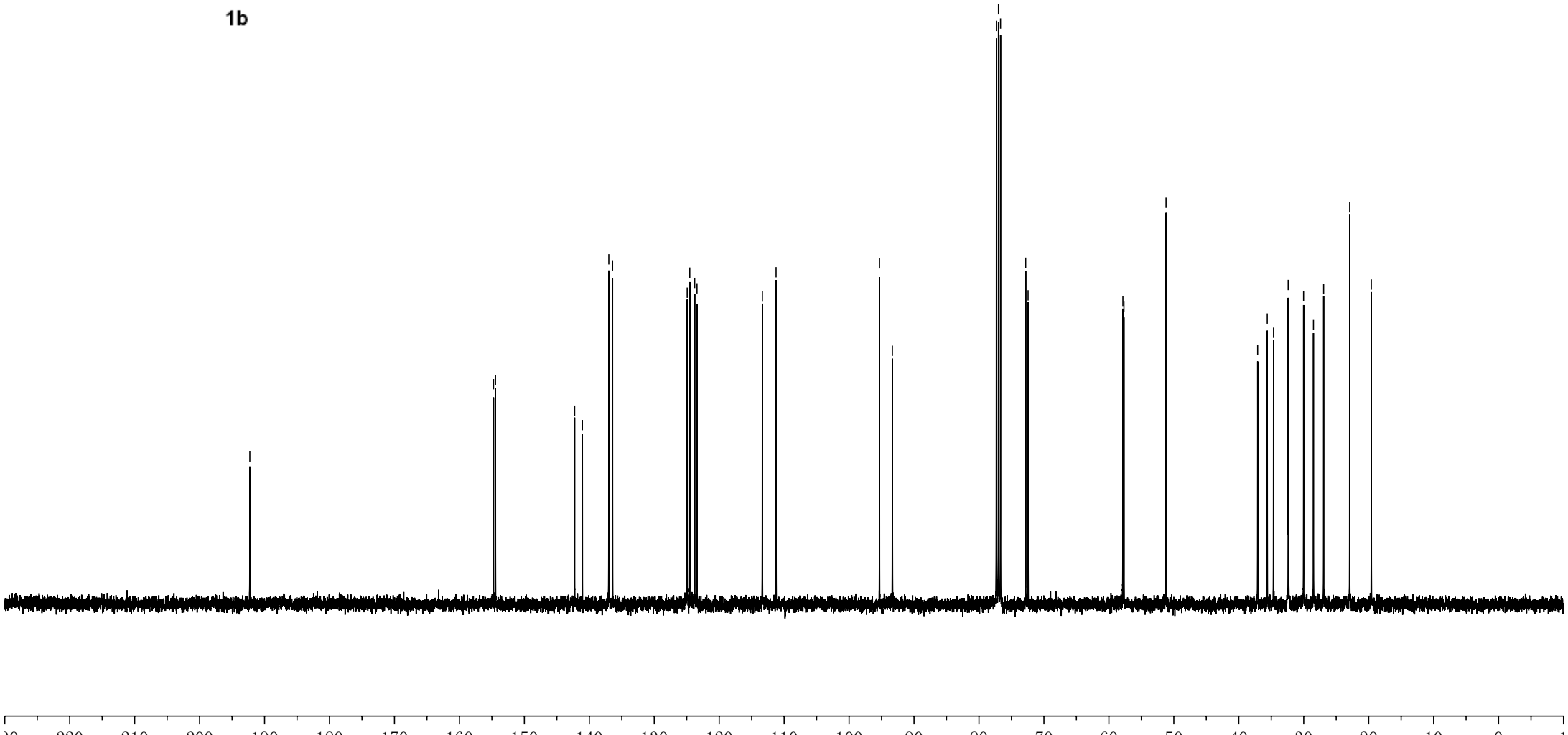


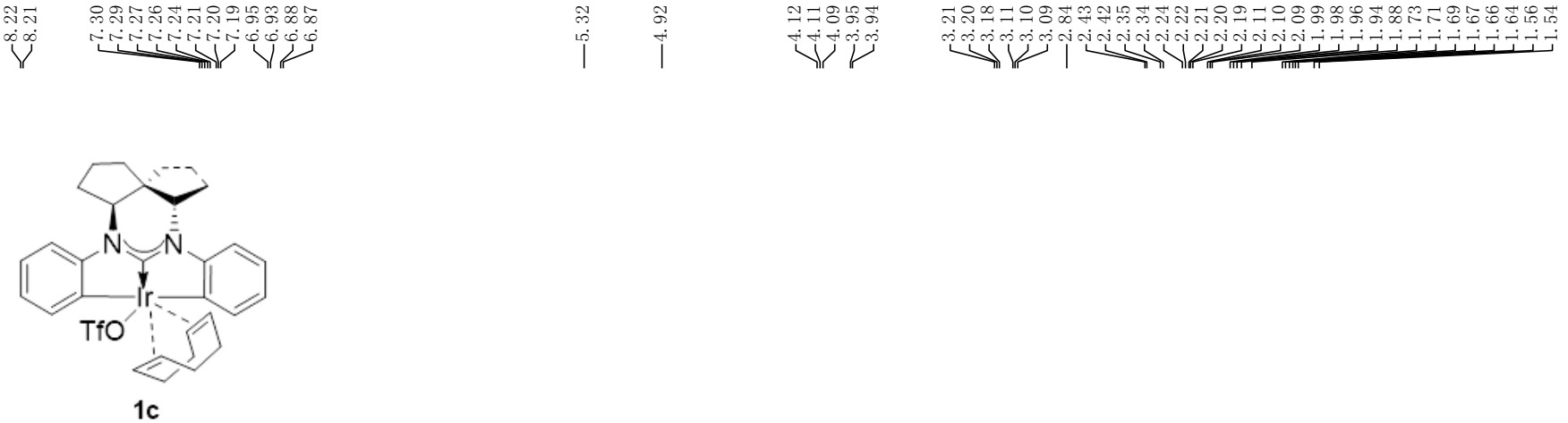
1b



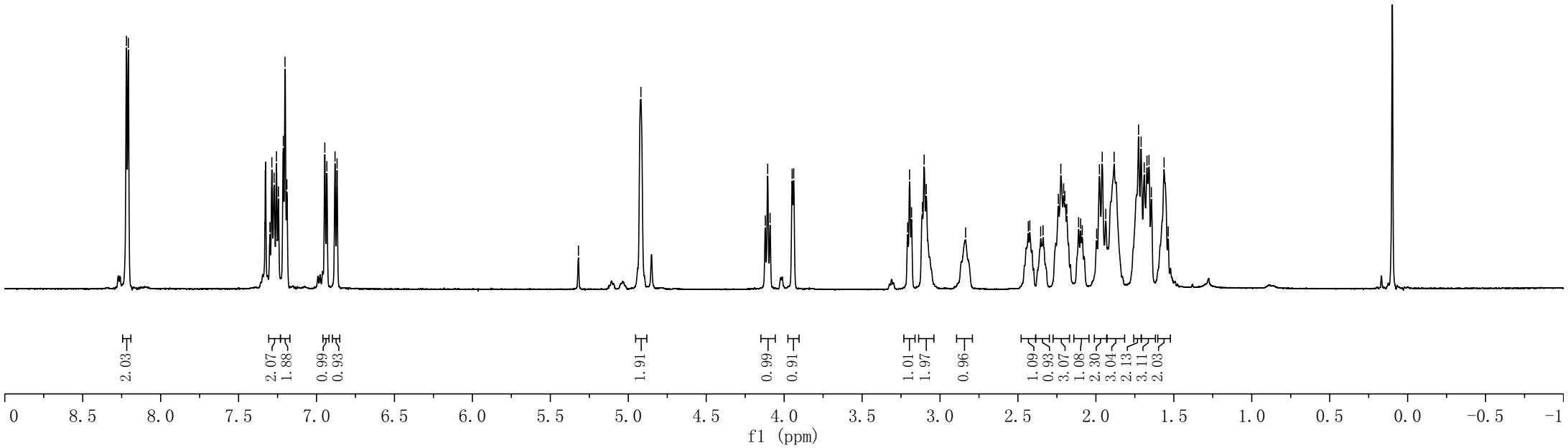
1b

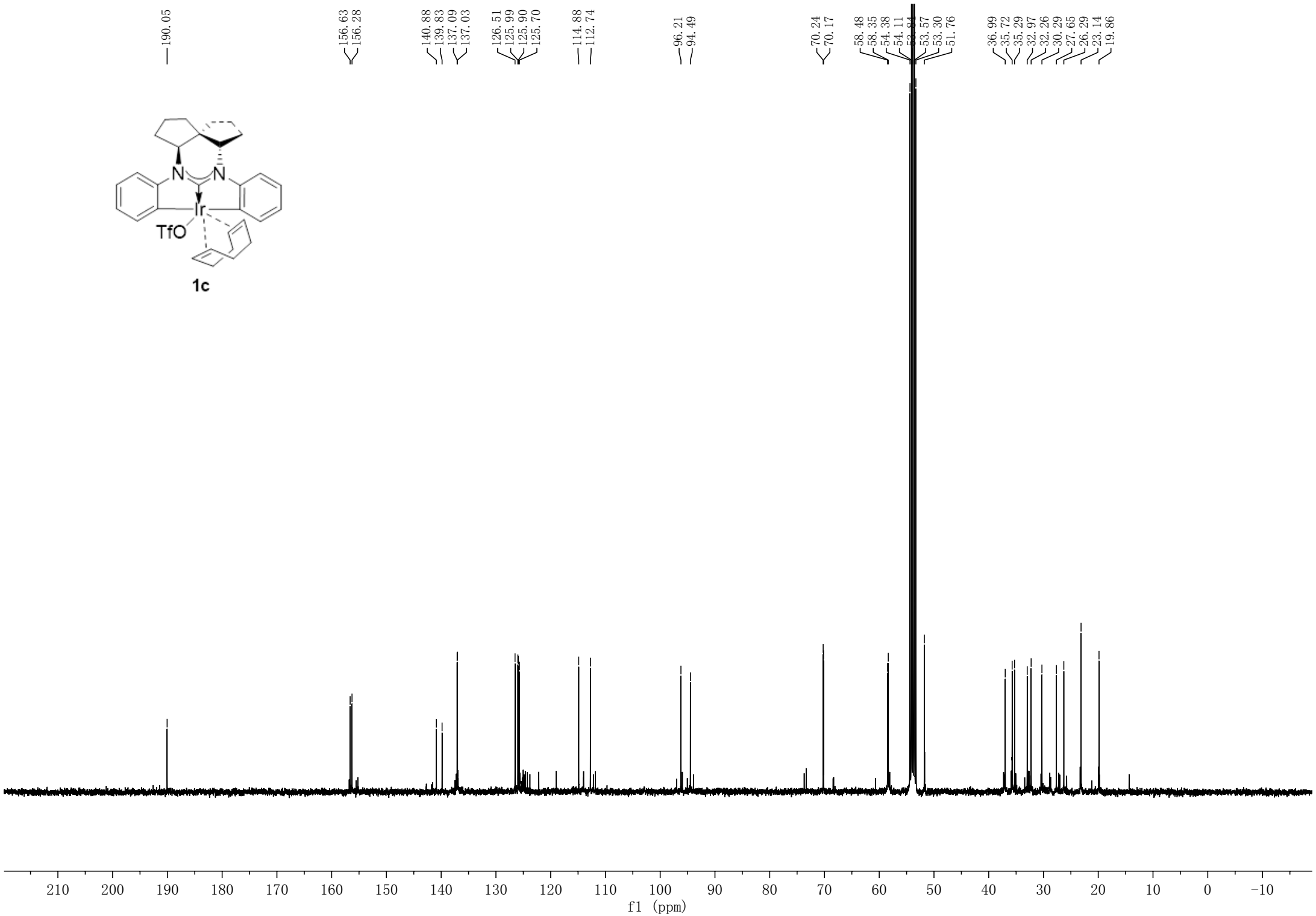
192.27
154.75
154.44
142.26
141.06
137.00
136.42
124.93
124.53
123.77
123.42
113.35
111.24
95.31
93.33
77.32
77.00
76.68
72.81
72.44
57.84
57.68
51.20
37.09
35.62
34.65
32.39
32.34
30.02
28.50
26.94
22.93
19.59

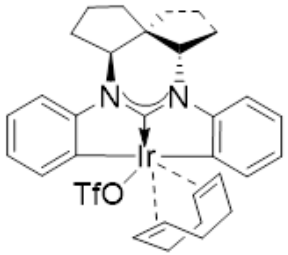



8.22
8.21
7.30
7.29
7.27
7.26
7.24
7.21
7.20
7.19
6.95
6.93
6.88
6.87
5.32
4.92
4.12
4.11
4.09
3.95
3.94
3.21
3.20
3.18
3.11
3.10
3.09
2.84
2.43
2.42
2.35
2.34
2.24
2.22
2.21
2.20
2.19
2.11
2.10
2.09
1.99
1.98
1.96
1.94
1.88
1.73
1.71
1.69
1.67
1.66
1.64
1.56
1.54
N
N
Ir
TfO

1c


2.03
2.07
1.88
0.99
0.93
1.91
0.99
0.91
1.01
1.97
0.96
1.09
0.93
3.07
1.08
2.30
3.04
2.13
3.11
2.03
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


190.05
156.63
156.28
140.88
139.83
137.09
137.03
126.51
125.99
125.90
125.70
114.88
112.74
96.21
94.49
70.24
70.17
58.48
58.35
54.38
54.11
53.57
53.30
51.76
36.99
35.72
35.29
32.97
32.26
30.29
27.65
26.29
23.14
19.86
N
N
Ir
TfO
1c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


N
N
Ir
TfO

1c

-79.01
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

4.2. UV−Visible spectra of 1a, 1b and 1c

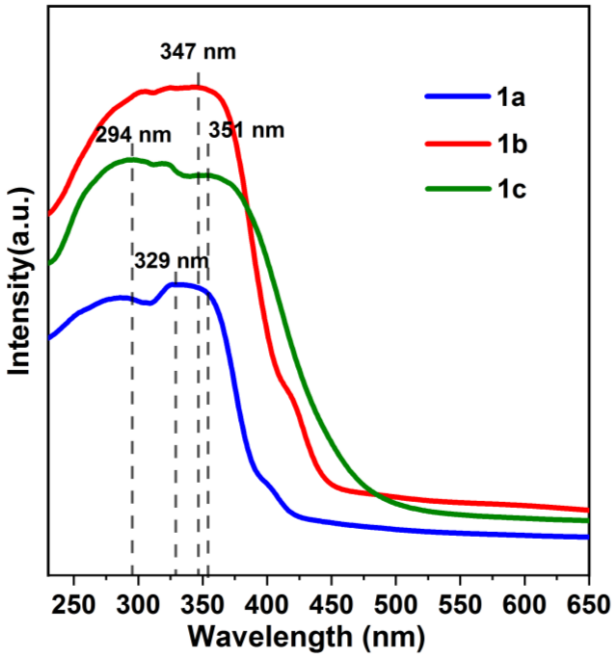


Fig. S1 UV−Visible absorption spectra of complexes **1a-1c**. By using $BaSO_4$ as reference, tests were conducted at 298 K. The UV−Visible absorption spectra of **1a-1c** showed high-energy absorption bands at ca. 250-400 nm. The maximum absorbance peak of **1a** was 329 nm. The maximum absorbance peak of **1b** was 347 nm. The maximum absorbance peak of **1c** was 294 nm, while the other high-energy absorption band at ca. 351 nm.

5. DFT calculation

5.1. Computational methods:

All DFT calculations were carried out by Gaussian 09 program package.[2] The B3LYP density functional[3,4] was employed for the computational study. The LANL2DZ basis set together with the LANL2DZ pseudopotential was used to describe Ir atom and 6-31G (d) basis set was utilized for other atoms. Vibrational frequency analyses were carried out to characterize the stationary points as local minima or transition states. To verify that each transition state connects to its appropriate reactant and product, the intrinsic reaction coordinate (IRC) calculations were employed. The solvent effect of toluene in the reaction was evaluated using the SMD solvation model. This model was used for single point energy calculations at a larger basis set (SDD for Ir atom and 6-311 + G (d, p) for other atoms). For the purpose of discussion, the solvation Gibbs free energy was used and it was obtained from the addition of solvation single point energy and gas-phase thermal correction to Gibbs free energy.

5.2. Coordinates and energies of S2 to 1a process:

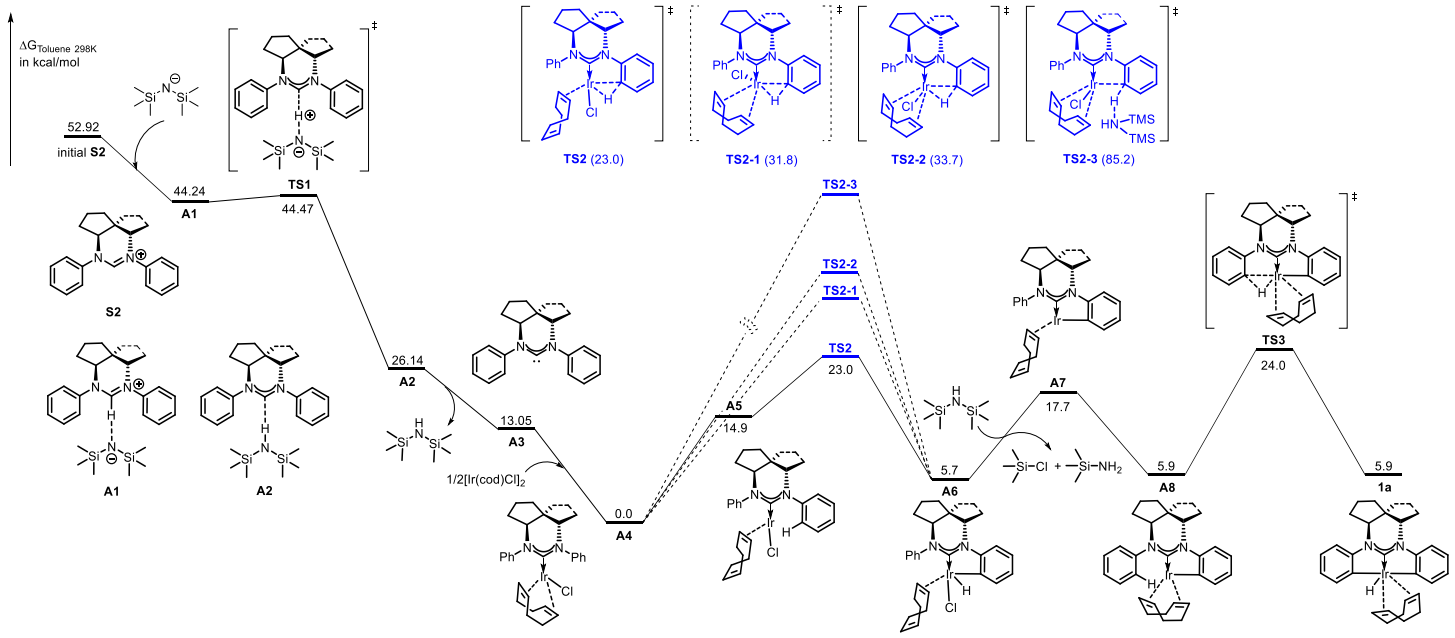


Fig. S2 Energy profiles for the formation of CCC pincer Ir(III) monohydride complex **1a** from **S2**. Bond distances were given in Å.

S2

Zero-point correction=	0.428704 (Hartree/Particle)
Thermal correction to Energy=	0.448263

Thermal correction to Enthalpy= 0.449207
Thermal correction to Gibbs Free Energy= 0.378771
Sum of electronic and zero-point Energies= -962.279834
Sum of electronic and thermal Energies= -962.260275
Sum of electronic and thermal Enthalpies= -962.259331
Sum of electronic and thermal Free Energies= -962.329767
SCF Done: E(RB3LYP) = -963.002011710

N	-0.21800281	0.24613220	0.00000000
N	-2.57105781	0.24595320	-0.03123500
C	-1.39394081	-0.35955580	-0.05449300
C	-0.07358581	1.72255720	0.21175600
C	-1.42469981	2.36208120	0.63792400
C	-2.62832681	1.72257020	-0.08617600
C	0.85174019	2.00721020	1.40645900
C	-0.03994481	1.77167120	2.63625300
C	-1.44995981	2.23797820	2.19405100
C	-1.50864081	3.81456120	0.11094100
C	-1.95793281	3.71362920	-1.36799300
C	-2.61556381	2.31303220	-1.51807000
C	0.97654119	-0.56319280	-0.15016300
C	1.81454619	-0.34622980	-1.24658400
C	2.96129419	-1.12653880	-1.39205500
C	3.26158819	-2.11836180	-0.45504700
C	2.41648719	-2.32932580	0.63541500
C	1.27233719	-1.54622980	0.79705600
C	-3.77498681	-0.54322380	0.07905300
C	-3.86565981	-1.51858380	1.07704000
C	-5.02268181	-2.29130280	1.17971200
C	-6.08928981	-2.07596580	0.30620400
C	-5.99640481	-1.08832780	-0.67706900
C	-4.83880081	-0.32087980	-0.80003300
H	0.31183019	2.13899020	-0.72395200
H	-3.54566081	2.00760520	0.43572600
H	-5.09364581	-3.04812780	1.95475400
H	4.15388719	-2.72486580	-0.57504400
H	2.64968319	-3.09546380	1.36832700
H	0.62340719	-1.68882780	1.65667100
H	-3.05213581	-1.65398780	1.78434000
H	-1.70122781	3.20818920	2.63374200
H	-2.22487081	1.53801020	2.52636500
H	-0.04790281	0.70708720	2.89737300
H	0.32357619	2.30772620	3.51672100
H	1.15550919	3.05833420	1.34444300

H	1.76558519	1.40830220	1.39561700
H	-0.56639981	4.35854920	0.23374100
H	-2.25926481	4.35206120	0.70152200
H	-2.65411681	4.51717020	-1.62133900
H	-1.10960081	3.81268520	-2.05175800
H	-2.02808681	1.66740220	-2.18024800
H	-3.62233181	2.36787220	-1.94024900
H	3.61401719	-0.96507280	-2.24432200
H	-6.82249581	-0.92012580	-1.36101700
H	-6.99225981	-2.67202080	0.39371600
H	-4.75967081	0.42484020	-1.58353200
H	1.56804619	0.41151220	-1.98427600
H	-1.39079581	-1.44119580	-0.13725900

A1

Zero-point correction=	0.654305 (Hartree/Particle)
Thermal correction to Energy=	0.691764
Thermal correction to Enthalpy=	0.692708
Thermal correction to Gibbs Free Energy=	0.582939
Sum of electronic and zero-point Energies=	-1835.520813
Sum of electronic and thermal Energies=	-1835.483353
Sum of electronic and thermal Enthalpies=	-1835.482409
Sum of electronic and thermal Free Energies=	-1835.592179

SCF Done: E(RB3LYP) = -1836.59296093

N	1.96202530	0.51336146	0.00000000
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C	1.22409530	-0.59286554	-0.11526900
C	3.45386930	0.54657946	0.07072200
C	4.07211230	-0.84597054	-0.21860400
C	3.19281030	-1.97556254	0.34504100
C	4.03769430	1.43210746	-1.04560300
C	3.98640530	0.53895746	-2.29493300
C	4.27989630	-0.88577354	-1.76401200
C	5.36529630	-1.03229054	0.60567600
C	4.90458630	-1.41959054	2.03244700
C	3.46337030	-1.97974554	1.87186700
C	1.29940330	1.79899546	0.06774300
C	1.41636130	2.55989146	1.23373500
C	0.82135030	3.81942546	1.29897600
C	0.11501430	4.31894246	0.20330500
C	0.00175330	3.55321846	-0.95761300
C	0.59614430	2.29303746	-1.03004200

C	1.00034030	-2.97672954	-0.34200900
C	0.20484530	-3.00009254	-1.48896200
C	-0.53538670	-4.14039654	-1.79502500
C	-0.47031870	-5.26562354	-0.97240000
C	0.33500430	-5.24194154	0.16700900
C	1.06924330	-4.09999454	0.48786800
H	3.72357330	0.91654746	1.06534100
H	3.51934230	-2.92288854	-0.09429700
H	-1.16090270	-4.14597154	-2.68280900
H	-0.35167170	5.29820246	0.25700200
H	-0.55407570	3.93127346	-1.81031900
H	0.50652530	1.69104146	-1.92762500
H	0.16426730	-2.13000854	-2.13334800
H	5.30876330	-1.18746354	-1.98932800
H	3.62524530	-1.62884254	-2.23235000
H	2.98802530	0.58265246	-2.74427600
H	4.69557130	0.85844146	-3.06443800
H	5.07686730	1.66357446	-0.78138200
H	3.51134630	2.38286146	-1.15700200
H	6.00593730	-0.14337854	0.59070900
H	5.94701030	-1.84779554	0.15844700
H	5.58182130	-2.15309754	2.47987700
H	4.90643630	-0.55074354	2.69849300
H	2.72834230	-1.34814654	2.38051800
H	3.35962930	-2.98321054	2.29387400
H	0.90175430	4.40387846	2.21094500
H	0.38552030	-6.10885854	0.81959300
H	-1.04572470	-6.15414354	-1.21536800
H	1.66805230	-4.07891954	1.39171900
H	1.94859030	2.16053446	2.09187400
H	0.03675330	-0.50569154	-0.12974800
N	-1.56540670	-0.44100654	0.17990400
Si	-2.67994070	-0.14230154	-1.07124800
Si	-1.93445470	-0.72492854	1.81736000
C	-1.86743370	-0.28804754	-2.80720000
H	-1.72303870	-1.33590654	-3.10049600
H	-2.51087170	0.16806746	-3.57103300
H	-0.89054570	0.21015846	-2.87365100
C	-4.15895970	-1.35334354	-1.14731000
H	-3.81344770	-2.39365454	-1.19956800
H	-4.79446470	-1.26723754	-0.25642300
H	-4.79688270	-1.16640554	-2.02234300
C	-3.47459370	1.59969046	-1.05173300
H	-2.71756670	2.39251546	-1.09663800

H	-4.15998170	1.74213146	-1.89894000
H	-4.05027770	1.75943546	-0.13160400
C	-3.13343870	0.53379246	2.61372000
H	-2.76322270	1.55974146	2.49325700
H	-4.12716670	0.49101846	2.14911900
H	-3.26704770	0.34733146	3.68820200
C	-2.67251370	-2.44958354	2.19106400
H	-3.64373770	-2.58305154	1.69852300
H	-2.01224270	-3.24544454	1.82301800
H	-2.82271270	-2.60824354	3.26813400
C	-0.34729070	-0.64363254	2.89469100
H	0.15762930	0.32690546	2.80276300
H	-0.59065670	-0.78661054	3.95555200
H	0.36958830	-1.42975254	2.62190600

TS1

Zero-point correction=	0.652911 (Hartree/Particle)
Thermal correction to Energy=	0.689822
Thermal correction to Enthalpy=	0.690766
Thermal correction to Gibbs Free Energy=	0.582445
Sum of electronic and zero-point Energies=	-1835.522192
Sum of electronic and thermal Energies=	-1835.485282
Sum of electronic and thermal Enthalpies=	-1835.484338
Sum of electronic and thermal Free Energies=	-1835.592659

SCF Done: E(RB3LYP) = -1836.59209330

N	-0.31645569	1.00562586	0.00000000
N	-0.50645569	-1.30902814	-0.05089300
C	-1.06300469	-0.09497214	-0.12732900
C	1.17476831	1.03261386	0.09327700
C	1.78958131	-0.35956214	-0.20324200
C	0.90144031	-1.48942714	0.34517400
C	1.78067131	1.92639286	-1.00449200
C	1.74024631	1.04862086	-2.26527800
C	2.00623331	-0.38668714	-1.74741000
C	3.07762731	-0.55866514	0.62631400
C	2.60866531	-0.96172014	2.04618000
C	1.16306731	-1.50629714	1.87315200
C	-0.97197569	2.29489186	0.05822600
C	-0.88018969	3.05041786	1.22994300
C	-1.46795669	4.31388686	1.28567900
C	-2.14205669	4.82359586	0.17451000
C	-2.23019169	4.06383186	-0.99263100

C	-1.64270769	2.79985786	-1.05506600
C	-1.28772669	-2.47709314	-0.36286100
C	-2.05777669	-2.50017214	-1.52717100
C	-2.79778469	-3.63692914	-1.84684400
C	-2.75726369	-4.76048714	-1.02023600
C	-1.97684069	-4.73801414	0.13637700
C	-1.24360669	-3.59911214	0.47050600
H	1.43243331	1.39057186	1.09570300
H	1.22738031	-2.43497014	-0.09883900
H	-3.40307069	-3.64178814	-2.74863700
H	-2.60288069	5.80603486	0.22063200
H	-2.76006569	4.45022386	-1.85814200
H	-1.71164769	2.20258886	-1.95773300
H	-2.07793169	-1.63117114	-2.17416300
H	3.03054931	-0.70498714	-1.97055700
H	1.34061031	-1.11276814	-2.22681700
H	0.75080531	1.11061286	-2.73186200
H	2.46712731	1.36840586	-3.01800600
H	2.81777631	2.14680286	-0.72327400
H	1.26381331	2.88270086	-1.11259600
H	3.72082031	0.32849886	0.62553300
H	3.65974331	-1.37040314	0.17280600
H	3.27772931	-1.70797214	2.48486100
H	2.61652231	-0.10277514	2.72488900
H	0.43208731	-0.86950814	2.38096300
H	1.04635931	-2.51100114	2.28874400
H	-1.40698969	4.89378486	2.20209100
H	-1.94531269	-5.60356014	0.79203200
H	-3.33199569	-5.64654814	-1.27364000
H	-0.66471069	-3.57921614	1.38732300
H	-0.37210769	2.64380586	2.09923800
H	-2.28063669	-0.00293914	-0.12556100
N	-3.81091569	0.06181986	0.18762400
Si	-4.92844269	0.37199786	-1.06319000
Si	-4.19279969	-0.23151514	1.82400200
C	-4.11923369	0.23004286	-2.79931900
H	-3.98181069	-0.81715714	-3.09734000
H	-4.76246269	0.69386286	-3.55859800
H	-3.14012169	0.72322386	-2.86501600
C	-6.40957369	-0.83514214	-1.13614300
H	-6.06597969	-1.87576214	-1.19268900
H	-7.04331269	-0.75034314	-0.24398300
H	-7.04872169	-0.64386214	-2.00926600
C	-5.71428969	2.11660886	-1.03032300

H	-4.95343669	2.90559486	-1.07523700
H	-6.40215869	2.26547886	-1.87436300
H	-6.28585769	2.27514286	-0.10755300
C	-5.40101469	1.02295086	2.61094700
H	-5.03182269	2.04985886	2.49633200
H	-6.39111869	0.97925886	2.13897700
H	-5.54235569	0.83294886	3.68375000
C	-4.93181769	-1.95846114	2.18031700
H	-5.89872669	-2.09052214	1.67923600
H	-4.26737269	-2.75138014	1.81372800
H	-5.09058769	-2.12262914	3.25528600
C	-2.61400169	-0.15200514	2.91034100
H	-2.10950369	0.81908486	2.82455300
H	-2.86433669	-0.29908614	3.96895300
H	-1.89520869	-0.93632714	2.63865500

A2

Zero-point correction=	0.655422 (Hartree/Particle)
Thermal correction to Energy=	0.693520
Thermal correction to Enthalpy=	0.694464
Thermal correction to Gibbs Free Energy=	0.580674
Sum of electronic and zero-point Energies=	-1835.549760
Sum of electronic and thermal Energies=	-1835.511662
Sum of electronic and thermal Enthalpies=	-1835.510718
Sum of electronic and thermal Free Energies=	-1835.624507

SCF Done: E(RB3LYP) = -1836.61954203

N	0.44225201	0.28770349	0.03247350
N	0.52675701	2.58102449	-0.12883450
C	1.15619101	1.38992149	-0.28578050
C	-1.01016099	0.19772949	0.38075550
C	-1.72006799	1.54998249	0.12063750
C	-0.80580199	2.73161649	0.48084650
C	-1.75054499	-0.76884651	-0.56322550
C	-1.92479699	0.04179649	-1.85706650
C	-2.15937899	1.49496249	-1.37405850
C	-2.88314299	1.74485349	1.11949450
C	-2.23649799	2.26070449	2.43150950
C	-0.83235099	2.78943149	2.02842450
C	1.15041801	-0.96361051	-0.04241850
C	1.10098501	-1.86865351	1.02367450
C	1.78243601	-3.08453651	0.94296750
C	2.51658501	-3.40783551	-0.19835350

C	2.56407301	-2.50439951	-1.26304550
C	1.88256301	-1.29055351	-1.18867350
C	1.20486501	3.76214849	-0.57192550
C	2.05368201	3.70304549	-1.68664550
C	2.70408401	4.84892449	-2.13643350
C	2.51118101	6.07581549	-1.49667450
C	1.66083001	6.13925749	-0.39429150
C	1.01168101	4.99292849	0.06966950
H	-1.10150599	-0.10637351	1.42973150
H	-1.25161799	3.64399649	0.06965650
H	3.35630401	4.78326849	-3.00347950
H	3.04684601	-4.35404451	-0.25856750
H	3.12814801	-2.74714251	-2.15963750
H	1.91749401	-0.57771451	-2.00498650
H	2.19351701	2.75053649	-2.18255250
H	-3.21506599	1.77589749	-1.46229050
H	-1.59026199	2.21100449	-1.97674650
H	-1.01002799	-0.01834951	-2.45687850
H	-2.74221499	-0.33569651	-2.47958650
H	-2.72815699	-0.99812051	-0.12022650
H	-1.22815999	-1.71801451	-0.70397650
H	-3.46933899	0.83027649	1.26452150
H	-3.56997899	2.49825749	0.71427650
H	-2.85090099	3.04245349	2.88912150
H	-2.14995499	1.46140949	3.17479350
H	-0.04089099	2.14732249	2.42814250
H	-0.63992099	3.79726649	2.40833050
H	1.74406901	-3.77514251	1.78118650
H	1.50229101	7.08315249	0.12064250
H	3.01539701	6.96896449	-1.85454050
H	0.37314501	5.06376549	0.94314350
H	0.54635801	-1.61943451	1.92327850
H	3.58010801	1.32698249	0.02798750
N	4.54912001	1.35824049	0.36712950
Si	5.75765201	0.98071549	-0.83540550
Si	4.68912701	1.83557749	2.04131150
C	4.96264001	1.09316849	-2.55130250
H	4.59918501	2.10749149	-2.75217650
H	5.68569201	0.83488549	-3.33514250
H	4.11239601	0.40786249	-2.64622750
C	7.19841101	2.21225049	-0.76443850
H	6.84821501	3.23417049	-0.95243450
H	7.70333801	2.20988049	0.20899150
H	7.95526001	1.97214249	-1.52232750

C	6.46267401	-0.76683951	-0.61775150
H	5.66284701	-1.51567651	-0.66561750
H	7.19917301	-1.00719551	-1.39583850
H	6.95906301	-0.87973651	0.35355650
C	6.18156501	0.99532749	2.85496750
H	6.08601801	-0.09645351	2.82867250
H	7.12902801	1.25812349	2.36966750
H	6.26343201	1.29815749	3.90679050
C	4.88670201	3.71169549	2.24107650
H	5.80147301	4.06637849	1.75040750
H	4.04426001	4.24578449	1.78496550
H	4.94116401	4.00634949	3.29748750
C	3.11772401	1.30089249	2.95450850
H	2.97335101	0.21622049	2.88982050
H	3.15930701	1.57743749	4.01551950
H	2.23411501	1.78053749	2.51807350

A3

Zero-point correction= 0.414602 (Hartree/Particle)
Thermal correction to Energy= 0.433850
Thermal correction to Enthalpy= 0.434794
Thermal correction to Gibbs Free Energy= 0.366016
Sum of electronic and zero-point Energies= -961.834361
Sum of electronic and thermal Energies= -961.815114
Sum of electronic and thermal Enthalpies= -961.814170
Sum of electronic and thermal Free Energies= -961.882947
SCF Done: E(RB3LYP) = -962.516038671

N	-0.48523206	0.83684950	0.00000000
N	-2.79055506	0.89680950	-0.00670800
C	-1.65581706	0.15875850	0.02789000
C	-0.28222906	2.31324350	0.11714600
C	-1.61396706	3.03720250	0.43834200
C	-2.81495406	2.35199850	-0.22390600
C	0.66534194	2.66757450	1.31013800
C	-0.19406206	3.42307350	2.35498200
C	-1.64253306	3.08304350	1.97584200
C	-1.63549406	4.43383850	-0.22549500
C	-2.10334606	4.20274950	-1.68777200
C	-2.75272106	2.79258850	-1.70752300
C	0.70357994	0.03512050	-0.13397200
C	1.86335294	0.55888250	-0.72212200
C	3.00682094	-0.23159650	-0.86199600

C	3.01636094	-1.55109450	-0.41717300
C	1.86169594	-2.07394850	0.17239900
C	0.71804294	-1.29480150	0.31513900
C	-4.03957706	0.19864950	0.07627600
C	-4.09453606	-1.06946150	0.67690600
C	-5.30297706	-1.75148150	0.77353200
C	-6.48577606	-1.18653150	0.28820500
C	-6.43607706	0.07252650	-0.30462500
C	-5.22595306	0.76206850	-0.41493000
H	0.12338294	2.67630150	-0.83368400
H	-3.72327106	2.74528150	0.24568000
H	-5.32095306	-2.73156250	1.24363200
H	3.90726794	-2.16341450	-0.52517300
H	1.85045494	-3.10042450	0.53026700
H	-0.18726206	-1.69771750	0.75068000
H	-3.17357906	-1.50016150	1.04861700
H	-2.37411706	3.80523150	2.35644100
H	-1.91895706	2.09618850	2.36889500
H	0.05592694	3.13659450	3.38165400
H	-0.03090006	4.50466750	2.27728200
H	1.51940494	3.26540850	0.97599900
H	1.07720794	1.74883750	1.73452800
H	-0.66653506	4.94179650	-0.16970600
H	-2.35615206	5.06690650	0.30749900
H	-2.80796706	4.98082250	-1.99798500
H	-1.26253206	4.25095950	-2.38747500
H	-2.13284706	2.08049450	-2.26250100
H	-3.73760606	2.78830450	-2.18406300
H	3.89174294	0.19627150	-1.32620000
H	-7.34130106	0.52907550	-0.69673100
H	-7.42826106	-1.72030750	0.37206600
H	-5.22030606	1.72842150	-0.90537800
H	1.88830594	1.58079550	-1.08270200

A4

Zero-point correction=	0.602135 (Hartree/Particle)
Thermal correction to Energy=	0.632611
Thermal correction to Enthalpy=	0.633555
Thermal correction to Gibbs Free Energy=	0.540150
Sum of electronic and zero-point Energies=	-1838.709184
Sum of electronic and thermal Energies=	-1838.678709
Sum of electronic and thermal Enthalpies=	-1838.677765
Sum of electronic and thermal Free Energies=	-1838.771169

SCF Done: E(RB3LYP) = -1839.40334002

Ir	-1.65322575	0.44354838	0.00000000
N	1.12549525	-0.56086562	-0.35514700
N	1.03631725	1.71763238	-0.53092400
C	0.34808325	0.55696838	-0.32799600
C	-4.43600675	1.67442838	-0.81418900
C	2.56200425	-0.57028262	0.03003400
C	-3.83230175	0.90677038	0.35459400
C	3.33269125	0.72915338	-0.37060300
C	-3.64556275	-0.47727262	0.38401800
C	2.39211125	1.69374638	-1.11690900
C	-3.93884275	-1.43904962	-0.75201900
C	2.76628825	-0.73653162	1.56302100
C	-3.43209475	-0.93904362	-2.12446500
C	4.04646425	0.05639738	1.86450900
C	-2.13528175	1.32317438	-1.87126900
C	3.89277525	1.28639338	0.95902300
C	-3.35553075	2.22264738	-1.77425900
C	4.40719325	0.43262138	-1.43872300
C	3.61285725	0.26950538	-2.74778100
C	2.44722425	1.28249438	-2.62436300
C	0.53247425	-1.87904462	-0.42955200
C	0.57153125	-2.54710862	-1.65826600
C	0.08014525	-3.84939362	-1.76606300
C	-0.44151875	-4.49281262	-0.64204900
C	-0.46738875	-3.82887862	0.58696400
C	0.02137525	-2.52571562	0.70081100
C	0.42235325	3.00653038	-0.36719800
C	-0.17078875	3.35893838	0.85078400
C	-0.72805675	4.62916038	1.00776100
C	-0.68451575	5.56016338	-0.03210300
C	-0.07857775	5.21201838	-1.24081400
C	0.47218925	3.94076238	-1.41049000
C	-2.15453075	-0.10290262	-2.00765700
H	2.99727425	-1.42676862	-0.49295700
H	2.78330225	2.70714538	-1.00225000
H	-1.18749675	4.89075238	1.95697300
H	-0.82371575	-5.50685662	-0.72282600
H	-4.20993775	-0.36156462	-2.63739400
H	-3.78665975	2.40477338	-2.77233900
H	-3.00900075	3.19553038	-1.40589100
H	-5.13955975	1.03375138	-1.35649800
H	-5.02896175	2.50984638	-0.42389200

H	-3.82781675	1.41973438	1.31409900
H	-3.54129075	-0.93823862	1.36411900
H	-3.43462875	-2.38241762	-0.51407600
H	-0.87224675	-4.32373662	1.46553000
H	-0.02418375	-1.99656962	1.64548700
H	-0.19753175	2.64096738	1.66239800
H	-1.29542475	-0.54758962	-2.50760900
H	4.82277425	1.84675838	0.81021000
H	3.16239725	1.97349338	1.40644000
H	4.14586925	0.31093538	2.92477400
H	4.93717425	-0.52037862	1.58086800
H	2.81762725	-1.78818962	1.86079400
H	1.91522425	-0.28567962	2.08702400
H	5.02142525	-0.44144162	-1.19319600
H	5.08510725	1.29373138	-1.51424300
H	4.23053325	0.43816338	-3.63560600
H	3.21984825	-0.75131662	-2.82355500
H	1.49456425	0.85230038	-2.94504000
H	2.62253125	2.16800838	-3.24527600
H	0.10668625	-4.35819762	-2.72591000
H	-0.03860875	5.92563138	-2.05939300
H	-1.11359675	6.54968738	0.09924500
H	-1.27103675	1.83496538	-2.29513300
H	-3.23339175	-1.80625662	-2.76484300
H	-5.01612375	-1.66528862	-0.79941200
H	0.92546525	3.67195138	-2.35990000
Cl	-1.19884375	0.32891238	2.41968700
H	0.98134325	-2.03869762	-2.52677200

A5

Zero-point correction=	0.600225 (Hartree/Particle)
Thermal correction to Energy=	0.631810
Thermal correction to Enthalpy=	0.632755
Thermal correction to Gibbs Free Energy=	0.534676
Sum of electronic and zero-point Energies=	-1838.670357
Sum of electronic and thermal Energies=	-1838.638772
Sum of electronic and thermal Enthalpies=	-1838.637828
Sum of electronic and thermal Free Energies=	-1838.735907

SCF Done: E(RB3LYP) = -1839.37417503

Ir	-1.58553540	-0.35465924	0.00000000
N	-4.14895040	-0.87978524	1.18496600
N	-3.56267740	1.33754376	1.29573100

C	-3.20469540	0.07279376	0.90053200
C	1.86981960	1.35133876	2.33033000
C	-5.60072940	-0.56591724	1.18730100
C	2.18683260	0.18498576	3.24565600
C	-5.94135240	0.80469476	1.86473800
C	2.26151060	-1.11950424	2.95229800
C	-4.63727540	1.51128676	2.29423800
C	2.06464960	-1.74316024	1.59262700
C	-6.22344940	-0.50889224	-0.23361300
C	0.58513860	-2.05511924	1.20309600
C	-7.37691840	0.49354276	-0.09487600
C	-0.35338740	0.37464376	1.56068900
C	-6.76415440	1.57805476	0.80479500
C	0.90958660	1.09880876	1.13653000
C	-6.66160340	0.60589476	3.21491700
C	-5.54527340	0.18488276	4.18857600
C	-4.30464040	0.99088676	3.72939000
C	-3.82788240	-2.28802724	1.11549000
C	-3.55730040	-2.96697624	2.30810800
C	-3.32155840	-4.34327824	2.29411100
C	-3.36822940	-5.04681024	1.08943000
C	-3.64898540	-4.36895024	-0.09959500
C	-3.88130340	-2.99292224	-0.09232200
C	-2.85036440	2.50861376	0.87146300
C	-2.65929640	2.77435076	-0.49061400
C	-2.00195040	3.94025776	-0.88357100
C	-1.54645840	4.85684776	0.06747900
C	-1.75022240	4.59797276	1.42356700
C	-2.39626640	3.42737776	1.82628400
C	-0.48032840	-1.05363224	1.65803300
H	-6.06670340	-1.37545824	1.75670500
H	-4.82918440	2.58556976	2.33270100
H	-1.85493340	4.13284276	-1.94258100
H	-3.18680040	-6.11810624	1.07652600
H	0.30056960	-3.03382324	1.60615600
H	0.64009460	2.07407676	0.71280900
H	1.42079160	0.55480576	0.33582900
H	1.42555860	2.14156476	2.95139300
H	2.80662460	1.78469876	1.94435200
H	2.37884760	0.46978776	4.28116400
H	2.48341360	-1.80628624	3.76968100
H	2.50800760	-1.09693124	0.82939200
H	-3.67977540	-4.90964924	-1.04141400
H	-4.06447240	-2.46012524	-1.01833100

H	-3.01544140	2.07003776	-1.23354000
H	-1.10300340	-1.43100624	2.46768600
H	-7.50562240	2.24115476	1.26419900
H	-6.09224440	2.20413976	0.20306500
H	-7.72342740	0.87917076	-1.05929900
H	-8.23879140	0.02514576	0.39928700
H	-6.53352040	-1.49626824	-0.58907300
H	-5.47615140	-0.12434924	-0.93773200
H	-7.48221740	-0.11851624	3.15702000
H	-7.09679840	1.56273276	3.53408200
H	-5.81005040	0.37066076	5.23434500
H	-5.35263740	-0.89019724	4.09428300
H	-3.39842640	0.37956876	3.72261700
H	-4.11250040	1.83953676	4.39544400
H	-3.10567340	-4.86247724	3.22400900
H	-1.39991240	5.30096076	2.17457800
H	-1.04076840	5.76585076	-0.24611200
H	-0.92367940	0.94575776	2.29659700
H	0.56243160	-2.18332724	0.10844400
H	2.62493760	-2.68531424	1.54200400
H	-2.53257840	3.22058376	2.88388200
Cl	-2.34644740	-0.46859824	-2.26459600
H	-3.52659240	-2.41107324	3.24076700

TS2

Zero-point correction=	0.596755 (Hartree/Particle)
Thermal correction to Energy=	0.627402
Thermal correction to Enthalpy=	0.628346
Thermal correction to Gibbs Free Energy=	0.532869
Sum of electronic and zero-point Energies=	-1838.658052
Sum of electronic and thermal Energies=	-1838.627406
Sum of electronic and thermal Enthalpies=	-1838.626462
Sum of electronic and thermal Free Energies=	-1838.721938

SCF Done: E(RB3LYP) = -1839.35945937

Ir	1.40472874	-0.25730180	0.00000000
N	-1.25917626	-0.70736280	0.96308500
N	-0.82818626	1.57081120	0.78540800
C	-0.36717826	0.28518520	0.64941400
C	4.74233974	2.25847920	2.01752600
C	-2.72411926	-0.53088180	1.06930100
C	5.28282174	1.35370320	3.09780000
C	-3.17499926	0.93826720	1.36206900

C	5.34028974	0.01753420	3.17345900
C	-1.97447826	1.85956320	1.65824200
C	4.84673374	-1.02474480	2.19326400
C	-3.45395826	-0.95500780	-0.23927500
C	3.34162874	-1.33231380	2.33541100
C	-4.61148226	0.04333220	-0.39081200
C	2.57637474	1.04622220	1.41597900
C	-3.99165026	1.35161020	0.11705200
C	3.87897274	1.63389220	0.90245200
C	-3.96559626	1.01383620	2.68740200
C	-2.88633326	0.96116520	3.78509700
C	-1.68248826	1.73192920	3.18738600
C	-0.76192526	-2.02814480	0.78564900
C	-1.39221726	-3.17530180	1.27359600
C	-0.79179226	-4.42231880	1.08781000
C	0.43225374	-4.52208080	0.41898300
C	1.06430874	-3.38133080	-0.07316000
C	0.47829774	-2.11456080	0.10662600
C	-0.11847526	2.65076320	0.18530200
C	0.41437774	2.50636420	-1.10630500
C	1.12750874	3.55344220	-1.69230800
C	1.29054374	4.76465420	-1.01803300
C	0.73844474	4.91830320	0.25536500
C	0.04476274	3.86931320	0.85999400
C	2.36439574	-0.20183780	2.04734200
H	-3.04878726	-1.16504780	1.89857100
H	-2.28116226	2.88262020	1.42788100
H	1.54170974	3.41950120	-2.68736000
H	0.89441374	-5.49528880	0.27589800
H	3.14938774	-1.64830380	3.37146600
H	3.62270874	2.43552220	0.19855500
H	4.44748074	0.90806520	0.32459700
H	4.16414074	3.05648720	2.51015800
H	5.59042474	2.77992120	1.54412100
H	5.70041074	1.90239020	3.94468000
H	5.77892774	-0.39078880	4.08544000
H	5.06800874	-0.76721580	1.15653700
H	2.00635774	-3.44627980	-0.60722600
H	0.55967074	-1.34376880	-1.03199900
H	0.24125774	1.58908120	-1.66251400
H	1.49457474	-0.23733380	2.70138500
H	-4.72669226	2.13017720	0.34968900
H	-3.31575926	1.75528120	-0.64934000
H	-4.97867226	0.10893020	-1.42017500

H	-5.46115526	-0.24830280	0.24036000
H	-3.77165626	-2.00109980	-0.21849200
H	-2.75707826	-0.84597280	-1.07902300
H	-4.71750926	0.22203320	2.78261700
H	-4.49946226	1.97272720	2.73030000
H	-3.23515526	1.38465220	4.73194700
H	-2.60315226	-0.07817180	3.98874800
H	-0.73762926	1.20800220	3.35761800
H	-1.57978926	2.72648720	3.63511800
H	-1.28459326	-5.31359080	1.46550500
H	0.86047474	5.85411620	0.79390600
H	1.83819074	5.58069920	-1.48011700
H	1.87229374	1.81741320	1.72797200
H	3.09291974	-2.19813880	1.71138500
H	5.38411174	-1.96146480	2.38869700
H	-0.34045626	3.99255120	1.86729700
Cl	3.41863474	-0.92176480	-1.25221400
H	-2.33248926	-3.11180480	1.81214500

TS2-1

Zero-point correction=	0.598843 (Hartree/Particle)
Thermal correction to Energy=	0.628559
Thermal correction to Enthalpy=	0.629503
Thermal correction to Gibbs Free Energy=	0.539019
Sum of electronic and zero-point Energies=	-1838.654826
Sum of electronic and thermal Energies=	-1838.625110
Sum of electronic and thermal Enthalpies=	-1838.624166
Sum of electronic and thermal Free Energies=	-1838.714650

SCF Done: E(RB3LYP) = -1839.35147439

Ir	1.85616447	-0.56164383	0.00000000
N	4.66967447	-1.21687683	-0.32420200
N	4.56300547	1.07171817	-0.04855900
C	3.88668147	-0.09855083	-0.16798600
C	-0.78710553	-0.43094183	1.76973500
C	6.08577247	-1.36480183	0.12423100
C	-0.17343353	-1.32867283	0.70196400
C	6.70175847	-0.02651283	0.59515500
C	-0.25897553	-1.08489883	-0.67010900
C	6.03525347	1.14078517	-0.12044800
C	-0.92101453	0.10125717	-1.34145600
C	6.18949047	-2.32180383	1.36128000
C	-0.55234353	1.43809917	-0.68398000

C	6.86168047	-1.50909483	2.48980500
C	1.18385547	1.11236817	1.21289200
C	6.54823947	-0.05281283	2.12594800
C	0.16842847	0.68169817	2.25778800
C	8.16502447	0.09450417	0.10587600
C	8.08599547	0.62000217	-1.35642400
C	6.63381147	1.13540717	-1.54826700
C	4.02622347	-2.39537583	-0.77885900
C	2.62560747	-2.32958383	-0.96771400
C	1.97254747	-3.49079483	-1.41801900
C	2.66716347	-4.66906683	-1.68095300
C	4.04932747	-4.70585183	-1.50392000
C	4.72927147	-3.57543783	-1.05091200
C	3.96706047	2.37055717	-0.23421900
C	3.87403047	3.25569217	0.84271900
C	3.42313447	4.56043717	0.63426200
C	3.08247447	4.98921817	-0.65036800
C	3.19300947	4.10870617	-1.72930900
C	3.63960847	2.80219317	-1.52458300
C	0.87512347	1.43958017	-0.13621100
H	6.64448747	-1.75046083	-0.73396200
H	6.31956547	2.07065617	0.38371700
H	3.33962147	5.24088117	1.47693800
H	2.13202947	-5.55093383	-2.02229400
H	-1.25550553	1.67892417	0.12164600
H	-0.40924953	1.55080717	2.61300600
H	0.73511447	0.30110017	3.11091800
H	-1.71892953	0.00006817	1.38456600
H	-1.07162953	-1.05578983	2.62264100
H	0.05750047	-2.34374083	1.01129700
H	-0.15599453	-1.94223383	-1.32658500
H	-0.58461553	0.11353117	-2.38461100
H	4.60854147	-5.61308983	-1.71513800
H	5.79953547	-3.64061783	-0.90557600
H	4.15101947	2.91533917	1.83622200
H	1.53296647	2.13510117	-0.63481900
H	7.19939447	0.67783517	2.62046700
H	5.50999647	0.17418117	2.39904800
H	6.47878047	-1.79053283	3.47526400
H	7.94683247	-1.67298583	2.49925800
H	6.74574947	-3.23354983	1.12271000
H	5.18005547	-2.61205383	1.66302200
H	8.71178447	-0.85110683	0.18358600
H	8.69111647	0.81704117	0.74178500

H	8.82046147	1.41450317	-1.52155000
H	8.31449747	-0.16870783	-2.08016800
H	6.05789247	0.45120017	-2.18058600
H	6.58757647	2.12379917	-2.01420400
H	0.89919747	-3.48131883	-1.57379200
H	2.93256547	4.43711017	-2.73168700
H	2.73481247	6.00592817	-0.81054100
H	2.05503447	1.59525317	1.64621200
H	-0.65430353	2.24379017	-1.42095100
H	-2.01362753	-0.04354583	-1.36767900
H	3.71993547	2.10563917	-2.35319000
H	2.16640247	-1.19407383	-1.57195200
Cl	2.64854447	-1.60499083	2.26570500

TS2-2

Zero-point correction=	0.598530 (Hartree/Particle)
Thermal correction to Energy=	0.628287
Thermal correction to Enthalpy=	0.629231
Thermal correction to Gibbs Free Energy=	0.538391
Sum of electronic and zero-point Energies=	-1838.652235
Sum of electronic and thermal Energies=	-1838.622479
Sum of electronic and thermal Enthalpies=	-1838.621534
Sum of electronic and thermal Free Energies=	-1838.712375

SCF Done: E(RB3LYP) = -1839.34781048

Ir	0.02778914	-0.60254255	-0.01469558
N	-2.52327686	-1.96426655	0.19530942
N	-2.85883786	0.24222345	0.66274042
C	-1.96223786	-0.71294755	0.26823642
C	2.63369114	1.29617545	0.71269042
C	-3.95325986	-2.15347455	-0.14206058
C	2.35632414	0.16930545	-0.26041958
C	-4.91950086	-1.18980155	0.61409642
C	2.36269314	-1.16557655	0.06071442
C	-4.07400486	-0.17722355	1.40707042
C	2.61106014	-1.74061755	1.44185242
C	-4.24029686	-1.96453855	-1.65216558
C	1.81670914	-1.04240955	2.56849442
C	-5.71391586	-1.53880755	-1.68453758
C	0.27255614	0.84318445	1.58974942
C	-5.80675086	-0.56711555	-0.49562458
C	1.34765514	1.88075745	1.32858742
C	-5.69545886	-1.92001155	1.72976542

C	-4.65919486	-2.11122955	2.85269842
C	-3.79620186	-0.82683555	2.80087342
C	-1.63494086	-3.06099255	0.04669642
C	-2.04643386	-4.39386155	0.17168142
C	-1.12398186	-5.42750255	0.02299442
C	0.20587214	-5.12353155	-0.26380158
C	0.60965514	-3.79366455	-0.37667058
C	-0.28529586	-2.72344955	-0.19532958
C	-2.75403286	1.66094245	0.43365542
C	-2.76813786	2.17298145	-0.86492458
C	-2.78733486	3.55488645	-1.06687058
C	-2.81309586	4.42985845	0.01830642
C	-2.81865286	3.91772145	1.31862442
C	-2.79223086	2.53982745	1.52644842
C	0.46347314	-0.47618555	2.12550442
H	-4.20934986	-3.17268455	0.14100142
H	-4.65858086	0.73349645	1.54133142
H	-2.78254586	3.94100345	-2.08190258
H	0.93249614	-5.91901655	-0.40744158
H	2.41379114	-0.24029555	3.01902642
H	1.59238114	2.43592445	2.24908742
H	0.92488714	2.60603545	0.62558542
H	3.30938214	0.94126745	1.49787942
H	3.17070314	2.08818545	0.17847342
H	2.33192814	0.43380245	-1.31118558
H	2.46044914	-1.85622755	-0.77157858
H	2.32692514	-2.79655555	1.41803442
H	1.64379414	-3.59772255	-0.63258058
H	-0.12169186	-1.67124755	-1.29829658
H	-2.74899986	1.49650045	-1.70873658
H	-0.37503586	-0.87323755	2.69553942
H	-6.83252286	-0.39593355	-0.15117058
H	-5.39763086	0.40625345	-0.79449958
H	-6.00627886	-1.08319955	-2.63616558
H	-6.36720686	-2.40684455	-1.52299258
H	-4.01987286	-2.86809055	-2.22913458
H	-3.60658086	-1.16047255	-2.04456558
H	-6.14655386	-2.85952755	1.38811042
H	-6.51505686	-1.27733655	2.07916642
H	-5.12454586	-2.27244555	3.83026742
H	-4.03623486	-2.98938455	2.64631042
H	-2.73345786	-1.04406255	2.93149442
H	-4.07946086	-0.12488555	3.59302342
H	-1.45079586	-6.45874255	0.12033642

H	-2.84074386	4.58889845	2.17285142
H	-2.83218686	5.50384645	-0.14502858
H	-0.67807486	1.30443445	1.83205942
H	1.64813014	-1.76921955	3.37142742
H	3.68976614	-1.71619655	1.66290542
H	-2.79740686	2.14194145	2.53774542
Cl	-0.08753686	1.05147545	-1.97376158
H	-3.07618986	-4.64684255	0.39931842

TS2-3

Zero-point correction=	0.841297 (Hartree/Particle)
Thermal correction to Energy=	0.888279
Thermal correction to Enthalpy=	0.889223
Thermal correction to Gibbs Free Energy=	0.763627
Sum of electronic and zero-point Energies=	-2712.310825
Sum of electronic and thermal Energies=	-2712.263843
Sum of electronic and thermal Enthalpies=	-2712.262899
Sum of electronic and thermal Free Energies=	-2712.388495

SCF Done: E(RB3LYP) = -2713.40076301

Ir	0.15753425	-0.20547945	0.00000000
N	0.31295925	2.67888455	0.22867900
N	2.22368425	1.96859855	-0.79598600
C	1.01887325	1.61494555	-0.24831600
C	1.01209525	-3.27719345	-0.00442400
C	0.40626425	4.01871755	-0.39041600
C	-0.20372175	-2.40893545	-0.30792700
C	1.87459325	4.45901755	-0.70449500
C	-1.08481375	-1.95795545	0.68008400
C	2.82017425	3.27565855	-0.42293900
C	-0.86328275	-2.19170645	2.16650900
C	-0.34279875	4.09604055	-1.74792900
C	0.54410625	-1.76884045	2.65363400
C	0.38862425	5.20418955	-2.51228900
C	2.01793425	-1.03309145	0.60675300
C	1.85878125	4.89857455	-2.19312800
C	2.29960925	-2.44082445	0.11070700
C	2.39138025	5.53802655	0.27001400
C	2.74533925	4.77475855	1.56025800
C	3.24536725	3.39134255	1.07614000
C	-0.76503675	2.37074755	1.13915400
C	-0.88324475	3.15561555	2.29178200
C	-1.79654475	2.80493855	3.28846300

C	-2.56496975	1.64876155	3.13127000
C	-2.42414275	0.88324855	1.97256700
C	-1.53674375	1.19987855	0.91134500
C	3.07461625	1.08692355	-1.54872500
C	2.58447425	0.38044355	-2.65091400
C	3.44741325	-0.42241445	-3.40028600
C	4.80143125	-0.51791945	-3.07636400
C	5.29232925	0.19488455	-1.98060000
C	4.43656325	0.99008455	-1.21911900
C	1.19773025	-0.70294345	1.76391600
H	-0.04400875	4.72027355	0.31603500
H	3.69814625	3.39160555	-1.05996100
H	3.05006925	-0.96600445	-4.25343100
H	-3.26961575	1.35186355	3.90557800
H	1.20438425	-2.64349545	2.72346600
H	3.03764225	-2.95275545	0.75212000
H	2.76139525	-2.35072545	-0.87911500
H	0.83665525	-3.84231745	0.91782600
H	1.12121125	-4.02454545	-0.79990000
H	-0.56171375	-2.44472745	-1.33330900
H	-2.10804575	-1.74093745	0.39518100
H	-1.61193775	-1.60872445	2.71033800
H	-3.05935575	0.00277955	1.86566800
H	-2.53766475	1.03564755	-0.27906000
H	1.53577225	0.45441755	-2.91226600
H	1.51114525	0.17915655	2.32506500
H	2.53374725	5.74146855	-2.37858200
H	2.19395225	4.06657255	-2.82556700
H	0.17164425	5.19896555	-3.58572600
H	0.10710025	6.19283255	-2.12425700
H	-1.41092575	4.28493255	-1.61936500
H	-0.23856975	3.13758655	-2.26957700
H	1.66793425	6.34688255	0.42876100
H	3.29636725	5.99591855	-0.15194900
H	3.48738725	5.30579755	2.16536700
H	1.85584125	4.65287055	2.18750700
H	2.81927925	2.57608955	1.66625500
H	4.33505325	3.31046055	1.15934200
H	-1.88626475	3.41580655	4.18289800
H	6.34208925	0.12771255	-1.70737700
H	5.46771725	-1.13792245	-3.67004300
H	2.85927525	-0.36648145	0.43442700
H	0.46115325	-1.37991845	3.67522500
H	-1.05299675	-3.24818045	2.41655500

H	4.82726225	1.51563555	-0.35321000
Cl	-0.79601175	0.22566655	-2.48914500
H	-0.24349575	4.02293455	2.43398200
N	-3.46479375	1.26577455	-1.11100900
Si	-4.28075775	-0.12431945	-2.07322400
Si	-4.59158275	2.62182655	-0.54277300
C	-4.16554075	0.38427755	-3.88557000
H	-3.11653075	0.45131055	-4.19127200
H	-4.65212075	-0.37465145	-4.51142800
H	-4.65307175	1.34331255	-4.09134700
C	-3.55933875	-1.83677245	-1.82456000
H	-2.48883075	-1.85920445	-2.02462400
H	-3.75697175	-2.24314245	-0.82759200
H	-4.05966175	-2.49606445	-2.54760100
C	-6.10221175	-0.32250545	-1.58181700
H	-6.73820775	0.55386855	-1.72950200
H	-6.49924675	-1.12104945	-2.22314200
H	-6.21708175	-0.66254645	-0.54694800
C	-5.54600175	3.28714155	-2.03839000
H	-4.85799375	3.67075255	-2.80201200
H	-6.20935475	2.56452055	-2.52152000
H	-6.16419075	4.13281155	-1.70991400
C	-5.73676675	1.98183055	0.81204100
H	-5.16783975	1.44435555	1.57696000
H	-6.19656175	2.84930455	1.30253100
H	-6.54329075	1.33643855	0.45935200
C	-3.67732775	4.10394055	0.16875400
H	-3.04102875	4.61255855	-0.56057400
H	-4.44856975	4.82404055	0.47578600
H	-3.07766775	3.86197055	1.04807100
H	-2.80054075	1.62651055	-1.81390400

A6

Zero-point correction=	0.598827 (Hartree/Particle)
Thermal correction to Energy=	0.630140
Thermal correction to Enthalpy=	0.631084
Thermal correction to Gibbs Free Energy=	0.534835
Sum of electronic and zero-point Energies=	-1838.686245
Sum of electronic and thermal Energies=	-1838.654932
Sum of electronic and thermal Enthalpies=	-1838.653988
Sum of electronic and thermal Free Energies=	-1838.750238

SCF Done: E(RB3LYP) = -1839.38890799

Ir	-0.08344923	0.45201668	0.00000000
N	-2.67848023	0.05827968	1.16491000
N	-2.23899223	2.31892168	0.87960900
C	-1.81839023	1.02524068	0.73637400
C	3.20102277	3.04126068	2.46707900
C	-4.13092023	0.22654268	1.36265400
C	3.95671977	2.08330768	3.35616500
C	-4.56629623	1.71858268	1.53865200
C	4.18724877	0.76998668	3.22810700
C	-3.35572223	2.63848768	1.78131500
C	3.74142277	-0.18365232	2.13973600
C	-4.94489923	-0.31554432	0.14536700
C	2.30111877	-0.70575732	2.32240100
C	-6.05361623	0.72107768	-0.10169700
C	1.16514977	1.61354768	1.91466100
C	-5.37012723	2.04492768	0.26245400
C	2.29903677	2.45032368	1.36146600
C	-5.36418823	1.90277568	2.84793500
C	-4.29670523	1.91621668	3.96217800
C	-3.03270923	2.53138168	3.30385200
C	-2.13712623	-1.25681732	1.07721500
C	-2.79304323	-2.41110432	1.51033200
C	-2.15634223	-3.64793932	1.36849700
C	-0.88836623	-3.72166032	0.79187300
C	-0.23478923	-2.55974132	0.36246600
C	-0.84469723	-1.31188732	0.51765000
C	-1.46861823	3.38419468	0.32095000
C	-1.01910523	3.30673468	-1.00714300
C	-0.25014623	4.33980168	-1.54684200
C	0.04795977	5.47298768	-0.78833900
C	-0.42653123	5.56453568	0.52194500
C	-1.17397023	4.52615968	1.07956000
C	1.17844577	0.30450468	2.30721400
H	-4.38548423	-0.33166232	2.26868300
H	-3.65866223	3.66155268	1.54109200
H	0.09963777	4.25852768	-2.57179000
H	-0.40422323	-4.68670932	0.66506500
H	2.23422677	-1.22202032	3.29156700
H	1.86333477	3.29141568	0.80883000
H	2.88429977	1.88707768	0.63645200
H	2.58920477	3.68769568	3.11543400
H	3.92199677	3.72403568	1.98952100
H	4.38183977	2.56536168	4.23864000
H	4.75974277	0.30571368	4.03242600

H	3.84737177	0.24125368	1.14085400
H	0.74011877	-2.62002532	-0.10979400
H	-0.78233623	0.15250368	-1.38959600
H	-1.29295023	2.45364768	-1.61757200
H	0.28454277	-0.03936732	2.82554400
H	-6.06721623	2.87625668	0.41696600
H	-4.68160223	2.33650168	-0.54244100
H	-6.42884623	0.69582768	-1.12993800
H	-6.90931023	0.54062968	0.56161900
H	-5.32662423	-1.32601732	0.31466700
H	-4.27835223	-0.36552032	-0.72290200
H	-6.12784923	1.13095068	2.99605200
H	-5.88578623	2.86848468	2.81256400
H	-4.63008923	2.47624068	4.84112200
H	-4.08544123	0.89596168	4.30119300
H	-2.15339823	1.89996968	3.46144100
H	-2.79616923	3.51715968	3.71794100
H	-2.66205123	-4.55022932	1.70096900
H	-0.20349023	6.44160068	1.12337600
H	0.63792177	6.27893668	-1.21472700
H	0.29837877	2.19030568	2.23307700
H	2.10092377	-1.47313532	1.56528800
H	4.40246977	-1.05907132	2.15920900
H	-1.50695623	4.59729068	2.10993300
Cl	2.01349377	-0.01314432	-1.15223000
H	-3.78467023	-2.36664932	1.94935000

A7

Zero-point correction=	0.587350 (Hartree/Particle)
Thermal correction to Energy=	0.616348
Thermal correction to Enthalpy=	0.617292
Thermal correction to Gibbs Free Energy=	0.526700
Sum of electronic and zero-point Energies=	-1377.838504
Sum of electronic and thermal Energies=	-1377.809506
Sum of electronic and thermal Enthalpies=	-1377.808562
Sum of electronic and thermal Free Energies=	-1377.899154

SCF Done: E(RB3LYP) = -1378.49051908

Ir	-0.08196721	-0.01366120	0.00000000
N	-2.64248821	-1.36632720	0.15020700
N	-2.89528121	0.94287080	0.19685100
C	-2.06257521	-0.14076520	0.07320400
C	4.40720079	0.69013380	-0.84683800

C	-4.08195521	-1.63681720	0.02704000
C	5.10301379	0.33428980	0.44749100
C	-4.98896221	-0.39731220	0.35275500
C	4.82440979	-0.61786720	1.34737100
C	-4.17583421	0.79668780	0.89855000
C	3.71462179	-1.64466220	1.32533000
C	-4.47460121	-2.08320120	-1.41472500
C	2.37412679	-1.15099120	1.92240300
C	-5.85201921	-1.45375020	-1.66704500
C	2.02166979	0.70988580	0.06704300
C	-5.72984621	-0.09378820	-0.96918500
C	2.94350879	0.22703480	-1.03380100
C	-5.92623721	-0.70939420	1.54064700
C	-5.02694321	-0.57858820	2.78360600
C	-4.05478921	0.57849180	2.44237600
C	-1.69349821	-2.42122820	0.01944900
C	-2.03213821	-3.77343420	0.01840700
C	-1.03233121	-4.73110320	-0.18698900
C	0.28139079	-4.31993020	-0.40350400
C	0.61009879	-2.95876320	-0.37899700
C	-0.35385021	-1.96907320	-0.13390700
C	-2.33046021	2.22693780	-0.01144500
C	-1.43395821	2.41382280	-1.08259700
C	-0.83067421	3.65890580	-1.28206800
C	-1.13367921	4.73637980	-0.44984500
C	-2.04800321	4.55875380	0.59186100
C	-2.63827221	3.31570080	0.81880400
C	1.74978779	0.09454080	1.30222400
H	-4.31149621	-2.43792120	0.73741100
H	-4.74743521	1.70697180	0.69556900
H	-0.14166821	3.78540880	-2.11273200
H	1.05942879	-5.05697520	-0.58881800
H	2.55107579	-0.91596720	2.98133100
H	2.58683779	0.63162480	-1.99061600
H	2.89484379	-0.85777820	-1.14178000
H	4.43353279	1.78614280	-0.94123800
H	5.00649479	0.31905980	-1.69455100
H	5.96626479	0.96662180	0.66275600
H	5.46934679	-0.65898320	2.22635000
H	3.55969879	-2.02839220	0.31443300
H	1.64156179	-2.66617220	-0.54973200
H	-1.26277721	1.60266180	-1.78541400
H	1.36335579	0.77568880	2.06275800
H	-6.69060021	0.40382380	-0.79476900

H	-5.11786521	0.57791280	-1.58676700
H	-6.09095121	-1.37405520	-2.73284800
H	-6.64425021	-2.05323320	-1.19937800
H	-4.46144421	-3.16961520	-1.53527800
H	-3.74044621	-1.67169620	-2.11718700
H	-6.40840221	-1.69002020	1.45667300
H	-6.72602221	0.04310680	1.57401900
H	-5.60248521	-0.39562020	3.69653200
H	-4.46460021	-1.50586720	2.94302200
H	-3.02348421	0.33813480	2.71465800
H	-4.32423921	1.49664080	2.97588400
H	-1.29057721	-5.78648420	-0.19074400
H	-2.29354121	5.38944280	1.24807900
H	-0.67357521	5.70609580	-0.61597400
H	1.86366979	1.79527980	0.04762300
H	1.66154579	-1.98206020	1.91638200
H	4.03125179	-2.51069920	1.92123400
H	-3.31168921	3.19054180	1.65977000
H	-3.05825121	-4.09714520	0.16461500

A8

Zero-point correction=	0.588658 (Hartree/Particle)
Thermal correction to Energy=	0.616928
Thermal correction to Enthalpy=	0.617872
Thermal correction to Gibbs Free Energy=	0.530037
Sum of electronic and zero-point Energies=	-1377.868708
Sum of electronic and thermal Energies=	-1377.840438
Sum of electronic and thermal Enthalpies=	-1377.839494
Sum of electronic and thermal Free Energies=	-1377.927330

SCF Done: E(RB3LYP) = -1378.51259555

Ir	-1.10958911	0.67123287	0.00000000
N	1.69979189	0.00530887	-0.03852000
N	1.54104789	2.31650087	0.00971600
C	0.90315889	1.11601987	-0.03051300
C	-3.33318011	0.06002087	2.11728300
C	3.12001289	-0.07228213	0.35821500
C	-2.90857411	-0.41272013	0.72957100
C	3.69990389	1.31341987	0.73850600
C	-3.23381611	0.22918687	-0.47557600
C	3.00778389	2.42494887	-0.04865900
C	-4.03781311	1.50342987	-0.62778300
C	3.29915789	-0.95759613	1.63949100

C	-3.66006011	2.58711487	0.40559000
C	3.89500289	-0.03853713	2.73260300
C	-1.57076611	1.89748887	1.78435800
C	3.54048089	1.38075687	2.26751800
C	-2.29539911	1.00213887	2.77473000
C	5.16250189	1.44146887	0.24906500
C	5.07925689	1.88154887	-1.24155400
C	3.61670489	2.35007887	-1.46915400
C	1.05844389	-1.18947013	-0.51668700
C	-0.32917911	-1.06148813	-0.76543200
C	-0.94989511	-2.17084213	-1.35718000
C	-0.25318211	-3.34776913	-1.66416800
C	1.10252589	-3.44569913	-1.36798500
C	1.77054789	-2.35961013	-0.78828000
C	0.84955689	3.53341687	-0.31525600
C	0.89611089	4.61474987	0.57066800
C	0.28738189	5.82324987	0.22933500
C	-0.36614511	5.95741687	-0.99801000
C	-0.40526011	4.87877887	-1.88475500
C	0.20712489	3.67001387	-1.55106800
C	-2.17156111	2.59127187	0.72326500
H	3.66956389	-0.49351813	-0.49067900
H	3.27011789	3.38789187	0.40329600
H	0.31569889	6.65546587	0.92719900
H	-0.77347611	-4.18485513	-2.12440100
H	-4.24805811	2.46180987	1.32163000
H	-2.78046411	1.60578987	3.55963000
H	-1.53701811	0.39219587	3.28008900
H	-4.31164011	0.54872787	2.06287800
H	-3.47164411	-0.81679113	2.76075100
H	-2.64347011	-1.46526513	0.66883200
H	-3.20334811	-0.37892713	-1.37944200
H	-3.84578111	1.89339087	-1.63503900
H	1.65361589	-4.35690013	-1.58615600
H	2.82852289	-2.45340113	-0.56905600
H	1.39156089	4.49971987	1.53074100
H	-1.62937211	3.43807487	0.32281900
H	4.16800989	2.15859887	2.71821200
H	2.49628889	1.61051087	2.51830300
H	3.50589689	-0.27130813	3.72903500
H	4.98476289	-0.15391513	2.77845700
H	3.93798689	-1.82475513	1.44551600
H	2.32207289	-1.34505913	1.94038400
H	5.73198789	0.51523787	0.38136500

H	5.66849389	2.21173387	0.84441100
H	5.79669289	2.68214187	-1.44719800
H	5.33064989	1.05793887	-1.91701400
H	3.05922289	1.61706687	-2.06196400
H	3.54723589	3.30795187	-1.99265000
H	-2.01285211	-2.13184213	-1.58704600
H	-0.91059111	4.97699987	-2.84154400
H	-0.84158611	6.89802287	-1.26182900
H	-0.63120611	2.29767087	2.16627000
H	-3.94032611	3.56963487	0.00642400
H	-5.11879611	1.28947187	-0.58272300
H	0.17514889	2.82334587	-2.22848700

A8 (calculated by M06-2X)

Zero-point correction=	0.594953 (Hartree/Particle)
Thermal correction to Energy=	0.622696
Thermal correction to Enthalpy=	0.623640
Thermal correction to Gibbs Free Energy=	0.537547
Sum of electronic and zero-point Energies=	-1377.219241
Sum of electronic and thermal Energies=	-1377.191498
Sum of electronic and thermal Enthalpies=	-1377.190554
Sum of electronic and thermal Free Energies=	-1377.276647

SCF Done: E(RM062X) = -1377.82845365

Ir	0.03660322	0.54904831	0.00000000
N	2.89078222	-0.00760769	-0.04979200
N	2.63361322	2.28087531	0.02046600
C	2.06220522	1.06439831	-0.04207700
C	-2.00362278	-0.06452569	2.22856700
C	4.32140222	-0.01890969	0.29687100
C	-1.58712978	-0.58709569	0.86001000
C	4.79523922	1.36670431	0.77146300
C	-2.02227378	-0.04147469	-0.35861500
C	4.08383122	2.47034331	0.00807900
C	-2.93879778	1.15129331	-0.50975400
C	4.59151122	-0.96082569	1.50931500
C	-2.57287878	2.30616431	0.43592900
C	5.04012622	-0.05839169	2.67849500
C	-0.38163978	1.83990731	1.70503300
C	4.55801422	1.33773131	2.28089200
C	-1.02216878	0.98715031	2.78228000
C	6.25951622	1.58219931	0.35609500
C	6.20483722	2.07977331	-1.11321300

C	4.72656422	2.44361631	-1.38807300
C	2.28785822	-1.22658769	-0.50198200
C	0.89111022	-1.17129269	-0.70160400
C	0.30891722	-2.32831969	-1.22760900
C	1.05169122	-3.47257069	-1.53855300
C	2.42071522	-3.48679669	-1.31277000
C	3.05130422	-2.35624869	-0.78730500
C	1.86852422	3.44458831	-0.30913800
C	1.78095222	4.49646031	0.60019200
C	1.05443422	5.63631531	0.26650400
C	0.42702222	5.72746331	-0.97504700
C	0.53518422	4.68067531	-1.88882500
C	1.26137122	3.53892231	-1.56137400
C	-1.07282878	2.41974531	0.63761200
H	4.87610722	-0.33539169	-0.59511900
H	4.28885422	3.43119531	0.49533200
H	0.96876122	6.44771831	0.98228600
H	0.55812722	-4.34833169	-1.95130200
H	-3.07652378	2.19251131	1.40117400
H	-1.52637878	1.62333831	3.52506000
H	-0.21461278	0.46922631	3.31127100
H	-3.01957578	0.33833631	2.17679000
H	-2.04985278	-0.90609969	2.92705600
H	-1.26315778	-1.62557069	0.84836000
H	-2.00995278	-0.69698369	-1.22904100
H	-2.84726778	1.50417031	-1.54383700
H	3.01044522	-4.36923569	-1.54272600
H	4.12237222	-2.38048069	-0.61848500
H	2.25960122	4.40350531	1.57165700
H	-0.61037578	3.26899831	0.14729800
H	5.08078822	2.14891131	2.79837300
H	3.48346022	1.44138631	2.48572500
H	4.63703822	-0.39390769	3.63725600
H	6.13218322	-0.05907169	2.76451300
H	5.34543822	-1.71553969	1.26828300
H	3.67086822	-1.49552869	1.75699100
H	6.85803722	0.67235431	0.47015900
H	6.70476322	2.34566831	1.00458100
H	6.85852722	2.94510231	-1.24825100
H	6.55059522	1.31227731	-1.81028100
H	4.23616922	1.66456231	-1.98310700
H	4.60439122	3.39101331	-1.91885400
H	-0.76552678	-2.35422169	-1.40163800
H	0.05206522	4.75067531	-2.85834700

H	-0.14340178	6.61475731	-1.23088000
H	0.55791722	2.30521331	2.00500400
H	-2.94609378	3.24544231	0.01383700
H	-3.99041578	0.85563731	-0.37405900
H	1.34800122	2.71036931	-2.25823800

TS3

Zero-point correction=	0.585024 (Hartree/Particle)
Thermal correction to Energy=	0.612186
Thermal correction to Enthalpy=	0.613131
Thermal correction to Gibbs Free Energy=	0.529653
Sum of electronic and zero-point Energies=	-1377.842504
Sum of electronic and thermal Energies=	-1377.815341
Sum of electronic and thermal Enthalpies=	-1377.814397
Sum of electronic and thermal Free Energies=	-1377.897874

SCF Done: E(RB3LYP) = -1378.48339721

Ir	-1.76697196	0.50650310	0.02976340
N	0.95526004	-0.50494690	0.15014240
N	0.80154404	1.84043210	0.23096440
C	0.20117404	0.62283910	0.19064440
C	-4.30102796	-1.26029490	0.92872440
C	2.39122404	-0.58427790	0.46852240
C	-3.92767896	-0.32953290	-0.22025360
C	2.96210504	0.79846710	0.88723240
C	-4.00047396	1.05555210	-0.13998860
C	2.25897404	1.96518610	0.17962140
C	-4.43772696	1.85534210	1.07537840
C	2.65516704	-1.52141790	1.69575540
C	-3.73664496	1.42971110	2.38063040
C	3.24135104	-0.63193890	2.81965140
C	-2.06188396	-0.50132690	1.92828940
C	2.84384504	0.79645810	2.42251140
C	-3.12322796	-1.58771390	1.87614240
C	4.41184404	0.95846610	0.37111140
C	4.28815904	1.42430610	-1.10431360
C	2.85605804	2.00968410	-1.24856560
C	0.26196504	-1.62472390	-0.39983860
C	-1.09439096	-1.37572990	-0.73693260
C	-1.75698796	-2.43416290	-1.37266960
C	-1.13343096	-3.65635890	-1.65542460
C	0.19355504	-3.86502490	-1.28813660
C	0.90198904	-2.84294390	-0.65220460

C	-0.03946296	2.94261410	-0.05588960
C	0.39546704	4.26879010	0.04036040
C	-0.47390396	5.31008610	-0.27763160
C	-1.77520396	5.02326110	-0.70372260
C	-2.20490196	3.70402110	-0.79549660
C	-1.36703496	2.61746610	-0.45755360
C	-2.32407896	0.89158510	2.14832440
H	2.89923004	-0.95872490	-0.42762360
H	2.52901804	2.87756710	0.72004940
H	-0.13040996	6.33802310	-0.20521360
H	-1.68887296	-4.44214290	-2.16266860
H	-4.33542696	0.67832410	2.91136740
H	-3.50183196	-1.80968990	2.88717340
H	-2.63372696	-2.50032190	1.52172040
H	-5.12827596	-0.81100690	1.49069640
H	-4.69441296	-2.19378690	0.51096240
H	-3.94469896	-0.75808490	-1.21600260
H	-4.07736196	1.58191910	-1.08958860
H	-4.20175496	2.90583110	0.88062740
H	0.68547104	-4.81168690	-1.49588960
H	1.93714404	-3.01003790	-0.37411360
H	1.40372704	4.50382110	0.36596640
H	-1.53247296	1.46107310	2.63086340
H	3.46824804	1.56829710	2.88728340
H	1.80386004	0.99614410	2.71280540
H	2.87196604	-0.91679590	3.80989540
H	4.33389404	-0.72132390	2.84810140
H	3.33189304	-2.34130590	1.43457640
H	1.71054904	-1.97735890	2.00446640
H	5.00078704	0.04092410	0.47458040
H	4.91473504	1.72769710	0.97106340
H	5.06083404	2.15986710	-1.34827960
H	4.42852704	0.58587210	-1.79407060
H	2.24359804	1.39266110	-1.91451060
H	2.84583104	3.02438610	-1.65648860
H	-2.79470196	-2.31934190	-1.67302660
H	-3.20848696	3.50446510	-1.15771760
H	-2.45240896	5.83125110	-0.96852060
H	-1.09926096	-0.86982790	2.28455140
H	-3.68608096	2.29421710	3.05284740
H	-5.53387296	1.79996410	1.18173940
H	-1.47846296	1.61013210	-1.33405060

1a

Zero-point correction=	0.588172 (Hartree/Particle)
Thermal correction to Energy=	0.615439
Thermal correction to Enthalpy=	0.616383
Thermal correction to Gibbs Free Energy=	0.533176
Sum of electronic and zero-point Energies=	-1377.874136
Sum of electronic and thermal Energies=	-1377.846869
Sum of electronic and thermal Enthalpies=	-1377.845924
Sum of electronic and thermal Free Energies=	-1377.929131

SCF Done: E(RB3LYP) = -1378.51568825

Ir	0.87671238	-0.41095890	0.00000000
N	3.60414138	-1.42592890	0.14458000
N	3.45197038	0.90672710	0.31455700
C	2.86194238	-0.29494290	0.15530600
C	-1.55247862	-2.15205190	1.15458400
C	5.03329638	-1.51609290	0.50731100
C	-1.22697762	-1.25453290	-0.04044600
C	5.58668538	-0.15299490	1.00827000
C	-1.32550762	0.14009710	0.00684100
C	4.90442838	1.04765910	0.33798500
C	-1.72075362	0.92762910	1.24517600
C	5.26129838	-2.50649190	1.69963000
C	-0.94108162	0.54426810	2.52359900
C	5.80629838	-1.66859490	2.88177600
C	0.70923438	-1.37247790	2.11066100
C	5.41634338	-0.22559790	2.53687500
C	-0.35023762	-2.45887890	2.07863100
C	7.05309038	0.02999210	0.55194800
C	6.97732038	0.55184510	-0.90568800
C	5.56568238	1.18256710	-1.05897100
C	2.89387138	-2.58048590	-0.31600500
C	1.50190638	-2.40095390	-0.49354100
C	0.81324938	-3.50080990	-1.01690900
C	1.44890238	-4.70998290	-1.33158400
C	2.81898638	-4.84876790	-1.13458000
C	3.55266838	-3.77413990	-0.62548300
C	2.58720538	2.02778110	0.11680800
C	3.07473838	3.33747610	0.09279700
C	2.20279538	4.38554110	-0.20948500
C	0.87294138	4.10258310	-0.50667100
C	0.40947138	2.78131610	-0.46108600
C	1.23010638	1.70182110	-0.11246300
C	0.45680738	-0.01090290	2.27135700

H	5.57335038	-1.84773190	-0.38686800
H	5.13586538	1.92949310	0.94392400
H	2.57442738	5.40645510	-0.23274900
H	0.86797238	-5.53683590	-1.73367100
H	-1.50919262	-0.18922390	3.10801000
H	-0.70525562	-2.66270090	3.10191400
H	0.13290538	-3.37566090	1.73140200
H	-2.36513162	-1.69091090	1.72863800
H	-1.95611262	-3.10051690	0.78306000
H	-1.33404062	-1.70965290	-1.01992500
H	-1.50497862	0.64949710	-0.93712900
H	-1.55641662	1.98774010	1.04333400
H	3.32551238	-5.77889290	-1.37806400
H	4.62359938	-3.88078690	-0.49075100
H	4.12071938	3.55771810	0.28194600
H	1.28429438	0.61894610	2.58558600
H	6.02133238	0.52660110	3.05606200
H	4.36644138	-0.04051790	2.80097900
H	5.40544938	-2.00078590	3.84479500
H	6.89750138	-1.75648090	2.94285000
H	5.94971638	-3.31100290	1.42261300
H	4.31217538	-2.98302890	1.95809100
H	7.64345738	-0.88839790	0.64052300
H	7.52978438	0.77767210	1.19879800
H	7.77708838	1.27082010	-1.10823600
H	7.10806038	-0.26715690	-1.62062500
H	4.96722538	0.63760210	-1.79638400
H	5.59699038	2.22504010	-1.38739700
H	-0.25543762	-3.43375490	-1.19735300
H	-0.62860462	2.60509310	-0.72524100
H	0.19132738	4.90487210	-0.77973400
H	1.71452138	-1.72542490	2.33125700
H	-0.85404162	1.43030510	3.16233300
H	-2.80348562	0.81519710	1.41812000
H	0.90983938	-0.25917090	-1.60011700

1a (calculated by M06-2X)

Zero-point correction=	0.594153 (Hartree/Particle)
Thermal correction to Energy=	0.620947
Thermal correction to Enthalpy=	0.621891
Thermal correction to Gibbs Free Energy=	0.539513
Sum of electronic and zero-point Energies=	-1377.226310
Sum of electronic and thermal Energies=	-1377.199516

Sum of electronic and thermal Enthalpies= -1377.198572
Sum of electronic and thermal Free Energies= -1377.280950
SCF Done: E(RM062X) = -1377.83669095

Ir	-0.12445094	0.25622254	0.00000000
N	2.57712806	-0.75902746	0.10845600
N	2.42882506	1.56218654	0.29795800
C	1.84522106	0.36868554	0.12442500
C	-2.48599794	-1.47893746	1.19530000
C	4.00699606	-0.85052946	0.44513600
C	-2.20418294	-0.57911446	-0.00240300
C	4.51914806	0.48629954	1.02271900
C	-2.30299094	0.80757354	0.06205000
C	3.87423706	1.69932954	0.35996400
C	-2.65804994	1.56770554	1.32386300
C	4.25065306	-1.88248546	1.58788700
C	-1.83659294	1.16145254	2.55988300
C	4.69790206	-1.07859846	2.82727800
C	-0.19365994	-0.71555246	2.06563300
C	4.25529706	0.35194054	2.52309100
C	-1.26163094	-1.78895746	2.07988800
C	5.99923106	0.67802354	0.65598600
C	6.00007006	1.28645054	-0.76848500
C	4.56660206	1.81771154	-1.00872000
C	1.85300806	-1.90619746	-0.33410600
C	0.46069006	-1.71858646	-0.47802900
C	-0.24508594	-2.82693746	-0.94924400
C	0.37646306	-4.04252446	-1.25445900
C	1.74935106	-4.18015746	-1.10515200
C	2.50074606	-3.10054646	-0.64342200
C	1.56277406	2.67781854	0.11573100
C	2.05354906	3.98079654	0.08116000
C	1.17478406	5.02719154	-0.19393700
C	-0.15950094	4.74569854	-0.45434200
C	-0.62085794	3.42651754	-0.40720400
C	0.20500006	2.34675054	-0.08795900
C	-0.44416894	0.63902854	2.24583100
H	4.54718506	-1.12134446	-0.47059400
H	4.10161406	2.57213754	0.98172800
H	1.54463806	6.04739554	-0.22556500
H	-0.21929794	-4.87727246	-1.61337400
H	-2.36959794	0.39768154	3.13715600
H	-1.58383694	-1.97120446	3.11571400
H	-0.79919894	-2.71473946	1.72950700

H	-3.28081694	-1.01699746	1.79225600
H	-2.89969794	-2.42507146	0.83205700
H	-2.32535994	-1.02565346	-0.98392300
H	-2.49669494	1.33089154	-0.87119200
H	-2.50592494	2.63250454	1.14022000
H	2.24471206	-5.11557846	-1.34652500
H	3.57602806	-3.20166446	-0.53830800
H	3.10587506	4.19328954	0.23973900
H	0.38956806	1.27790654	2.52539800
H	4.78655206	1.11237454	3.10455000
H	3.17992306	0.47044554	2.71746800
H	4.26808206	-1.47308346	3.75142200
H	5.78728006	-1.11265546	2.93426100
H	4.99582606	-2.62722246	1.29424200
H	3.32315706	-2.42425946	1.78986000
H	6.56683406	-0.25634146	0.71456300
H	6.44956606	1.37636854	1.37096600
H	6.74508206	2.08196154	-0.84748700
H	6.26056006	0.53592254	-1.51965600
H	4.02791106	1.18931454	-1.72670100
H	4.54259006	2.83984954	-1.39446900
H	-1.32089394	-2.76476146	-1.08933200
H	-1.66582794	3.25158854	-0.64582500
H	-0.84713194	5.54914354	-0.70372100
H	0.82332106	-1.07171346	2.22684600
H	-1.74300994	2.02798654	3.22150100
H	-3.73148594	1.44175254	1.52867400
H	-0.11735094	0.41517354	-1.58449900

Bis(trimethylsilyl)amine anion

Zero-point correction=	0.226025 (Hartree/Particle)
Thermal correction to Energy=	0.242742
Thermal correction to Enthalpy=	0.243687
Thermal correction to Gibbs Free Energy=	0.181196
Sum of electronic and zero-point Energies=	-873.126104
Sum of electronic and thermal Energies=	-873.109387
Sum of electronic and thermal Enthalpies=	-873.108443
Sum of electronic and thermal Free Energies=	-873.170934

SCF Done: E(RB3LYP) = -873.554147728

N	-0.35864979	1.03375526	0.00000000
Si	1.28534621	1.03414626	-0.00429800
Si	-2.00272279	1.03486526	-0.00385200

C	2.09243521	0.30119226	1.58268400
H	1.77875221	-0.74077474	1.73270100
H	3.19223121	0.31772626	1.54481000
H	1.78037121	0.86349126	2.47317500
C	2.08476421	0.02339926	-1.43556300
H	1.77185121	-1.02855274	-1.38875800
H	1.76399121	0.41191326	-2.41169600
H	3.18485221	0.04613126	-1.41108900
C	2.08734821	2.77829326	-0.16378500
H	1.76424721	3.42976126	0.65954700
H	3.18742121	2.74402726	-0.15060800
H	1.78026121	3.26536326	-1.09930400
C	-2.80191679	2.51871526	-0.93564500
H	-2.48490379	3.47209026	-0.49159500
H	-2.48434679	2.53167526	-1.98719100
H	-3.90198179	2.49105926	-0.91904600
C	-2.80519779	-0.51146474	-0.82449500
H	-2.48817079	-0.60467174	-1.87202200
H	-2.49263279	-1.43037974	-0.31007700
H	-3.90519579	-0.47737874	-0.80928600
C	-2.80862479	1.09684026	1.74429300
H	-2.50301179	2.00413726	2.28297000
H	-3.90862379	1.08570226	1.70590100
H	-2.48738279	0.23875426	2.35007500

Bis(trimethylsilyl)amine

Zero-point correction=	0.239796 (Hartree/Particle)
Thermal correction to Energy=	0.256677
Thermal correction to Enthalpy=	0.257622
Thermal correction to Gibbs Free Energy=	0.195612
Sum of electronic and zero-point Energies=	-873.707812
Sum of electronic and thermal Energies=	-873.690931
Sum of electronic and thermal Enthalpies=	-873.689987
Sum of electronic and thermal Free Energies=	-873.751996

SCF Done: E(RB3LYP) = -874.105313345

N	0.86293980	0.09589041	0.01129650
Si	2.47713280	0.10644041	-0.67605550
Si	-0.75123820	0.08852841	-0.67612950
C	3.65211380	0.73741341	0.66715750
H	3.61602180	0.10773741	1.56543050
H	4.69037880	0.73627541	0.31342250
H	3.40440880	1.76227941	0.96786250

C	3.03369180	-1.62260959	-1.21286350
H	3.04001880	-2.31880359	-0.36536050
H	2.36291480	-2.03892859	-1.97388950
H	4.04575180	-1.60501559	-1.63757650
C	2.54118680	1.25118341	-2.18129950
H	2.27735480	2.27985541	-1.90954150
H	3.54849580	1.26668241	-2.61616350
H	1.85356580	0.93025341	-2.97340550
C	-1.30896820	1.82066141	-1.20165150
H	-1.31689820	2.51100641	-0.34939150
H	-0.63770920	2.24281241	-1.95903050
H	-2.32053220	1.80502841	-1.62762450
C	-0.81438820	-1.04644359	-2.18877150
H	-0.12690420	-0.71992959	-2.97870050
H	-0.54992520	-2.07669759	-1.92369850
H	-1.82165020	-1.05976159	-2.62380950
C	-1.92585520	-0.55201859	0.66286950
H	-1.88985320	0.07151741	1.56542150
H	-2.96417220	-0.54878459	0.30929150
H	-1.67777220	-1.57883259	0.95653050
H	0.86293380	0.09292241	1.02792050

[Ir(cod)Cl]$_2$

Zero-point correction=	0.372139 (Hartree/Particle)
Thermal correction to Energy=	0.393130
Thermal correction to Enthalpy=	0.394074
Thermal correction to Gibbs Free Energy=	0.320765
Sum of electronic and zero-point Energies=	-1753.694545
Sum of electronic and thermal Energies=	-1753.673554
Sum of electronic and thermal Enthalpies=	-1753.672610
Sum of electronic and thermal Free Energies=	-1753.745919

SCF Done: E(RB3LYP) = -1753.70550193

Ir	-1.10949402	-0.30136986	0.01452407
C	-3.23462602	-0.99651086	2.13955107
C	-2.34240202	-1.66581186	1.09285007
C	-2.65526602	-1.70947986	-0.30038393
C	-3.86542802	-1.06009586	-0.95039293
C	-4.05949102	0.40825014	-0.50723893
C	-2.18575802	1.10974214	1.16533507
C	-2.81136402	0.46783714	2.39219007
C	-2.72781302	1.07369814	-0.15617493
H	-4.74053702	0.46739114	0.34911507

H	-3.66267502	1.06564514	2.75307507
H	-2.05933802	0.49070914	3.18942607
H	-4.28183402	-1.04646186	1.82128007
H	-3.17710402	-1.56012386	3.07717907
H	-1.71037202	-2.46912586	1.47091107
H	-2.25049202	-2.55163586	-0.86344893
H	-3.70477002	-1.08835586	-2.03428493
H	-2.42439802	1.87847714	-0.82555793
H	-1.52155302	1.94466214	1.39274807
H	-4.54137002	0.97058514	-1.31442493
H	-4.77431902	-1.65058386	-0.75673693
Cl	0.65516698	1.35412214	-0.55168193
Ir	2.41374898	-0.31182486	0.01446607
C	5.36372698	-1.02133686	-0.50752693
C	4.03206498	-1.68685786	-0.15653693
C	3.49005898	-1.72313986	1.16498507
C	4.11570598	-1.08145286	2.39193107
C	4.53897398	0.38293214	2.13952307
C	3.95950298	1.09635014	-0.30024793
C	5.16963998	0.44708414	-0.95042093
C	3.64669798	1.05242414	1.09299007
H	5.58616398	0.43292214	1.82119707
H	6.07853598	1.03754314	-0.75669893
H	5.00893498	0.47553314	-2.03429993
H	6.04479898	-1.08062086	0.34879907
H	5.84558698	-1.58352786	-1.31482493
H	3.72863398	-2.49152186	-0.82605093
H	2.82586898	-2.55810586	1.39227507
H	3.36370198	-1.10445486	3.18918407
H	3.01468198	1.85566614	1.47122707
H	3.55470298	1.93860514	-0.86314493
H	4.48151398	0.94638314	3.07725307
H	4.96702198	-1.67932986	2.75268907
Cl	0.64906998	-1.96720986	-0.55199193

Chlorotrimethylsilane

Zero-point correction=	0.113456 (Hartree/Particle)
Thermal correction to Energy=	0.122088
Thermal correction to Enthalpy=	0.123032
Thermal correction to Gibbs Free Energy=	0.080757
Sum of electronic and zero-point Energies=	-869.409103
Sum of electronic and thermal Energies=	-869.400472
Sum of electronic and thermal Enthalpies=	-869.399528

Sum of electronic and thermal Free Energies= -869.441802
SCF Done: E(RB3LYP) = -869.622659220

Si	-0.68493155	-0.28767123	0.00000000
C	-1.24500655	-1.72138523	-1.08193100
H	-0.88017055	-2.67837823	-0.69342000
H	-2.34091655	-1.76875623	-1.11992000
H	-0.87717755	-1.61247223	-2.10799500
C	-1.24374655	-0.50739523	1.78303700
H	-0.87490555	-1.45014323	2.20155700
H	-0.87914855	0.30786477	2.41732600
H	-2.33958655	-0.51734923	1.84336500
C	-1.24164255	1.36737077	-0.70056200
H	-0.87229455	1.51089577	-1.72179300
H	-2.33737355	1.42473077	-0.72688400
H	-0.87554855	2.20004877	-0.09015900
Cl	1.42587645	-0.28899023	0.00020100

Trimethylsilanamine

Zero-point correction= 0.137506 (Hartree/Particle)
Thermal correction to Energy= 0.146765
Thermal correction to Enthalpy= 0.147709
Thermal correction to Gibbs Free Energy= 0.105100
Sum of electronic and zero-point Energies= -465.109498
Sum of electronic and thermal Energies= -465.100239
Sum of electronic and thermal Enthalpies= -465.099295
Sum of electronic and thermal Free Energies= -465.141904
SCF Done: E(RB3LYP) = -465.344110138

N	0.32876714	0.34246575	0.00000000
Si	0.32841814	1.09797675	-1.58045500
C	0.32814114	2.99584375	-1.54330300
H	-0.55598386	3.38779275	-1.02494600
H	1.21287814	3.38807975	-1.02621400
H	0.32733914	3.41686475	-2.55718600
C	1.88537514	0.50539975	-2.47036500
H	2.79670614	0.79097075	-1.92986100
H	1.88720214	-0.58578625	-2.57039400
H	1.95694414	0.93714875	-3.47613600
C	-1.22856386	0.50489975	-2.46999300
H	-2.13984086	0.78961175	-1.92894600
H	-1.30083686	0.93709475	-3.47551900
H	-1.22972786	-0.58624025	-2.57053000

H	−0.49865686	0.44118175	0.57907500
H	1.15654614	0.44102875	0.57859600

5.3. Coordinates and energies of spirobicycle and *N,N*-diphenyl hexahydro-pyrimidine and 1,3-imidazole frameworks

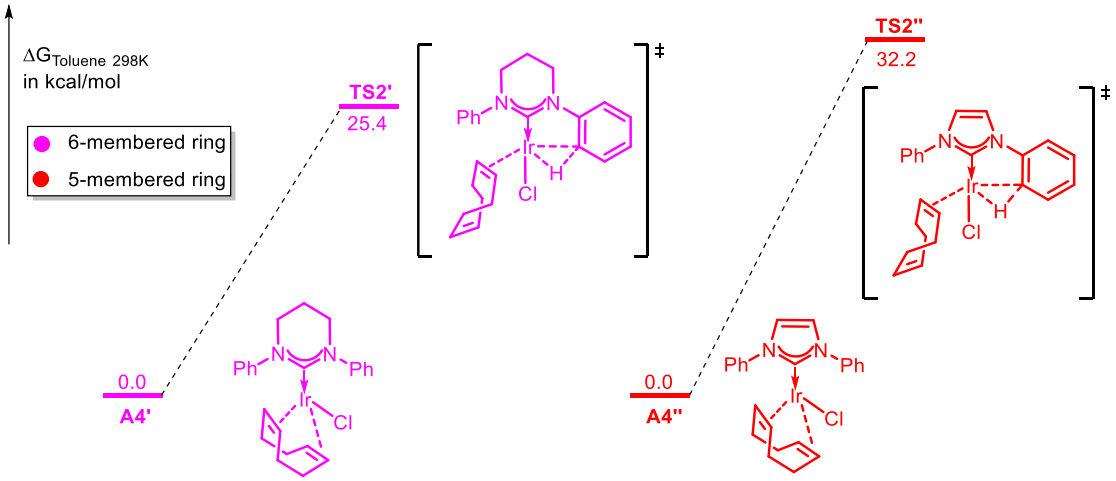


Fig. S3 Energy profiles for the *N,N*-diphenyl hexahydro-pyrimidine and 1,3-imidazole frameworks. Bond distances were given in Å.

A4' (*N,N*-diphenyl hexahydro-pyrimidine frameworks)

Zero-point correction=	0.473060 (Hartree/Particle)
Thermal correction to Energy=	0.498844
Thermal correction to Enthalpy=	0.499788
Thermal correction to Gibbs Free Energy=	0.415954
Sum of electronic and zero-point Energies=	−1605.381353
Sum of electronic and thermal Energies=	−1605.355570
Sum of electronic and thermal Enthalpies=	−1605.354625
Sum of electronic and thermal Free Energies=	−1605.438460

SCF Done: E(RB3LYP) = −1605.88584438

Ir	−1.08219185	−0.08219178	0.00000000
N	−0.12374085	2.67593422	−0.52607000
N	−2.43441085	2.55245822	−0.56387900
C	−1.24317185	1.91136722	−0.42742000
C	−2.18598885	−2.96151778	−0.62522700
C	−0.10278685	4.15121922	−0.61040300
C	−1.45791185	−2.24494678	0.50445400
C	−1.40899085	4.73107622	−0.09508000
C	−0.08274485	−1.99183978	0.52225100
C	−2.55833485	4.00913322	−0.78001000
C	0.90092615	−2.33003378	−0.58217200
C	0.39686715	−1.93964678	−1.99030400

C	-1.91715585	-0.72593278	-1.84140300
C	-2.76484485	-1.97486278	-1.66547500
C	1.19500415	2.08408122	-0.52346200
C	1.90138615	2.00963722	-1.72806600
C	3.21016415	1.52283622	-1.74096900
C	3.81782015	1.12277122	-0.54919400
C	3.11453415	1.21657122	0.65495000
C	1.80690415	1.70409822	0.67550200
C	-3.69294585	1.85083222	-0.49945700
C	-4.12497785	1.25191922	0.68771900
C	-5.38046985	0.64139922	0.73109100
C	-6.20994185	0.63902822	-0.39275800
C	-5.78004485	1.25162122	-1.57175100
C	-4.52374585	1.85796322	-1.62579300
C	-0.49120285	-0.69285878	-1.96567400
H	0.07596915	4.46153822	-1.64971400
H	-3.52145785	4.32195222	-0.37009900
H	-5.71077585	0.17271922	1.65397300
H	4.83621015	0.74372622	-0.55766500
H	-0.14403085	-2.77347778	-2.45300100
H	-2.91585885	-2.48176378	-2.63274600
H	-3.75612185	-1.64545978	-1.33225500
H	-1.51066585	-3.67484078	-1.11005500
H	-3.00219685	-3.55904978	-0.20263000
H	-1.97623585	-2.20235978	1.45982000
H	0.36642215	-1.79728278	1.49432800
H	1.82200715	-1.77463878	-0.37321500
H	3.58325015	0.90915522	1.58574100
H	1.24496015	1.75874722	1.60132600
H	-3.47552285	1.25568422	1.55599700
H	-0.08044385	0.14842722	-2.52112400
H	3.75170815	1.45739622	-2.68075700
H	-6.41707785	1.25467122	-2.45207100
H	-7.18742985	0.16635722	-0.34966100
H	-2.46208985	0.08335022	-2.32770000
H	1.26214615	-1.74979978	-2.63595000
H	1.16696415	-3.39876078	-0.55003900
H	-4.18204685	2.32707922	-2.54457900
Cl	-1.06643385	0.52282722	2.38540800
H	1.42120015	2.32355922	-2.65093600
H	0.74550515	4.50181722	-0.01505700
H	-1.45350685	5.80529722	-0.30329200
H	-1.48067285	4.59111122	0.98951100
H	-2.56606485	4.23445922	-1.85617400

TS2' (*N,N*-diphenyl hexahydro-pyrimidine frameworks)

Zero-point correction=	0.468200 (Hartree/Particle)
Thermal correction to Energy=	0.493812
Thermal correction to Enthalpy=	0.494756
Thermal correction to Gibbs Free Energy=	0.411930
Sum of electronic and zero-point Energies=	-1605.329952
Sum of electronic and thermal Energies=	-1605.304340
Sum of electronic and thermal Enthalpies=	-1605.303396
Sum of electronic and thermal Free Energies=	-1605.386222

SCF Done: E(RB3LYP) = -1605.84133711

Ir	0.10928961	0.32786885	0.00000000
N	1.99809361	2.02510585	-1.31713700
N	-0.11110739	3.04224485	-1.21719900
C	0.67656061	1.95193285	-0.95382100
C	-3.84317939	-1.34381515	-1.77485000
C	2.64813361	3.18897985	-1.93387100
C	-3.39793939	-2.49056815	-2.64970100
C	1.83434161	4.45147685	-1.68835900
C	-2.33336839	-3.29857515	-2.55934300
C	0.37195661	4.18280885	-2.01596100
C	-1.20787939	-3.29894115	-1.54754100
C	-0.09276839	-2.28306715	-1.87156100
C	-1.61860639	-0.16144115	-1.36046100
C	-2.85103839	-0.78767415	-0.73244800
C	2.78796161	0.90695985	-0.95160000
C	4.07299661	0.66989685	-1.44319800
C	4.75872861	-0.47909415	-1.04064200
C	4.15891561	-1.38450815	-0.16065100
C	2.87207461	-1.15397315	0.32598700
C	2.16086161	-0.00669815	-0.06860300
C	-1.41655939	3.13538785	-0.64619100
C	-1.64571039	2.73226085	0.67847800
C	-2.93057039	2.81183685	1.22030500
C	-3.98697139	3.32212085	0.46453000
C	-3.75243939	3.74873185	-0.84483000
C	-2.47733439	3.65171585	-1.40277500
C	-0.46451539	-0.80731115	-1.86566300
H	2.77108161	3.01135385	-3.01123800
H	-0.24649139	5.04916585	-1.77374900
H	-3.09445839	2.48588385	2.24317700
H	4.69672361	-2.27674515	0.14885100

H	0.28925961	-2.49948015	-2.88019200
H	-3.37117339	0.00042985	-0.17384200
H	-2.58901939	-1.54407615	0.00472800
H	-4.15780239	-0.52244415	-2.43824300
H	-4.76316239	-1.64512515	-1.24751200
H	-4.07716139	-2.67958315	-3.48368300
H	-2.23831839	-4.05250215	-3.34257500
H	-1.55912939	-3.13919615	-0.52731200
H	2.39991261	-1.84480715	1.01642000
H	1.49680861	0.57485685	0.99253900
H	-0.81491939	2.39967085	1.29715000
H	0.06340761	-0.25029015	-2.63805600
H	5.75997461	-0.66339915	-1.41925500
H	-4.56728539	4.14561885	-1.44394600
H	-4.98286439	3.39115285	0.89220100
H	-1.84773039	0.77557485	-1.86877400
H	0.75085461	-2.45116915	-1.19296300
H	-0.74419139	-4.29362015	-1.55061500
H	-2.31416839	3.95250985	-2.43348700
Cl	-0.48505939	-1.45374715	1.59251500
H	4.53494861	1.34905485	-2.15323300
H	0.25176661	3.97283185	-3.08827000
H	1.92185661	4.75838685	-0.63962300
H	2.21943361	5.26688085	-2.30952900
H	3.64728261	3.28868385	-1.50057500

A4'' (*N,N*-diphenyl 1,3-imidazole frameworks)

Zero-point correction=	0.420330 (Hartree/Particle)
Thermal correction to Energy=	0.444306
Thermal correction to Enthalpy=	0.445251
Thermal correction to Gibbs Free Energy=	0.365542
Sum of electronic and zero-point Energies=	-1564.922324
Sum of electronic and thermal Energies=	-1564.898347
Sum of electronic and thermal Enthalpies=	-1564.897403
Sum of electronic and thermal Free Energies=	-1564.977111

SCF Done: E(RB3LYP) = -1565.36300166

Ir	-0.27322403	0.84699452	0.00000000
N	-1.28206403	-2.02032148	-0.40853900
N	0.87753697	-1.97975948	-0.40092700
C	-0.21851803	-1.16406148	-0.27238400
C	0.98739197	3.54561052	-1.00363200
C	-0.85196503	-3.33048848	-0.61999500
C	0.25490197	3.02239452	0.22590100

C	-1.13172403	2.86925652	0.31326500
C	0.49851097	-3.30518848	-0.61576900
C	-2.13038803	3.13564752	-0.79755600
C	-1.70263203	2.54400952	-2.16034200
C	0.53230197	1.20440852	-1.93011700
C	1.46167197	2.40577852	-1.93504000
C	-2.67135403	-1.66218748	-0.37283300
C	-3.49682003	-2.06964648	-1.42478000
C	-4.85881303	-1.76673148	-1.38949300
C	-5.38913703	-1.05451648	-0.31217200
C	-4.55458403	-0.65186248	0.73339800
C	-3.19278303	-0.95777648	0.71552500
C	2.25150197	-1.56964348	-0.34760300
C	2.72636397	-0.82748748	0.73703900
C	4.07442097	-0.46663048	0.77073400
C	4.94146897	-0.85197448	-0.25467400
C	4.45782997	-1.60259048	-1.32797800
C	3.10993097	-1.96063448	-1.37953300
C	-0.89754803	1.25086952	-2.00672200
H	4.44670497	0.11128152	1.61178700
H	-6.44881803	-0.81611148	-0.28656000
H	-1.12536803	3.27690752	-2.73556000
H	1.60744197	2.78361252	-2.96013100
H	2.44279297	2.05376452	-1.59442800
H	0.34309497	4.24240252	-1.55065300
H	1.85574597	4.13056852	-0.67899400
H	0.80247397	3.06064652	1.16504700
H	-1.55697203	2.82662552	1.31419900
H	-3.07880103	2.67634352	-0.49642200
H	-4.96333203	-0.10445748	1.57795800
H	-2.53872403	-0.65767948	1.52726600
H	2.04783897	-0.54036448	1.53335400
H	-1.38388003	0.37579952	-2.43753600
H	-5.49987303	-2.08052348	-2.20850200
H	5.12408197	-1.90310848	-2.13170700
H	5.99000697	-0.56996048	-0.21687600
H	1.00824897	0.30512052	-2.32478700
H	-2.60007603	2.33951052	-2.75561300
H	-2.32541803	4.21594152	-0.89072200
H	2.72047197	-2.52543648	-2.22188600
Cl	-0.27241803	0.50552452	2.42426800
H	-3.07157303	-2.60508948	-2.26899800
H	-1.54876603	-4.14785948	-0.71270300
H	1.22588997	-4.09603248	-0.70344900

TS2'' (*N,N*-diphenyl 1,3-imidazole frameworks)

Zero-point correction=	0.414648 (Hartree/Particle)
Thermal correction to Energy=	0.438788
Thermal correction to Enthalpy=	0.439732
Thermal correction to Gibbs Free Energy=	0.359623
Sum of electronic and zero-point Energies=	-1564.860384
Sum of electronic and thermal Energies=	-1564.836244
Sum of electronic and thermal Enthalpies=	-1564.835300
Sum of electronic and thermal Free Energies=	-1564.915409

SCF Done: E(RB3LYP) = -1565.30577345

Ir	0.08196721	0.16393442	0.00000000
N	-0.60145079	-2.28408758	-1.34320000
N	1.56266921	-2.33275058	-1.16164500
C	0.46840321	-1.54672858	-0.88791800
C	3.17779821	3.37298442	-1.27422200
C	-0.18917579	-3.49308758	-1.88715600
C	2.45164721	4.19992942	-2.30678500
C	1.14571621	4.44668442	-2.47429800
C	1.16104621	-3.52334758	-1.77929300
C	-0.04158879	3.93913042	-1.68388400
C	-0.49760279	2.52849942	-2.10881800
C	1.65853621	1.32642542	-1.11712500
C	2.34772521	2.44872642	-0.36014300
C	-1.88137079	-1.72901858	-1.13236200
C	-3.05428179	-2.21413758	-1.70345500
C	-4.24969479	-1.53370158	-1.46560800
C	-4.25191379	-0.38145458	-0.67192800
C	-3.07359179	0.09886442	-0.09889800
C	-1.85443279	-0.56633058	-0.32165000
C	2.90819521	-2.04806058	-0.78059700
C	3.17912121	-1.53689258	0.49351400
C	4.49865821	-1.26917458	0.85817400
C	5.54485821	-1.52857158	-0.03028700
C	5.26714621	-2.05061958	-1.29535000
C	3.94982021	-2.30535058	-1.67771300
C	0.47285421	1.38055342	-1.88280100
H	4.70678421	-0.86846158	1.84595500
H	-5.18436779	0.14712642	-0.49247800
H	-0.71193579	2.54182642	-3.18775700
H	3.04272721	1.98510242	0.35197500
H	1.64848021	3.02131142	0.24626700
H	3.93217421	2.76793842	-1.80184200

H	3.76238321	4.05343642	-0.63382000
H	3.12660321	4.67539042	-3.02147600
H	0.88558321	5.08165942	-3.32265100
H	0.12957121	3.95440442	-0.60671700
H	-3.07923179	0.98031942	0.53317300
H	-1.10751879	-0.69067258	0.87367700
H	2.36204721	-1.35893258	1.18574100
H	0.39472121	0.61687542	-2.65444400
H	-5.17363979	-1.90135558	-1.90189900
H	6.07461921	-2.24895158	-1.99429400
H	6.57096221	-1.32507458	0.26177100
H	2.36337921	0.56786442	-1.45972500
H	-1.45110579	2.29734642	-1.62011100
H	-0.88672779	4.61606142	-1.86125900
H	3.72772821	-2.68094858	-2.67228400
Cl	-0.45565579	2.03549842	1.47642200
H	-3.03845079	-3.09166358	-2.34446000
H	-0.87749879	-4.22280958	-2.28210600
H	1.87132021	-4.28985958	-2.04415300

6. Catalytic homo and hetero addition of styrene derivatives

Procedure A:

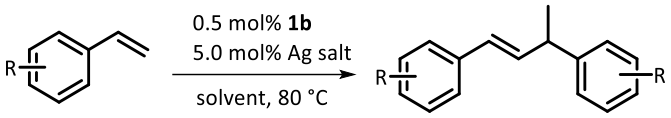
In glove box, to dry THF (0.5 mL) were added **1b** (3.3 mg, 0.005 mmol, 0.5 mol%) and AgOTf (12.8 mg, 0.05 mmol, 5.0 mol%) in a 10.0 mL dry Schlenk tube at room temperature. The system was stirred for 10 min. Then the styrene derivative **2** (1.0 mmol, 1.0 equiv.) was subsequently added. The tube was taken out from the glove box and placed in a preheated oil bath (80 °C) and the mixture was stirred for about 16-36 h. The resulting solution was concentrated *in vacuo*, and the residual was purified by silica gel column chromatography (eluting with PE) to give the desired products **4**.

Procedure B:

In glove box, to dry dioxane (0.5 mL) were added **1b** (3.3 mg, 0.005 mmol, 1.0 mol%) and AgOTf (6.5 mg, 0.025 mmol, 5.0 mol%) in a 10.0 mL dry Schlenk tube at room temperature. The system was stirred for 10 min. Then the styrene derivative **2** (0.5 mmol, 1.0 equiv.) and **3** (1.25 mmol, 2.5 equiv.) were subsequently added. The tube was taken out from the glove box and placed in a preheated oil bath (100 °C) and the mixture was stirred for 8 h. The resulting solution was concentrated *in vacuo*, and the residual was purified by silica gel column chromatography (eluting with PE) to give the desired products **4**.

6.1. Screening of homo addition conditions and substituent effect

Table S21. Screening of conditions[a]



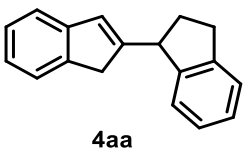
2 **product 4**

Entry	**2** (R=)	Ag salt	Solvent	t (h)	Product (**4**)	Yield[b] (%)
1	H, 2c	$AgSbF_6$	DCE	16	4cc	23
2	H, 2c	$AgSbF_6$	hexane	16	4cc	20
3	H, 2c	$AgSbF_6$	EtOH	16	-	ND[c]
4	H, 2c	$AgSbF_6$	dioxane	16	4cc	31
5	H, 2c	$AgSbF_6$	THF	16	4cc	50
6	H, 2c	$AgPF_6$	dioxane	16	4cc	29
7	H, 2c	$AgPF_6$	THF	16	4cc	55
8	H, 2c	$AgBF_4$	THF	16	-	ND
9	H, 2c	AgOTf	THF	16	4cc	89
10[d]	H, 2c	AgOTf	THF	16	-	ND
11[e]	H, 2c	AgOTf	THF	16	4cc	86
12	4-Me, 2b	AgOTf	THF	16	4bb	83
13	3-Me, 2g	AgOTf	THF	24	4gg	72
14	2-Me, 2e	AgOTf	THF	24	4ee	81
15	4-^{t}Bu, 2h	AgOTf	THF	16	4hh	79
16[f]	4-OMe	AgOTf	THF	16	-	<5
17	4-F, 2f	AgOTf	THF	20	4ff	90
18	2-F, 2i	AgOTf	THF	36	4ii	38
19	4-Cl, 2j	AgOTf	THF	36	4jj	78
20	4-CF_3, 2d	AgOTf	THF	24	4dd	33
21	4-CF_3, 2d	AgOTf	DCE	24	4dd	85

[a]Conditions: Unless otherwise specified, reactions were conducted using: **2** (1.0 mmol), **1b** (0.5 mol%) and Ag salt (5.0 mol%) in solvent (0.5 mL) at 80 °C for 16-36 h. [b]Isolated yields. [c]Not detected by GC-MS. [d]**1a** was used as catalyst. [e]**1c** was used as catalyst. [f]Yield determined by GC-MS.

6.2. Catalytic homo addition of styrene derivatives

2,3-dihydro-1H,1'H-1,2'-biindene **(4aa)**

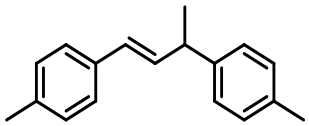


4aa

The reaction of **2a** (116.6 μL, 1.0 mmol) was conducted under procedure A for 16 h to give the desired product **4aa** (107.1 mg, 92% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33

(d, *J* = 7.3 Hz, 1H), 7.26 (t, *J* = 6.4 Hz, 2H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.18-7.05 (m, 4H), 6.59 (s, 1H), 4.30 (t, *J* = 7.7 Hz, 1H), 3.38-3.19 (m, 2H), 3.08-2.97 (m, 1H), 2.97-2.84 (m, 1H), 2.50-2.37 (m, 1H), 2.15-1.98 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.3, 145.7, 145.1, 143.8, 143.3, 127.2, 126.6, 126.3, 126.3, 124.6, 124.5, 123.8, 123.5, 120.2, 47.3, 38.6, 33.7, 31.7; **HRMS (MALDI)** calcd for $[M]^+$ $C_{18}H_{16}$, m/z: 232.1252, found: 232.1247, Error 2.2 ppm.

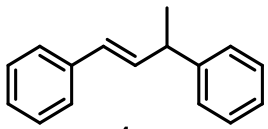
(*E*)-4,4'-(but-1-ene-1,3-diyl)bis(methylbenzene) **(4bb)**



4bb

The reaction of **2b** (131.7 μL, 1.0 mmol) was conducted under procedure A for 16 h to give the desired product **4bb** (97.6 mg, 83% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 8.1 Hz, 2H), 7.18-7.05 (m, 6H), 6.41-6.26 (m, 2H), 3.58 (m, 1H), 2.31 (d, *J* = 5.2 Hz, 6H), 1.43 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.8, 136.7, 135.6, 134.8, 134.4, 129.1, 129.1, 128.1, 127.2, 126.0, 42.1, 21.3, 21.1, 21.0; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{18}H_{20}Na$, m/z: 259.1457, found: 259.1454, Error 1.3 ppm.

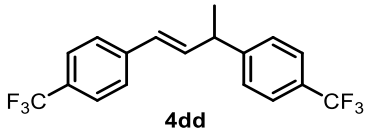
(*E*)-but-1-ene-1,3-diyldibenzene **(4cc)**



4cc

The reaction of **2c** (114.9 μL, 1.0 mmol) was conducted under procedure A for 16 h to give the desired product **4cc** (92.9 mg, 89% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37-7.22 (m, 8H), 7.22-7.13 (m, 2H), 6.45-6.31 (m, 2H), 3.68-3.56 (m, 1H), 1.45 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.6, 137.5, 135.2, 128.5, 128.4, 127.3, 127.0, 126.2, 126.1, 42.5, 21.2; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{16}H_{16}Na$, m/z: 231.1144, found: 231.1145, Error 0.3 ppm.

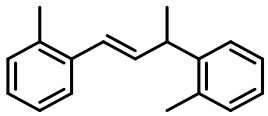
(*E*)-4,4'-(but-1-ene-1,3-diyl)bis((trifluoromethyl)benzene) **(4dd)**



4dd

The reaction of **2d** (147.7 μL, 1.0 mmol) was conducted under procedure A in 0.5 mL DCE for 24 h to give the desired product **4dd** (146.2 mg, 85% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.1 Hz, 2H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 2H), 6.44 (d, *J* = 3.0 Hz, 2H), 3.77-3.64 (m, 1H), 1.48 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.1, 140.7, 136.8, 129.6, 129.3, 129.0, 129.0, 128.6, 128.3, 128.1, 127.7, 126.4, 125.7, 125.6, 125.6, 125.6, 125.5, 125.5, 125.5, 125.4, 123.0, 122.9, 42.5, 20.8; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.29, -62.38; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{18}H_{14}F_6Na$, m/z: 367.0892, found: 367.0866, Error 7.1 ppm.

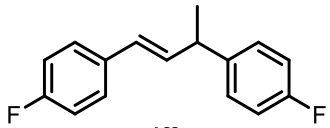
(*E*)-2,2'-(but-1-ene-1,3-diyl)bis(methylbenzene) **(4ee)**



4ee

The reaction of **2e** (129.3 μL, 1.0 mmol) was conducted under procedure A for 24 h to give the desired product **4ee** (96.6 mg, 81% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 5.0 Hz, 1H), 7.25 (d, *J* = 7.6 Hz, 1H), 7.21-7.03 (m, 6H), 6.56 (d, *J* = 15.8 Hz, 1H), 6.20 (dd, *J* = 15.8, 6.5 Hz, 1H), 3.92-3.80 (m, 1H), 2.37 (s, 3H), 2.29 (s, 3H), 1.44 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.5, 136.7, 136.2, 135.5, 135.0, 130.4, 130.1, 126.9, 126.3, 126.2, 126.2, 126.0, 126.0, 125.5, 38.4, 20.5, 19.8, 19.5; **HRMS (MALDI)** calcd for $[M]^+$ $C_{18}H_{20}$, m/z: 236.1565, found: 236.1560, Error 2.1 ppm.

(*E*)-4,4'-(but-1-ene-1,3-diyl)bis(fluorobenzene) **(4ff)**

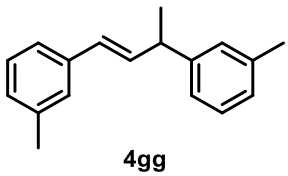


4ff

The reaction of **2f** (119.3 μL, 1.0 mmol) was conducted under procedure A for 20 h to give the desired product **4ff** (109.9 mg, 90% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30-7.23 (m, 2H), 7.21-7.14 (m, 2H), 7.02-6.89 (m, 4H), 6.37-6.18 (m, 2H), 3.57 (m, 1H), 1.41 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.3, 162.6, 160.8, 160.2, 141.1, 141.1, 134.7, 134.7, 128.7, 128.6, 127.6, 127.5, 127.5, 115.4, 115.3, 115.2, 115.1, 41.7, 21.2; **^{19}F NMR** (376 MHz,

$CDCl_3$) δ -114.97, -116.83; **HRMS (MALDI)** calcd for $[M]^+$ $C_{16}H_{14}F_2$, m/z: 244.1064, found: 244.1058, Error 2.5 ppm.

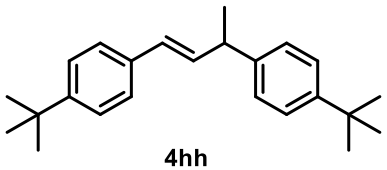
(*E*)-3,3'-(but-1-ene-1,3-diyl)bis(methylbenzene) **(4gg)**



4gg

The reaction of **2g** (131.2 μL, 1.0 mmol) was conducted under procedure A for 24 h to give the desired product **4gg** (85.0 mg, 72% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.26-7.12 (m, 4H), 7.11-7.04 (m, 2H), 7.04-6.96 (m, 2H), 6.44-6.30 (m, 2H), 3.66-3.49 (m, 1H), 2.33 (s, 3H), 2.31 (s, 3H), 1.44 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.6, 138.0, 138.0, 137.5, 135.1, 128.4, 128.4, 128.1, 127.8, 126.9, 126.8, 124.3, 123.3, 42.5, 21.5, 21.4, 21.2; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{18}H_{20}Na$, m/z: 259.1457, found: 259.1449, Error 3.1 ppm.

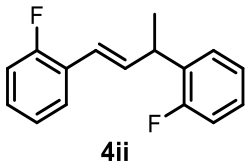
(*E*)-4,4'-(but-1-ene-1,3-diyl)bis(tert-butylbenzen*e)* **(4hh)**



4hh

The reaction of **2h** (183.2 μL, 1.0 mmol) was conducted under procedure A for 16 h to give the desired product **4hh** (127.1 mg, 79% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35-7.27 (m, 6H), 7.22-7.17 (m, 2H), 6.46-6.27 (m, 2H), 3.66-3.54 (m, 1H), 1.44 (d, *J* = 7.0 Hz, 3H), 1.31 (s, 9H), 1.30 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.0, 148.9, 142.7, 134.9, 134.7, 128.0, 126.9, 125.8, 125.4, 125.3, 42.0, 34.5, 34.4, 31.4, 31.3, 21.2; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{24}H_{32}Na$, m/z: 343.2396, found: 343.2383, Error 3.9 ppm.

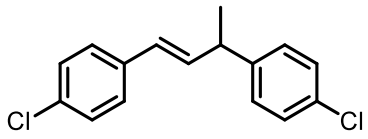
(*E*)-2,2'-(but-1-ene-1,3-diyl)bis(fluorobenzene) **(4ii)**



4ii

The reaction of **2i** (119.2 μL, 1.0 mmol) was conducted under procedure A for 36 h to give the desired product **4ii** (46.5 mg, 38% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48-7.38 (m, 1H), 7.30-7.22 (m, 1H), 7.22-7.13 (m, 2H), 7.13-6.96 (m, 4H), 6.66-6.42 (m, 2H), 4.04-3.94 (m, 1H), 1.47 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.7, 161.3, 159.3, 158.8, 136.1, 136.0, 128.4, 128.3, 128.3, 127.8. 127.7, 127.1, 127.1, 124.2, 124.2, 124.0, 124.0, 121.4, 121,4, 115.7, 115.6, 115.5, 115.4, 36.1, 36.0, 20.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -118.52, -118.54; **HRMS (MALDI)** calcd for $[M]^+$ $C_{16}H_{14}F_2$, m/z: 244.1064, found: 244.1058, Error 2.5 ppm.

(*E*)-4,4'-(but-1-ene-1,3-diyl)bis(chlorobenzene) **(4jj)**

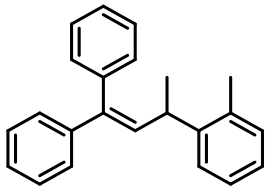


4jj

The reaction of **2j** (120.0 μL, 1.0 mmol) was conducted under procedure A 36 h to give the desired product **4jj** (107.9 mg, 78% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32-7.21 (m, 6H), 7.21-7.11 (m, 2H), 6.38-6.25 (m, 2H), 3.66-3.54 (m, 1H), 1.43 (d, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.7, 135.8, 135.3, 132.7, 132.0, 128.6, 128.6, 128.6, 127.7, 127.3, 41.9, 21.0; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{16}H_{14}Cl_2Na$, m/z: 299.0365, found: 299.0355, Error 3.3 ppm.

6.3. Catalytic hetero addition of styrene derivatives

(3-(o-tolyl)but-1-ene-1,1-diyl)dibenzene **(4ea)**

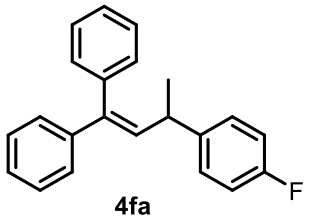


4ea

The reaction of **2e** (64.6 μL, 0.5 mmol, 1.0 equiv.) and **3a** (220.6 μL, 1.25 mmol, 2.5 equiv.) was conducted under procedure B for 8 h to give the desired product **4ea** (123.7 mg, 83% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39-7.27 (m, 4H), 7.27-7.16 (m, 6H), 7.16-7.11 (m, 2H), 7.10-7.05 (m, 2H), 6.24 (d, *J* = 10.0 Hz, 1H), 3.83-3.69 (m, 1H), 1.96 (s, 3H), 1.37 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.9, 142.4, 140.3, 140.1, 135.2, 134.1, 130.3, 129.7,

128.1, 128.0, 127.3, 127.1, 127.0, 126.2, 125.9, 125.7, 35.3, 22.7, 19.2; **IR** (KBr): 3078, 2925, 1491, 1444, 1265, 1030, 778, 701 cm^{-1}; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{23}H_{22}Na$, m/z: 321.1614, found: 321.1610, Error 1.1 ppm.

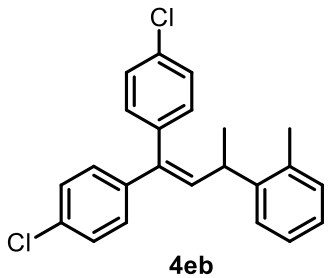
(3-(4-fluorophenyl)but-1-ene-1,1-diyl)dibenzene **(4fa)**



4fa

The reaction of **2f** (59.7 μL, 0.5 mmol, 1.0 equiv.) and **3a** (220.6 μL, 1.25 mmol, 2.5 equiv.) was conducted under procedure B for 8 h to give the desired product **4fa** (113.3 mg, 75% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40-7.31 (m, 3H), 7.27-7.19 (m, 5H), 7.19-7.10 (m, 4H), 7.00-6.90 (m, 2H), 6.16 (d, *J* = 10.3 Hz, 1H), 3.63-3.52 (m, 1H), 1.36 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.4, 160.0, 142.1, 141.8, 141.8, 140.3, 139.9, 133.8, 129.7, 128.3, 128.2, 128.1, 127.2, 127.1, 127.1, 115.3, 115.0, 38.5, 22.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -117.20; **IR** (KBr): 2963, 2926, 1508, 1444, 1224, 1159, 834, 701 cm^{-1}; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{22}H_{19}FNa$, m/z: 325.1363, found: 325.1363, Error 0 ppm.

4,4'-(3-(o-tolyl)but-1-ene-1,1-diyl)bis(chlorobenzene) **(4eb)**

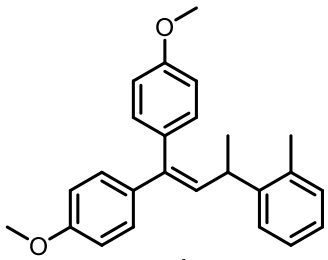


4eb

The reaction of **2e** (64.6 μL, 0.5 mmol, 1.0 equiv.) and **3b** (310 mg, 1.25 mmol, 2.5 equiv.) was conducted under procedure B for 8 h to give the desired product **4eb** (161.6 mg, 88% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36-7.28 (m, 3H), 7.23-7.16 (m, 3H), 7.11-7.06 (m, 4H), 7.06-7.01 (m, 2H), 6.23 (d, *J* = 10.0 Hz, 1H), 3.75-3.65 (m, 1H), 1.98 (s, 3H), 1.37 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.4, 140.5, 138.1, 138.0, 135.1, 135.1, 133.2, 133.0, 131.0, 130.4, 128.6, 128.5, 128.2, 126.4, 125.9, 125.8, 35.4, 22.6, 19.3; **IR** (KBr): 2963, 2925, 1490,

1460, 1264, 1091, 830, 737 cm^{-1}; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{23}H_{20}Cl_2Na$, m/z: 389.0834, found: 389.0844, Error 2.6 ppm.

4,4'-(3-(o-tolyl)but-1-ene-1,1-diyl)bis(methoxybenzene) **(4ec)**



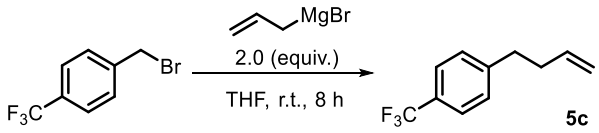
4ec

The reaction of **2e** (64.6 μL, 0.5 mmol, 1.0 equiv.) and **3c** (300 mg, 1.25 mmol, 2.5 equiv.) was conducted under procedure B for 8 h to give the desired product **4ec** (115.0 mg, 64% yield) as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.6 Hz, 1H), 7.23-7.16 (m, 1H), 7.13 (d, *J* = 8.7 Hz, 2H), 7.11-7.01 (m, 4H), 6.89 (d, *J* = 8.6 Hz, 2H), 6.78 (d, *J* = 8.7 Hz, 2H), 6.09 (d, *J* = 10.0 Hz, 1H), 3.84 (s, 3H), 3.78 (s, 3H), 3.77-3.70 (m, 1H), 2.00 (s, 3H), 1.37 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.7, 158.5, 145.3, 139.2, 135.6, 135.3, 132.7, 132.3, 130.8, 130.3, 128.5, 126.2, 125.9, 125.6, 113.4, 113.3, 55.2, 55.2, 35.4, 22.8, 19.3; **IR** (KBr): 2958, 2929, 1511, 1462, 1247, 1035, 832, 736 cm^{-1}; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{25}H_{26}O_2Na$, m/z: 381.1825, found: 381.1834, Error 2.3 ppm.

7. Catalytic olefin isomerization reaction

7.1. Synthesis of substrates

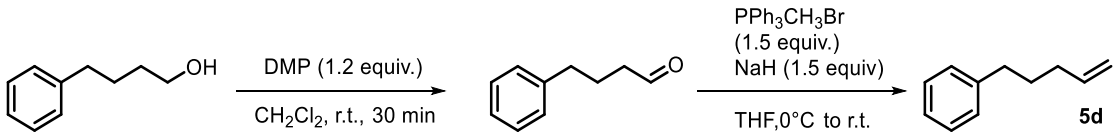
1-(But-3-en-1-yl)-4-(trifluoromethyl) benzene **(5c)**



Following a reported procedure:[5]

To a solution of 4-trifluoromethylbenzyl bromide (2.39 g, 10 mmol, 1.0 equiv.) in dry THF (30.0 mL), allylmagnesium bromide (1.0 mol/L in Et_2O, 20.0 mL, 20 mmol, 2.0 equiv.) was added dropwise and the resulting mixture was stirred for 8 h at room temperature under argon atmosphere. After the reaction was completed, the system was quenched by saturated aqueous NH_4Cl (15.0 mL) at 0 °C. Then the mixture was extracted with EA (3 × 15.0 mL), the combined organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give the crude product, which was purified by column chromatography on silica gel (eluting with PE) to afford the desired product **5c** as a colorless oil (1.82 g, 91% yield). The spectral data is consistent with the literature.[5] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46 (d, J = 7.9 Hz, 2H), 7.25-7.17 (m, 2H), 5.81-5.71 (m, 1H), 5.02-4.88 (m, 2H), 2.69 (t, J = 7.8 Hz, 2H), 2.37-2.26 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.8, 137.3, 128.7, 128.3, 128.0, 125.7, 125.2, 125.2, 125.1, 125.1, 122.9, 115.4, 35.1, 35.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.29; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{11}H_{11}F_3$, m/z: 223.0705, found: 223.0716, Error 4.9 ppm.

Pent-4-en-1-ylbenzene **(5d)**



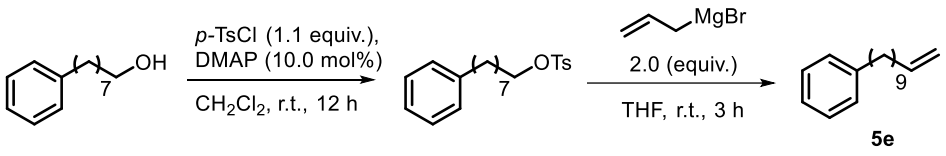
Following a reported procedure:[6]

Step 1: Under argon atmosphere, 4-phenylbutan-1-ol (1.5 g, 10 mmol, 1.0 equiv.) was dissolved in DCM (30.0 mL) and then Dess-Martin periodinane (5.1 g, 12.0 mmol, 1.2 equiv.) was slowly added to the solution. The reaction mixture was stirred at room temperature for 30 min. After the reaction was complete, saturated aqueous $NaHCO_3$ was added, and the aqueous phase was extracted

with DCM (3 × 20.0 mL). The combined organic layer was dried over anhydrous Na_2SO_4 and then concentrated under reduced pressure. The obtained crude prodect was further purified by flash column chromatography to afford the desired product (1.35 g, 91% yield), which can be used directly in the next step.

Step 2: Methyltriphenylphosp honium bromide (4.88 g, 13.7 mmol, 1.0 equiv.) was dissolved in THF (20.0 mL) under a nitrogen atmosphere and cooled to 0 °C. After that, sodium hydride (328 mg, 13.7 mmol, 1.0 equiv.) was added, the mixture was stirred for 3 h (the system was allowed to rise to room temperature). After the reaction was completed, the reaction mixture was quenched by saturated aqueous NH_4Cl (15.0 mL) at 0 °C. The organic layer was separated and the aqueous layer was extracted with EA (3 × 15.0 mL). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluting with PE) to afford the product **5d** as a colorless oil (930.0 mg, 64% yield). The spectral data is consistent with the literature.[6] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (q, *J* = 6.1, 4.4 Hz, 3H), 7.22-7.15 (m, 3H), 5.89-5.79 (m, 1H), 5.10-4.89 (m, 2H), 2.62 (t, *J* = 7.8 Hz, 2H), 2.12-2.07 (m, 2H), 1.76-1.68 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.4, 138.5, 128.4, 128.2, 125.6, 114.6, 35.3, 33.2, 30.6; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{11}H_{15}$, m/z: 147.1168, found: 147.1177, Error 6.1 ppm.

Undec-10-en-1-ylbenzene **(5e)**



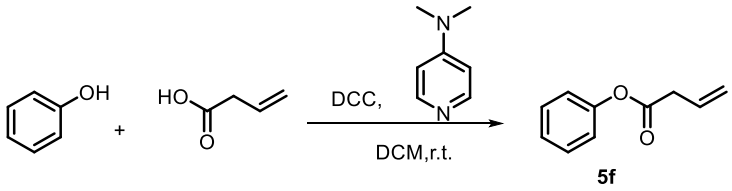
Following a reported procedure:[7]

Step 1: Under argon atmosphere, to a solution of 8-phenyl-1-octanol (0.45 g, 2.16 mmol, 1.0 equiv.) in DCM (8.0 mL), DMAP (26 mg, 0.22 mmol, 10.0 mol%), *para*-toluenesulfonylchloride (*p*-TsCl, 0.45 g, 2.37 mmol, 1.1 equiv.) and Et_3N (0.6 mL, 4.32 mmol, 2.0 equiv.) were added. The reaction mixture was stirred for 12 h at room temperature. After the reaction was completed, the reaction system was diluted with water (20.0 mL) and extracted with DCM (3 × 20.0 mL). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated *in vacuo* to give the crude product, which was purified by silica chromatography (eluting with PE:EA = 8:1) to give the

product as colorless oil (493 mg, 63% yield). The product can be used directly for the next step.

Step 2: To a solution of tosylate (493.0 mg, 1.37 mmol, 1.0 equiv.) in dry THF (8.0 mL), allylmagnesium bromide (1.0 mol/L in Et_2O, 2.8 mL, 2.8 mmol, 2.0 equiv.) was added dropwise and the resulting mixture was stirred for 3 h at room temperature under argon atmosphere. After the reaction was completed, the reaction mixture was quenched by NH_4Cl (15.0 mL, saturated aqueous solution) at 0 °C. The organic layer was separated and the aqueous layer was extracted with EA (3 × 15.0 mL). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give the crude product as colorless oil, which was purified by column chromatography on silica gel (eluting with petroleum ether) to afford the desired product **5e** as a colorless oil (258.0 mg, 82% yield). The spectral data is consistent with the literature.[7] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.23-7.15 (m, 2H), 7.14-7.04 (m, 3H), 5.80-5.63 (m, 1H), 4.98-4.80 (m, 2H), 2.51 (t, *J* = 7.9 Hz, 2H), 1.95 (q, *J* = 7.2 Hz, 2H), 1.56-1.49 (m, 2H), 1.29-1.15 (m, 12H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.8, 139.1, 128.3, 128.1, 125.5, 114.0, 35.9, 33.8, 31.5, 29.5, 29.5, 29.3, 29.1, 28.9; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{17}H_{27}$, m/z: 231.2102, found: 231.2107, Error 2.3 ppm.

But-3-enoic acid phenyl ester **(5f)**



5f

Following a reported procedure:[8]

To a solution of vinylaceticacid (860.0 mg, 10 mmol, 1.0 equiv.) and phenol (1.18 g, 12.0 mmol, 1.2 equiv.) in DCM (10.0 mL), dicyclohexylcarbodiimide (1.3 g, 10.5 mmol, 1.05 equiv.) and 4-dimethyaminopyridine (122 mg, 1.0 mmol, 0.1 equiv.) were added. The reaction mixture was stirred at room temperature for 8 h and then concentrated *in vacuo* to afford the crude product, which was triturated with PE:Et_2O (9:1), and then filtered by a pad of celite. The filtrate was concentrated *in vacuo*, and the residue was purified by flash chromatography (eluting with PE:EA = 40:1) to afford the desired product **5f** as a colorless oil (1.3 g, 78% yield). The spectral data is consistent with the literature.[8] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 (t, *J* = 7.8 Hz, 2H), 7.28-7.17 (m, 1H), 7.14-7.04 (m, 2H), 6.08-5.98 (m, 1H), 5.34-5.17 (m, 2H), 3.33 (d, *J* = 6.9 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$)

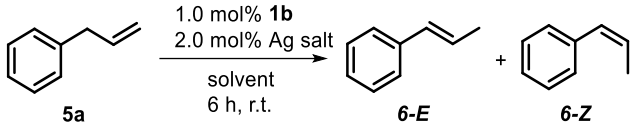
δ 169.9, 150.5, 129.5, 129.3, 125.8, 121.4, 119.1, 39.0; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{10}H_{10}O_2Na$, m/z: 185.0576, found: 185.0573, Error 1.4 ppm.

7.2. Catalytic olefin isomerization reaction

General procedure: In an argon-filled glove box, terminal alkene, cat.**1b**, $AgPF_6$, and acetone-d_6 were added to a Schlenk tube, the reaction mixture was stirred at room temperature inside the glove box for several hours and monitored by GC-MS analysis. The obtained solution was directly loaded onto a short silica column for purification, eluting with PE or the mixture of PE and EA. The yield and *E*/*Z* ratio were determined by integration of suitable ^1H NMR signals (see below).

7.2.1. Effects of solvent and Ag salt on conversion and selectivity

Table S22. Screening of conditions[a]

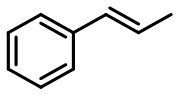


Entry	Ag salt	Solvent	Conv. (%)	**6** yield[b] (%)	*E*:*Z*[b]
1	AgOTf	$CHCl_3$	90	80	86:14
2	AgOTf	THF	95	78	85:15
3	AgOTf	hexane	0	NR	-
4	AgOTf	acetone	98	93	97:3
5	AgOTf	DMSO	0	NR	-
6	AgOTf	DMF	0	NR	-
7	AgOAc	acetone	70	65	97:3
8	Ag_2CO_3	acetone	0	NR	-
9	$AgPF_6$	acetone	98	95	98:2

[a]Conditions: Unless other specified, reactions conducted using: **3a** (0.5 mmol), **1b** (1.0 mol%), Ag salt (2.0 mol%), solvent (1.0 mL). [b]Yield and *E*/*Z* ratios were determined by GC-MS analysis using 1,3,5-trimethylbenzene.

7.2.2. Characterization data of *E*-olefins

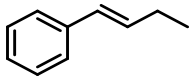
(*E*)-prop-1-en-1-ylbenzene **(6a):**



6a

The reaction was carried out according to the general procedure by using **5a** (59.0 mg, 0.5 mmol, 1.0 equiv.), iridium complex **1b** (3.3 mg, 5 μmol, 1.0 mol%), $AgPF_6$ (2.5 mg, 10 μmol, 2.0 mol%) and acetone-d_6 (1.0 mL) resulting in 54.0 mg (92% yield) of the title product obtained as a colorless oil. **^{1}H NMR** (400 MHz, Acetone-d_6) δ 7.38-7.35 (m, 2H), 7.31-7.27 (m, 2H), 7.21-7.16 (m, 1H), 6.46-6.41 (m, 1H), 6.34-6.25 (m, 1H), 1.85 (dd, *J* = 6.5, 1.6 Hz, 3H); **^{13}C NMR** (100 MHz, Acetone-d_6) δ 138.5, 131.6, 129.1, 127.4, 126.4, 125.8, 18.4; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_9H_{10}Na$, m/z: 141.0675, found: 141.0679, Error 3.4 ppm.

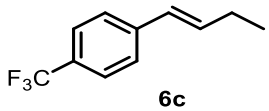
(*E*)-1-(but-1-en-1-yl) benzene **(6b):**



6b

The reaction was carried out according to the general procedure by using **5b** (66.0 mg, 0.5 mmol, 1.0 equiv.), iridium complex **1b** (8.3 mg, 12.5 μmol, 2.5 mol%), $AgPF_6$ (6.3 mg, 25 μmol, 5.0 mol%) and acetone-d_6 (1.0 mL) resulting in 62.0 mg (94% yield) of the title product obtained as a colorless oil. **^{1}H NMR** (400 MHz, Acetone-d_6) δ 7.40-7.37 (m, 2H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.23-7.14 (m, 1H), 6.47-6.25 (m, 2H), 2.26-2.18 (m, 2H), 1.07 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (100 MHz, Acetone-d_6) δ 138.5, 132.7, 129.4, 129.1, 127.4, 126.5, 26.5, 13.8; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{10}H_{13}$, m/z: 133.1012, found: 133.1009, Error 2.1 ppm.

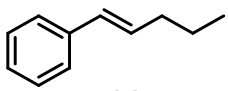
(*E*)-1-(but-1-en-1-yl)-4-(trifluoromethyl) benzene **(6c):**



6c

The reaction was carried out according to the general procedure by using **5c** (100.0 mg, 0.5 mmol, 1.0 equiv.), iridium complex **1b** (8.3 mg, 12.5 μmol, 2.5 mol%), $AgPF_6$ (6.3 mg, 25 μmol, 5.0 mol%) and acetone-d_6 (1.0 mL) resulting in 92.0 mg (92% yield) of the title product obtained as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.1 Hz, 2H), 7.39 (d, *J* = 8.1 Hz, 2H), 6.41-6.31 (m, 2H), 2.28-2.20 (m, 2H), 1.09 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.4, 135.4, 128.8, 128.7, 128.4, 127.7, 126.0, 125.7, 125.4, 125.4, 125.4, 125.3, 123.0, 26.1, 13.3; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.38; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{11}H_{11}F_3Na$, m/z: 233.0705, found: 233.0727, Error 8.8 ppm.

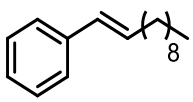
(*E*)-pent-1-en-1-ylbenzene **(6d):**



6d

The reaction was carried out according to the general procedure by using **5d** (73.1 mg, 0.5 mmol, 1.0 equiv.), iridium complex **1b** (8.3 mg, 12.5 μmol, 2.5 mol%), $AgPF_6$ (6.3 mg, 25 μmol, 5.0 mol%) and acetone-d_6 (1.0 mL) resulting in 59.9 mg (82% yield) of the title product obtained as a colorless oil. **^{1}H NMR** (400 MHz, Acetone-d_6) δ 7.40-7.38 (m, 2H), 7.31-7.27 (m, 2H), 7.22-7.15 (m, 1H), 6.46-6.41 (m, 1H), 6.36-6.25 (m, 1H), 2.22-2.14 (m, 2H), 1.53-1.44 (m, 2H), 0.94 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, Acetone-d_6) δ 138.4, 130.9, 130.4, 129.0, 127.4, 126.5, 35.5, 23.0, 13.8; **HRMS (ESI)** calcd for $[M+H]^+$ $C_{11}H_{15}$, m/z: 147.1168, found: 147.1168, Error 0.2 ppm.

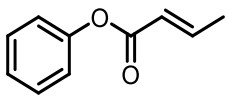
(*E*)-non-1-en-1-ylbenzene **(6e):**



6e

The reaction was carried out according to the general procedure by using **5e** (115.1 mg, 0.5 mmol, 1.0 equiv.), iridium complex **1b** (16.6 mg, 25 μmol, 5.0 mol%), $AgPF_6$ (12.6 mg, 50 μmol, 10.0 mol%) and acetone-d_6 (1.0 mL) resulting in 65% yield of the title product (determined by **^{1}H NMR** using 0.50 mmol CH_2Br_2 as internal standard). **HRMS (ESI)** calcd for $[M+H]^+$ $C_{17}H_{27}$, m/z: 231.2107, found: 231.2112, Error 2.0 ppm.

(*E*)-2-butenoic acid phenyl ester **(6f):**

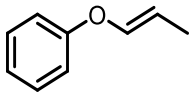


6f

The reaction was carried out according to the general procedure by using **5f** (40.5 mg, 0.25 mmol, 1.0 equiv.), iridium complex **1b** (8.3 mg, 12.5 μmol, 5.0 mol%), $AgPF_6$ (6.3 mg, 25 μmol, 10.0 mol%) and acetone-d_6 (1.0 mL) resulting in 38.7 mg (96% yield) of the title product obtained as a colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35-7.23 (m, 2H), 7.22-7.07 (m, 2H), 7.07-6.98 (m,

2H), 6.00-5.94 (m, 1H), 1.88 (dd, *J* = 7.0, 1.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.8, 150.7, 146.9, 129.3, 125.6, 122.0, 121.6, 18.2; **HRMS (ESI)** calcd for $[M+Na]^+$ $C_{10}H_{10}O_2Na$, m/z: 185.0573, found: 185.0581, Error 4.2 ppm.

(*E*)-(prop-1-en-1-yloxy) benzene **(6g)**



6g

The reaction was carried out according to the general procedure by using **5g** (67.0 mg, 0.5 mmol, 1.0 equiv.), iridium complex **1b** (3.3 mg, 5 μmol, 1.0 mol%), $AgPF_6$ (2.5 mg, 10 μmol, 2.0 mol%) and acetone-d_6 (1.0 mL) resulting in 63.7 mg (95% yield) of the title product obtained as a colorless oil. The ratio between *E* and *Z* was determined to be 85:15. The spectral data is consistent with the literature.[9] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35-7.25 (m, 2H), 7.05-6.96 (m, 3H), 6.43-6.36 (m, 1H), 5.41-5.33 (m, 0.15H *Z*), 4.91-4.84 (m, 0.85H *E*), 1.71 (dd, J = 6.9, 1.8 Hz, 2.5H *E*), 1.67(dd, J = 6.9, 1.7 Hz, 0.5H *Z*); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.5, 141.9(*Z*), 140.8, 129.5, 122.4(*Z*), 122.3, 116.3(*Z*), 116.1, 108.2(*Z*), 107.4, 12.2(*Z*), 9.3.

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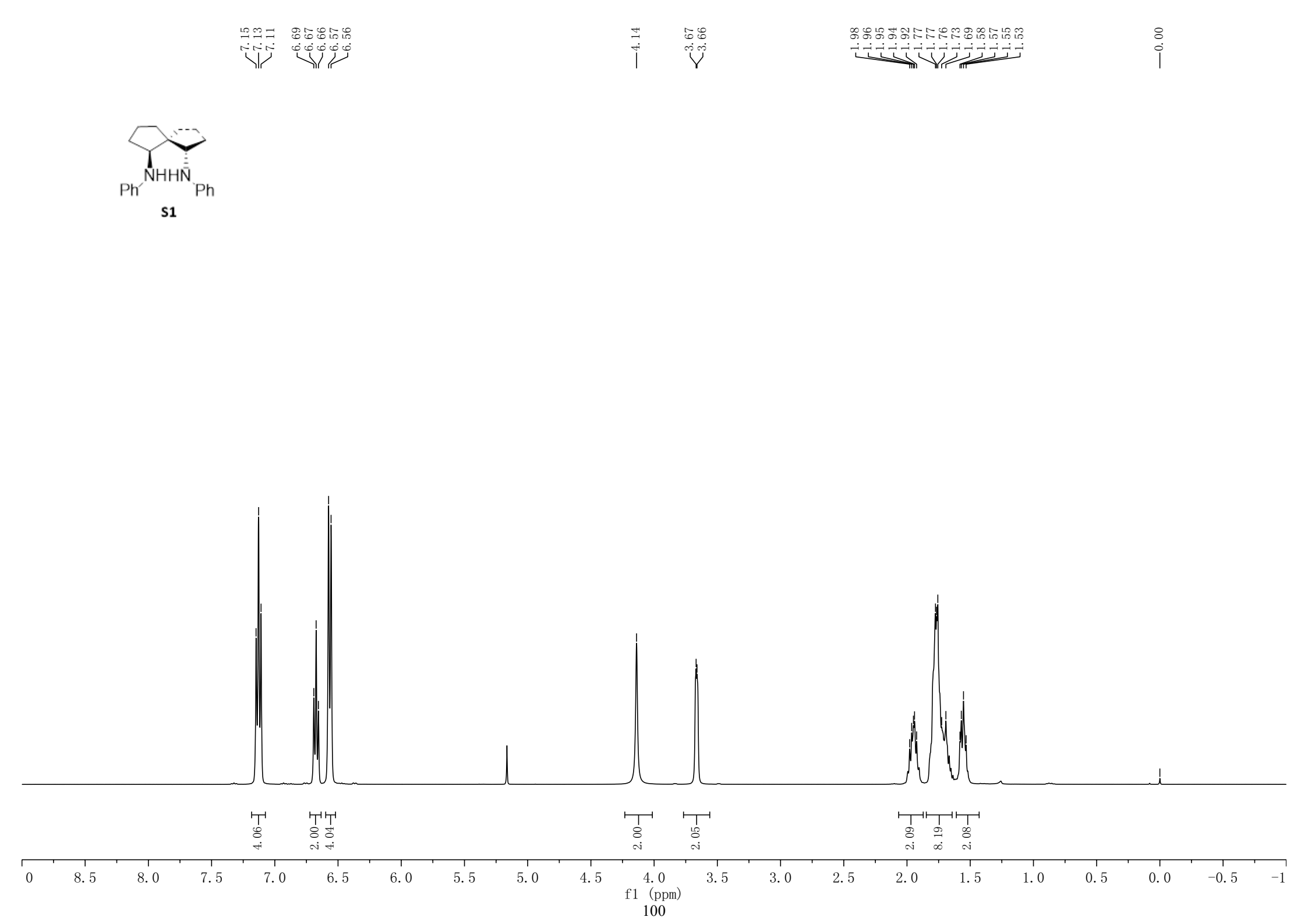
9. Copies of NMR spectroscopy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1.58
1.57
1.55
1.53
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NHHN
Ph
Ph
S1
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2.00
4.04
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2.05
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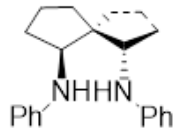

S1

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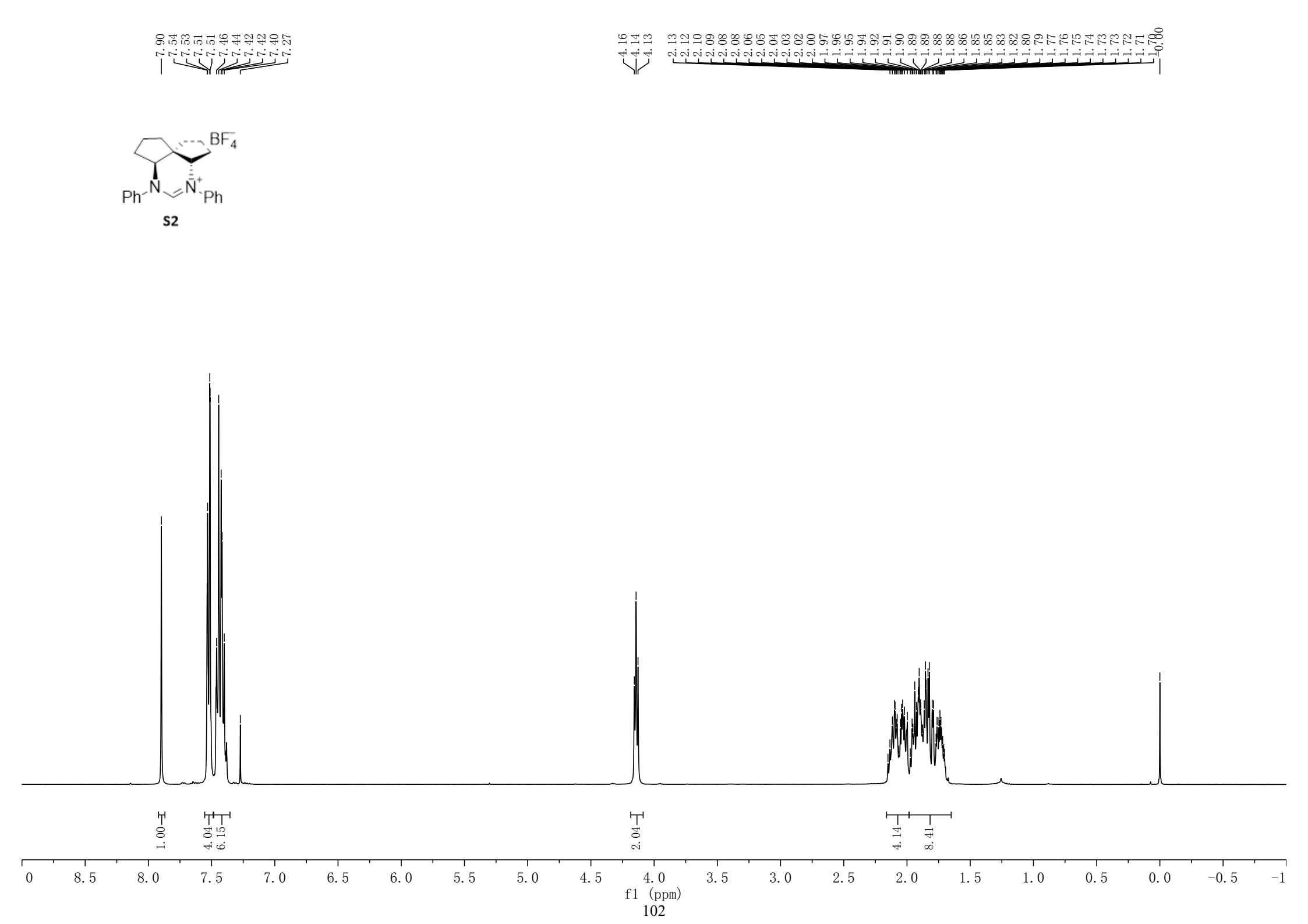
20.11

f1 (ppm)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2.02
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1.72
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0.00
BF4
Ph
N
N+
Ph
S2
1.00
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2.04
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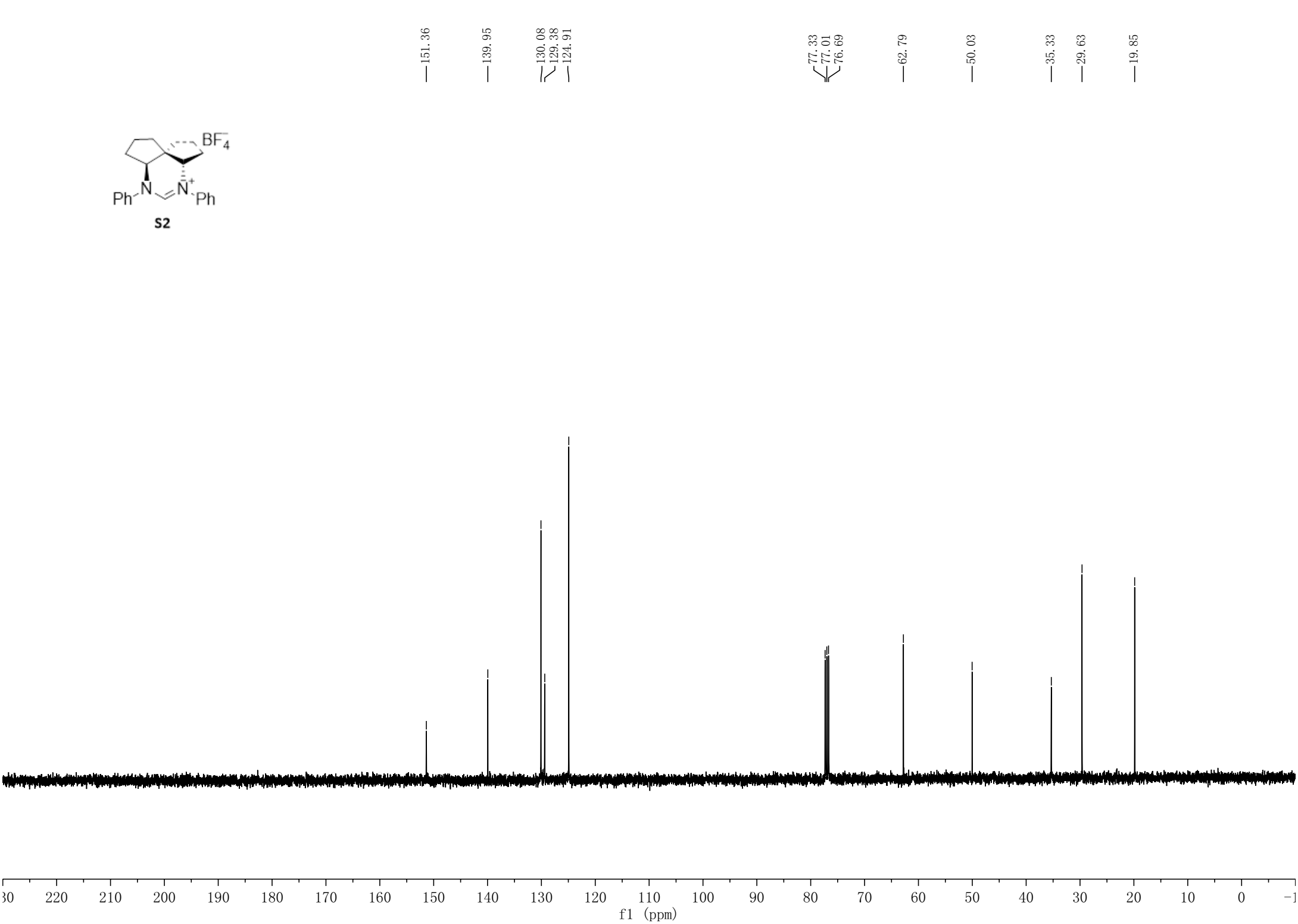
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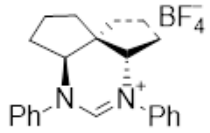
N+
Ph
S2
f1 (ppm)


BF4
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N
N+
Ph

S2

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-60
-70
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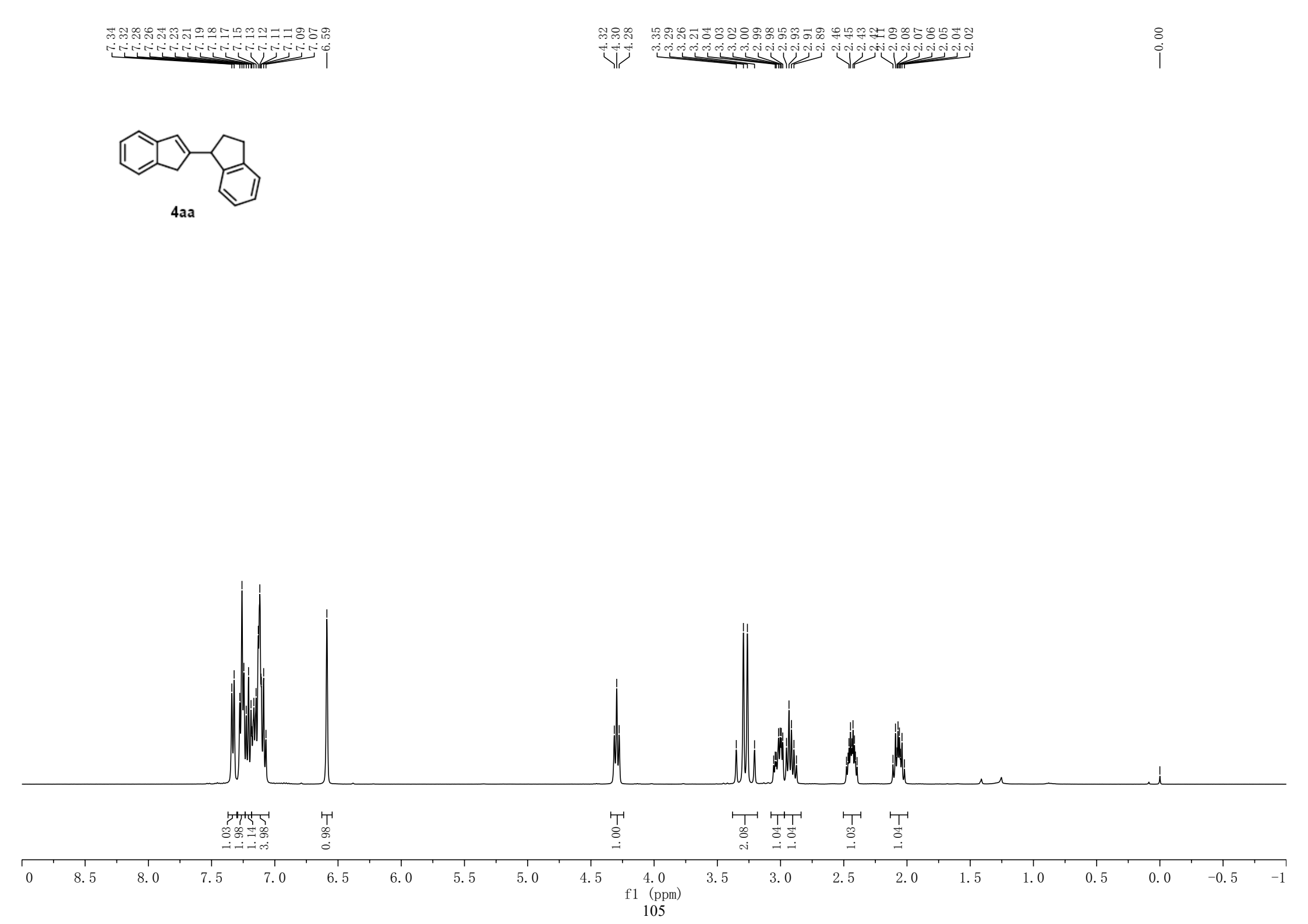
f1 (ppm)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7.09
7.07
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3.03
3.02
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2.95
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2.91
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2.09
2.08
2.07
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2.05
2.04
2.02
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1.03
1.98
1.14
3.98
0.98
1.00
2.08
1.04
1.04
1.03
1.04
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6.0
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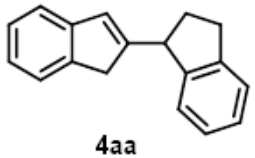
f1 (ppm)



4aa

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143.26
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126.62
126.26
126.25
124.59
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123.53
120.18
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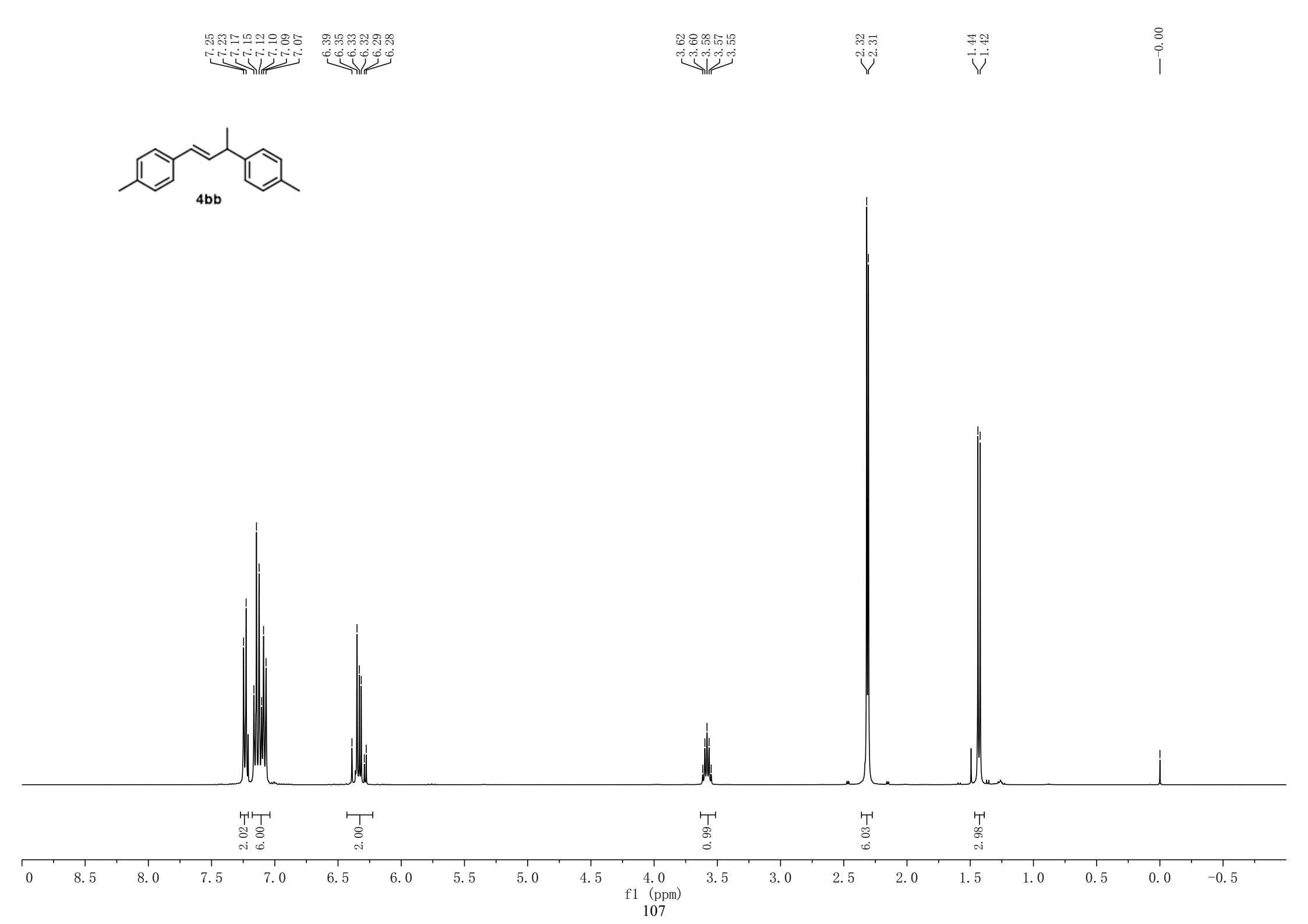
f1 (ppm)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6.28
3.62
3.60
3.58
3.57
3.55
2.32
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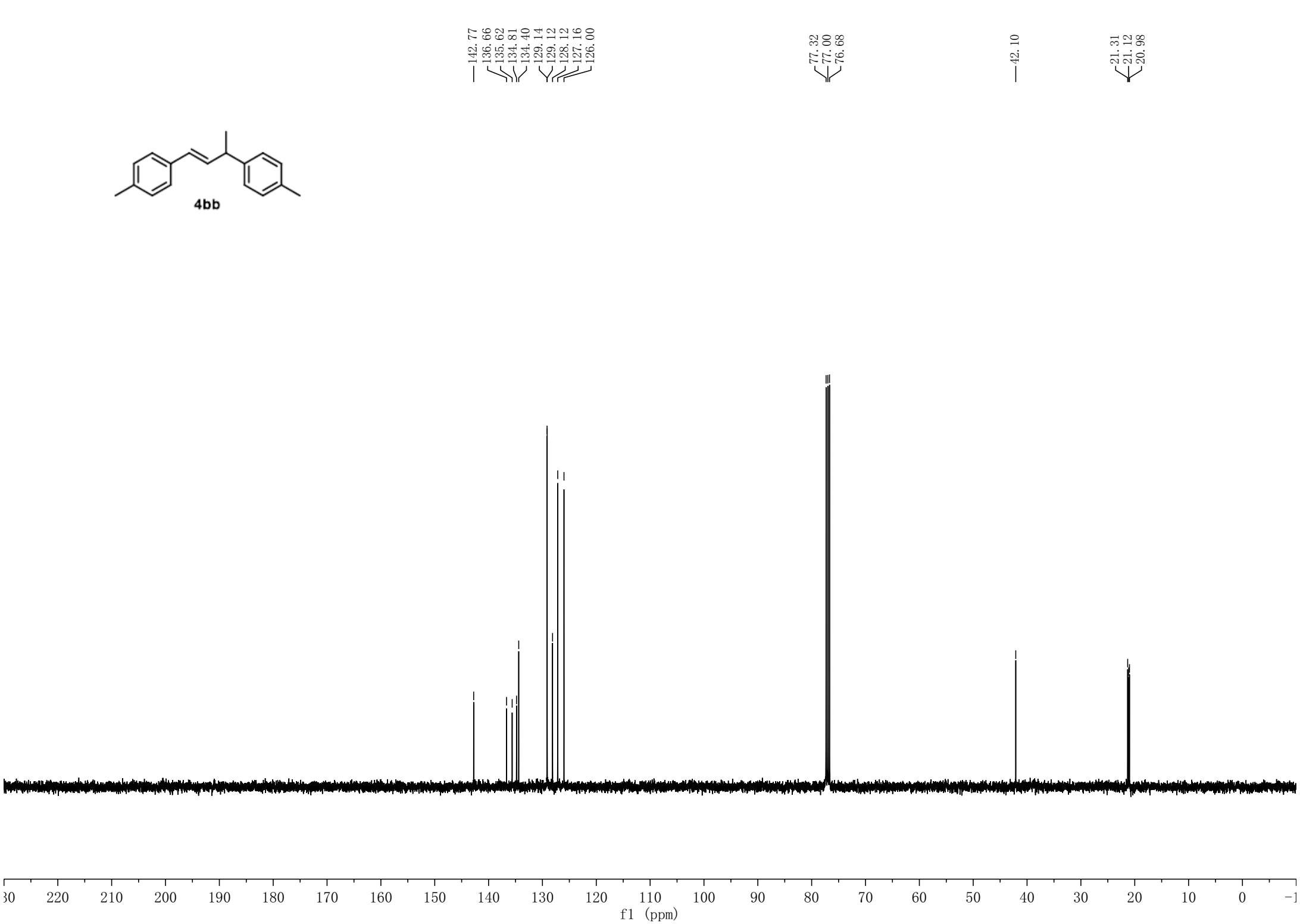
2.98
f1 (ppm)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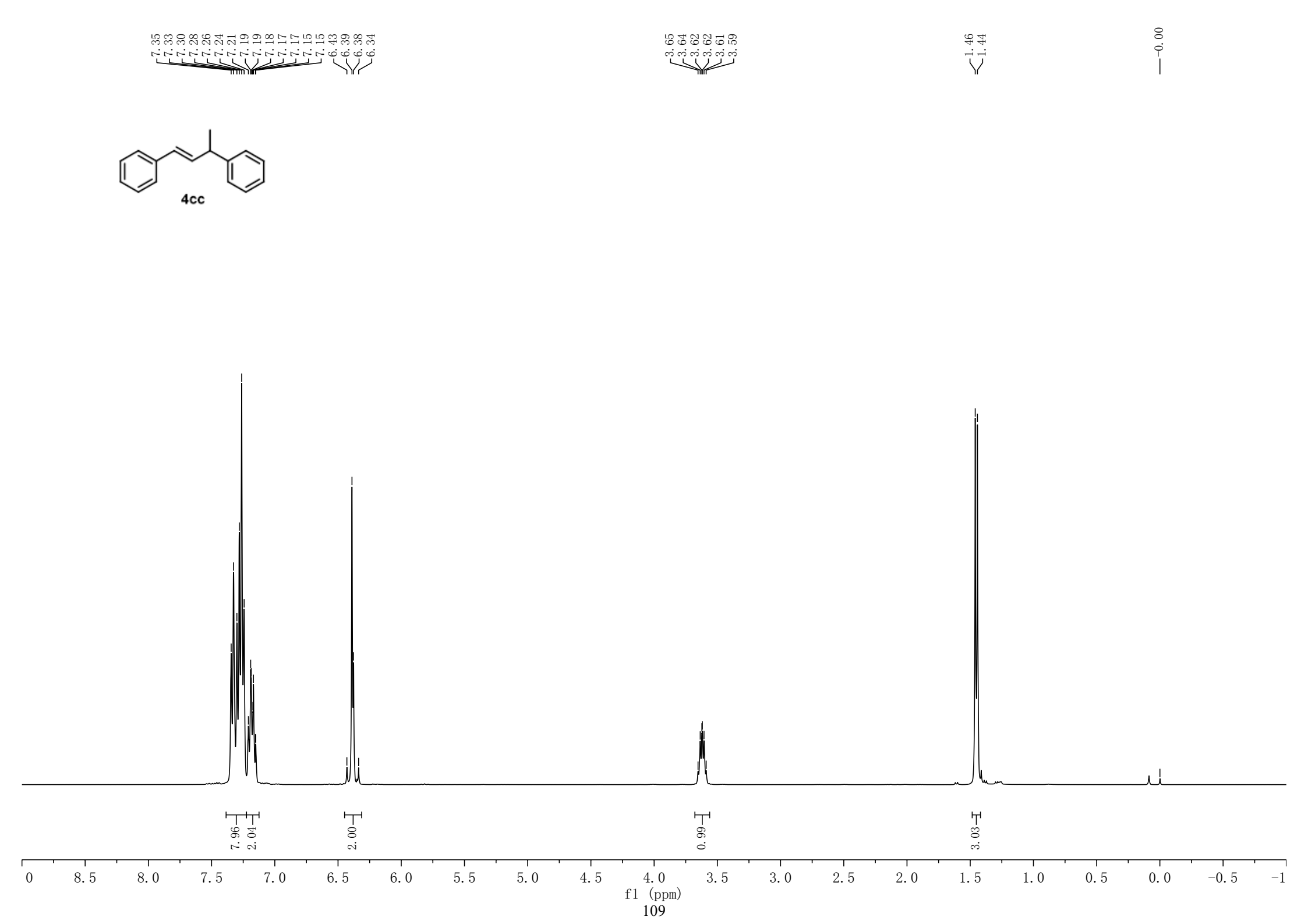
f1 (ppm)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6.43
6.39
6.38
6.34
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3.64
3.62
3.62
3.61
3.59
1.46
1.44
0.00
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2.00
0.99
3.03
0
8.5
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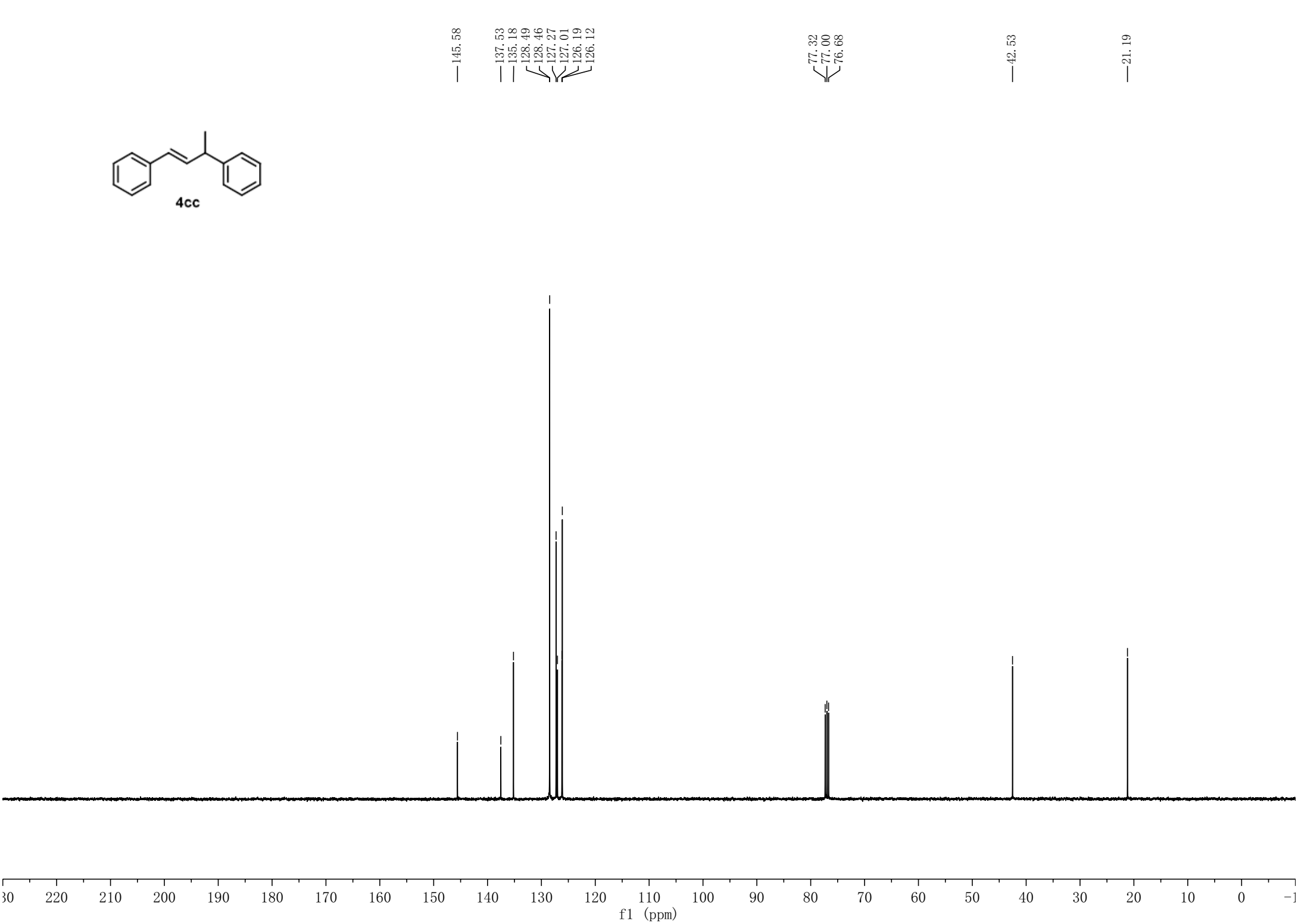
f1 (ppm)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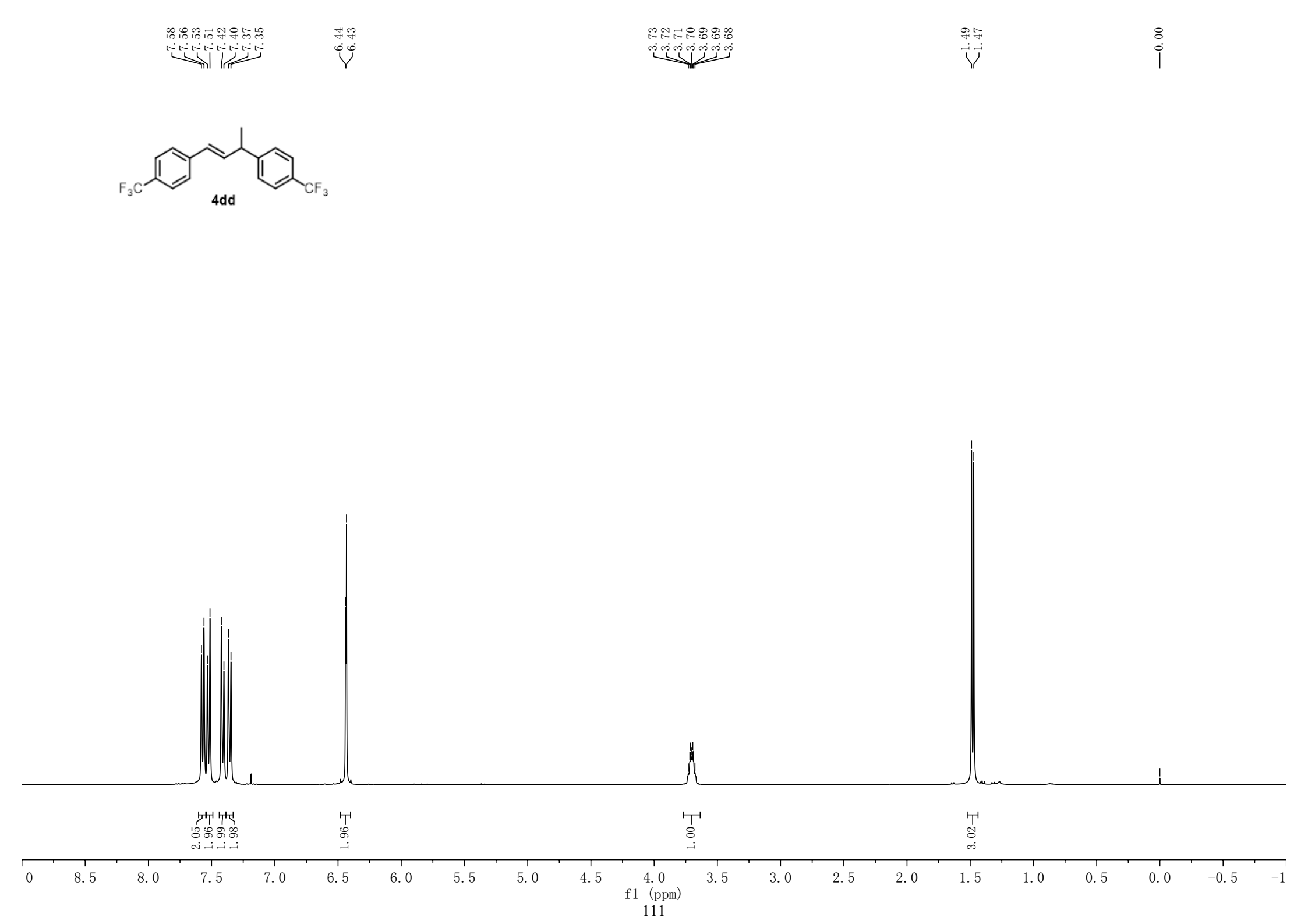
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3.69
3.68
1.49
1.47
0.00
F3C
CF3
4dd
2.05
1.96
1.99
1.98
1.96
1.00
3.02
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8.0
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7.0
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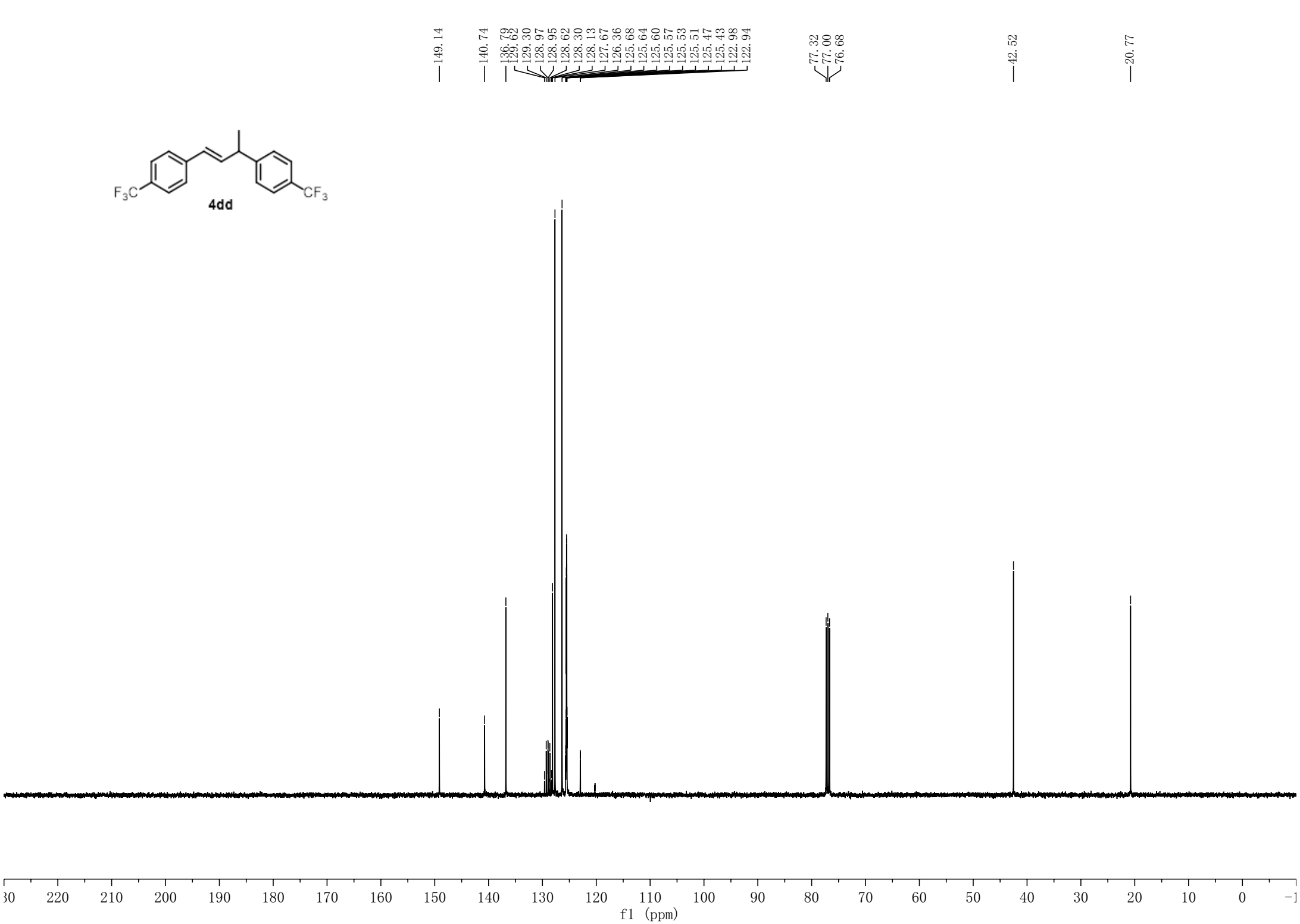
f1 (ppm)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125.60
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125.51
125.47
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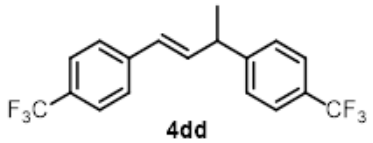
20.77
F3C
CF3
4dd
f1 (ppm)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CF3

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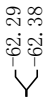
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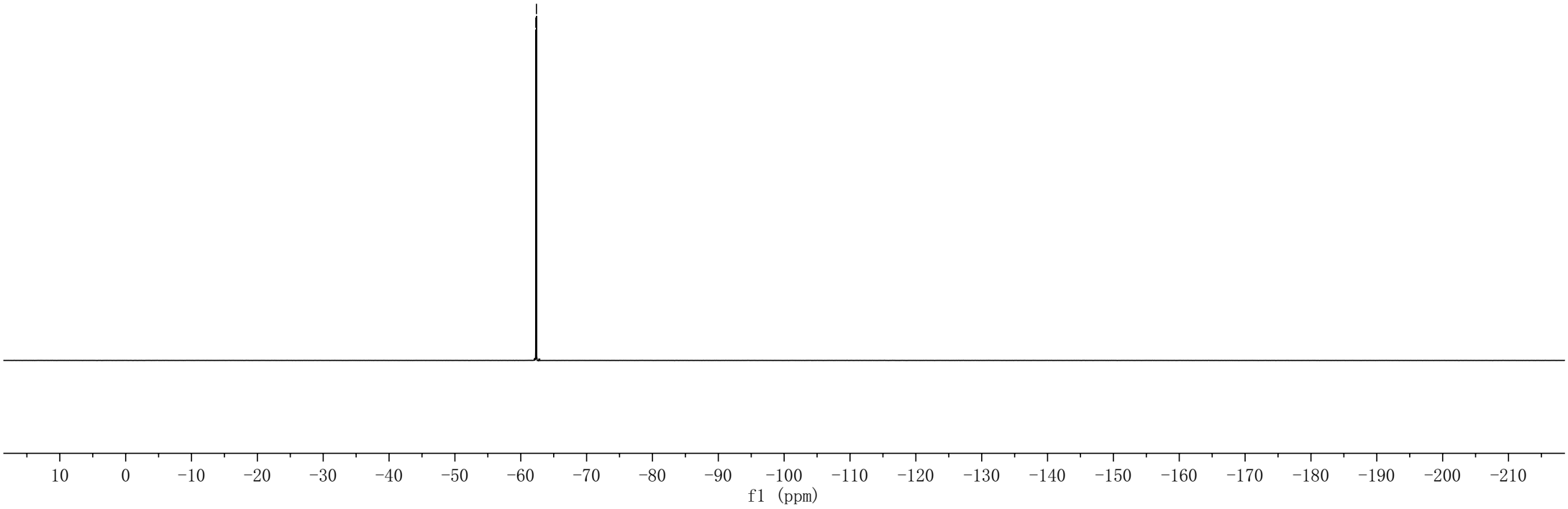
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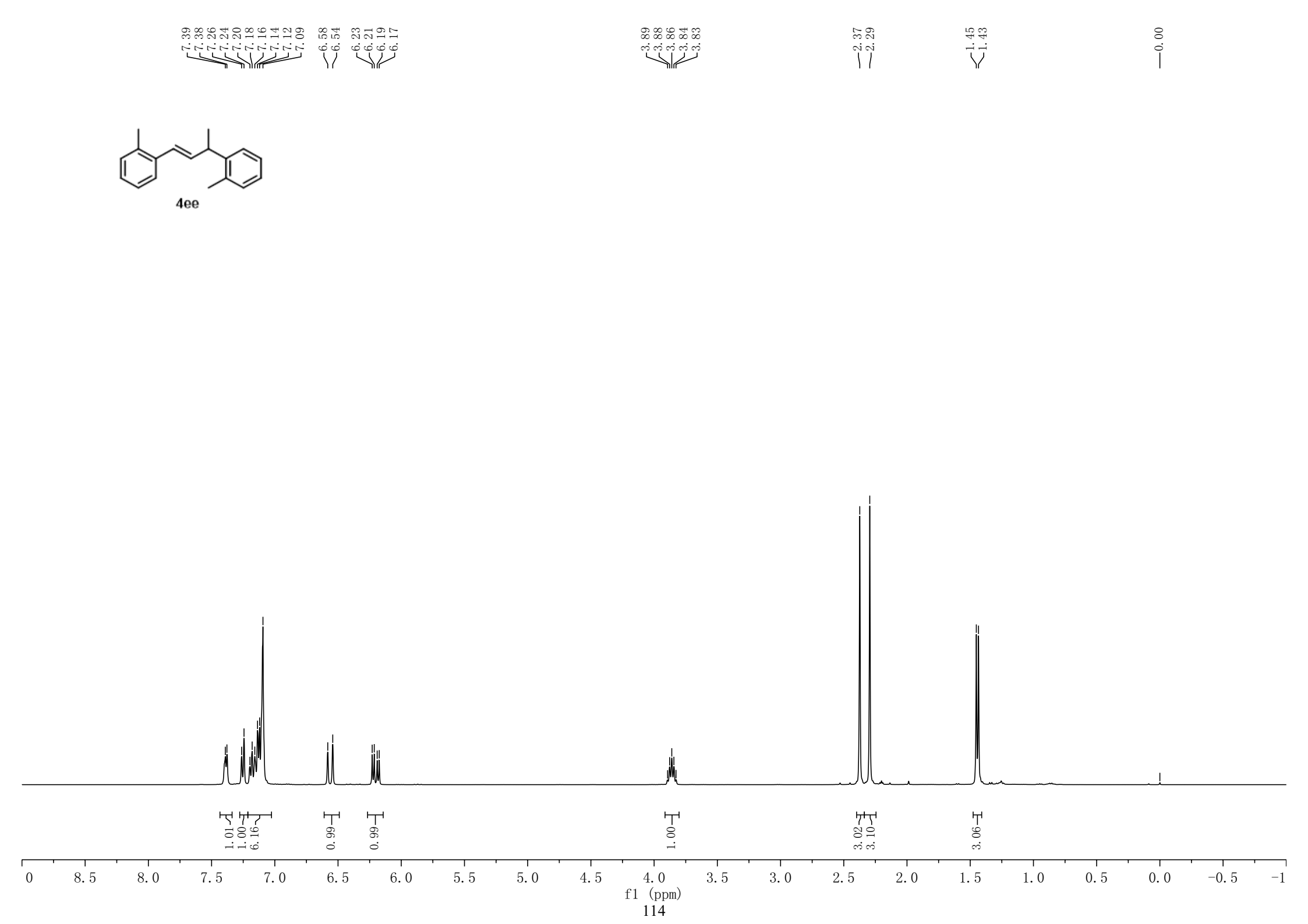
-200
-210
f1 (ppm)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6.19
6.17
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3.88
3.86
3.84
3.83
2.37
2.29
1.45
1.43
0.00
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1.01
1.00
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0.99
1.00
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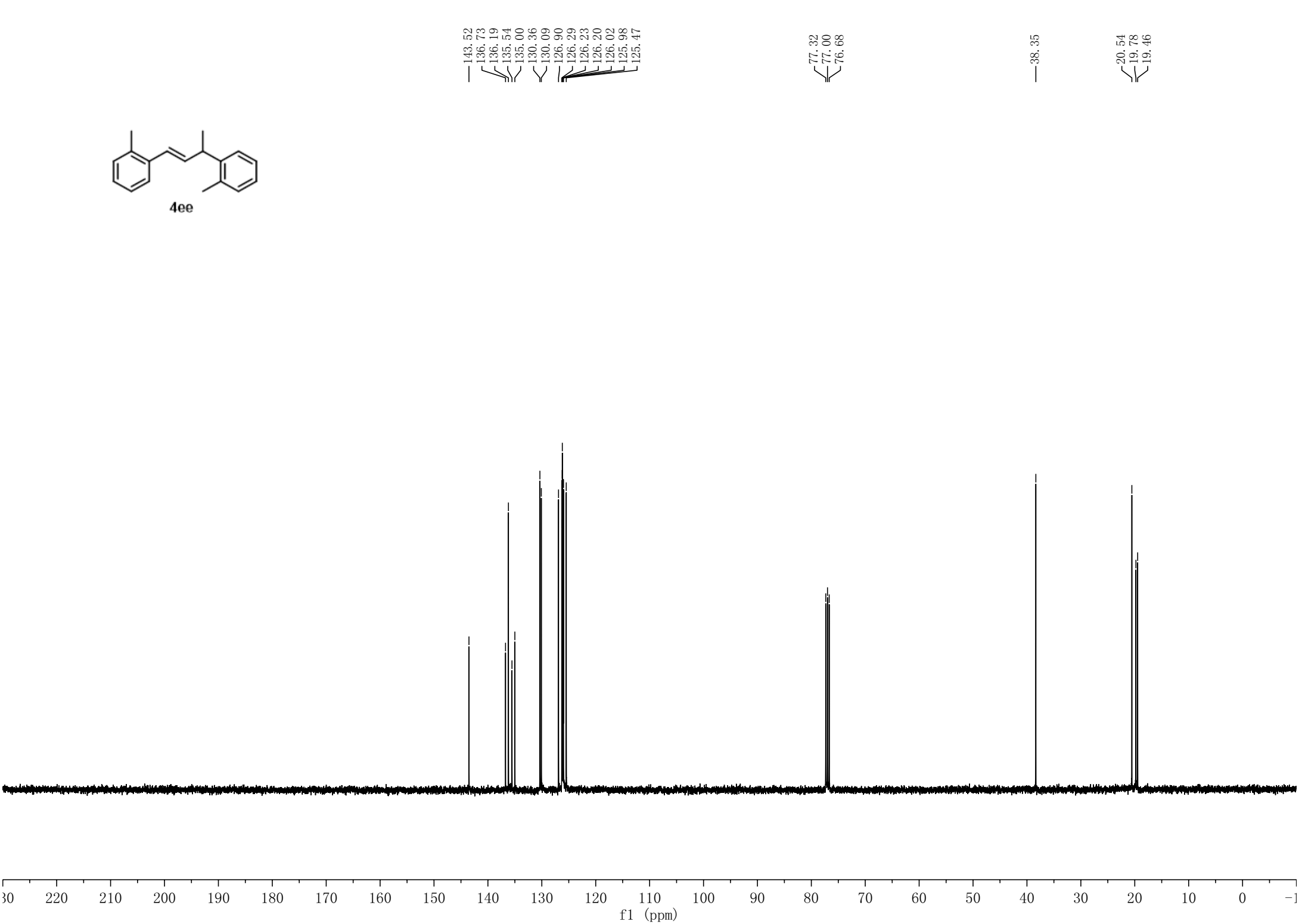
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77.00
76.68
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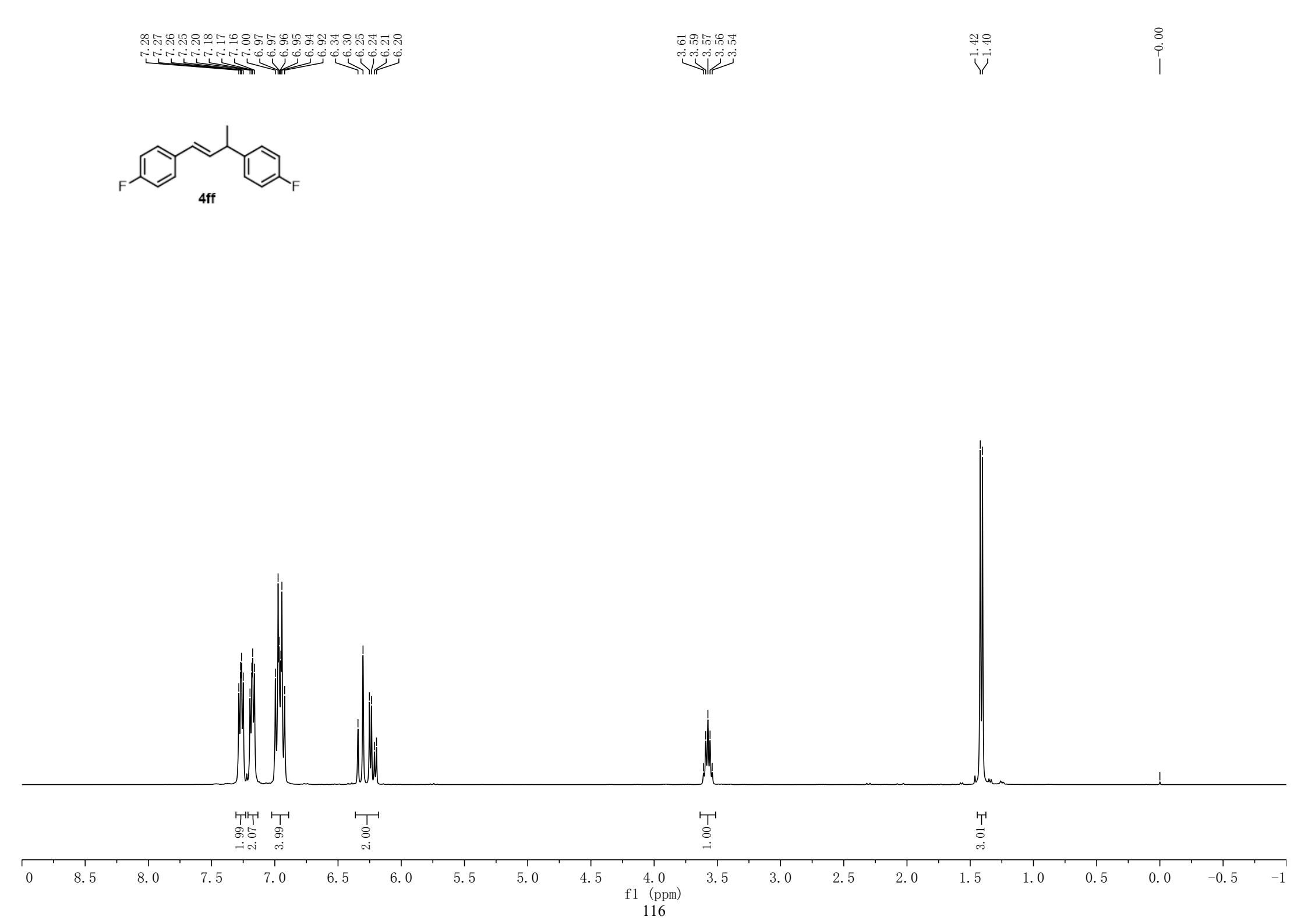
20.54
19.78
19.46
4ee
f1 (ppm)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6.94
6.92
6.34
6.30
6.25
6.24
6.21
6.20
3.61
3.59
3.57
3.56
3.54
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1.40
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F
F
4ff
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2.07
3.99
2.00
1.00
3.01
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8.5
8.0
7.5
7.0
6.5
6.0
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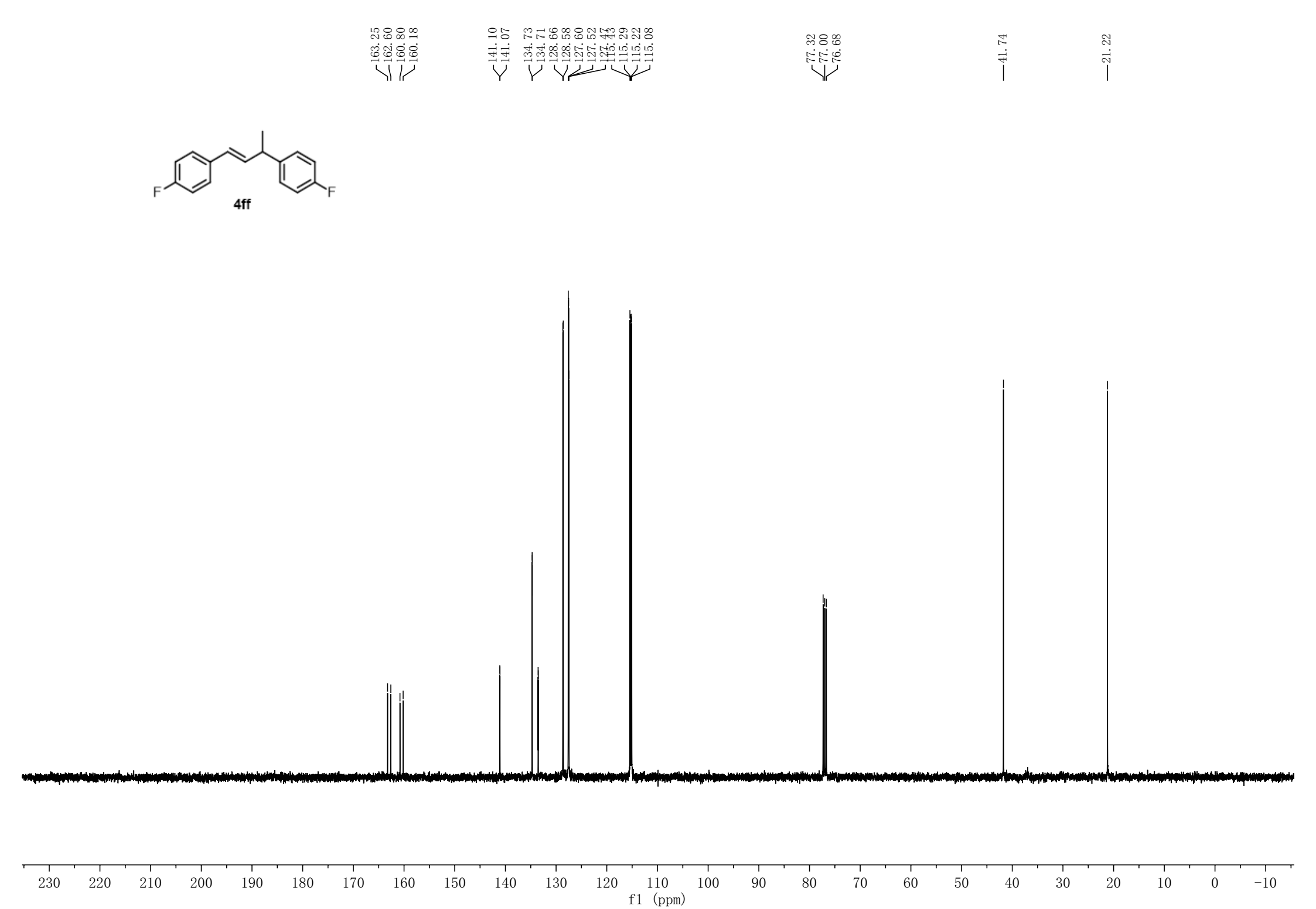
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115.08
77.32
77.00
76.68
41.74
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F
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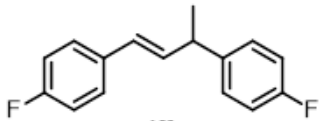
f1 (ppm)


F
F

4ff

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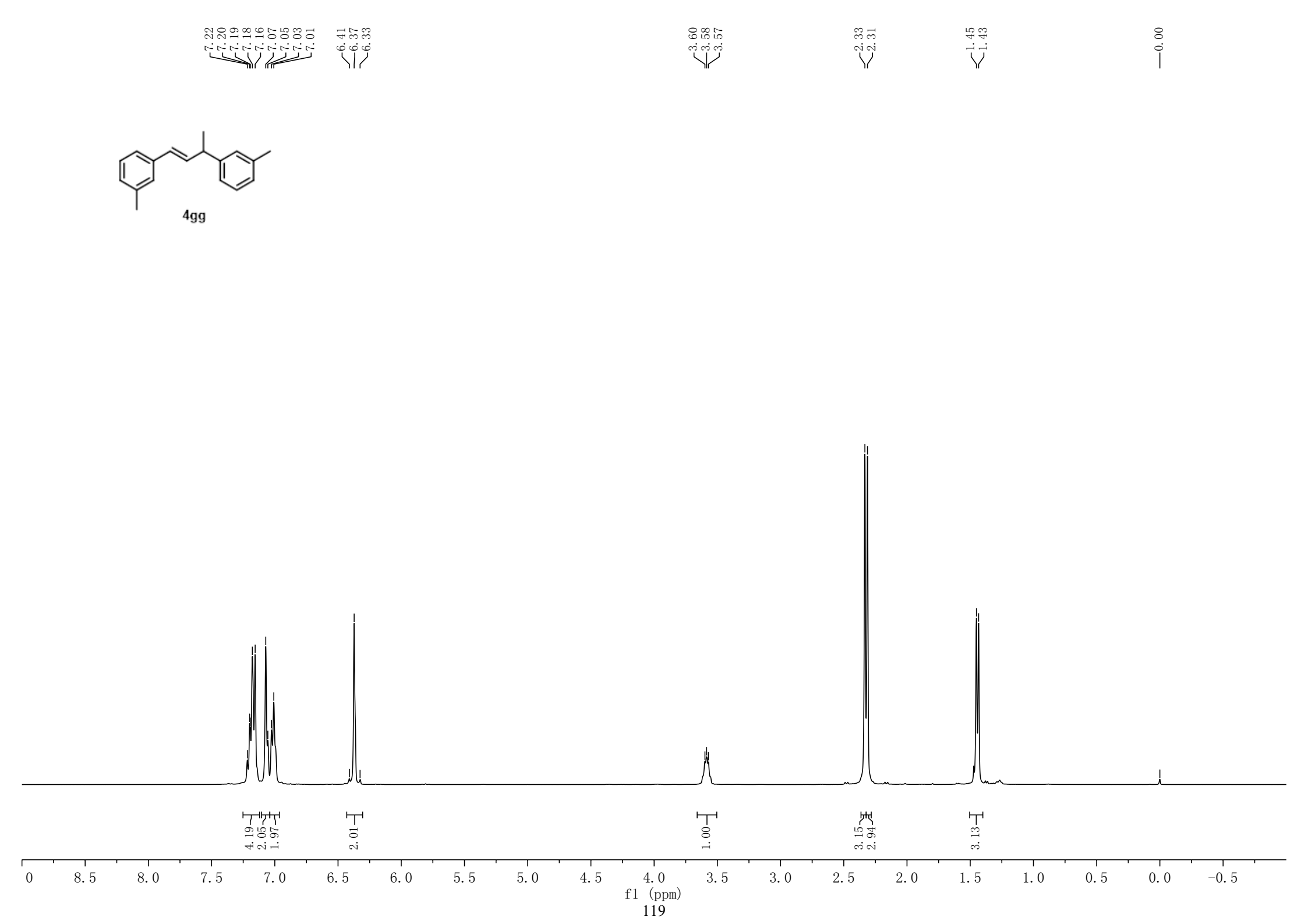
f1 (ppm)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3.58
3.57
2.33
2.31
1.45
1.43
0.00
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4.19
2.05
1.97
2.01
1.00
3.15
2.94
3.13
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8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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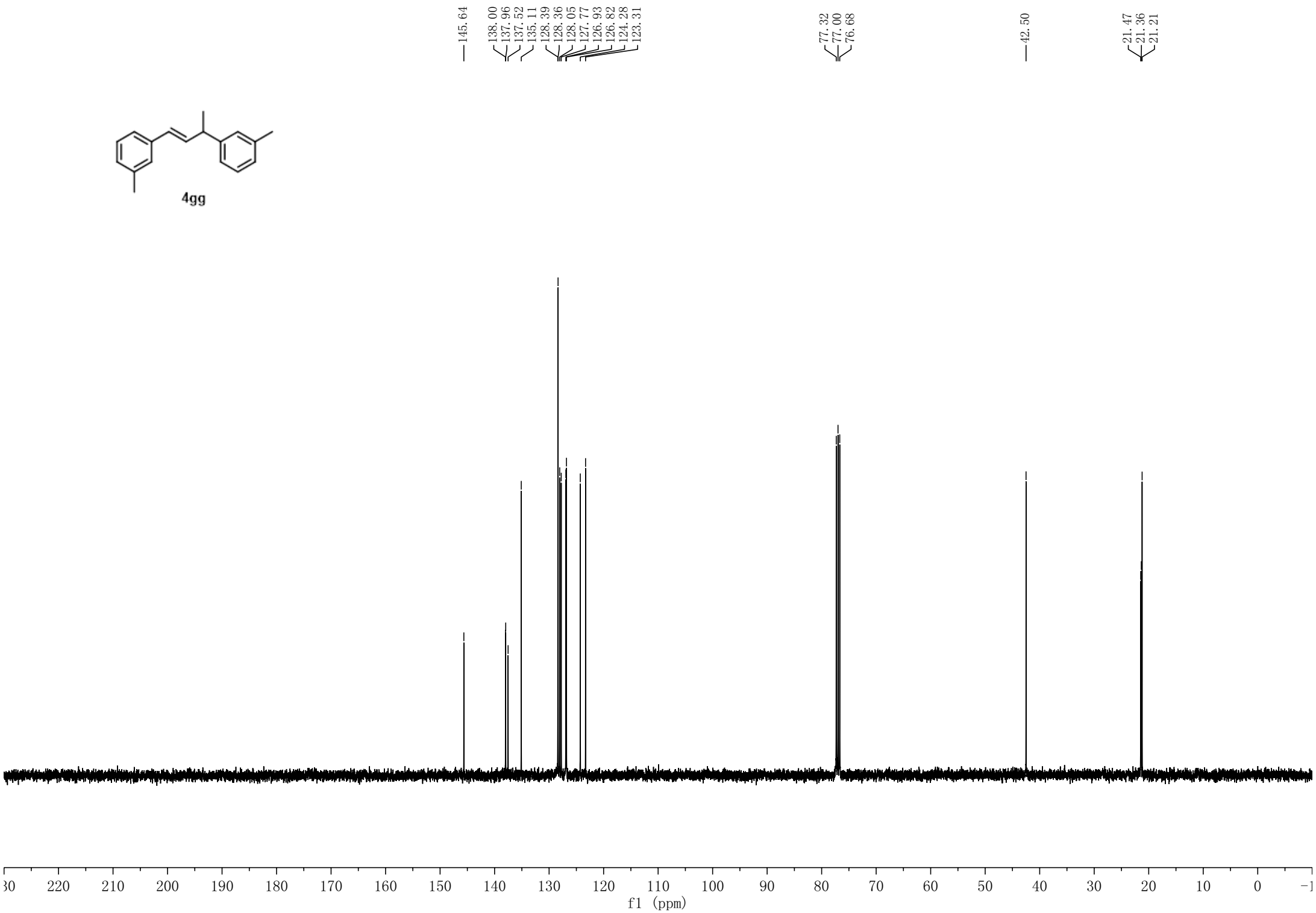
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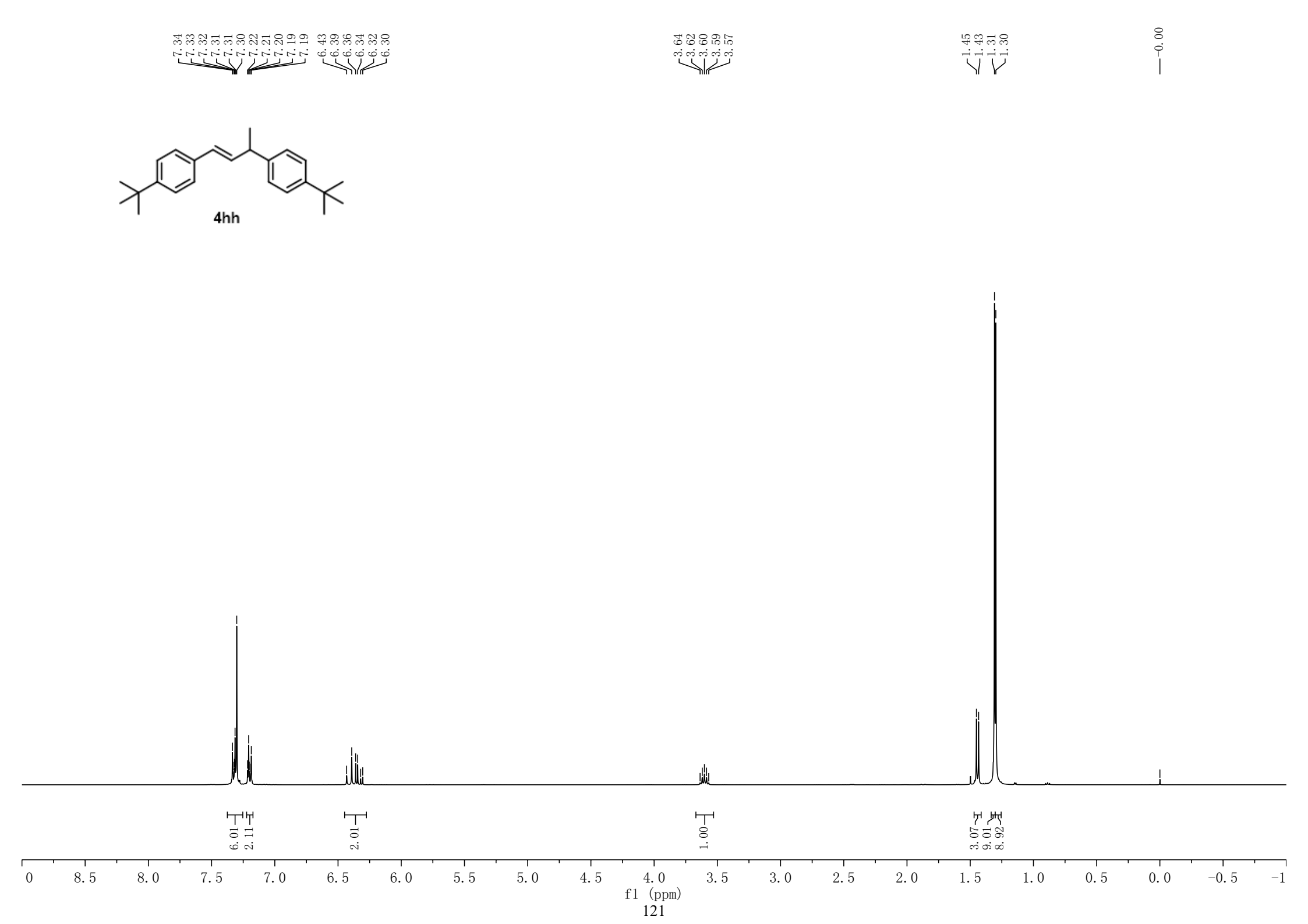
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6.36
6.34
6.32
6.30
3.64
3.62
3.60
3.59
3.57
1.45
1.43
1.31
1.30
0.00
4hh
6.01
2.11
2.01
1.00
3.07
9.01
8.92
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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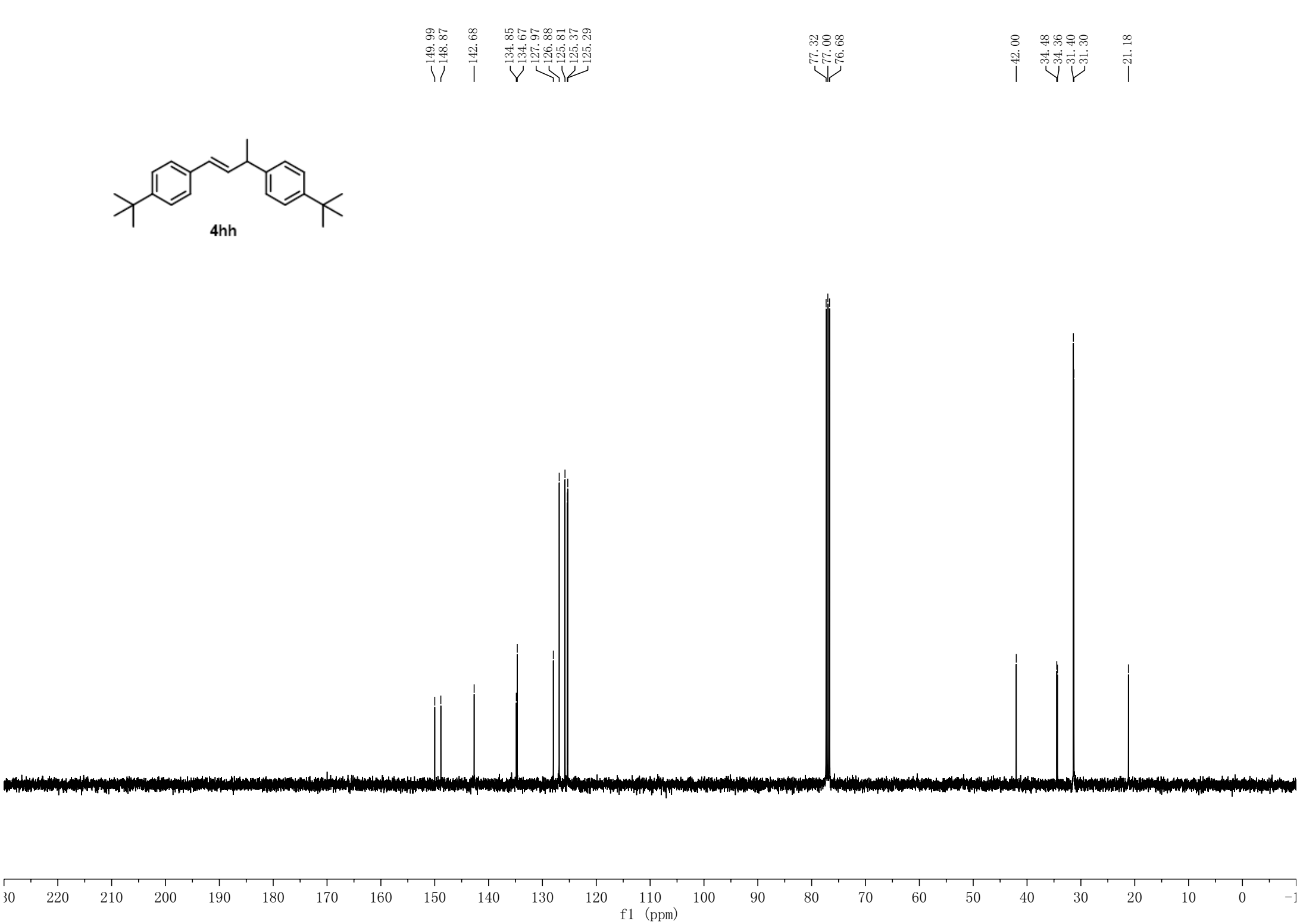
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76.68
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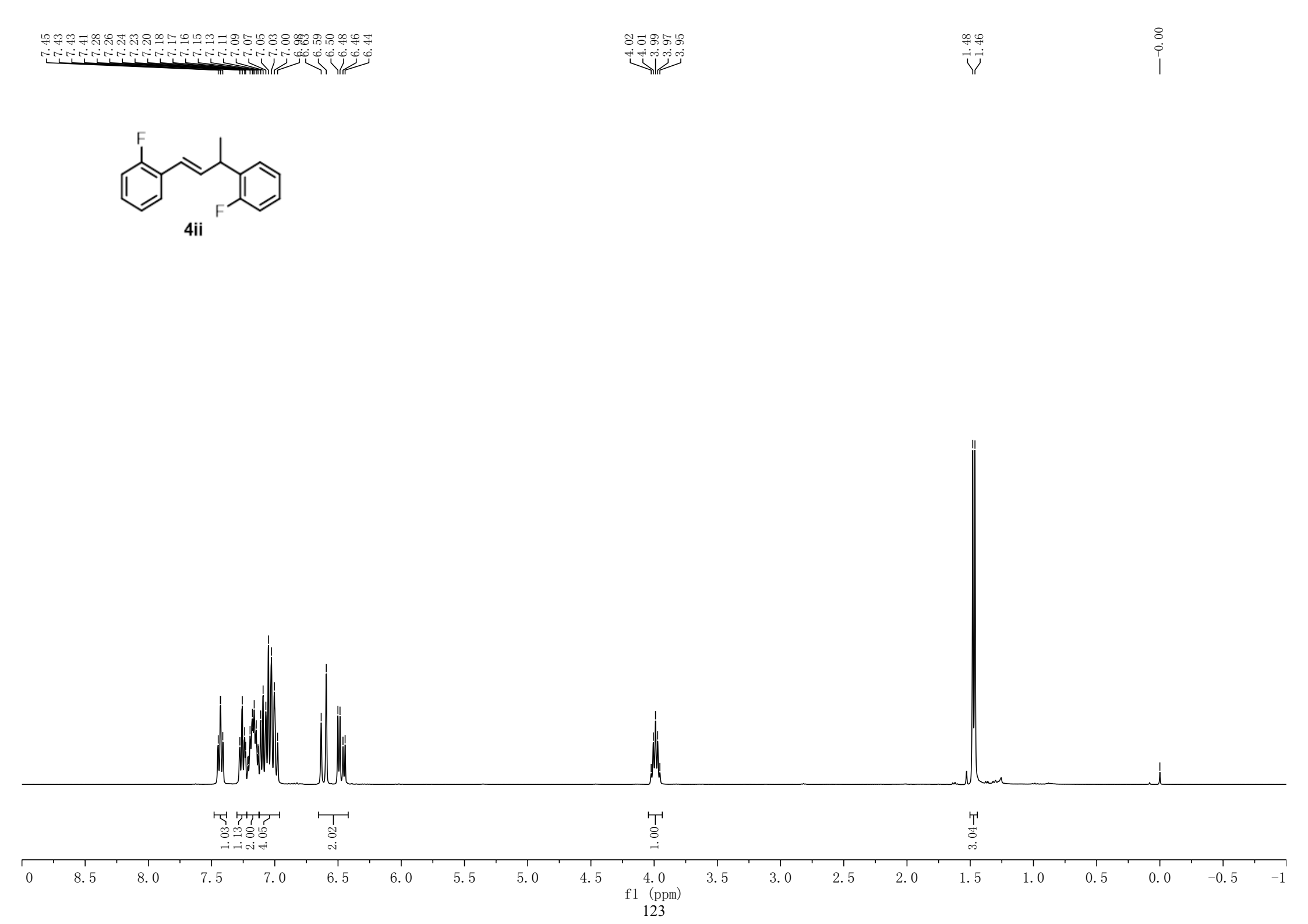
34.36
31.40
31.30
21.18
4hh
f1 (ppm)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1.46
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F
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5.5
5.0
4.5
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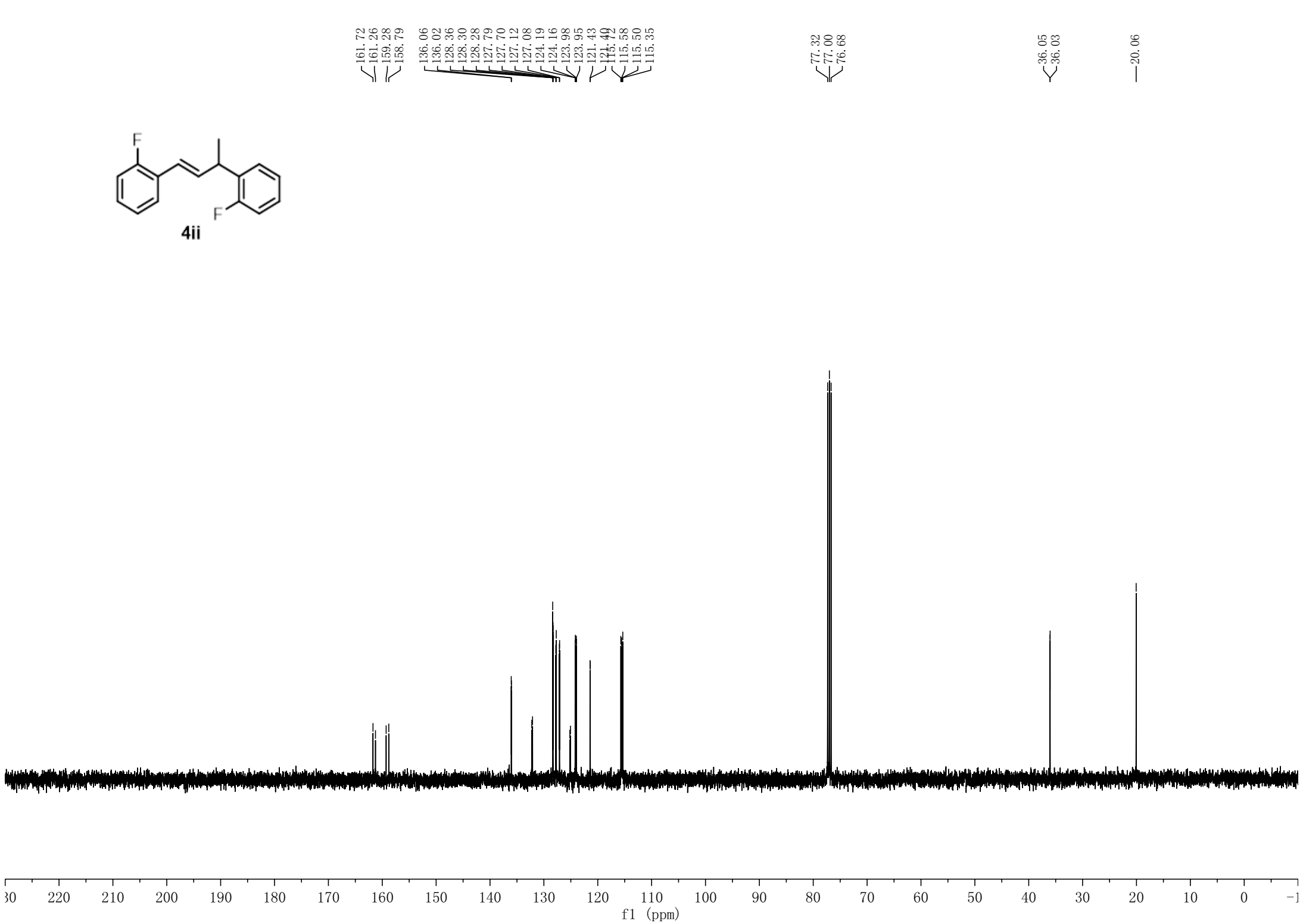
f1 (ppm)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136.02
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127.79
127.70
127.12
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124.19
124.16
123.98
123.95
121.43
121.40
115.72
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76.68
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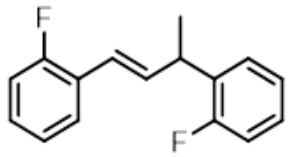
36.03
20.06
F
F
4ii
f1 (ppm)


F
F

4ii

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-118.54
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-170
-180
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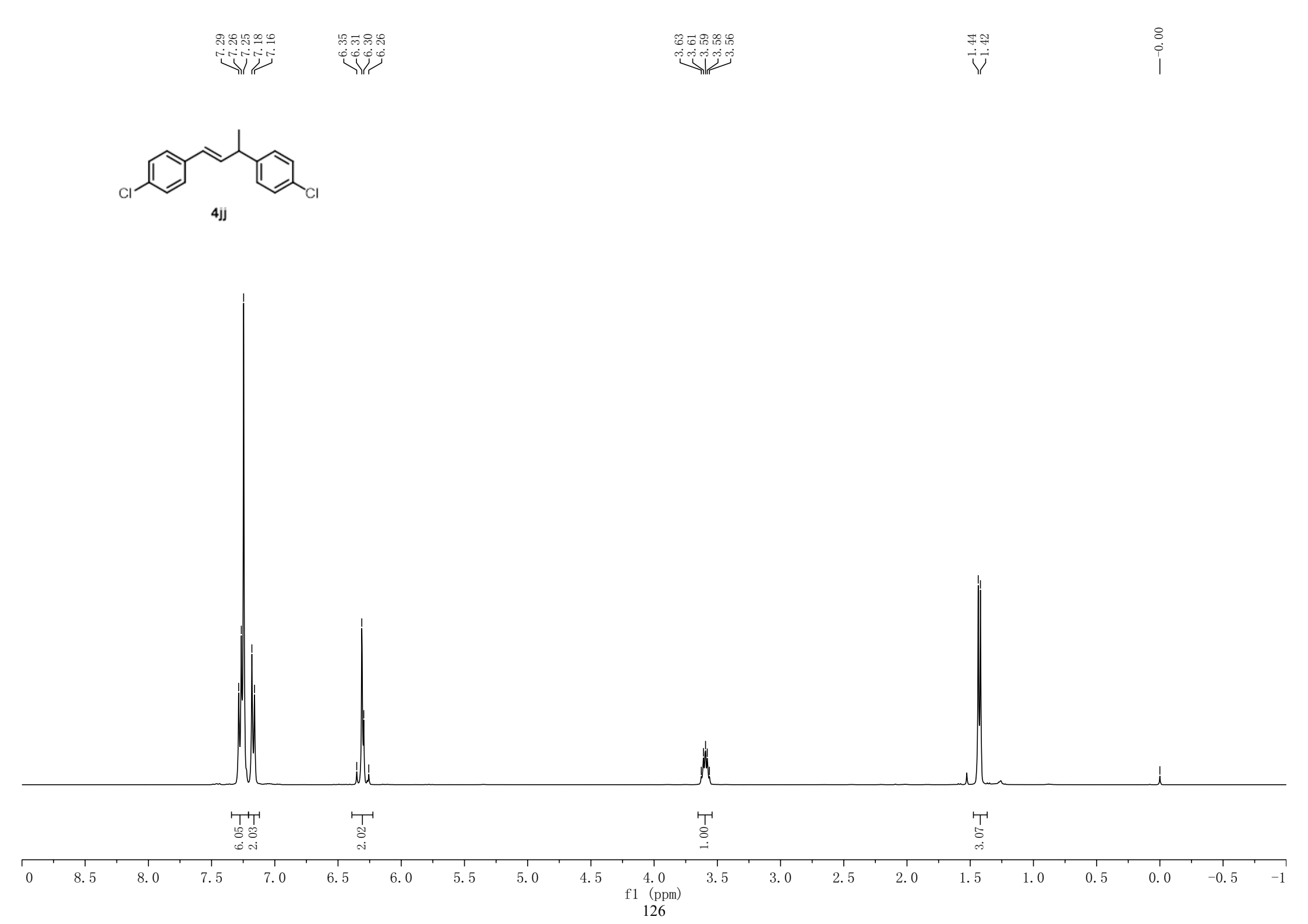
-210
f1 (ppm)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3.58
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Cl
4jj
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2.02
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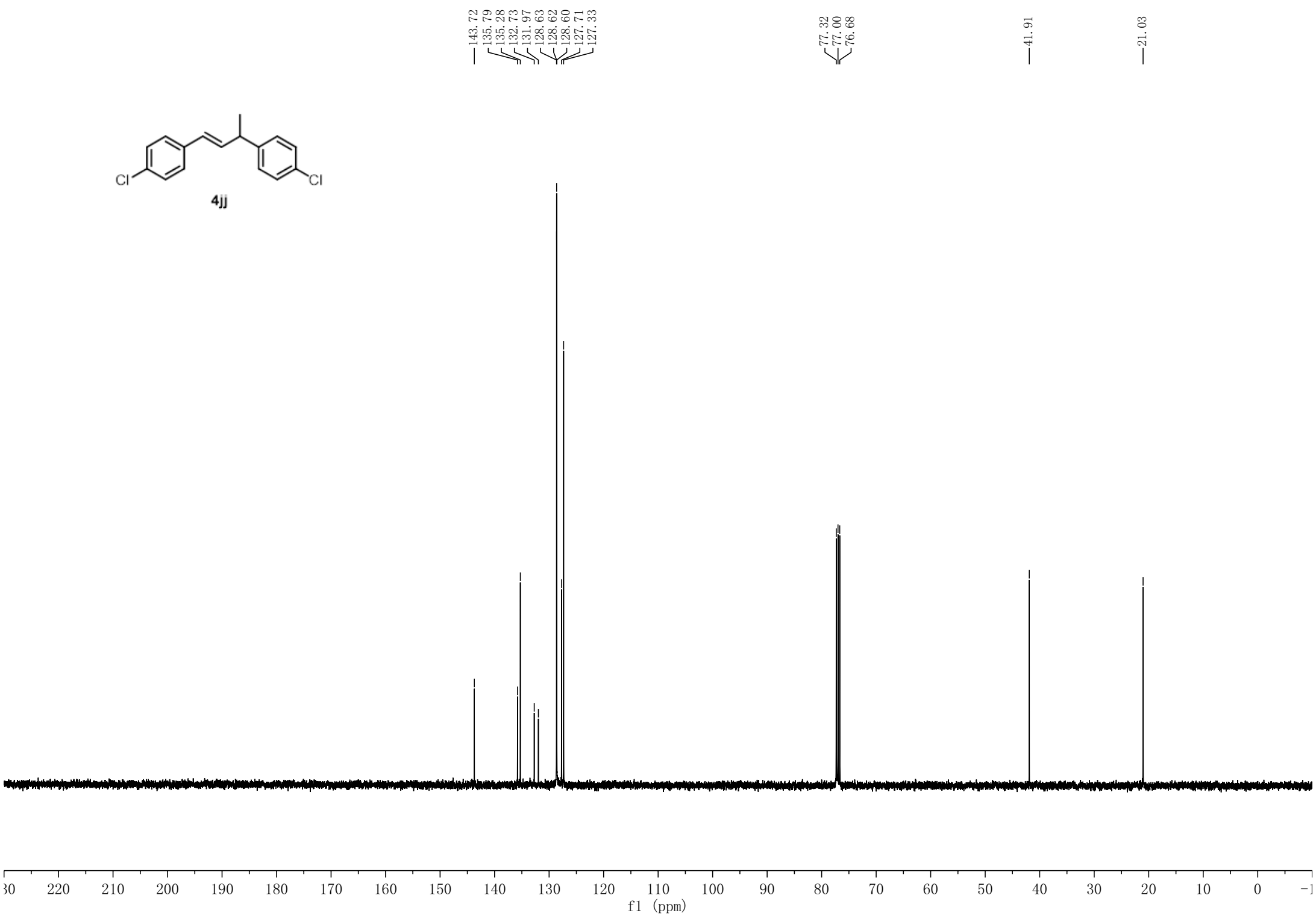
3.07
f1 (ppm)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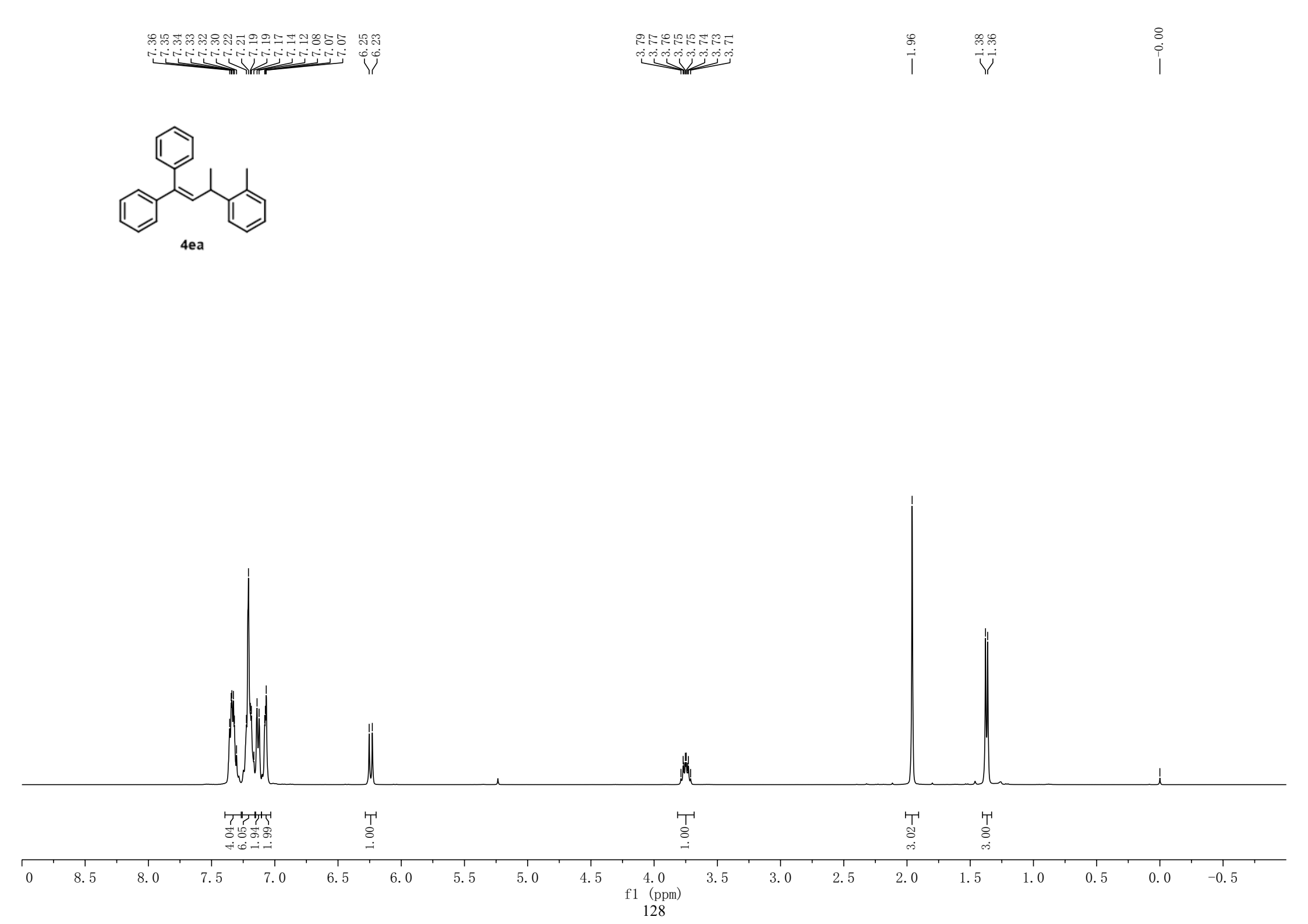
Cl
Cl
4jj
f1 (ppm)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7.12
7.08
7.07
7.07
6.25
6.23
3.79
3.77
3.76
3.75
3.75
3.74
3.73
3.71
1.96
1.38
1.36
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4ea
4.04
6.05
1.94
1.99
1.00
1.00
3.02
3.00
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
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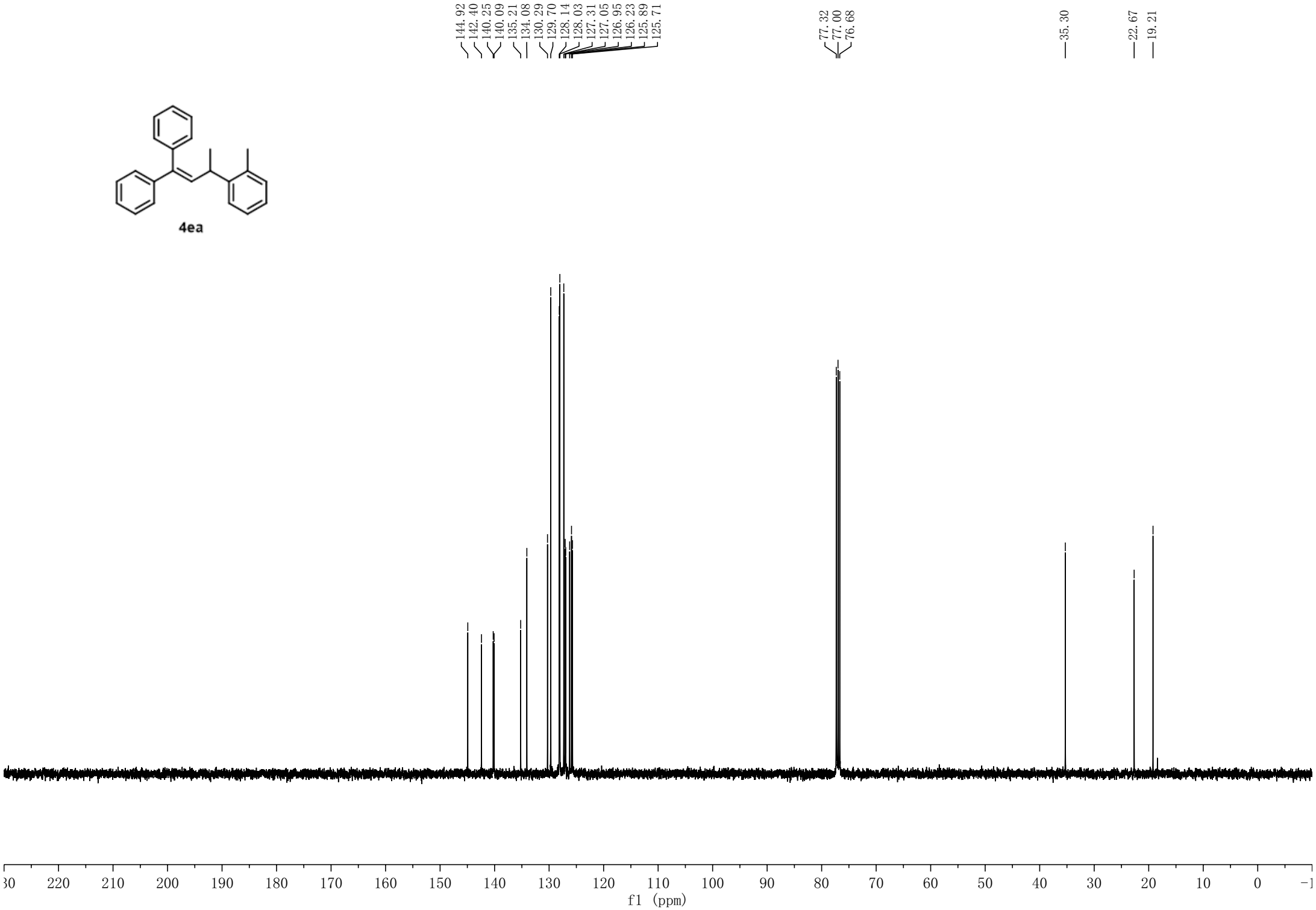
-0.5
f1 (ppm)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127.05
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77.00
76.68
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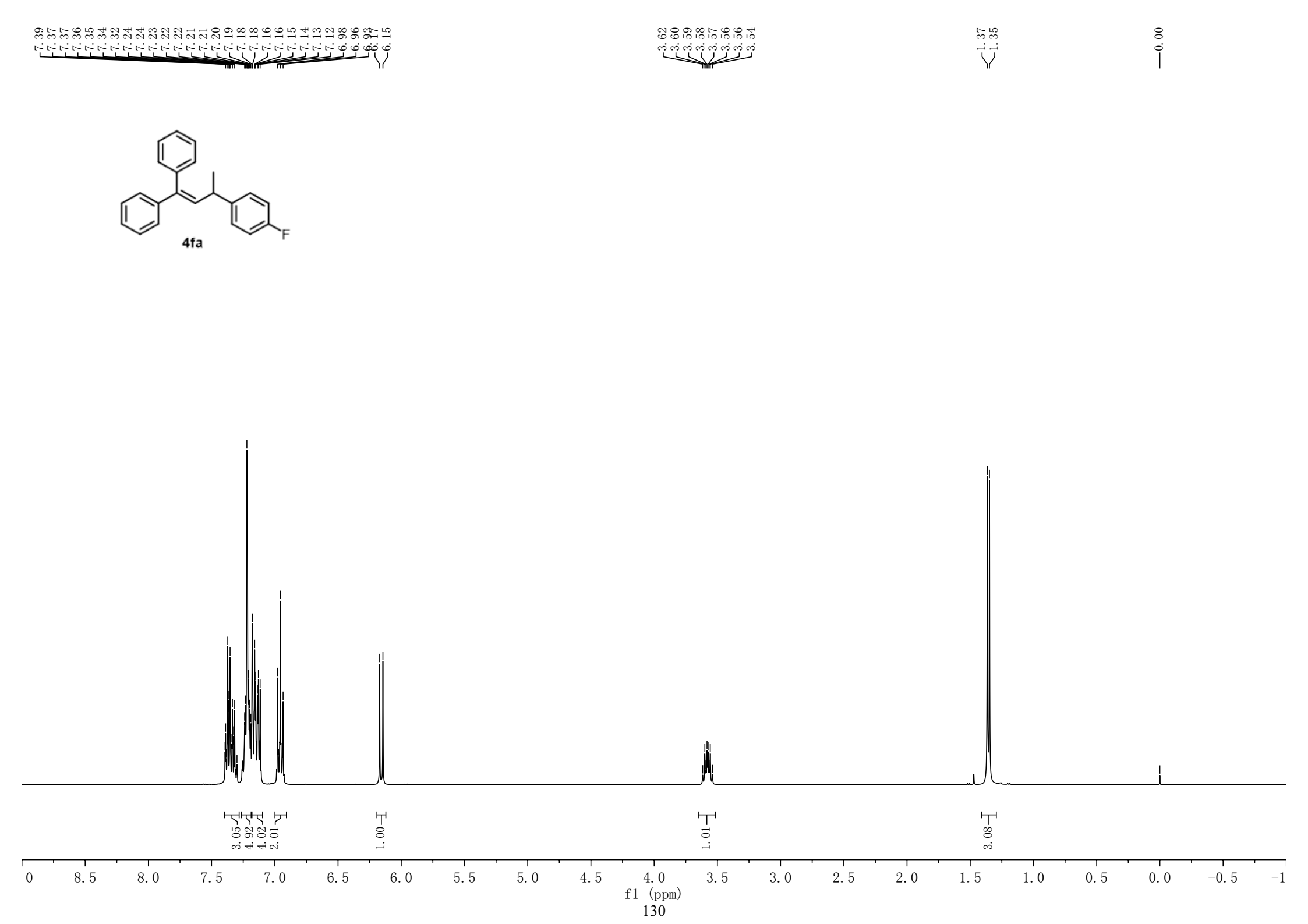
19.21
4ea
f1 (ppm)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7.19
7.18
7.18
7.16
7.16
7.15
7.14
7.13
7.12
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6.96
6.93
6.17
6.15
3.62
3.60
3.59
3.58
3.57
3.56
3.56
3.54
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1.35
0.00
F
4fa
3.05
4.92
4.02
2.01
1.00
1.01
3.08
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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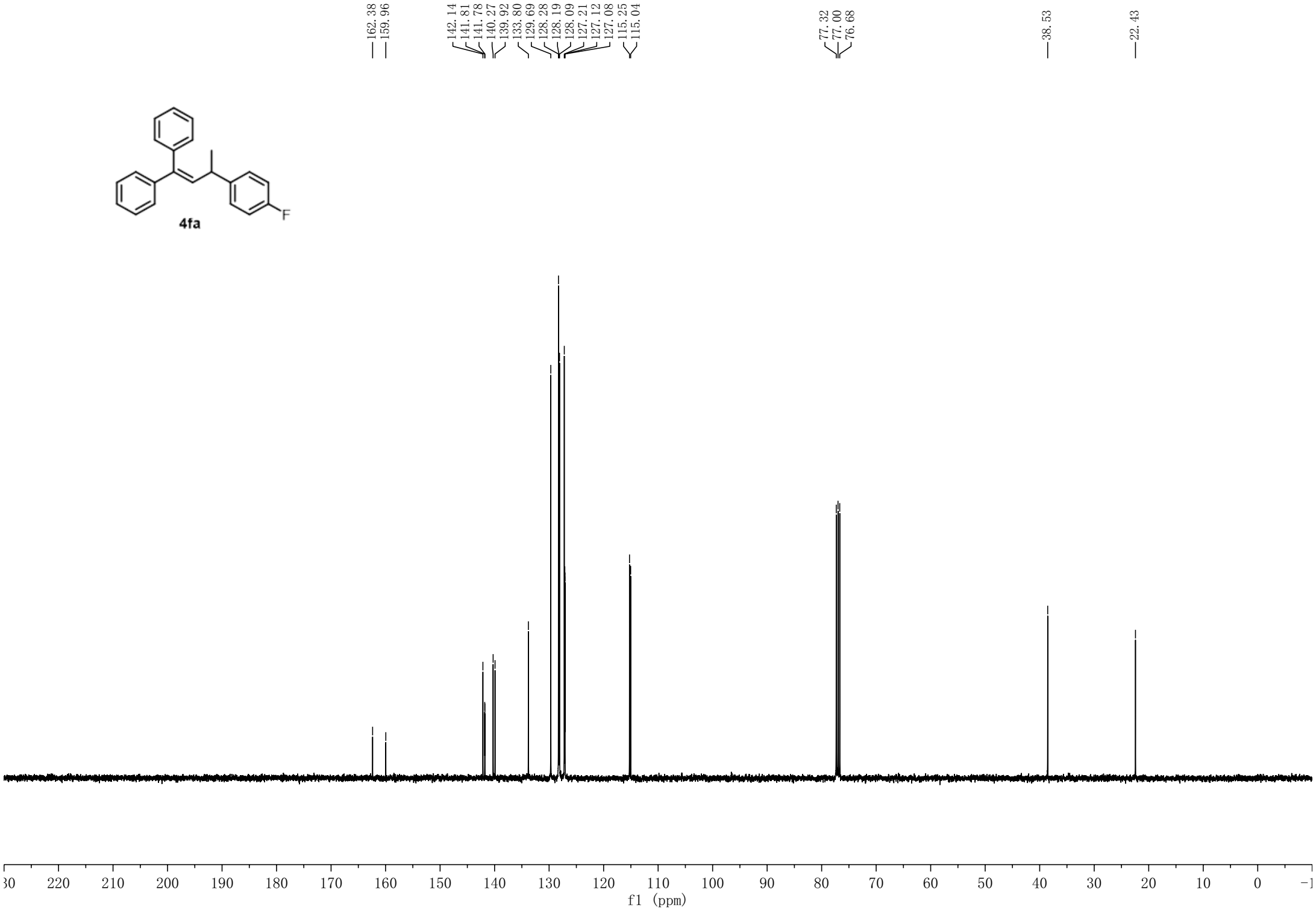
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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140.27
139.92
133.80
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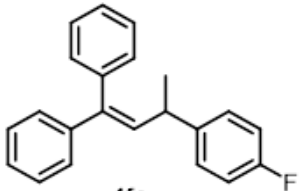
128.28
128.19
128.09
127.21
127.12
127.08
115.25
115.04
77.32
77.00
76.68
38.53
22.43
F
4fa
f1 (ppm)


F

4fa

-117.20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
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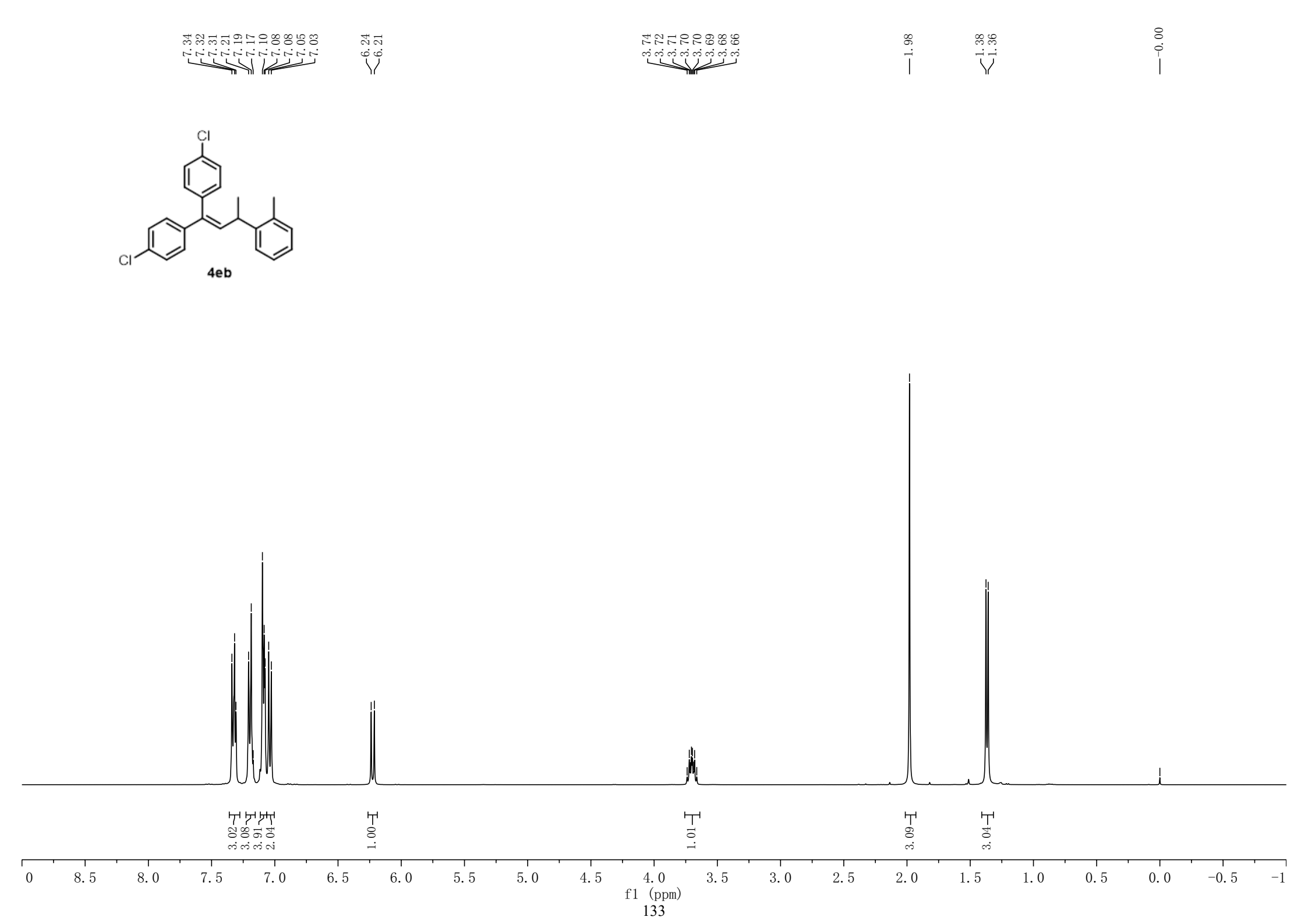
-170
-180
-190
-200
-210
f1 (ppm)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7.03
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6.21
3.74
3.72
3.71
3.70
3.70
3.69
3.68
3.66
1.98
1.38
1.36
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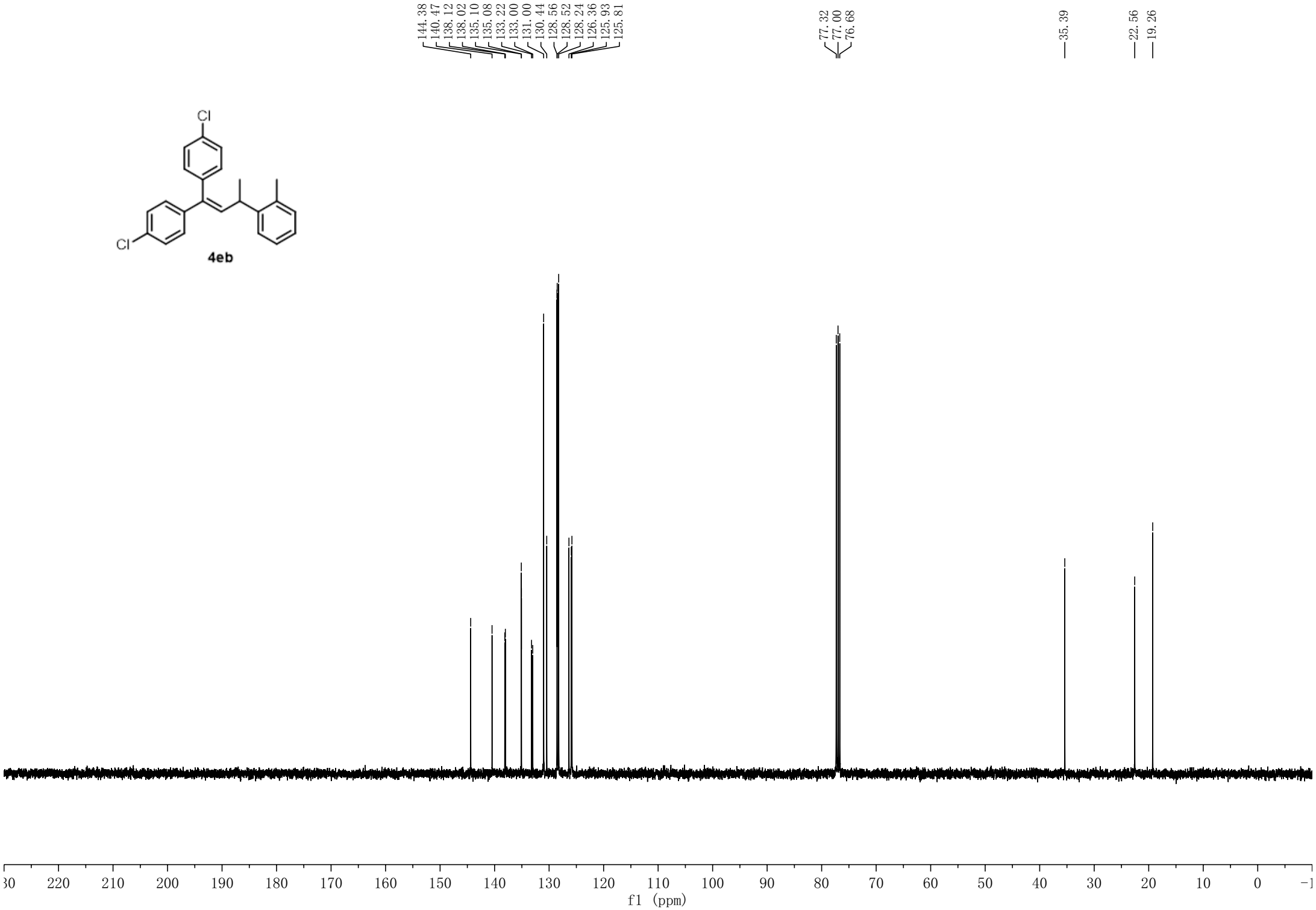
Cl
Cl
4eb
3.02
3.08
3.91
2.04
1.00
1.01
3.09
3.04
f1 (ppm)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133.00
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77.00
76.68
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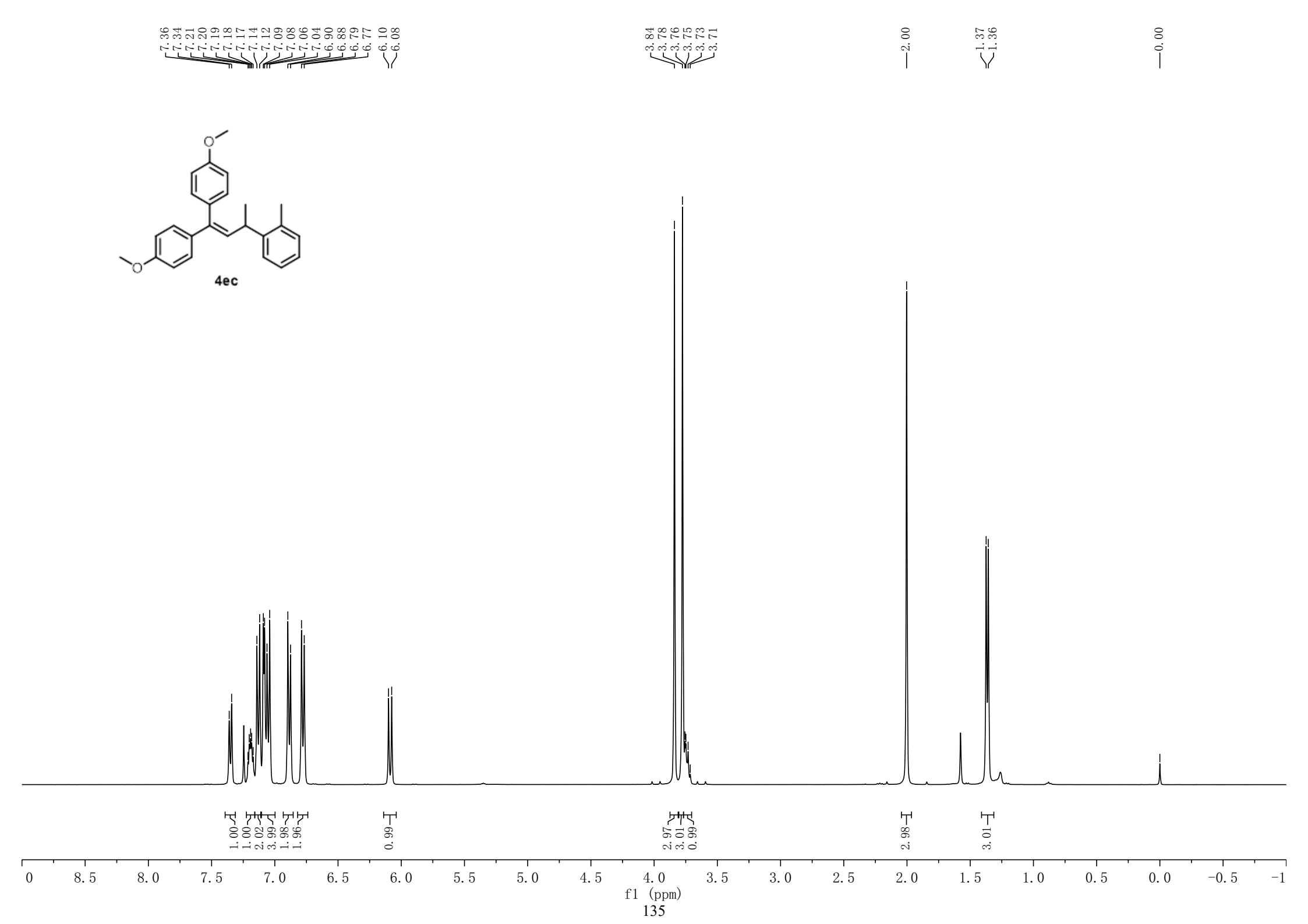
22.56
19.26
Cl
Cl
4eb
f1 (ppm)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7.08
7.06
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6.79
6.77
6.10
6.08
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3.78
3.76
3.75
3.73
3.71
2.00
1.37
1.36
0.00
4ec
1.00
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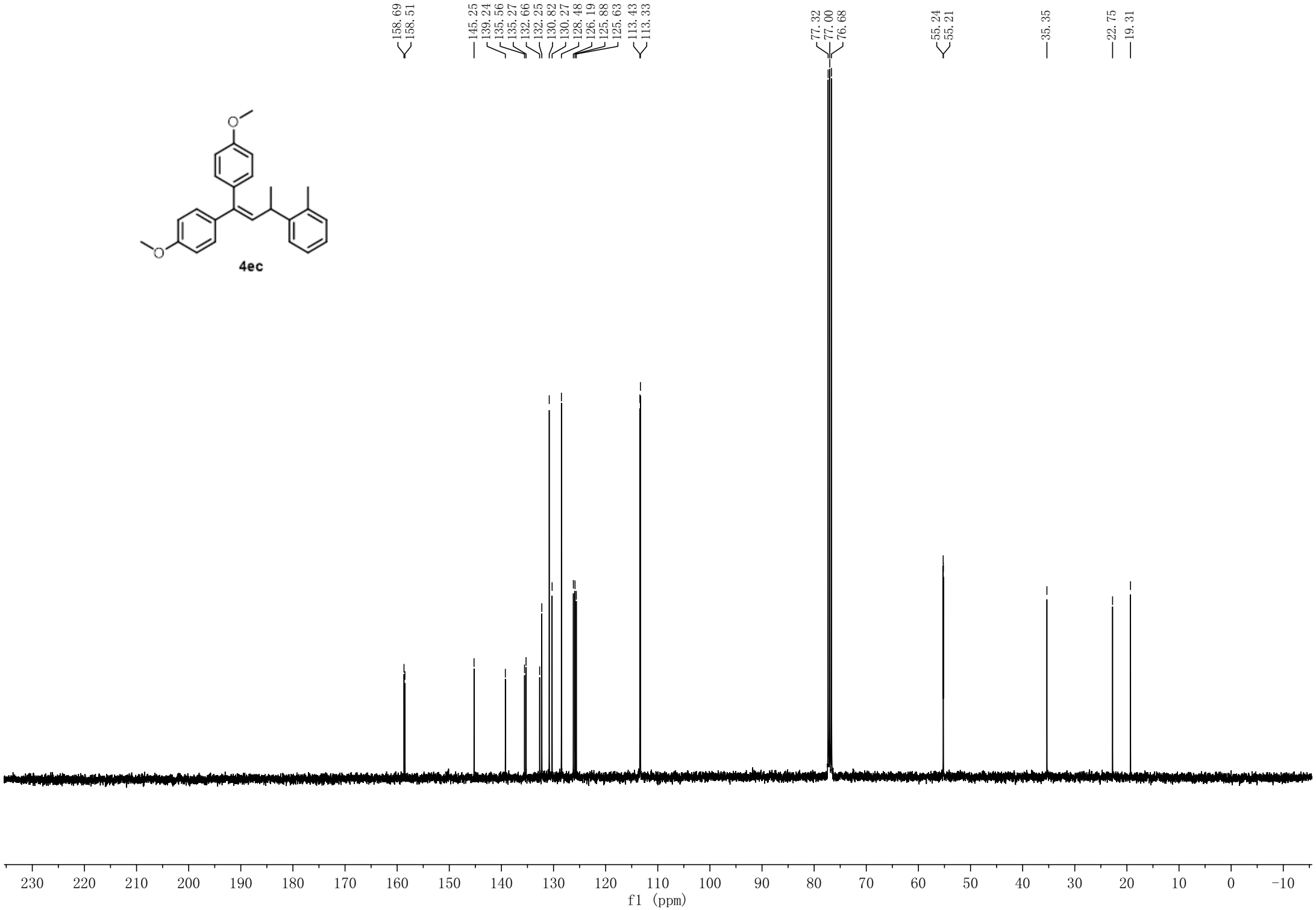
0.99
2.97
3.01
0.99
2.98
3.01
f1 (ppm)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130.82
130.27
128.48
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125.88
125.63
113.43
113.33
77.32
77.00
76.68
55.24
55.21
35.35
22.75
19.31
4ec
230
220
210
200
190
180
170
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100
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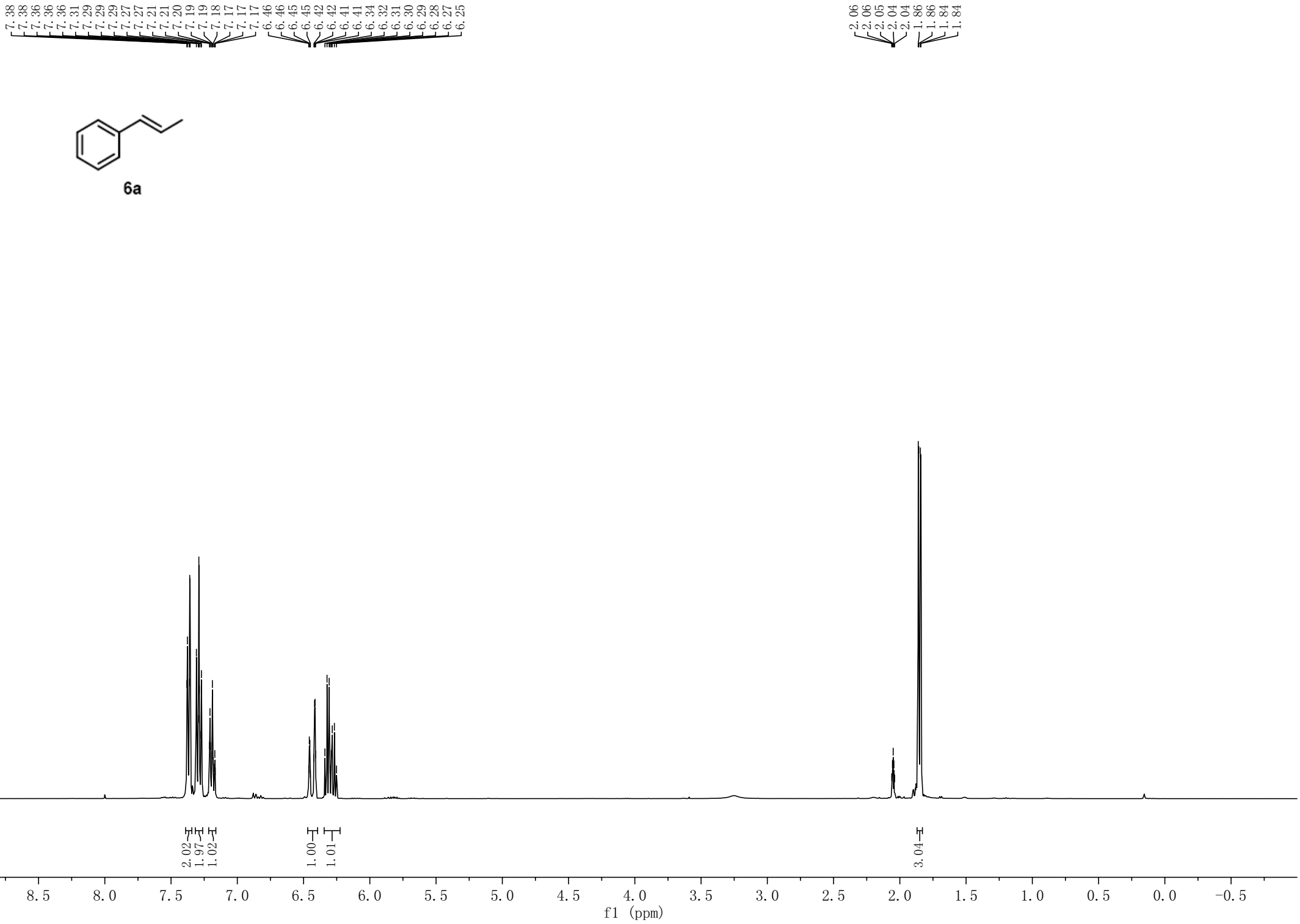
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.19
7.19
7.18
7.17
7.17
7.17
6.46
6.45
6.45
6.42
6.42
6.41
6.41
6.34
6.32
6.31
6.30
6.29
6.28
6.27
6.25
2.06
2.06
2.05
2.04
2.04
1.86
1.86
1.84
1.84
1.84
6a
2.02
1.97
1.02
1.00
1.01
3.04
0
8.5
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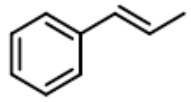
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

206.14

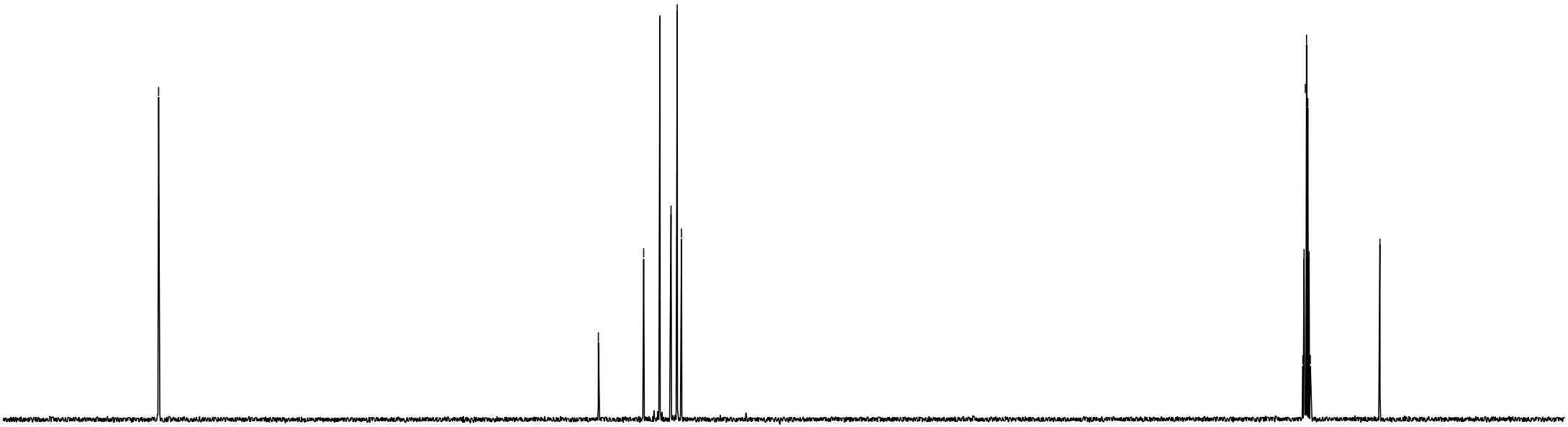
138.54
131.58
129.08
127.38
126.43
125.77

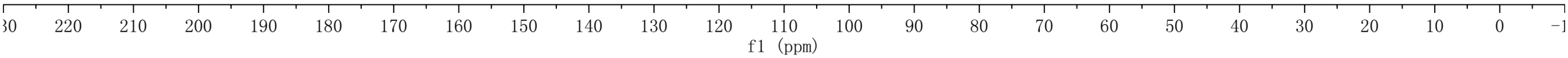
30.28
30.08
29.89
29.70
29.51
29.31
29.12

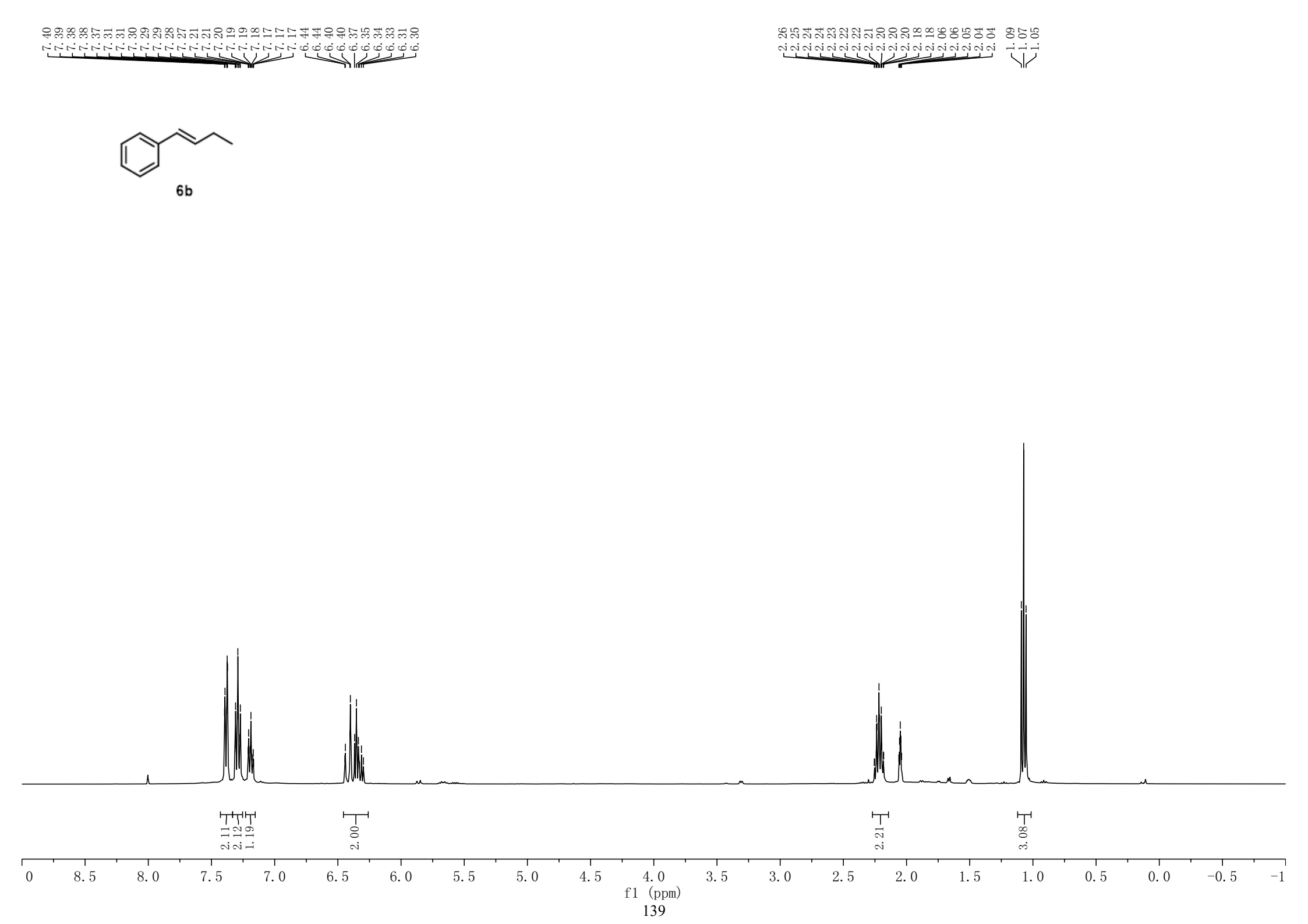
18.42



6a



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7.19
7.19
7.18
7.17
7.17
7.17
6.44
6.44
6.40
6.40
6.37
6.35
6.34
6.33
6.31
6.30
2.26
2.25
2.24
2.24
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2.22
2.22
2.21
2.20
2.20
2.20
2.18
2.18
2.06
2.06
2.05
2.04
2.04
1.09
1.07
1.05
6b
2.11
2.12
1.19
2.00
2.21
3.08
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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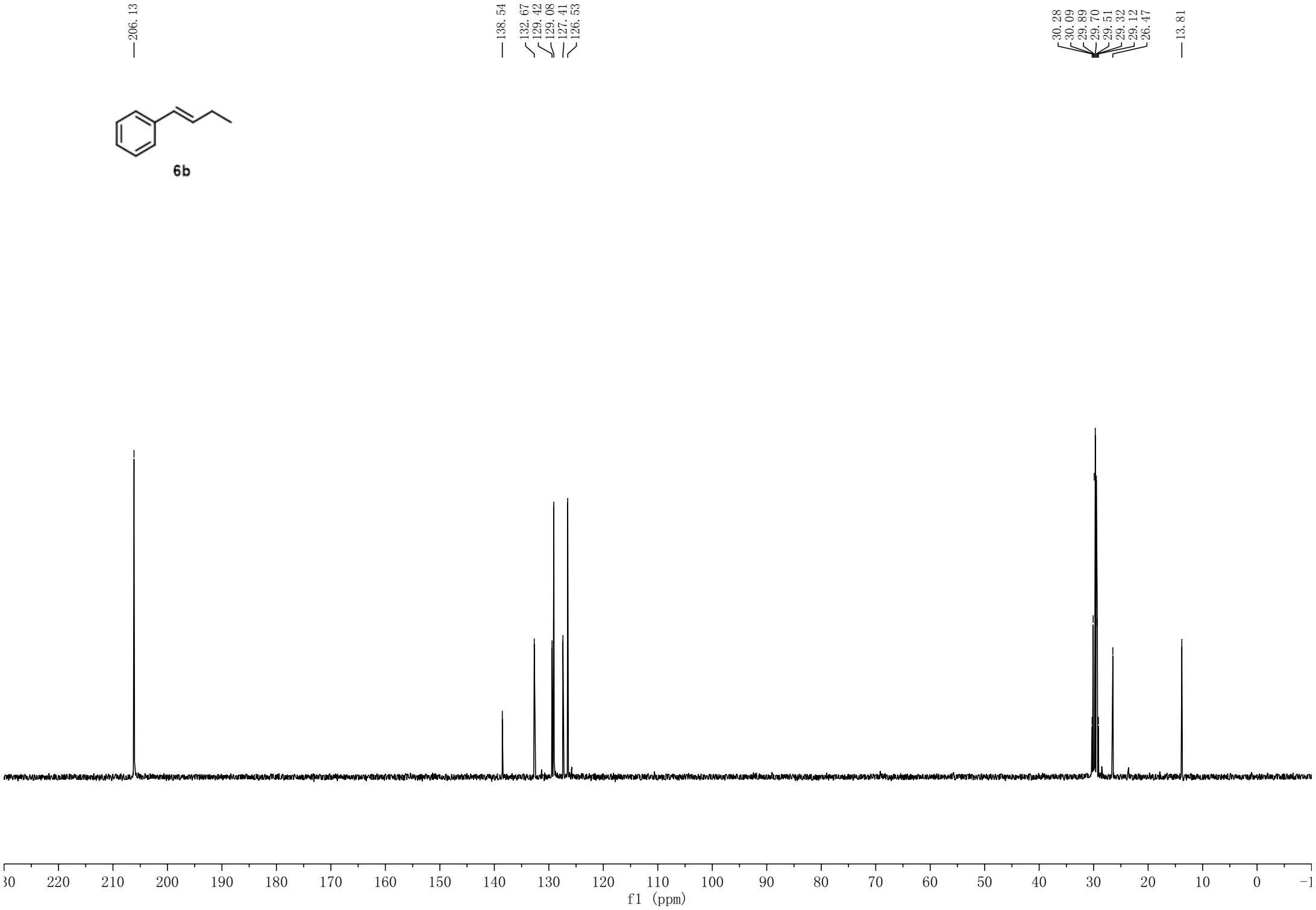
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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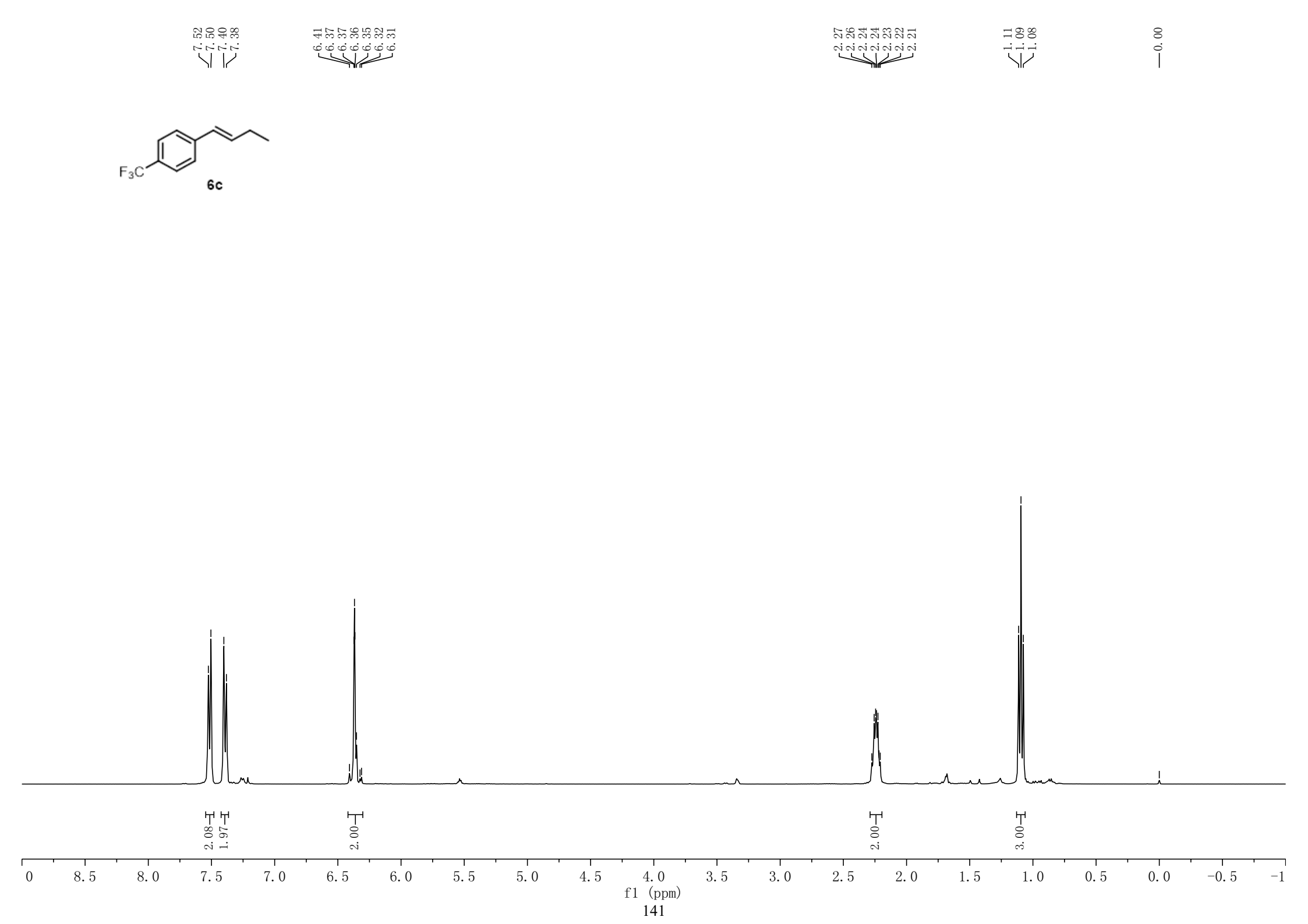
30.09
29.89
29.70
29.51
29.32
29.12
26.47
13.81
6b
f1 (ppm)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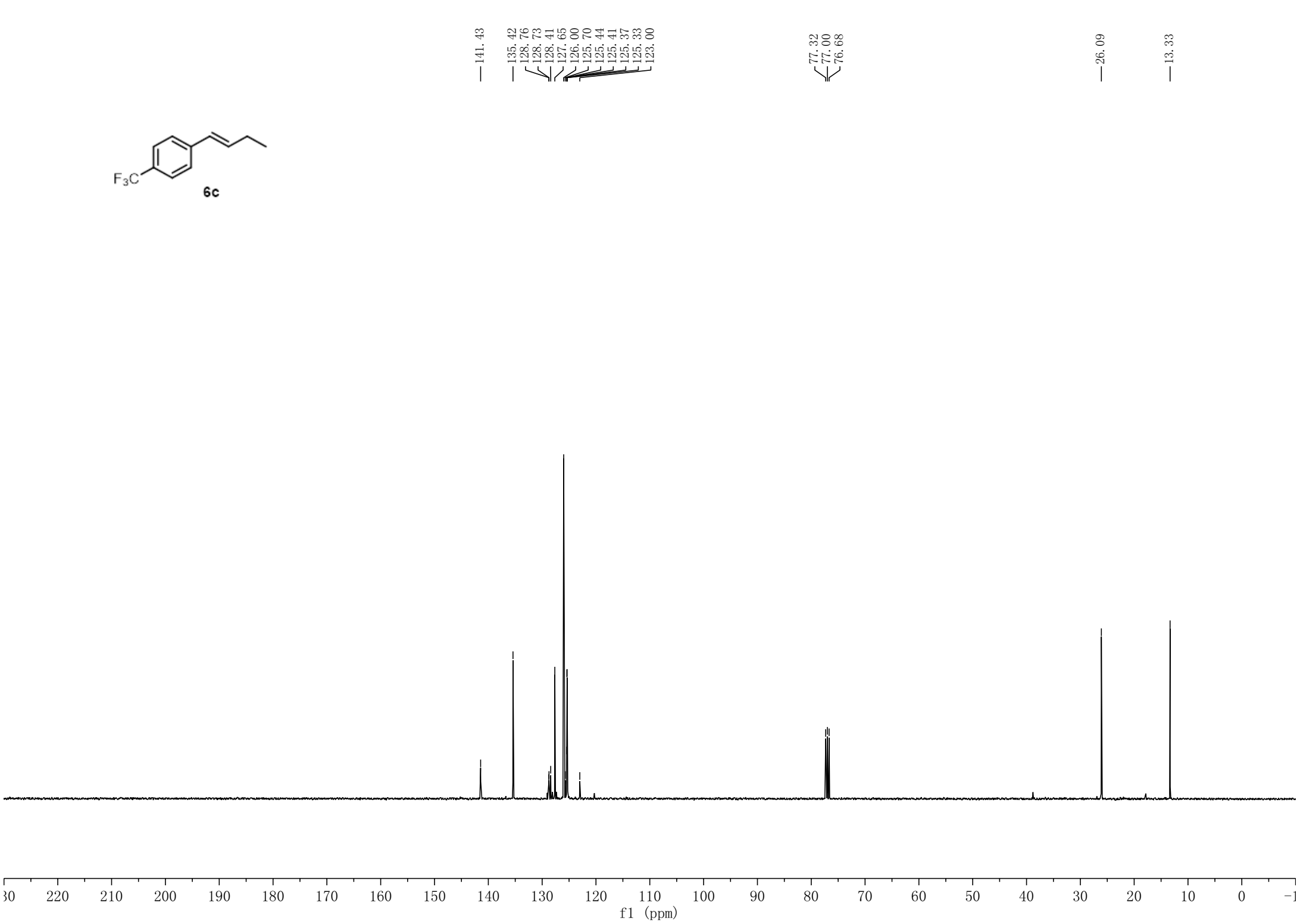
6.36
6.35
6.32
6.31
2.27
2.26
2.24
2.24
2.23
2.22
2.21
1.11
1.09
1.08
0.00
F3C
6c
2.08
1.97
2.00
2.00
3.00
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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127.65
126.00
125.70
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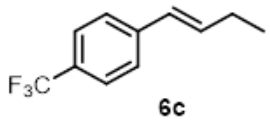
125.37
125.33
123.00
77.32
77.00
76.68
26.09
13.33
F3C
6c
f1 (ppm)


F3C

6c

-62.38
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-2
f1 (ppm)


7.40
7.40
7.39
7.38
7.38
7.38
7.31
7.31
7.30
7.29
7.29
7.27
7.27
7.21
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7.19
7.19
7.18
7.17
7.17
7.17
6.45
6.42
6.41
6.41
6.35
6.33
6.31
6.31
6.29
6.27


2.21
2.21
2.19
2.19
2.18
2.17
2.17
2.16
2.06
2.06
2.05
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2.04
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1.50
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1.46
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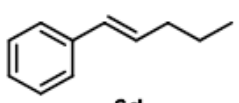
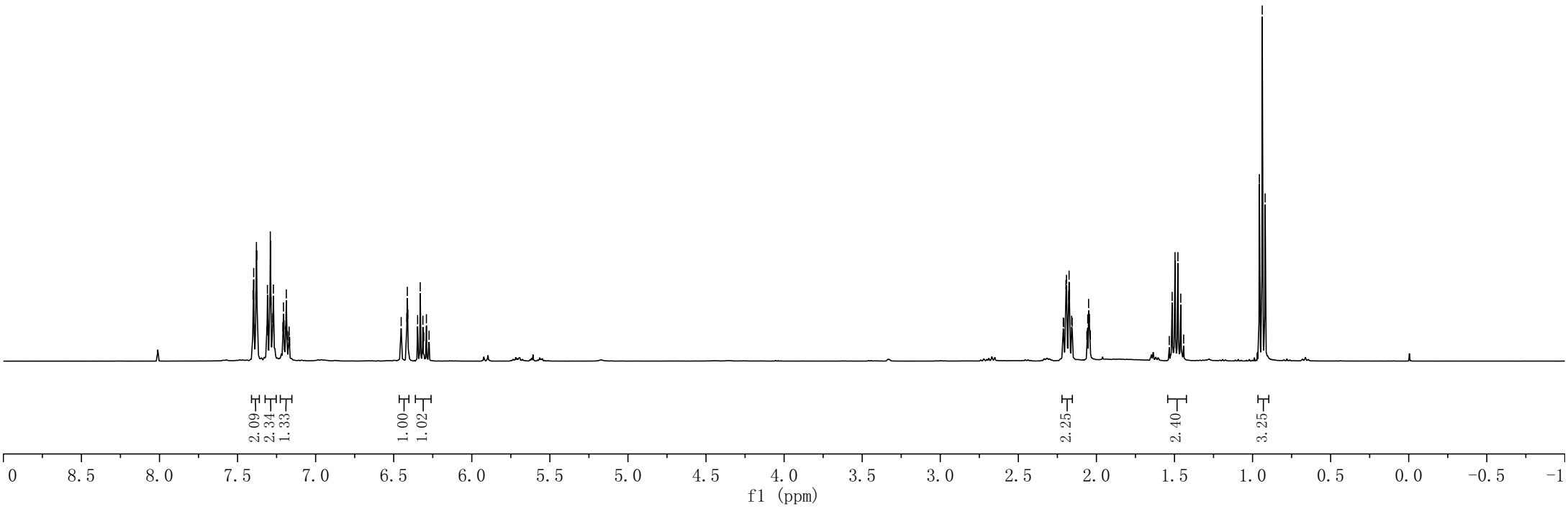
0.94
0.92



6d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0
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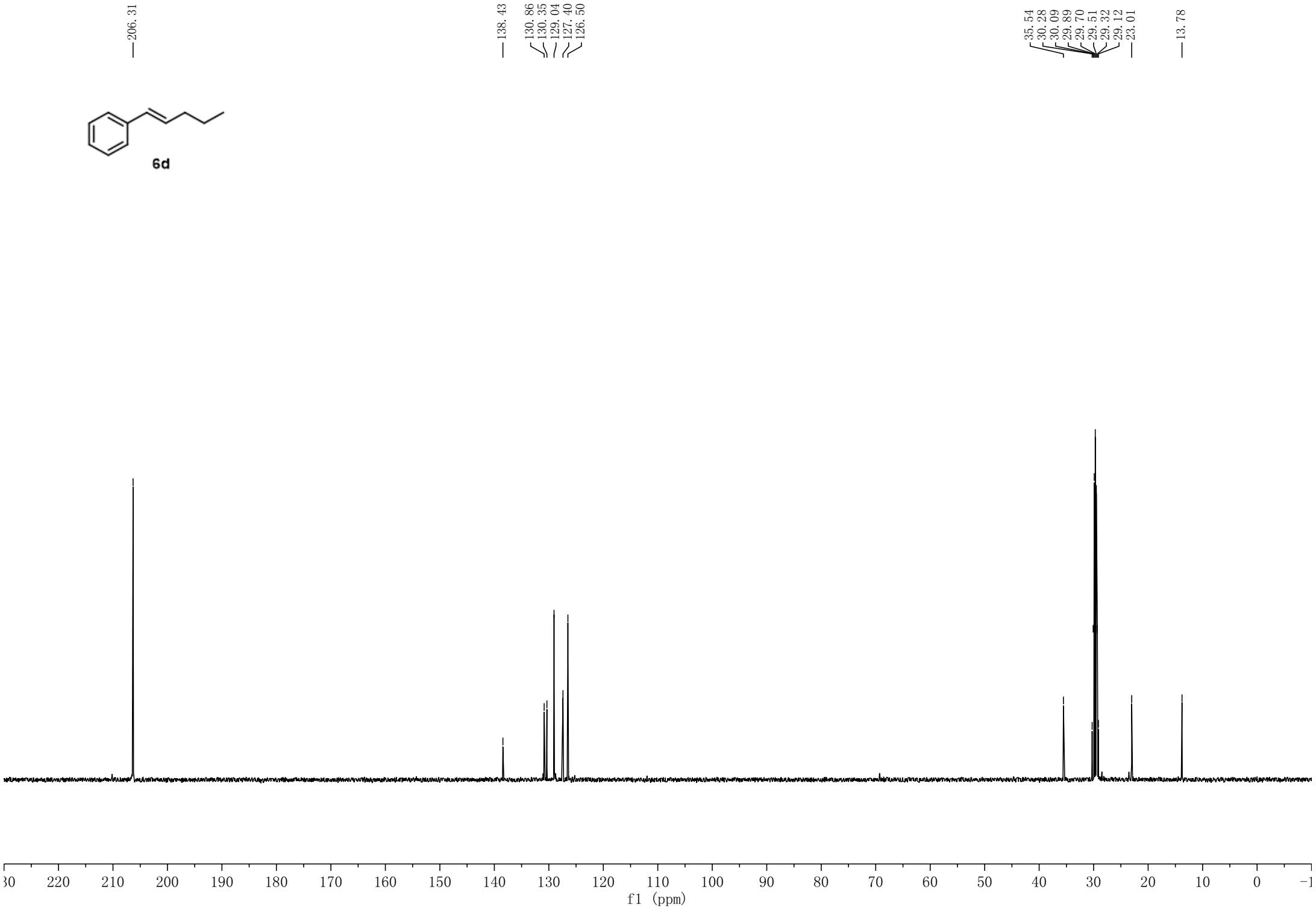
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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126.50
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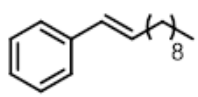
29.12
23.01
13.78
6d
f1 (ppm)


8

6e

2.09
3.30
2.61
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2.30
1.27
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18.02
4.53
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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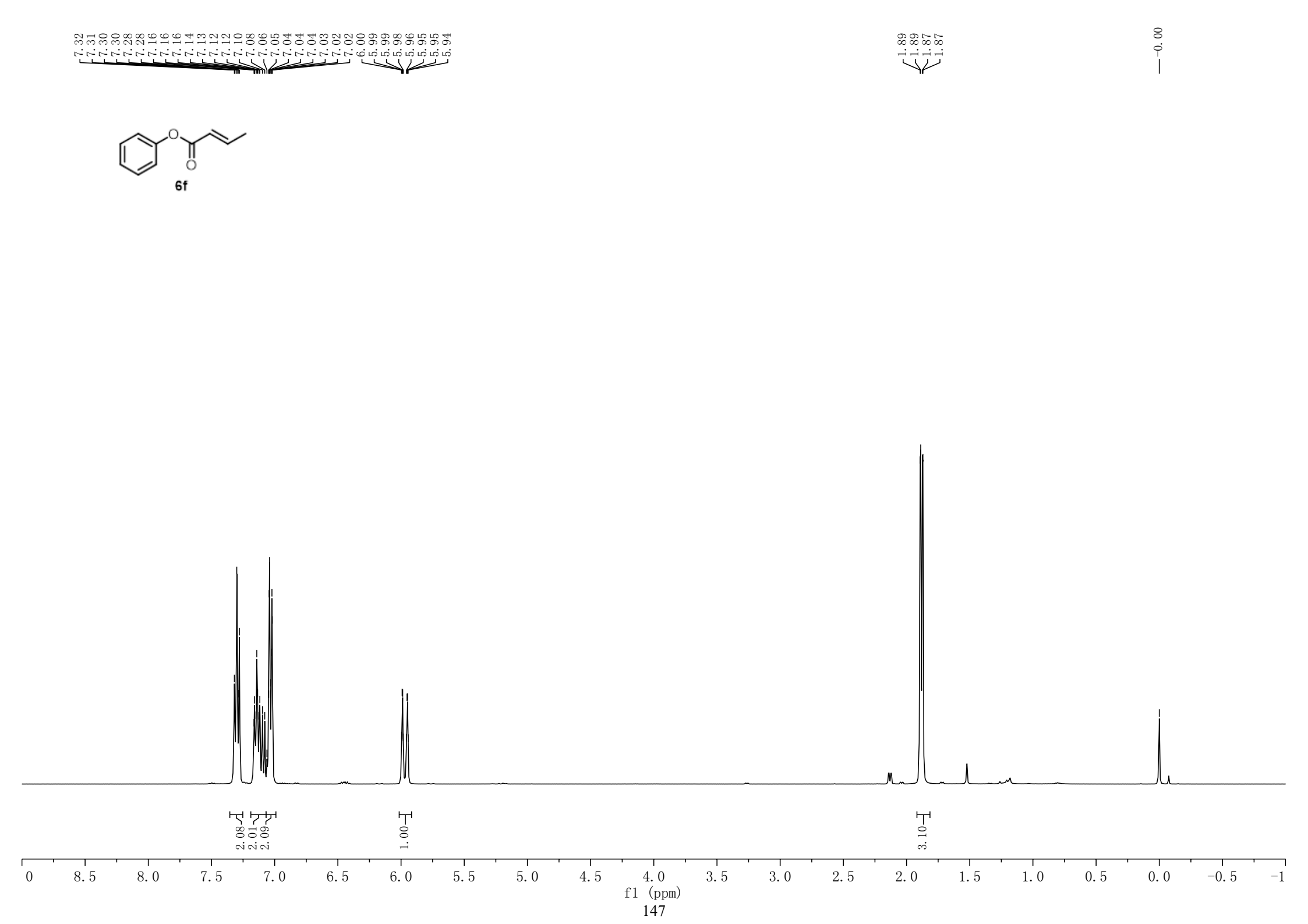
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)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7.08
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6.00
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5.99
5.98
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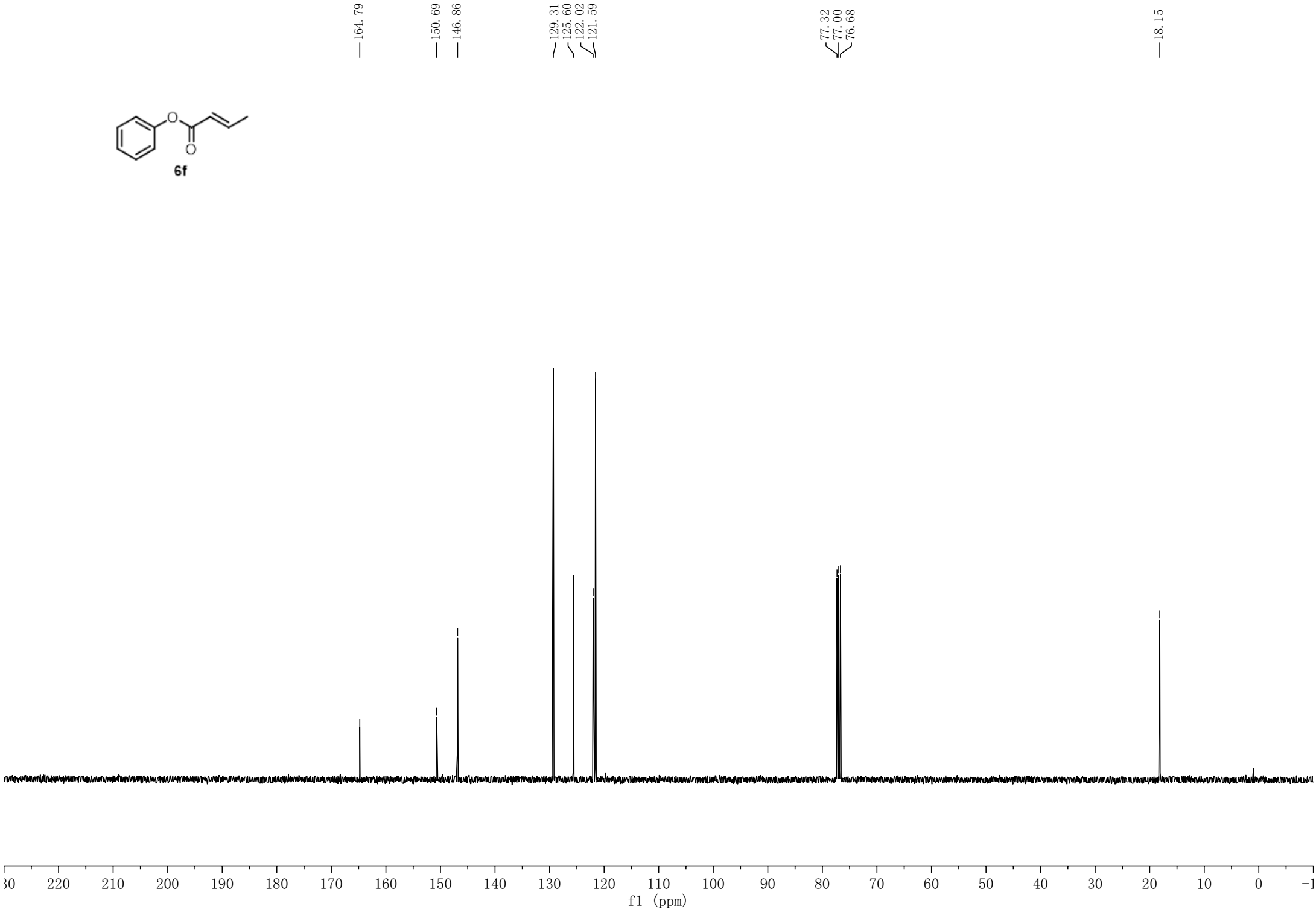
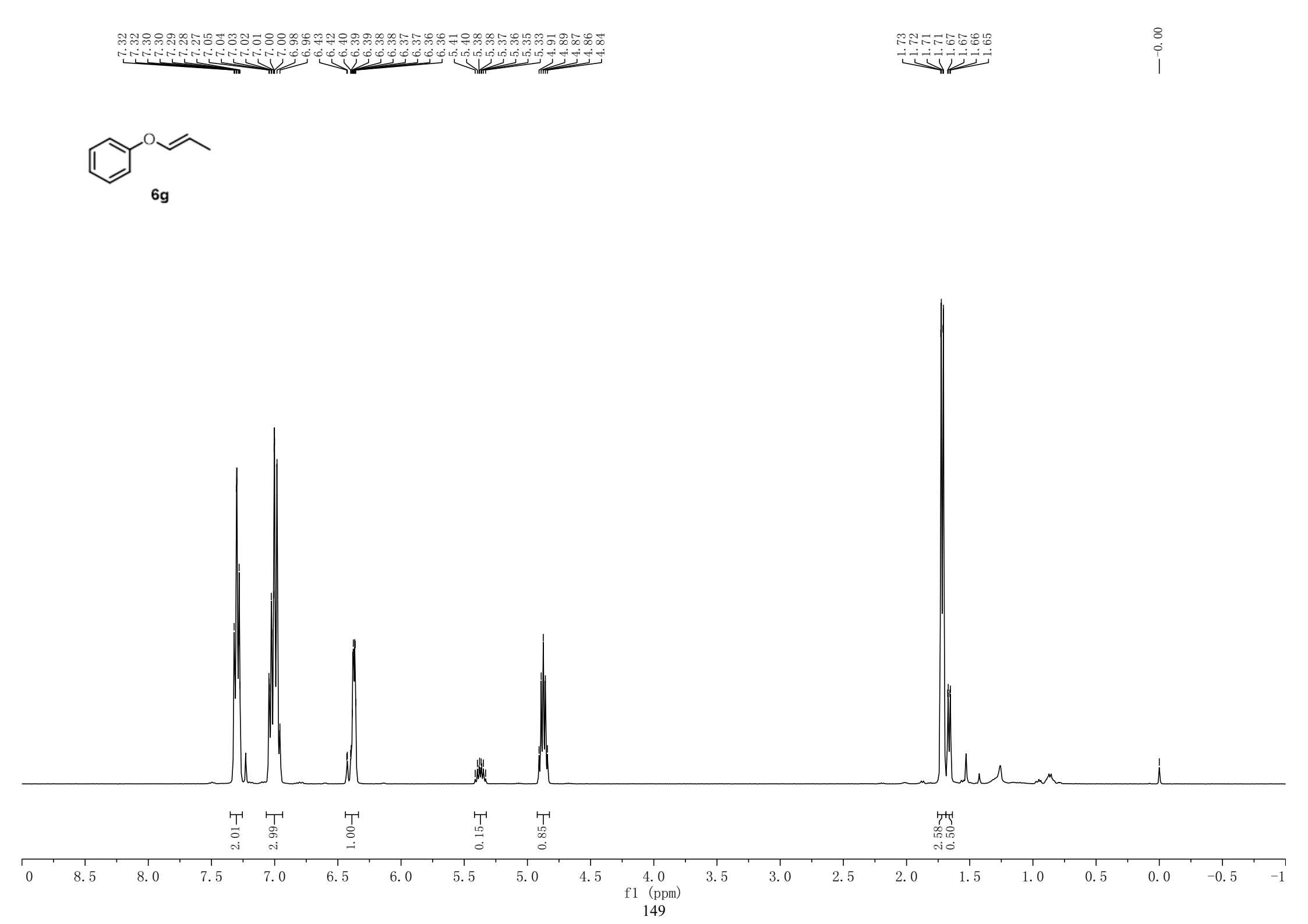
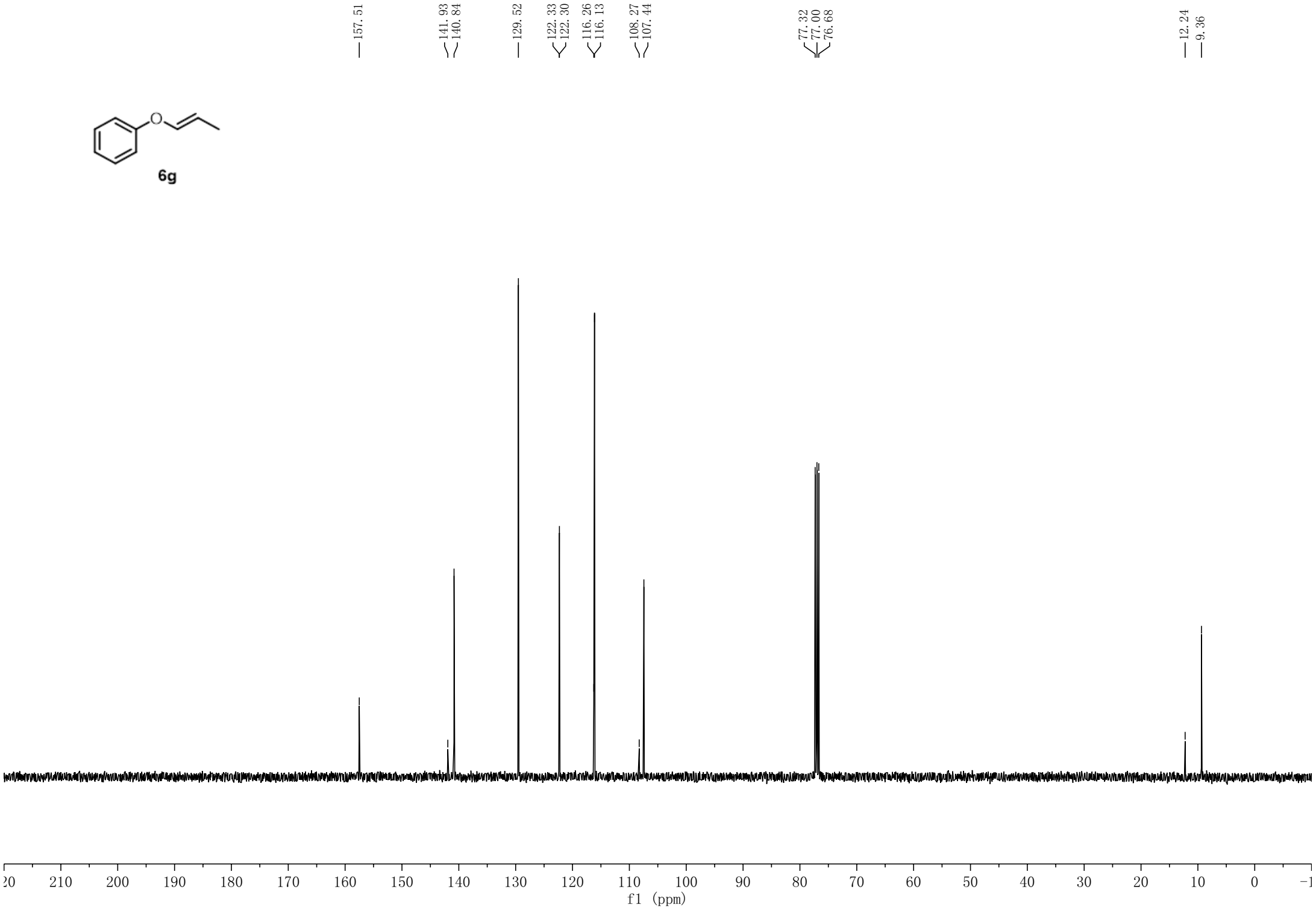
5.95
5.95
5.94
1.89
1.89
1.87
1.87
0.00
6f
2.08
2.01
2.09
1.00
3.10
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


164.79
150.69
146.86
129.31
125.60
122.02
121.59
77.32
77.00
76.68
18.15
6f
f1 (ppm)


7.32
7.32
7.30
7.30
7.29
7.28
7.27
7.05
7.04
7.03
7.02
7.01
7.00
7.00
6.98
6.96
6.43
6.42
6.40
6.39
6.39
6.38
6.38
6.37
6.37
6.36
6.36
5.41
5.40
5.38
5.38
5.37
5.36
5.35
5.33
4.91
4.89
4.87
4.86
4.84
1.73
1.72
1.71
1.71
1.67
1.67
1.66
1.65
0.00
O
6g
2.01
2.99
1.00
0.15
0.85
2.58
0.50
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


157.51
141.93
140.84
129.52
122.33
122.30
116.26
116.13
108.27
107.44
77.32
77.00
76.68
12.24
9.36
6g
f1 (ppm)