

Electronic Supporting Information

Palladium-catalyzed intramolecular dehydrogenative coupling of BH and OH: synthesis of carborane-fused benzoxaboroles

Chun-Xiao Cui,^a Jie Zhang,^b Zaozao Qiu,^{*acd} and Zuowei Xie^{*ab}

^aShanghai-Hong Kong Joint Laboratory in Chemical Synthesis, Shanghai Institute of Organic Chemistry, University of Chinese Academy of Sciences, Chinese Academy of Sciences, 345 Lingling Rd, Shanghai 200032, China

^bDepartment of Chemistry and State Key Laboratory of Synthetic Chemistry, The Chinese University of Hong Kong, Shatin, N. T., Hong Kong, China

^cCAS Key Laboratory of Energy Regulation Materials, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Rd, Shanghai 200032, China

^dFujian Innovation Academy, Chinese Academy of Sciences, 155 Yangqiao Rd West, Fuzhou, 350002, China

Email Address: qiuzz@sioc.ac.cn; zxie@cuhk.edu.hk

Table of Contents

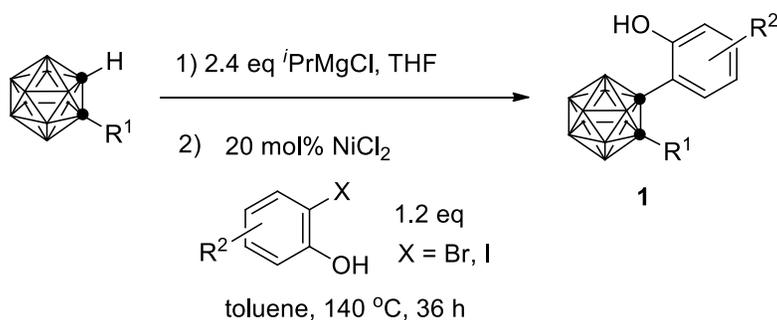
1. General Information	S2
2. Experimental Section	S2
3. Crystal Data and Summary of Data Collection and Refinements	S21
4. References	S22
5. NMR Spectra	S24

1. General Information

All reactions were carried out in oven-dried glassware under an atmosphere of dry N₂ with the rigid exclusion of air and moisture using standard Schlenk techniques or in a glovebox. Toluene and THF were freshly distilled from sodium benzophenone ketyl immediately prior to use. All chemicals were purchased from either Aldrich or J&K Chemical Co. and used as received unless otherwise specified. ¹H and ¹³C{¹H} NMR spectra were recorded on a Varian 400 or Agilent 400 spectrometer at 400 MHz and 100 MHz, respectively. ¹¹B and ¹⁹F NMR spectra were recorded on a Bruker 400 spectrometer at 128 MHz and 376 MHz, respectively. All signals were reported in ppm unit with references to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, to external BF₃ OEt₂ (0.00) for boron chemical shifts, and to external CFCl₃ (0.00) for fluorine chemical shifts. Mass spectra were obtained on a Thermo Fisher Scientific LTQ FTICR-MS spectrometer. Elemental analyses were performed with an elementary VARIO EL III elemental analyzer, Shanghai Institute of Organic Chemistry, CAS.

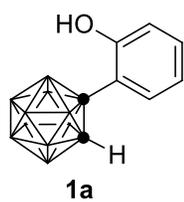
2. Experimental Section

Preparation of Starting Materials (1a-p).



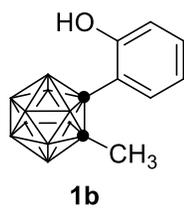
Typical procedure for the preparation of 1-(*o*'-HOC₆H₃R²)-2-R¹-*o*-C₂B₁₀H₁₀ (1). ⁱPrMgCl (2.0 M in THF, 6.0 mL, 12.0 mmol) was slowly added to a THF solution (25 mL) of *o*-carborane (5.0 mmol) at 0 °C, and the mixture was stirred at 0 °C for 1 h. After replacement of THF with toluene (25 mL), and the addition of 2-iodophenols or 2-bromophenols (6.0 mmol) and NiCl₂ (130 mg, 1.0 mmol), the reaction mixture was heated at 140 °C under stirring for 36 h in a closed flask. Then, the reaction was

quenched with water (50 mL) and extracted with ethyl acetate (100 mL x 3). The organic portions were combined and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (300–400 mesh) using hexane/EtOAc (20/1(v/v)) as eluent to give product **1**.



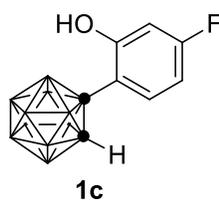
1a: Yield 48%. White solid. mp: 186-188 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.57 (d, J = 8.0 Hz, 1H), 7.21 (t, J = 8.0 Hz, 1H), 6.94 (t, J = 8.0 Hz, 1H), 6.68 (d, J = 8.0 Hz, 1H) (aromatic CH), 5.44 (s, 1H) (cage H), 5.14 (s, 1H) (OH). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 151.7, 132.7, 130.7, 121.9, 120.0, 117.3 (aromatic C), 74.9, 60.0 (cage C).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.3 (2B), -8.7 (2B), -9.3 (2B), -11.0 (2B), -13.0 (2B). IR (KBr): ν (cm^{-1}) 3559, 3103, 2566, 1502, 1453, 1334, 1186, 750. Anal. Calcd for $\text{C}_8\text{H}_{16}\text{B}_{10}\text{O}$: C, 40.66; H, 6.82. Found: C, 40.77; H, 6.84.



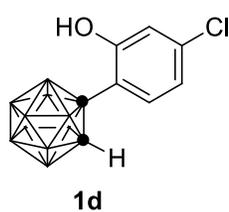
1b: Yield 28%. White solid. mp: 113-115 °C. ^1H NMR (300 MHz, CDCl_3): δ 7.68 (d, J = 10.8 Hz, 1H), 7.33 (t, J = 10.8 Hz, 1H), 6.97 (t, J = 10.8 Hz, 1H), 6.87 (d, J = 10.8 Hz, 1H) (aromatic CH), 5.71 (s, 1H) (OH), 1.74 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 155.6, 134.2, 132.4, 121.5, 119.0, 115.7 (aromatic C), 80.0, 79.6 (cage C), 23.5 (CH_3).

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -2.0 (1B), -5.1 (1B), -9.5 (8B). IR (KBr): ν (cm^{-1}) 3586, 2568, 1605, 1453, 1303, 1175, 1094, 751. Anal. Calcd for $\text{C}_9\text{H}_{18}\text{B}_{10}\text{O}$: C, 43.18; H, 7.25. Found: C, 43.47; H, 7.02.

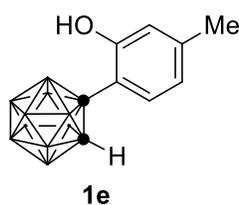


1c: Yield 36%. White solid. mp: 191-192 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.55 (dd, J = 8.8, 6.0 Hz, 1H), 6.67 (td, J = 8.2, 2.8 Hz, 1H), 6.46 (dd, J = 8.8, 2.8 Hz, 1H) (aromatic CH), 5.75 (s, 1H) (cage H), 5.37 (s, 1H) (OH). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 163.2 (d, $^1J_{\text{C-F}}$ = 250.7 Hz), 152.8 (d, $^3J_{\text{C-F}}$ = 10.4 Hz), 134.2 (d, $^3J_{\text{C-F}}$ = 10.0 Hz), 116.3 (d, $^4J_{\text{C-F}}$ = 3.6 Hz), 109.3 (d, $^2J_{\text{C-F}}$ = 21.2 Hz), 104.6 (d, $^2J_{\text{C-F}}$ = 24.5 Hz) (aromatic C),

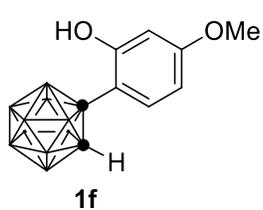
74.2, 59.6 (cage C). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.5 (2B), -8.8 (2B), -9.5 (2B), -11.1 (2B), -13.1 (2B). ^{19}F NMR (376 MHz, CDCl_3): δ -109.7 (m, 1F). IR (KBr): ν (cm^{-1}) 3547, 3103, 2575, 1609, 1516, 1425, 1189, 991, 835, 729. Anal. Calcd for $\text{C}_8\text{H}_{15}\text{B}_{10}\text{FO}$: C, 37.78; H, 5.95. Found: C, 37.93; H, 6.00.



1d: Yield 43%. White solid. mp: 203-205 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.50 (d, $J = 8.8$ Hz, 1H), 6.93 (d, $J = 8.4$ Hz, 1H), 6.74 (s, 1H) (aromatic CH), 5.77 (s, 1H) (cage H), 5.37 (s, 1H) (OH). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 152.4, 136.0, 133.6, 122.1, 118.8, 117.3 (aromatic C), 74.2, 59.7 (cage C). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.3 (2B), -8.7 (2B), -9.4 (2B), -11.1 (2B), -13.0 (2B). IR (KBr): ν (cm^{-1}) 3543, 3102, 2571, 1584, 1499, 1411, 1243, 1192, 913, 733. Anal. Calcd for $\text{C}_8\text{H}_{15}\text{B}_{10}\text{ClO}$: C, 35.49; H, 5.58. Found: C, 35.53; H, 5.59.

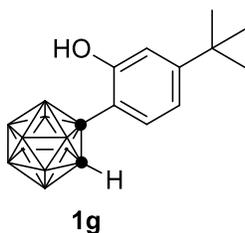


1e: Yield 48%. White solid. mp: 190-192 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.43 (d, $J = 8.0$ Hz, 1H), 6.75 (d, $J = 8.0$ Hz, 1H), 6.50 (s, 1H) (aromatic CH), 5.42 (s, 1H) (cage H), 5.28 (s, 1H) (OH), 2.27 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 151.5, 141.4, 132.3, 122.8, 117.7, 117.1 (aromatic C), 75.1, 59.9 (cage C), 20.9 (CH_3). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.6 (2B), -8.9 (2B), -9.4 (2B), -11.0 (2B), -13.2 (2B). IR (KBr): ν (cm^{-1}) 3547, 3105, 2921, 2567, 1619, 1420, 1305, 1190, 1116, 813, 724. Anal. Calcd for $\text{C}_9\text{H}_{18}\text{B}_{10}\text{O}$: C, 43.18; H, 7.25. Found: C, 43.21; H, 7.32.

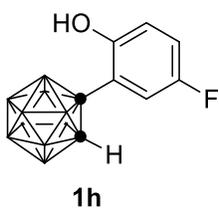


1f: Yield 57%. White solid. mp: 180-183 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.47 (d, $J = 8.8$ Hz, 1H), 6.49 (dd, $J = 9.2, 2.4$ Hz, 1H), 6.21 (d, $J = 2.4$ Hz, 1H) (aromatic CH), 5.51 (s, 1H) (cage H), 5.37 (s, 1H) (OH), 3.77 (s, 3H) (OCH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 161.1, 152.8, 133.5, 112.7, 107.2, 102.9 (aromatic C), 75.0, 59.7 (cage C), 55.6 (OCH_3). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.9 (2B), -9.1

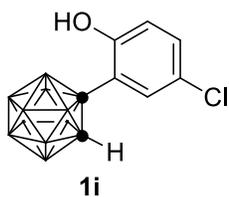
(2B), -9.6 (2B), -11.1 (2B), -13.3 (2B). IR (KBr): ν (cm⁻¹) 3415, 3113, 2562, 1619, 1520, 1422, 1316, 1213, 1113, 829, 728. Anal. Calcd for C₉H₁₈B₁₀O₂: C, 40.58; H, 6.81. Found: C, 40.69; H, 6.82.



1g: Yield 56%. White solid. mp: 136-138 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.47 (d, J = 8.8 Hz, 1H), 6.95 (d, J = 8.4 Hz, 1H), 6.65 (s, 1H) (aromatic CH), 5.41 (s, 1H) (cage H), 5.00 (s, 1H) (OH), 1.27 (s, 9H) ((CH₃)₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 154.6, 151.3, 132.2, 119.2, 117.0, 114.3 (aromatic C), 75.0, 59.9 (cage C), 34.6, 31.1 (C(CH₃)₃). ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -3.7 (2B), -9.0 (4B), -11.1 (2B), -13.2 (2B). IR (KBr): ν (cm⁻¹) 3570, 3118, 2966, 2575, 1615, 1409, 1309, 1191, 1023, 821, 723. Anal. Calcd for C₁₂H₂₄B₁₀O: C, 49.29; H, 8.27. Found: C, 49.35; H, 8.34.

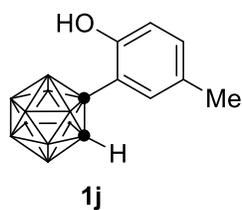


1h: Yield 47%. White solid. mp: 148-151 °C. ¹H NMR (300 MHz, CDCl₃): δ 7.32 (dd, J = 9.9, 2.7 Hz, 1H), 6.94 (td, J = 8.0, 3.0 Hz, 1H), 6.66 (dd, J = 8.7, 4.5 Hz, 1H) (aromatic CH), 5.41 (s, 1H) (cage H), 5.15 (s, 1H) (OH). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 156.9 (d, ¹ J_{C-F} = 239.3 Hz), 148.0 (d, ⁴ J_{C-F} = 1.7 Hz), 121.1 (d, ³ J_{C-F} = 7.7 Hz), 119.2 (d, ² J_{C-F} = 26.4 Hz), 118.3 (d, ³ J_{C-F} = 8.0 Hz), 117.4 (d, ² J_{C-F} = 23.1 Hz) (aromatic C), 73.9, 59.6 (cage C). ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -3.4 (2B), -8.9 (2B), -9.6 (2B), -11.2 (2B), -13.2 (2B). ¹⁹F NMR (376 MHz, CDCl₃): δ -121.3 (s, 1F). IR (KBr): ν (cm⁻¹) 3570, 3108, 2563, 1508, 1422, 1334, 1173, 812, 762. Anal. Calcd for C₈H₁₅B₁₀FO: C, 37.78; H, 5.95. Found: C, 37.65; H, 5.94.

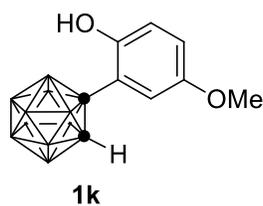


1i: Yield 57%. White solid. mp: 132-134 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.56 (s, 1H), 7.18 (d, J = 8.4 Hz, 1H), 6.65 (d, J = 8.4 Hz, 1H) (aromatic CH), 5.37 (s, 1H) (cage H), 5.24 (s, 1H) (OH). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 150.4, 132.3, 130.5, 126.9, 121.4, 118.5 (aromatic C), 73.7, 59.6 (cage C). ¹¹B{¹H} NMR (128 MHz, CDCl₃): δ -3.5 (2B), -8.9 (2B), -9.6 (2B), -11.4 (2B), -13.3 (2B). IR (KBr): ν (cm⁻¹) 3549, 3106, 2594, 1491, 1402, 1324, 1188, 1118, 808, 728. Anal. Calcd for C₈H₁₅B₁₀ClO: C, 35.49; H, 5.58. Found:

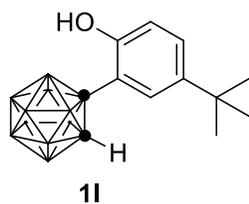
C, 35.35; H, 5.64.



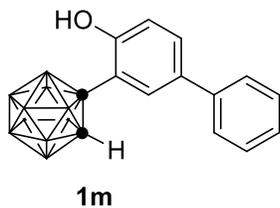
1j: Yield 43%. White solid. mp: 77-78 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.35 (s, 1H), 7.00 (d, $J = 7.6$ Hz, 1H), 6.57 (d, $J = 8.0$ Hz, 1H) (aromatic CH), 5.45 (s, 1H) (cage H), 4.92 (s, 1H) (OH), 2.27 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 149.5, 132.9, 131.4, 131.2, 119.6, 117.2 (aromatic C), 75.0, 59.9 (cage C), 20.6 (CH_3). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.6 (2B), -9.0 (2B), -9.5 (2B), -11.1 (2B), -13.3 (2B). IR (KBr): ν (cm^{-1}) 3631, 3102, 2922, 2589, 1607, 1513, 1409, 1349, 1198, 1079, 813, 727. Anal. Calcd for $\text{C}_9\text{H}_{18}\text{B}_{10}\text{O}$: C, 43.18; H, 7.25. Found: C, 43.08; H, 7.19.



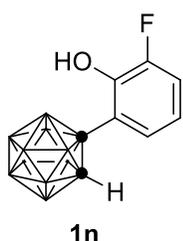
1k: Yield 50%. White solid. mp: 181-183 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.12 (s, 1H), 6.77 (d, $J = 8.8$ Hz, 1H), 6.62 (d, $J = 8.8$ Hz, 1H) (aromatic CH), 5.48 (s, 1H) (cage H), 5.20 (s, 1H) (OH), 3.77 (s, 3H) (OCH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 153.8, 145.8, 120.5, 118.1, 117.7, 116.3 (aromatic C), 74.8, 59.7 (cage C), 56.0 (OCH_3). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.6 (2B), -9.0 (2B), -9.6 (2B), -11.2 (2B), -13.3 (2B). IR (KBr): ν (cm^{-1}) 3362, 3115, 2589, 1512, 1427, 1352, 1279, 1219, 1040, 812, 739. Anal. Calcd for $\text{C}_9\text{H}_{18}\text{B}_{10}\text{O}_2$: C, 40.58; H, 6.81. Found: C, 40.83; H, 6.79.



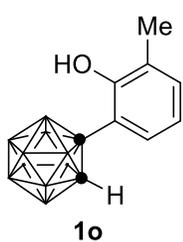
1l: Yield 64%. White solid. mp: 131-132 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.57 (s, 1H), 7.21 (d, $J = 8.4$ Hz, 1H), 6.60 (d, $J = 8.4$ Hz, 1H) (aromatic CH), 5.46 (s, 1H) (cage H), 4.95 (s, 1H) (OH), 1.28 (s, 9H) ($(\text{CH}_3)_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 149.3, 144.8, 129.7, 127.6, 119.1, 116.8 (aromatic C), 75.5, 59.9 (cage C), 34.4, 31.4 ($\text{C}(\text{CH}_3)_3$). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.6 (2B), -8.9 (4B), -11.1 (2B), -13.2 (2B). IR (KBr): ν (cm^{-1}) 3578, 3107, 2965, 2575, 1516, 1404, 1332, 1128, 818, 723. Anal. Calcd for $\text{C}_{12}\text{H}_{24}\text{B}_{10}\text{O}$: C, 49.29; H, 8.27. Found: C, 49.59; H, 8.24.



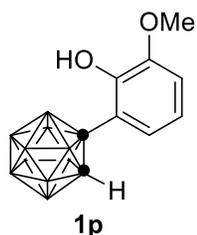
1m: Yield 57%. White solid. mp: 150-152 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.79 (s, 1H), 7.50 (d, $J = 7.2$ Hz, 2H), 7.44 (m, 3H), 7.36 (t, $J = 7.6$ Hz, 1H), 6.76 (d, $J = 8.4$ Hz, 1H) (aromatic CH), 5.47 (s, 1H) (cage H), 5.19 (s, 1H) (OH). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 151.0, 139.5, 135.2, 131.4, 129.2, 129.1, 127.6, 126.9, 120.2, 117.7 (aromatic C), 74.9, 59.8 (cage C). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.3 (2B), -8.7 (4B), -11.0 (2B), -13.1 (2B). IR (KBr): ν (cm^{-1}) 3416, 3101, 2587, 1597, 1523, 1488, 1260, 833, 758, 688. Anal. Calcd for $\text{C}_{14}\text{H}_{20}\text{B}_{10}\text{O}$: C, 53.82; H, 6.45. Found: C, 53.82; H, 6.57.



1n: Yield 40%. White solid. mp: 171-173 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.35 (d, $J = 8.4$ Hz, 1H), 7.12 (t, $J = 8.4$ Hz, 1H), 6.86 (dd, $J = 14.4, 8.0$ Hz, 1H) (aromatic CH), 5.82 (s, 1H) (cage H), 5.40 (s, 1H) (OH). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 151.1 (d, $^1J_{\text{C-F}} = 235.4$ Hz), 141.1 (d, $^2J_{\text{C-F}} = 17.3$ Hz), 127.5 (d, $^3J_{\text{C-F}} = 3.4$ Hz), 121.4, 120.6 (d, $^3J_{\text{C-F}} = 7.8$ Hz), 116.2 (d, $^2J_{\text{C-F}} = 18.6$ Hz) (aromatic C), 73.8, 59.5 (cage C). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.2 (2B), -8.7 (2B), -9.4 (2B), -11.1 (2B), -13.0 (2B). ^{19}F NMR (376 MHz, CDCl_3): δ -139.7 (m, 1F). IR (KBr): ν (cm^{-1}) 3530, 3104, 2579, 1470, 1554, 1268, 1178, 717. Anal. Calcd for $\text{C}_8\text{H}_{15}\text{B}_{10}\text{FO}$: C, 37.78; H, 5.95. Found: C, 37.95; H, 6.03.

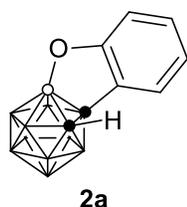


1o: Yield 31%. White solid. mp: 184-185 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.45 (d, $J = 8.0$ Hz, 1H), 7.13 (d, $J = 7.2$ Hz, 1H), 6.85 (t, $J = 8.0$ Hz, 1H) (aromatic CH), 5.49 (s, 1H) (cage H), 5.02 (s, 1H) (OH), 2.25 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 150.4, 131.9, 130.7, 123.7, 121.2, 119.7 (aromatic C), 75.3, 60.1 (cage C), 15.8 (CH_3). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.5 (2B), -8.9 (4B), -11.1 (2B), -13.2 (2B). IR (KBr): ν (cm^{-1}) 3577, 3109, 2983, 2576, 1460, 1332, 1208, 724. Anal. Calcd for $\text{C}_9\text{H}_{18}\text{B}_{10}\text{O}$: C, 43.18; H, 7.25. Found: C, 43.31; H, 7.25.

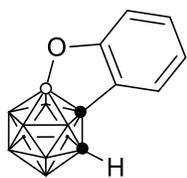


1p: Yield 55%. White solid. mp: 167-169 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.14 (d, J = 7.2 Hz, 1H), 6.84 (m, 2H) (aromatic CH), 6.31 (s, 1H) (OH), 5.50 (s, 1H) (cage H), 3.91 (s, 3H) (OCH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 146.6, 142.7, 123.6, 120.0, 118.8, 111.1 (aromatic C), 74.7, 59.6 (cage C), 56.6 (OCH_3). $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ -3.9 (2B), -9.4 (2B), -10.0 (2B), -11.5 (2B), -13.6 (2B). IR (KBr): ν (cm^{-1}) 3496, 3106, 2940, 2599, 1472, 1441, 1370, 1294, 1245, 1092, 725. Anal. Calcd for $\text{C}_9\text{H}_{18}\text{B}_{10}\text{O}_2$: C, 40.58; H, 6.81. Found: C, 40.51; H, 6.91.

Preparation of 1,3- or 1,4-*o*-carboranobenzofurans. A Representative Procedure. An oven-dried Schlenk flask equipped with a stir bar was charged with 1-(*o*'-HOC₆H₄)-*o*-C₂B₁₀H₁₁ (**1a**, 118 mg, 0.50 mmol), Pd(OAc)₂ (5.6 mg, 0.025 mmol), AgOAc (250 mg, 1.50 mmol) and dry toluene (3 mL) under an atmosphere of dry nitrogen. The flask was closed, and then stirred at 80 °C for 12 h. After hydrolysis with water (3 mL) and extraction with diethyl ether (5 mL x 3), the ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (200-300 mesh) using *n*-hexane as eluent to give the products **2a/3a**.

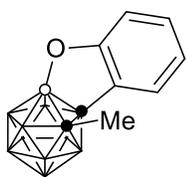


2a: Yield 85%. White solid. mp: 101-102 °C. ^1H NMR (300 MHz, CDCl_3): δ 7.41 (m, 2H), 7.15 (d, J = 8.4 Hz, 1H), 7.06 (t, J = 7.5 Hz, 1H) (aromatic CH), 2.90 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 167.7, 131.8, 126.2, 123.4, 122.1, 115.9 (aromatic C), 78.9, 61.8 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 0.5 (s, 1B) ($B_{\text{cage-O}}$), -3.3 (d, J_{BH} = 149 Hz, 1B), -9.2 (d, J_{BH} = 136 Hz, 1B), -10.2 (d, J_{BH} = 143 Hz, 1B), -12.4 (d, J_{BH} = 147 Hz, 1B), -13.3 (m, 1B), -14.1 (m, 1B), -14.9 (m, 1B), -15.7 (m, 1B), -18.1 (d, J_{BH} = 152 Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3057, 2589, 1608, 1459, 1192, 1156, 1094, 756. Anal. Calcd for $\text{C}_8\text{H}_{14}\text{B}_{10}\text{O}$: C, 41.01; H, 6.02. Found: C, 41.34; H, 5.98.



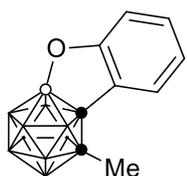
3a

3a: Yield 9%. White solid. mp: 117-118 °C. ^1H NMR (300 MHz, CDCl_3): δ 7.40 (t, $J = 8.1$ Hz, 1H), 7.25 (d, $J = 8.1$ Hz, 1H), 7.18 (d, $J = 8.4$ Hz, 1H), 7.02 (t, $J = 7.8$ Hz, 1H) (aromatic CH), 4.23 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 167.3, 131.2, 125.3, 121.1, 119.9, 115.8 (aromatic C), 78.0, 56.4 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 3.3 (s, 1B) ($B_{\text{cage-O}}$), -4.1 (d, $J_{\text{BH}} = 151$ Hz, 1B), -10.2 (d, $J_{\text{BH}} = 167$ Hz, 3B), -11.5 (d, $J_{\text{BH}} = 159$ Hz, 2B), -15.0 (d, $J_{\text{BH}} = 164$ Hz, 1B), -15.8 (d, $J_{\text{BH}} = 179$ Hz, 1B), -21.5 (d, $J_{\text{BH}} = 166$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3062, 2591, 1605, 1456, 1145, 1104, 751. Anal. Calcd for $\text{C}_8\text{H}_{14}\text{B}_{10}\text{O}$: C, 41.01; H, 6.02. Found: C, 41.29; H, 6.12.



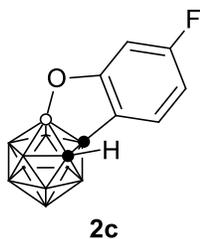
2b

2b: Yield 54%. White solid. mp: 83-85 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.45 (t, $J = 10.8$ Hz, 1H), 7.37 (d, $J = 10.0$ Hz, 1H), 7.17 (d, $J = 11.2$ Hz, 1H), 7.10 (t, $J = 10.0$ Hz, 1H) (aromatic CH), 1.21 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 167.3, 132.1, 124.7, 124.3, 122.4, 115.7 (aromatic C), 82.4, 71.0 (cage C), 19.4 (CH_3). ^{11}B NMR (128 MHz, CDCl_3): δ 0.3 (s, 1B) ($B_{\text{cage-O}}$), -5.8 (d, $J_{\text{BH}} = 149$ Hz, 1B), -8.9 (d, $J_{\text{BH}} = 144$ Hz, 1B), -10.0 (d, $J_{\text{BH}} = 143$ Hz, 1B), -10.8 (d, $J_{\text{BH}} = 185$ Hz, 1B), -12.3 (d, $J_{\text{BH}} = 168$ Hz, 1B), -13.0 (m, 2B), -14.5 (d, $J_{\text{BH}} = 169$ Hz, 1B), -18.1 (d, $J_{\text{BH}} = 151$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 2941, 2569, 1606, 1456, 1144, 1096, 756. Anal. Calcd for $\text{C}_9\text{H}_{16}\text{B}_{10}\text{O}$: C, 43.53; H, 6.49. Found: C, 43.56; H, 6.44.

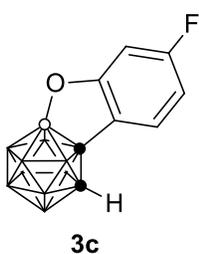


3b

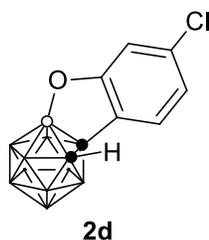
3b: Yield 39%. White solid. mp: 99-100 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.43 (t, $J = 10.8$ Hz, 1H), 7.31 (d, $J = 10.0$ Hz, 1H), 7.22 (d, $J = 10.8$ Hz, 1H), 7.05 (d, $J = 10.0$ Hz, 1H) (aromatic CH), 2.28 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 167.8, 131.1, 125.2, 121.0, 120.6, 116.0 (aromatic C), 80.8, 72.8 (cage C), 22.7 (CH_3). ^{11}B NMR (128 MHz, CDCl_3): δ 4.2 (s, 1B) ($B_{\text{cage-O}}$), -8.0 (d, $J_{\text{BH}} = 139$ Hz, 2B), -9.1 (d, $J_{\text{BH}} = 149$ Hz, 2B), -11.9 (d, $J_{\text{BH}} = 142$ Hz, 3B), -12.7 (d, $J_{\text{BH}} = 131$ Hz, 1B), -18.3 (d, $J_{\text{BH}} = 161$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3057, 2575, 1613, 1459, 1180, 752. Anal. Calcd for $\text{C}_9\text{H}_{16}\text{B}_{10}\text{O}$: C, 43.53; H, 6.49. Found: C, 43.40; H, 6.45.



2c: Yield 80%. White solid. mp: 91-93 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.35 (dd, $J = 8.4, 5.6$ Hz, 1H), 6.87 (dd, $J = 8.8, 2.0$ Hz, 1H), 6.78 (td, $J = 8.8, 2.0$ Hz, 1H) (aromatic CH), 2.92 (s, 1H) (Cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 168.8, (d, $^3J_{\text{C-F}} = 13.4$ Hz), 165.0 (d, $^1J_{\text{C-F}} = 249.9$ Hz), 124.1 (d, $^3J_{\text{C-F}} = 10.8$ Hz), 122.3 (d, $^4J_{\text{C-F}} = 2.9$ Hz), 109.5 (d, $^2J_{\text{C-F}} = 23.5$ Hz), 104.3 (d, $^2J_{\text{C-F}} = 26.3$ Hz) (aromatic C), 78.1, 62.1 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 0.6 (s, 1B) ($B_{\text{cage-O}}$), -3.2 (d, $J_{\text{BH}} = 151$ Hz, 1B), -9.1 (d, $J_{\text{BH}} = 135$ Hz, 1B), -10.1 (d, $J_{\text{BH}} = 146$ Hz, 1B), -12.3 (d, $J_{\text{BH}} = 141$ Hz, 1B), -13.3 (m, 1B), -14.1 (m, 1B), -14.8 (m, 1B), -15.6 (m, 1B), -17.9 (d, $J_{\text{BH}} = 149$ Hz, 1B) (B_{cageH}). ^{19}F NMR (376 MHz, CDCl_3): δ -106.6 (m, 1F). IR (KBr): ν (cm^{-1}) 3068, 2602, 1620, 1487, 1430, 1195, 1136, 1099, 962, 848. Anal. Calcd for $\text{C}_8\text{H}_{13}\text{B}_{10}\text{FO}$: C, 38.08; H, 5.19. Found: C, 38.35; H, 5.25.

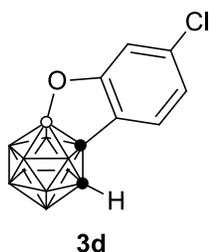


3c: Yield 11%. White solid. mp: 144-145 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.18 (dd, $J = 8.4, 5.6$ Hz, 1H), 6.90 (dd, $J = 9.2, 2.4$ Hz, 1H), 6.74 (td, $J = 8.8, 2.4$ Hz, 1H) (aromatic CH), 4.21 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 168.4 (d, $^3J_{\text{C-F}} = 13.5$ Hz), 164.9 (d, $^1J_{\text{C-F}} = 248.1$ Hz), 121.3 (d, $^4J_{\text{C-F}} = 2.7$ Hz), 120.4 (d, $^3J_{\text{C-F}} = 10.9$ Hz), 108.4 (d, $^2J_{\text{C-F}} = 23.7$ Hz), 104.2 (d, $^2J_{\text{C-F}} = 26.0$ Hz) (aromatic C), 77.4, 56.4 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 3.6 (s, 1B) ($B_{\text{cage-O}}$), -3.9 (d, $J_{\text{BH}} = 144$ Hz, 1B), -9.9 (d, $J_{\text{BH}} = 182$ Hz, 3B), -11.4 (d, $J_{\text{BH}} = 165$ Hz, 2B), -14.8 (d, $J_{\text{BH}} = 154$ Hz, 1B), -15.7 (d, $J_{\text{BH}} = 169$ Hz, 1B), -21.1 (d, $J_{\text{BH}} = 166$ Hz, 1B) (B_{cageH}). ^{19}F NMR (376 MHz, CDCl_3): δ -108.2 (m, 1F). IR (KBr): ν (cm^{-1}) 3061, 2878, 1621, 1482, 1139, 1096, 984, 847. HRMS (EI): m/z Calcd for $\text{C}_8\text{H}_{13}\text{B}_{10}\text{FO}^-$: 252.1963. Found: 252.1966.



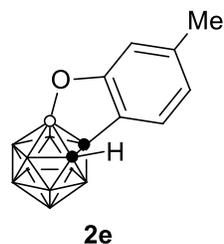
2d: Yield 22%. White solid. mp: 116-118 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.32 (d, $J = 8.4$ Hz, 1H), 7.16 (d, $J = 1.6$ Hz, 1H), 7.05 (dd, $J = 8.4, 1.6$ Hz, 1H) (aromatic CH), 2.91 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 168.1, 138.0, 124.8, 123.8, 122.6, 116.6 (aromatic C), 78.0, 61.8 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ

0.3 (s, 1B) ($B_{\text{cage-O}}$), -3.3 (d, $J_{\text{BH}} = 151$ Hz, 1B), -9.1 (d, $J_{\text{BH}} = 151$ Hz, 1B), -10.4 (d, $J_{\text{BH}} = 167$ Hz, 1B), -12.4 (d, $J_{\text{BH}} = 149$ Hz, 1B), -13.5 (m, 1B), -14.2 (m, 1B), -15.0 (m, 1B), -15.7 (m, 1B), -18.1 (d, $J_{\text{BH}} = 153$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3046, 2571, 1605, 1474, 1415, 1193, 1063, 853, 823. Anal. Calcd for $\text{C}_8\text{H}_{13}\text{B}_{10}\text{ClO}$: C, 35.75; H, 4.88. Found: C, 35.37; H, 4.97.



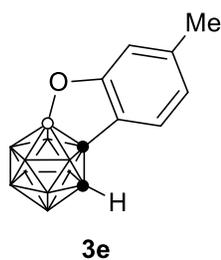
3d: Yield 6%. White solid. mp: 135-138 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.19 (s, 1H), 7.15 (d, $J = 8.0$ Hz, 1H), 7.01 (d, $J = 8.0$ Hz, 1H) (aromatic CH), 4.20 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 167.7, 137.4, 123.9, 121.5, 120.3, 116.6 (aromatic C), 56.4 (cage C), another cage C was not observed. ^{11}B NMR (128 MHz, CDCl_3): δ 3.6 (s, 1B) ($B_{\text{cage-O}}$), -3.7 (d, $J_{\text{BH}} = 149$ Hz, 1B), -9.7 (d, $J_{\text{BH}} = 182$

Hz, 3B), -11.2 (d, $J_{\text{BH}} = 157$ Hz, 2B), -14.7 (d, $J_{\text{BH}} = 162$ Hz, 1B), -15.5 (d, $J_{\text{BH}} = 164$ Hz, 1B), -21.1 (d, $J_{\text{BH}} = 160$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3046, 2571, 1605, 1473, 1415, 1193, 1062, 823. HRMS (EI): m/z Calcd for $\text{C}_8\text{H}_{14}\text{B}_{10}\text{ClO}^+$: 270.1708. Found: 270.1701.



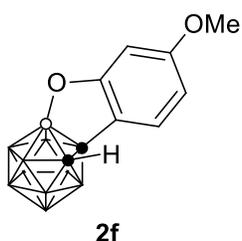
2e: Yield 79%. White solid. mp: 119-122 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.26 (d, $J = 8.0$ Hz, 1H), 6.96 (s, 1H), 6.85 (d, $J = 8.0$ Hz, 1H) (aromatic CH), 2.87 (s, 1H) (cage H), 2.37 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 167.9, 142.8, 123.4, 122.9, 122.8, 116.3 (aromatic C), 79.0, 62.2 (cage C), 21.8 (CH_3). ^{11}B NMR (128 MHz, CDCl_3): δ 0.4 (s, 1B) ($B_{\text{cage-O}}$), -3.6 (d, $J_{\text{BH}} = 150$ Hz, 1B), -9.7 (m, 2B),

-12.7 (d, $J_{\text{BH}} = 153$ Hz, 1B), -13.5 (m, 1B), -14.3 (m, 1B), -15.1 (m, 1B), -15.9 (m, 1B), -18.4 (d, $J_{\text{BH}} = 153$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3046, 2922, 2571, 1619, 1424, 1197, 1117, 1063, 823, 725. Anal. Calcd for $\text{C}_9\text{H}_{16}\text{B}_{10}\text{O}$: C, 43.53; H, 6.49. Found: C, 43.92; H, 6.57.



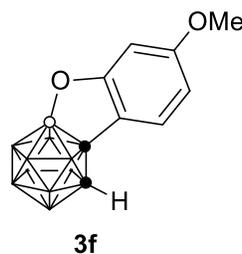
3e: Yield 13%. White solid. mp: 151-154 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.10 (d, $J = 8.0$ Hz, 1H), 6.99 (s, 1H), 6.82 (d, $J = 7.6$ Hz, 1H) (aromatic CH), 4.19 (s, 1H) (cage H), 2.38 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 167.5, 142.0,

122.4, 121.9, 119.3, 116.4 (aromatic C), 78.1, 56.2 (cage C), 21.9 (CH₃). ¹¹B NMR (128 MHz, CDCl₃): δ 3.3 (s, 1B) (*B*_{cage-O}), -4.2 (d, *J*_{BH} = 159 Hz, 1B), -10.3 (d, *J*_{BH} = 161 Hz, 3B), -11.7 (d, *J*_{BH} = 157 Hz, 2B), -15.1 (d, *J*_{BH} = 158 Hz, 1B), -15.9 (d, *J*_{BH} = 164 Hz, 1B), -21.6 (d, *J*_{BH} = 169 Hz, 1B) (*B*_{cage-H}). IR (KBr): ν (cm⁻¹) 3074, 2919, 2571, 1618, 1440, 1258, 1159, 1108, 985, 812. Anal. Calcd for C₉H₁₆B₁₀O: C, 43.53; H, 6.49. Found: C, 43.80; H, 6.54.



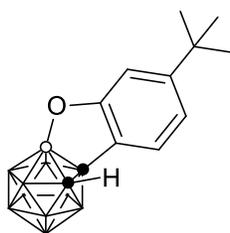
2f: Yield 80%. White solid. mp: 106-107 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.26 (d, *J* = 8.4 Hz, 1H), 6.68 (d, *J* = 2.0 Hz, 1H), 6.57 (dd, *J* = 8.4, 2.0 Hz, 1H) (aromatic CH), 3.80 (s, 3H) (OCH₃), 2.90 (s, 1H) (cage H). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 169.3, 163.0, 123.5, 118.5, 108.5, 101.6 (aromatic C), 79.2, 62.8 (cage C), 55.9 (OCH₃). ¹¹B NMR (128 MHz, CDCl₃): δ 0.4 (s, 1B) (*B*_{cage-O}), -3.6

(d, *J*_{BH} = 150 Hz, 1B), -9.8 (d, *J*_{BH} = 156 Hz, 2B), -12.7 (d, *J*_{BH} = 149 Hz, 1B), -13.5 (m, 1B), -14.4 (m, 1B), -15.2 (m, 1B), -15.9 (m, 1B), -18.3 (d, *J*_{BH} = 153 Hz, 1B) (*B*_{cage-H}). IR (KBr): ν (cm⁻¹) 3051, 2930, 2586, 1613, 1440, 1297, 1190, 1150, 1102, 848, 825. Anal. Calcd for C₉H₁₆B₁₀O₂: C, 40.89; H, 6.10. Found: C, 40.64; H, 6.06.



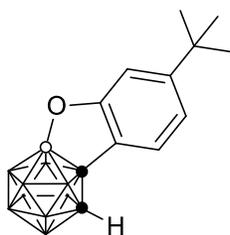
3f: Yield 6%. White solid. mp: 128-129 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.10 (d, *J* = 8.4 Hz, 1H), 6.72 (s, 1H), 6.55 (d, *J* = 8.4 Hz, 1H) (aromatic CH), 4.18 (s, 1H) (cage H), 3.80 (s, 3H) (OCH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 168.9, 162.7, 120.0, 117.5, 107.9, 101.4 (aromatic C), 78.3, 56.2 (cage C), 55.8 (OCH₃). ¹¹B

NMR (128 MHz, CDCl₃): δ 3.6 (s, 1B) (*B*_{cage-O}), -4.1 (d, *J*_{BH} = 150 Hz, 1B), -9.5 (d, *J*_{BH} = 129 Hz, 2B), -10.3 (d, *J*_{BH} = 135 Hz, 1B), -11.6 (d, *J*_{BH} = 155 Hz, 2B), -14.9 (d, *J*_{BH} = 155 Hz, 1B), -16.0 (d, *J*_{BH} = 143 Hz, 1B), -21.3 (d, *J*_{BH} = 166 Hz, 1B) (*B*_{cage-H}). IR (KBr): ν (cm⁻¹) 3051, 2929, 2578, 1613, 1495, 1440, 1296, 1190, 1151, 1102, 1029, 848, 825. HRMS (EI): *m/z* Calcd for C₉H₁₇B₁₀O₂⁺: 265.2231. Found: 265.2236.



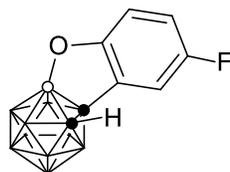
2g

2g: Yield 75%. White solid. mp: 177-179 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.30 (d, $J = 8.4$ Hz, 1H), 7.16 (d, $J = 1.6$ Hz, 1H), 7.07 (dd, $J = 8.4, 1.6$ Hz, 1H) (aromatic CH), 2.89 (s, 1H) (cage H), 1.30 (s, 9H) ($(\text{CH}_3)_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 168.0, 156.2, 123.2, 122.5, 119.3, 113.0 (aromatic C), 79.0, 62.2 (cage C). 35.4, 31.4 ($\text{C}(\text{CH}_3)_3$). ^{11}B NMR (128 MHz, CDCl_3): δ 0.6 (s, 1B) ($B_{\text{cage-O}}$), -3.4 (d, $J_{\text{BH}} = 154$ Hz, 1B), -9.4 (d, $J_{\text{BH}} = 136$ Hz, 1B), -10.0 (d, $J_{\text{BH}} = 157$ Hz, 1B), -12.5 (d, $J_{\text{BH}} = 150$ Hz, 1B), -13.3 (m, 1B), -14.1 (m, 1B), -14.9 (m, 1B), -15.7 (m, 1B), -18.2 (d, $J_{\text{BH}} = 156$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3047, 2963, 2585, 1617, 1487, 1423, 1204, 864, 829, 652. Anal. Calcd for $\text{C}_{12}\text{H}_{22}\text{B}_{10}\text{O}$: C, 49.63; H, 7.64. Found: C, 50.08; H, 7.64.



3g

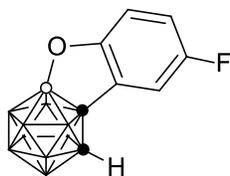
3g: Yield 10%. White solid. mp: 197-200 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.20 (s, 1H), 7.15 (d, $J = 8.0$ Hz, 1H), 7.04 (d, $J = 8.0$ Hz, 1H) (aromatic CH), 4.20 (s, 1H) (cage H), 1.31 (s, 9H) ($(\text{CH}_3)_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 167.5, 155.4, 122.2, 119.0, 118.3, 113.1 (aromatic C), 78.2, 56.2 (cage C). 35.3, 31.4 ($\text{C}(\text{CH}_3)_3$). ^{11}B NMR (128 MHz, CDCl_3): δ 3.7 (s, 1B) ($B_{\text{cage-O}}$), -3.9 (d, $J_{\text{BH}} = 142$ Hz, 1B), -9.9 (d, $J_{\text{BH}} = 169$ Hz, 3B), -11.3 (d, $J_{\text{BH}} = 162$ Hz, 2B), -14.8 (d, $J_{\text{BH}} = 135$ Hz, 1B), -15.6 (d, $J_{\text{BH}} = 145$ Hz, 1B), -21.2 (d, $J_{\text{BH}} = 162$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3063, 2963, 2596, 1615, 1485, 1420, 1165, 862, 830, 703, 651. Anal. Calcd for $\text{C}_{12}\text{H}_{22}\text{B}_{10}\text{O}$: C, 49.63; H, 7.64. Found: C, 49.60; H, 7.75.



2h

2h: Yield 51%. White solid. mp: 120-123 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.11 (m, 3H) (aromatic CH), 2.91 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 163.7, 157.6 (d, $^1J_{\text{C-F}} = 242.7$ Hz), 126.8 (d, $^3J_{\text{C-F}} = 9.4$ Hz), 118.8 (d, $^2J_{\text{C-F}} = 24.1$ Hz), 116.6 (d, $^3J_{\text{C-F}} = 8.4$ Hz), 110.8 (d, $^2J_{\text{C-F}} = 25.8$ Hz) (aromatic C), 78.0, 61.5 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 0.6 (s, 1B) ($B_{\text{cage-O}}$), -3.3 (d, $J_{\text{BH}} = 148$ Hz, 1B), -9.1 (d, $J_{\text{BH}} = 156$ Hz, 1B), -10.4 (d, $J_{\text{BH}} = 181$ Hz, 1B), -12.3 (d, $J_{\text{BH}} = 145$ Hz, 1B), -13.4 (m, 1B), -14.2 (m, 1B),

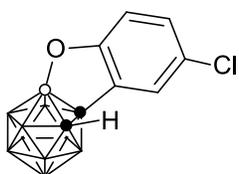
-14.8 (m, 1B), -15.7 (m, 1B), -18.1 (d, $J_{\text{BH}} = 153$ Hz, 1B) (B_{cageH}). ^{19}F NMR (282 MHz, CDCl_3): δ -120.4 (m, 1F). IR (KBr): ν (cm^{-1}) 3064, 2963, 2579, 1592, 1476, 1260, 1172, 1098, 877, 823. Anal. Calcd for $\text{C}_8\text{H}_{13}\text{B}_{10}\text{FO}$: C, 38.08; H, 5.19. Found: C, 38.25; H, 5.56.



3h

3h: Yield 5%. White solid. mp: 138-140 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.13 (m, 2H), 6.97, (m, 1H) (aromatic CH), 4.21 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 163.3 (d, $^4J_{\text{C-F}} = 1.8$ Hz), 157.0 (d, $^1J_{\text{C-F}} = 241.1$ Hz), 125.6 (d, $^3J_{\text{C-F}} = 9.2$ Hz), 118.1 (d, $^2J_{\text{C-F}} = 23.9$ Hz), 116.3 (d, $^3J_{\text{C-F}} = 8.3$ Hz), 107.4 (d, $^2J_{\text{C-F}} = 25.9$ Hz)

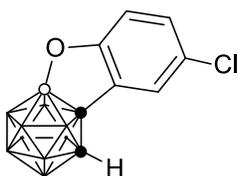
(aromatic C), 77.4, 56.3 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 3.4 (s, 1B) ($B_{\text{cage-O}}$), -4.0 (d, $J_{\text{BH}} = 156$ Hz, 1B), -10.1 (d, $J_{\text{BH}} = 166$ Hz, 3B), -11.5 (d, $J_{\text{BH}} = 158$ Hz, 2B), -15.0 (d, $J_{\text{BH}} = 151$ Hz, 1B), -15.8 (d, $J_{\text{BH}} = 167$ Hz, 1B), -21.4 (d, $J_{\text{BH}} = 174$ Hz, 1B) (B_{cageH}). ^{19}F NMR (282 MHz, CDCl_3): δ -121.8 (m, 1F). IR (KBr): ν (cm^{-1}) 3065, 2589, 1590, 1475, 1257, 1155, 984, 873, 772. Anal. Calcd for $\text{C}_8\text{H}_{13}\text{B}_{10}\text{FO}$: C, 38.08; H, 5.19. Found: C, 38.50; H, 5.39.



2i

2i: Yield 25%. White solid. mp: 118-121 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.37 (m, 2H), 7.08 (d, $J = 8.4$ Hz, 1H) (aromatic CH), 2.90 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 166.1, 131.9, 127.6, 127.3, 123.6, 116.9 (aromatic C), 77.7, 61.5 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 0.4 (s, 1B) ($B_{\text{cage-O}}$), -3.3 (d,

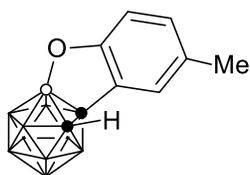
$J_{\text{BH}} = 149$ Hz, 1B), -9.0 (d, $J_{\text{BH}} = 160$ Hz, 1B), -10.5 (d, $J_{\text{BH}} = 191$ Hz, 1B), -12.4 (d, $J_{\text{BH}} = 151$ Hz, 1B), -13.4 (m, 1B), -14.2 (m, 1B), -15.0 (m, 1B), -15.7 (m, 1B), -18.1 (d, $J_{\text{BH}} = 153$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3046, 2578, 1453, 1264, 1194, 1076, 821, 694, 651. Anal. Calcd for $\text{C}_8\text{H}_{13}\text{B}_{10}\text{ClO}$: C, 35.75; H, 4.88. Found: C, 35.84; H, 4.99.



3i

3i: Yield 9%. White solid. mp: 131-133 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.36 (d, $J = 8.8$ Hz, 1H), 7.24 (s, 1H), 7.10 (d, $J = 8.8$ Hz, 1H) (aromatic CH), 4.21 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 165.8, 131.3, 126.5, 126.4, 120.3,

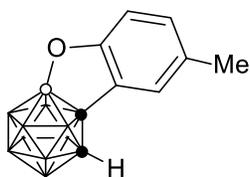
116.7 (aromatic C), 77.4, 56.4 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 3.5 (s, 1B) ($B_{\text{cage-O}}$), -3.7 (d, $J_{\text{BH}} = 144$ Hz, 1B), -9.8 (d, $J_{\text{BH}} = 176$ Hz, 3B), -11.2 (d, $J_{\text{BH}} = 155$ Hz, 2B), -14.8 (d, $J_{\text{BH}} = 148$ Hz, 1B), -15.5 (d, $J_{\text{BH}} = 165$ Hz, 1B), -21.2 (d, $J_{\text{BH}} = 167$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3046, 2578, 1453, 1264, 1194, 1076, 821, 694, 651. HRMS (EI): m/z Calcd for $\text{C}_8\text{H}_{14}\text{B}_{10}\text{ClO}^+$: 270.1708. Found: 270.1709.



2j

2j: Yield 28%. White solid. mp: 68-70 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.19 (m, 2H), 7.02 (d, $J = 8.8$ Hz, 1H) (aromatic CH), 2.88 (s, 1H) (cage H), 2.34 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 165.6, 132.4, 131.9, 125.9, 123.6, 115.4 (aromatic C), 78.9, 61.9 (cage C), 20.8 (CH_3). ^{11}B NMR (128 MHz, CDCl_3):

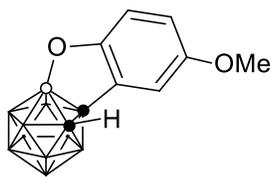
δ 0.6 (s, 1B) ($B_{\text{cage-O}}$), -3.4 (d, $J_{\text{BH}} = 147$ Hz, 1B), -9.4 (d, $J_{\text{BH}} = 132$ Hz, 1B), -10.1 (d, $J_{\text{BH}} = 112$ Hz, 1B), -12.5 (d, $J_{\text{BH}} = 148$ Hz, 1B), -13.4 (m, 1B), -14.2 (m, 1B), -14.9 (m, 1B), -15.7 (m, 1B), -18.2 (d, $J_{\text{BH}} = 152$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3053, 2922, 2591, 1478, 1267, 1202, 1063, 816. Anal. Calcd for $\text{C}_9\text{H}_{16}\text{B}_{10}\text{O}$: C, 43.53; H, 6.49. Found: C, 43.76; H, 6.48.



3j

3j: Yield 6%. White solid. mp: 84-87 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.19 (d, $J = 8.4$ Hz, 1H), 7.05 (d, $J = 8.8$ Hz, 2H) (aromatic CH), 4.19 (s, 1H) (Cage H), 2.34 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 165.3, 131.8, 130.8, 125.0, 120.2, 115.3 (aromatic C), 78.0, 56.2 (cage C), 20.9 (CH_3). ^{11}B NMR (128 MHz, CDCl_3): δ 3.5 (s, 1B) ($B_{\text{cage-O}}$), -4.0 (d, $J_{\text{BH}} = 146$ Hz, 1B), -10.2 (d, $J_{\text{BH}} = 165$ Hz,

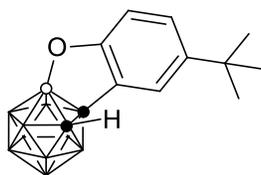
3B), -11.5 (d, $J_{\text{BH}} = 162$ Hz, 2B), -14.9 (d, $J_{\text{BH}} = 152$ Hz, 1B), -15.8 (d, $J_{\text{BH}} = 144$ Hz, 1B), -21.4 (d, $J_{\text{BH}} = 163$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3064, 2923, 2584, 1475, 1259, 1209, 1143, 810. Anal. Calcd for $\text{C}_9\text{H}_{16}\text{B}_{10}\text{O}$: C, 43.53; H, 6.49. Found: C, 43.83; H, 6.60.



2k

2k: Yield 12%. White solid. mp: 69-70 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.04 (d, $J = 9.2$ Hz, 1H), 6.94 (dd, $J = 9.2, 2.8$ Hz, 1H), 6.90 (d, $J = 2.8$ Hz, 1H) (aromatic CH), 3.79 (s, 3H) (OCH_3), 2.89 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100

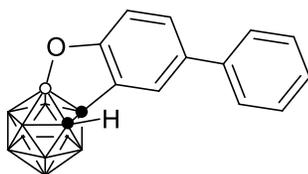
MHz, CDCl₃): δ 161.5, 154.9, 126.4, 117.8, 116.2, 108.4 (aromatic C), 78.8, 61.8 (cage C), 56.2 (OCH₃). ¹¹B NMR (128 MHz, CDCl₃): δ 0.8 (s, 1B) (*B*_{cage-O}), -3.3 (d, *J*_{BH} = 140 Hz, 1B), -9.4 (m, 1B), -10.1 (m, 1B), -12.3 (d, *J*_{BH} = 151 Hz, 1B), -13.3 (m, 1B), -14.2 (m, 1B), -14.7(m, 1B), -15.6 (m, 1B), -18.2 (d, *J*_{BH} = 152 Hz, 1B) (*B*_{cageH}). IR (KBr): ν (cm⁻¹) 2924, 2590, 1476, 1193, 1037, 805, 548. Anal. Calcd for C₉H₁₆B₁₀O₂: C, 40.89; H, 6.10. Found: C, 41.12; H, 6.18.



2l

2l: Yield 25%. White solid. mp: 117-119 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.42 (d, *J* = 8.8 Hz, 1H), 7.35 (s, 1H), 7.05 (d, *J* = 8.8 Hz, 1H) (aromatic CH), 2.90 (s, 1H) (cage H), 1.31 (s, 9H) ((CH₃)₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 165.4, 145.6, 129.0, 125.6, 119.8, 115.1 (aromatic C), 79.3, 62.0 (cage C). 34.7, 31.6

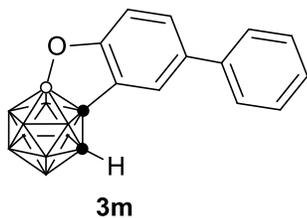
(C(CH₃)₃). ¹¹B NMR (128 MHz, CDCl₃): δ 0.6 (s, 1B) (*B*_{cage-O}), -3.4 (d, *J*_{BH} = 147 Hz, 1B), -9.5 (d, *J*_{BH} = 133 Hz, 1B), -10.1 (m, 1B), -12.5 (d, *J*_{BH} = 153 Hz, 1B), -13.4 (m, 1B), -14.2 (m, 1B), -15.0 (m, 1B), -15.7 (m, 1B), -18.3 (d, *J*_{BH} = 152 Hz, 1B) (*B*_{cageH}). IR (KBr): ν (cm⁻¹) 3055, 2963, 2608, 1616, 1479, 1364, 1199, 825, 809, 698. Anal. Calcd for C₁₂H₂₂B₁₀O: C, 49.63; H, 7.64. Found: C, 49.55; H, 7.71.



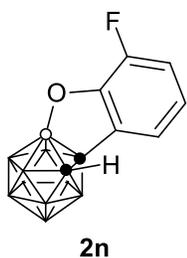
2m

2m: Yield 29%. White solid. mp: 142-145 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.61 (d, *J* = 8.8 Hz, 1H), 7.58 (s, 1H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.45 (t, *J* = 7.2 Hz, 2H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 1H) (aromatic CH), 2.96 (s, 1H) (cage H). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ 167.0, 139.5,

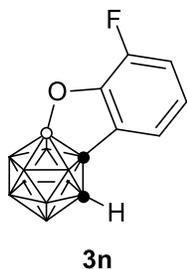
135.9, 130.7, 129.2, 127.8, 127.2, 126.6, 121.9, 116.0 (aromatic C), 78.7, 61.9 (cage C). ¹¹B NMR (128 MHz, CDCl₃): δ 0.6 (s, 1B) (*B*_{cage-O}), -3.3 (d, *J*_{BH} = 149 Hz, 1B), -9.1 (d, *J*_{BH} = 130 Hz, 1B), -10.1 (d, *J*_{BH} = 142 Hz, 1B), -12.4 (d, *J*_{BH} = 153 Hz, 1B), -14.1 (m, 2B), -14.9 (m, 1B), -15.5 (m, 1B), -18.1 (d, *J*_{BH} = 148 Hz, 1B) (*B*_{cageH}). IR (KBr): ν (cm⁻¹) 3050, 2594, 1467, 1199, 835, 762, 694. Anal. Calcd for C₁₄H₁₈B₁₀O: C, 54.17; H, 5.84. Found: C, 54.59; H, 5.98.



3m: Yield 8%. White solid. mp: 155-157 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.62 (dd, $J = 8.8, 2.0$ Hz, 1H), 7.51 (m, 2H), 7.44 (m, 3H), 7.36 (t, $J = 7.6$ Hz, 1H), 7.23 (d, $J = 8.8$ Hz, 1H) (aromatic CH), 4.27 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 166.6, 139.9, 134.8, 130.1, 129.1, 127.6, 127.1, 125.7, 118.5, 115.9 (aromatic C), 77.9, 56.3 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 3.6 (s, 1B) ($B_{\text{cage-O}}$), -3.9 (d, $J_{\text{BH}} = 151$ Hz, 1B), -9.9 (d, $J_{\text{BH}} = 177$ Hz, 3B), -11.3 (d, $J_{\text{BH}} = 156$ Hz, 2B), -14.8 (m, 2B), -21.3 (d, $J_{\text{BH}} = 168$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3063, 2582, 1466, 1198, 1119, 825, 758, 693. Anal. Calcd for $\text{C}_{14}\text{H}_{18}\text{B}_{10}\text{O}$: C, 54.17; H, 5.84. Found: C, 53.79; H, 5.91.

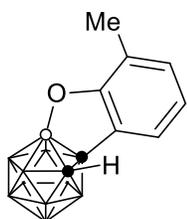


2n: Yield 68%. White solid. mp: 123-124 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.21 (m, 2H), 7.02 (m, 1H) (aromatic CH), 2.97 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 154.7 (d, $^2J_{\text{C-F}} = 12.3$ Hz), 149.9 (d, $^1J_{\text{C-F}} = 251.1$ Hz), 128.7 (d, $^3J_{\text{C-F}} = 10.8$ Hz), 122.8 (d, $^3J_{\text{C-F}} = 6.2$ Hz), 118.9 (d, $^4J_{\text{C-F}} = 2.3$ Hz), 118.8 (d, $^2J_{\text{C-F}} = 10.5$ Hz) (aromatic C), 78.3, 61.6 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 0.4 (s, 1B) ($B_{\text{cage-O}}$), -3.3 (d, $J_{\text{BH}} = 148$ Hz, 1B), -9.0 (d, $J_{\text{BH}} = 157$ Hz, 1B), -10.5 (d, $J_{\text{BH}} = 194$ Hz, 1B), -12.3 (d, $J_{\text{BH}} = 145$ Hz, 1B), -13.4 (m, 1B), -14.2 (m, 1B), -14.9 (m, 1B), -15.6 (m, 1B), -18.1 (d, $J_{\text{BH}} = 148$ Hz, 1B) (B_{cageH}). ^{19}F NMR (376 MHz, CDCl_3): δ -133.0 (m, 1F). IR (KBr): ν (cm^{-1}) 3055, 2580, 1628, 1487, 1450, 1263, 1185, 1093, 782, 726. Anal. Calcd for $\text{C}_8\text{H}_{13}\text{B}_{10}\text{FO}$: C, 38.08; H, 5.19. Found: C, 38.57; H, 5.28.



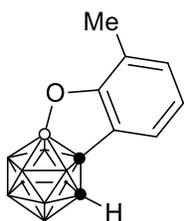
3n: Yield 9%. White solid. mp: 137-140 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.19 (d, $J = 8.8$ Hz, 1H), 7.03 (d, $J = 7.6$ Hz, 1H), 6.97 (td, $J = 8.0, 4.0$ Hz, 1H) (aromatic CH), 4.23 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 154.4 (d, $^2J_{\text{C-F}} = 12.8$ Hz), 150.1 (d, $^1J_{\text{C-F}} = 249.8$ Hz), 127.9 (d, $^3J_{\text{C-F}} = 3.7$ Hz), 121.6 (d, $^3J_{\text{C-F}} = 6.3$ Hz), 118.0 (d, $^2J_{\text{C-F}} = 17.0$ Hz), 115.5 (d, $^4J_{\text{C-F}} = 3.9$ Hz) (aromatic C), 77.4, 56.3 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 3.5 (s, 1B) ($B_{\text{cage-O}}$), -3.7 (d, $J_{\text{BH}} = 144$ Hz, 1B), -9.9 (d, $J_{\text{BH}} = 185$ Hz, 3B), -11.2 (d, $J_{\text{BH}} = 151$ Hz, 2B), -14.8 (d, $J_{\text{BH}} = 165$ Hz, 1B), -15.6 (d, $J_{\text{BH}} = 159$ Hz, 1B), -21.2 (d, $J_{\text{BH}} =$

168 Hz, 1B) (B_{cageH}). ^{19}F NMR (376 MHz, CDCl_3): δ -133.5 (m, 1F). IR (KBr): ν (cm^{-1}) 3062, 2588, 1628, 1594, 1488, 1446, 1140, 782, 729. HRMS (EI): m/z Calcd for $\text{C}_8\text{H}_{13}\text{B}_{10}\text{FO}^-$: 252.1963. Found: 252.1966.



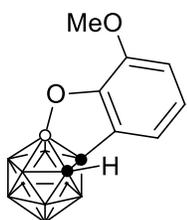
2o

2o: Yield 30%. White solid. mp: 97-98 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.22 (d, J = 7.6 Hz, 2H), 6.94 (t, J = 7.6 Hz, 1H) (aromatic CH), 2.88 (s, 1H) (cage H), 2.34 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 166.3, 132.8, 126.0, 125.6, 121.8, 120.7 (aromatic C), 79.3, 61.8 (cage C), 15.4 (CH_3). ^{11}B NMR (128 MHz, CDCl_3): δ 0.4 (s, 1B) ($B_{\text{cage-O}}$), -3.4 (d, J_{BH} = 153 Hz, 1B), -9.5 (d, J_{BH} = 144 Hz, 1B), -10.2 (m, 1B), -12.5 (d, J_{BH} = 158 Hz, 1B), -13.2 (m, 1B), -14.1 (m, 1B), -15.0 (m, 1B), -15.8 (m, 1B), -18.3 (d, J_{BH} = 156 Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3047, 2956, 2584, 1607, 1456, 1197, 1096, 775. Anal. Calcd for $\text{C}_9\text{H}_{16}\text{B}_{10}\text{O}$: C, 43.53; H, 6.49. Found: C, 43.87; H, 6.50.



3o

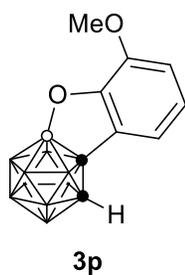
3o: Yield 6%. White solid. mp: 87-89 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.22 (d, J = 7.2 Hz, 1H), 7.06 (d, J = 7.2 Hz, 1H), 6.91 (t, J = 7.2 Hz, 1H) (aromatic CH), 4.20 (s, 1H) (cage H), 2.37 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 165.9, 132.1, 125.9, 124.6, 120.7, 117.2 (aromatic C), 78.4, 56.4 (cage C), 15.6 (CH_3). ^{11}B NMR (128 MHz, CDCl_3): δ 3.3 (s, 1B) ($B_{\text{cage-O}}$), -4.0 (d, J_{BH} = 158 Hz, 1B), -10.2 (d, J_{BH} = 159 Hz, 3B), -11.5 (d, J_{BH} = 154 Hz, 2B), -14.9 (d, J_{BH} = 153 Hz, 1B), -15.7 (d, J_{BH} = 176 Hz, 1B), -21.5 (d, J_{BH} = 169 Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3057, 2926, 2583, 1608, 1458, 1263, 1166, 1143, 836, 739. Anal. Calcd for $\text{C}_9\text{H}_{16}\text{B}_{10}\text{O}$: C, 43.53; H, 6.49. Found: C, 43.87; H, 6.53.



2p

2p: Yield 37%. White solid. mp: 162-165 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.00 (m, 3H) (aromatic CH), 3.94 (s, 3H) (OCH_3), 2.93 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 156.5, 147.6, 127.1, 122.8, 115.2, 113.9 (aromatic C), 79.0, 61.7 (cage C), 56.4 (OCH_3). ^{11}B NMR (128 MHz, CDCl_3): δ 0.5 (s, 1B) ($B_{\text{cage-O}}$), -3.3 (d, J_{BH} =

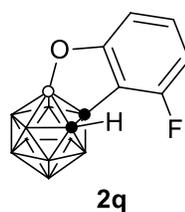
150 Hz, 1B), -9.3 (d, $J_{\text{BH}} = 138$ Hz, 1B), -10.2 (d, $J_{\text{BH}} = 132$ Hz, 1B), -12.2 (d, $J_{\text{BH}} = 145$ Hz, 1B), -13.3 (m, 1B), -14.2 (m, 1B), -14.7 (m, 1B), -15.7 (m, 1B), -18.1 (d, $J_{\text{BH}} = 147$ Hz, 1B) ($B_{\text{cage}}\text{H}$). IR (KBr): ν (cm^{-1}) 3106, 2939, 2599, 1591, 1472, 1441, 1370, 1294, 1245, 1092, 1009, 725, 484. HRMS (EI): m/z Calcd for $\text{C}_9\text{H}_{16}\text{B}_{10}\text{O}_2^-$: 264.2164. Found: 264.2161.



3p: Yield 9%. White solid. mp: 148-150 °C. ^1H NMR (400 MHz, CDCl_3): δ 6.98 (m, 2H), 6.85 (m, 1H) (aromatic CH), 4.22 (s, 1H) (cage H), 3.94 (s, 3H) (OCH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 156.3, 147.7, 126.2, 121.8, 113.2, 111.9 (aromatic C), 78.1, 56.2 (cage C), 56.3 (OCH_3). ^{11}B NMR (128 MHz, CDCl_3): δ 3.5 (s, 1B) ($B_{\text{cage}}\text{-O}$), -3.8 (d, $J_{\text{BH}} = 142$ Hz, 1B), -10.1 (d, $J_{\text{BH}} = 161$ Hz, 3B), -11.4 (d, $J_{\text{BH}} = 155$ Hz, 2B), -14.9

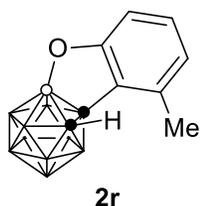
(d, $J_{\text{BH}} = 149$ Hz, 1B), -15.7 (d, $J_{\text{BH}} = 164$ Hz, 1B), -21.4 (d, $J_{\text{BH}} = 163$ Hz, 1B) ($B_{\text{cage}}\text{H}$). IR (KBr): ν (cm^{-1}) 3106, 2926, 2599, 1591, 1472, 1441, 1370, 1294, 1245, 1193, 1092, 1009, 725. HRMS (EI): m/z Calcd for $\text{C}_9\text{H}_{17}\text{B}_{10}\text{O}_2^+$: 265.2231. Found: 265.2228.

One-pot preparation of 2q-t. $i\text{PrMgCl}$ (2.0 M in THF, 6.0 mL, 12.0 mmol) was slowly added to a THF solution (25 mL) of *o*-carborane (720 mg, 5.0 mmol) at 0 °C, and the mixture was stirred at 0 °C for 1 h. After replacement of THF with toluene (25 mL), and addition of **1q-t** (6.0 mmol) and NiCl_2 (130 mg, 1.0 mmol), the reaction mixture was heated at 140 °C under stirring for 36 h in a closed flask. Then, the reaction was quenched with water (50 mL) and extracted with ethyl acetate (100 mL x 3). The organic portions were combined and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (300–400 mesh) using hexane as eluent to give **2q-t**.

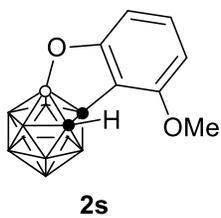


2q: Yield 5%. White solid. mp: 64-66 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.36 (dd, $J = 15.2, 8.4$ Hz, 1H), 6.95 (d, $J = 8.4$ Hz, 1H), 6.19 (t, $J = 8.4$ Hz, 1H) (aromatic CH), 2.96 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 169.3 (d, $^3J_{\text{C-F}} = 4.7$ Hz), 157.5 (d, $^1J_{\text{C-F}} = 254.5$ Hz), 132.8 (d, $^3J_{\text{C-F}} = 8.9$ Hz), 114.2 (d, $^2J_{\text{C-F}} = 17.9$ Hz), 111.7 (d,

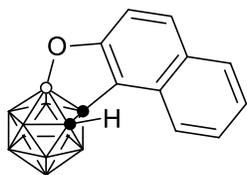
$^4J_{C-F} = 3.7$ Hz), 109.5 (d, $^2J_{C-F} = 18.8$ Hz) (aromatic C), 75.0, 62.2 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 0.5 (s, 1B) ($B_{\text{cage-O}}$), -3.6 (d, $J_{\text{BH}} = 148$ Hz, 1B), -8.5 (d, $J_{\text{BH}} = 164$ Hz, 1B), -10.1 (d, $J_{\text{BH}} = 195$ Hz, 1B), -12.4 (d, $J_{\text{BH}} = 146$ Hz, 1B), -13.5 (d, $J_{\text{BH}} = 177$ Hz, 2B), -15.0 (d, $J_{\text{BH}} = 160$ Hz, 1B), -16.0 (d, $J_{\text{BH}} = 170$ Hz, 1B), -17.5 (d, $J_{\text{BH}} = 163$ Hz, 1B) (B_{cageH}). ^{19}F NMR (376 MHz, CDCl_3): δ -116.8 (m, 1F). IR (KBr): ν (cm^{-1}) 3044, 2926, 2577, 1634, 1589, 1447, 1197, 1023, 784. HRMS (EI): m/z Calcd for $\text{C}_8\text{H}_{13}\text{B}_{10}\text{FO}^-$: 252.1963. Found: 252.1966.



2r: Yield 10%. White solid. mp: 82-84 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.26 (m, 1H), 6.98 (d, $J = 8.4$ Hz, 1H), 6.84 (d, $J = 7.6$ Hz, 1H) (aromatic CH), 2.93 (s, 1H) (cage H), 2.50 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 168.2, 135.5, 131.3, 124.4, 124.1, 113.5 (aromatic C), 78.9, 62.9 (cage C), 18.1 (CH_3). ^{11}B NMR (128 MHz, CDCl_3): δ 0.3 (s, 1B) ($B_{\text{cage-O}}$), -4.2 (d, $J_{\text{BH}} = 148$ Hz, 1B), -9.1 (d, $J_{\text{BH}} = 150$ Hz, 1B), -10.2 (d, $J_{\text{BH}} = 148$ Hz, 1B), -12.6 (d, $J_{\text{BH}} = 150$ Hz, 1B), -14.0 (d, $J_{\text{BH}} = 172$ Hz, 2B), -15.1 (d, $J_{\text{BH}} = 157$ Hz, 1B), -16.5 (d, $J_{\text{BH}} = 195$ Hz, 1B), -18.0 (d, $J_{\text{BH}} = 165$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3046, 2922, 2571, 1619, 1424, 1196, 1117, 1063, 823. Anal. Calcd for $\text{C}_9\text{H}_{16}\text{B}_{10}\text{O}$: C, 43.53; H, 6.49. Found: C, 43.62; H, 6.93.



2s: Yield 25%. White solid. mp: 93-95 °C. ^1H NMR (400 MHz, CDCl_3): δ 7.30 (t, $J = 8.4$ Hz, 1H), 6.74 (d, $J = 8.4$ Hz, 1H), 6.55 (d, $J = 8.4$ Hz, 1H) (aromatic CH), 3.88 (s, 3H) (OCH_3), 2.90 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 169.2, 155.9, 132.5, 114.1, 108.3, 104.6 (aromatic C), 77.1, 63.1 (cage C), 56.0 (OCH_3). ^{11}B NMR (128 MHz, CDCl_3): δ 0.4 (s, 1B) ($B_{\text{cage-O}}$), -4.2 (d, $J_{\text{BH}} = 148$ Hz, 1B), -9.2 (d, $J_{\text{BH}} = 140$ Hz, 1B), -9.8 (m, 1B), -12.8 (d, $J_{\text{BH}} = 128$ Hz, 2B), -13.5 (d, $J_{\text{BH}} = 159$ Hz, 1B), -15.3 (d, $J_{\text{BH}} = 185$ Hz, 1B), -16.5 (d, $J_{\text{BH}} = 161$ Hz, 1B), -17.7 (d, $J_{\text{BH}} = 152$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3054, 2944, 2571, 1609, 1494, 1437, 1282, 1201, 1081, 776. Anal. Calcd for $\text{C}_9\text{H}_{16}\text{B}_{10}\text{O}_2$: C, 40.89; H, 6.10. Found: C, 40.95; H, 6.14.



2t

2t: Yield 28%. White solid. mp: 102-104 °C. ^1H NMR (400 MHz, CDCl_3): δ 8.18 (d, $J = 8.4$ Hz, 1H), 7.89 (t, $J = 9.2$ Hz, 2H), 7.65 (t, $J = 8.4$ Hz, 1H) 7.48 (t, $J = 7.6$ Hz, 1H), 7.35 (d, $J = 9.2$ Hz, 1H) (aromatic CH), 2.92 (s, 1H) (cage H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 167.5, 133.0, 129.2, 129.0, 128.7, 128.6, 125.2, 121.8, 119.0, 116.2 (aromatic C), 79.2, 62.6 (cage C). ^{11}B NMR (128 MHz, CDCl_3): δ 0.5 (s, 1B) ($B_{\text{cage-O}}$), -3.9 (d, $J_{\text{BH}} = 152$ Hz, 1B), -9.2 (d, $J_{\text{BH}} = 136$ Hz, 1B), -10.0 (d, $J_{\text{BH}} = 112$ Hz, 1B), -12.3 (d, $J_{\text{BH}} = 156$ Hz, 1B), -13.8 (d, $J_{\text{BH}} = 172$ Hz, 2B), -14.8 (d, $J_{\text{BH}} = 169$ Hz, 1B), 16.6 (d, $J_{\text{BH}} = 189$ Hz, 1B), -17.7 (d, $J_{\text{BH}} = 146$ Hz, 1B) (B_{cageH}). IR (KBr): ν (cm^{-1}) 3056, 2573, 1625, 1587, 1521, 1200, 1061, 816, 750. Anal. Calcd for $\text{C}_{12}\text{H}_{16}\text{B}_{10}\text{O}$: C, 50.68; H, 5.67. Found: C, 50.65; H, 5.72.

3. Crystal Data and Summary of Data Collection and Refinements

X-ray Structure Determination. All data were collected at 293K on a Bruker SMART 1000 CCD diffractometer using Mo-K α radiation. An empirical absorption correction was applied using the SADABS program.² All structures were solved by direct methods and subsequent Fourier difference techniques and refined anisotropically for all non-hydrogen atoms by full-matrix least squares calculations on F2 using the SHELXTL program package.³ All hydrogen atoms were geometrically fixed using the riding model. Crystal data and details of data collection and structure refinements are given in Table S1.

CCDC 1961649-1961653 (**2b**, **2g**, **2s**, **3b** and **3h**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

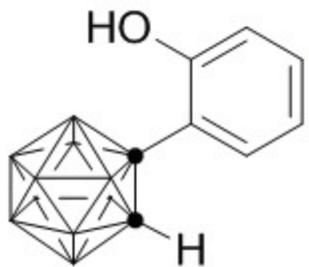
Table S1. Crystal Data and Summary of Data Collection and Refinement for **2b**, **3b**, **2g**, **3h** and **2s**.

compound	2b	3b	2g	3h	2s
formula	C ₉ H ₁₆ B ₁₀ O	C ₉ H ₁₆ B ₁₀ O	C ₁₂ H ₂₂ B ₁₀ O	C ₈ H ₁₃ B ₁₀ FO	C ₉ H ₁₆ B ₁₀ O ₂
crystal size (mm)	0.11 × 0.1 × 0.05	0.2 × 0.15 × 0.12	0.22 × 0.2 × 0.18	0.12 × 0.1 × 0.08	0.3 × 0.25 × 0.22
fw	248.47	248.47	290.39	252.43	264.47
crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	P-1	P2 ₁ /n	P2 ₁ /m	P2 ₁ /n	P2 ₁ /n
<i>a</i> Å	6.678(1)	12.865(1)	6.703(1)	6.681(1)	10.104(1)
<i>b</i> Å	7.725(1)	7.029(1)	9.329(1)	20.124(2)	10.567(2)
<i>c</i> Å	14.170(2)	14.895(1)	13.382(1)	9.432(1)	26.989(4)
<i>α</i> , deg	83.442(3)	90	90	90	90
<i>β</i> , deg	89.351(3)	90.789(2)	92.850(2)	92.779(2)	95.920(2)
<i>γ</i> , deg	67.197(3)	90	90	90	90
<i>V</i> , Å ³	669.0(2)	1346.8(2)	835.7(2)	1266.7(2)	2866.1(7)
<i>Z</i>	2	4	2	4	8
<i>D</i> _{calcd} , Mg/m ³	1.233	1.225	1.154	1.323	1.225
radiation (λ) Å	0.71073	0.71073	0.71073	0.71073	0.71073
2θ range, deg	5.76 to 60.98	5.48 to 61.32	4.36 to 61.30	4.04 to 61.46	4.14 to 57.96
μ, mm ⁻¹	0.063	0.063	0.060	0.079	0.068
<i>F</i> (000)	256	512	304	512	1088
no. of obsd reflns	4034	4167	2736	3944	7574
no. of params refnd	182	182	126	181	381
goodness of fit	1.057	1.051	1.076	1.047	1.0194
R1	0.0569	0.0435	0.0587	0.0455	0.0550
wR2	0.1326	0.1266	0.1472	0.1202	0.1441

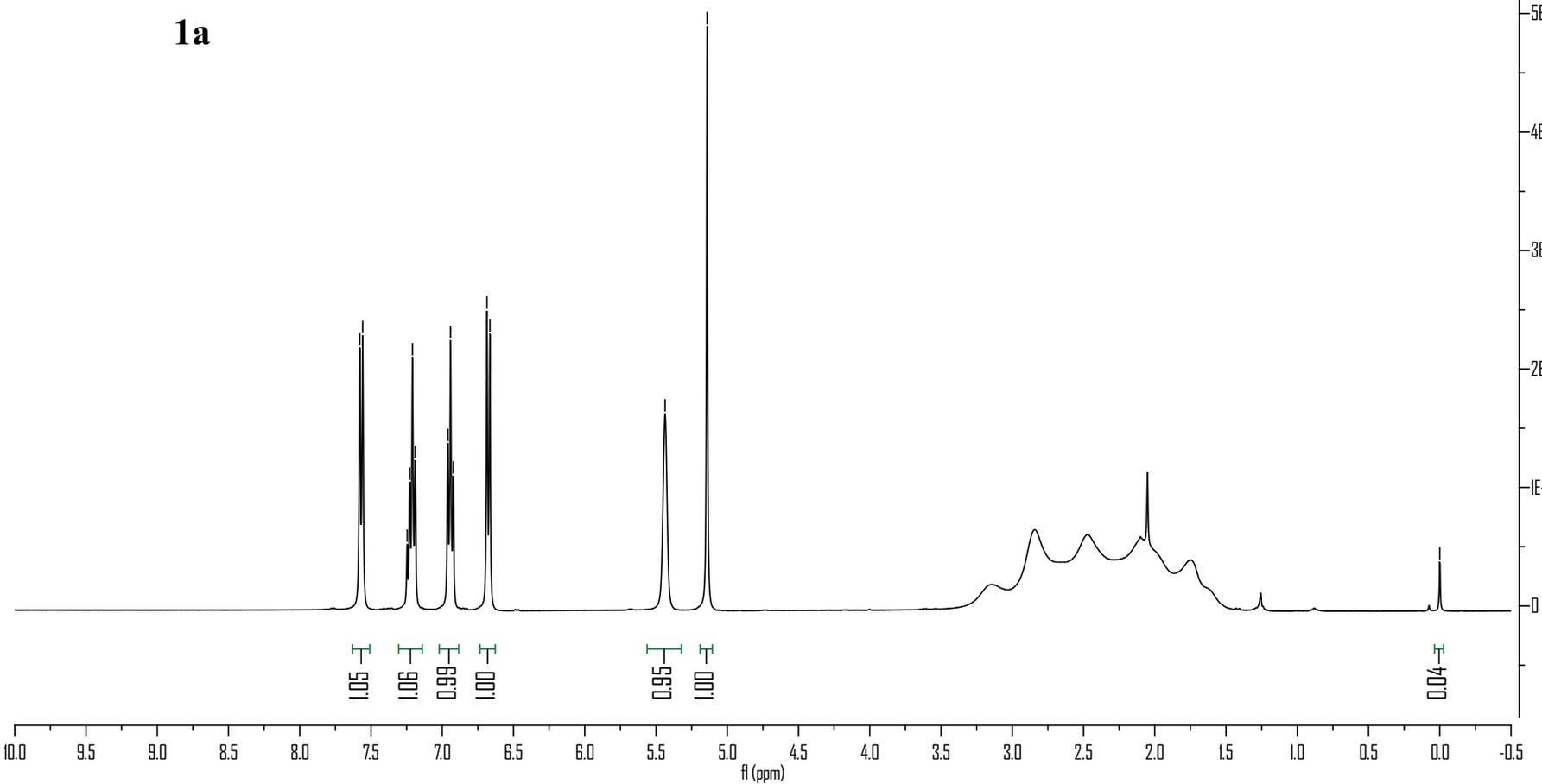
4. References

- 1 C. Tang, Z. Xie, *Angew. Chem. Int. Ed.* 2015, **54**, 7662–7665.
- 2 G. M. Sheldrick, *SADABS: Program for Empirical Absorption Correction of Area Detector Data*; University of Göttingen: Germany, 1996.

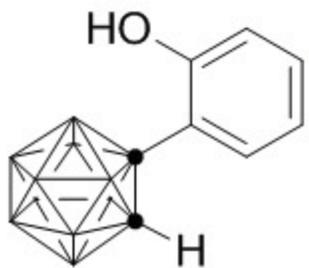
- 3 G. M. Sheldrick, SHELXTL 5.10 for Windows NT: *Structure Determination Software Programs*; Bruker Analytical X-ray Systems, Inc.: Madison, WI, USA, 1997.



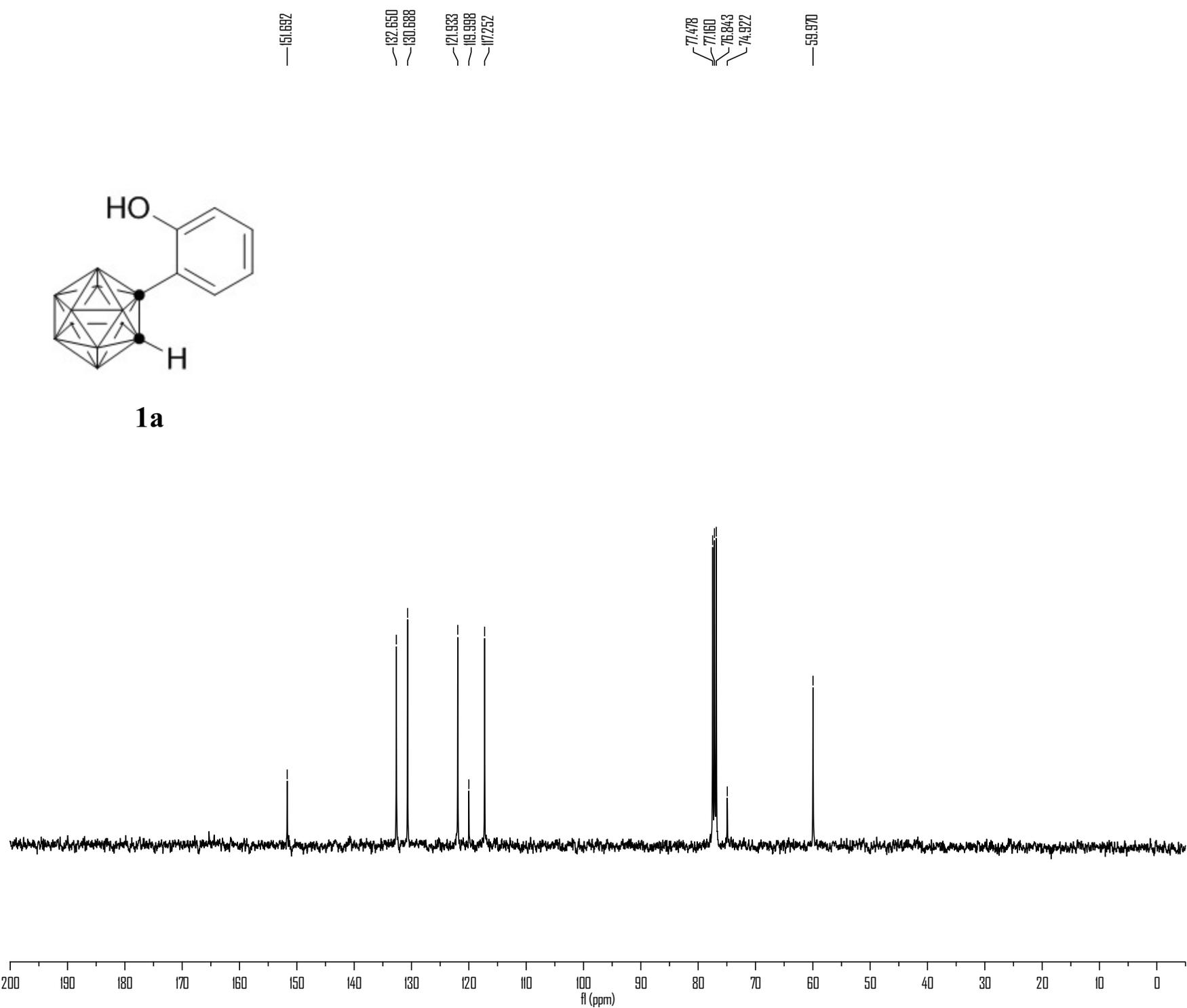
1a



Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/5-43-1/h-cx-5-43-1/pdata/1/1r
Title	5-43-1
Comment	
Origin	UXMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	zg
Number of Scans	8
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	4.0000
Acquisition Time	1.3631
Acquisition Date	2015-11-02T22:54:47
Modification Date	2015-11-02T15:54:00
Spectrometer Frequency	400.13
Spectral Width	12019.2
Lowest Frequency	-4470.3
Nucleus	¹ H
Acquired Size	16384
Spectral Size	32768

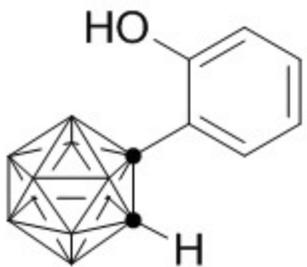


1a

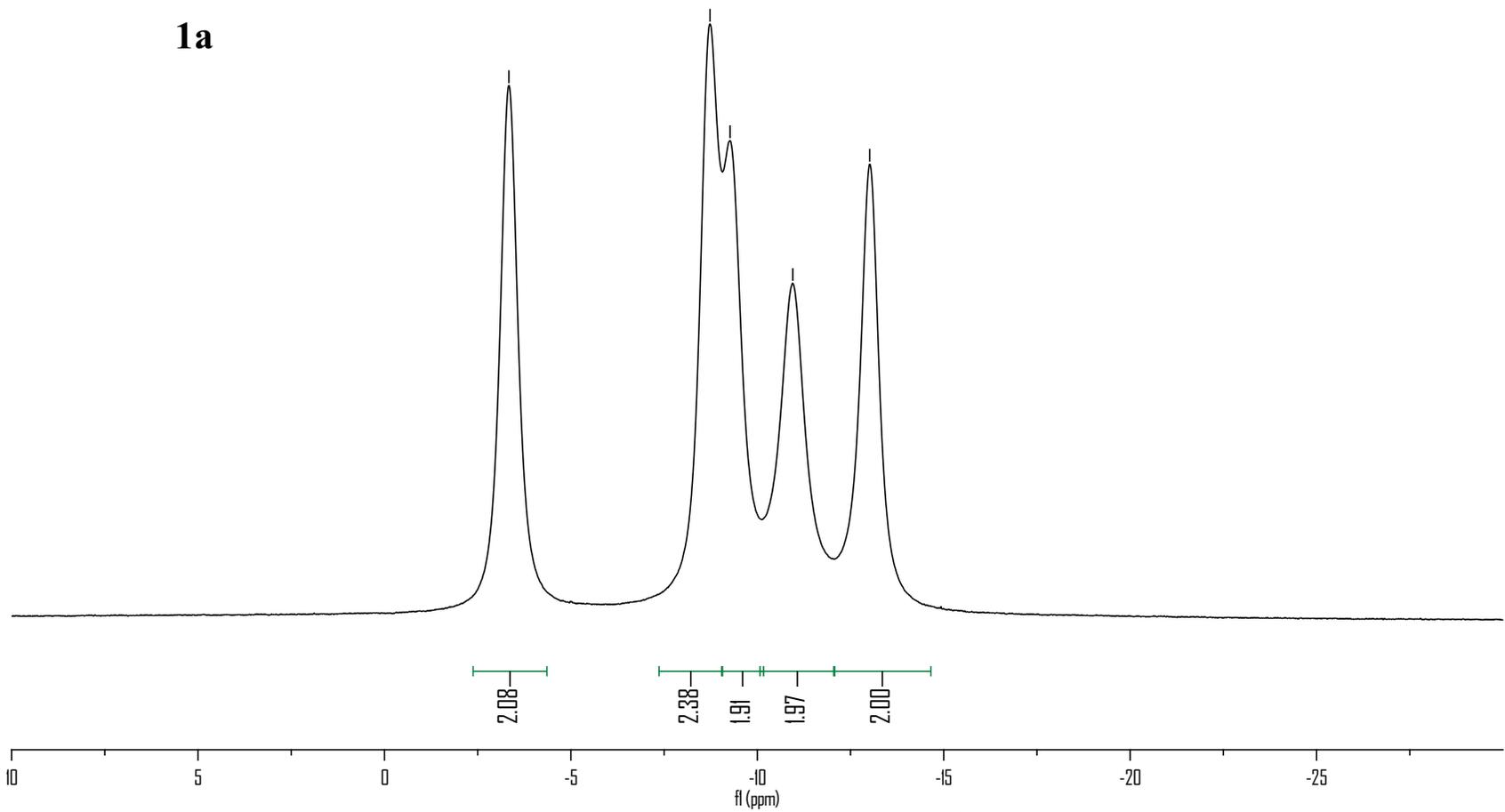


S25

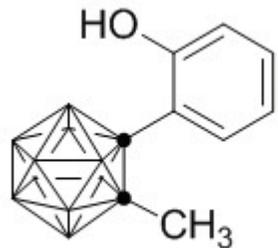
Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/5-43-1/c-cx-5-43-1/pdata/1/1r
Title	cl3
Comment	
Origin	UXNMR Bruker
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgdc
Number of Scans	297
Receiver Gain	16384
Relaxation Delay	2.0000
Pulse Width	6.0000
Acquisition Time	0.4654
Acquisition Date	2015-11-02T23:04:16
Modification Date	2015-11-02T16:15:00
Spectrometer Frequency	100.61
Spectral Width	35211.3
Lowest Frequency	-6255.3
Nucleus	¹³ C
Acquired Size	16384
Spectral Size	65536



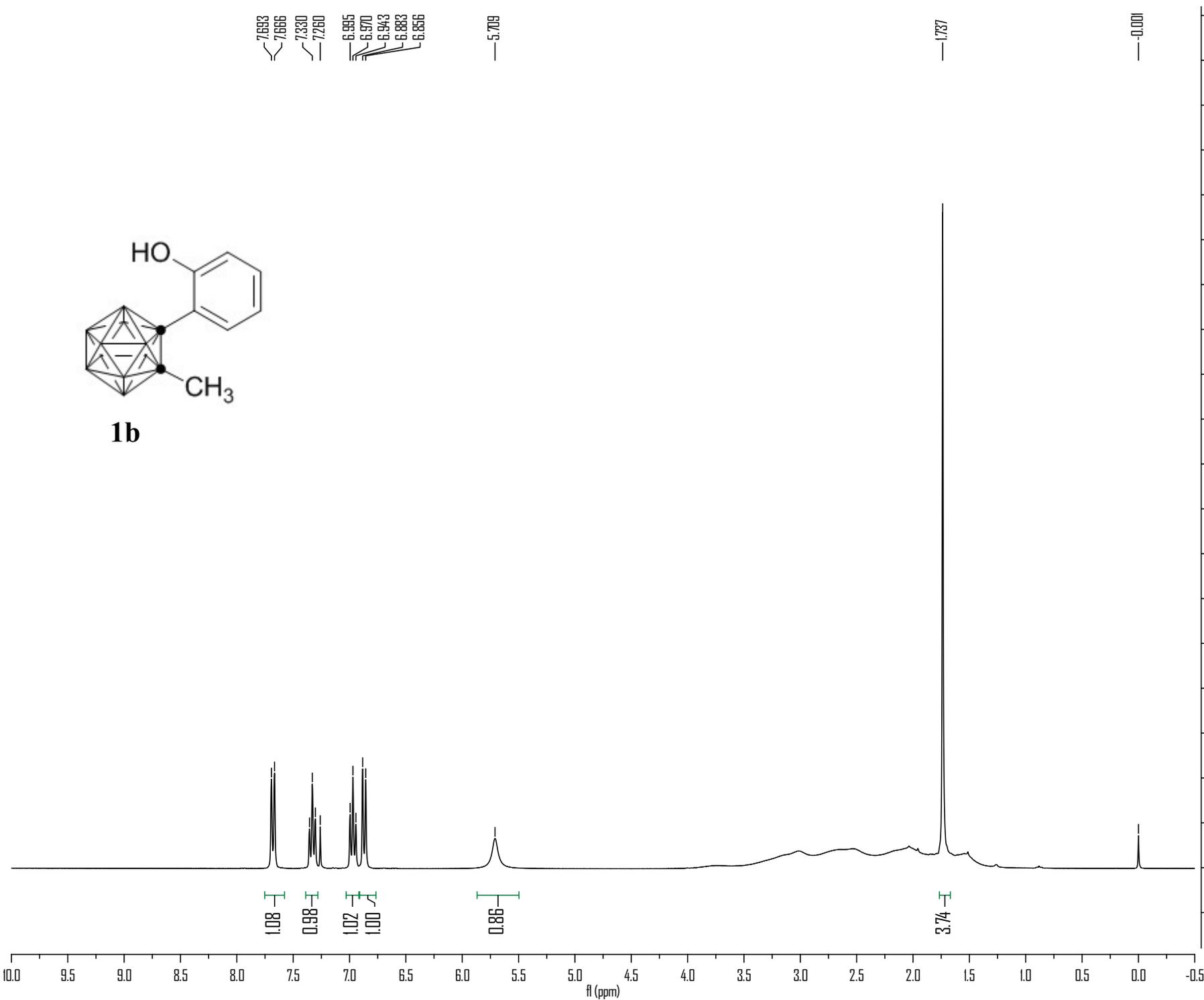
1a



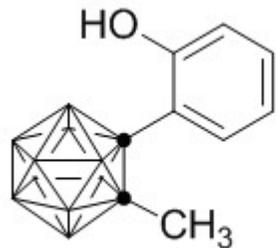
Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/5-43-1/b-ccx-5-43-1/pdata/1/1r
Title	5-43-1
Comment	
Origin	UNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	256
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	13.4000
Acquisition Time	0.5112
Acquisition Date	2015-11-02T22:56:37
Modification Date	2015-11-02T15:57:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16666.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



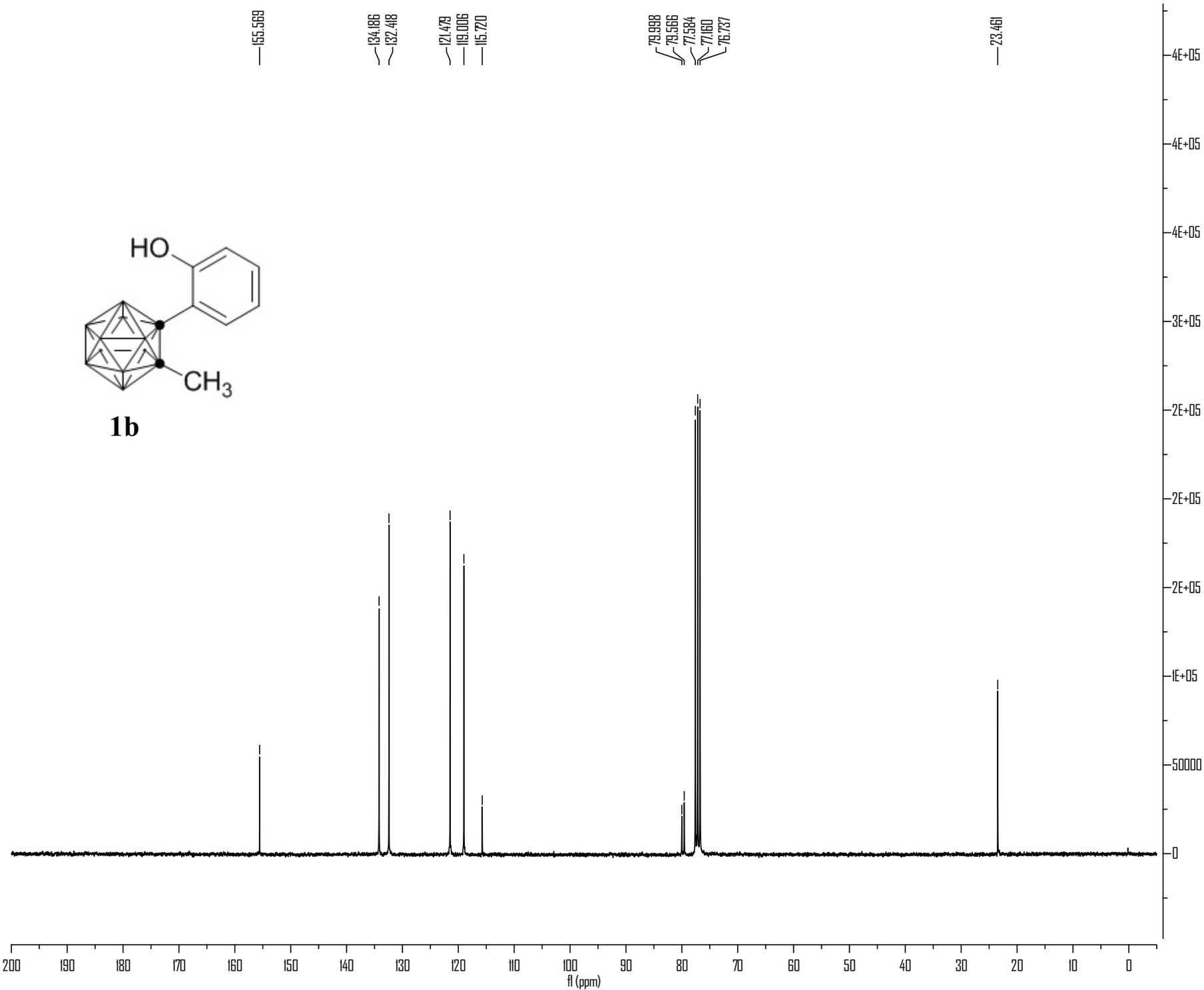
1b



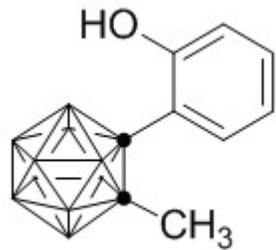
Parameter	Value
Title	ccx-6-1-1H
Comment	STANDARD 1H OBSERVE
Origin	Varian
Owner	
Site	
Spectrometer	mercury
Author	omc
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Number of Scans	24
Receiver Gain	24
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.0000
Acquisition Date	2016-01-13T23:11:43
Modification Date	2016-01-13T23:13:00
Spectrometer	300.03
Frequency	
Spectral Width	5494.5
Lowest Frequency	-709.6
Nucleus	1H
Acquired Size	10989
Spectral Size	32768



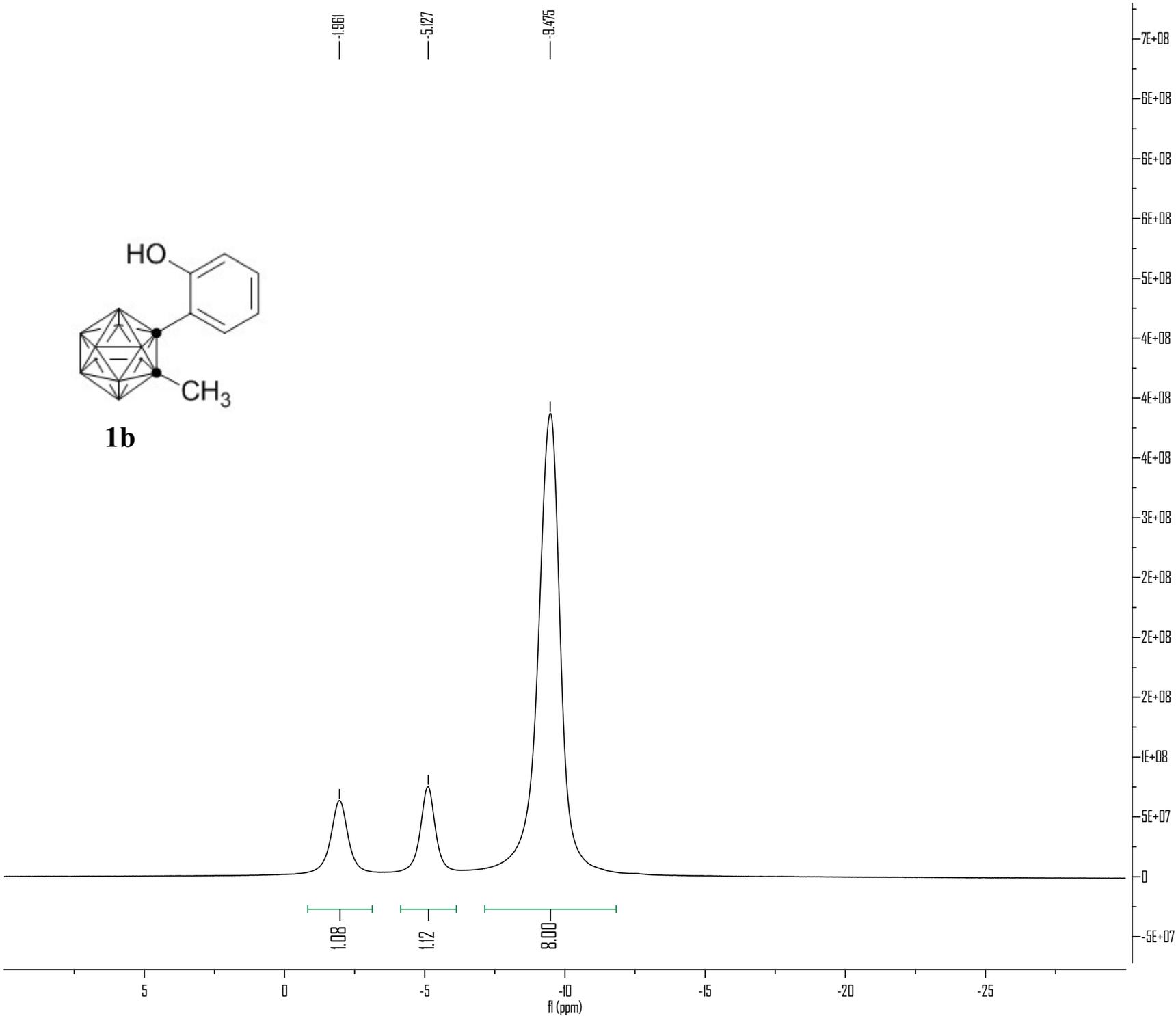
1b



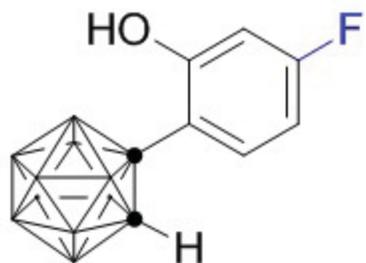
Parameter	Value
Title	ccx-61-1C
Comment	13C OBSERVE
Origin	Varian
Owner	
Site	
Spectrometer	mercury
Author	omc
Solvent	CDCl ₃
Temperature	29.0
Pulse Sequence	s2pul
Number of Scans	11308
Receiver Gain	34
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.5000
Acquisition Date	2016-01-14T00:30:30
Modification Date	2016-01-14T08:22:00
Spectrometer	75.45
Frequency	
Spectral Width	19011.4
Lowest Frequency	-1742.9
Nucleus	13C
Acquired Size	28617
Spectral Size	65536



1b



Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/原料数据/6-1-1/2012060b-ccx-6-1-1/2012060b-ccx-6-1-1/pdata/1/1r
Title	2012060b-ccx-6-1-1
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	256
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	13.4000
Acquisition Time	0.512
Acquisition Date	2016-01-14T20:07:02
Modification Date	2016-01-14T15:01:32
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16682.0
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

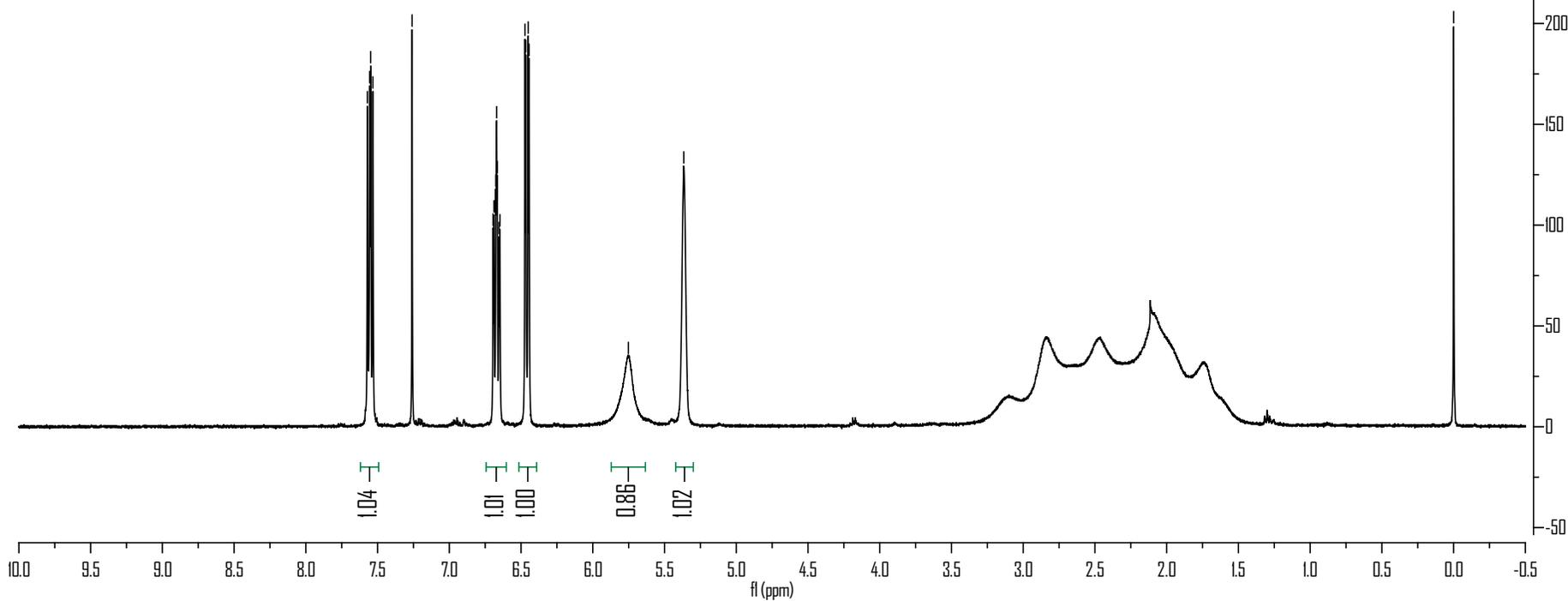


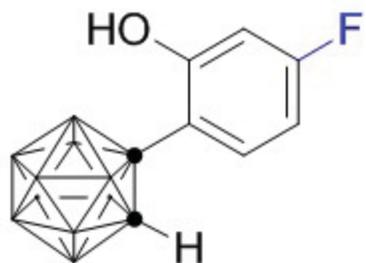
1c

7.571
7.556
7.549
7.533
7.260
6.676
6.666
6.647
6.473
6.450
6.444
5.752
5.366

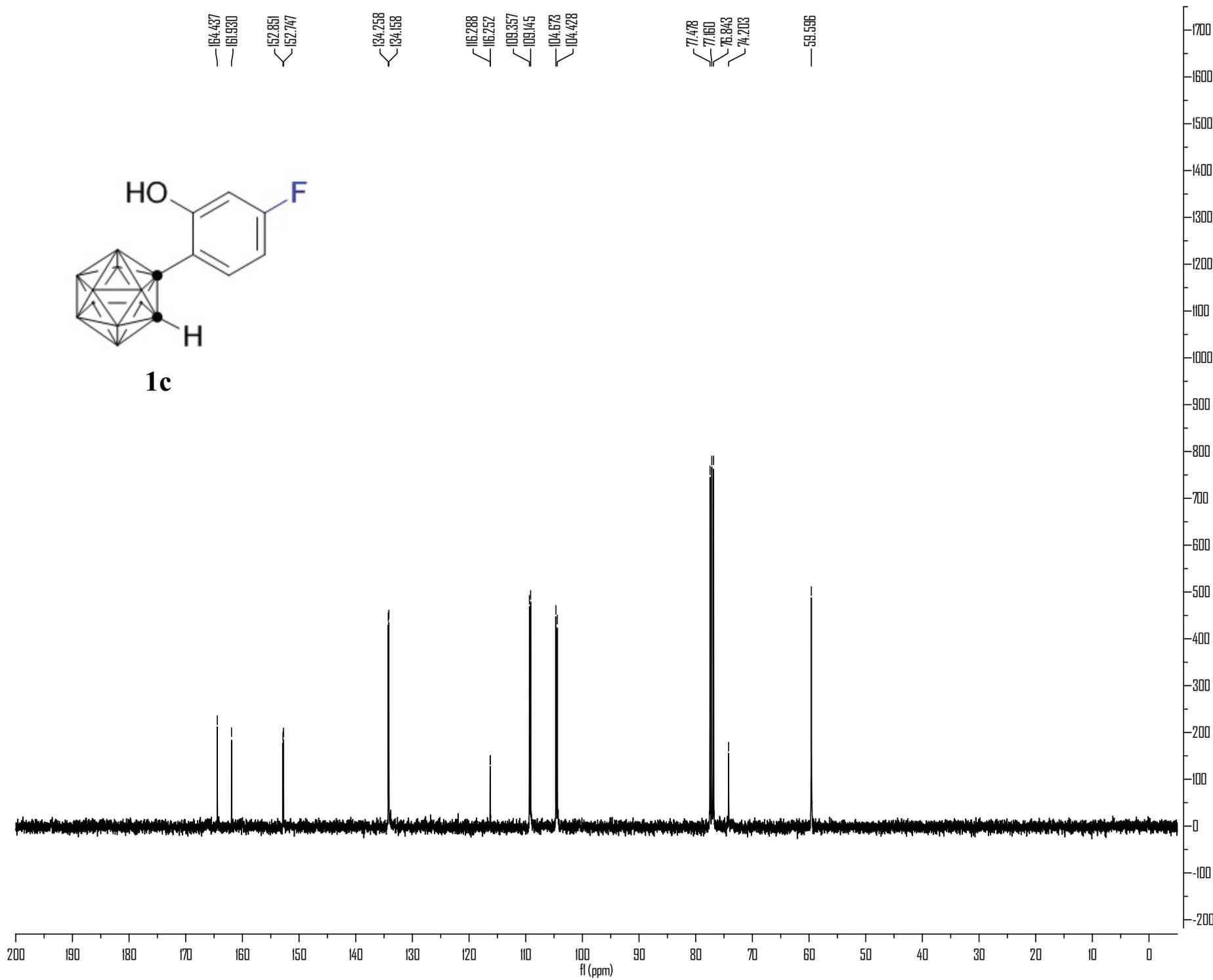
0.000

Parameter	Value
Title	ccx-7-2-1H
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	
Solvent	CDCl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	46
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-09-27T19:16:23
Modification Date	2016-09-27T11:17:00
Spectrometer	399.72
Frequency	
Spectral Width	7183.9
Lowest Frequency	-793.9
Nucleus	1H
Acquired Size	21552
Spectral Size	65536



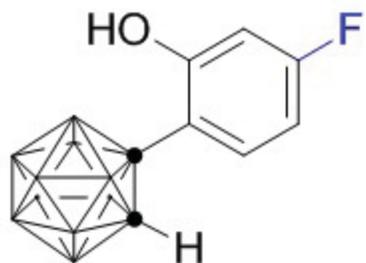


1c

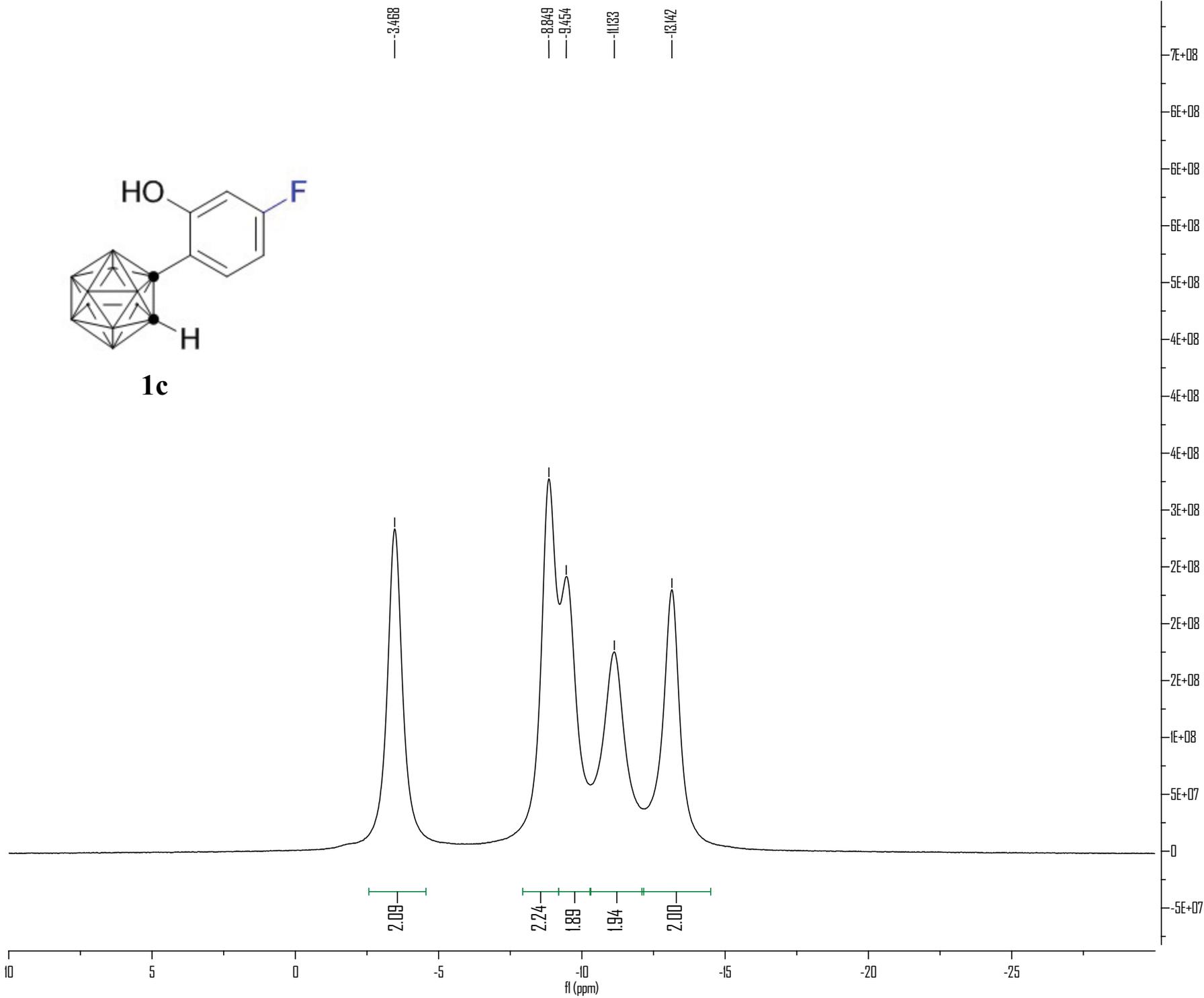


164.437
161.930
152.851
152.747
134.258
134.158
116.288
116.252
109.357
109.145
104.678
104.428
77.478
77.160
76.843
74.203
59.596

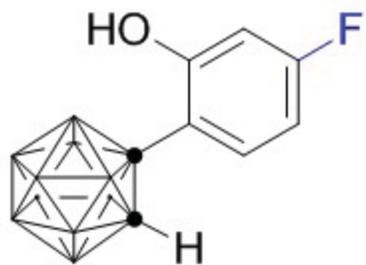
Parameter	Value
Title	ccx-7-2-1-CCC
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	304
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Acquisition Date	2017-11-21 06:21:38
Modification Date	2017-11-20 12:33:00
Spectrometer	100.52
Frequency	
Spectral Width	25000.0
Lowest Frequency	-1432.0
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



1c

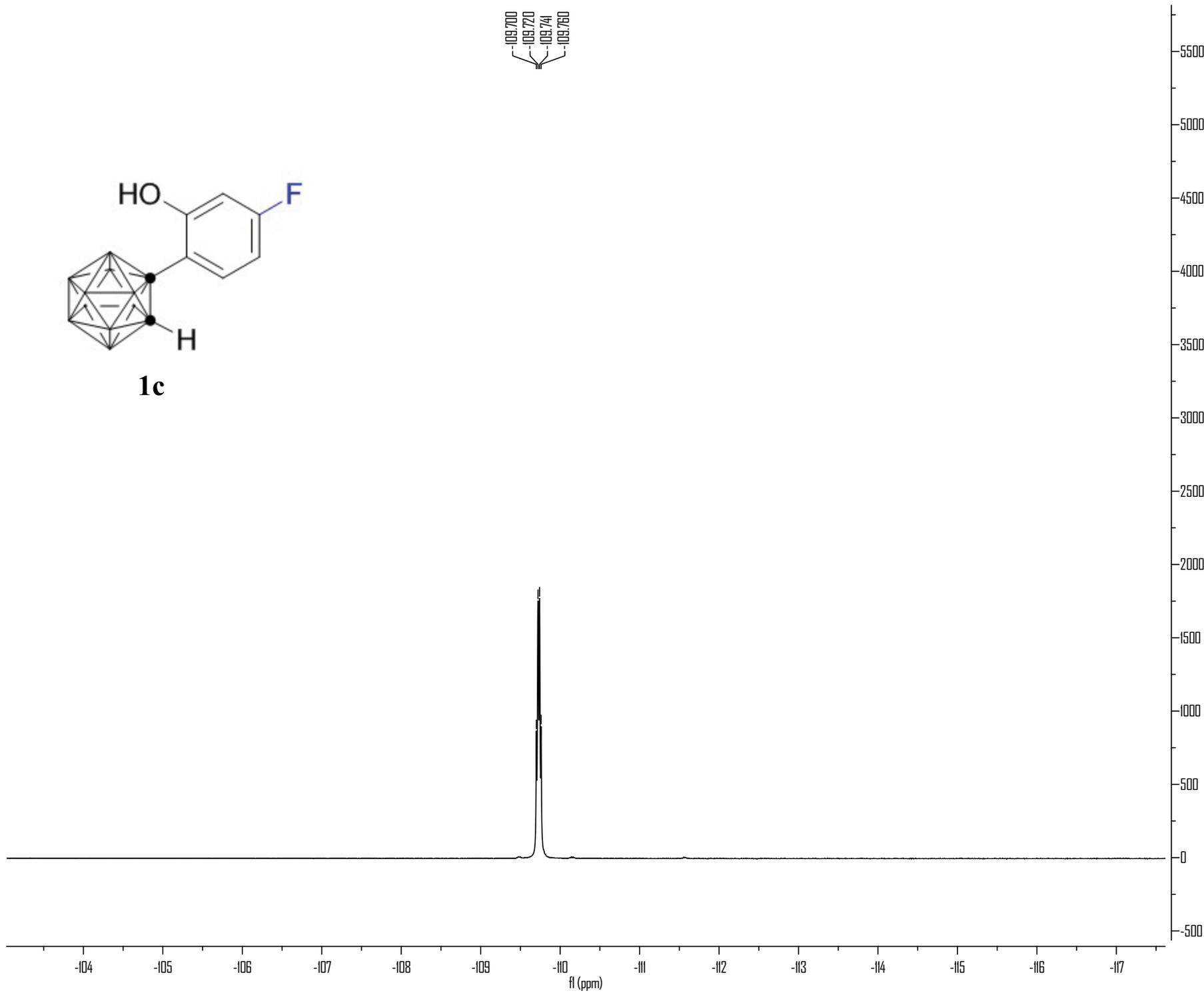


Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/7-2-1/b-cx-7-2-1 (1)/pdata/1/1r
Title	7-2-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	143
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-09-28T17:55:42
Modification Date	2016-09-28T11:58:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16404.2
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

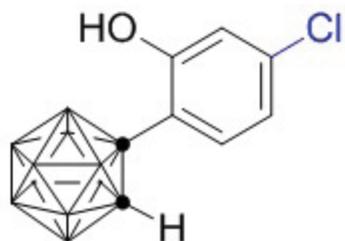


1c

109.700
109.770
109.741
109.760



Parameter	Value
Title	ccx-7-2-1F
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	52
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	1.0000
Acquisition Date	2016-09-28T09:24:09
Modification Date	2016-09-28T01:25:00
Spectrometer Frequency	376.08
Spectral Width	147058.8
Lowest Frequency	-110727.0
Nucleus	19F
Acquired Size	147058
Spectral Size	524288



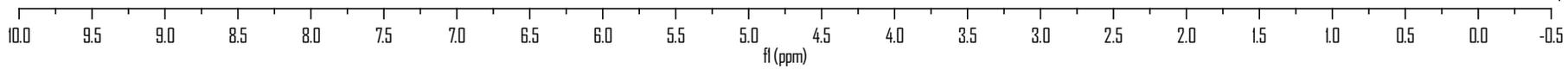
1d

7.511
7.489
7.260
6.940
6.919
6.743

5.773
5.367

2.013

0.001



1.00

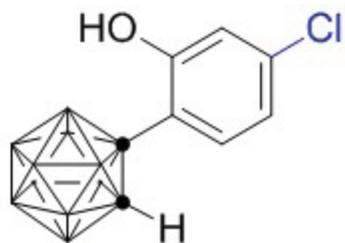
1.02

1.01

0.97

1.06

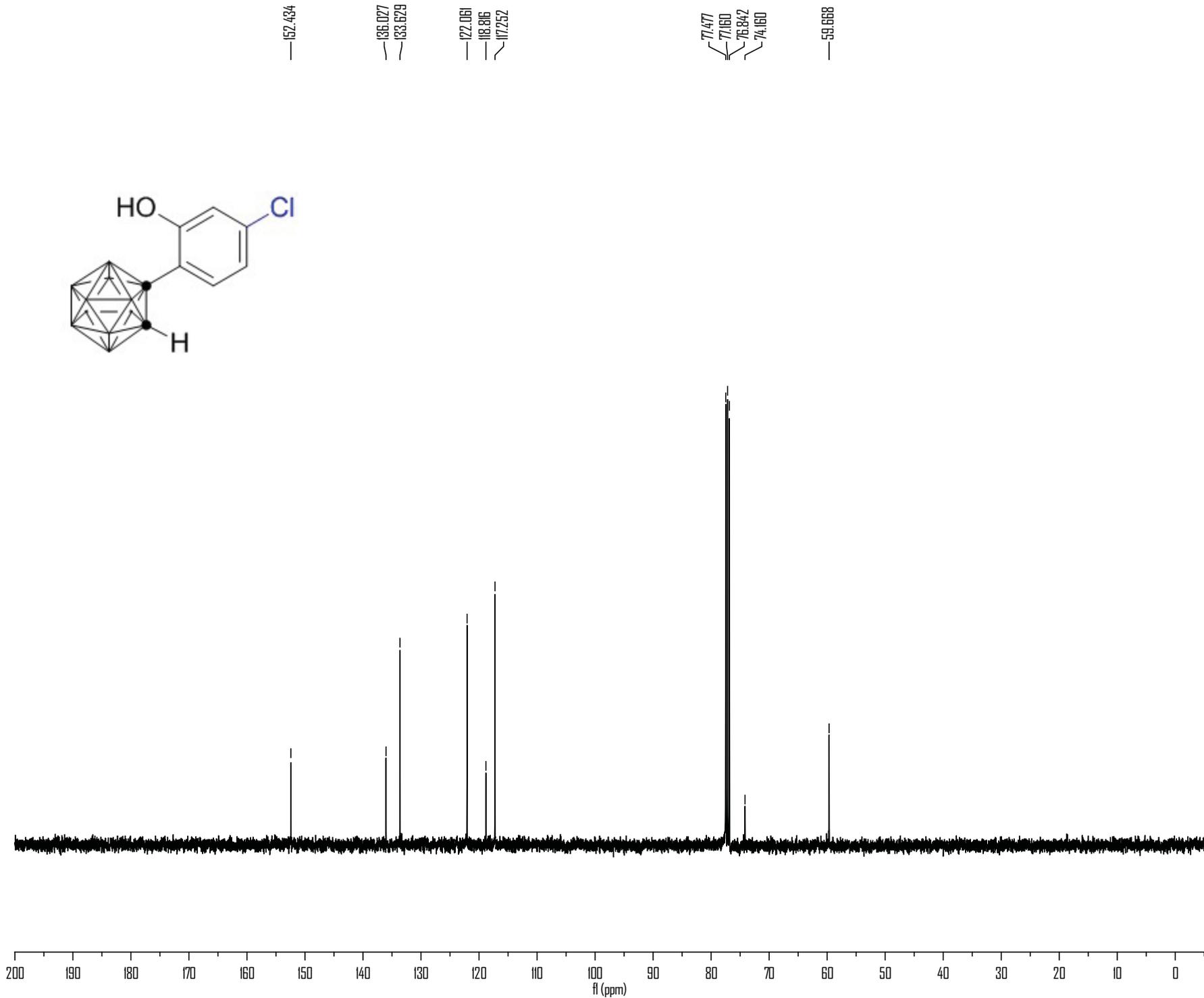
Parameter	Value
Title	H-CDX-6103-1
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmr's
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	20
Receiver Gain	20
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5559
Acquisition Date	2016-09-22T09:40:42
Modification Date	2016-09-22T09:43:00
Spectrometer Frequency	399.67
Spectral Width	6410.3
Lowest Frequency	-794.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



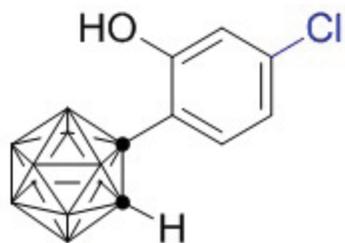
152.434

136.027
133.629122.061
118.816
117.25271.477
71.160
70.842
71.160

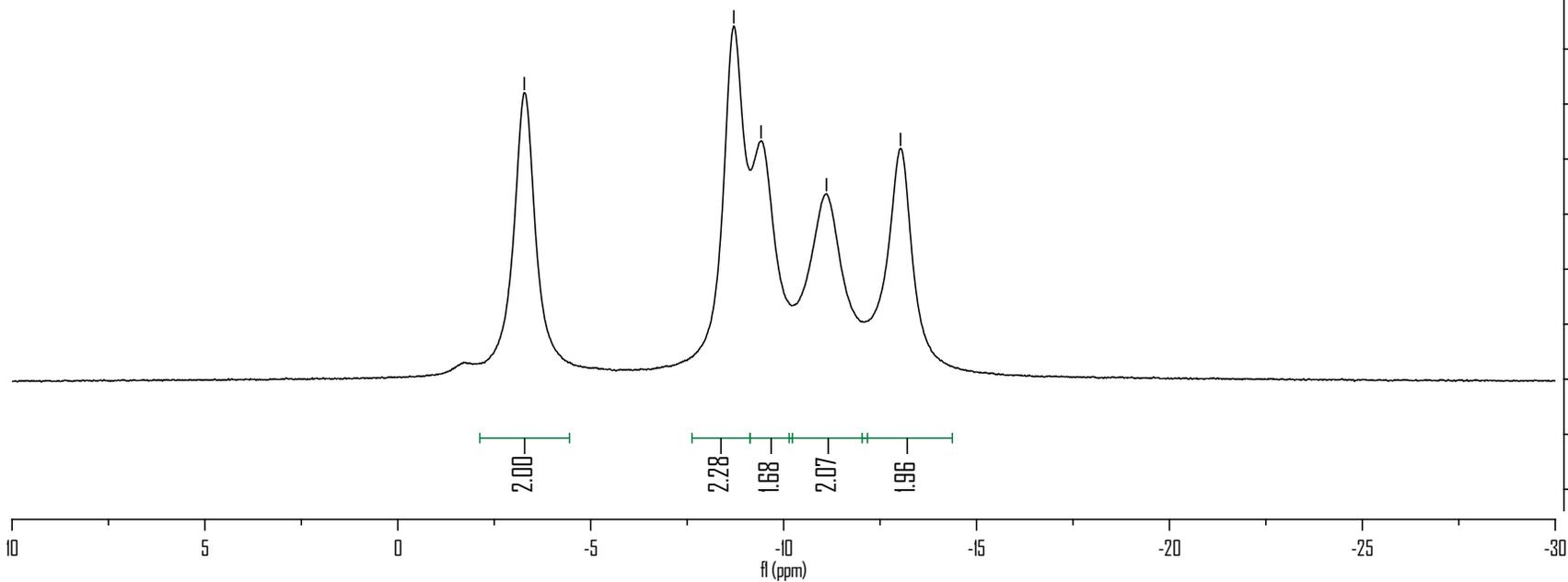
59.668



Parameter	Value
Title	CCX-6-103-1C
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	cdcl3
Temperature	21.0
Pulse	s2pul
Sequence	
Number of Scans	292
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3000
Acquisition Date	2016-10-07T18:55:24
Modification Date	2016-10-07T11:07:00
Spectrometer Frequency	100.52
Spectral Width	25000.0
Lowest frequency	-1429.1
Nucleus	^{13}C
Acquired Size	32500
Spectral Size	65536

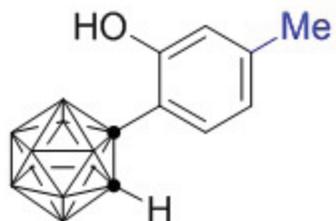


-3.279
 -8.709
 -9.414
 -11.111
 -13.031



S36

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/6-103/2012060b-ccx-6-103-1/2012060b-ccx-6-103-1/1/pdata/1/1r
Title	2012060b-ccx-6-103-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	256
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2016-09-23T15:41:20
Modification Date	2016-09-23T08:57:52
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16392.4
Nucleus	1H
Acquired Size	16394
Spectral Size	32768



1e

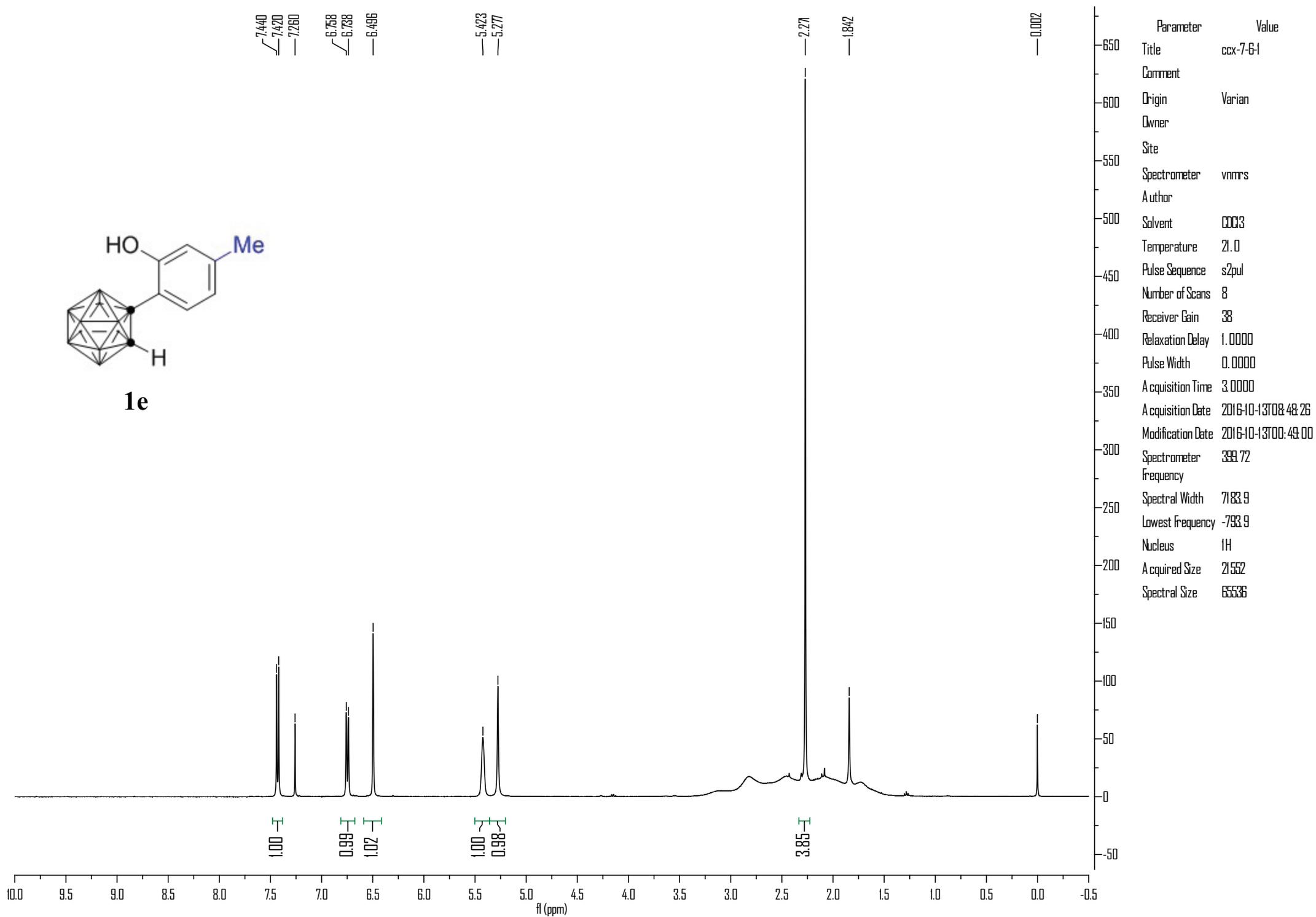
7.440
7.420
7.260

6.758
6.738
6.496

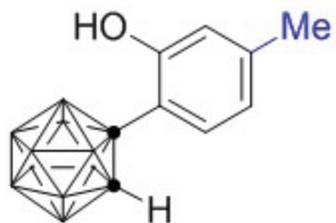
5.423
5.277

2.271
1.842

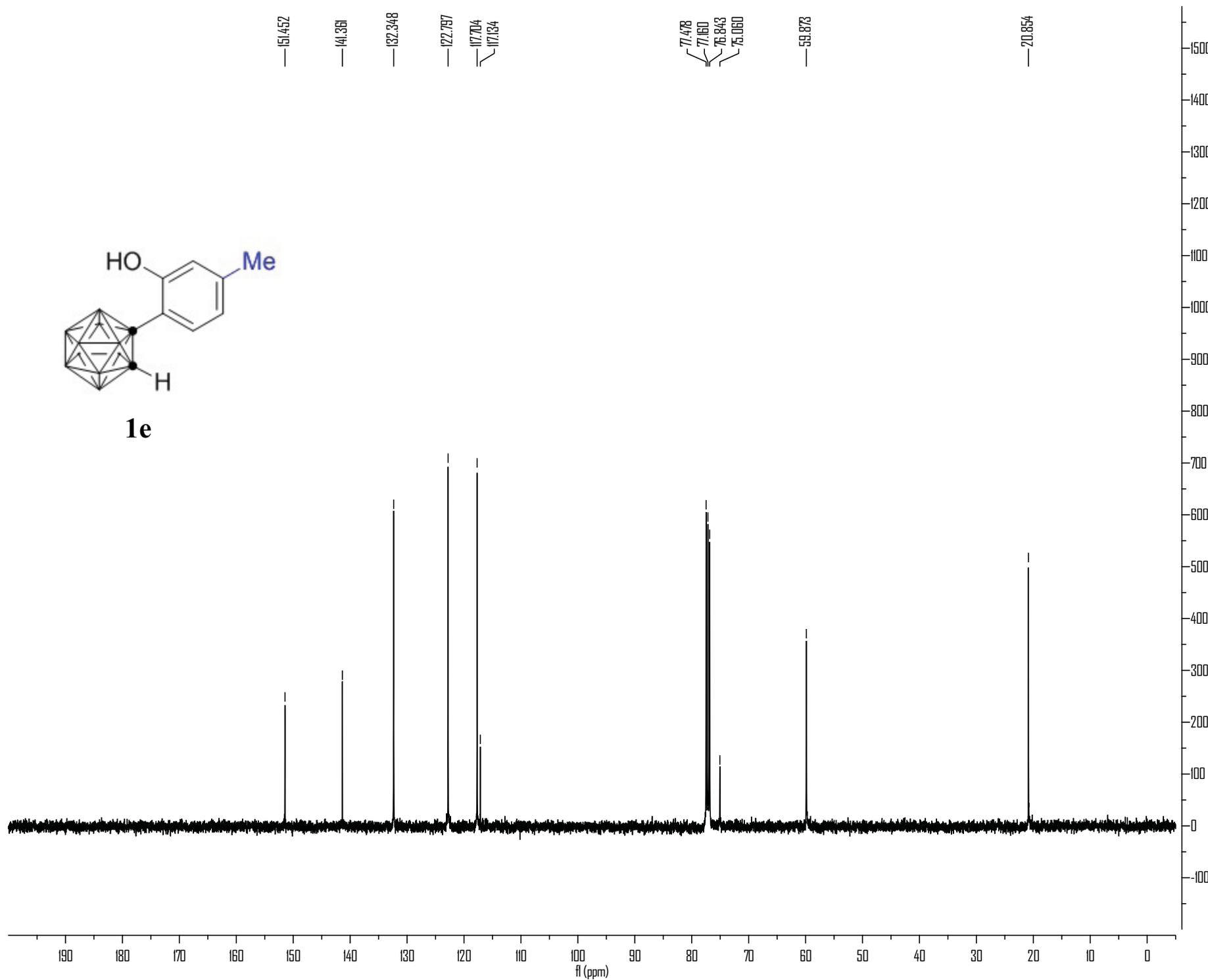
0.002



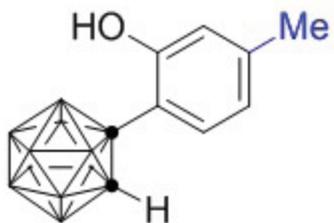
Parameter	Value
Title	ccx-7-6-1
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	CDCl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	38
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-10-13T08:48:26
Modification Date	2016-10-13T00:49:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-793.9
Nucleus	1H
Acquired Size	21552
Spectral Size	65536



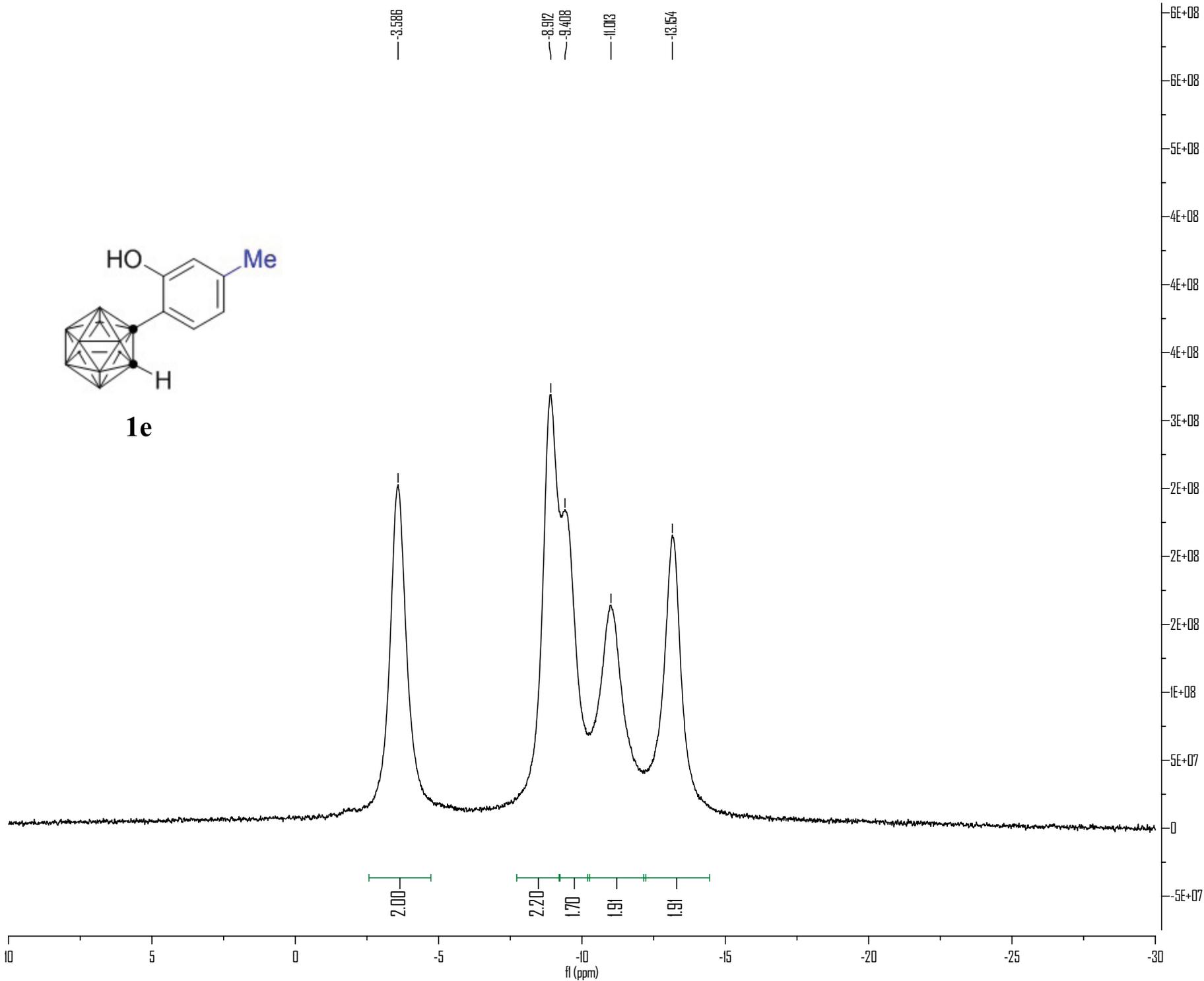
1e



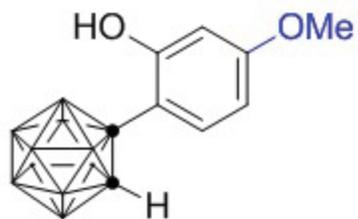
Parameter	Value
Title	-CCX-7-6-1C
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	nmrns
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse	s2pul
Sequence	
Number of Scans	240
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-10-13T11:36:57
Modification Date	2016-10-13T11:50:00
Spectrometer Frequency	100.51
Spectral Width	25510.2
Lowest Frequency	-1682.4
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



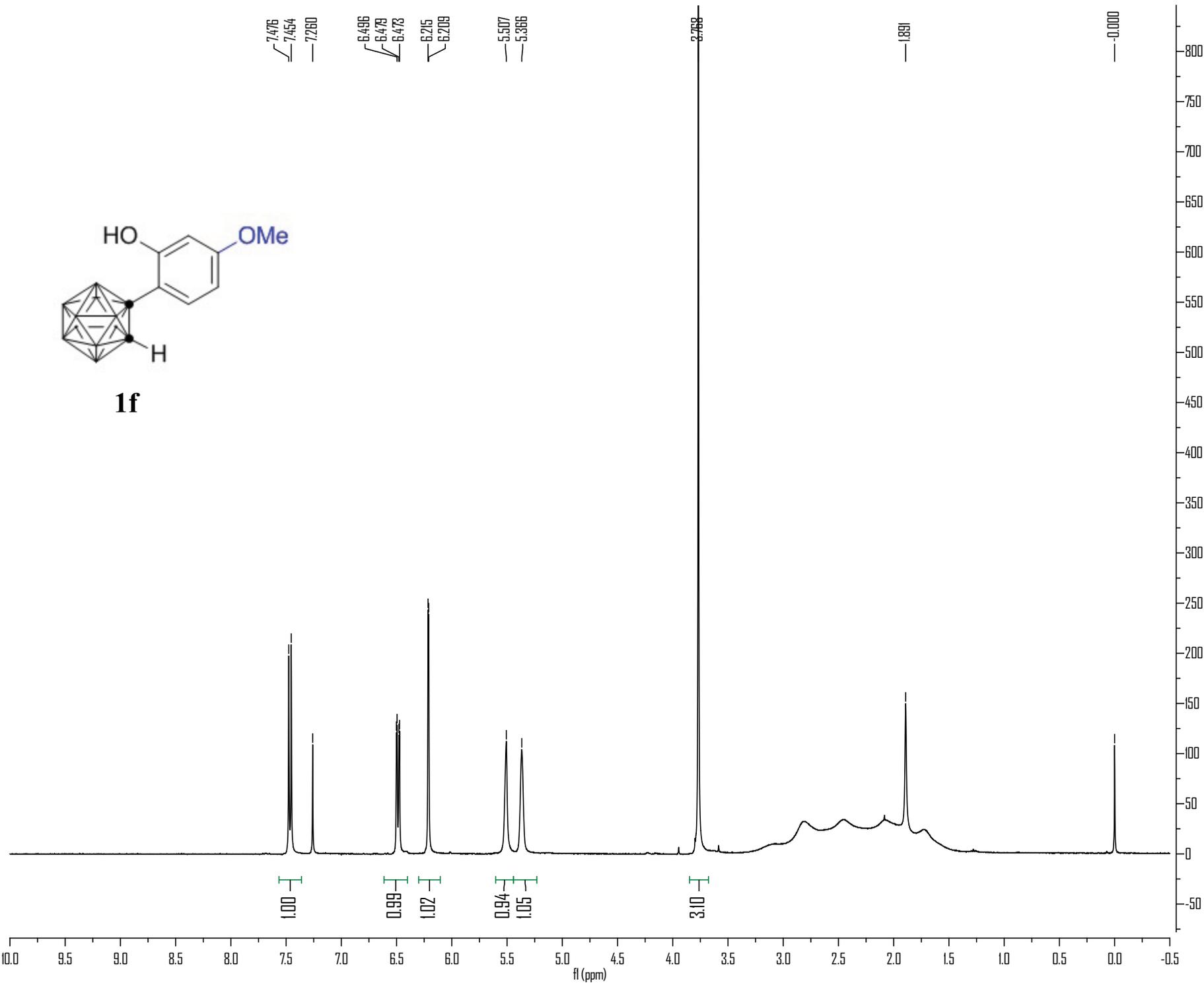
1e



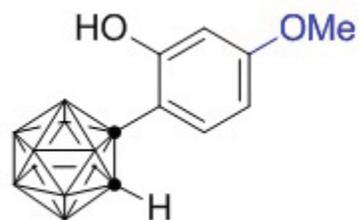
Parameter	Value
Data file Name	C:/Users/cwichunxia/Desktop/原料数据/7-6-1/bccx-7-6-1/pdata/1/1r
Title	7-6-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	32
Receiver Gain	181
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-10-13T17:03:05
Modification Date	2016-10-13T11:03:00
Spectrometer Frequency	128.38
Spectral Width	32051.3



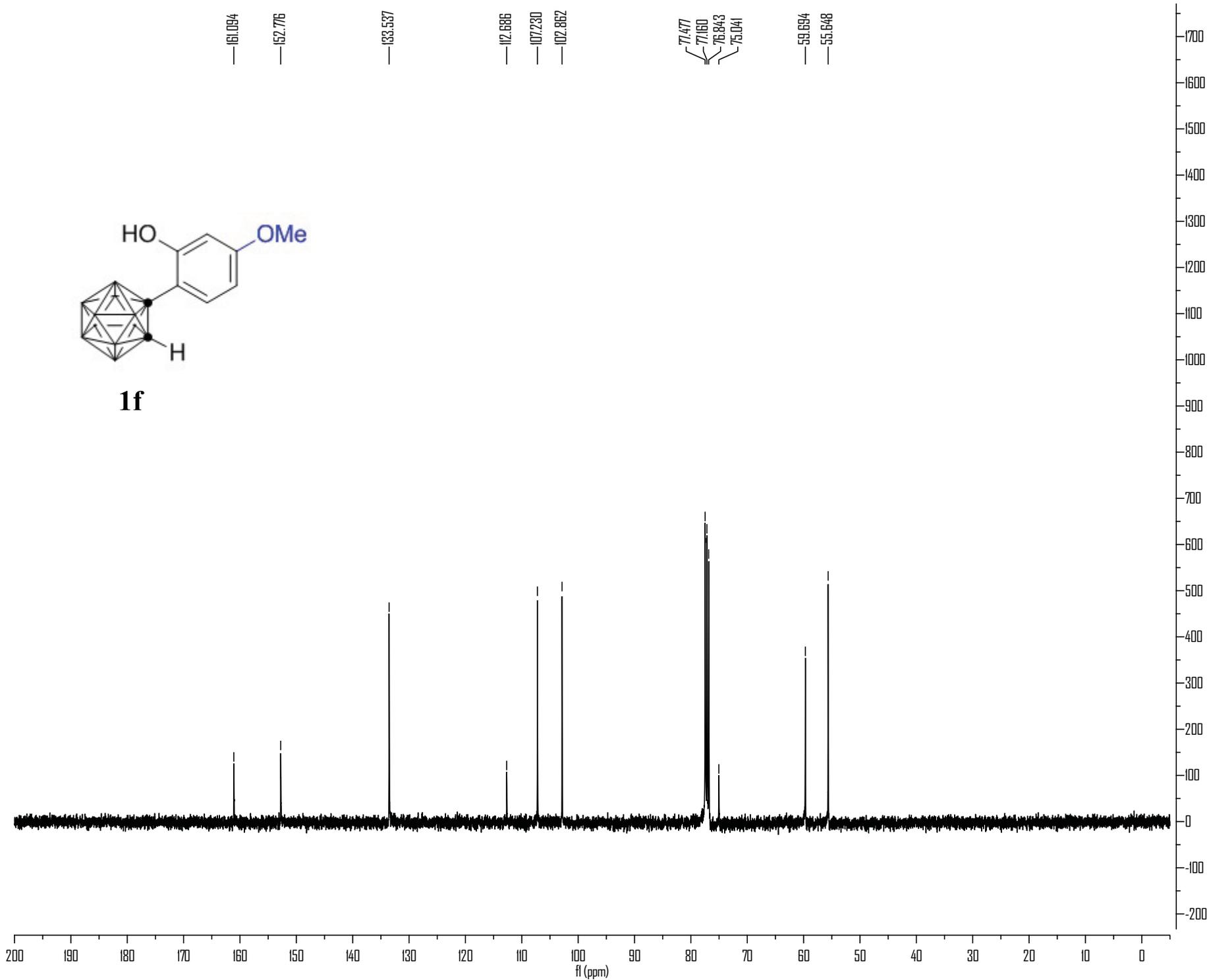
1f



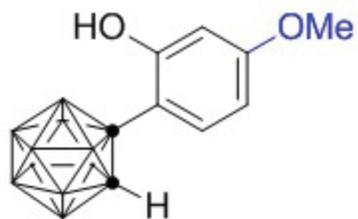
Parameter	Value
Title	ccx-7-8-1
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	
Solvent	CDCl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	44
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-10-21T09:37:29
Modification Date	2016-10-21T01:38:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-793.9
Nucleus	1H
Acquired Size	21552
Spectral Size	65536



1f

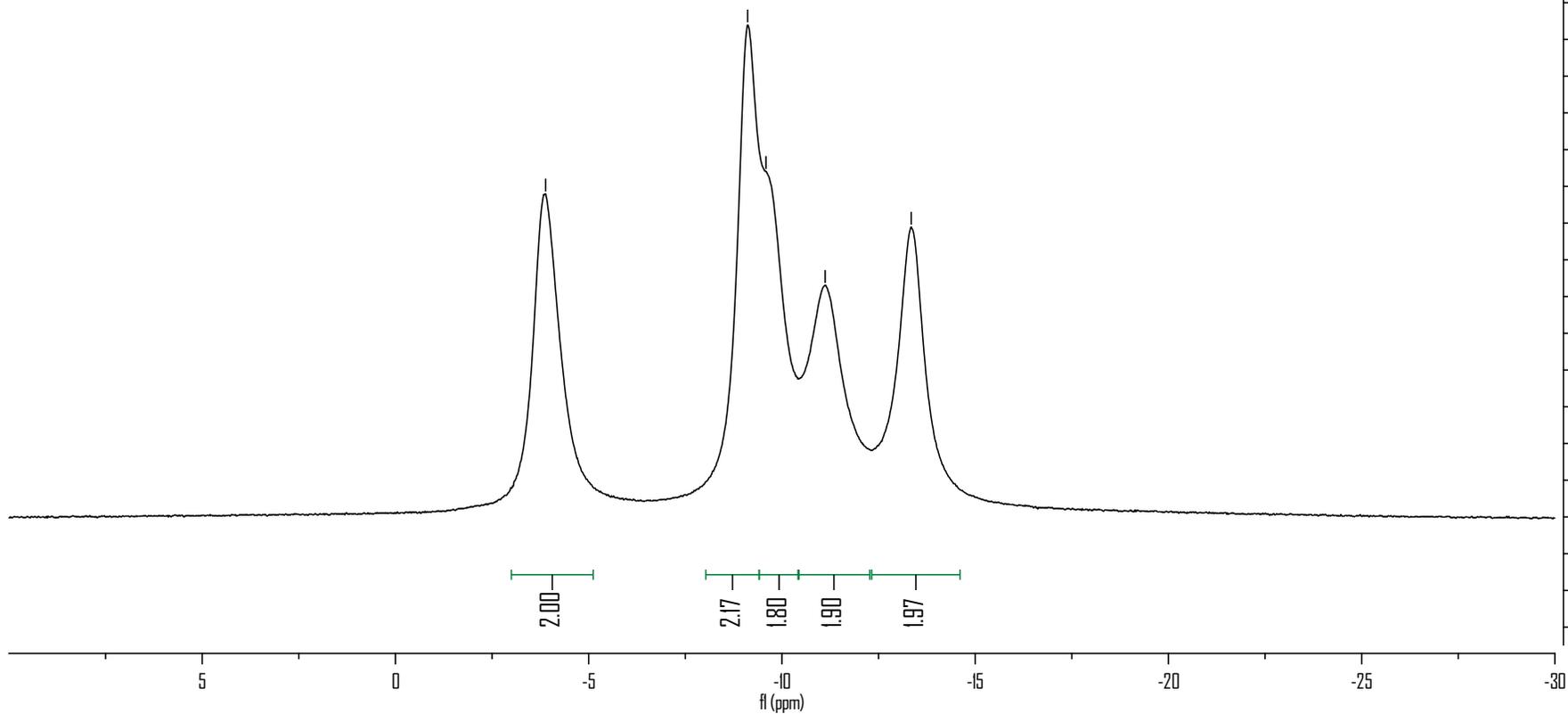


Parameter	Value
Title	-CCX-7-8-1C
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	stu
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	400
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-10-21T10:57:26
Modification Date	2016-10-21T11:19:00
Spectrometer	100.51
Frequency	
Spectral Width	25510.2
Lowest Frequency	-1683.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



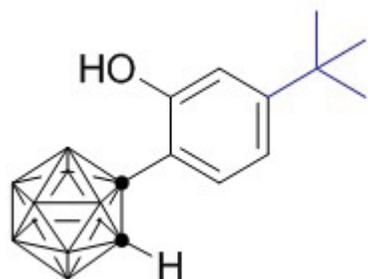
1f

3.886
9.112
9.587
11.118
13.345



S42

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/7-8-1/ b-ccx-7-8-1/ pdata/1/ 1r
Title	7-8-1
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	128
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2016-10-21T21:22:52
Modification Date	2016-10-21T15:22:00
Spectrometer	128.38
Frequency	
Spectral Width	32051.3
Lowest Frequency	-16419.8
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



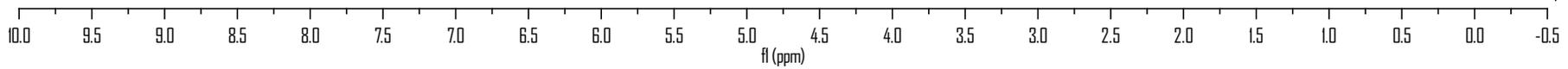
1g

7.477
7.455
7.260
6.942
6.653

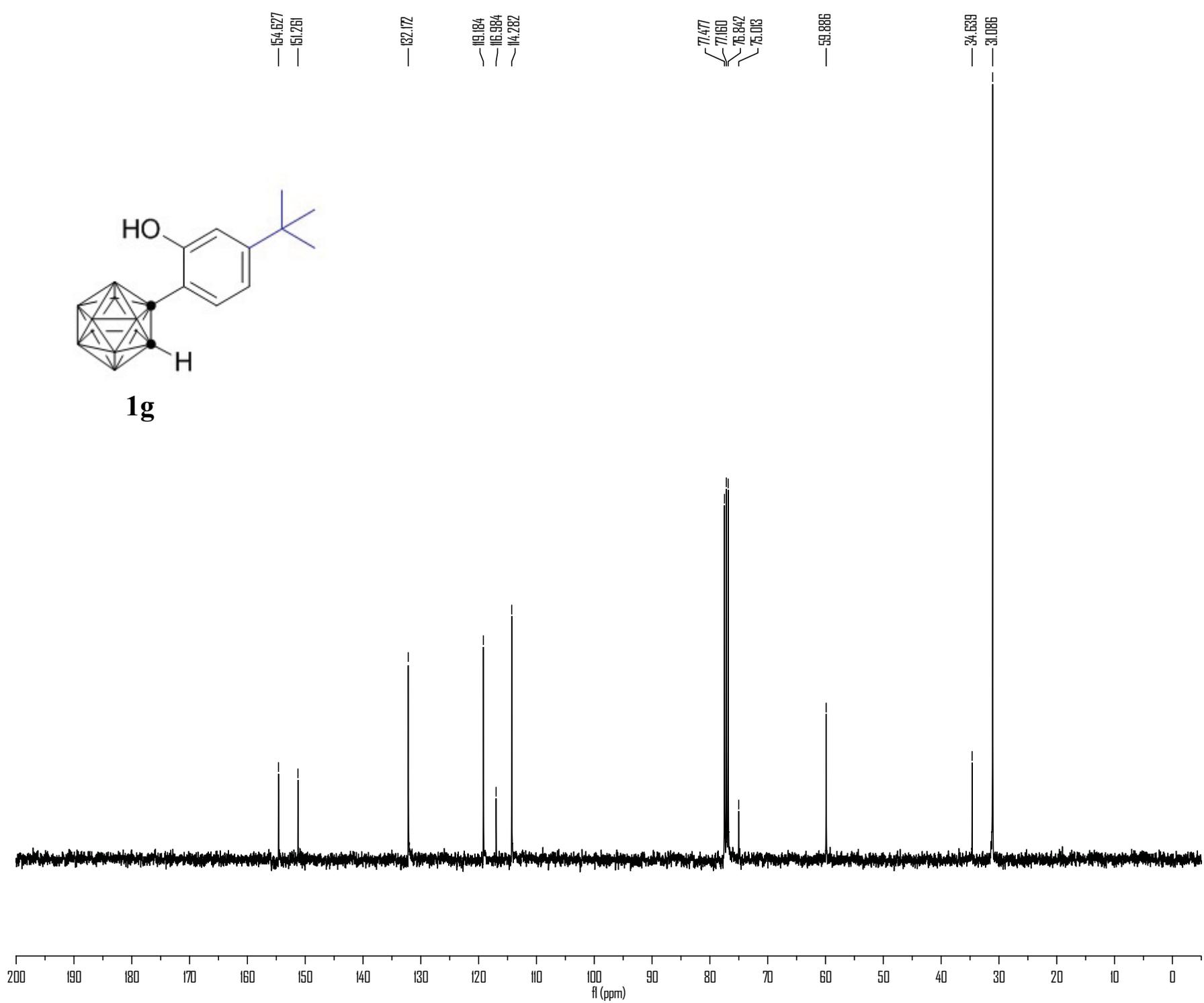
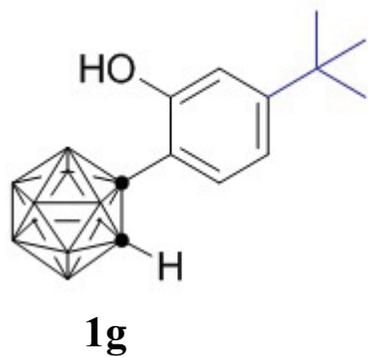
5.412
5.002

1.272

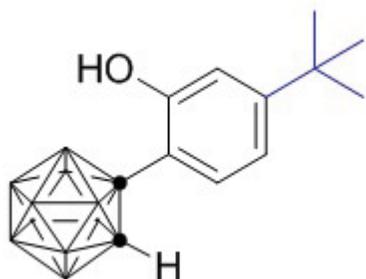
0.001



Parameter	Value
Title	ccx-7-68-1
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse	s2pul
Sequence	
Number of Scans	8
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-03-03T13:32:04
Modification Date	2017-03-03T05:32:00
Spectrometer Frequency	400.03
Spectral Width	7225.4
Lowest Frequency	-804.5
Nucleus	1H
Acquired Size	21676
Spectral Size	65536



Parameter	Value
Title	cc-cx-6-36-1-cc
Comment	STA NDA RD PROTON PARA METERSga
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	nmr1
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	172
Receiver Gain	30
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-04-13T07:40:14
Modification Date	2016-04-12T23:51:00
Spectrometer Frequency	100.51
Spectral Width	25510.2
Lowest Frequency	-1684.9
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



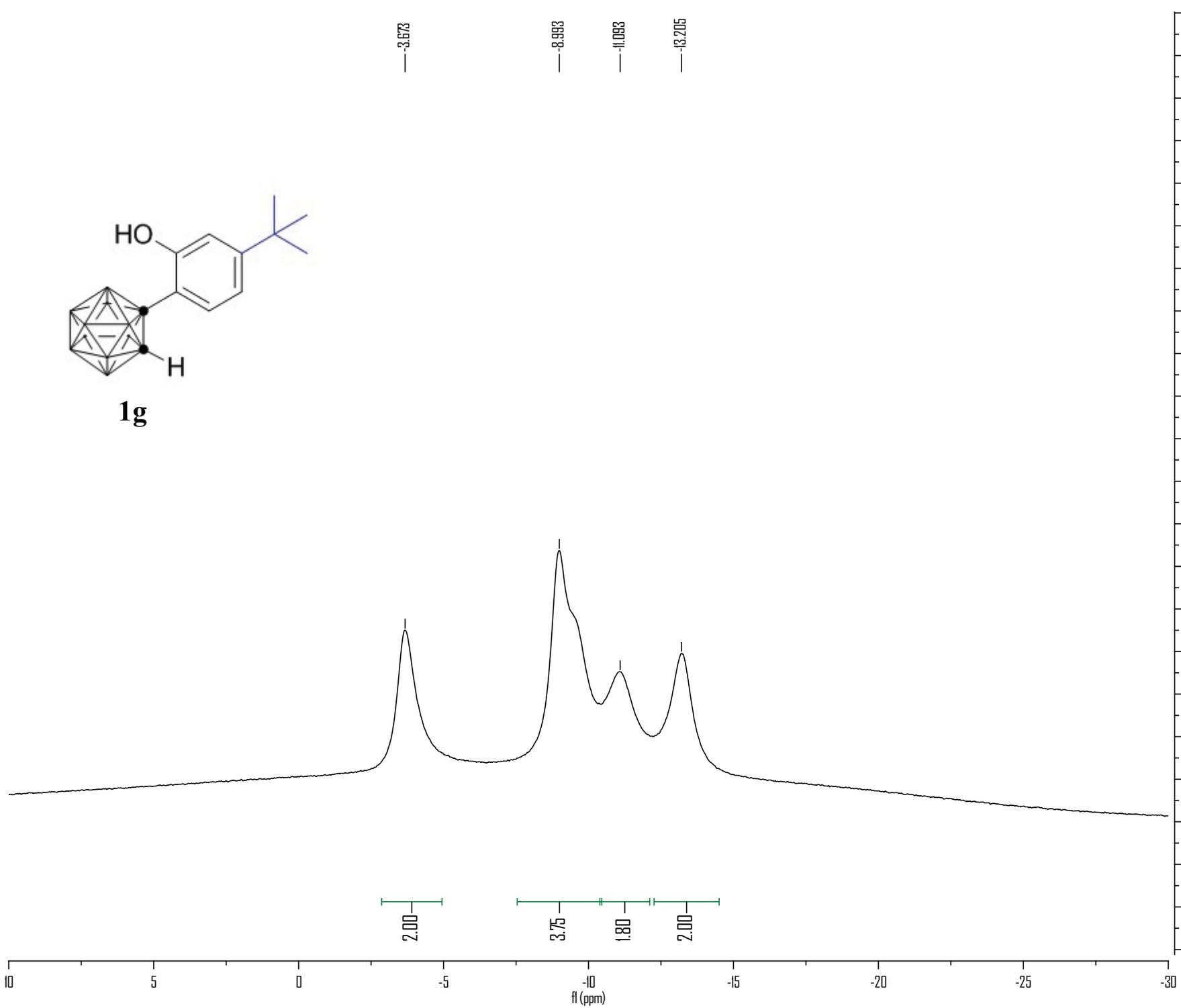
1g

3.673

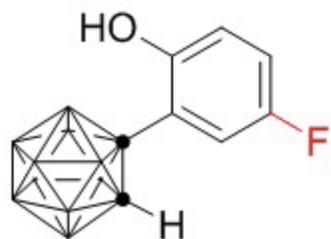
8.993

11.093

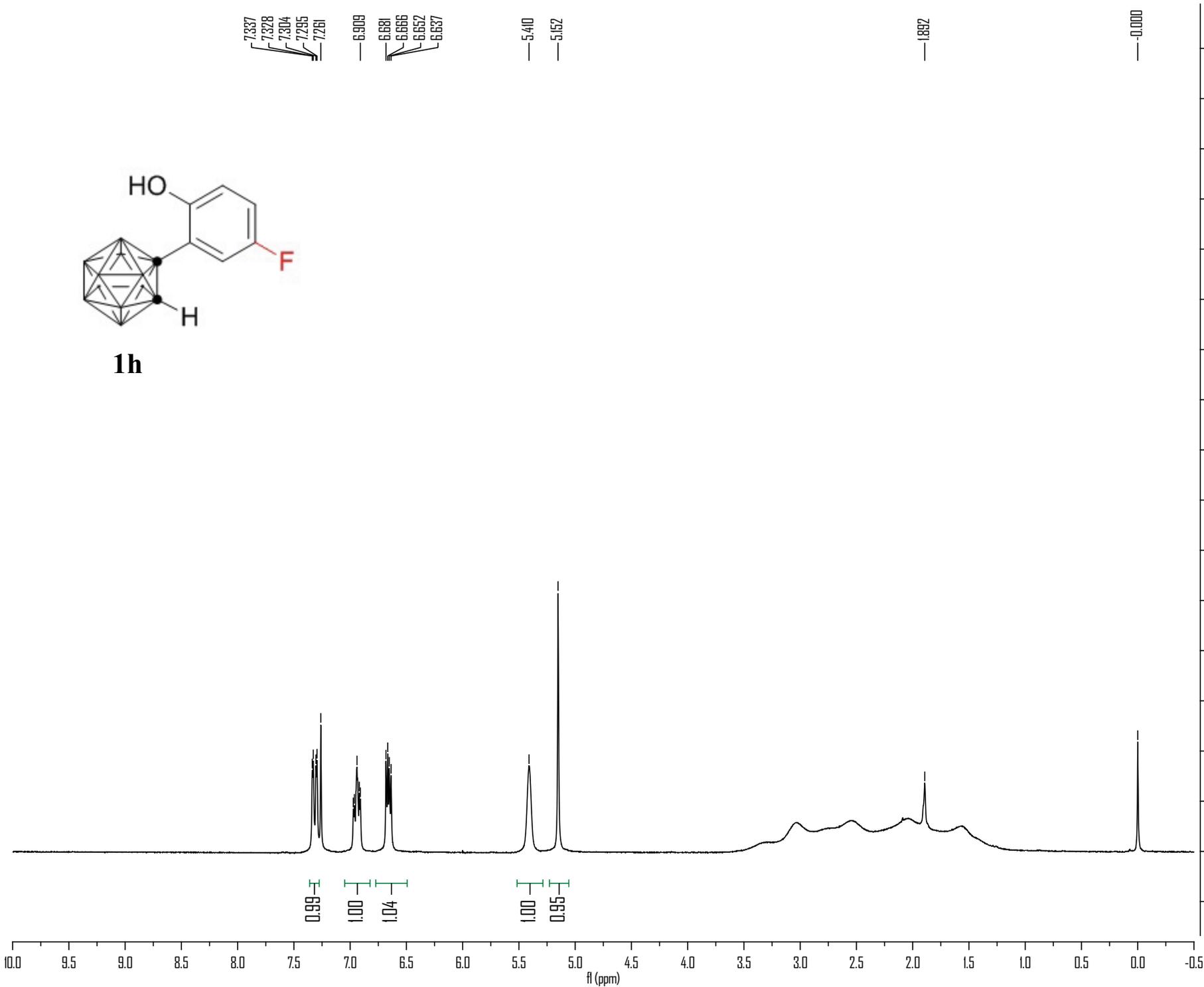
13.205



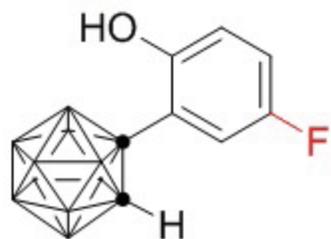
Parameter	Value
Title	b-cx-6-36-1
Comment	STANDARD CARBORANE PARAMETERS
Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	
Solvent	cdcl3
Temperature	19.0
Pulse Sequence	s2pul
Number of Scans	128
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2583
Acquisition Date	2016-04-14T10:34:51
Modification Date	2016-04-14T02:35:00
Spectrometer	128.23
Frequency	
Spectral Width	26041.7
Lowest Frequency	-13541.5
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



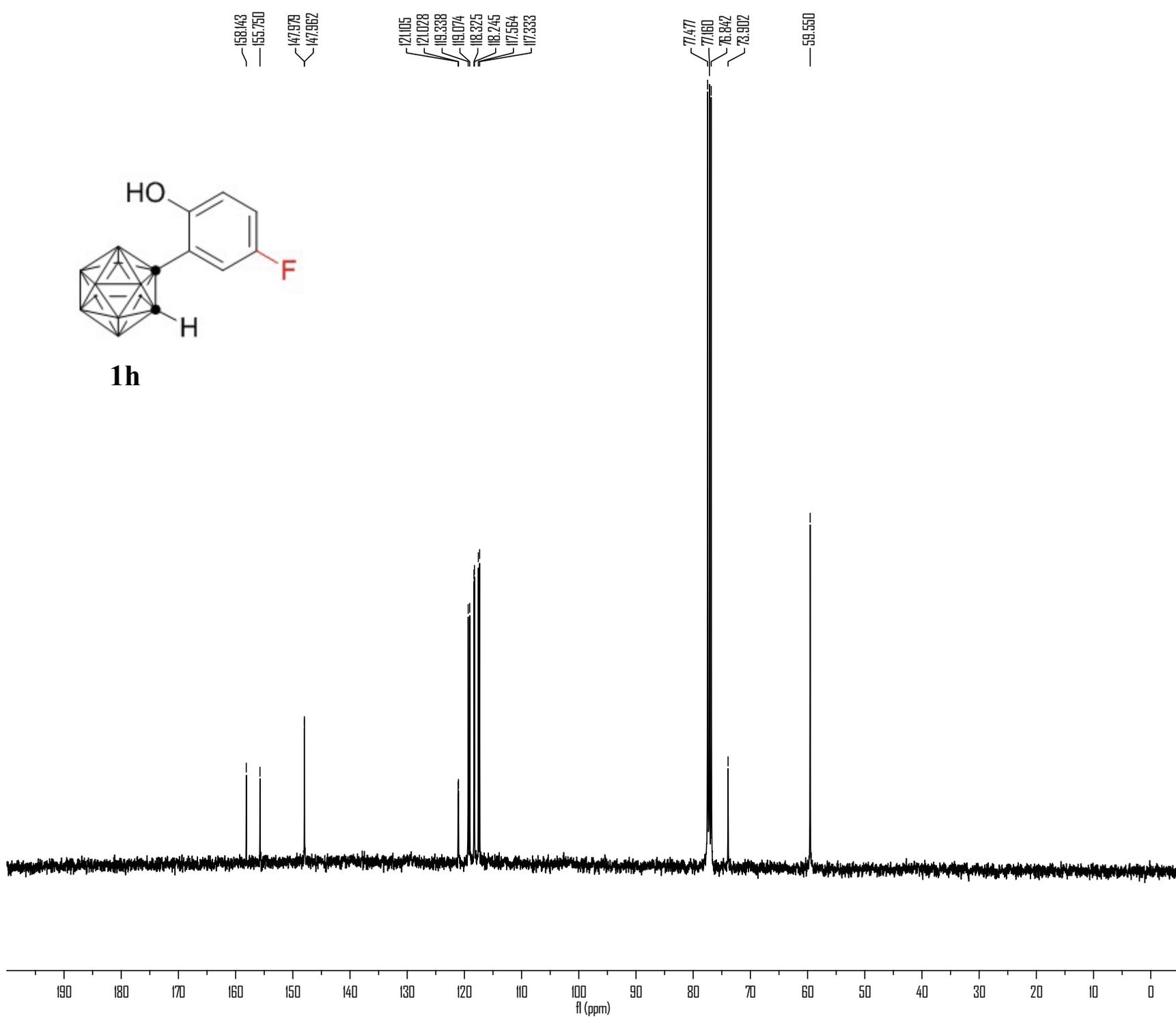
1h



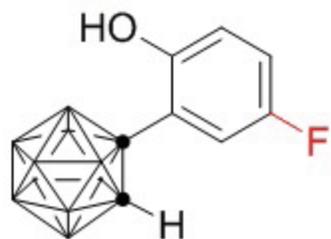
Parameter	Value
Title	ccx-6-15-2H_07Mar2016
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	mercury
Author	
Solvent	CDCl3
Temperature	3.0
Pulse Sequence	s2pul
Number of Scans	32
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.9971
Acquisition Date	1969-11-13T16:23:44
Modification Date	2016-03-07T14:34:00
Spectrometer Frequency	300.04
Spectral Width	4803.1
Lowest Frequency	-600.7
Nucleus	1H
Acquired Size	9592
Spectral Size	32768



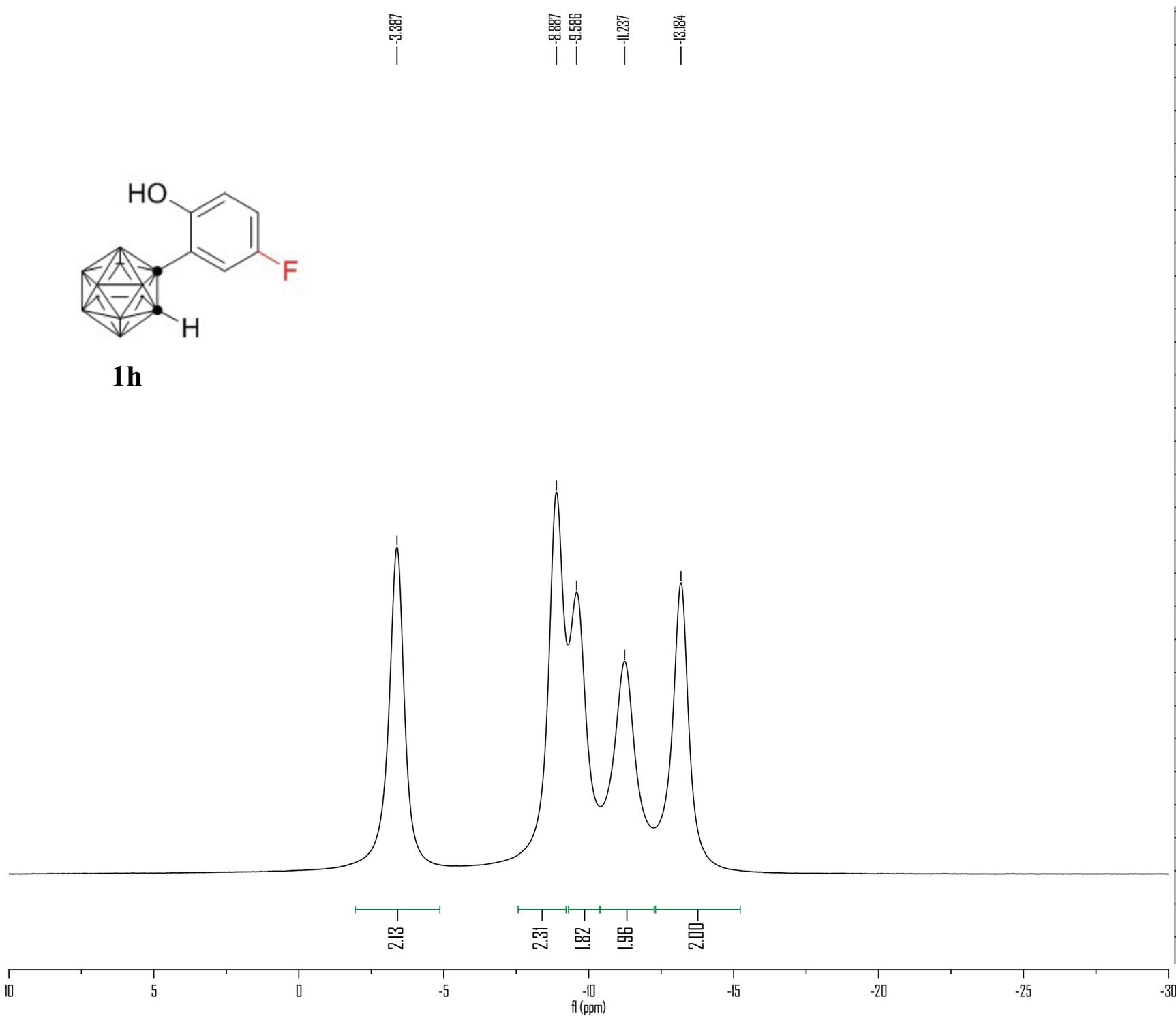
1h



Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/6-15-1/2012060c-ccx-6-15-2/3/pdata/1/1r
Title	2012060c-ccx-6-15-2
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgdc
Number of Scans	438
Receiver Gain	16384
Relaxation Delay	3.0000
Pulse Width	4.0000
Acquisition Time	0.4653
Acquisition Date	2016-03-08T15:21:43
Modification Date	2016-03-08T09:56:56
Spectrometer Frequency	100.61
Spectral Width	35211.3
Lowest Frequency	-6979.7
Nucleus	13C
Acquired Size	16384
Spectral Size	65536

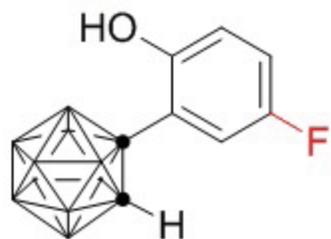


1h

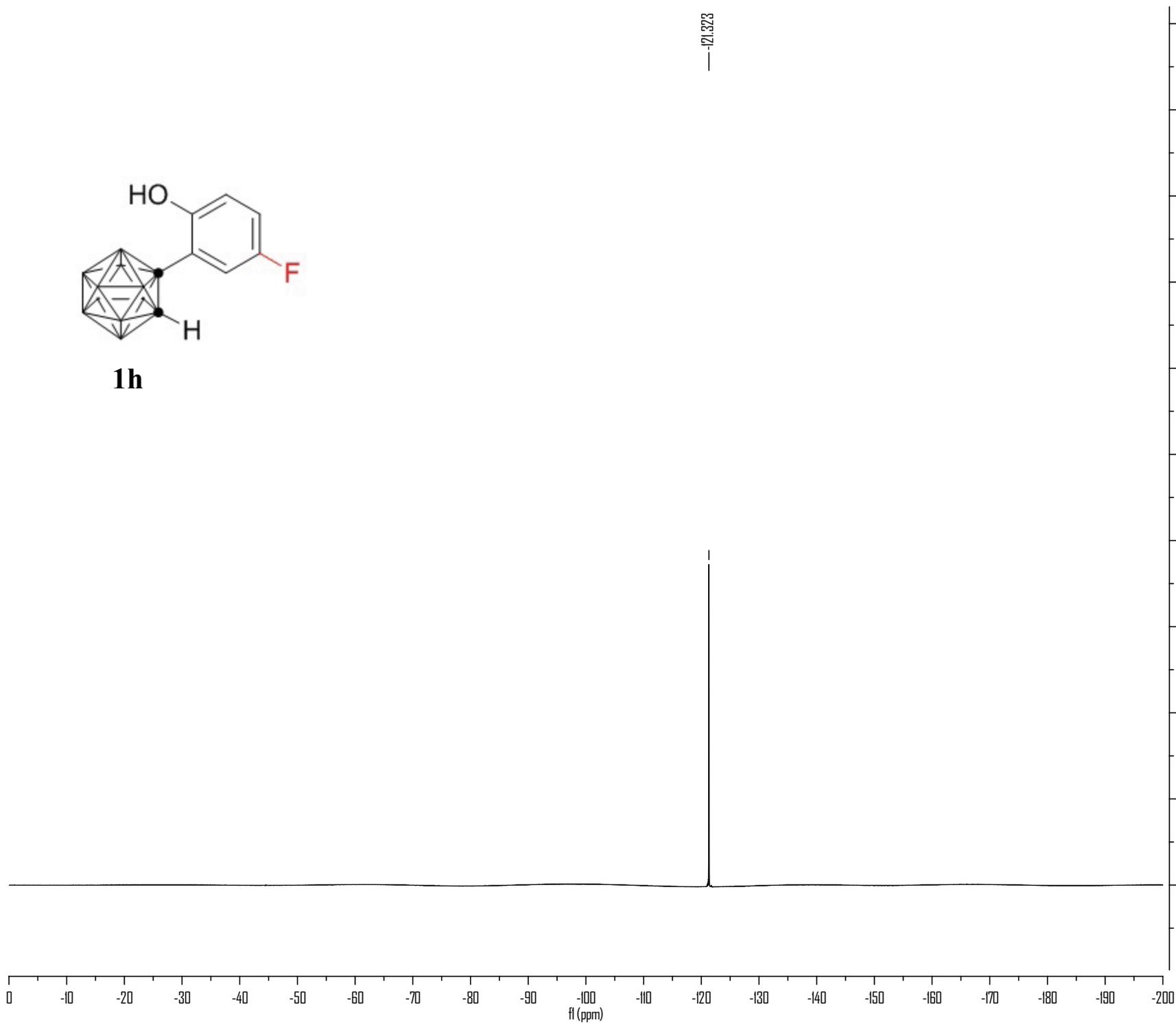


S48

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/6-15-1/2012060b-ccx-6-15-2/1/pdata/1/1r
Title	2012060b-ccx-6-15-2
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	128
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	8.5000
Acquisition Time	0.512
Acquisition Date	2016-03-08 15:54:49
Modification Date	2016-03-08 09:56:50
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16415.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



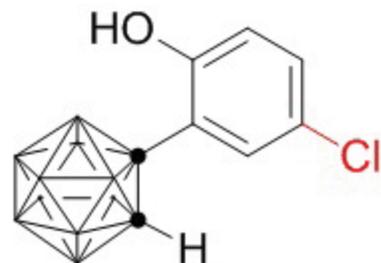
1h



-121.323

S49

Parameter	Value
Title	f-cxx-6-15-2
Comment	H autocalibration done on Dec 13, 2013 pwx calibrated as 12.0 at pwxlvl 61 H pwxlvl compression factor calibrated as 0.922
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	vnmr1
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	28
Receiver Gain	10
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	0.1049
Acquisition Date	2016-03-08T11:22:39
Modification Date	2016-03-08T03:23:00
Spectrometer Frequency	376.03
Spectral Width	156250.0
Lowest Frequency	-114960.6
Nucleus	19F
Acquired Size	16384
Spectral Size	32768



1i

7.557
7.280
7.171
6.660
6.639

5.368
5.241

1.814

0.002

1.00

0.98

1.03

1.07

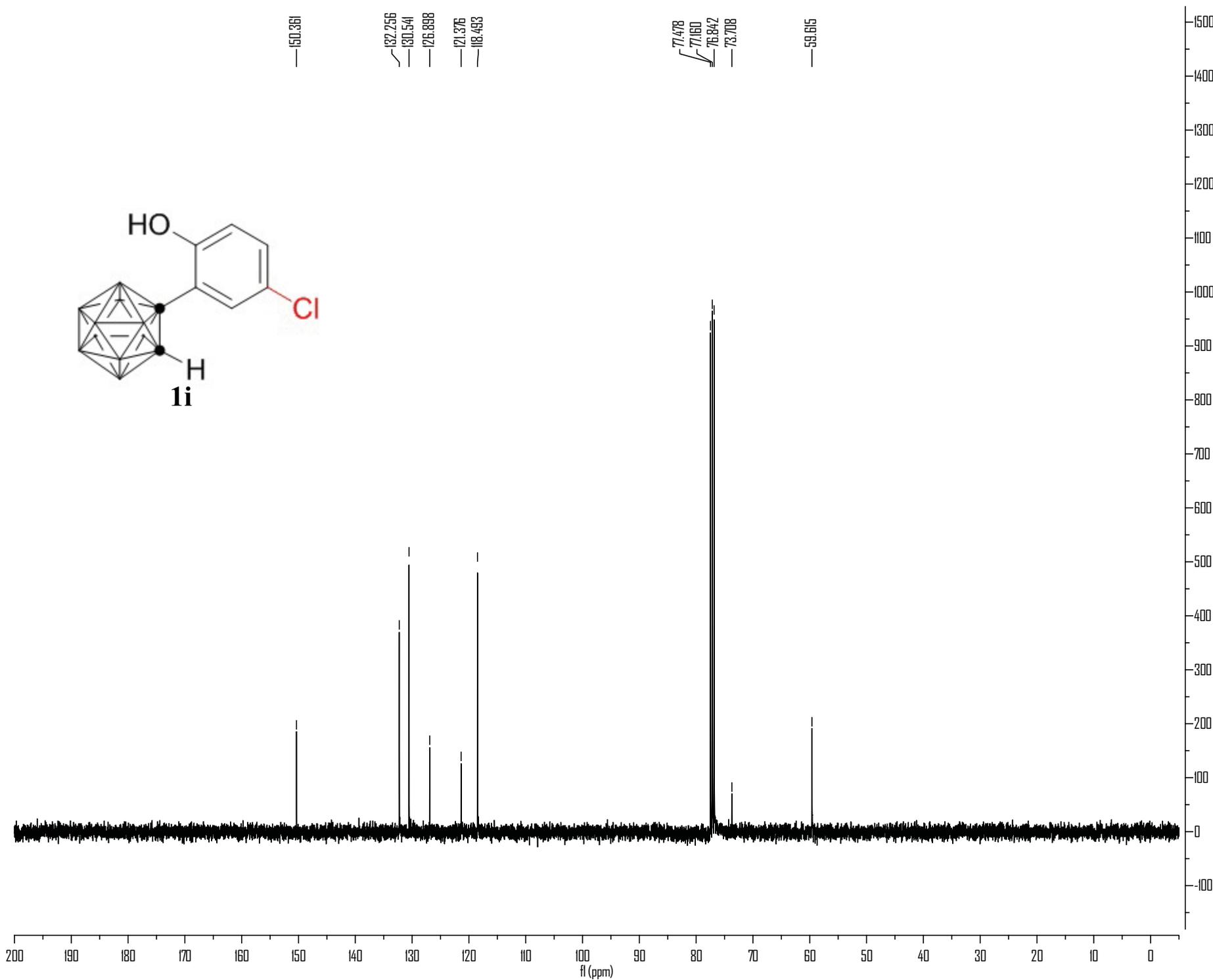
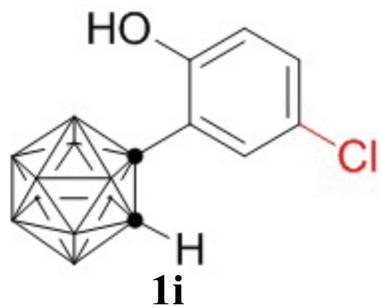
1.12

10.0 9.5 9.0 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

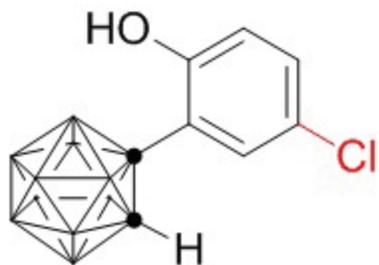
fl (ppm)

S50

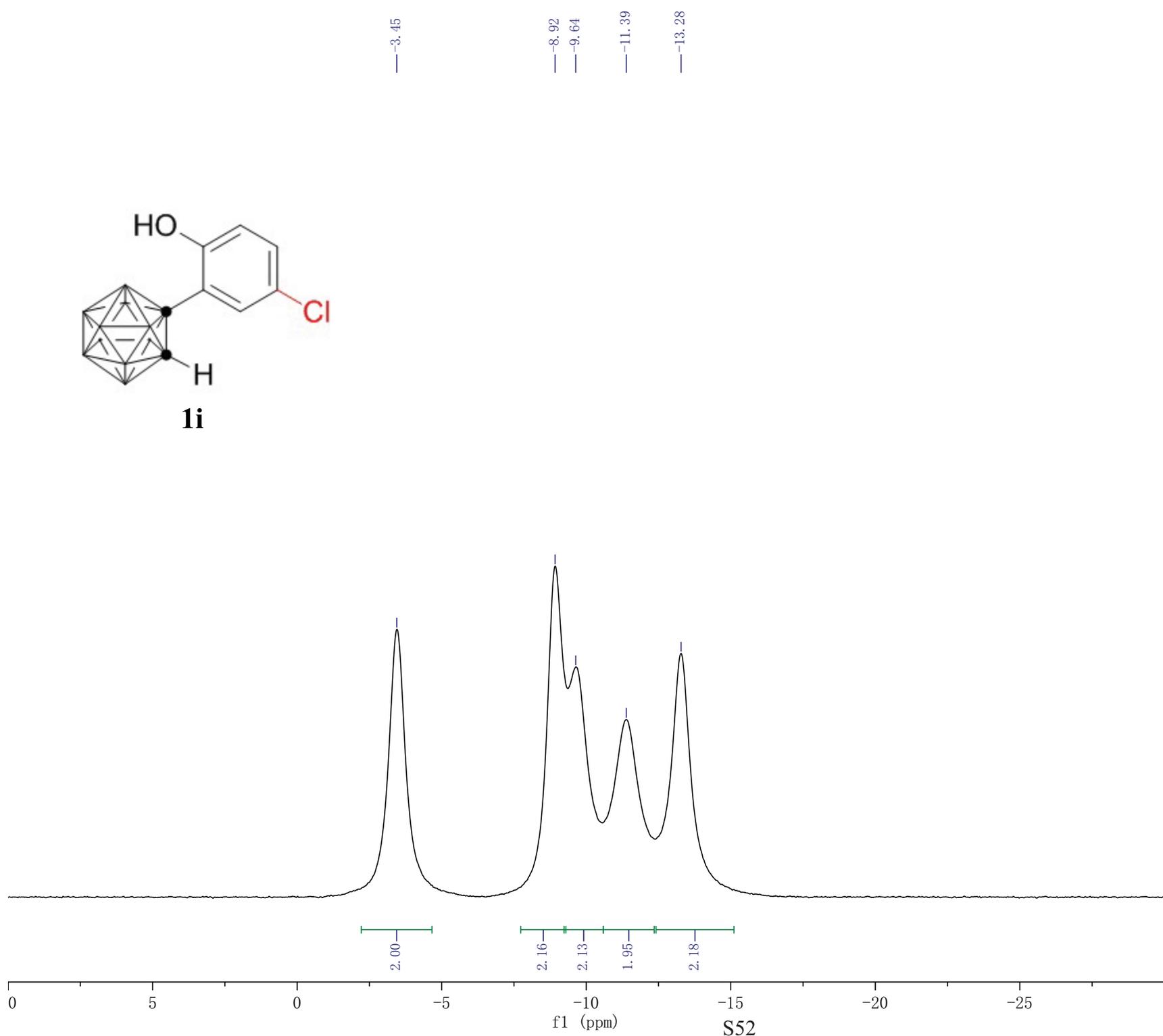
Parameter	Value
Title	ccx-7-47-1
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	vnmr-s
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-03-03T13:23:55
Modification Date	2017-03-03T05:24:00
Spectrometer Frequency	400.03
Spectral Width	7225.4
Lowest Frequency	-804.5
Nucleus	¹ H
Acquired Size	21676
Spectral Size	65536



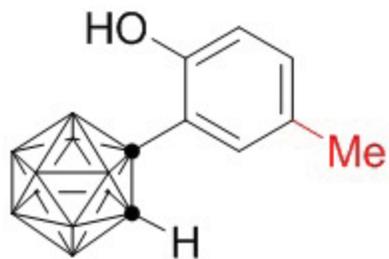
Parameter	Value
Title	ccx-6-43-4C
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	omcl
Solvent	cdcl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	244
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3000
Acquisition Date	2016-08-29T13:04:09
Modification Date	2016-08-29T05:14:00
Spectrometer Frequency	100.52
Spectral Width	25000.0
Lowest Frequency	-1429.4
Nucleus	¹³ C



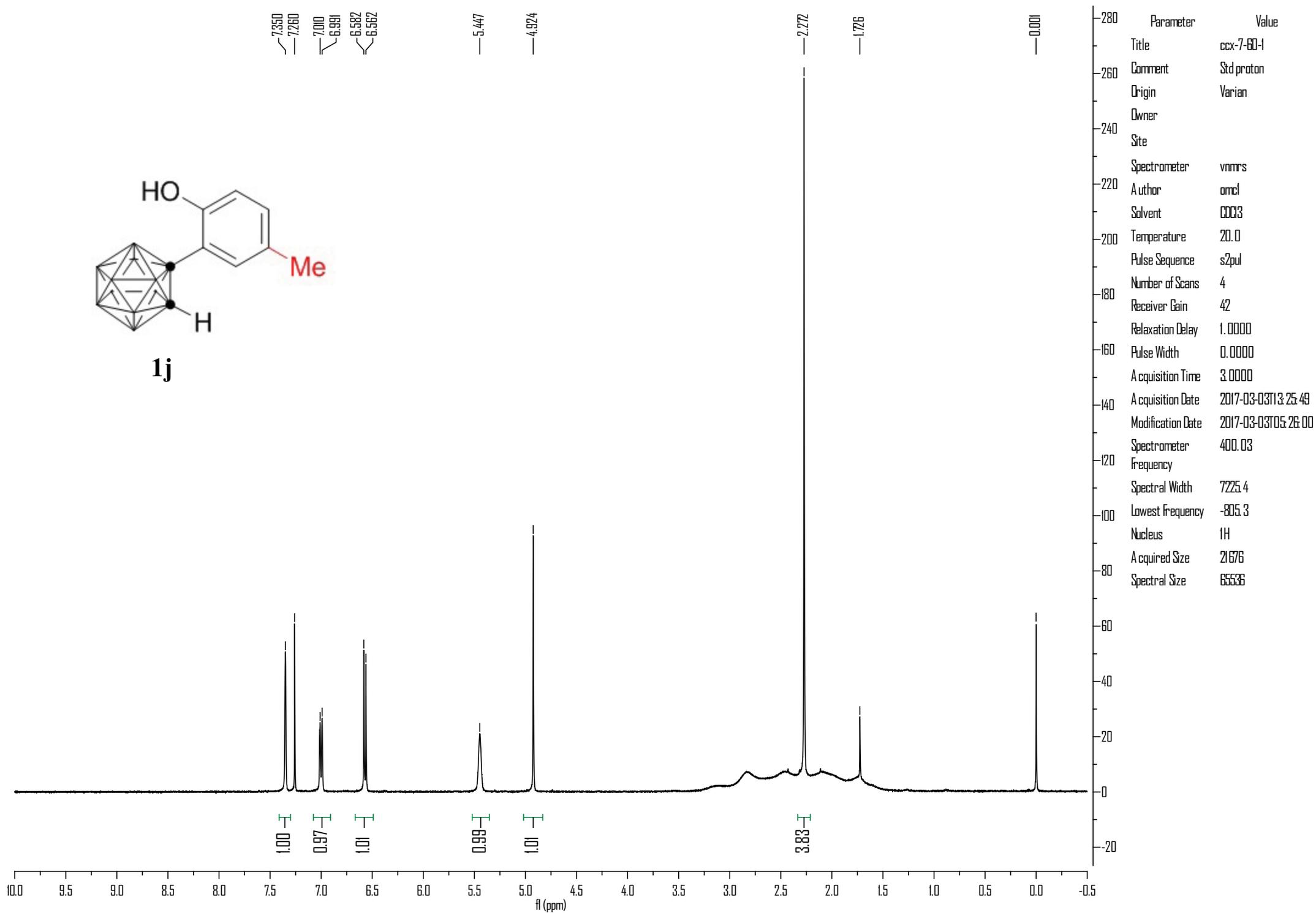
1i



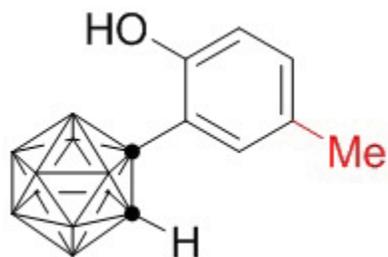
Parameter	Value
Data File Name	H / 2013156b-ccx-6-43-1.fid/ fid
Title	2013156b-ccx-6-43-1
Comment	STANDARD CARBON PARAMETERS
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	vnmr1
Solvent	cdcl3
Temperature	19.0
Pulse Sequence	s2pul
Experiment	10
Number of Scans	256
Receiver Gain	30
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	0.5000
Acquisition Date	2016-04-18 10:28:36
Modification Date	2016-04-18 10:30:00
Spectrometer Frequency	128.23
Spectral Width	26041.7
Lowest Frequency	-13020.9
Nucleus	11B
Acquired Size	13021
Spectral Size	32768



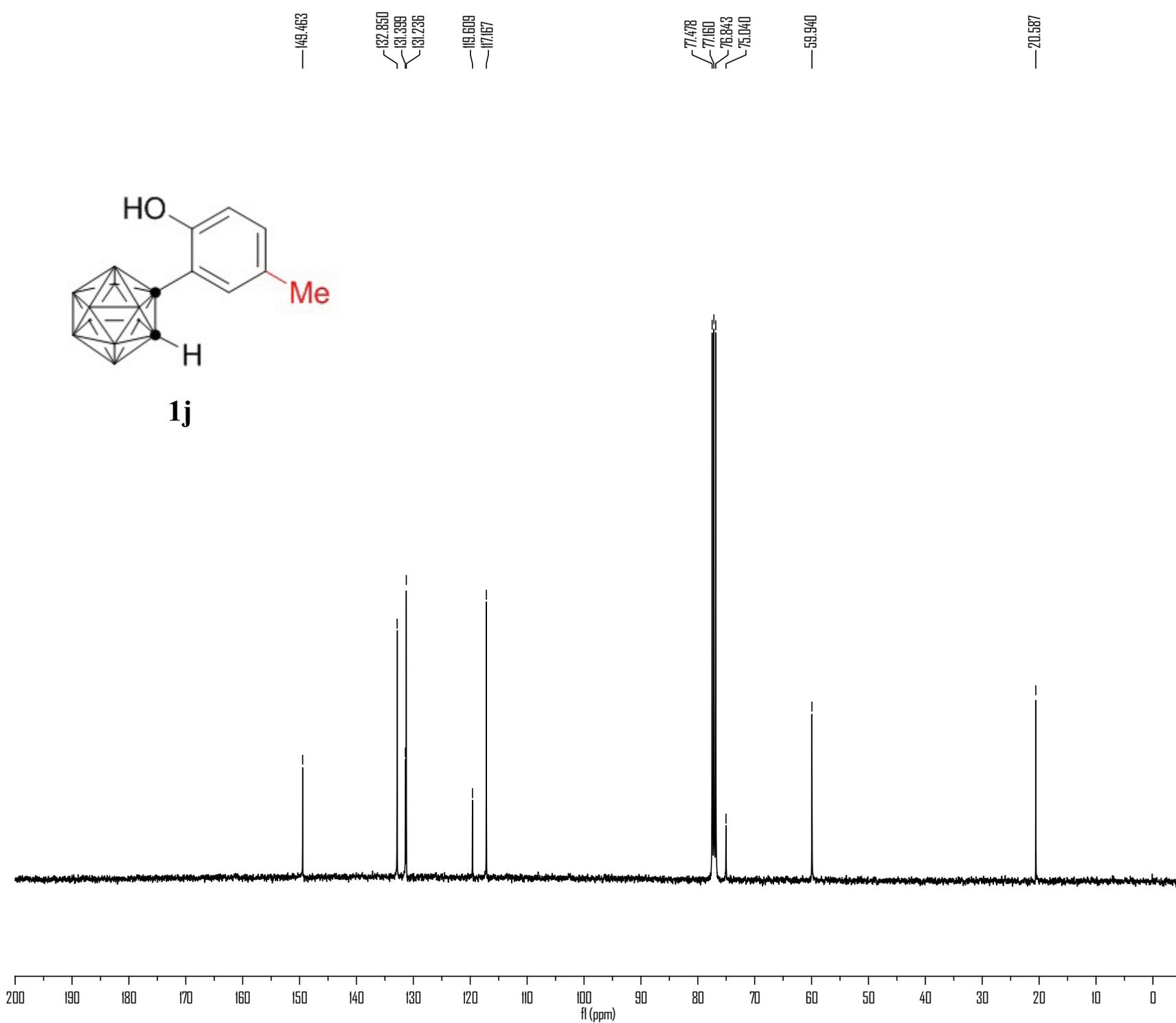
1j



Parameter	Value
Title	ccx-7-60-1
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	4
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-03-03T13:25:49
Modification Date	2017-03-03T05:26:00
Spectrometer Frequency	400.03
Spectral Width	7225.4
Lowest Frequency	-805.3
Nucleus	1H
Acquired Size	21676
Spectral Size	65536



1j



149.463

132.850

131.339

131.236

119.609

117.167

77.478

77.160

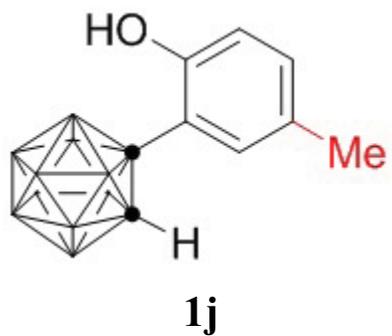
76.843

75.040

59.940

20.587

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/6-25-1/cc-cx-6-25-1/pdata/1/1r
Title	6-25-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgdc
Number of Scans	647
Receiver Gain	16384
Relaxation Delay	3.0000
Pulse Width	4.0000
Acquisition Time	0.4653
Acquisition Date	2016-03-25T20:24:02
Modification Date	2016-03-25T13:25:00
Spectrometer Frequency	100.61
Spectral Width	35211.3
Lowest Frequency	-6979.0
Nucleus	13C
Acquired Size	16384
Spectral Size	65536



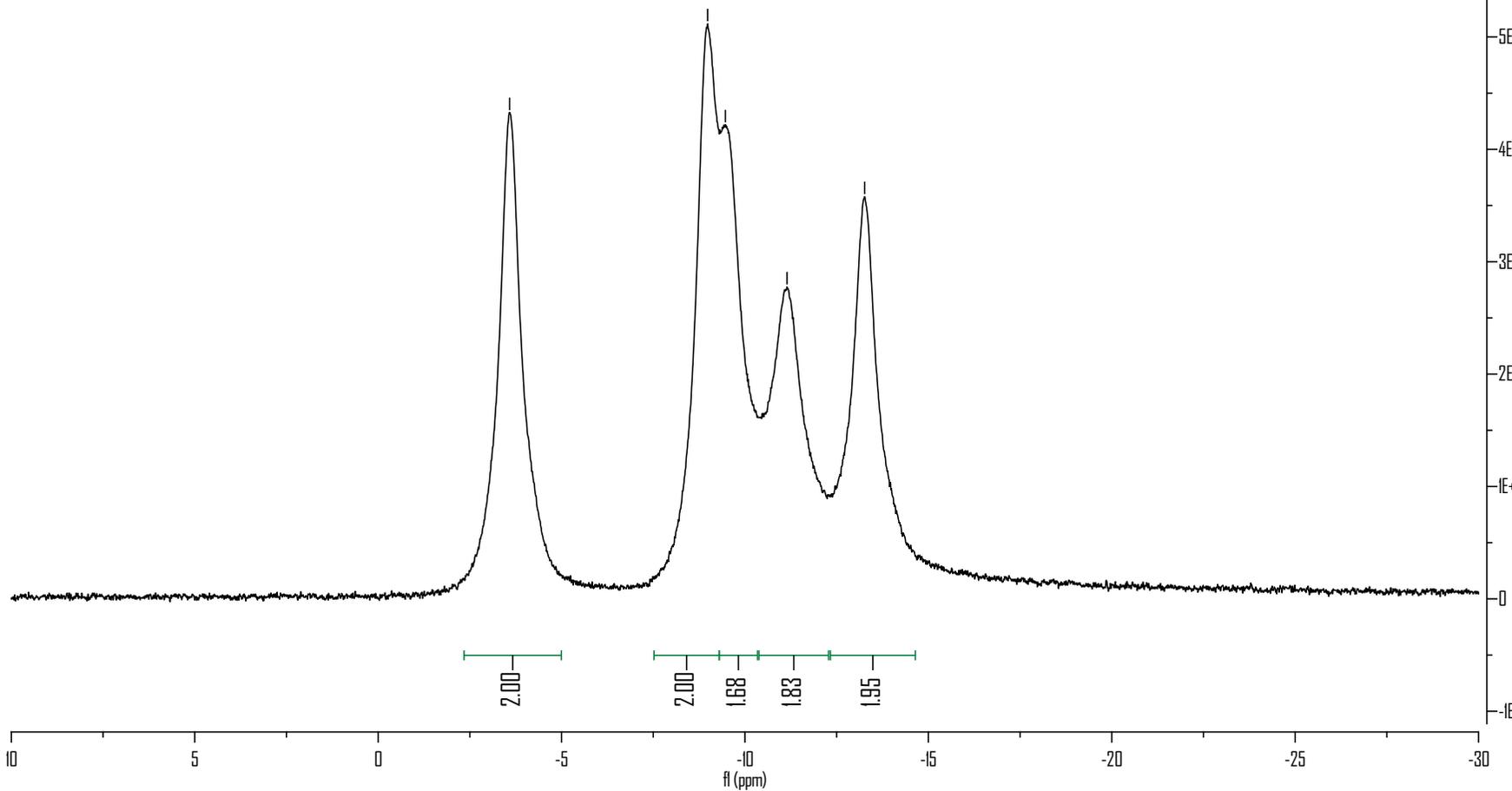
— 3.584

— 8.982

— 9.466

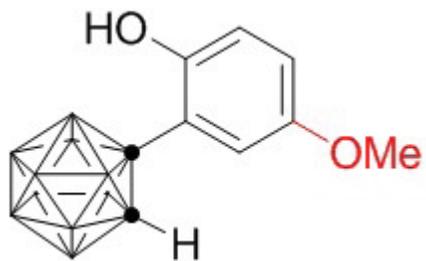
— 11.147

— 13.264

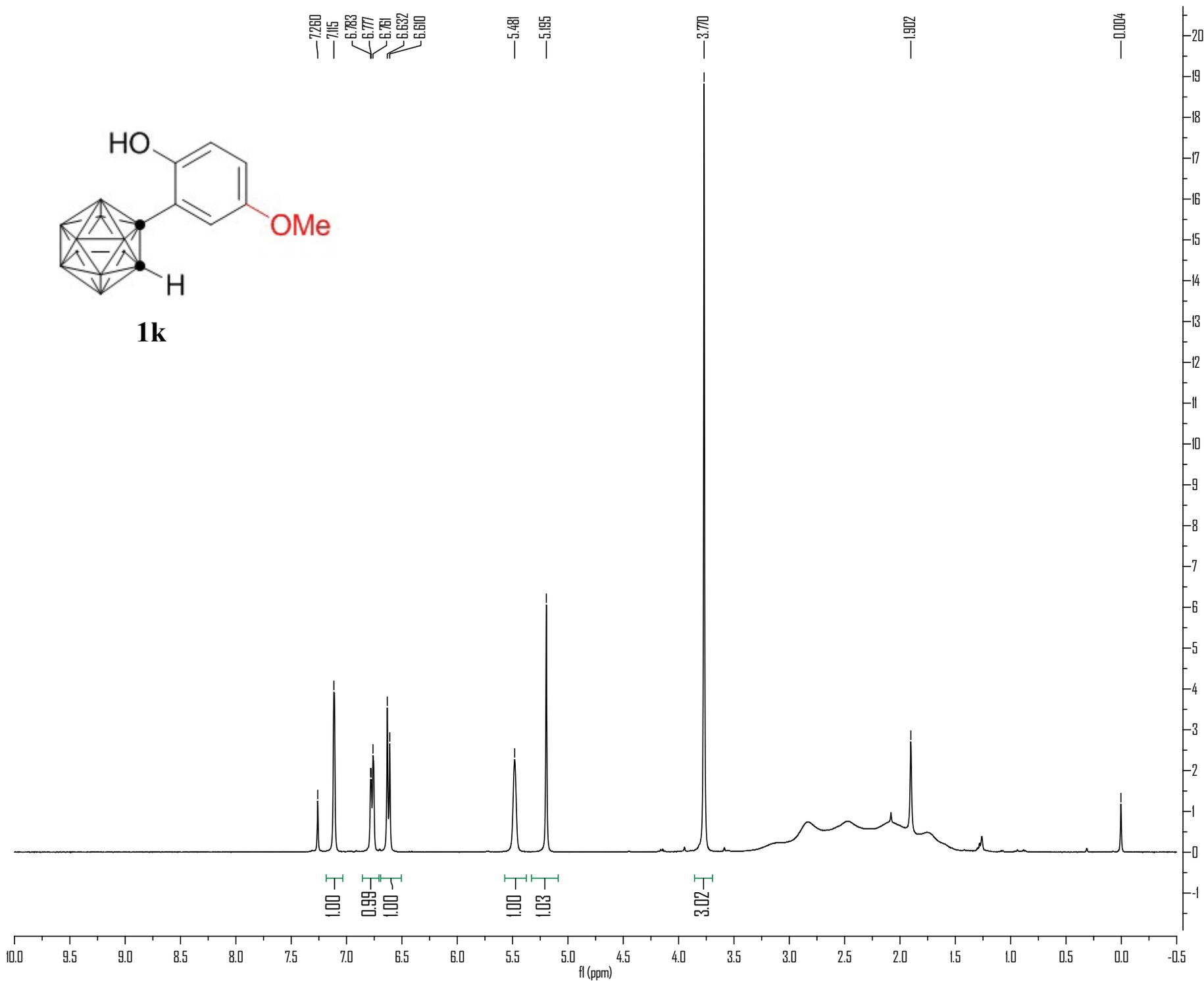


S55

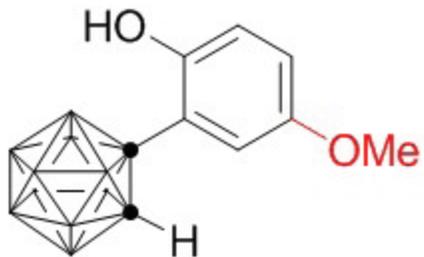
Parameter	Value
Data file Name	G:/Users/cuichunxiao/Desktop/原料数据/6-25-1/b-ccx-6-25-1/pdata/1/1r
Title	6-25-1
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	0003
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	73
Receiver Gain	362
Relaxation Delay	0.0000
Pulse Width	13.4000
Acquisition Time	0.512
Acquisition Date	2016-03-25T22:12:16
Modification Date	2016-03-25T15:12:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16408.1
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



1k



Parameter	Value
Title	H-cvx-6-82-1
Comment	STA NDA RD PROTON PA RA METERS
Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	vnm1
Solvent	cdcl3
Temperature	25.0
Pulse	s2pul
Sequence	
Number of Scans	12
Receiver Gain	10
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.7224
Acquisition Date	2016-07-07T12:06:07
Modification Date	2016-07-07T04:07:00
Spectrometer Frequency	399.68
Spectral Width	8802.8
Lowest Frequency	-797.5
Nucleus	1H
Acquired Size	32768
Scanned Size	88000



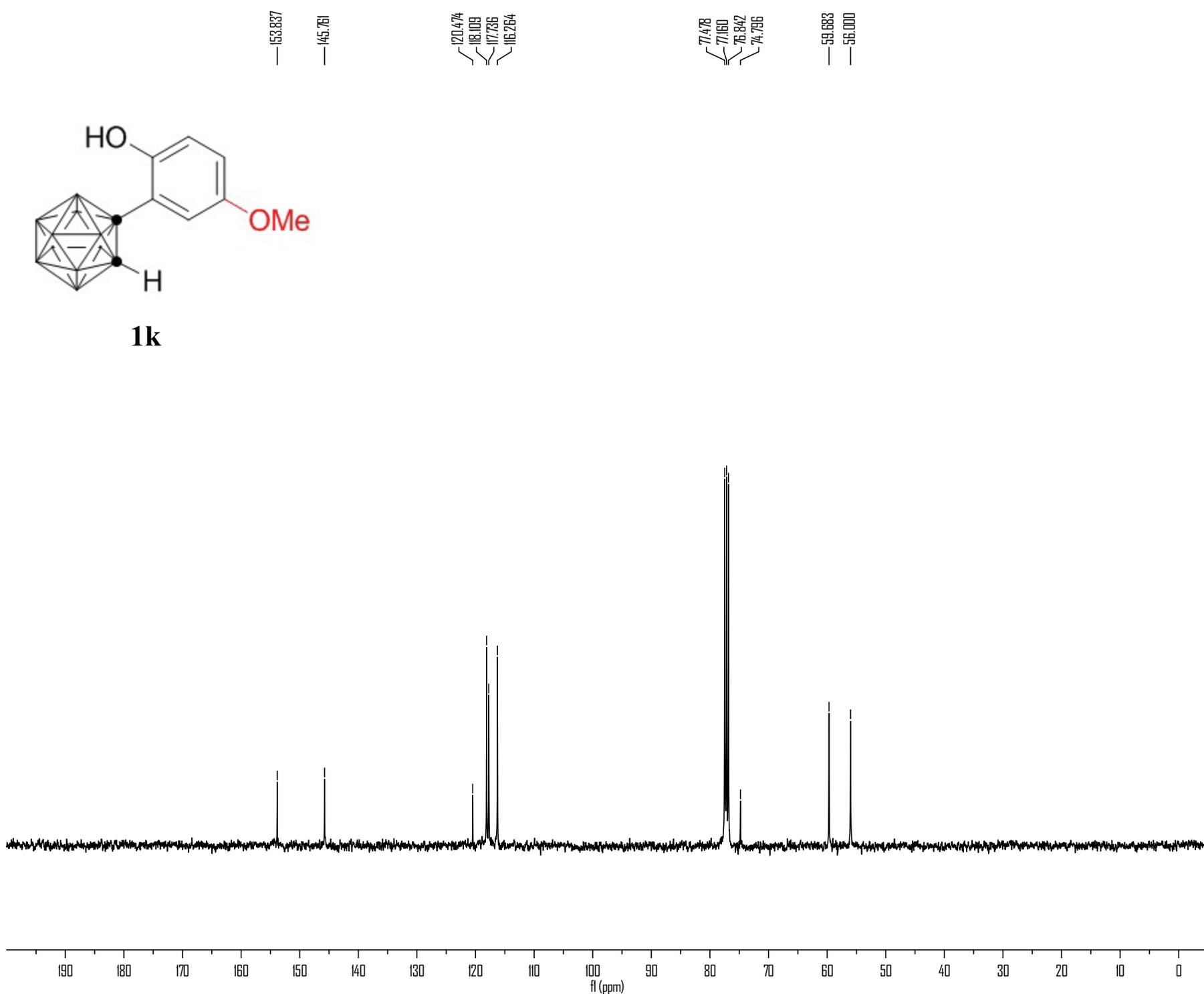
1k

153.837
145.761

120.474
118.109
117.736
116.264

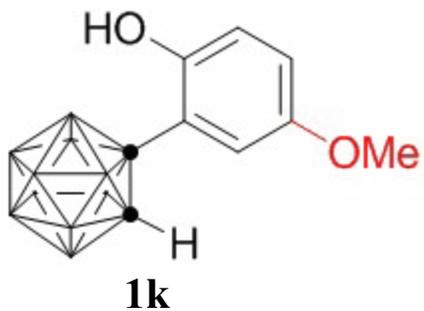
77.478
77.160
76.842
74.796

59.683
56.000

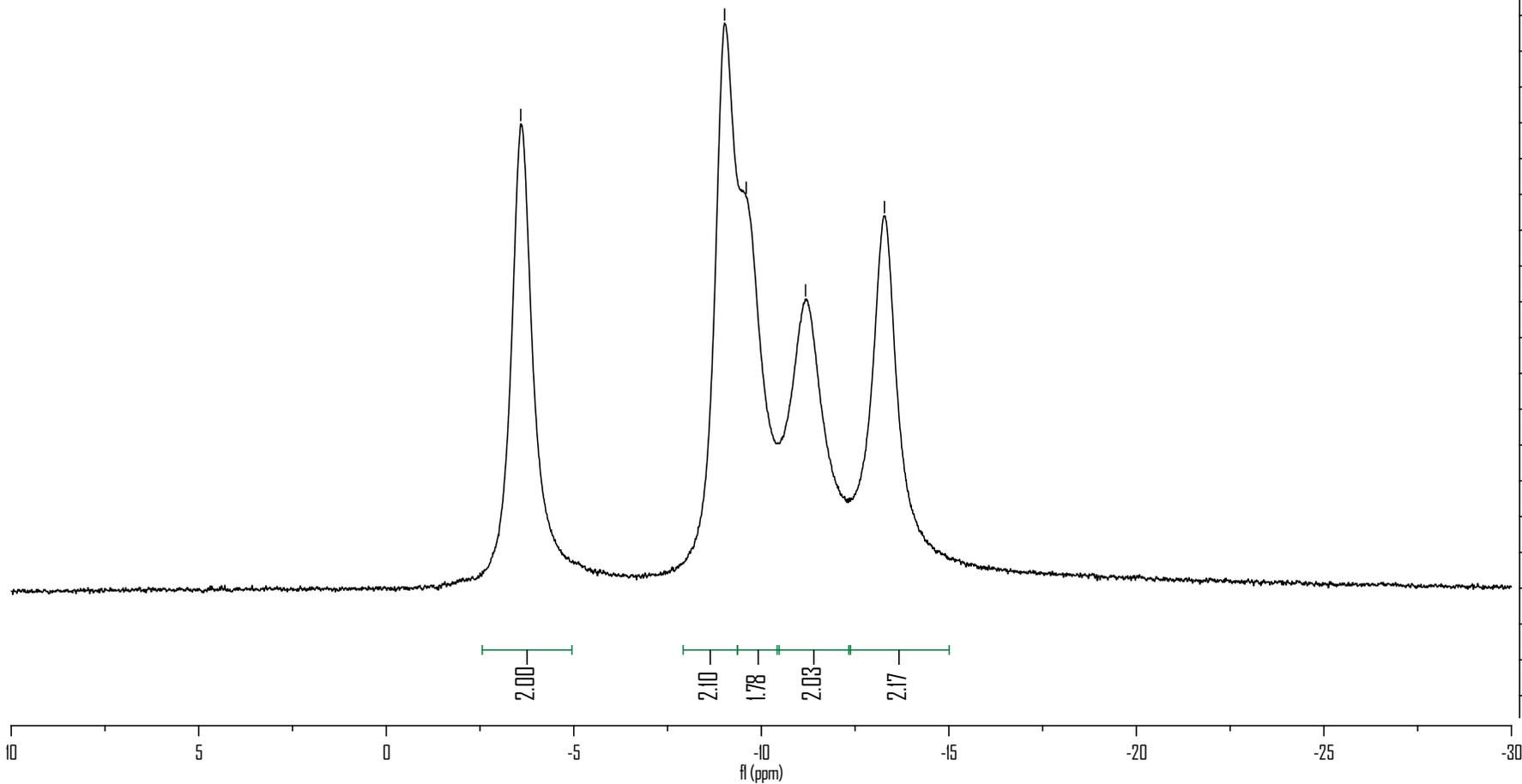


S57

Parameter	Value
Title	C-cxx-6-82-1
Comment	STANDARD CARBON PARAMETERS
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	nmr1
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	228
Receiver Gain	30
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-07-07T11:50:59
Modification Date	2016-07-07T04:04:00
Spectrometer Frequency	100.51
Spectral Width	25510.2
Lowest Frequency	-1683.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

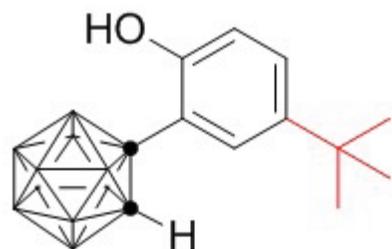


3.586
9.071
9.598
11.179
18.288

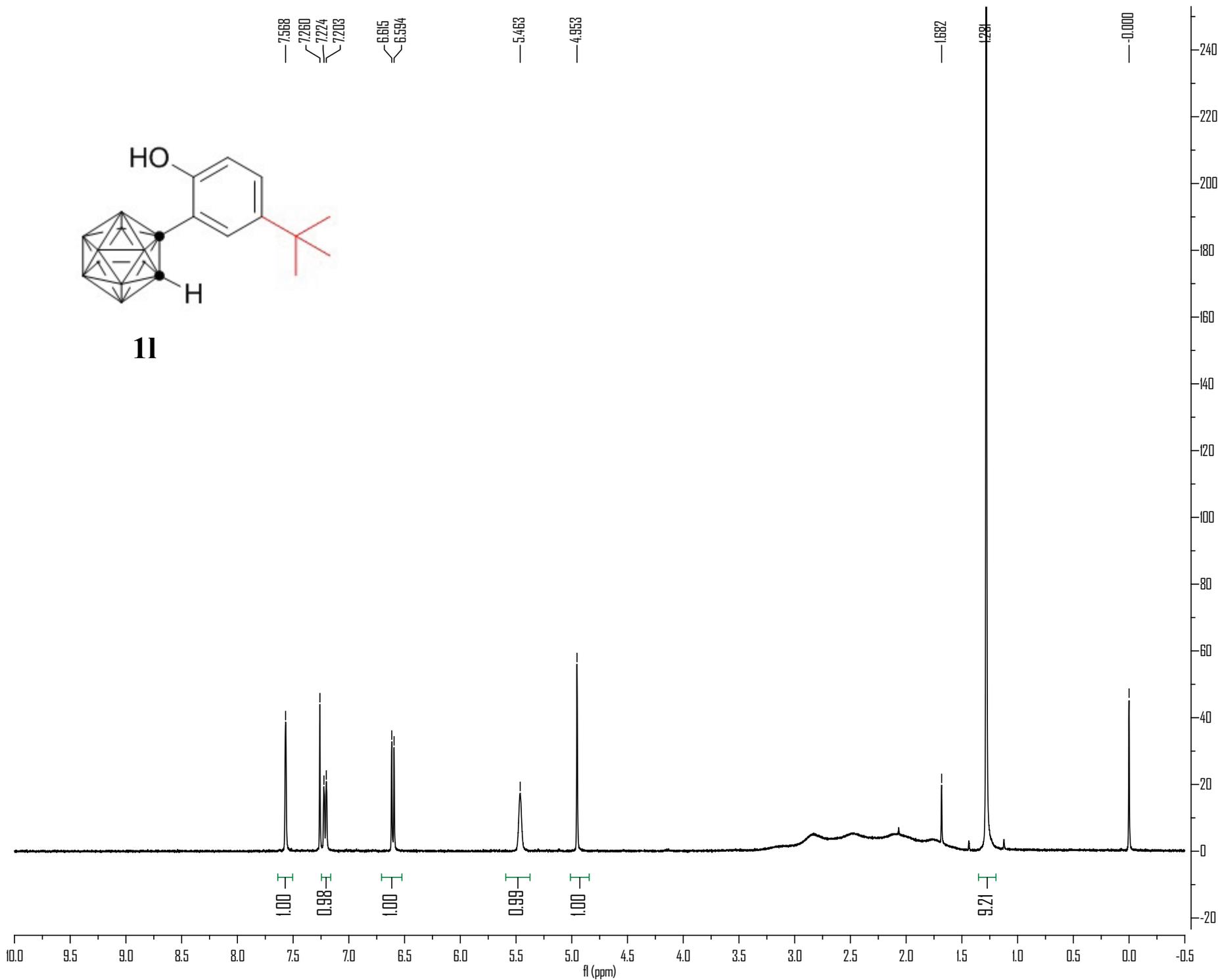


S58

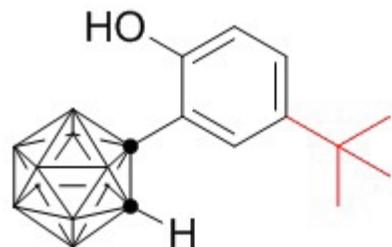
Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/6-82-1/b-cx-6-82-1/pdata/1/1r
Title	6-82-1
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	24
Receiver Gain	362
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-07-07T22:04:15
Modification Date	2016-07-07T16:04:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest	-16414.9



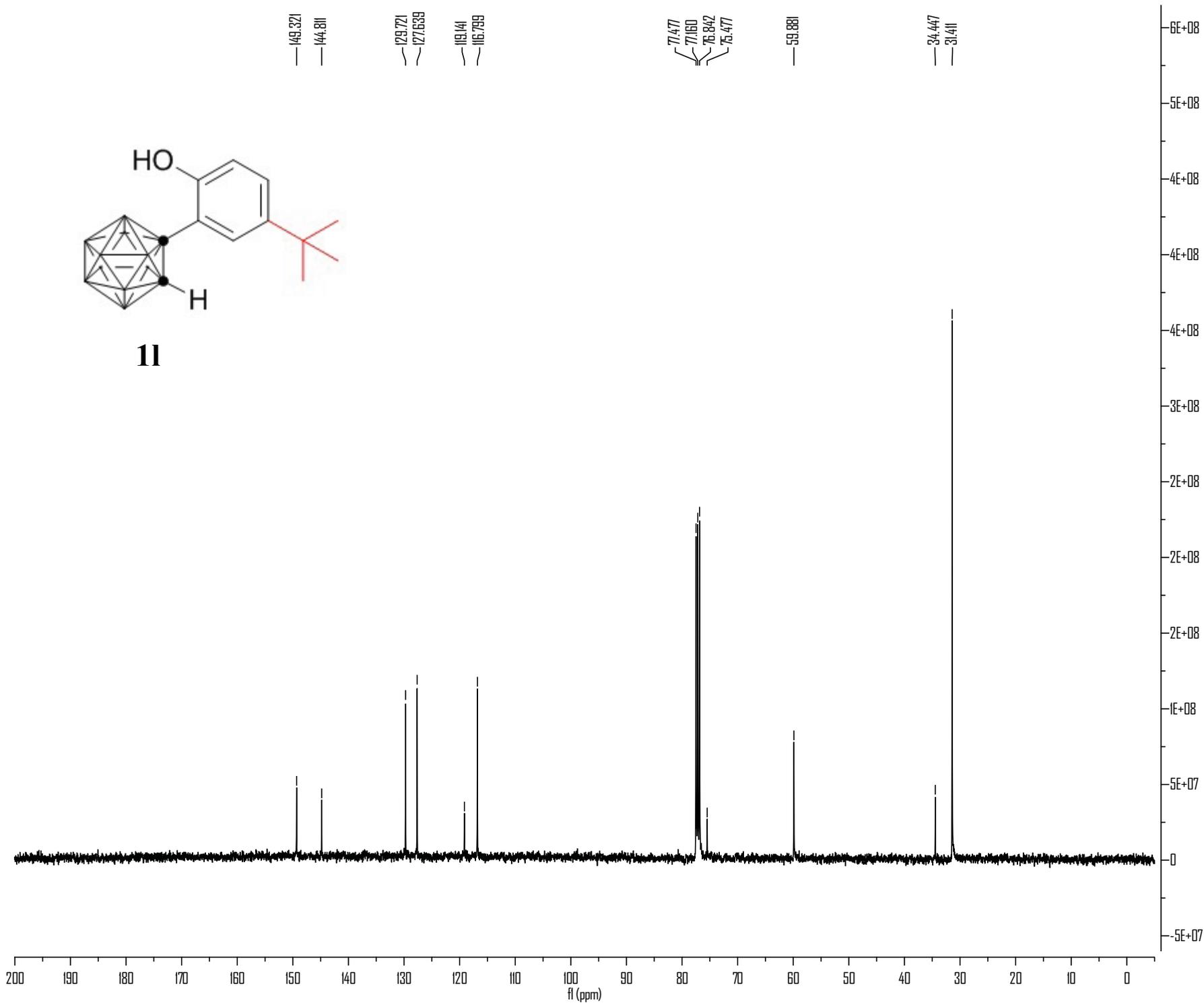
11



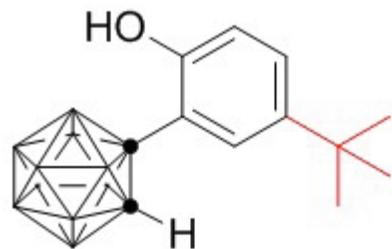
Parameter	Value
Title	ccx-7-53-1
Comment	td proton
Origin	Varian
Owner	
Site	
Spectrometer	nmrns
Author	omel
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	4
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-03-03T13:22:13
Modification Date	2017-03-03T05:22:00
Spectrometer Frequency	400.03
Spectral Width	7225.4
Lowest Frequency	-804.5
Nucleus	1H
Acquired Size	21676
Spectral Size	65536



11



Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/6-19-1/2012060c-ccx-6-19-1/3/pdata/1/1r
Title	2012060c-ccx-6-19-1
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgdc
Number of Scans	193
Receiver Gain	16384
Relaxation Delay	3.0000
Pulse Width	4.0000
Acquisition Time	0.4653
Acquisition Date	2016-03-11T21:27:08
Modification Date	2016-03-11T16:35:02
Spectrometer Frequency	100.61
Spectral Width	35211.3
Lowest Frequency	-6978.8
Nucleus	¹³ C
Acquired Size	16384
Spectral Size	65536



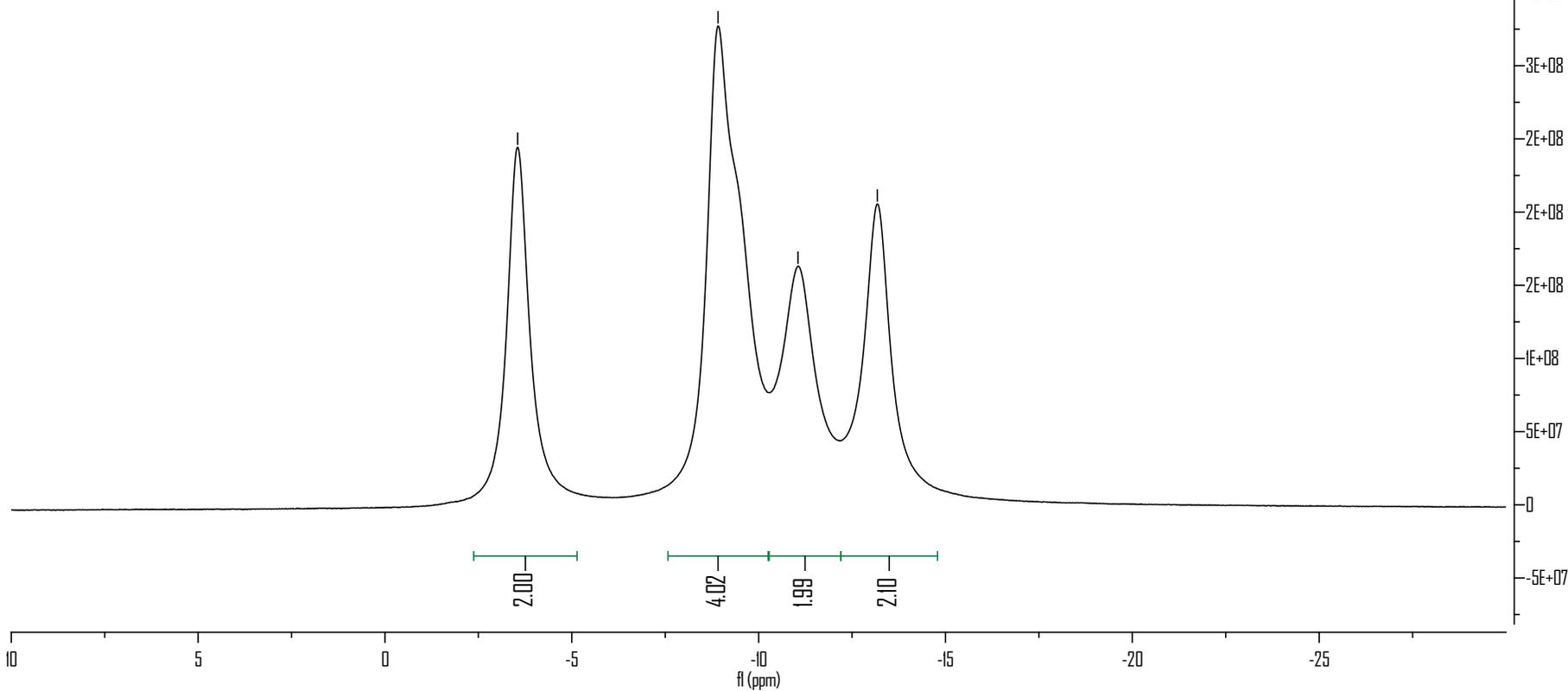
11

3.552

8.913

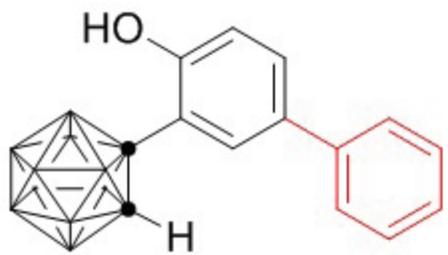
11.054

13.177



S61

Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/原料数据/6-19-1/2012060b-ccx-6-19-1/1/pdata/1/1r
Title	2012060b-ccx-6-19-1
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	256
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	8.5000
Acquisition Time	0.512
Acquisition Date	2016-03-11T21:14:14
Modification Date	2016-03-11T16:35:06
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16391.5
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

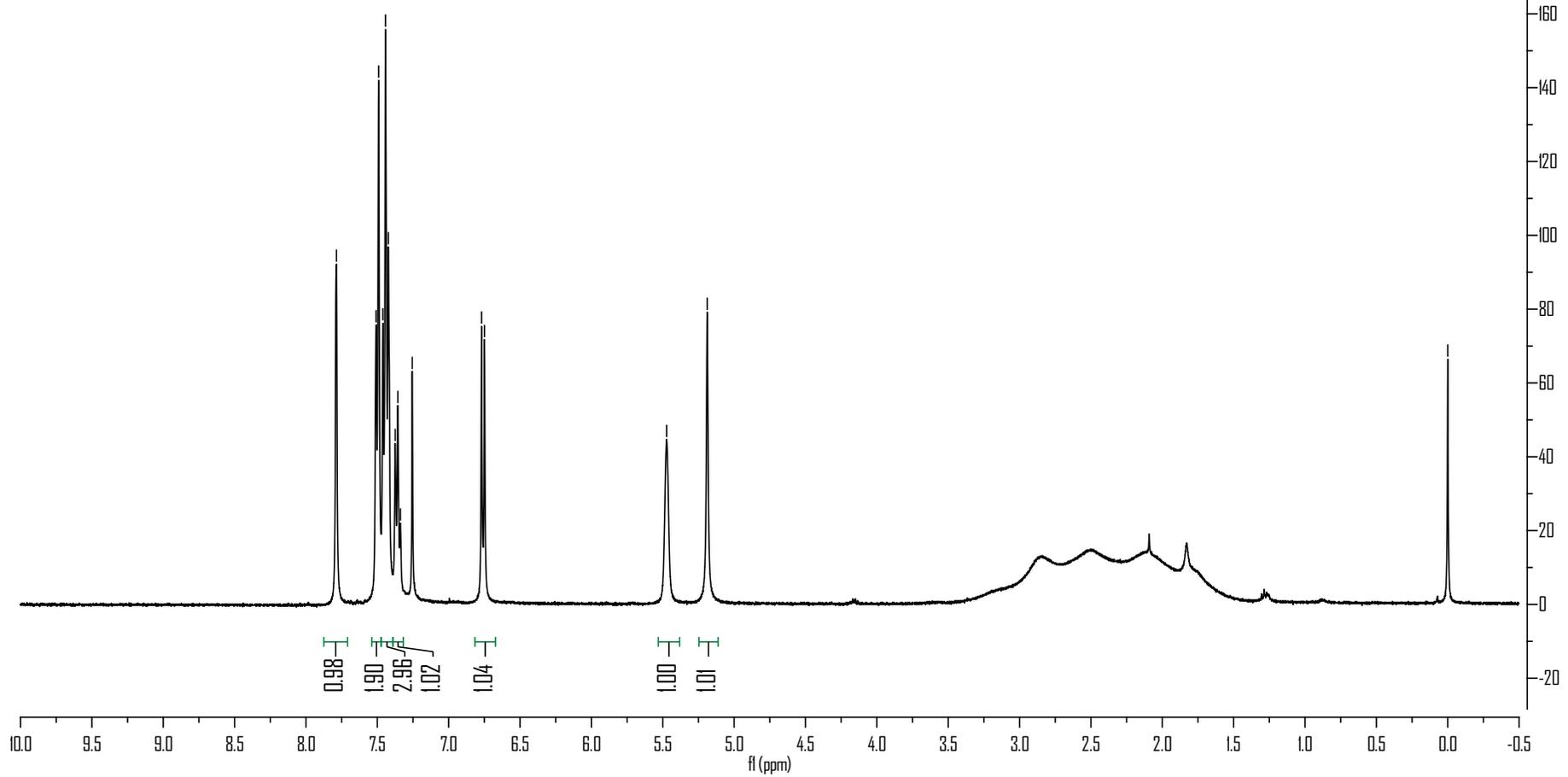


1m

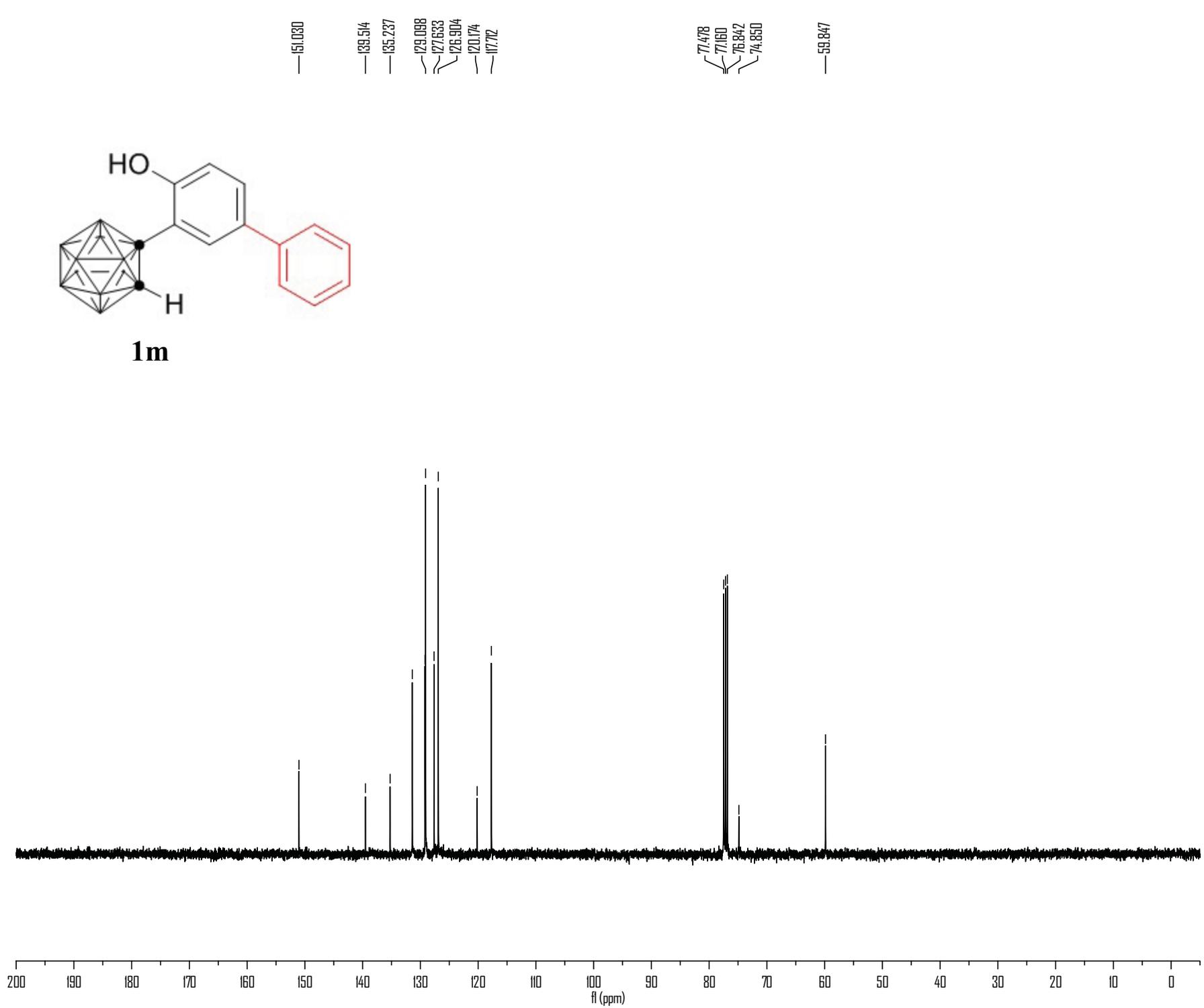
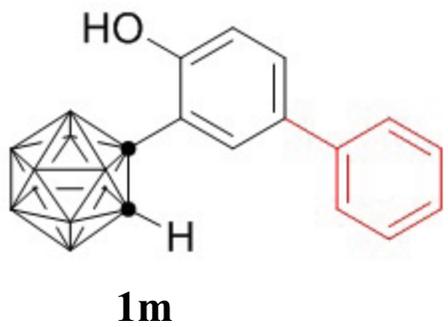
7.786
7.462
7.375
7.255
6.770
6.749

5.473
5.189

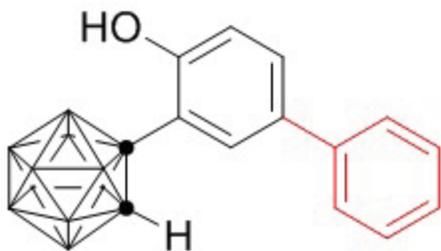
0.000



Parameter	Value
Title	ccx-6-62-1-2
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	omcl
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	40
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-02-22T14:16:14
Modification Date	2017-02-22T06:17:00
Spectrometer	399.72
Frequency	
Spectral Width	7183.9
Lowest Frequency	-795.8
Nucleus	1H
Acquired Size	21552
Spectral Size	65536

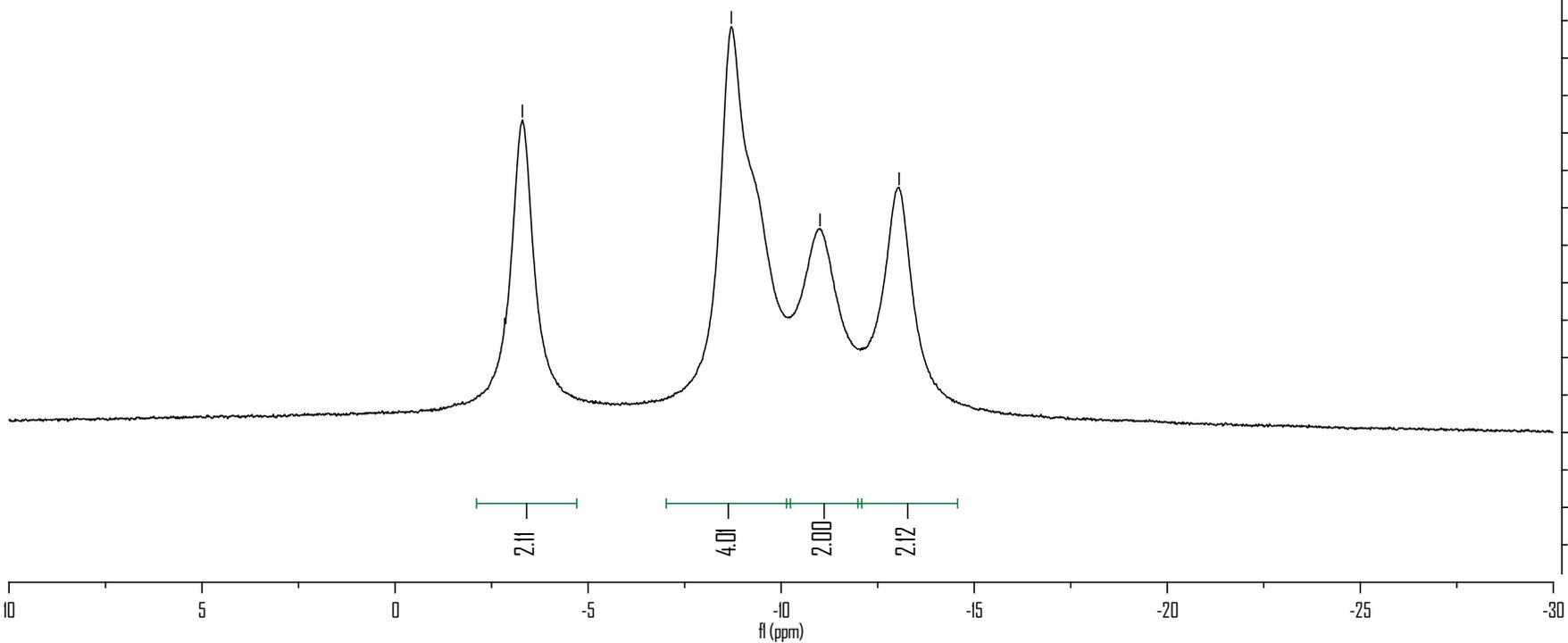


Parameter	Value
Title	ccx-6-62-1-2000
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omcl
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	372
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Acquisition Date	2017-02-24T13:34:23
Modification Date	2017-02-24T05:48:00
Spectrometer Frequency	100.52
Spectral Width	25000.0
Lowest Frequency	-1430.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



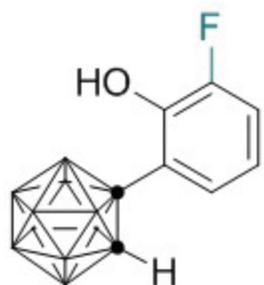
1m

— 3.298
— 8.70
— 11.007
— 13.055

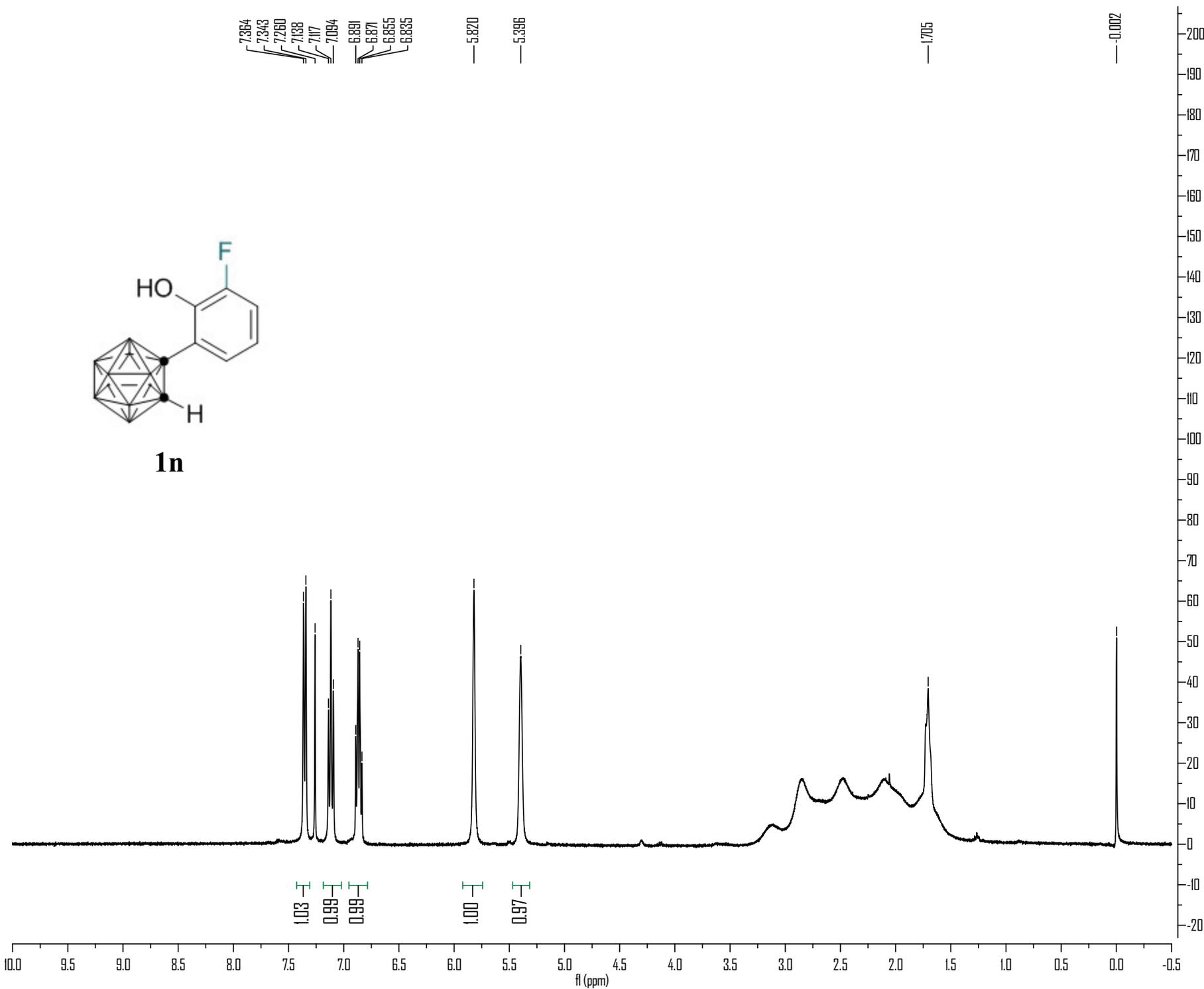


S64

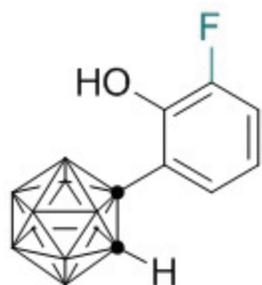
Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/原料数据/6-62-1/b-cx-6-62-1 (1)/pdata/1/1r
Title	6-62-1
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring1gy
Number of Scans	256
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	8.5000
Acquisition Time	0.512
Acquisition Date	2016-05-30T23:16:55
Modification Date	2016-05-30T17:22:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16391.5
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



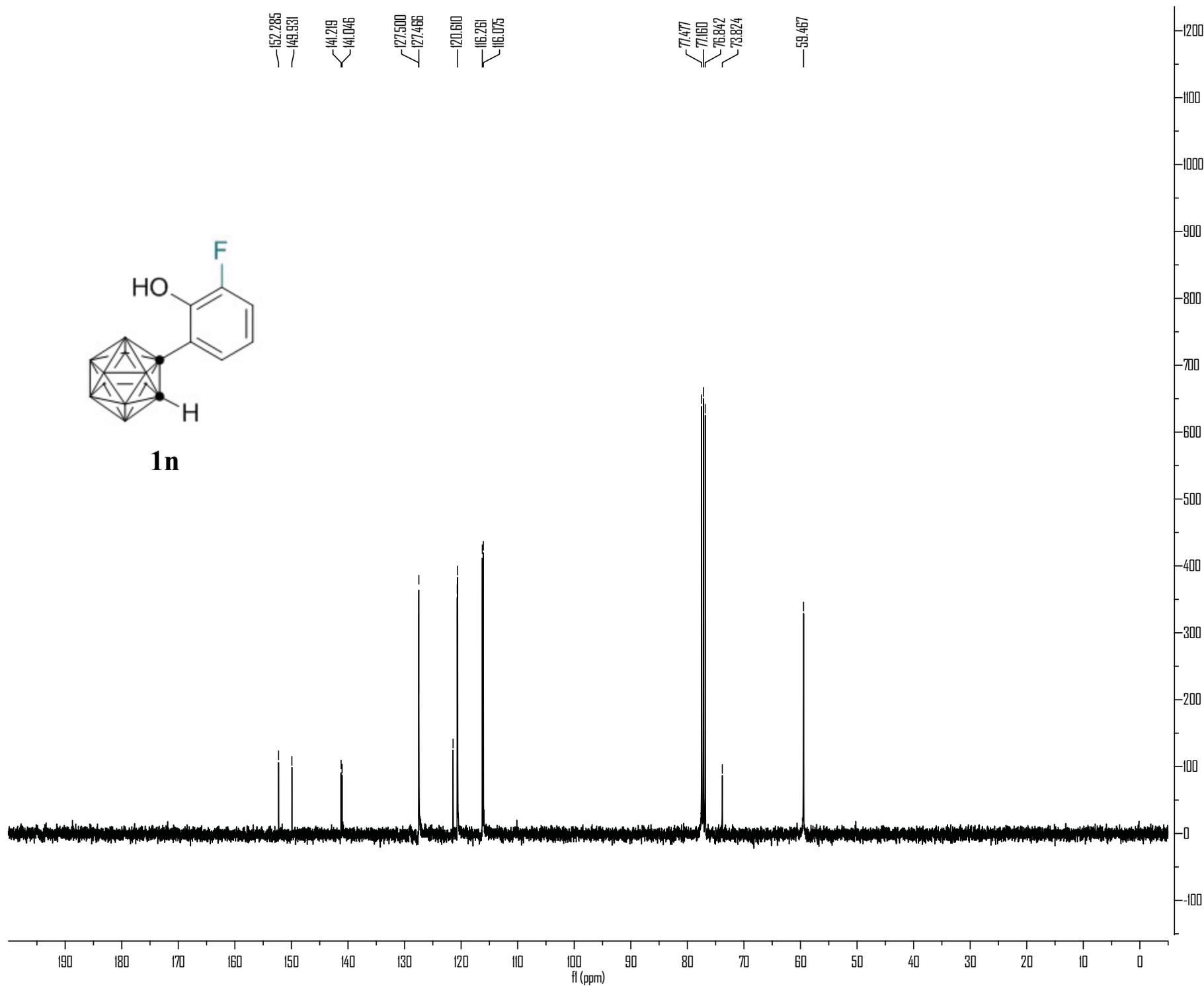
1n



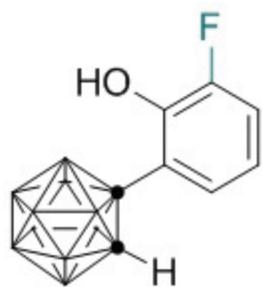
Parameter	Value
Title	ccx-7-3-1
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	36
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-10-12T11:45:46
Modification Date	2016-10-12T03:46:00
Spectrometer Frequency	400.03
Spectral Width	7309.9
Lowest Frequency	-807.3
Nucleus	1H
Acquired Size	21930
Spectral Size	65536



1n

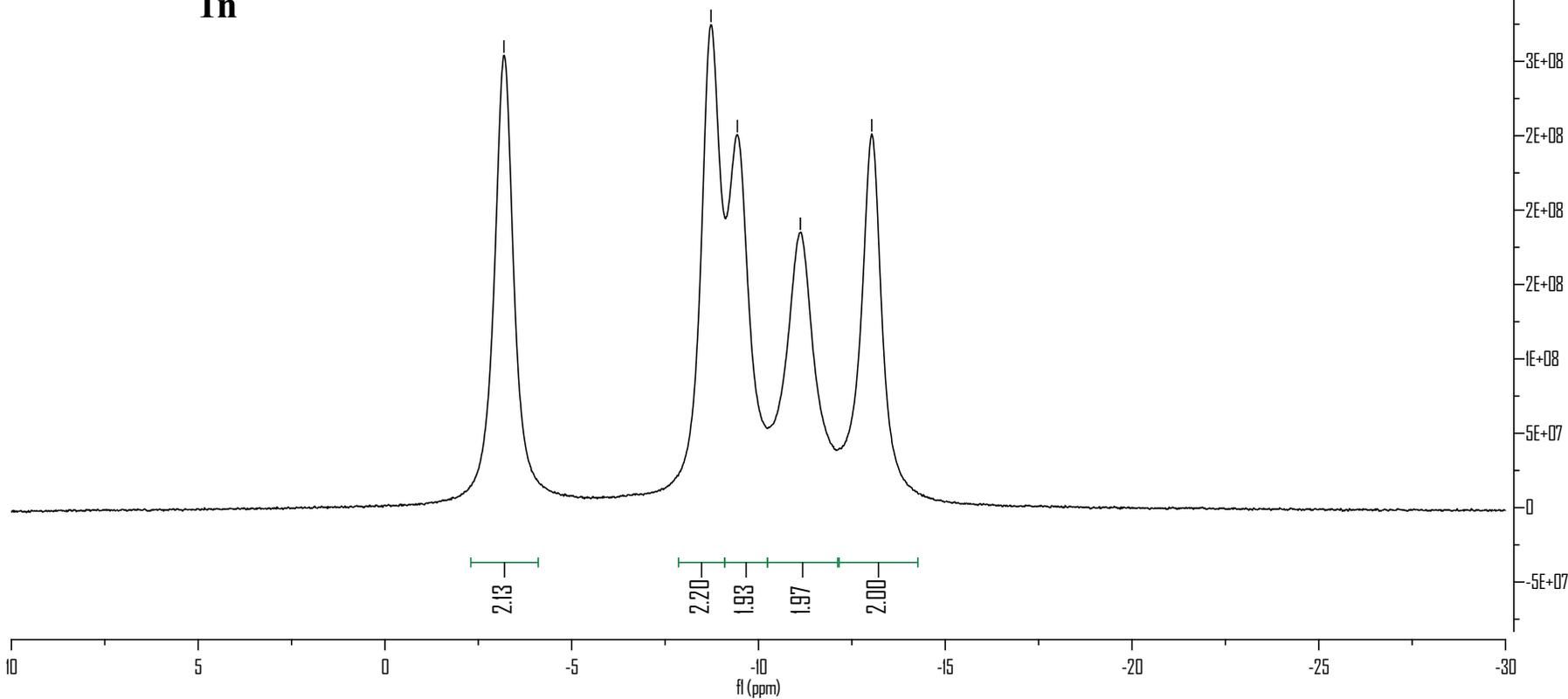


Parameter	Value
Title	-CCX-7-3-1C
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	nmr's
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	220
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-10-13 10:50:38
Modification Date	2016-10-13 10:03:00
Spectrometer	100.51
Frequency	
Spectral Width	25510.2
Lowest Frequency	-1682.4
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



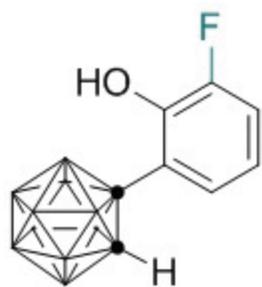
1n

3.186
8.729
9.435
11.122
13.033



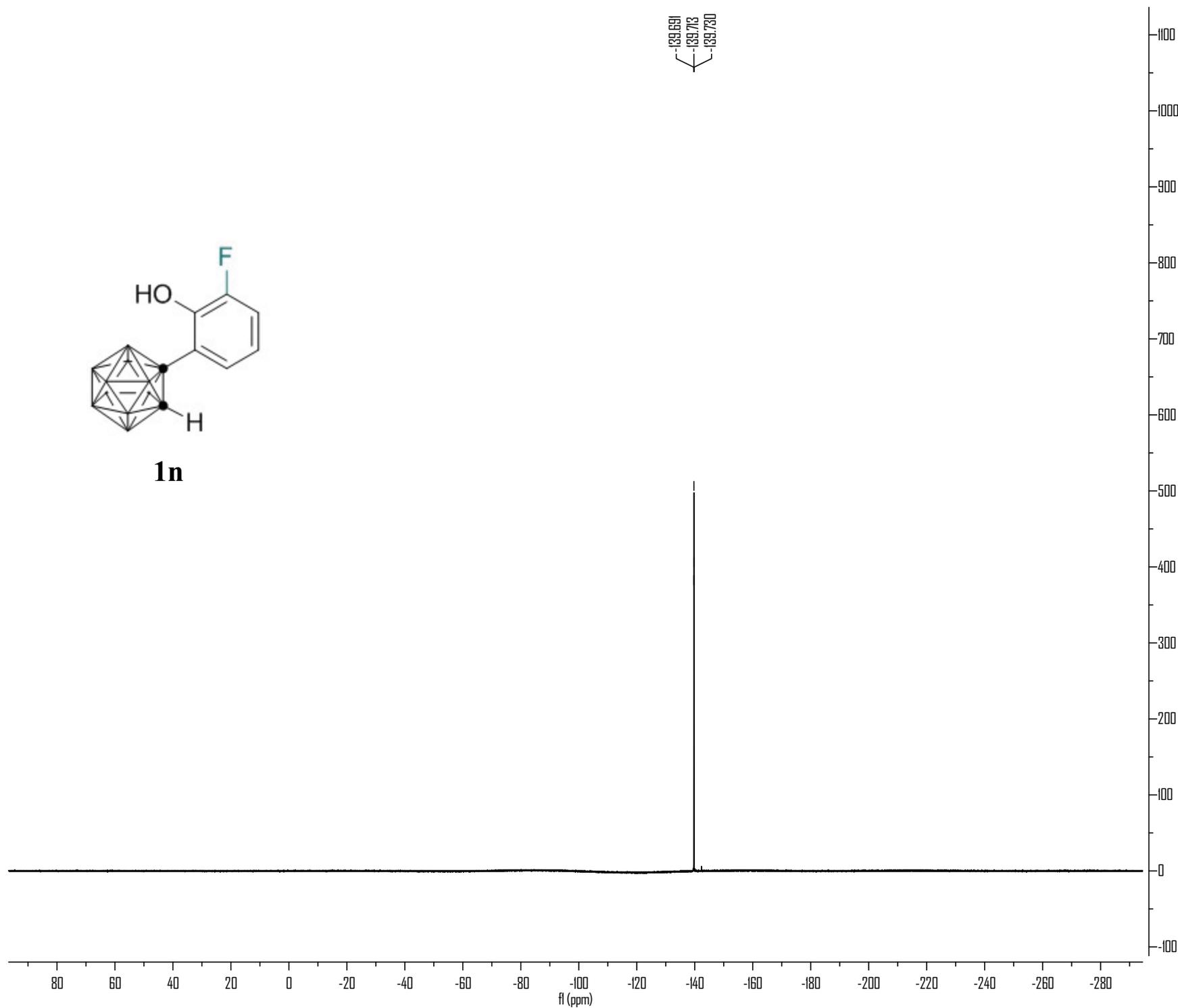
S67

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/7-3-1/b-cx-7-3-1 (1)/pdata/1/1r
Title	7-3-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	23
Receiver Gain	203
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-10-13 16:54:47
Modification Date	2016-10-13 10:55:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16337.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

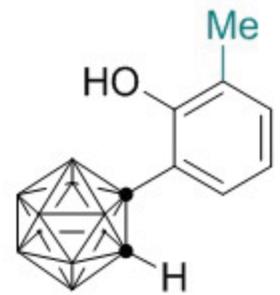
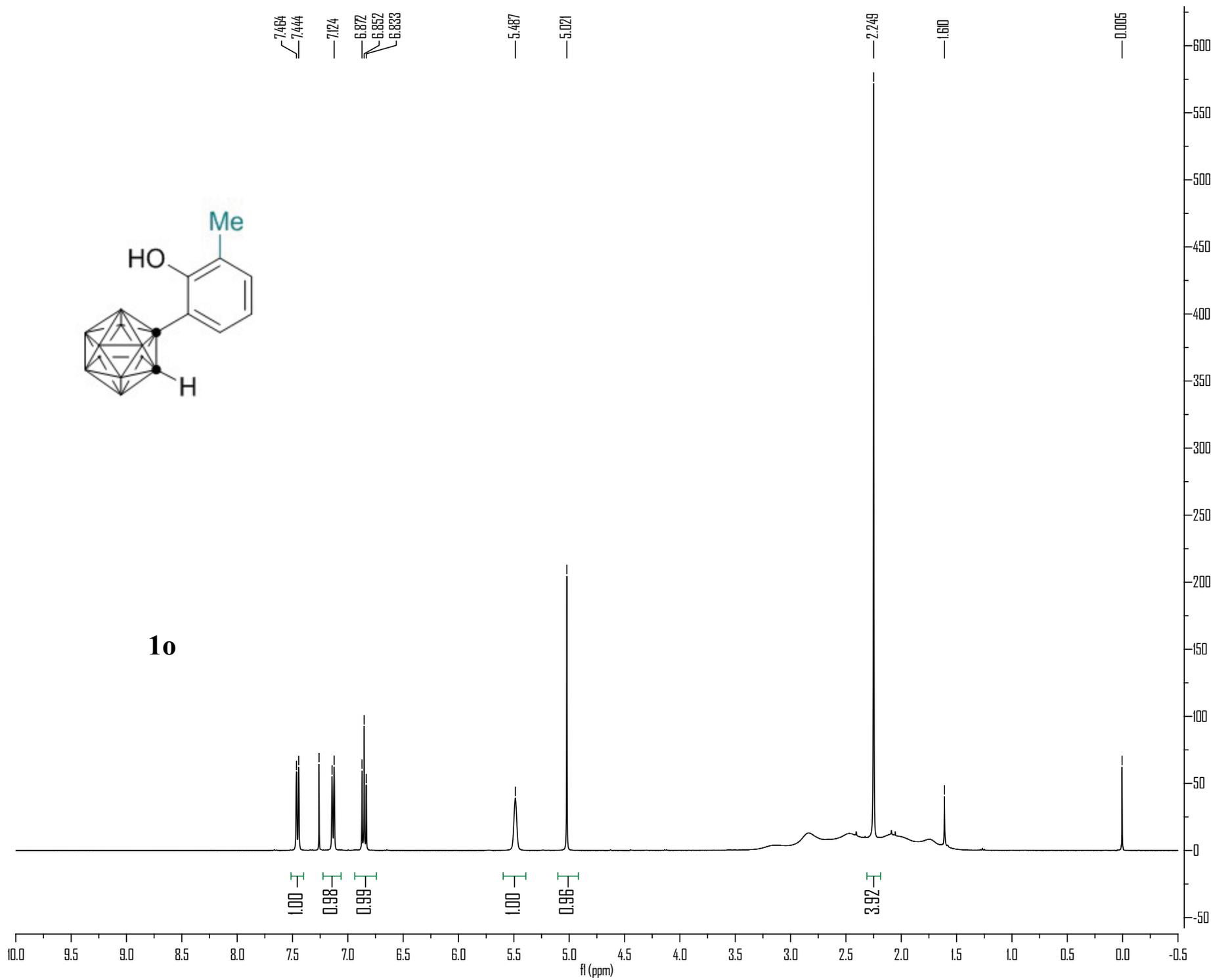


1n

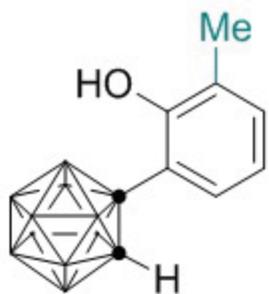
139.691
139.713
139.730



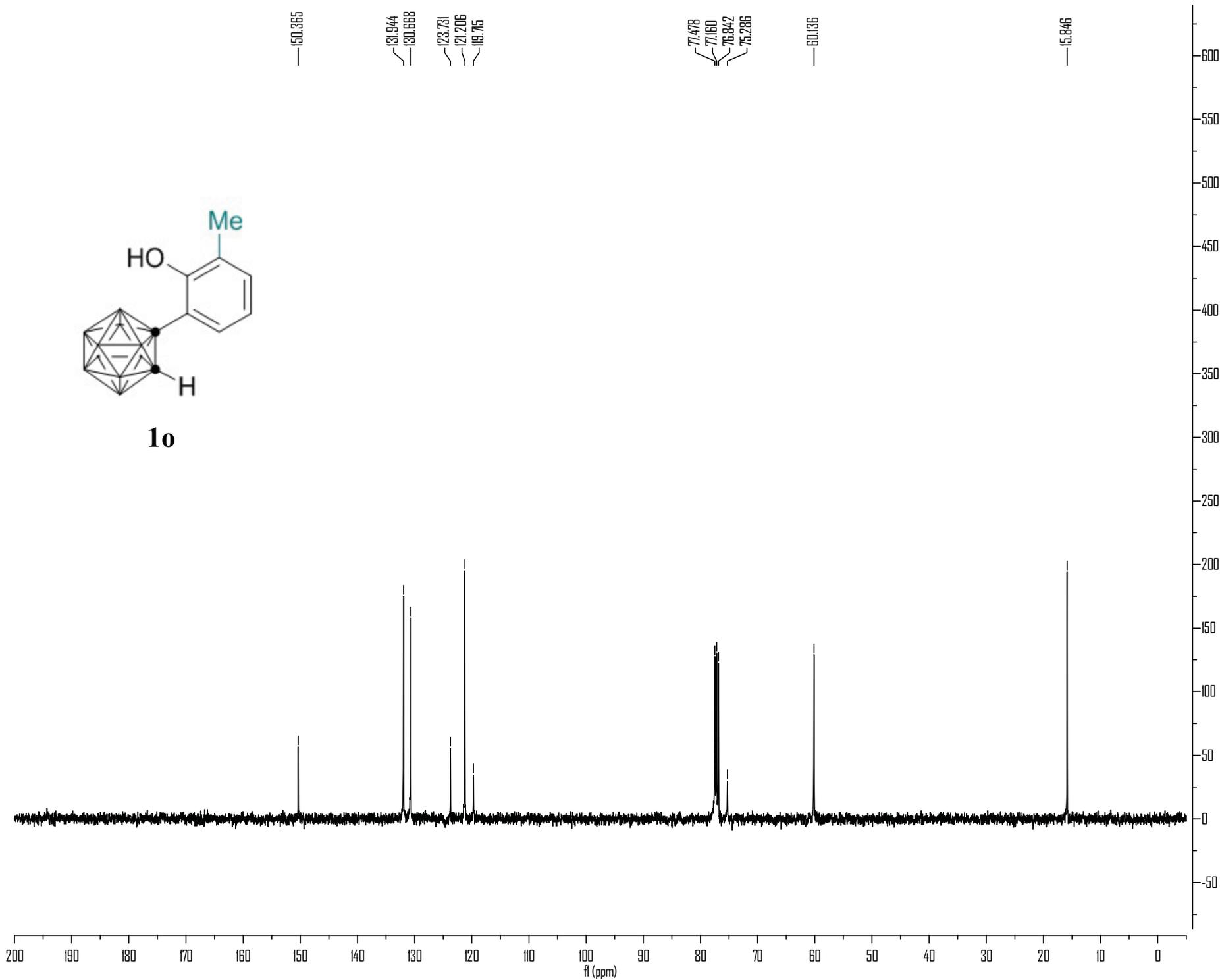
Parameter	Value
Title	ccx-7-3-1F
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	44
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	1.0000
Acquisition Date	2016-10-13T08:54:18
Modification Date	2016-10-13T00:55:00
Spectrometer Frequency	376.08
Spectral Width	147058.8
Lowest Frequency	-110727.0
Nucleus	19F
Acquired Size	147059
Spectral Size	524288



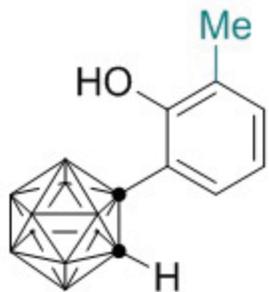
Parameter	Value
Title	ccx-7-30-1
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	
Solvent	CDCl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	34
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-11-29T18:54:33
Modification Date	2016-11-29T10:55:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-793.9
Nucleus	¹ H
Acquired Size	21552
Spectral Size	65536



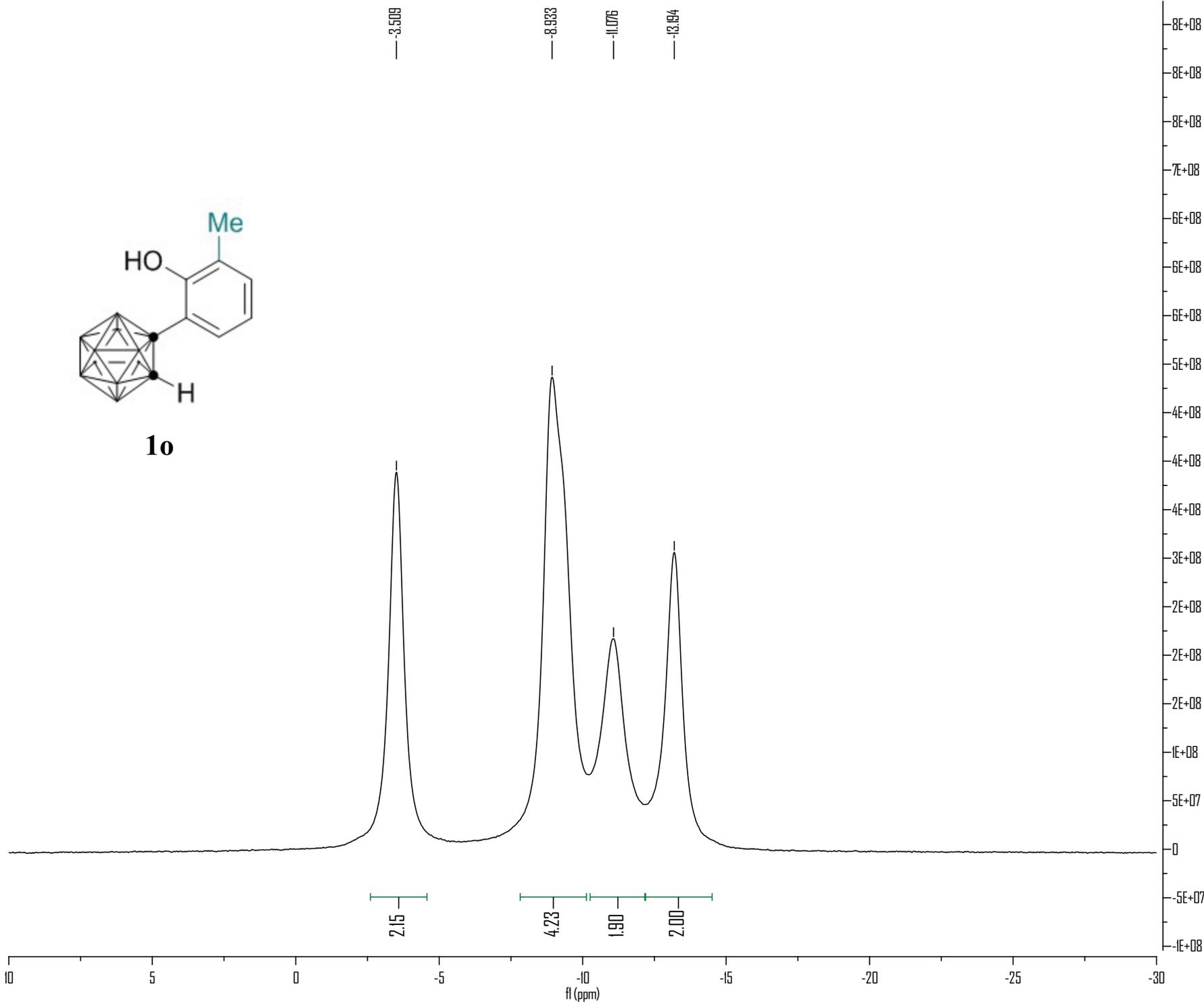
1o



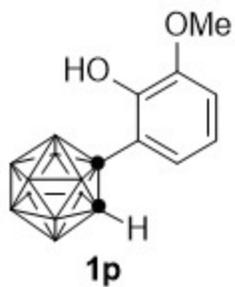
Parameter	Value
Title	CDX-7-30-1-1000
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	80
Receiver Gain	60
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-12-13T15:36:39
Modification Date	2016-12-13T15:42:00
Spectrometer	100.51
Frequency	
Spectral Width	25510.2
Lowest Frequency	-1683.4
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



1o



Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/7-30-1/2012060b-ccx-7-30-1/1/pdata/1/1r
Title	2012060b-ccx-7-30-1
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	35
Receiver Gain	181
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-11-30T17:33:39
Modification Date	2016-11-30T11:03:19
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16400.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



7.260
7.153
7.148
7.135
7.130

6.844
6.807

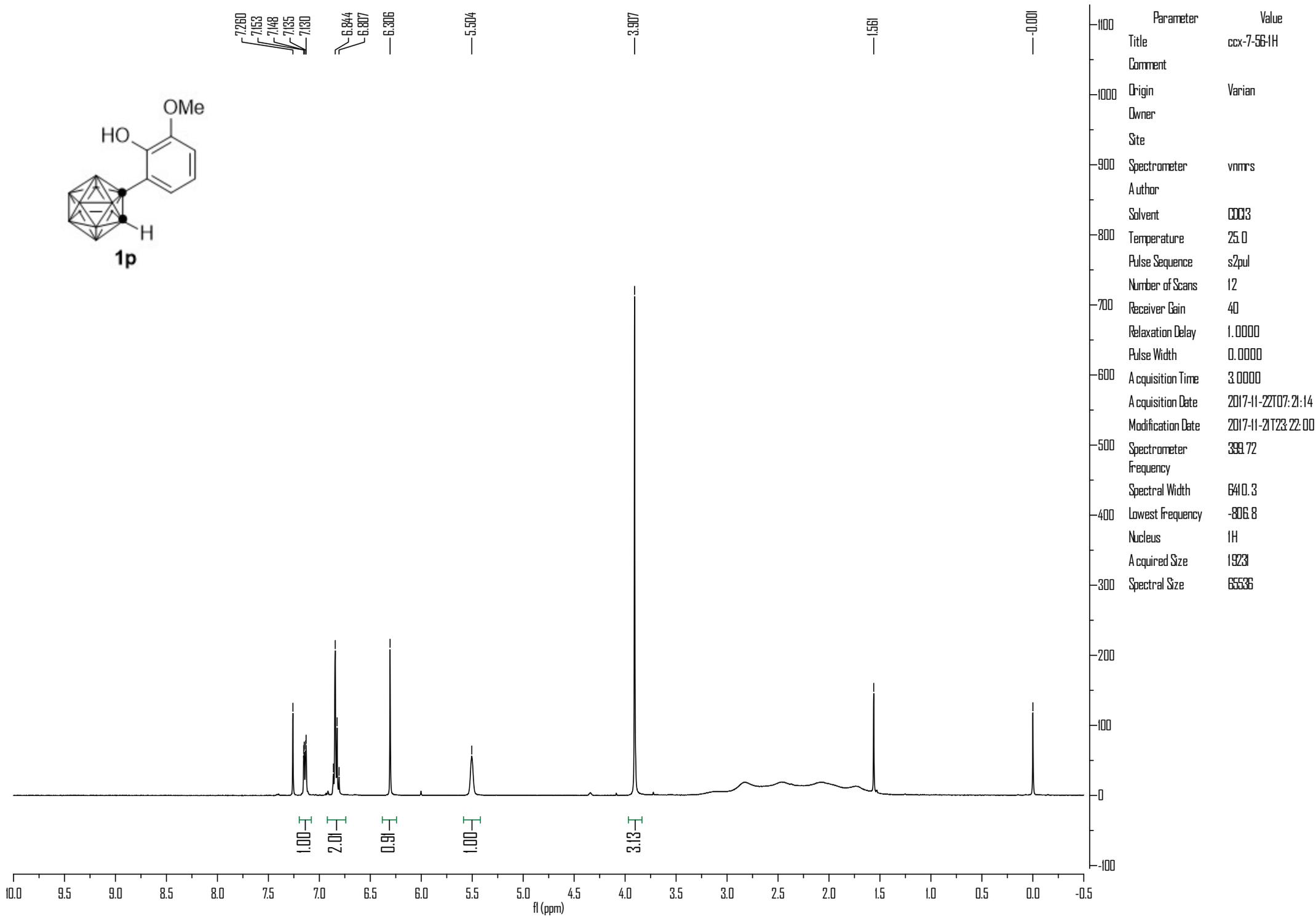
6.306

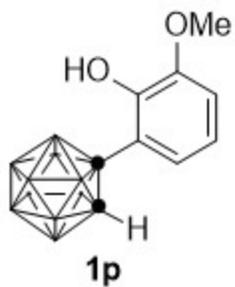
5.504

3.907

1.561

0.001





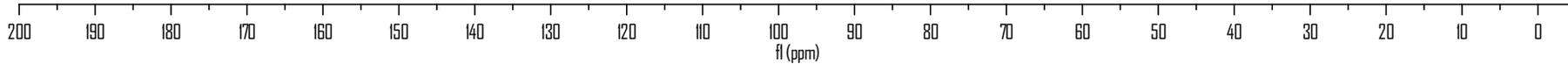
146.636
142.744

123.595
120.014
118.793

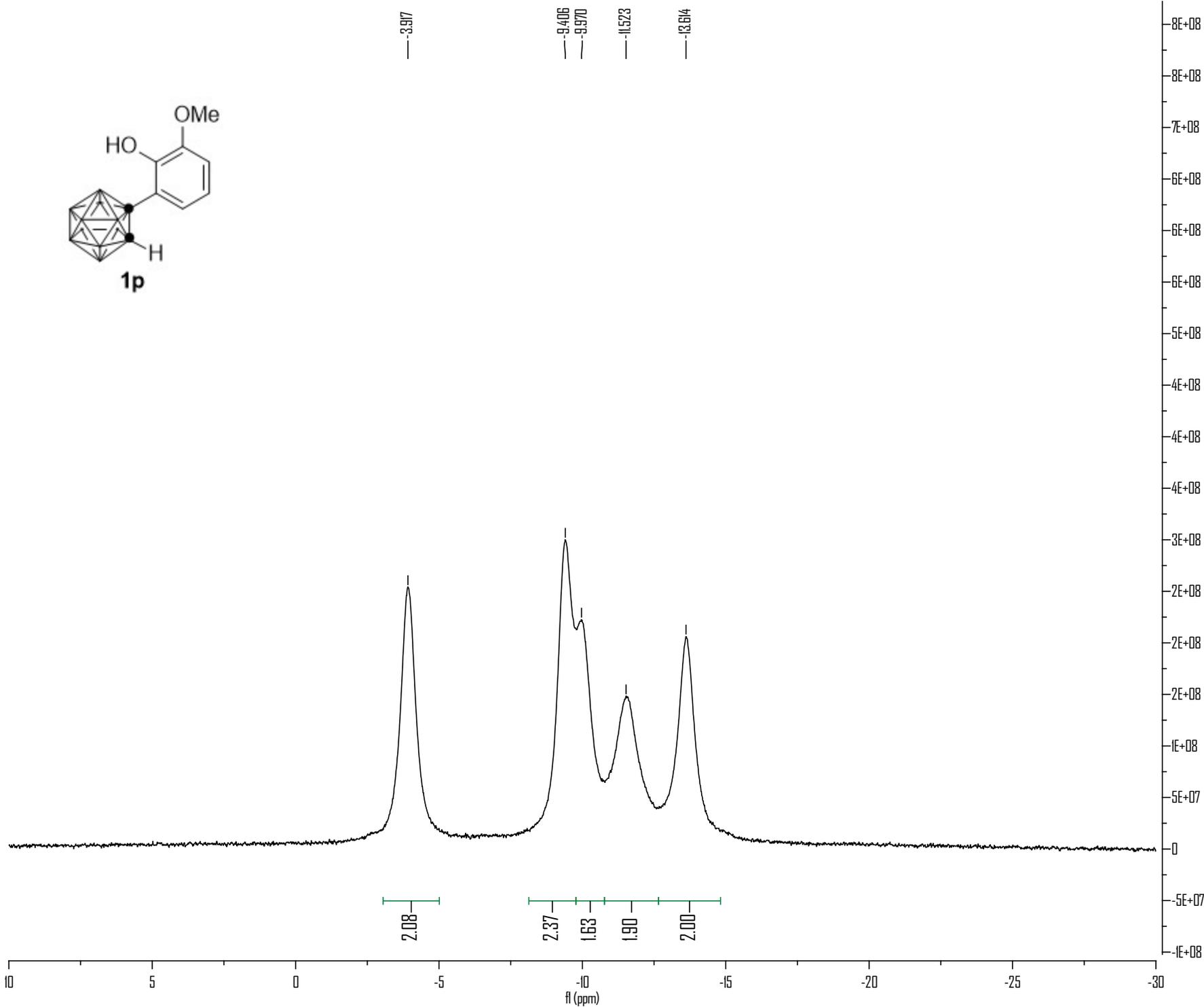
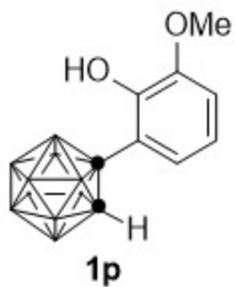
111.099

77.478
77.160
76.842
74.716

59.621
56.568



Parameter	Value
Title	-CCX-7-12-1-1000
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	232
Receiver Gain	60
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-12-13 11:58:48
Modification Date	2016-12-13 14:16:00
Spectrometer Frequency	100.51
Spectral Width	25510.2
Lowest Frequency	-1685.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



S74

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/原料数据/7-12-1/2012060b-ccx-7-56-1/1/pdata/1/1r
Title	2012060b-ccx-7-56-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	90
Receiver Gain	362
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.4260
Acquisition Date	2017-11-22T22:52:05
Modification Date	2017-11-22T15:57:04
Spectrometer Frequency	128.38
Spectral Width	38461.5
Lowest Frequency	-19665.1
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

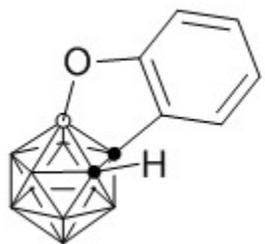
7.429
7.420
7.405
7.395
7.380
7.260
7.160
7.132
7.080
7.055
7.030

2.895

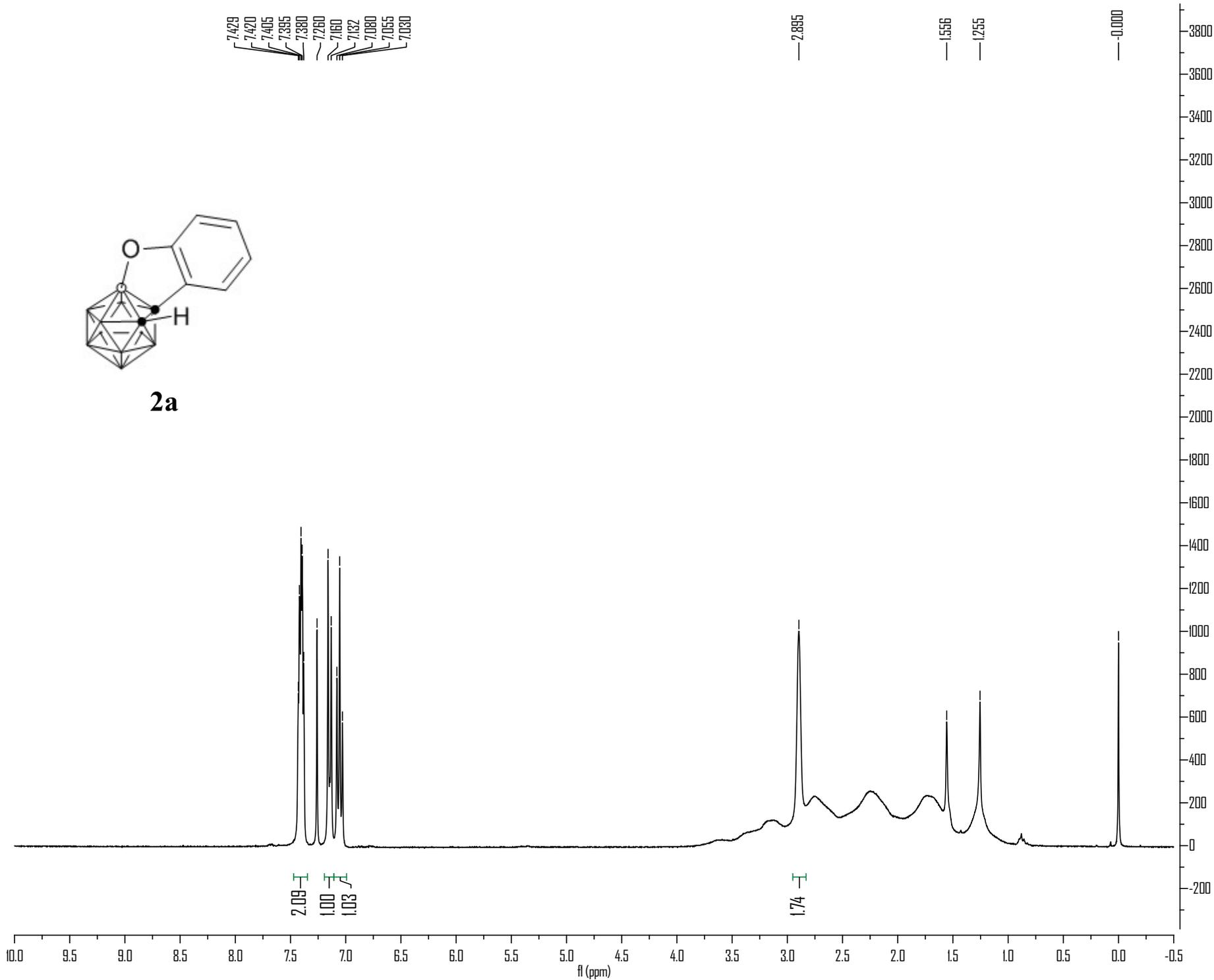
1.556

1.255

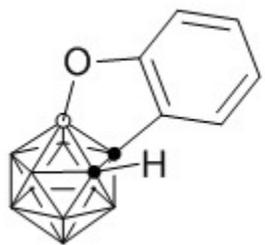
0.000



2a



Parameter	Value
Title	ccx-5-101-3a-2H
Comment	STANDARD 1H OBSERVE
Origin	Varian
Owner	
Site	
Spectrometer	mercury
Author	omc
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Number of Scans	40
Receiver Gain	34
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.0000
Acquisition Date	2016-03-17T14:19:28
Modification Date	2016-03-17T14:24:00
Spectrometer Frequency	300.03
Spectral Width	5494.5
Lowest Frequency	-709.9
Nucleus	1H
Acquired Size	10989
Spectral Size	32768



2a

167.71

131.831

123.359

122.114

115.863

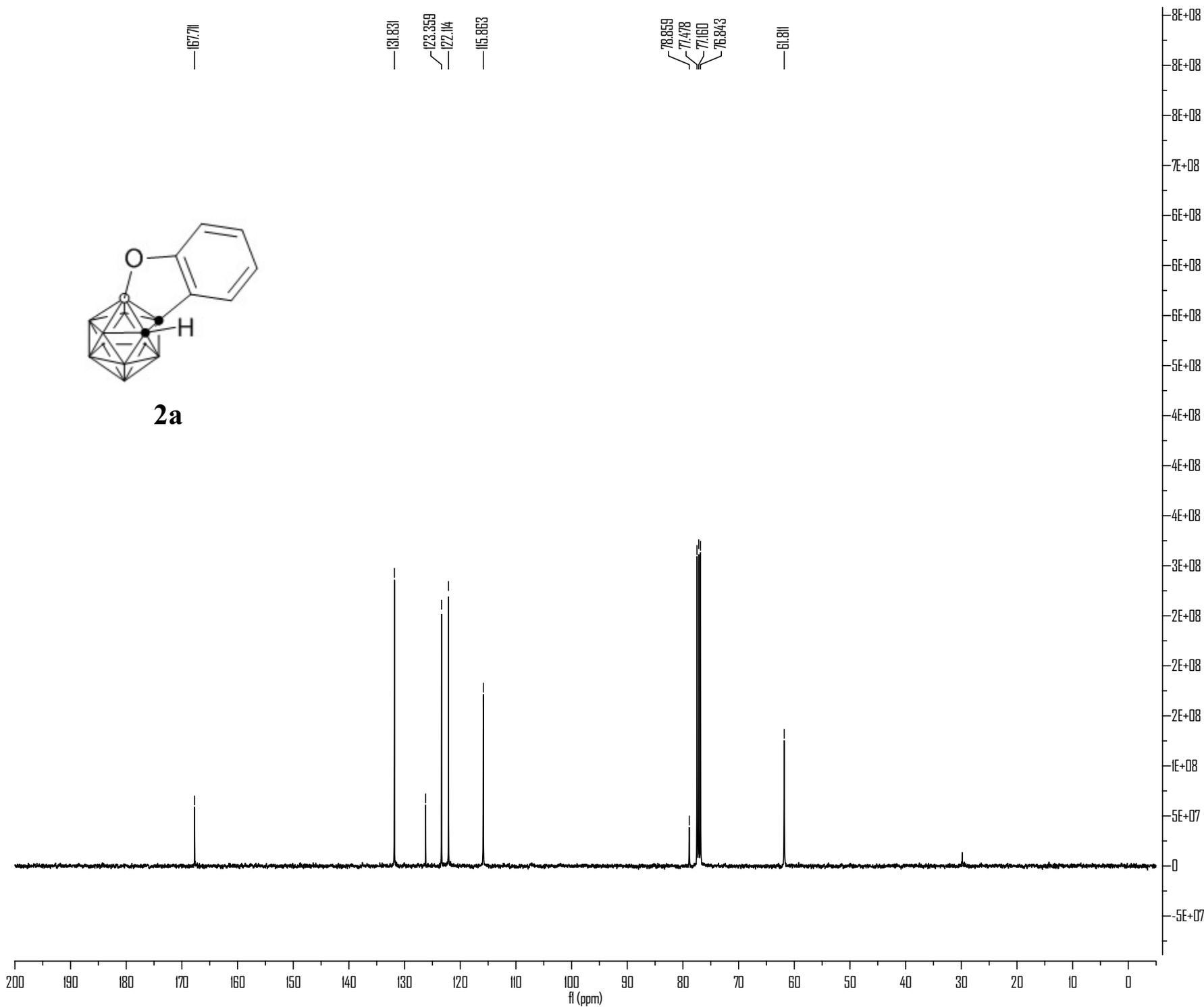
78.859

77.478

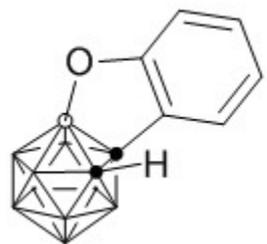
77.160

76.843

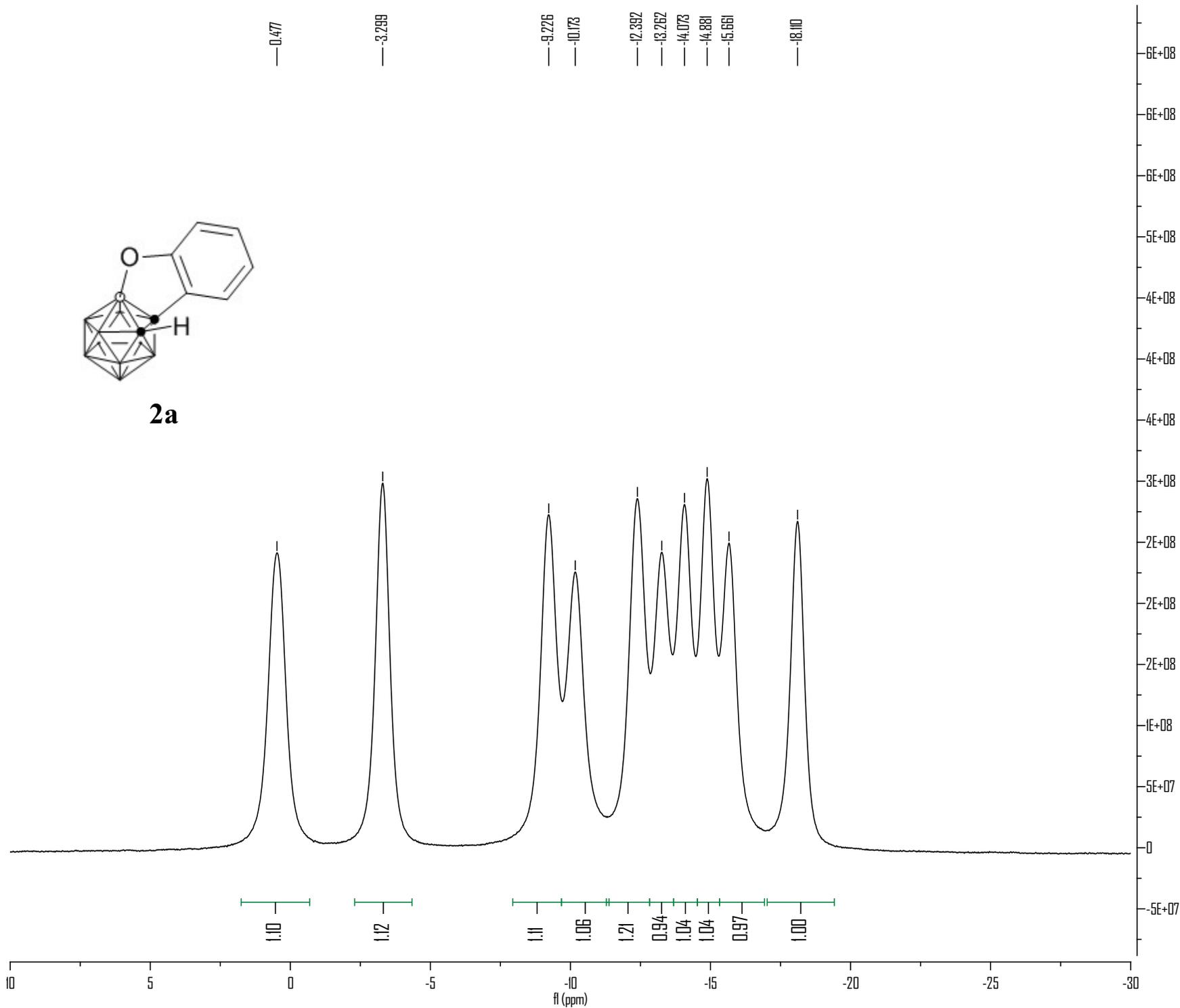
61.811



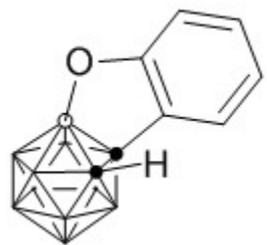
Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/产物数据/5-101-a/cc-cx-5-101-1-0104/pdata/1/1r
Title	5-101-a
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgdc
Number of Scans	1494
Receiver Gain	16384
Relaxation Delay	3.0000
Pulse Width	6.0000
Acquisition Time	0.4653
Acquisition Date	2016-01-05T17:17:41
Modification Date	2016-01-05T10:18:00
Spectrometer	100.61
Frequency	
Spectral Width	35211.3
Lowest Frequency	-6049.0
Nucleus	13C
Acquired Size	16384
Spectral Size	65536



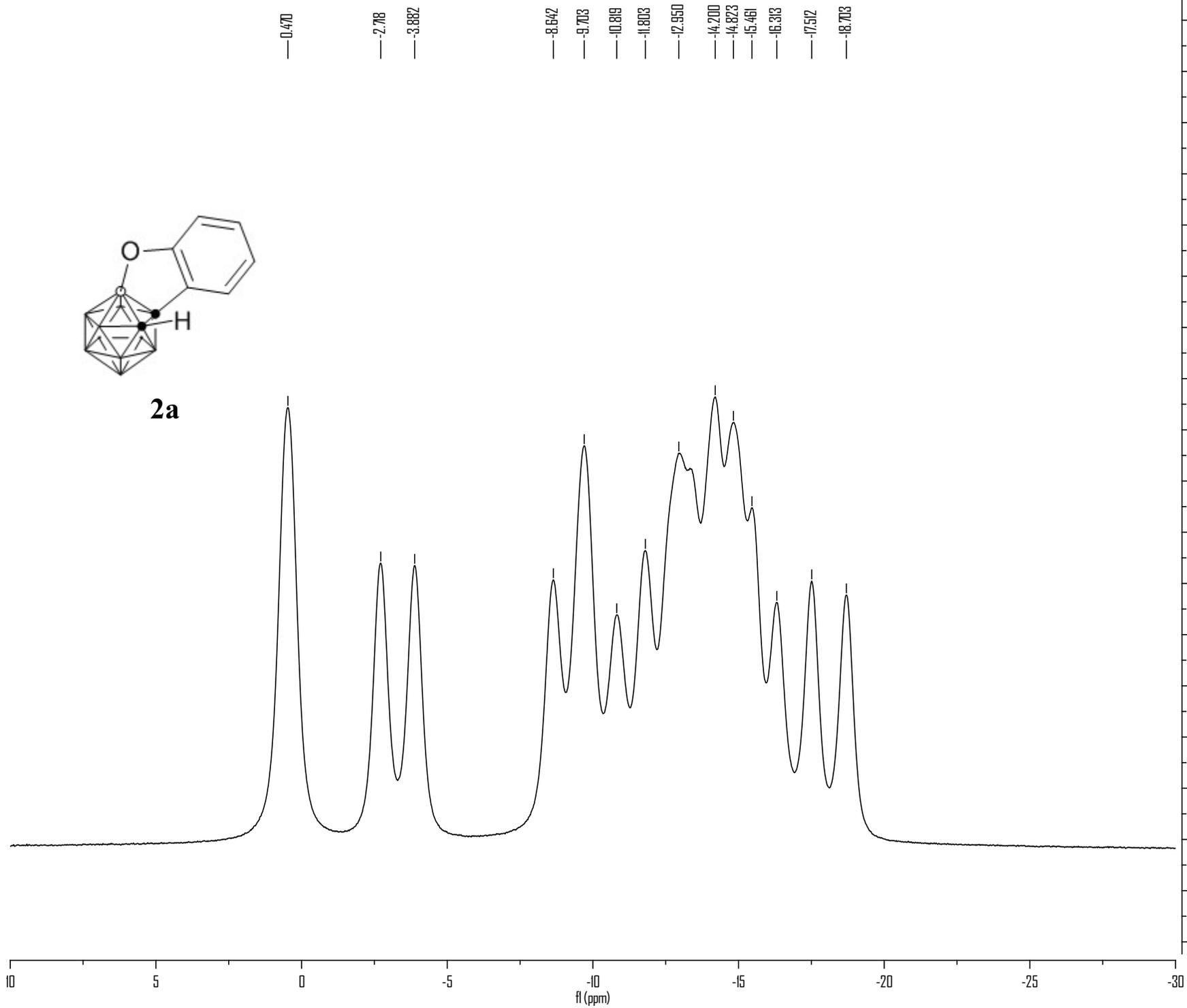
2a



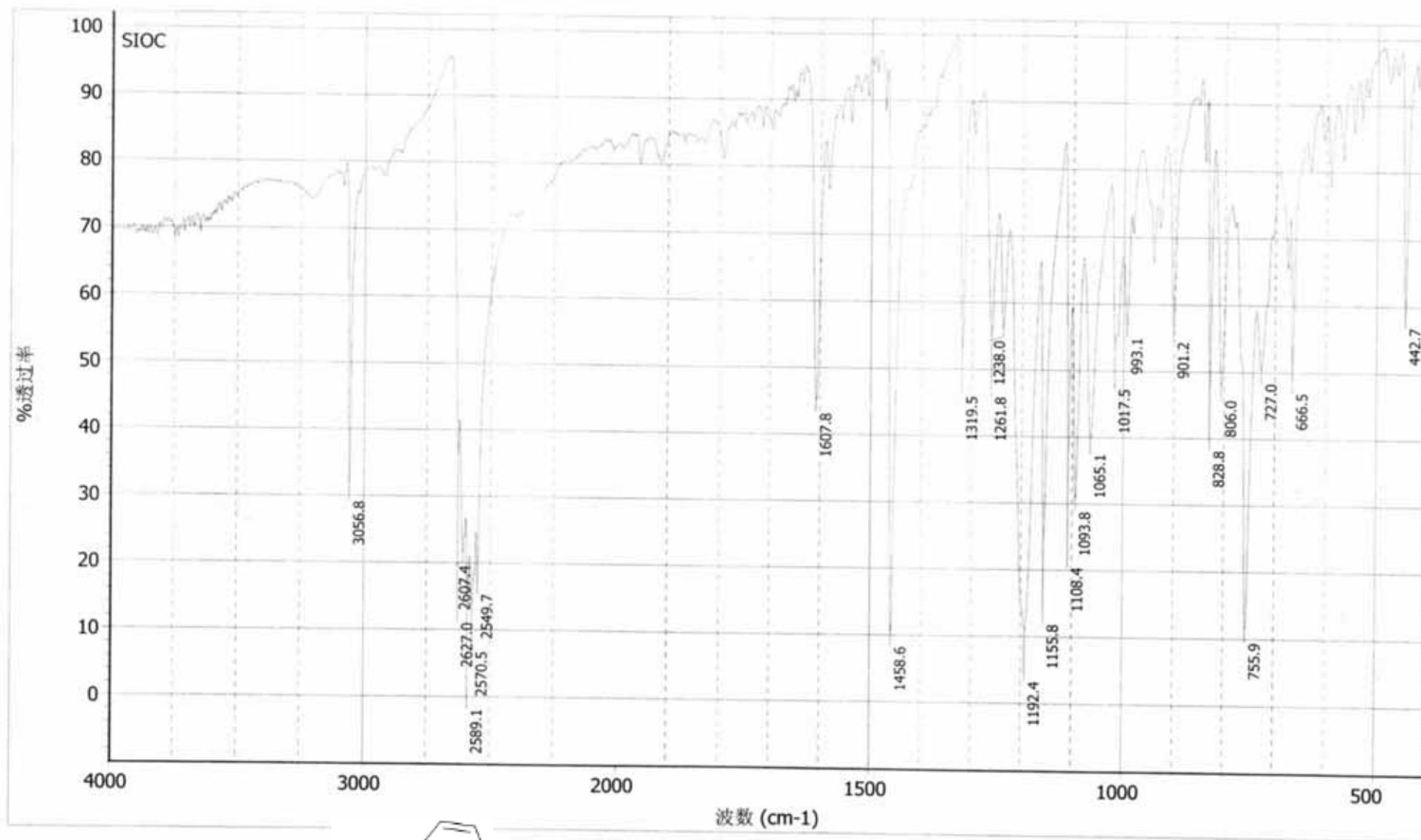
Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/5-101-a/b-ccx-5101-1/pdata/1/1r
Title	5-101-a
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	140
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	13.4000
Acquisition Time	0.3195
Acquisition Date	2016-01-04T18:00:15
Modification Date	2016-01-04T11:00:00
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-25747.6
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



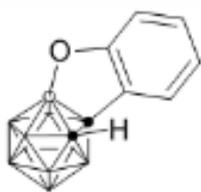
2a



Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/5-101-a/b-cx-5-101-1-coupling/pdata/1/1r
Title	5-101-a
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	243
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	13.4000
Acquisition Time	0.3195
Acquisition Date	2016-01-04T18:02:07
Modification Date	2016-01-04T11:02:00
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-26010.4
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



CCX-5-101-A 2015806 JS



2a

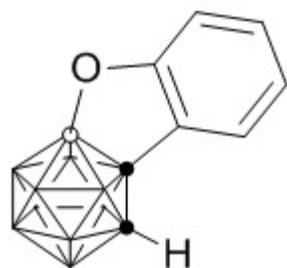
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329

7.428
7.401
7.376
7.259
7.232
7.190
7.162
7.044
7.018
6.993

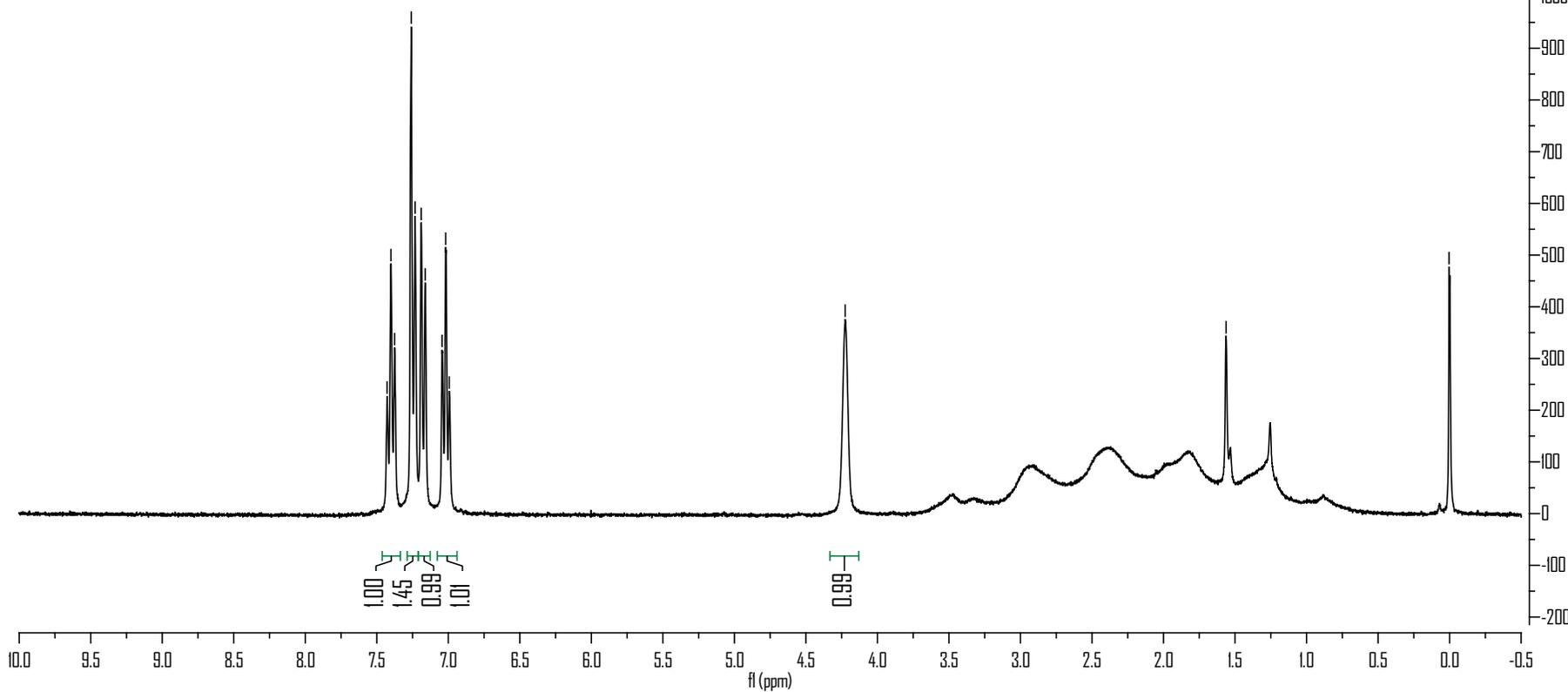
4.225

1.562

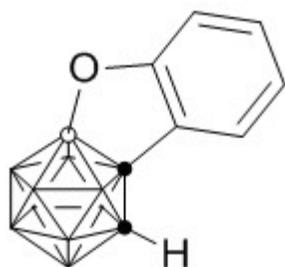
0.004



3a



Parameter	Value
Title	CCX-6-10-3b-2H_17Mar2016
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	mercury
Author	
Solvent	CDCl3
Temperature	3.0
Pulse Sequence	s2pul
Number of Scans	32
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.9971
Acquisition Date	1999-11-13T16:23:44
Modification Date	2016-03-17T11:21:00
Spectrometer Frequency	300.04
Spectral Width	4803.1
Lowest Frequency	-600.1
Nucleus	1H
Acquired Size	9592
Spectral Size	32768



3a

167.332

131.167

125.283

119.887

115.827

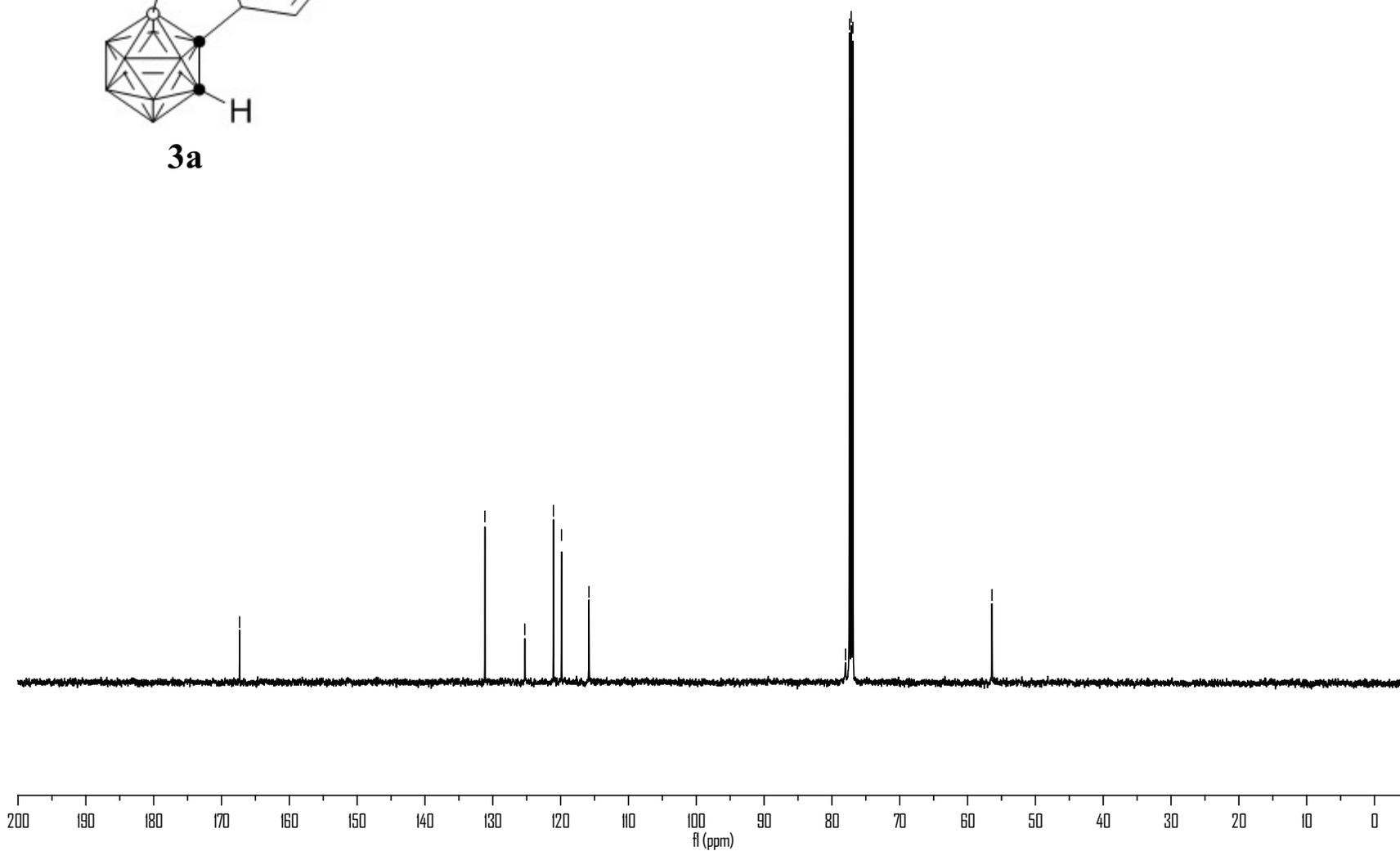
77.997

77.414

77.160

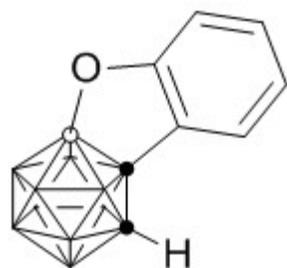
76.905

56.401



S81

Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/产物数据/5-101-b/cc-cx-5-101-3b-3/pdata/1/1r
Title	qnp-cl3
Comment	
Origin	Bruker BioSpin GmbH
Owner	slp
Site	
Spectrometer	spect
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgpg30
Number of Scans	246
Receiver Gain	16384
Relaxation Delay	2.0000
Pulse Width	9.4000
Acquisition Time	0.7472
Acquisition Date	2016-03-18T13:28:05
Modification Date	2016-03-18T13:34:00
Spectrometer	125.76
Frequency	
Spectral Width	43859.6
Lowest Frequency	-9331.9
Nucleus	13C
Acquired Size	32768
Spectral Size	32768



3a

3.259

4.088

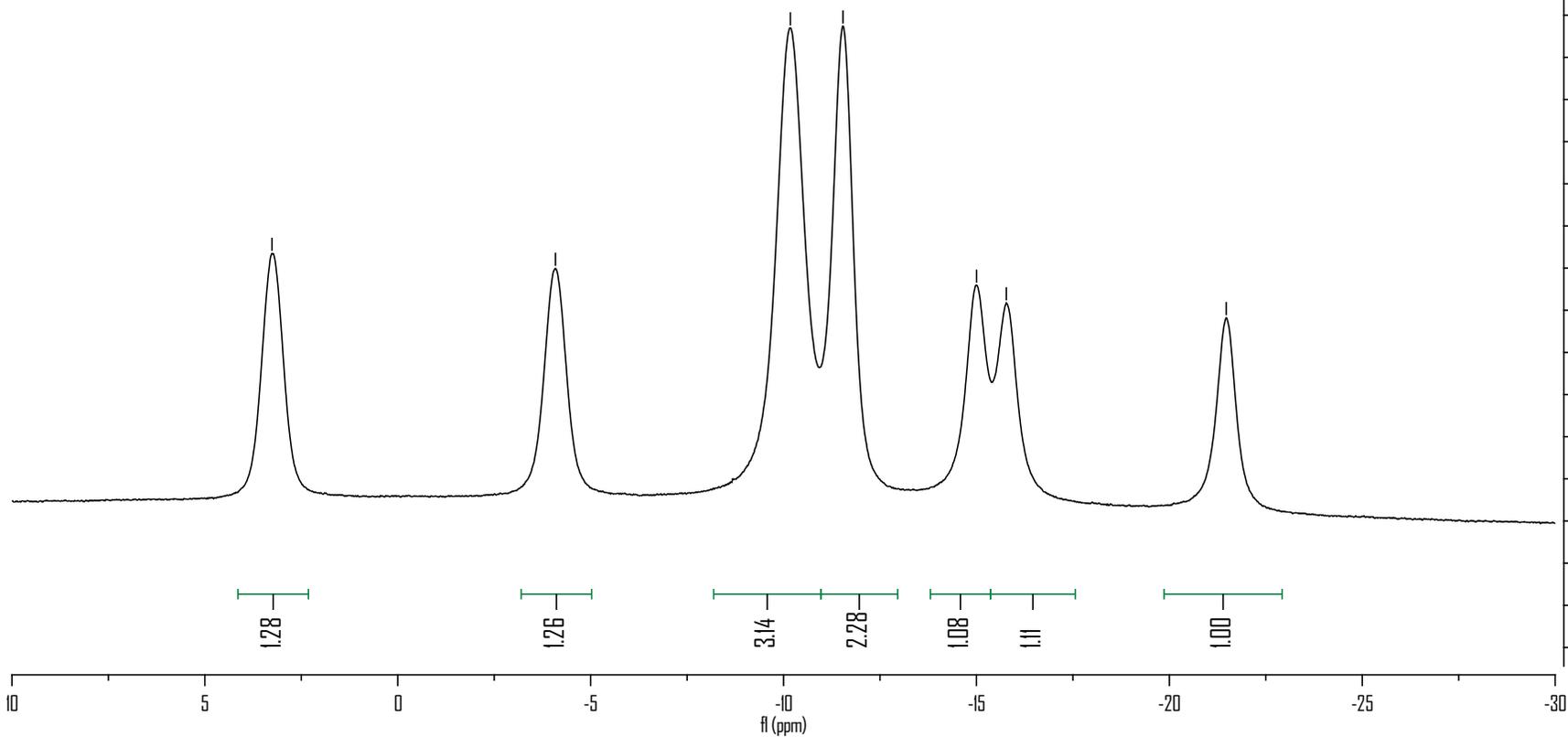
10.178

11.541

15.003

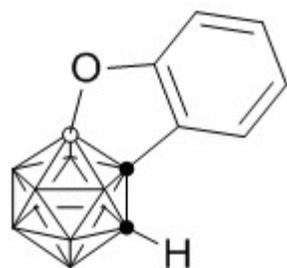
15.775

21.476

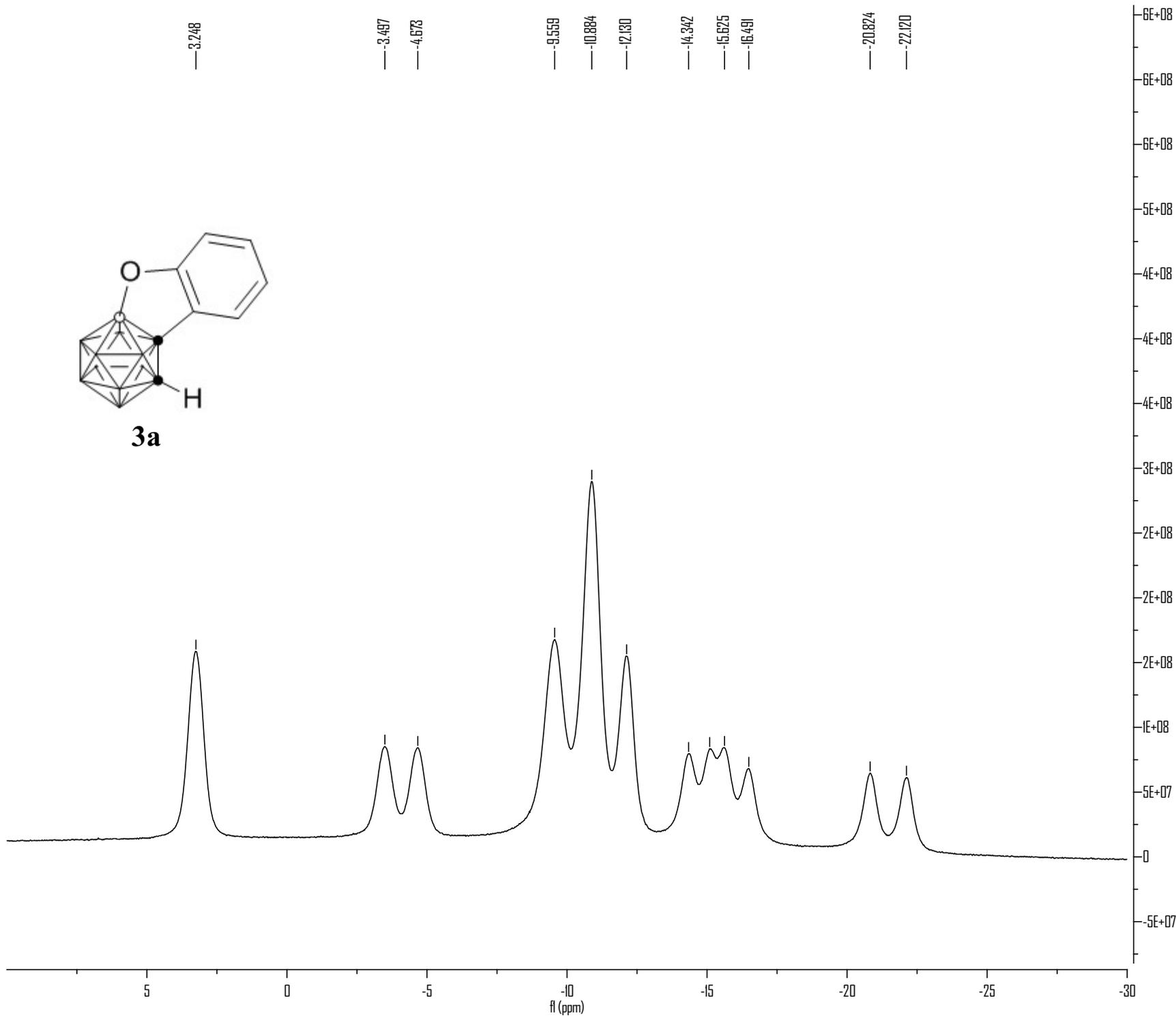


S82

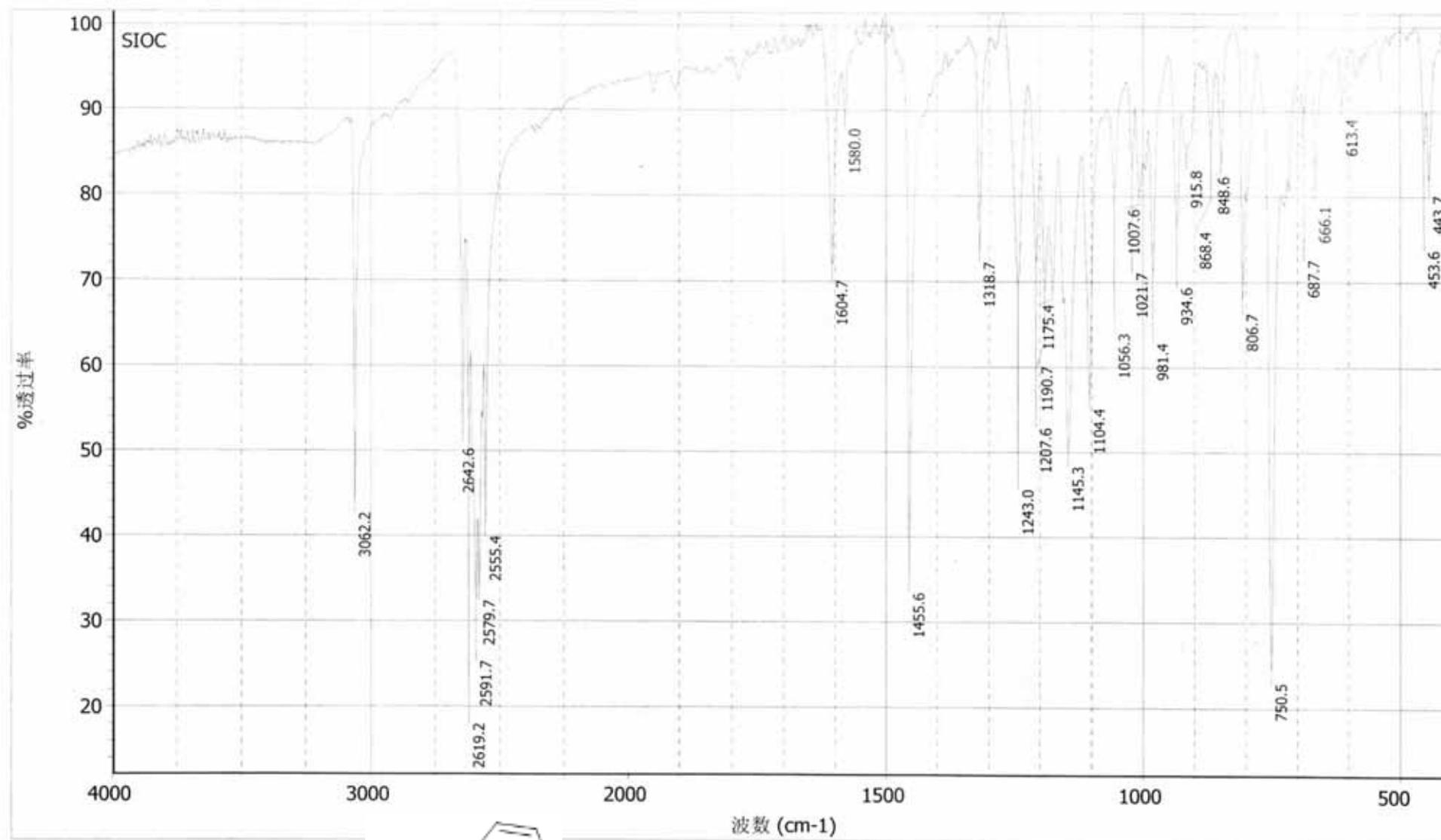
Parameter	Value
Data file Name	G:/Users/cuichunxiao/Desktop/产物数据/5-101-b/2012060b-ccx-6-10-3b/1/pdata/1/1r
Title	2012060b-ccx-6-10-3b
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	256
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	12.0000
Acquisition Time	0.512
Acquisition Date	2016-02-19 19:16:54
Modification Date	2016-02-19 13:01:55
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-17138.7
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



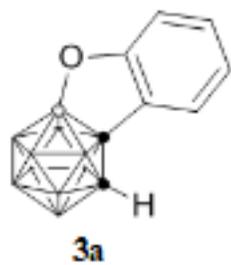
3a



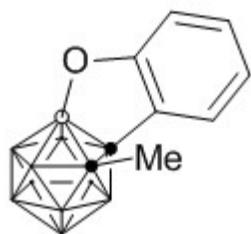
Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/5-10-b/2012060b-ccx-6-10-3b-coupling/1/pdata/1/1r
Title	2012060b-ccx-6-10-3b-coupling
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring.lgy
Number of Scans	256
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	12.0000
Acquisition Time	0.512
Acquisition Date	2016-02-19T19:25:01
Modification Date	2016-02-19T13:01:49
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-17138.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



CCX-5-101-B 2015806 JS

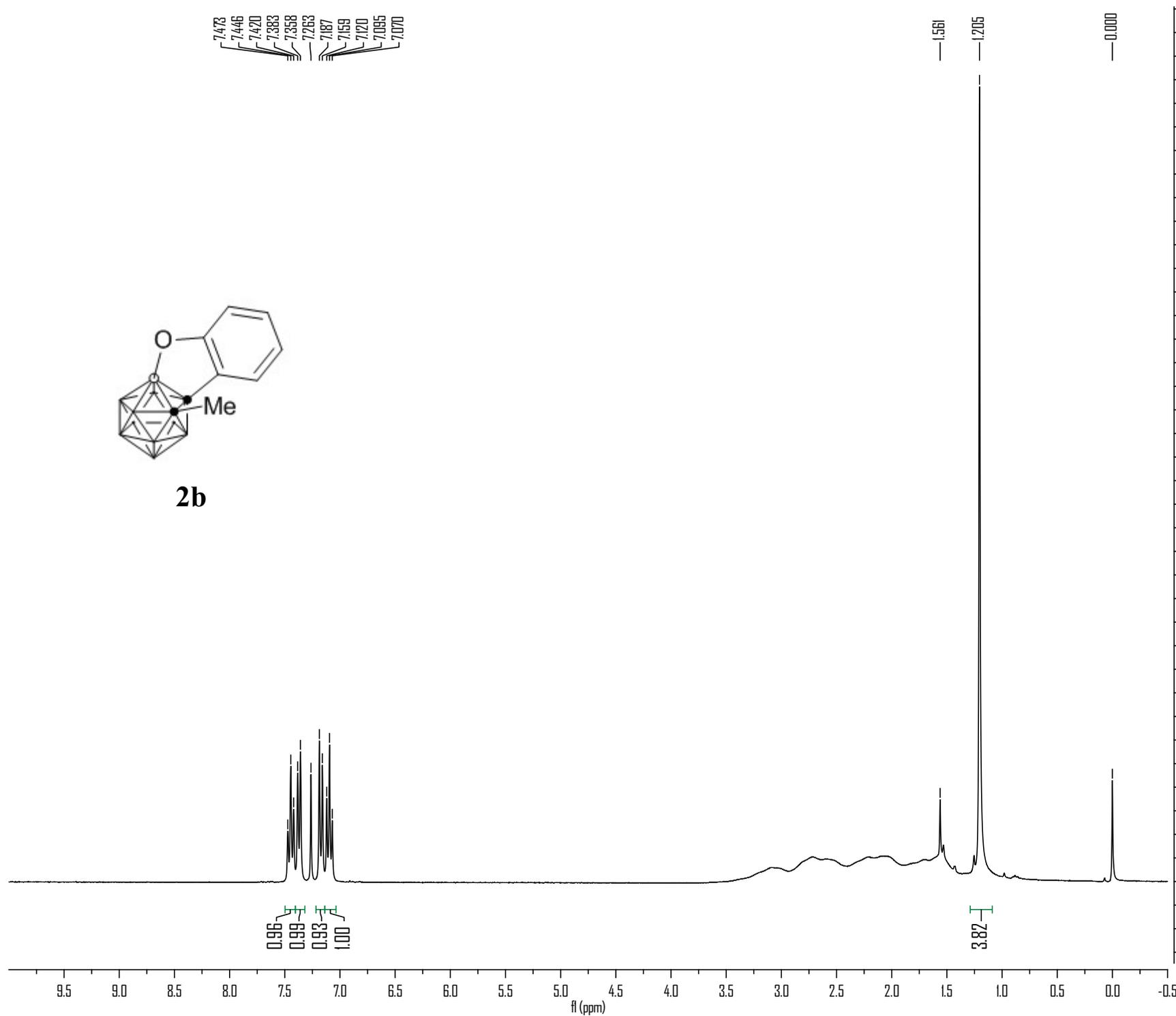


样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



2b

7.478
7.446
7.420
7.388
7.358
7.283
7.187
7.159
7.120
7.095
7.070



0.96
0.99
0.93
1.00

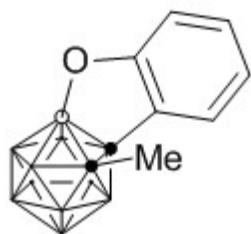
1.561

1.205

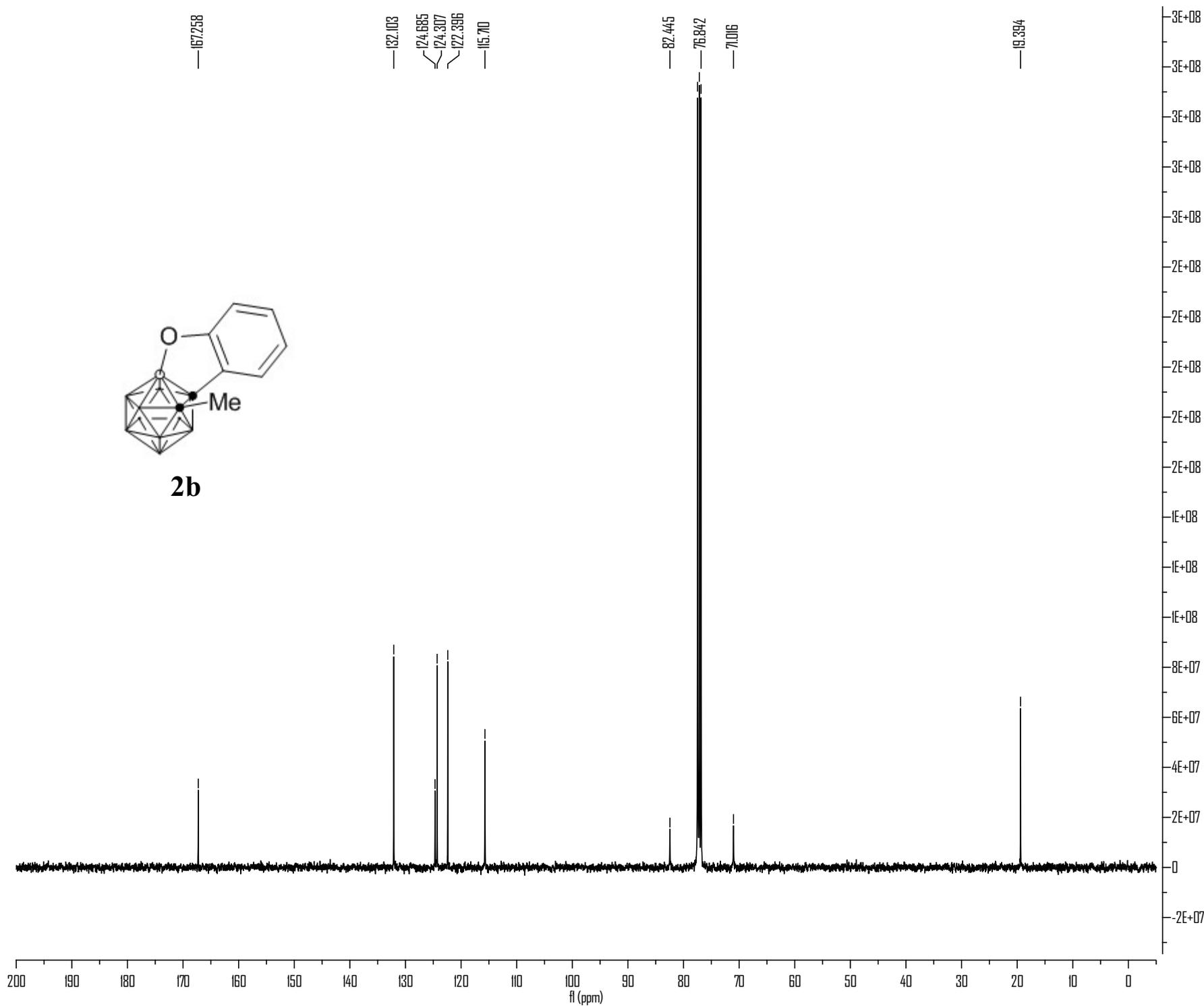
0.000

3.82

Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/6-30-a/ccx-6-30-aH.fid/fid
Title	ccx-6-30-aH
Comment	STANDARD 1H OBSERVE
Origin	Varian
Owner	
Site	
Spectrometer	mercury
Author	omc
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Number of Scans	32
Receiver Gain	28
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.0000
Acquisition Date	2016-03-30T08:40:00
Modification Date	2016-03-30T08:42:00
Spectrometer Frequency	300.03
Spectral Width	5494.5
Lowest Frequency	-709.3
Nucleus	1H
Acquired Size	10989
Spectral Size	32768

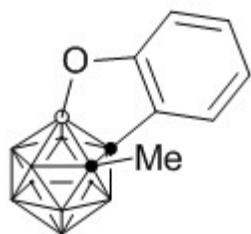


2b

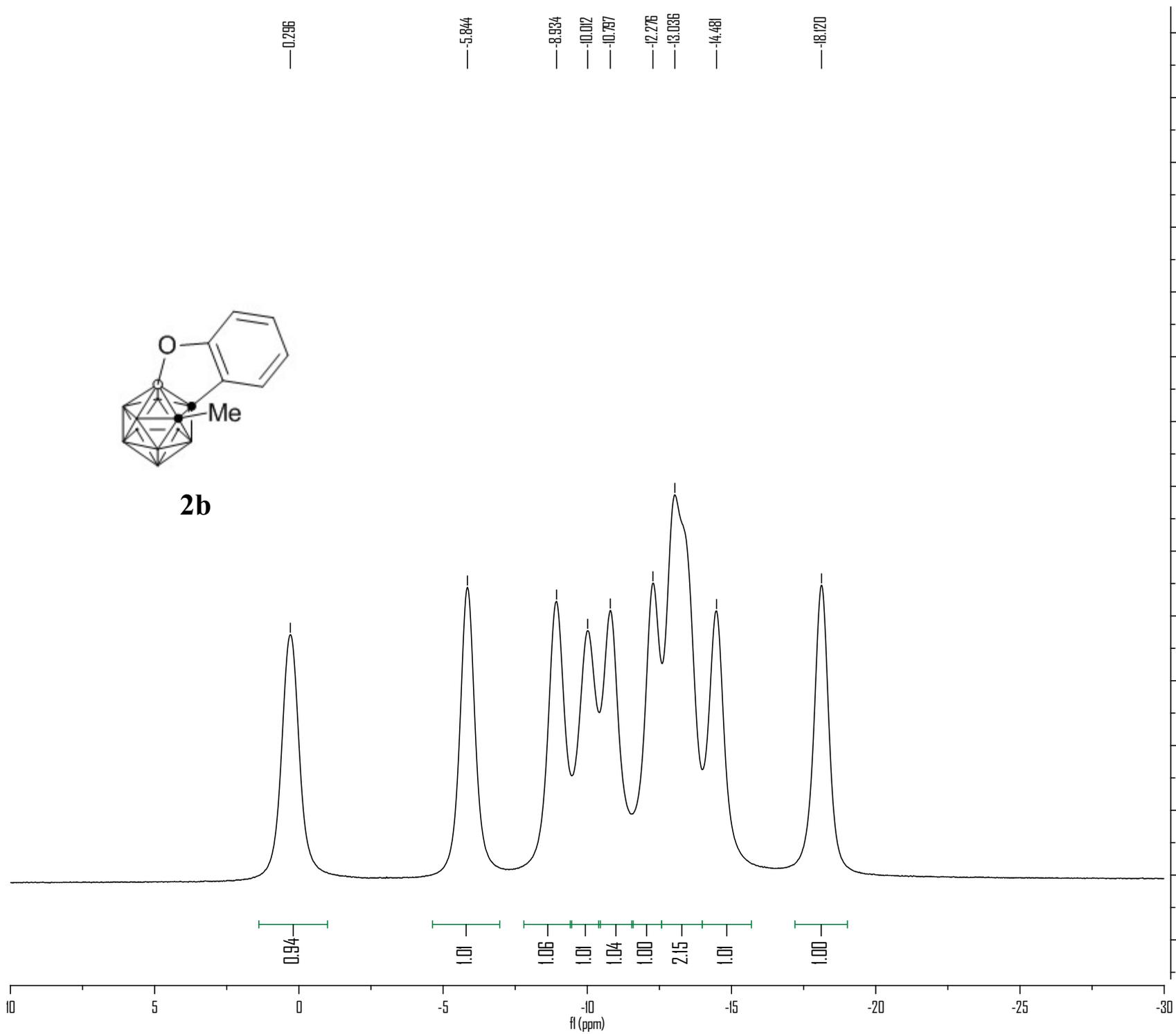


S86

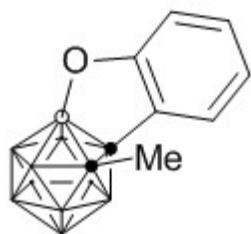
Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/6-30-a/2012060cc-cx-cx-6-30-a/3/pdata/1/1r
Title	2012060cc-cx-cx-6-30-a
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	zgdc
Number of Scans	936
Receiver Gain	16384
Relaxation Delay	3.0000
Pulse Width	4.0000
Acquisition Time	0.4653
Acquisition Date	2016-03-30T21:35:20
Modification Date	2016-03-30T14:43:47
Spectrometer Frequency	100.61
Spectral Width	35211.3
Lowest Frequency	-6677.9
Nucleus	¹³ C
Acquired Size	16384
Spectral Size	65536



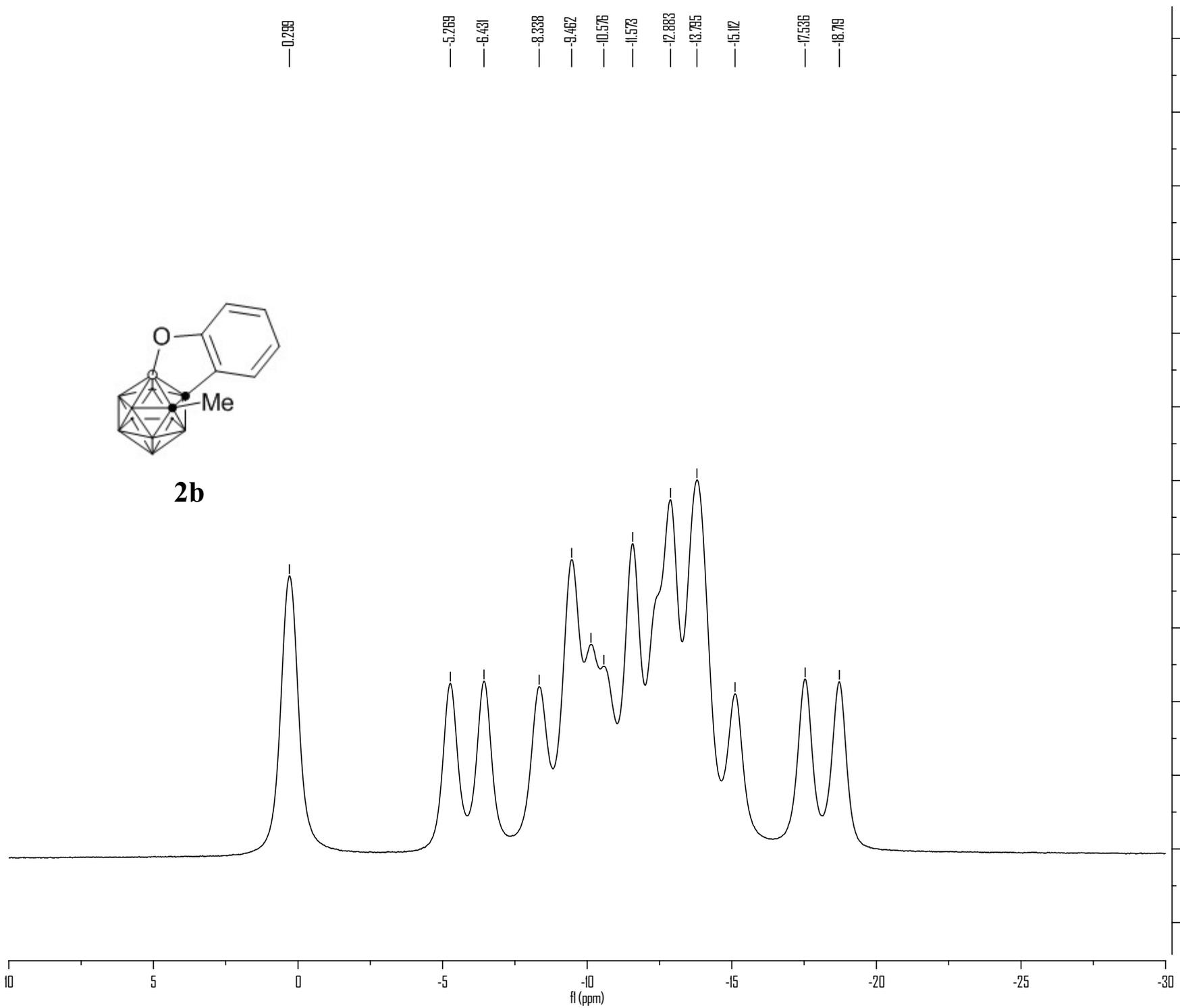
2b



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/6-30-a/2012060b-ccx-6-30a/1/pdata/1/1r
Title	2012060b-ccx-6-30a
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	128
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	8.5000
Acquisition Time	0.512
Acquisition Date	2016-03-30T18:42:58
Modification Date	2016-03-30T14:44:16
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16415.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

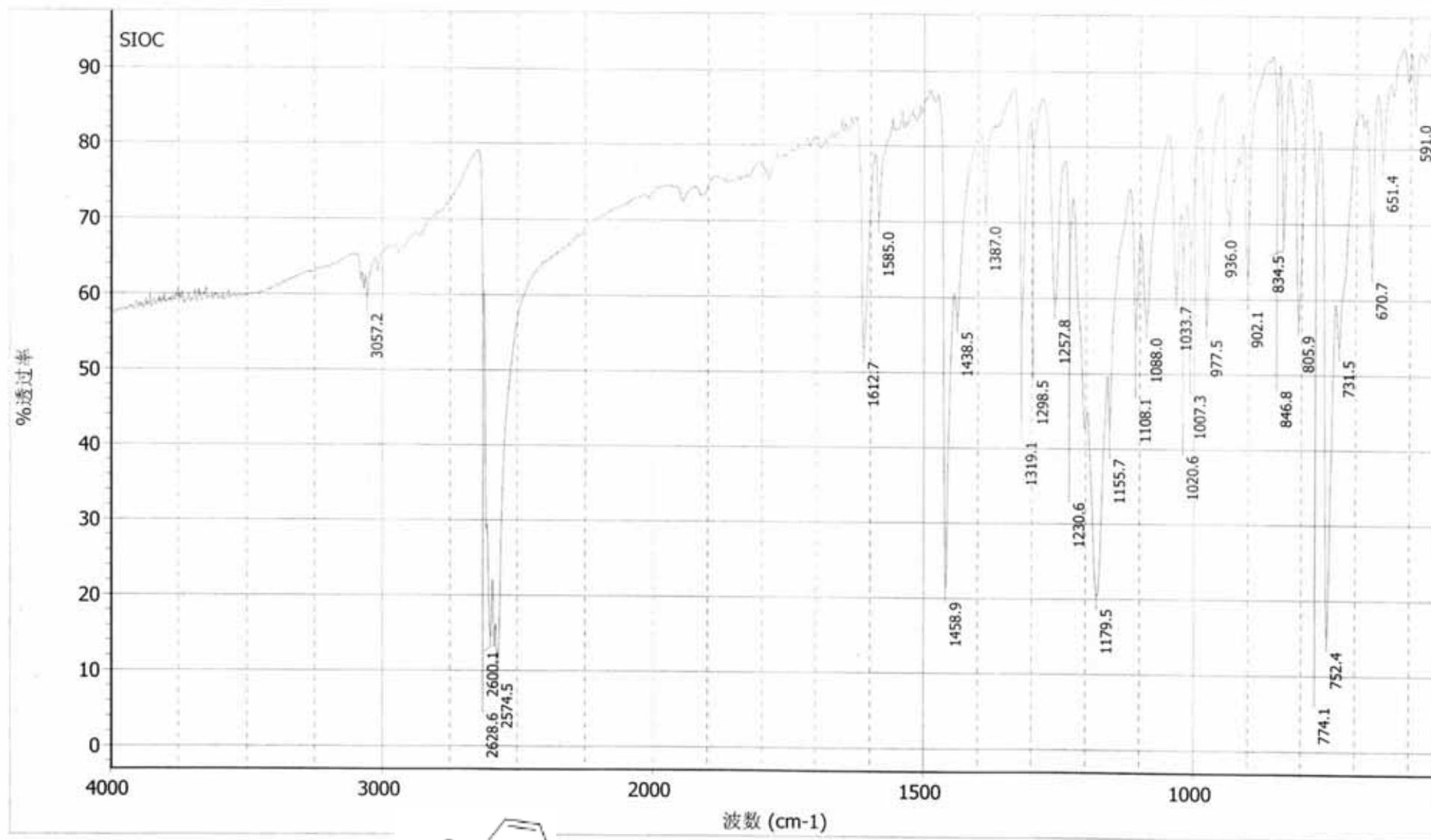


2b

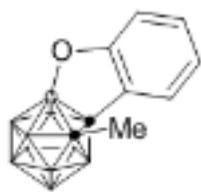


S88

Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/6-30-a/20120160b-cx-6-30a-coupling/1/pdata/1/1r
Title	20120160b-cx-6-30a-coupling
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	128
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	8.5000
Acquisition Time	0.5112
Acquisition Date	2016-03-30T18:49:04
Modification Date	2016-03-30T14:44:10
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16415.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



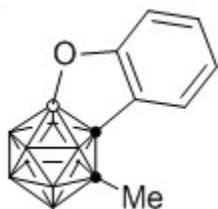
CCX-6-30-a 2015806 JS



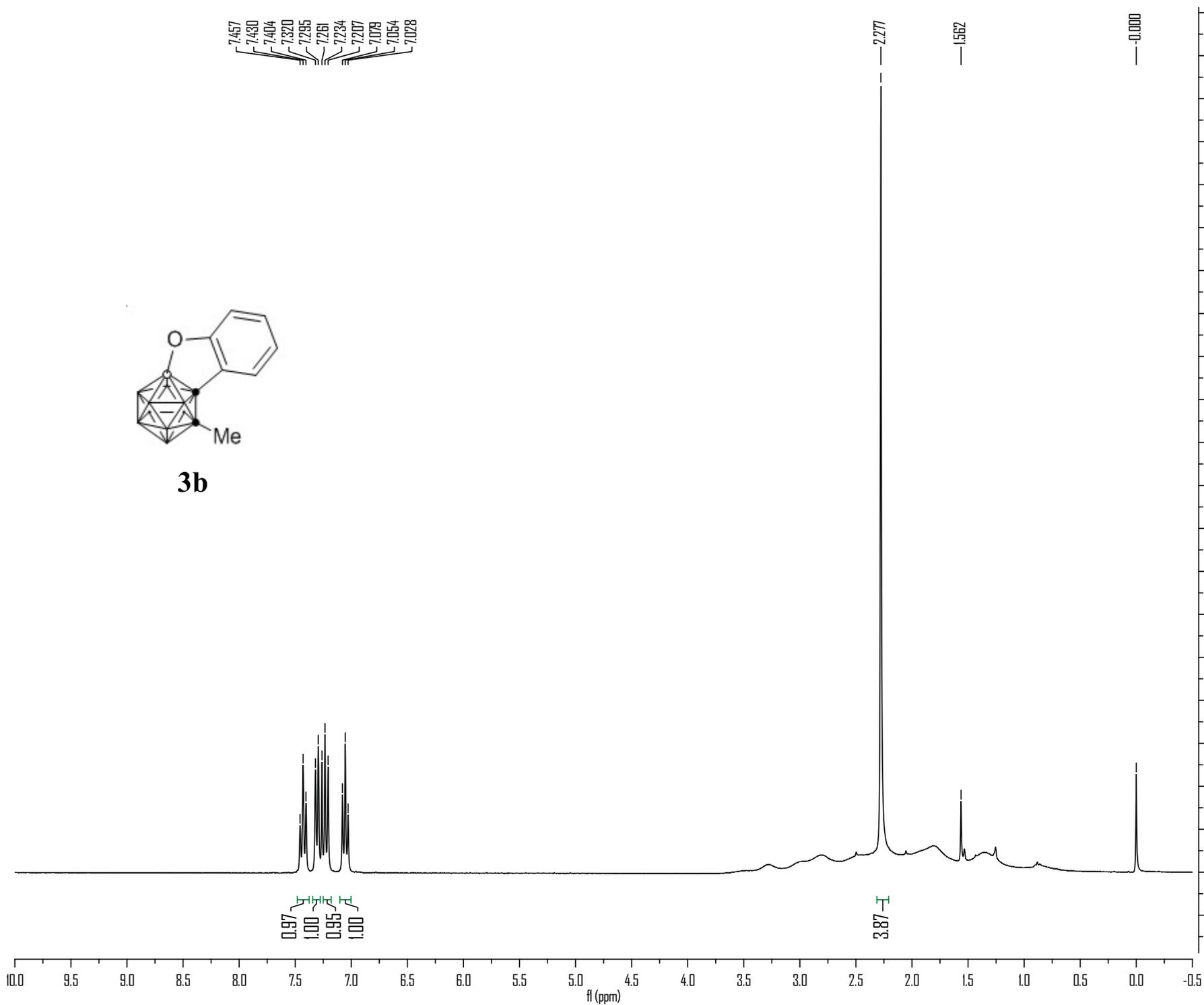
2b

样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329

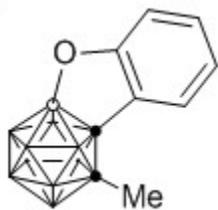
7.457
7.430
7.404
7.320
7.295
7.261
7.234
7.207
7.079
7.054
7.028



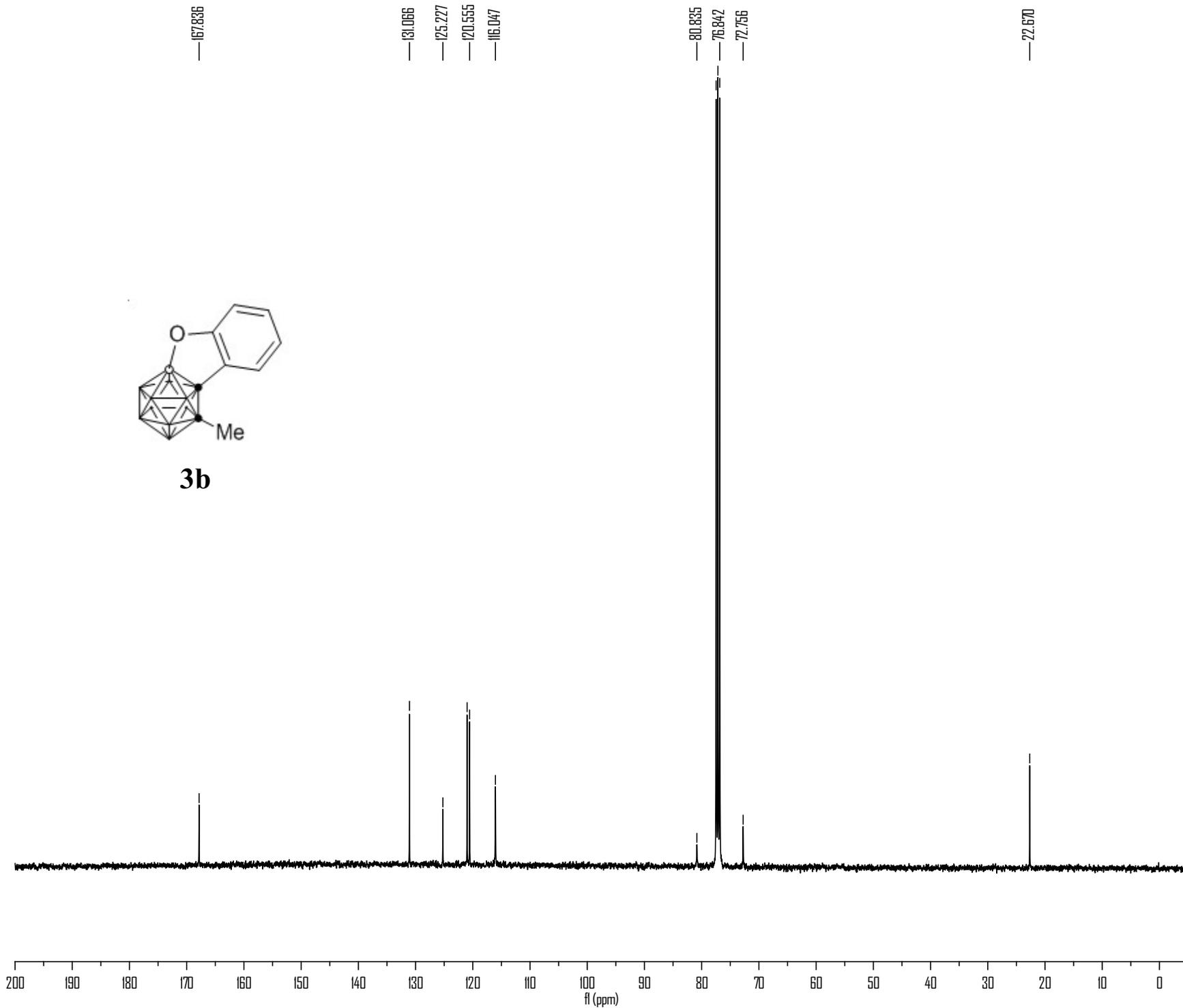
3b



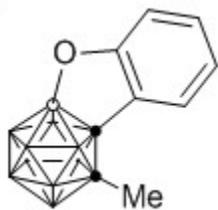
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/6-30-b/ccx-6-30-bH.fid/fid
Title	ccx-6-30-bH
Comment	STANDARD OBSERVE
Origin	Varian
Owner	
Site	
Spectrometer	mercury
Author	omc
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Number of Scans	32
Receiver Gain	28
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.0000
Acquisition Date	2016-03-30T08:43:56
Modification Date	2016-03-30T08:45:00
Spectrometer Frequency	300.03
Spectral Width	5494.5
Lowest Frequency	-709.6
Nucleus	¹ H
Acquired Size	10988
Spectral Size	32768



3b



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/6-30-b/2012060cc-cx-ccx-6-30-b/3/pdata/1/1r
Title	2012060cc-cx-ccx-6-30-b
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgdc
Number of Scans	1500
Receiver Gain	16384
Relaxation Delay	3.0000
Pulse Width	4.0000
Acquisition Time	0.4653
Acquisition Date	2016-03-30T19:05:20
Modification Date	2016-03-30T14:43:53
Spectrometer Frequency	100.61
Spectral Width	35211.3
Lowest Frequency	-6978.3
Nucleus	¹³ C
Acquired Size	16384
Spectral Size	65536



3b

4.160

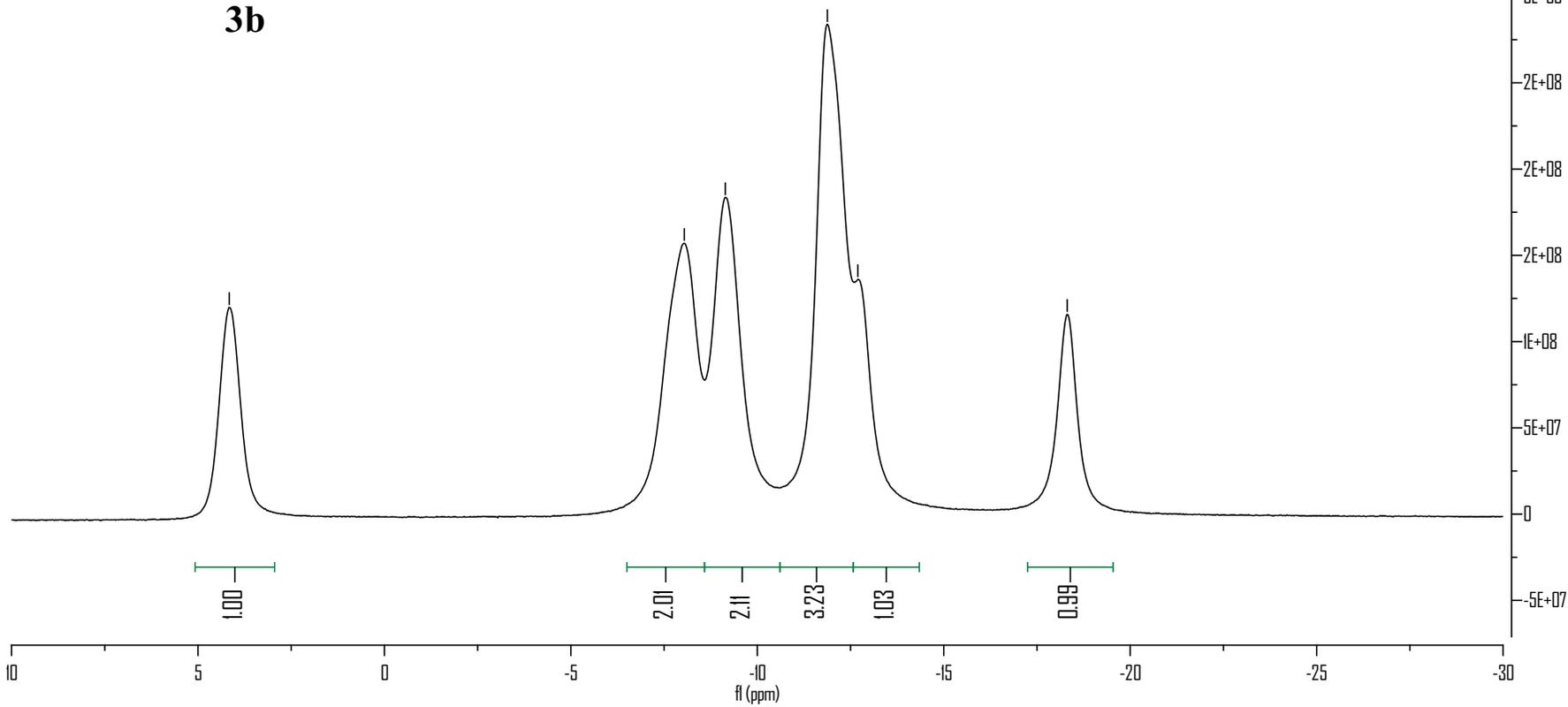
8.042

9.141

11.878

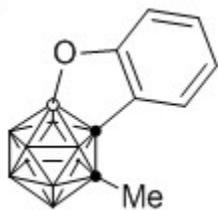
12.696

18.310



S92

Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/6-30-b/2012060b-ccx-6-30b/1/pdata/1/1r
Title	2012060b-ccx-6-30b
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	128
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	8.5000
Acquisition Time	0.512
Acquisition Date	2016-03-30T18:56:16
Modification Date	2016-03-30T14:44:04
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16415.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



3b

4.152

7.486

8.584

9.746

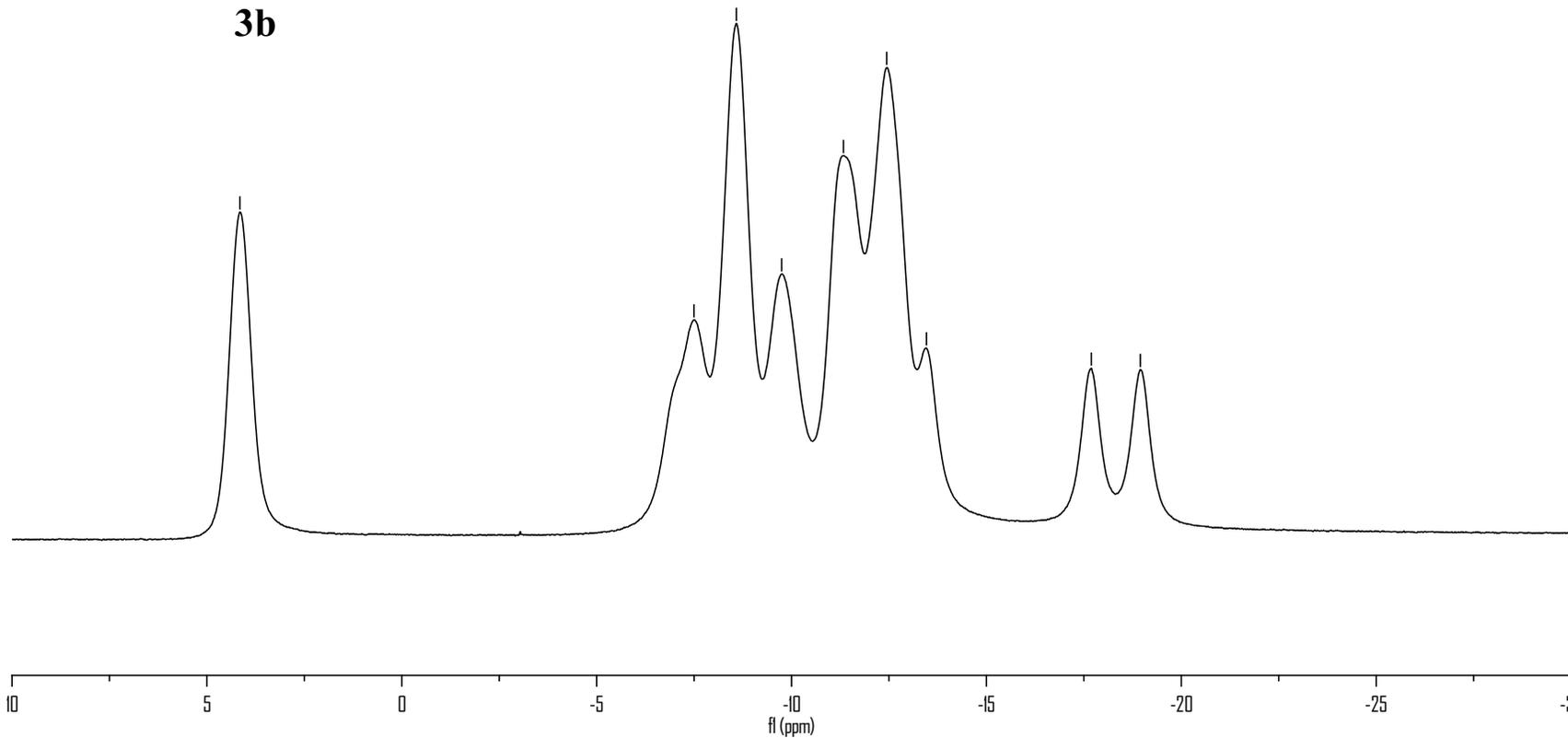
11.332

12.442

13.462

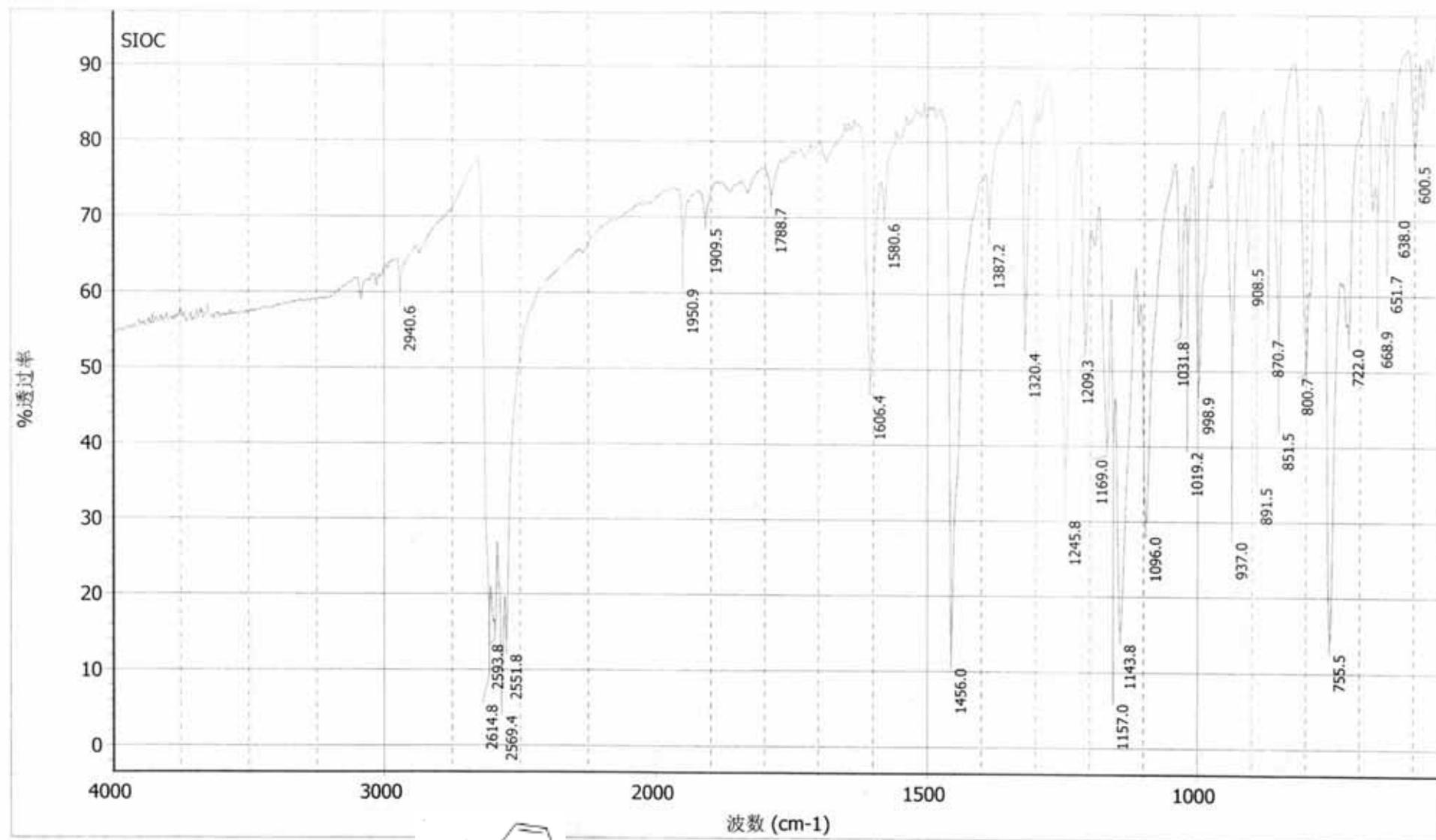
17.691

18.949

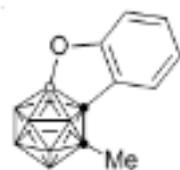


S93

Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/6-30-b/201606-cx-6-30b-coupling/1/pdata/1/1r
Title	201606-cx-6-30b-coupling
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	128
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	8.5000
Acquisition Time	0.512
Acquisition Date	2016-03-30T19:00:17
Modification Date	2016-03-30T14:43:58
Spectrometer	128.38
Frequency	
Spectral Width	32051.3
Lowest Frequency	-16415.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



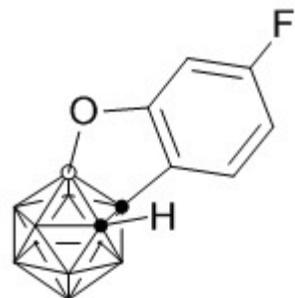
CCX-6-30-b 2015806 JS



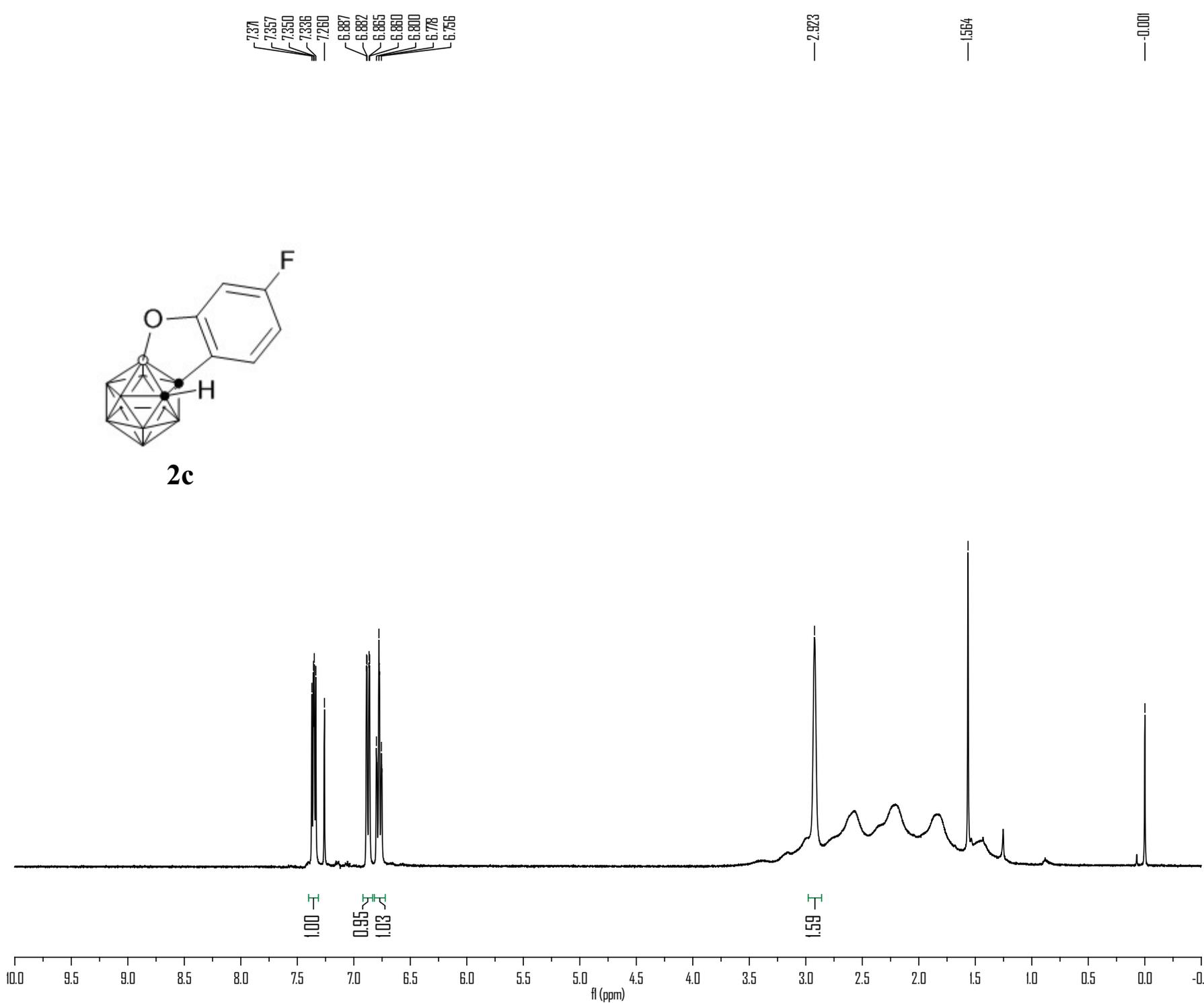
3b

样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329

7.37
7.357
7.350
7.336
7.280
6.887
6.882
6.865
6.860
6.800
6.778
6.756



2c



Parameter	Value
Title	ccx-7-74
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	36
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-10-12T11:37:34
Modification Date	2016-10-12T03:38:00
Spectrometer	400.03
Frequency	
Spectral Width	7309.9
Lowest Frequency	-806.9
Nucleus	1H
Acquired Size	21930
Spectral Size	65536

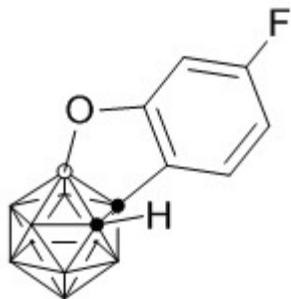
168.866
168.732
166.285
163.786

124.126
124.018
122.330
122.301

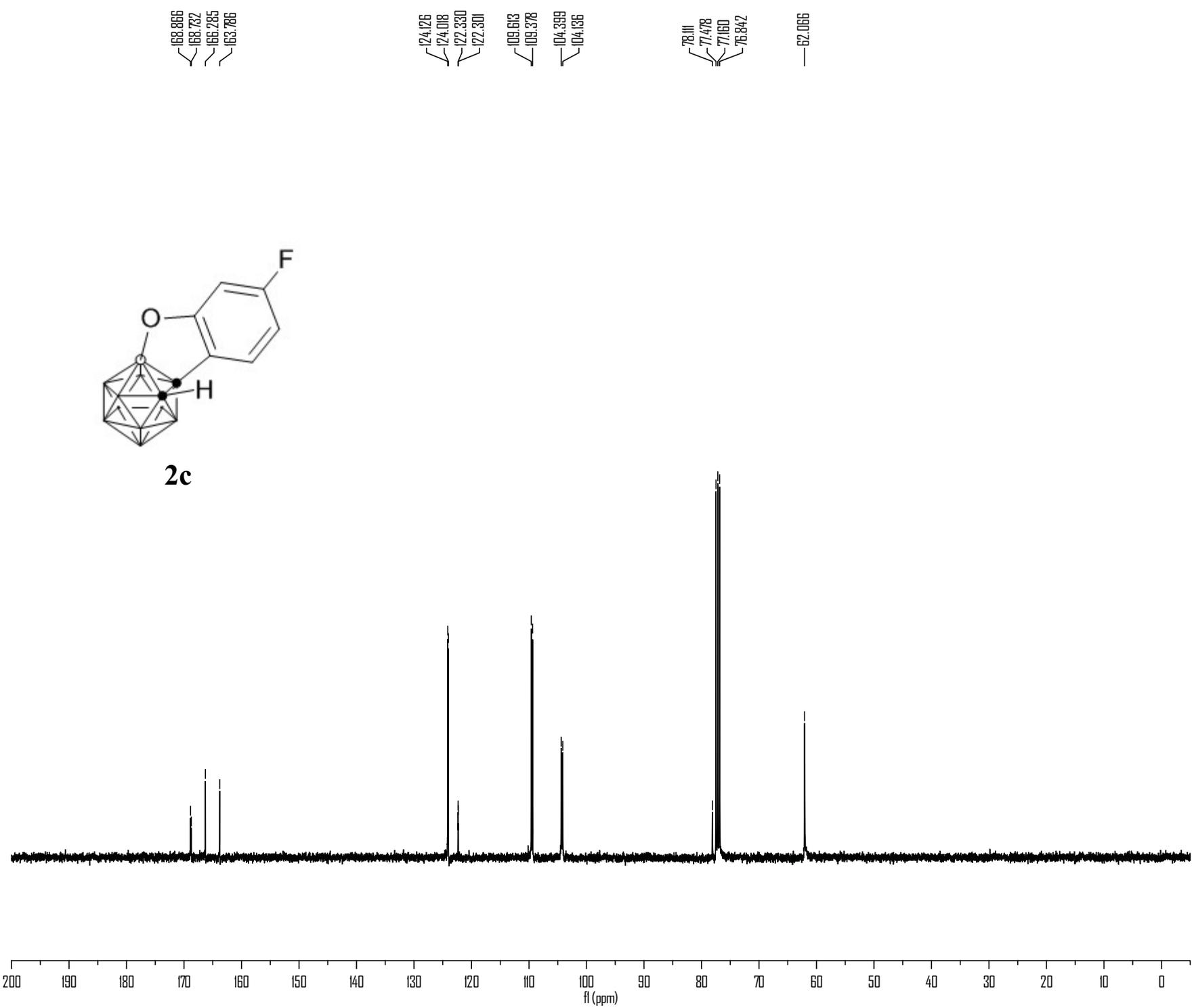
109.613
109.378
104.399
104.136

78.111
77.478
77.160
76.842

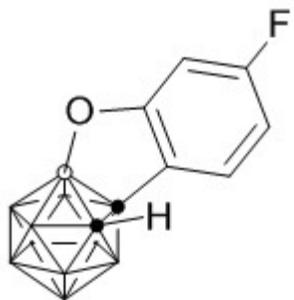
62.066



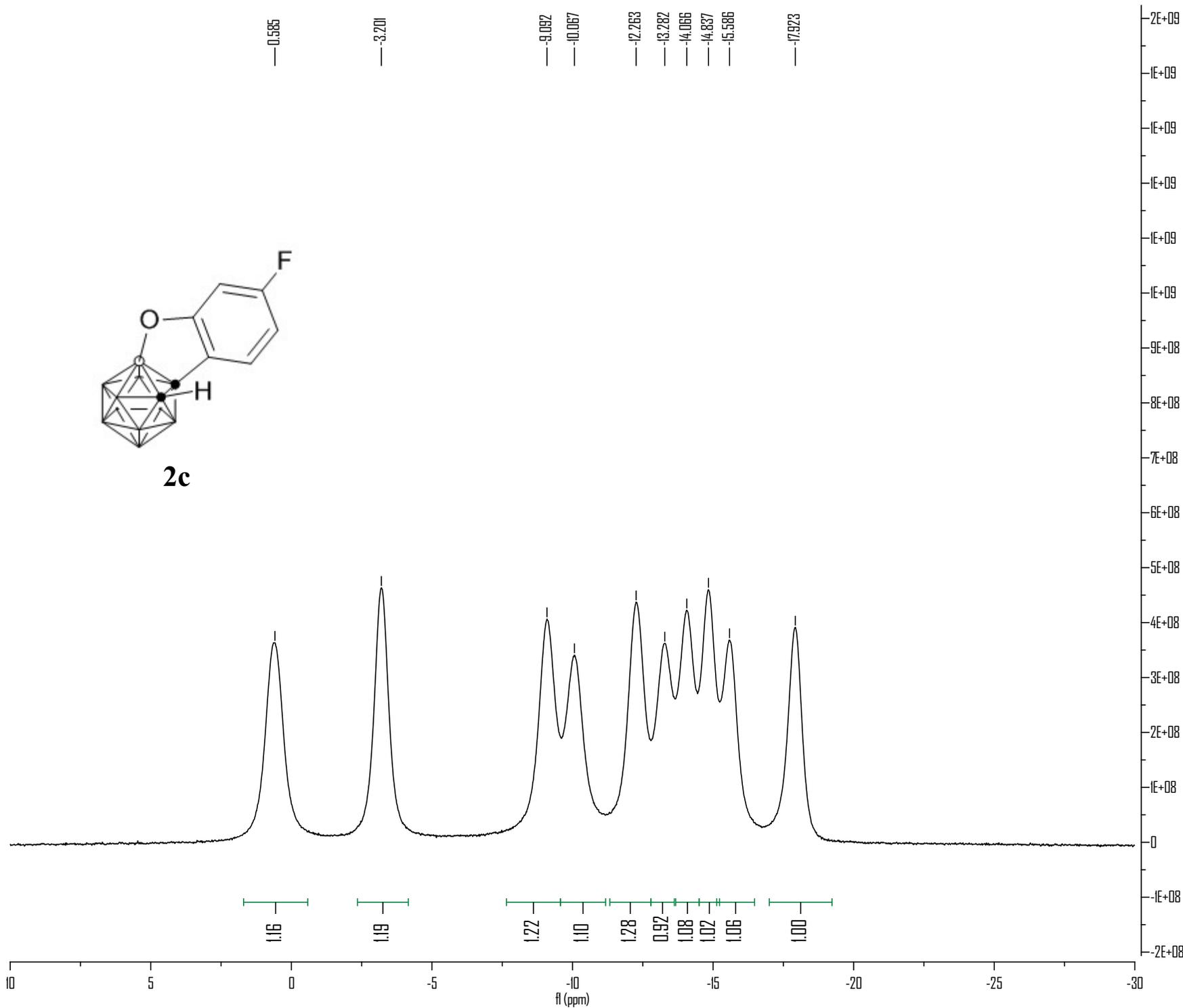
2c



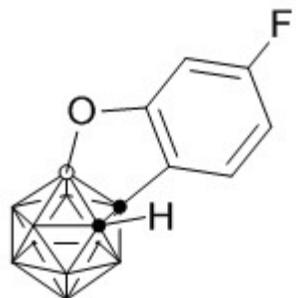
Parameter	Value
Title	-CCX-7-7-1C
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	460
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-10-13T09:22:35
Modification Date	2016-10-13T09:48:00
Spectrometer Frequency	100.51
Spectral Width	25510.2
Lowest Frequency	-1681.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



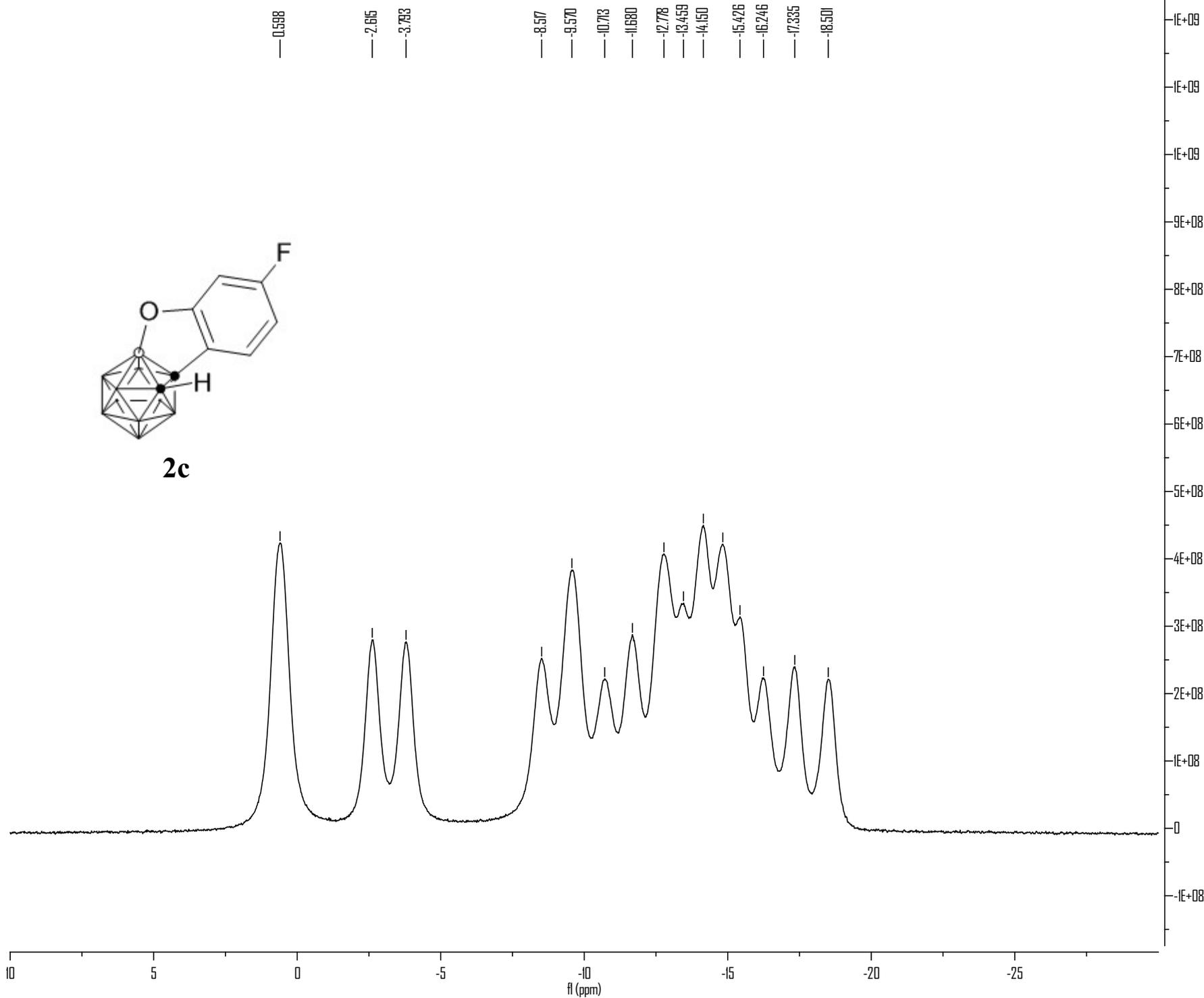
2c



Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/产物数据/7-7-a/b-ccx-7-7-1/pdata/1/1r
Title	7-7-a
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	37
Receiver Gain	181
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2016-10-13 16:58:35
Modification Date	2016-10-13 10:59:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16397.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

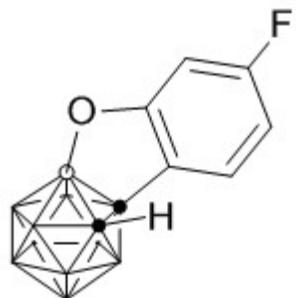


2c



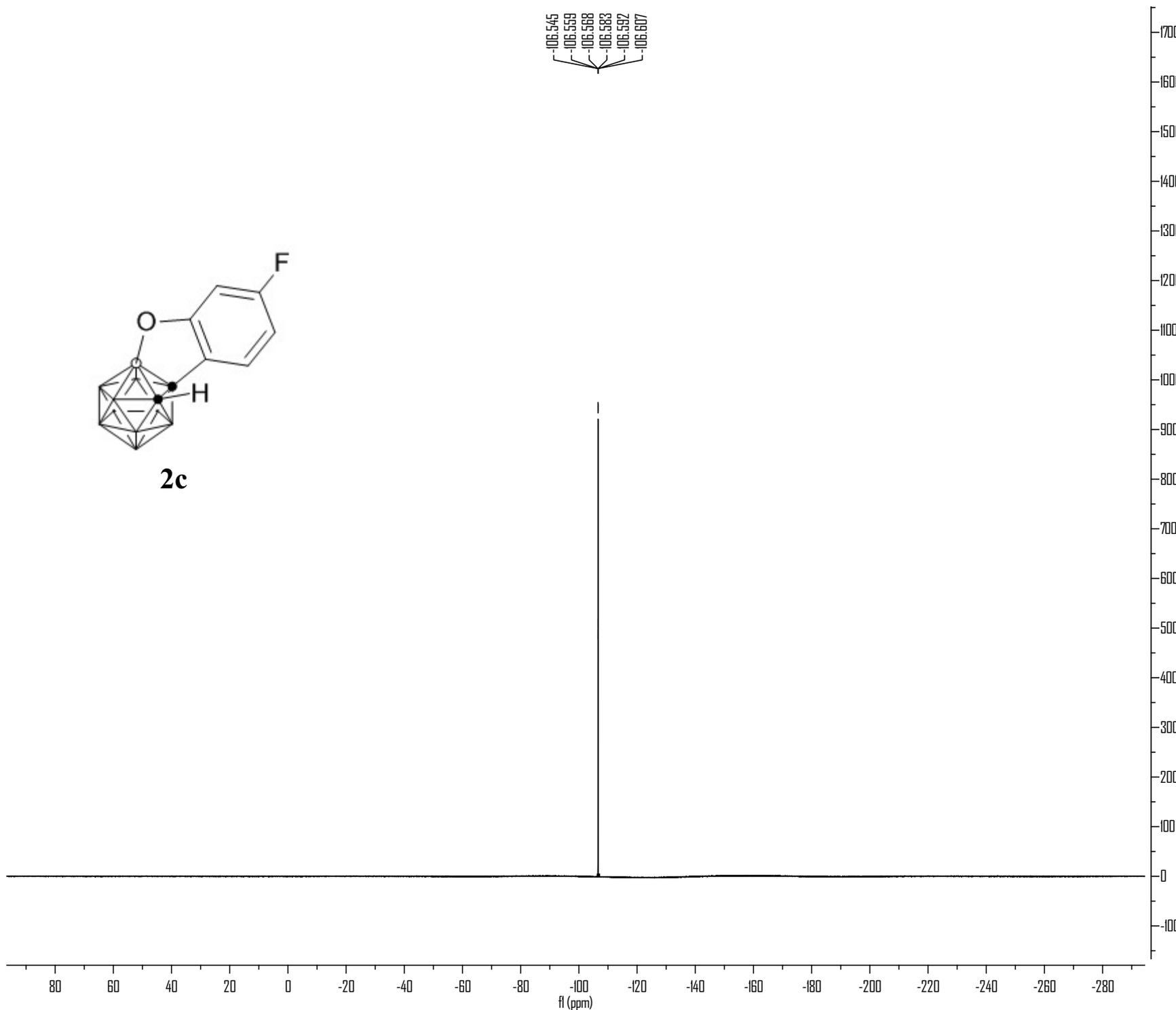
S98

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-7-a/b-cx-7-7-1-coupling/pdata/1/1r
Title	7-7-a
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	116
Receiver Gain	181
Relaxation Delay	0.0000
Pulse Width	4.0000
Acquisition Time	0.4260
Acquisition Date	2016-10-13T17:00:35
Modification Date	2016-10-13T11:01:00
Spectrometer	128.38
Frequency	
Spectral Width	38461.5
Lowest Frequency	-20607.7
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



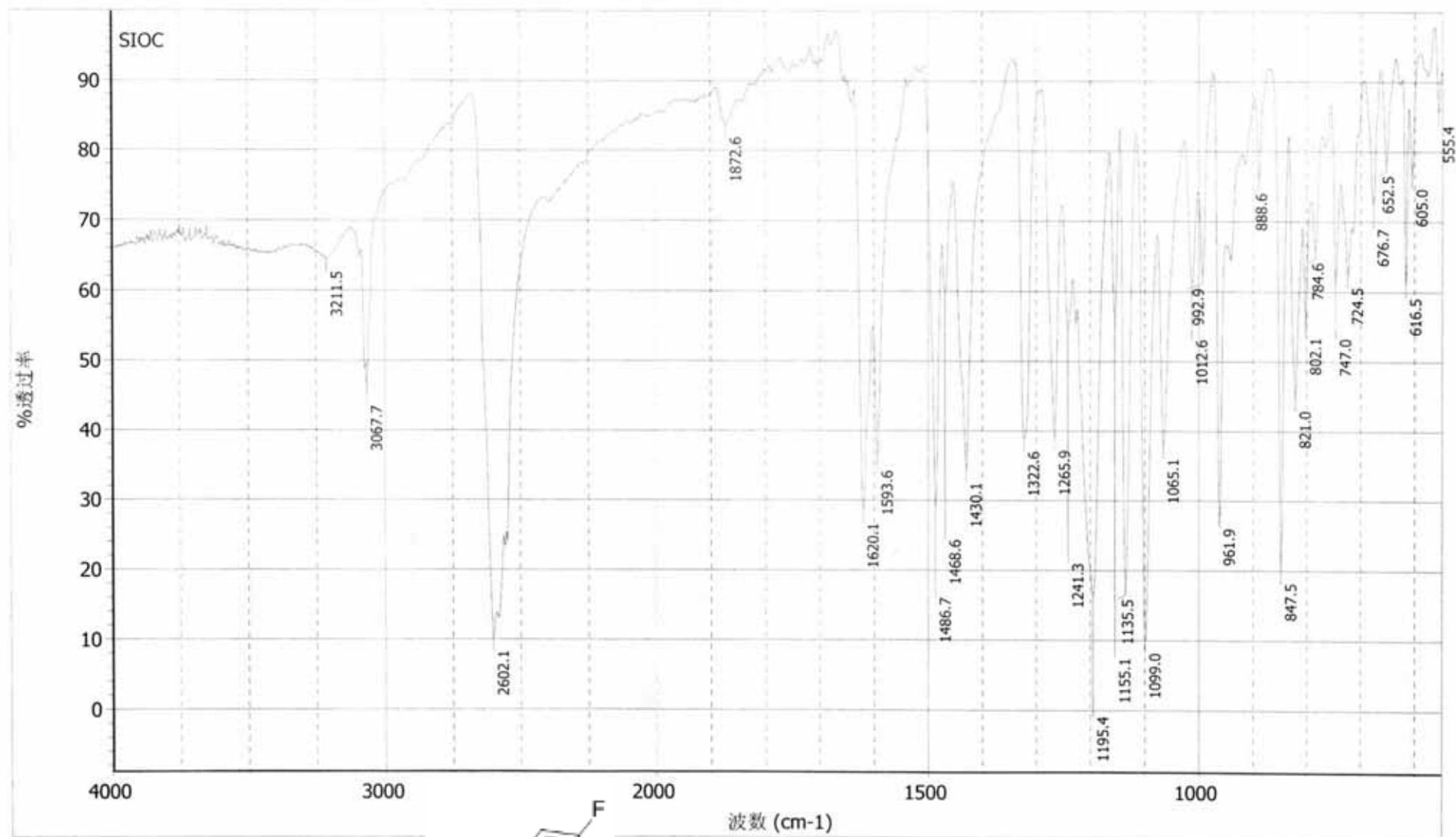
2c

106.545
106.559
106.568
106.583
106.592
106.607

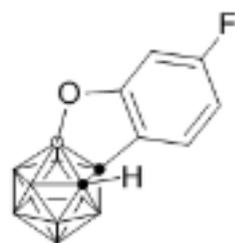


S99

Parameter	Value
Title	ccx-7-7-1F
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
A uthor	omcl
Solvent	CDCl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	44
Relaxation Delay	3.0000
Pulse Width	0.0000
A cquisition Time	1.0000
A cquisition Date	2016-10-13T08:56:28
Modification Date	2016-10-13T00:57:00
Spectrometer Frequency	376.08
Spectral Width	147058.8
Lowest Frequency	-110727.0
Nucleus	¹⁹ F
A cquired Size	147058
Spectral Size	524288

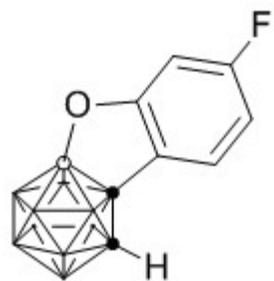


CCX-7-7-a 2015806 JS

**2c**

S100

样品扫描次数: 32
背景扫描次数: 32
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.6329



3c

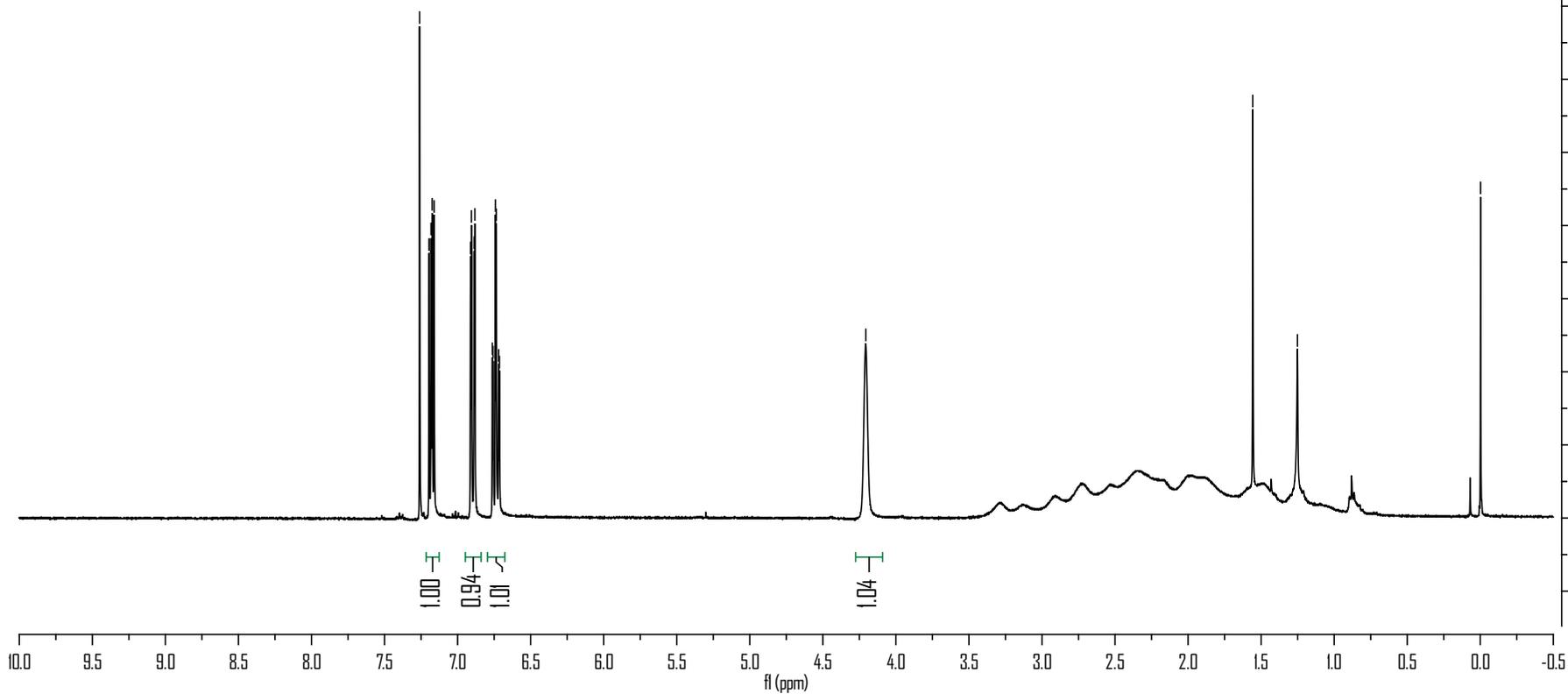
7.260
7.186
7.182
7.175
7.161
6.911
6.906
6.888
6.882
6.763
6.757
6.741
6.735
6.719
6.714

4.206

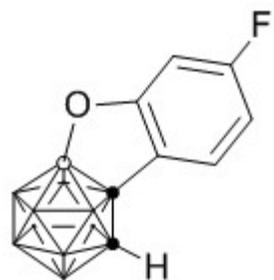
1.557

1.252

0.002



Parameter	Value
Title	ccx-7-69-2
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omcl
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	46
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-03-03T22:23:08
Modification Date	2017-03-03T14:23:00
Spectrometer	399.72
Frequency	
Spectral Width	7183.9
Lowest Frequency	-793.8
Nucleus	1H
Acquired Size	21552
Spectral Size	65536



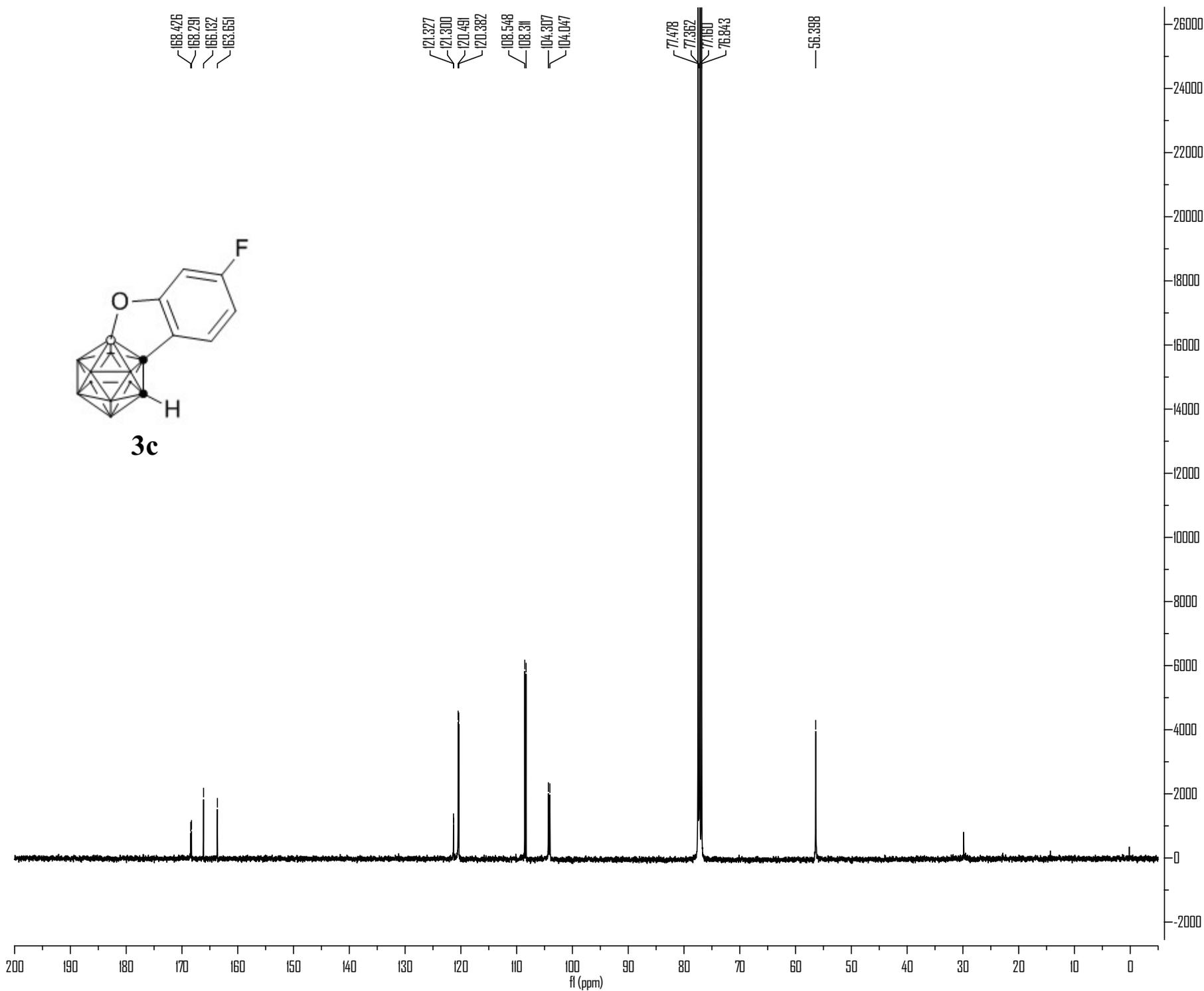
3c

168.426
168.291
166.132
163.651

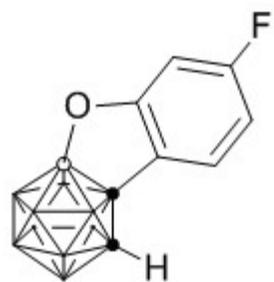
121.327
121.300
120.491
120.382
108.548
108.31
104.307
104.047

77.478
77.362
77.161
76.843

56.398



Parameter	Value
Title	ccx-7-69-2-C
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	13200
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-03-03T22:46:40
Modification Date	2017-03-03T23:13:00
Spectrometer Frequency	100.60
Spectral Width	25510.2
Lowest Frequency	-1673.7
Nucleus	¹³ C
Acquired Size	33176
Spectral Size	131072



3c

3.607

-3.890

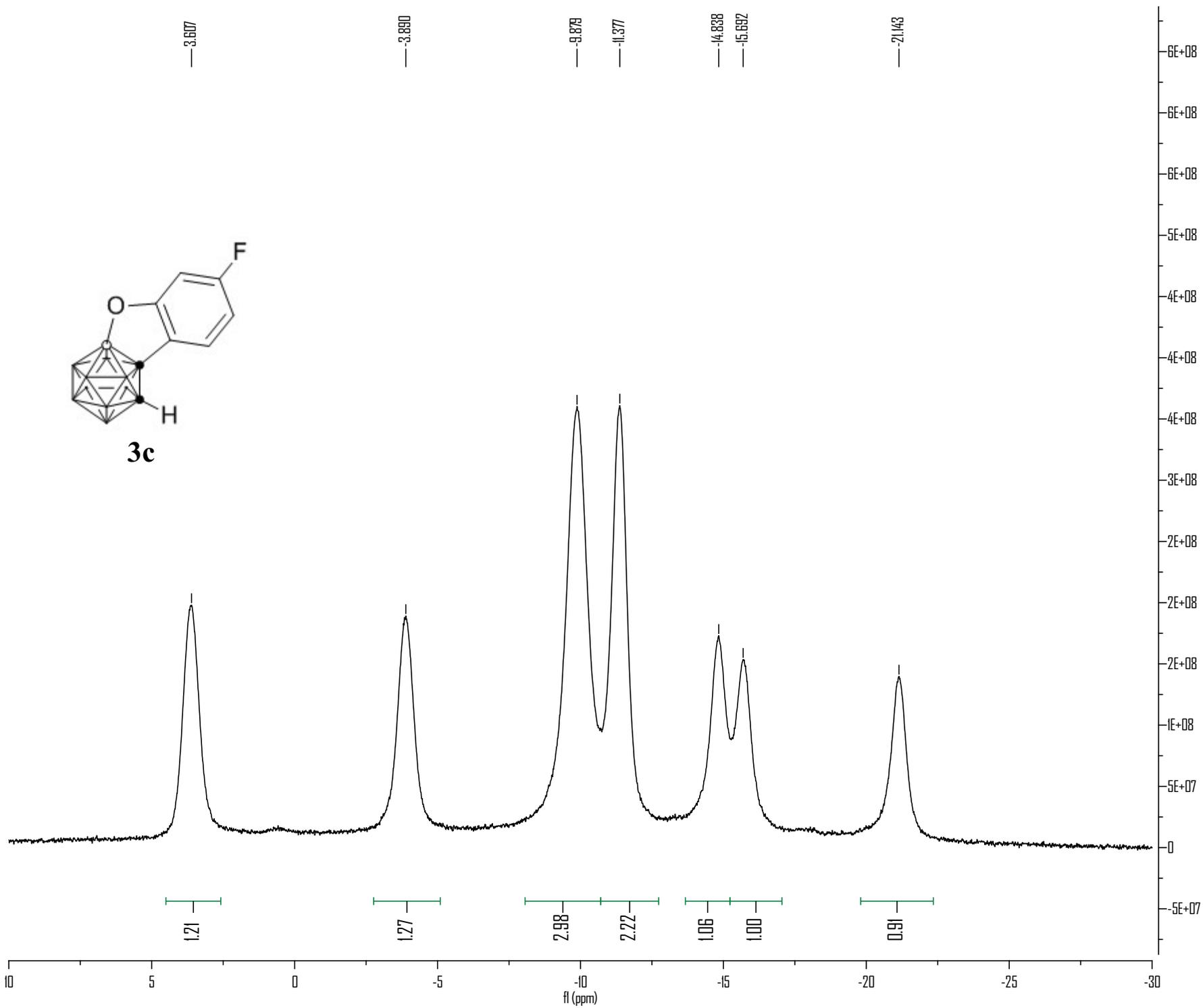
-9.879

-11.377

-14.838

-15.692

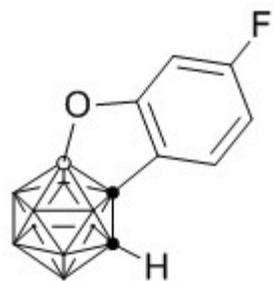
-21.143



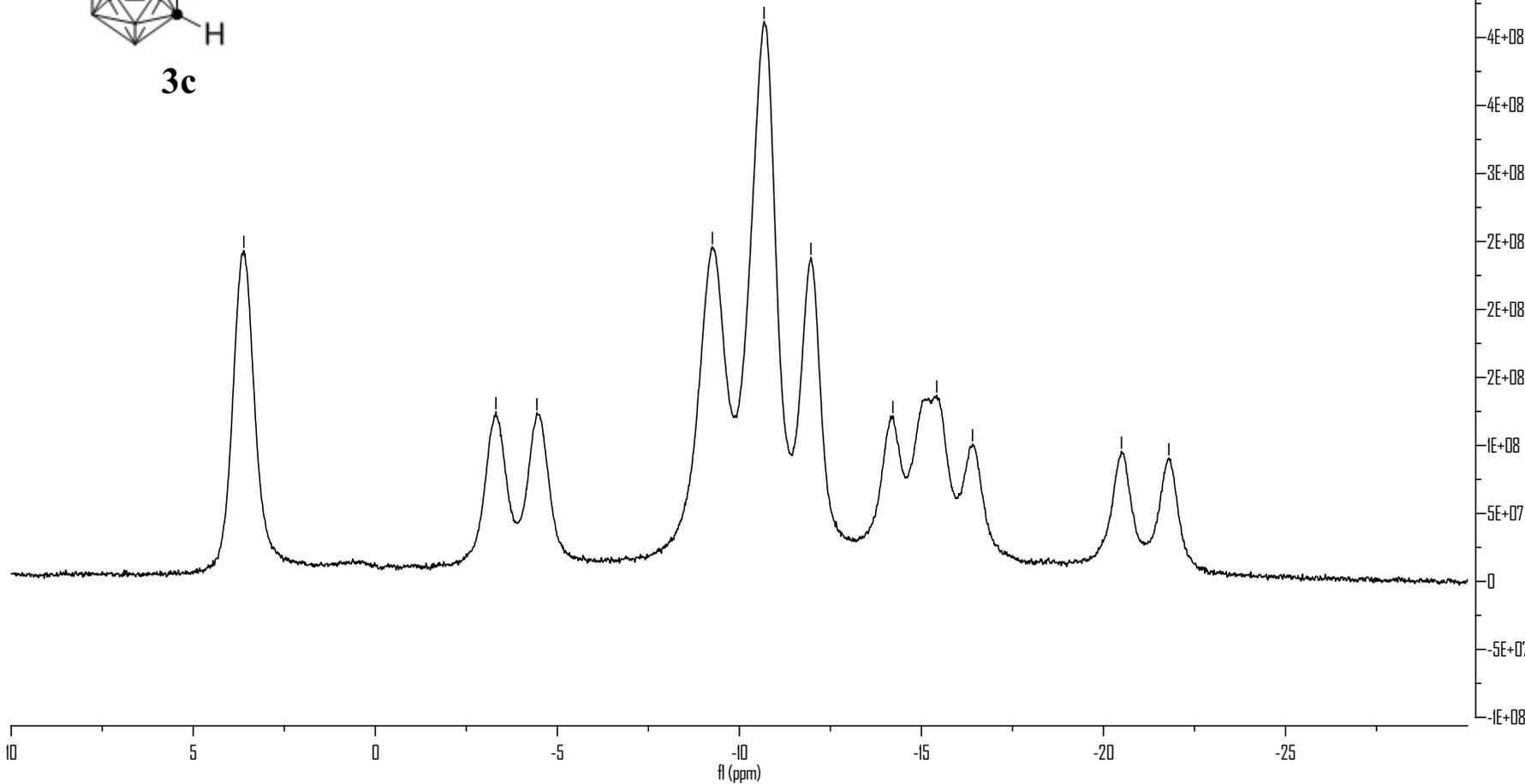
fl (ppm)

S103

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-7-b/b-cxx-7-7-2/pdata/1/1r
Title	7-7-b
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	62
Receiver Gain	287
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2016-10-13 17:06:24
Modification Date	2016-10-13 11:07:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16397.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

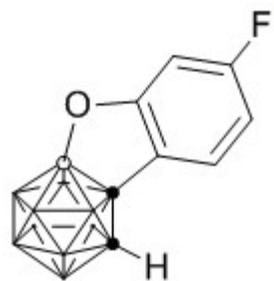


3c



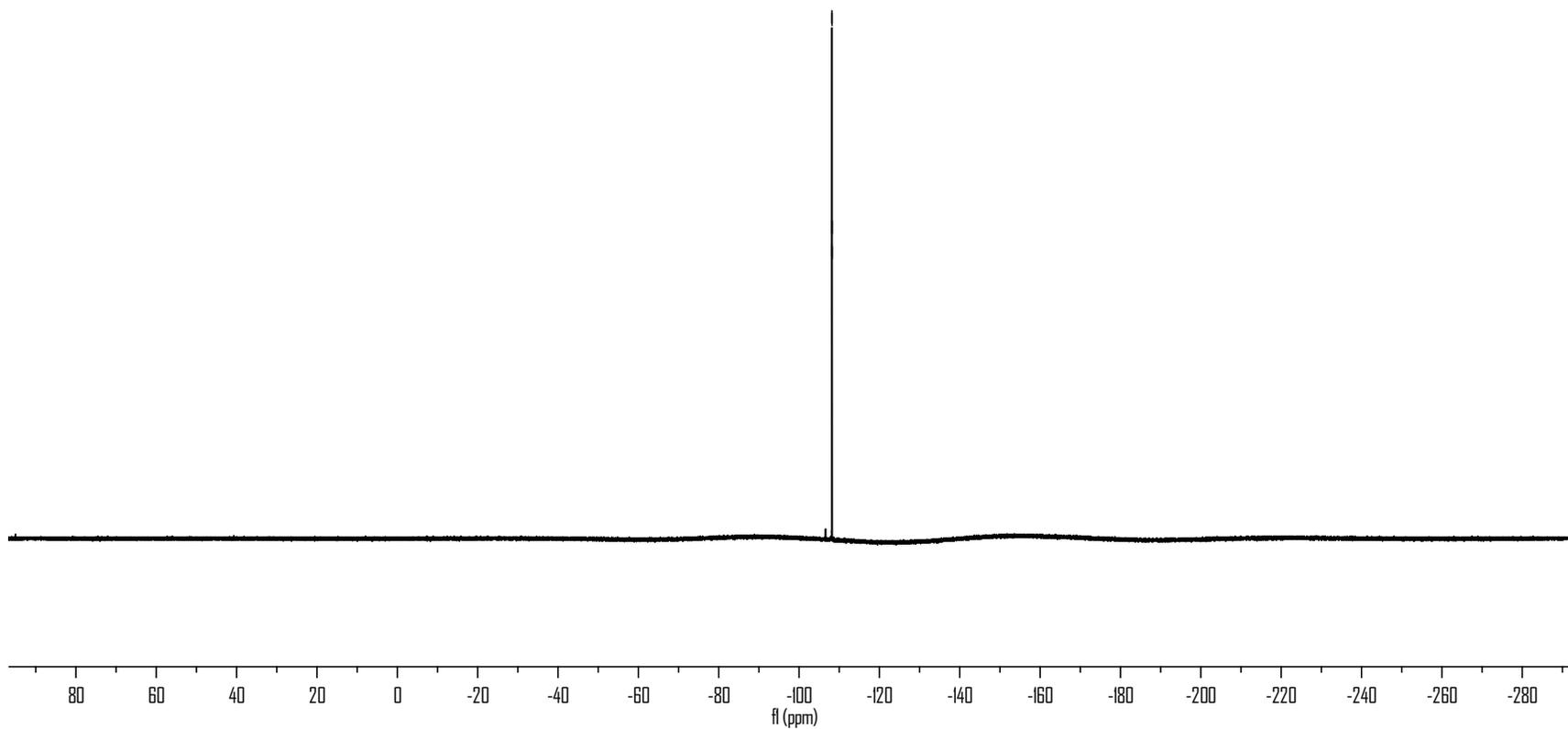
S104

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-7-b/b-cx-7-7-2-coupling/pdata/1/1r
Title	7-7-b
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	204
Receiver Gain	287
Relaxation Delay	0.0000
Pulse Width	4.0000
Acquisition Time	0.4260
Acquisition Date	2016-10-13T17:09:16
Modification Date	2016-10-13T11:09:00
Spectrometer Frequency	128.38
Spectral Width	38461.5
Lowest Frequency	-20607.7
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



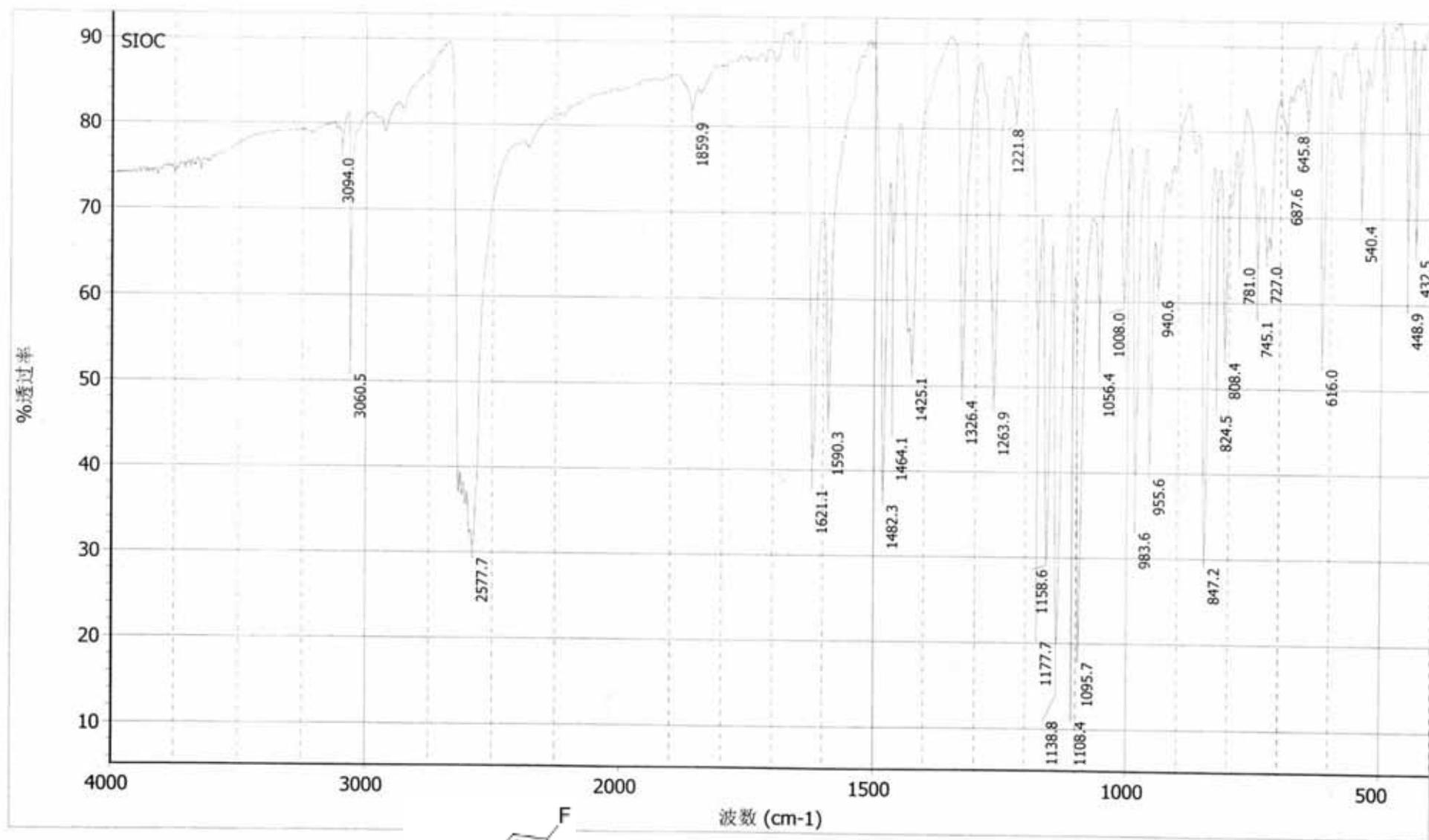
3c

-108.156
-108.17
-108.181
-108.195
-108.205
-108.219

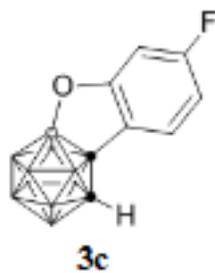


S105

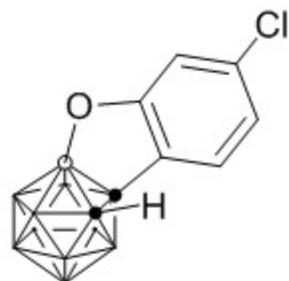
Parameter	Value
Title	ccx-7-7-2f
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omel
Solvent	CDCl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	44
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	1.0000
Acquisition Date	2016-10-13T08:50:38
Modification Date	2016-10-13T00:52:00
Spectrometer Frequency	376.08
Spectral Width	147058.8
Lowest Frequency	-110727.0
Nucleus	19F
Acquired Size	147059
Spectral Size	524288



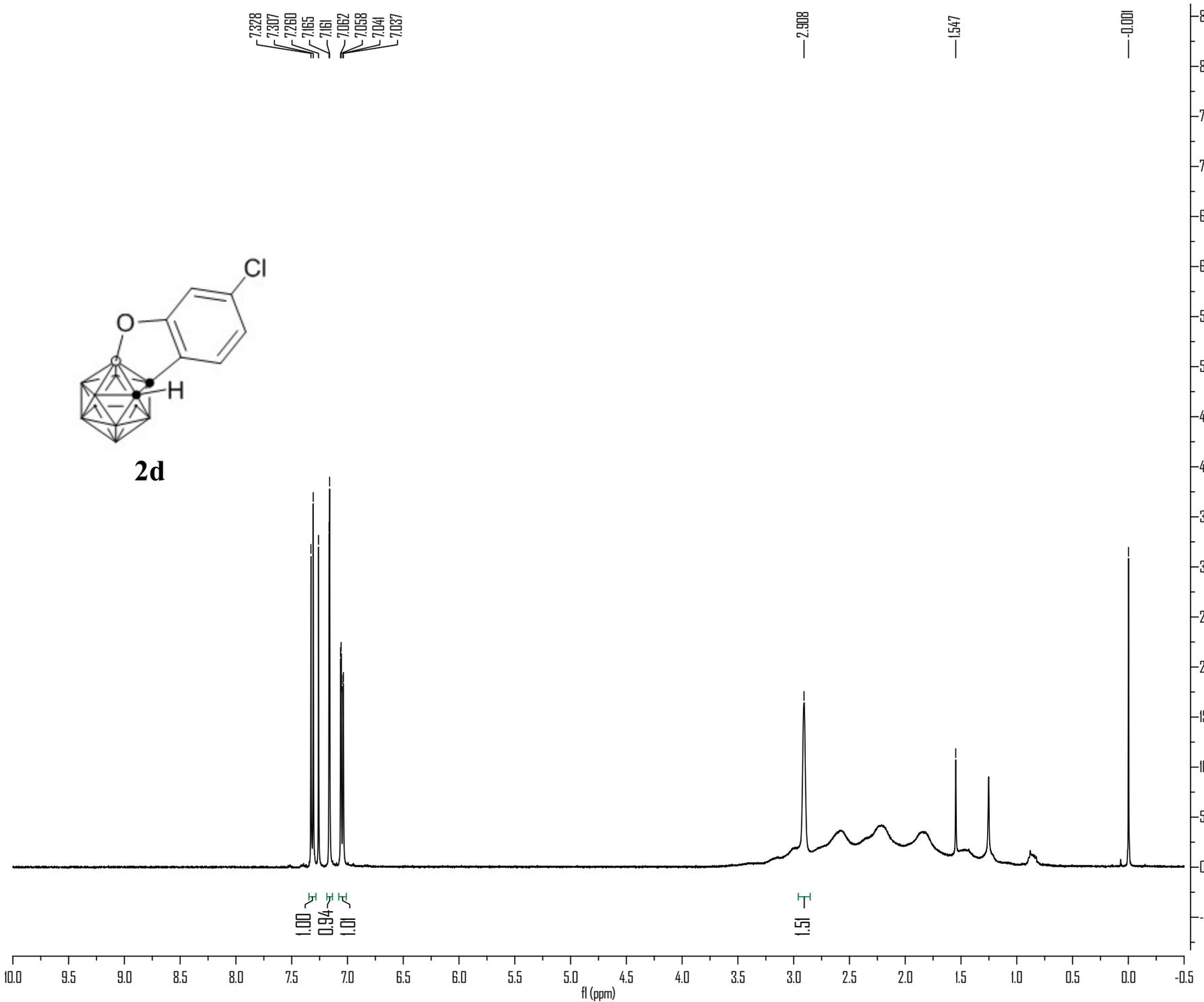
CCX-7-7-B 2015806 JS



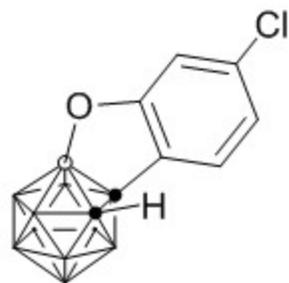
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



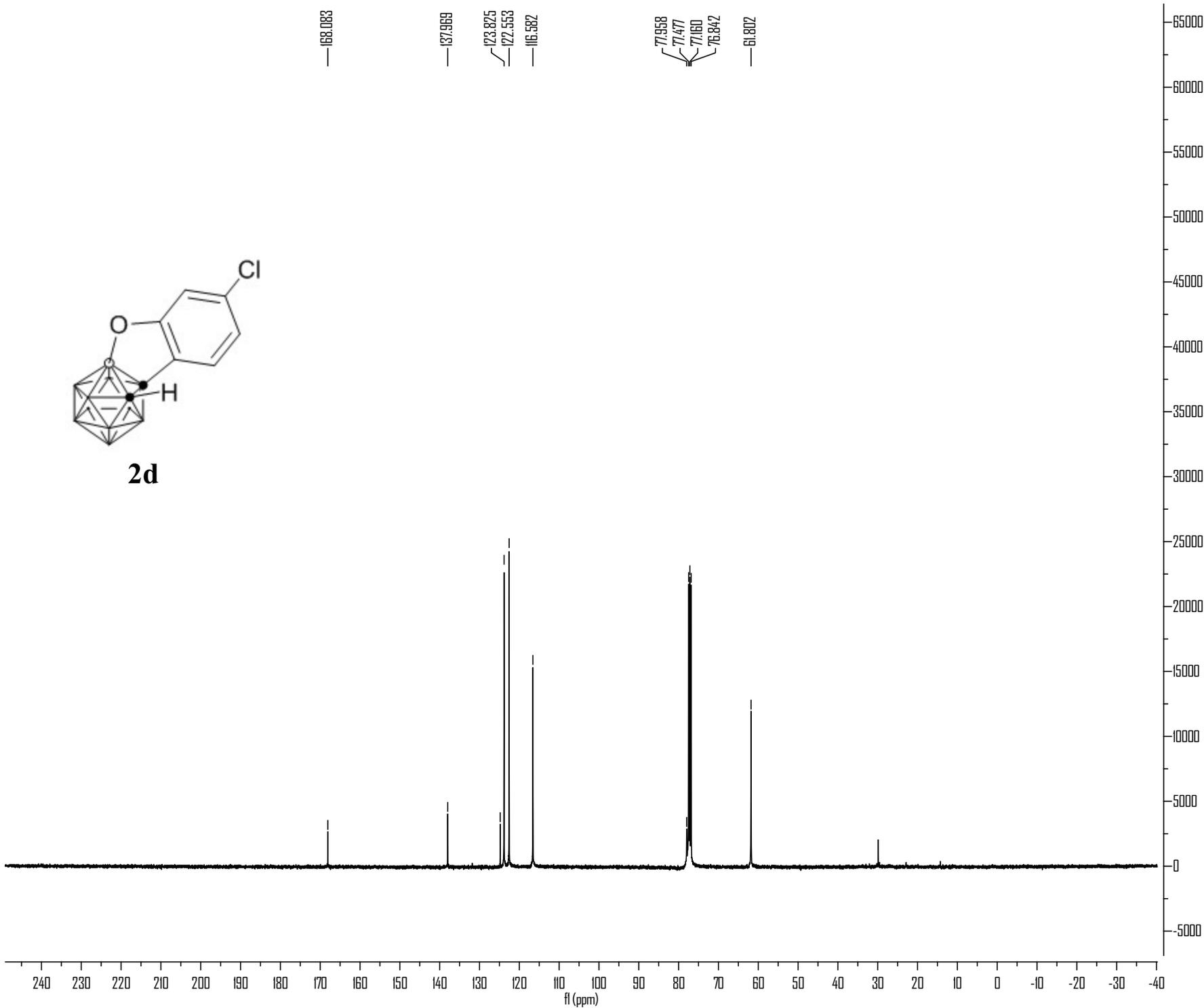
2d



Parameter	Value
Title	ccx-7-55-1
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	48
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-02-12T16:53:45
Modification Date	2017-02-12T08:54:00
Spectrometer	399.72
Frequency	
Spectral Width	7183.9
Lowest Frequency	-793.8
Nucleus	1H
Acquired Size	21552
Spectral Size	65536

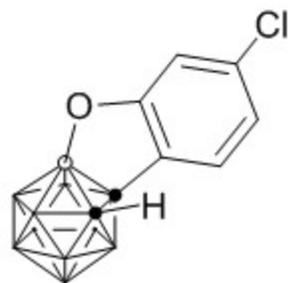


2d

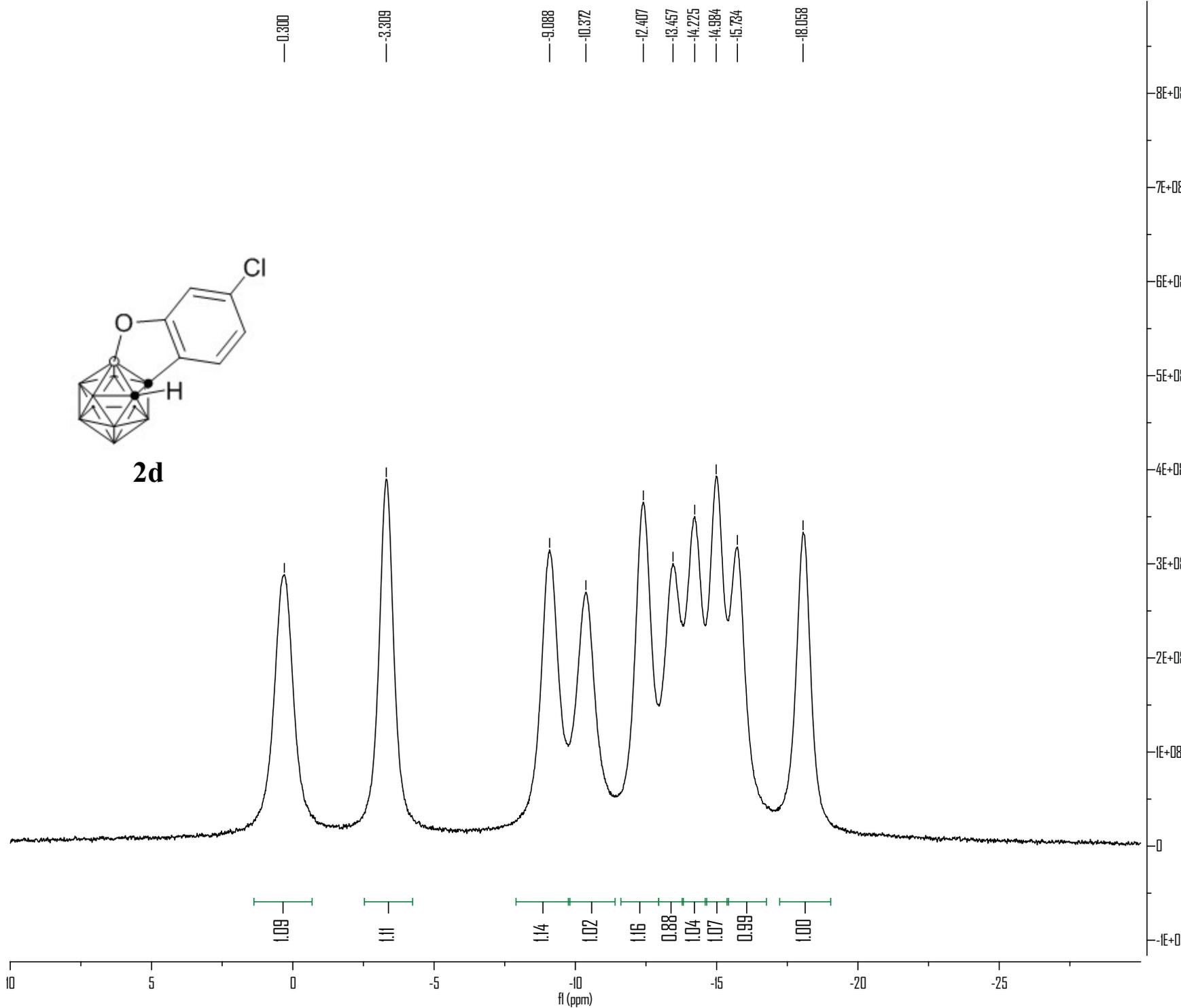


S108

Parameter	Value
Title	-CDX-7-55-1-CC
Comment	shimileneu experiment
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	26886
Receiver Gain	56
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.1272
Acquisition Date	2017-02-21 16:00:26
Modification Date	2017-02-22 07:55:00
Spectrometer Frequency	100.51
Spectral Width	29069.8
Lowest Frequency	-4040.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

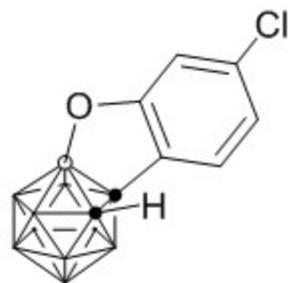


2d

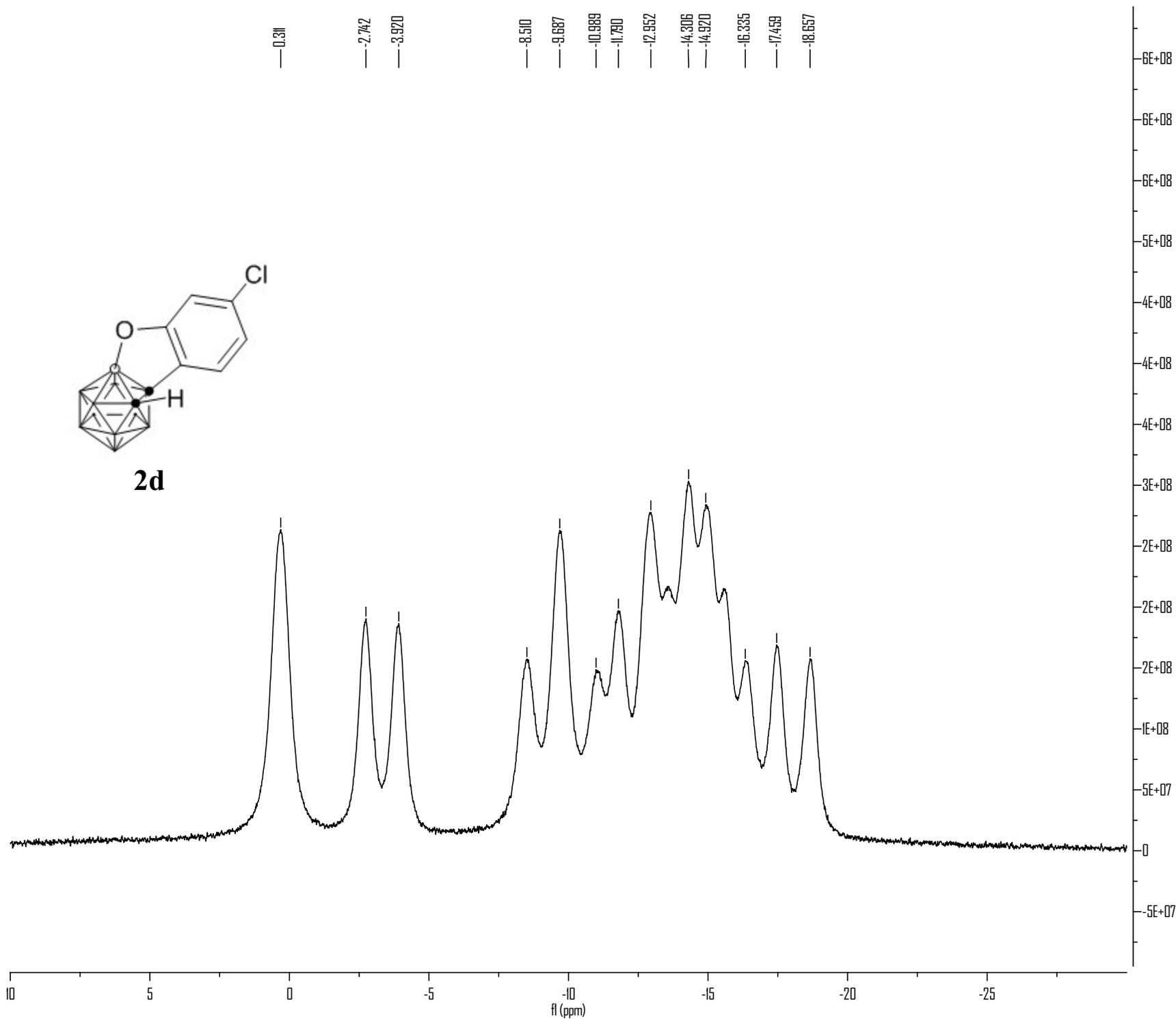


S109

Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/产物数据/7-1-1/2012060b-cxx-7-55-a/1/pdata/1/1r
Title	2012060b-cxx-7-55-a
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.lgy
Number of Scans	211
Receiver Gain	322
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-02-14T19:38:52
Modification Date	2017-02-14T15:04:50
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16416.9
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

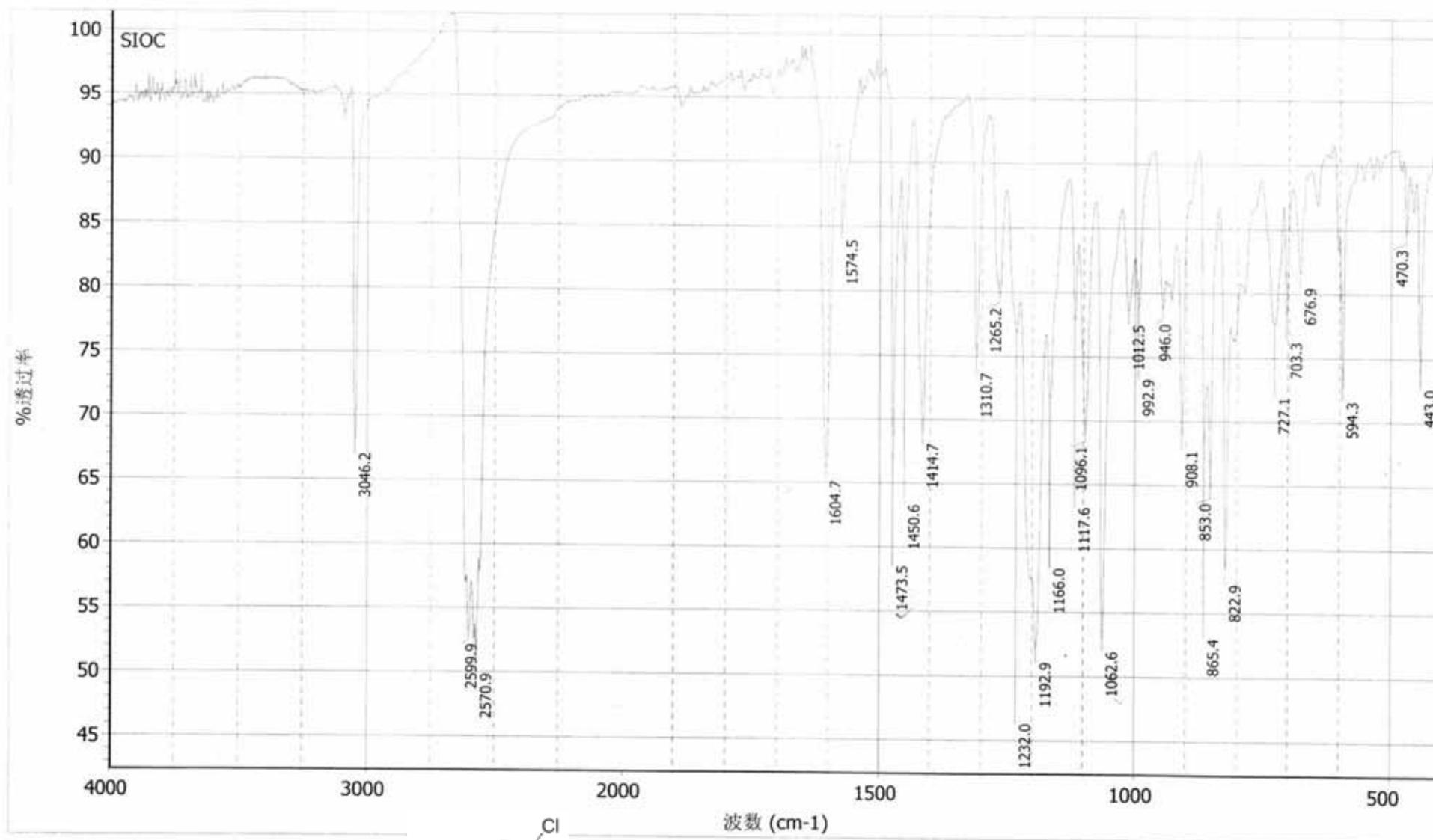


2d

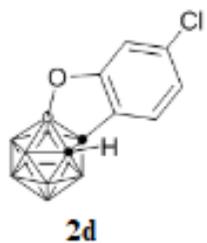


S110

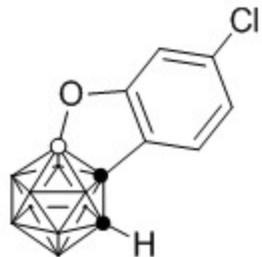
Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/产物数据/7-1-1/2012060b-ccx-7-55-a-coupling/1/pdata/1/1r
Title	2012060b-ccx-7-55-a-coupling
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	138
Receiver Gain	228
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-02-14T19:36:06
Modification Date	2017-02-14T15:05:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16416.9
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



CCX-7-57-A 2015806 JS



样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



3d

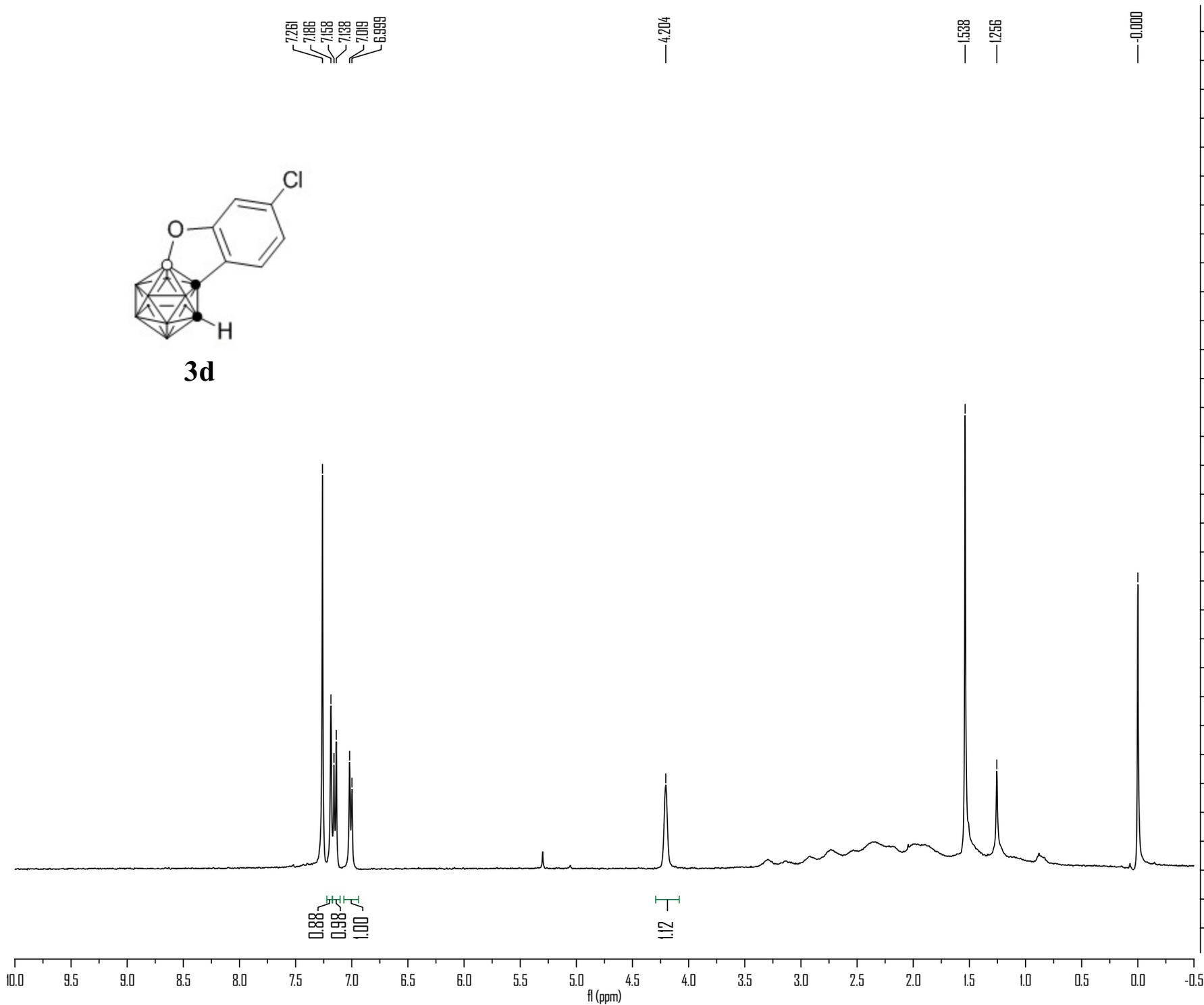
7.261
7.186
7.158
7.138
7.019
6.999

4.204

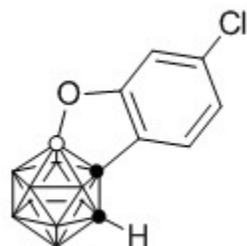
1.538

1.256

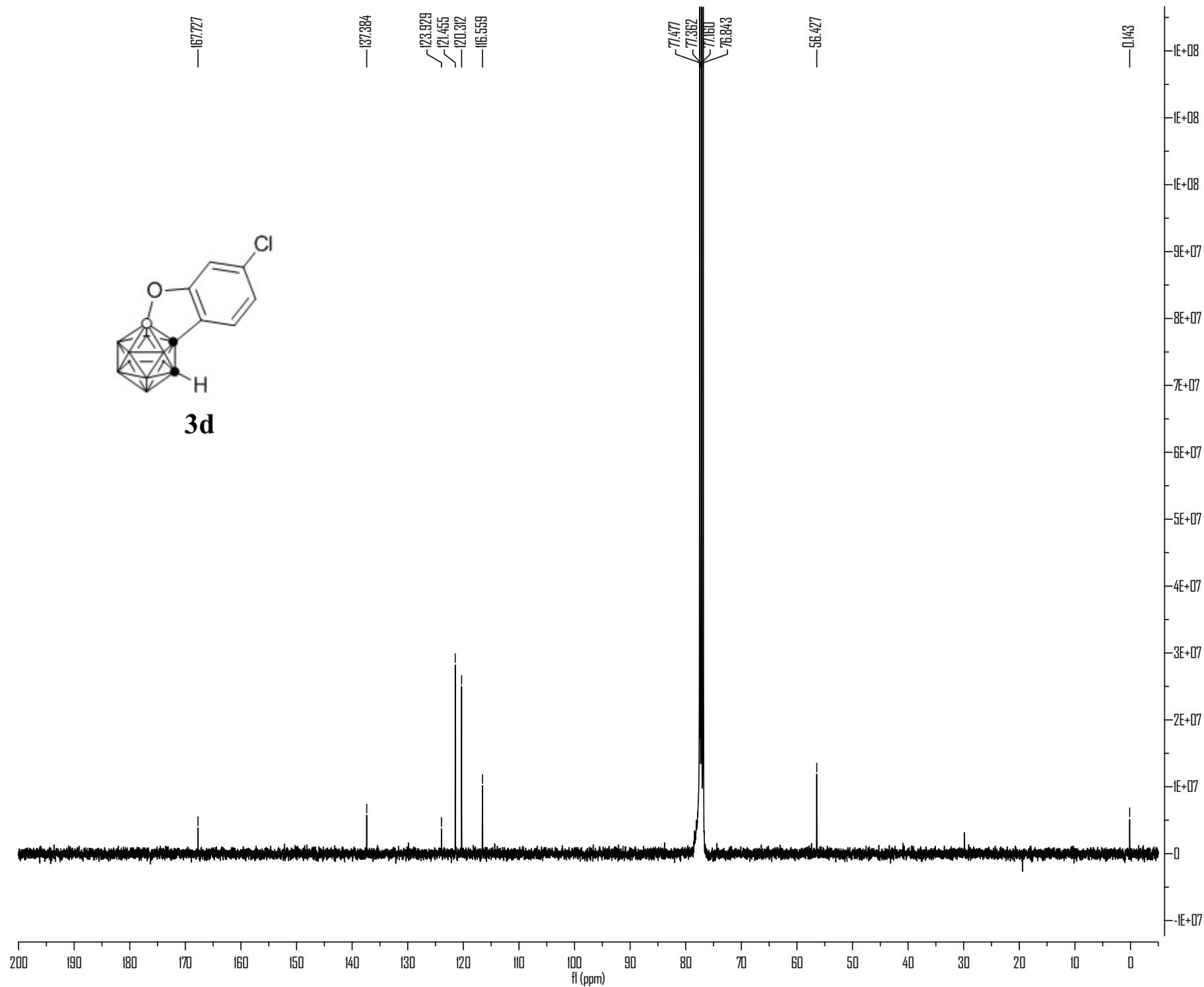
0.000



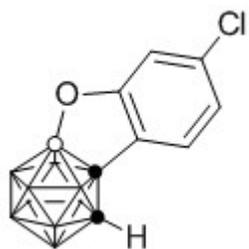
Parameter	Value
Data file Name	H-CCX-7-57-ab-3.fid/ fid
Title	-H-CCX-7-57-ab-3
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.5558
Acquisition Date	2018-12-13T08:23:58
Modification Date	2018-12-13T08:24:00
Spectrometer Frequency	399.70
Spectral Width	6410.3
Lowest Frequency	-800.9
Nucleus	¹ H
Acquired Size	16384
Spectral Size	32768



3d



Parameter	Value
Data file Name	2012060cccc-cx-7-57-ab-3/ 3/ pdata/ 1/ 1r
Title	2012060cccc-cx-7-57-ab-3
Comment	
Origin	LXNMR Bruker
	Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgdc
Number of Scans	23076
Receiver Gain	32768
Relaxation Delay	2.0000
Pulse Width	4.0000
Acquisition Time	0.9306
Acquisition Date	2018-12-13T20:40:38
Modification Date	2018-12-14T10:25:57
Spectrometer Frequency	100.61
Spectral Width	35211.3
Lowest Frequency	-6858.2
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



3d

3.553

3.691

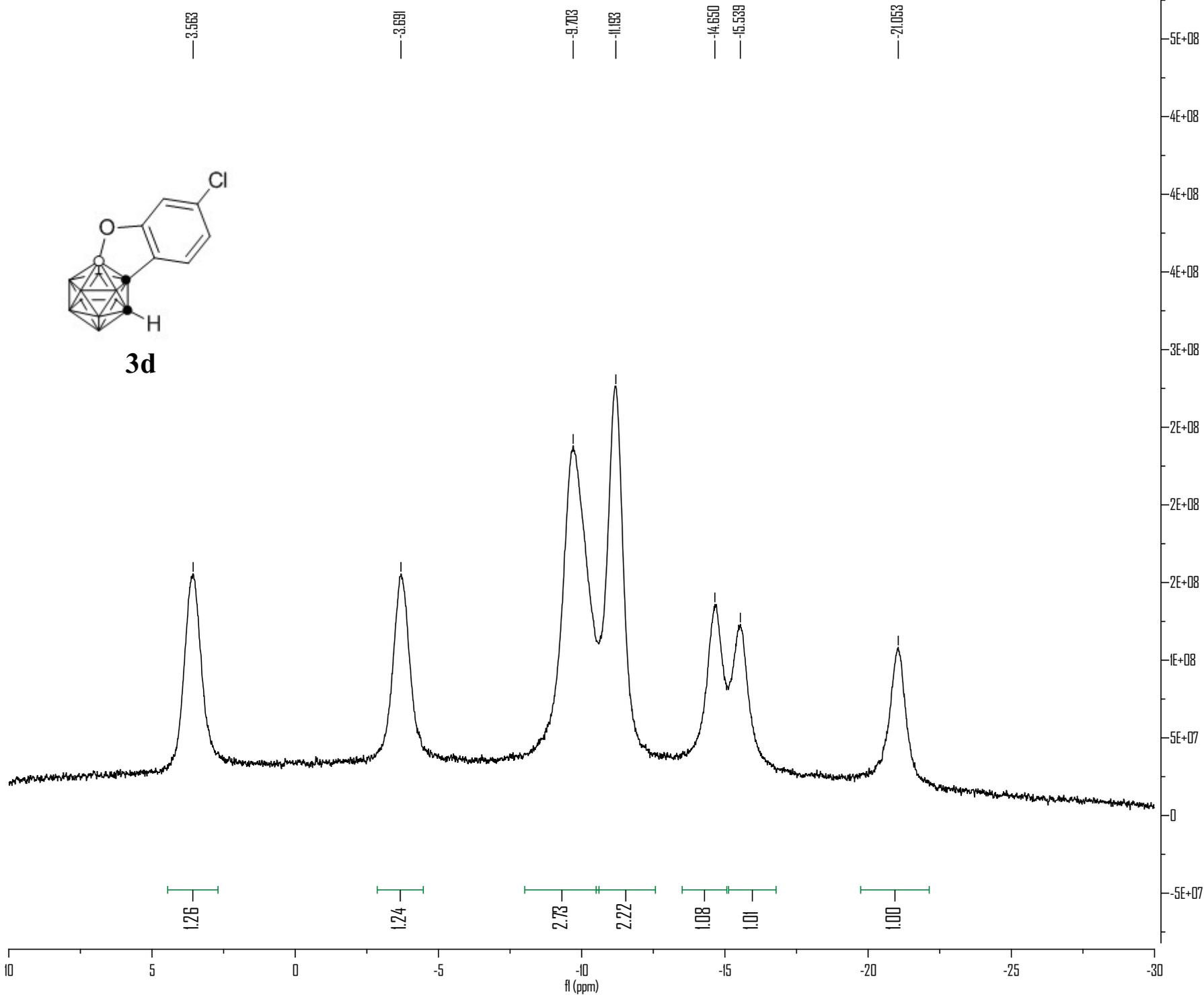
9.703

11.193

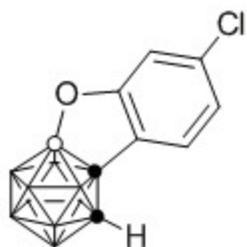
14.650

15.539

21.053

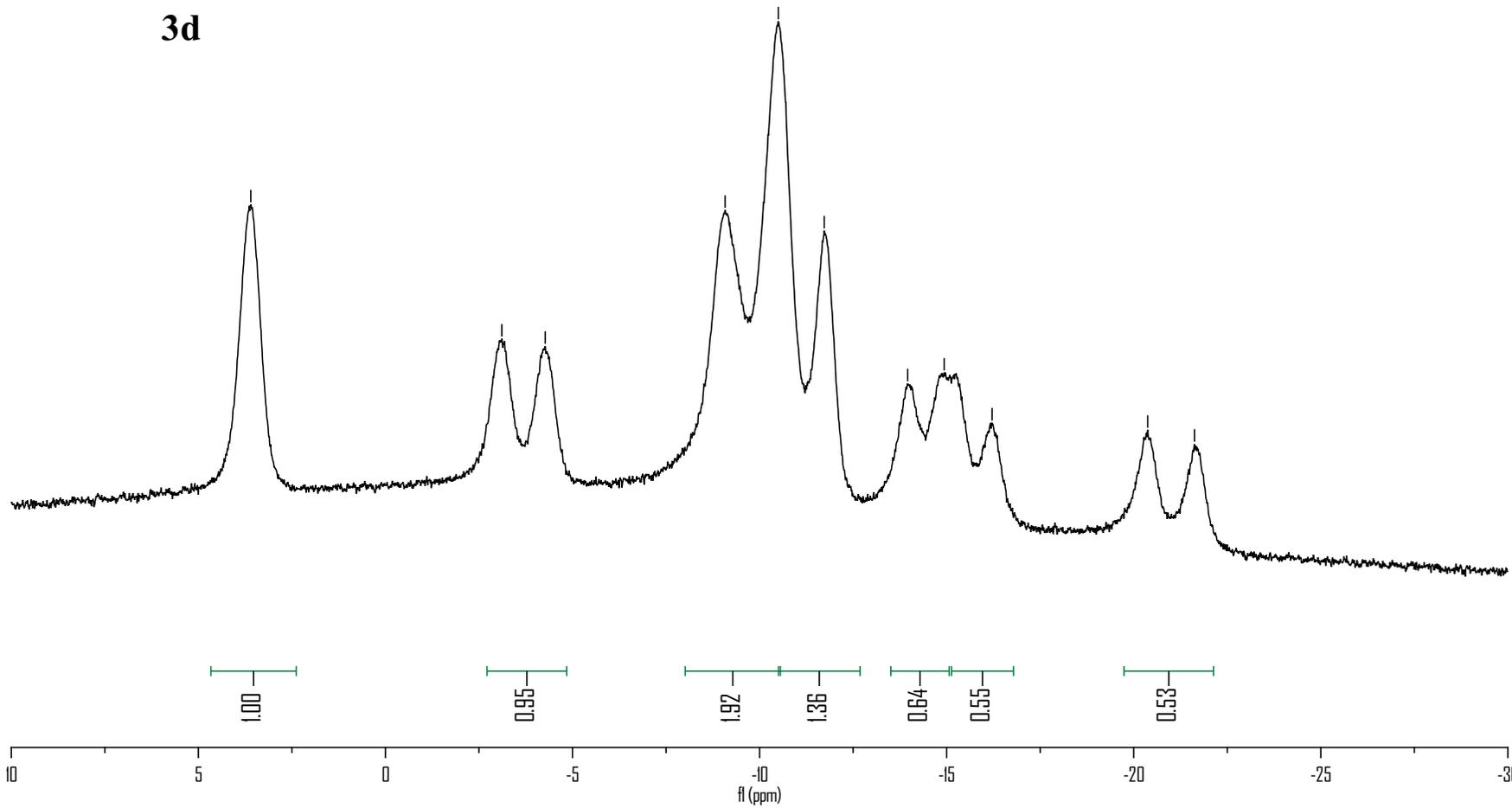


Parameter	Value
Data File Name	2012060b-ccx-7-57-ab-3/1/pdata/1/1r
Title	2012060b-ccx-7-57-ab-3
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	THF
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	790
Receiver Gain	645
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.4260
Acquisition Date	2018-12-13 11:52:15
Modification Date	2018-12-13 11:33:28
Spectrometer Frequency	128.38
Spectral Width	38461.5
Lowest Frequency	-19585.2
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

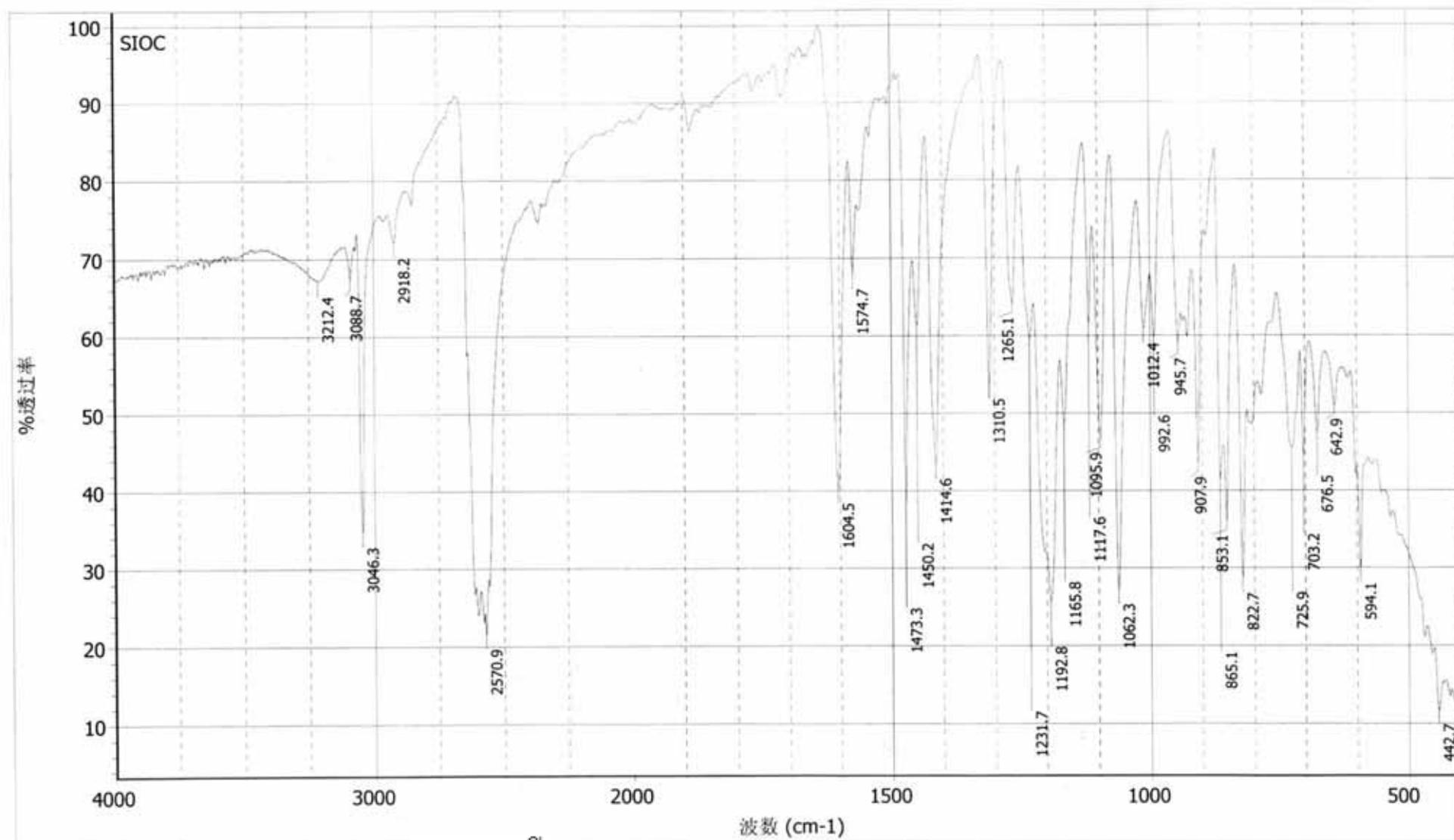


3d

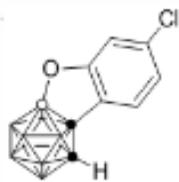
3.588 3.10 4.272 9.078 10.503 11.728 13.959 14.934 16.214 20.373 21.624



Parameter	Value
Data File Name	2012060b-ccx-7-57-ab-3/ 2012060b-ccx-7-57-ab-3-coupling/ 1/ pdata/ 1/ 1r
Title	2012060b-ccx-7-57-ab-3-coupling
Comment	
Origin	LXNMR Bruker
Owner	Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	THF
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	1216
Receiver Gain	645
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.4260
Acquisition Date	2018-12-13T20:01:33
Modification Date	2018-12-13T13:33:24
Spectrometer Frequency	128.38
Spectral Width	38461.5
Lowest Frequency	-19565.2
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

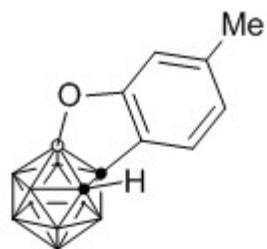


CCX-7-57-4 2015806 JS

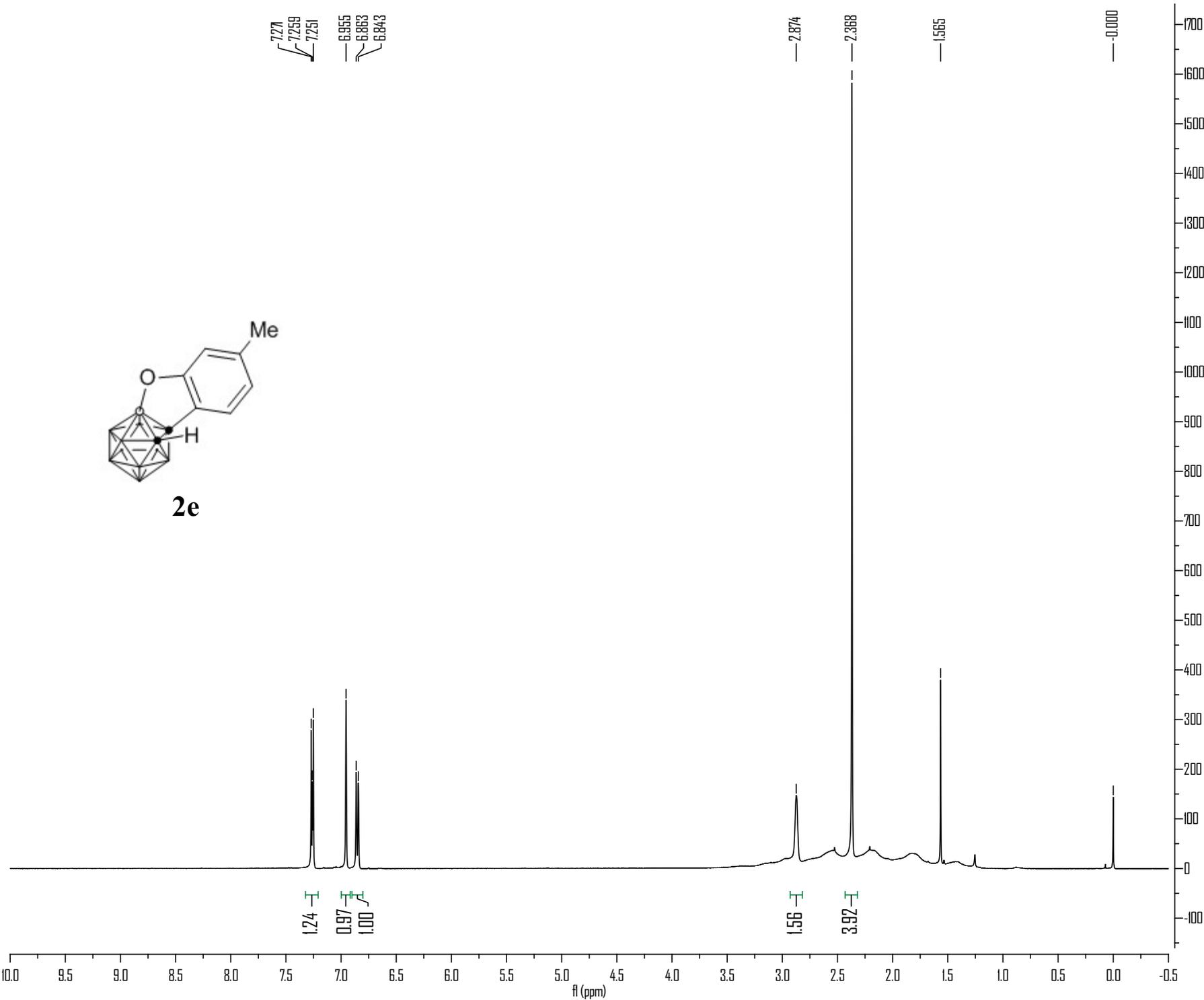


3d

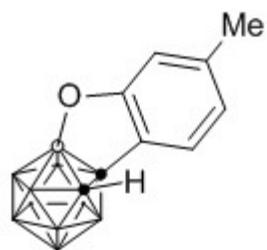
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.4747



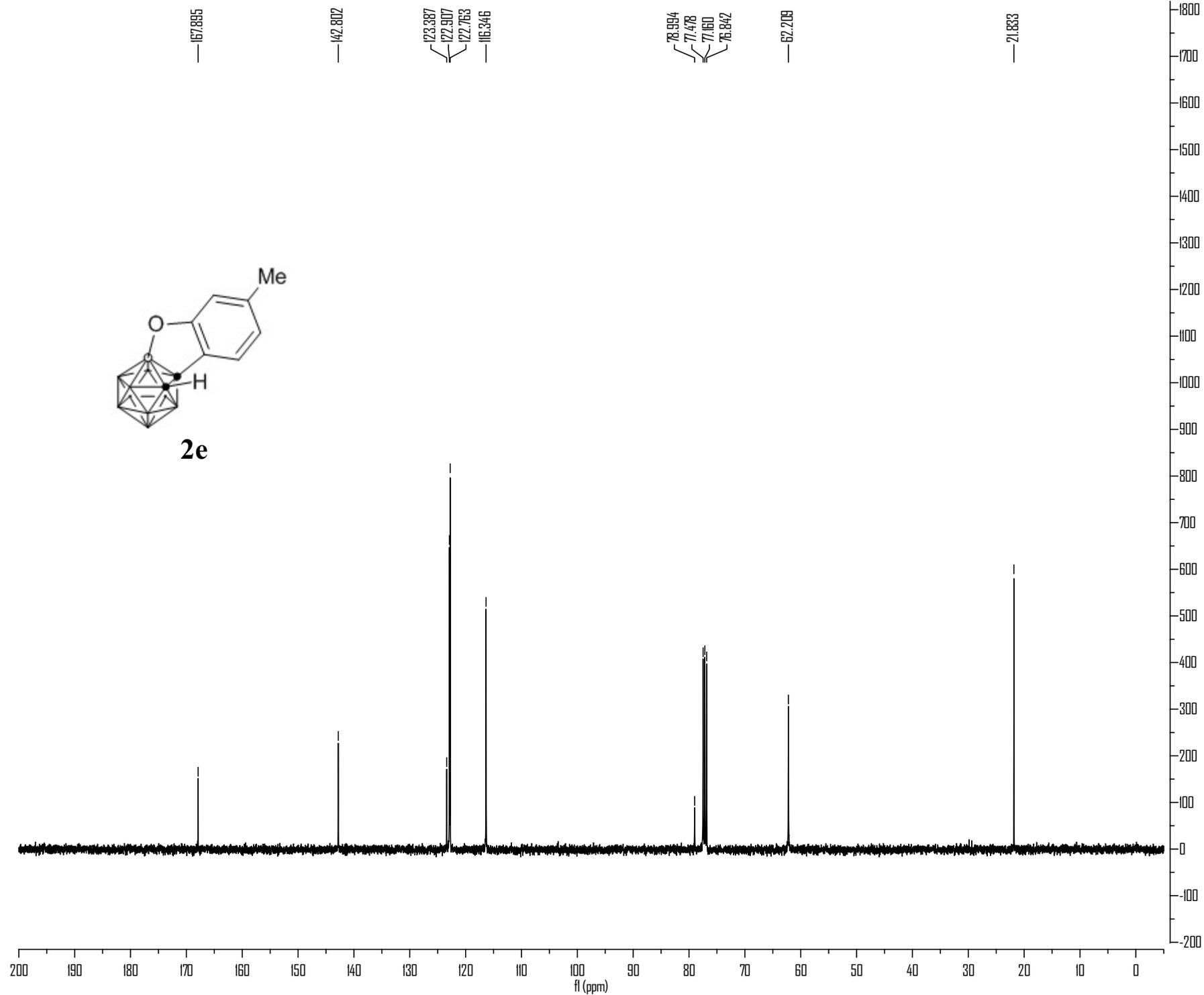
2e



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-9-1/ccx-7-9-1.fid/ fid
Title	ccx-7-9-1
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	
Solvent	CDCl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	44
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-10-21T09:35:27
Modification Date	2016-10-21T01:36:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-793.9
Nucleus	1H
Acquired Size	21552
Spectral Size	65536

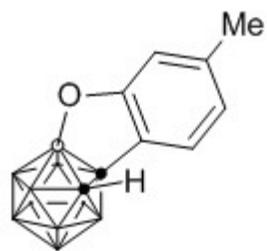


2e

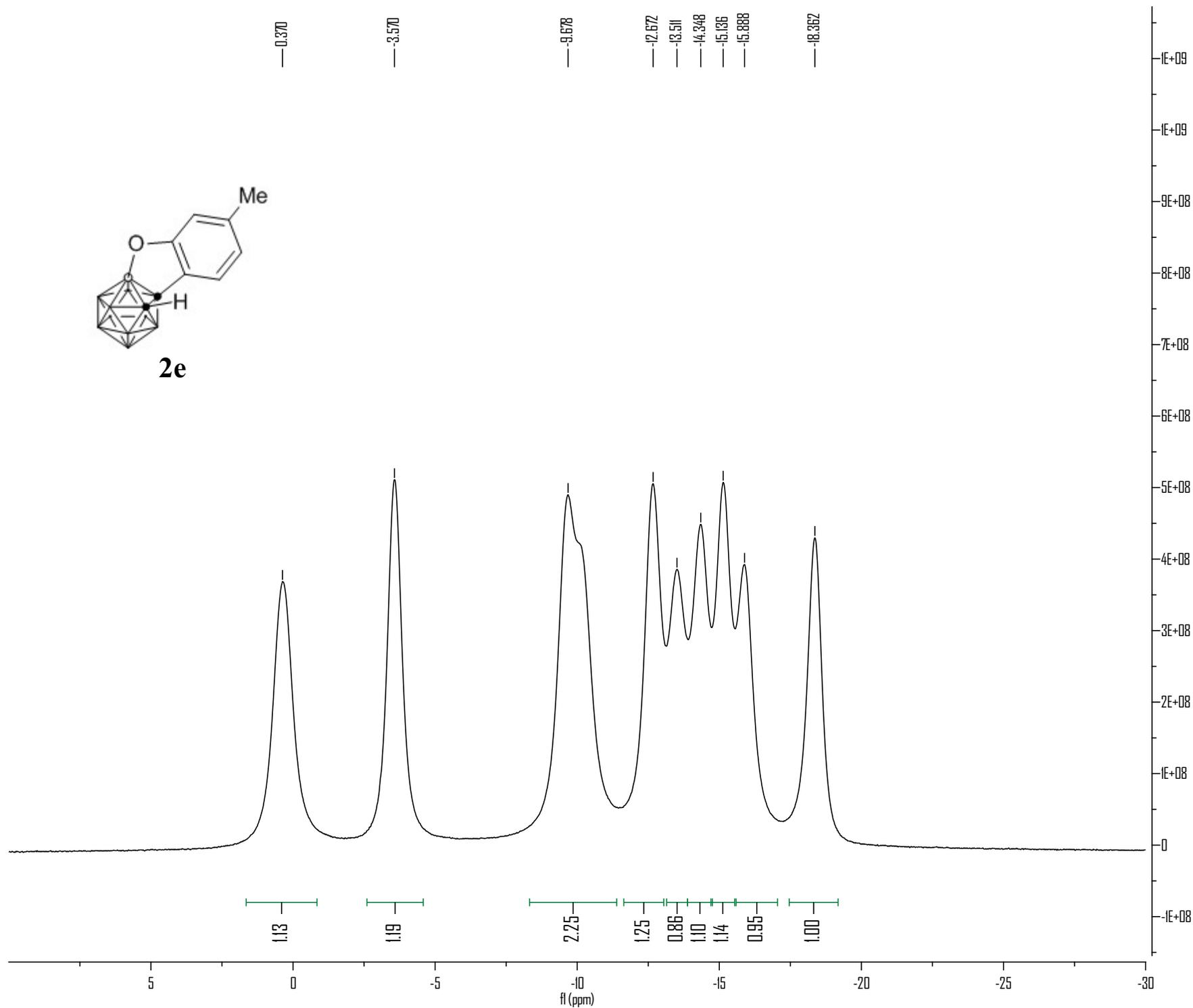


S118

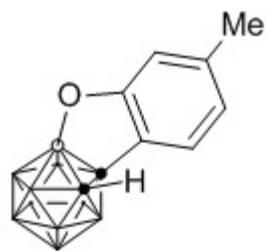
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-91/-CCX-7-9-1C.fid/ fid
Title	-CCX-7-9-1C
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	stu
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	172
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-10-21T11:22:54
Modification Date	2016-10-21T11:32:00
Spectrometer Frequency	100.51
Spectral Width	25510.2
Lowest Frequency	-1684.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



2e

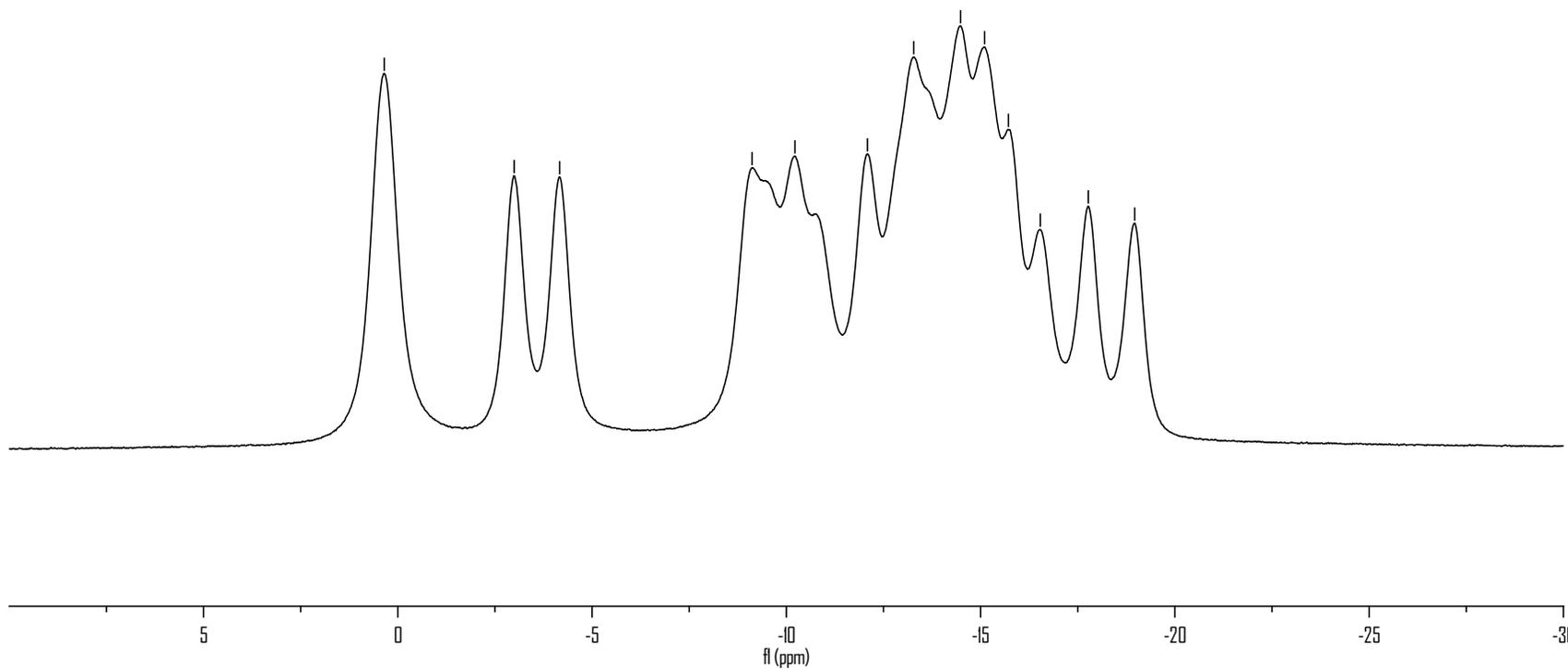


Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-9-1/bccx-7-9-1/pdata/1/1r
Title	7-9-1
Comment	
Origin	UXMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	256
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-10-21T21:05:24
Modification Date	2016-10-21T15:10:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16419.8
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



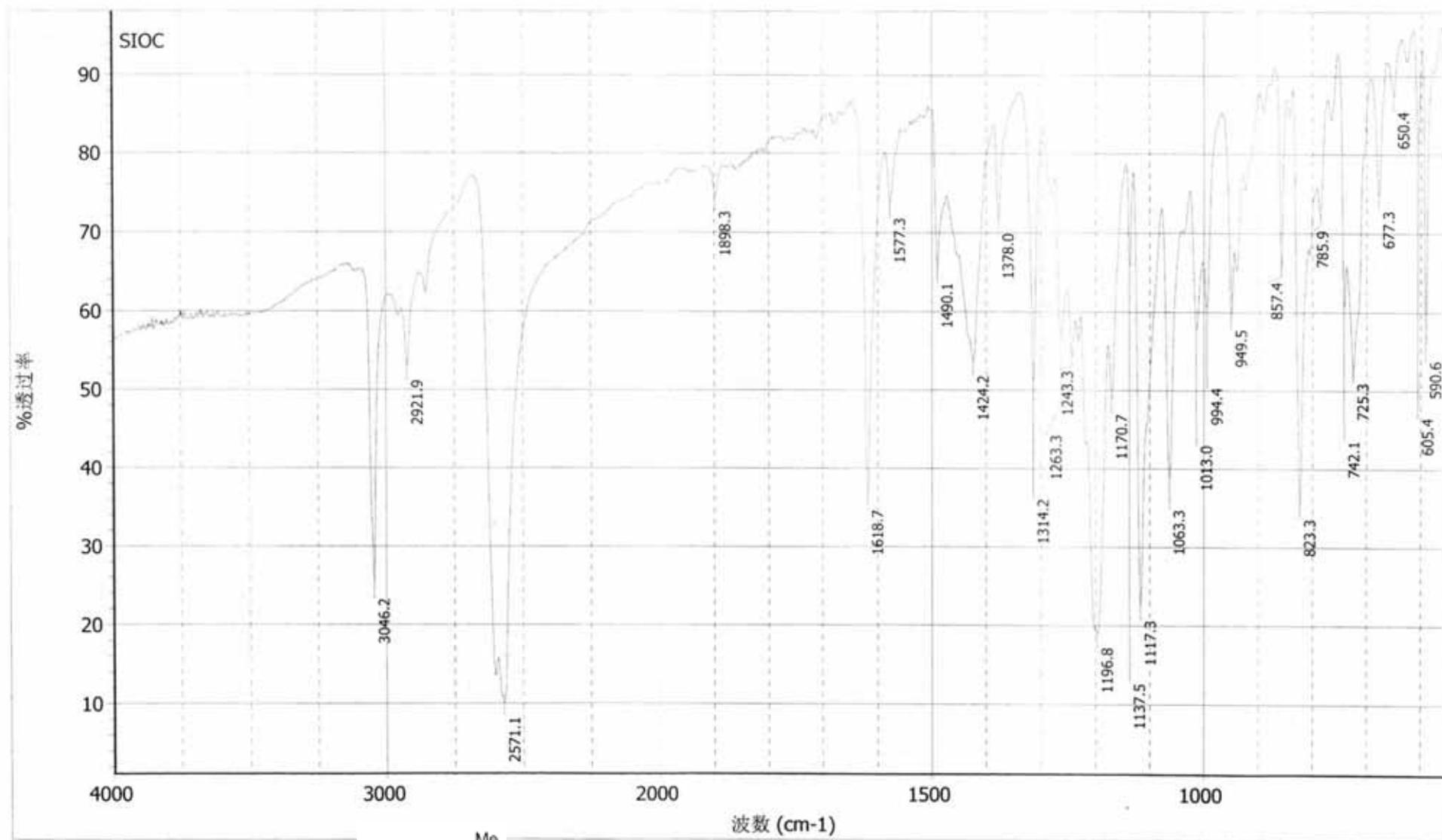
2e

0.350
-2.896
-4.166
-9.116
-10.222
-12.087
-13.278
-14.484
-15.716
-16.536
-17.771
-18.964

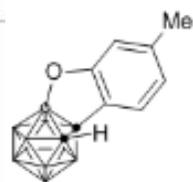


S120

Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/7-9-1/b-cx-7-9-1-coupling/pdata/1/1r
Title	7-9-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	256
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-10-21T21:10:57
Modification Date	2016-10-21T15:17:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16419.8
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

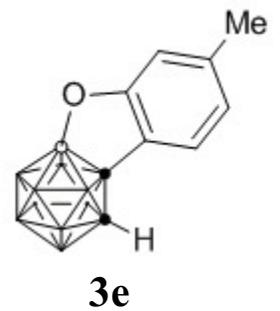
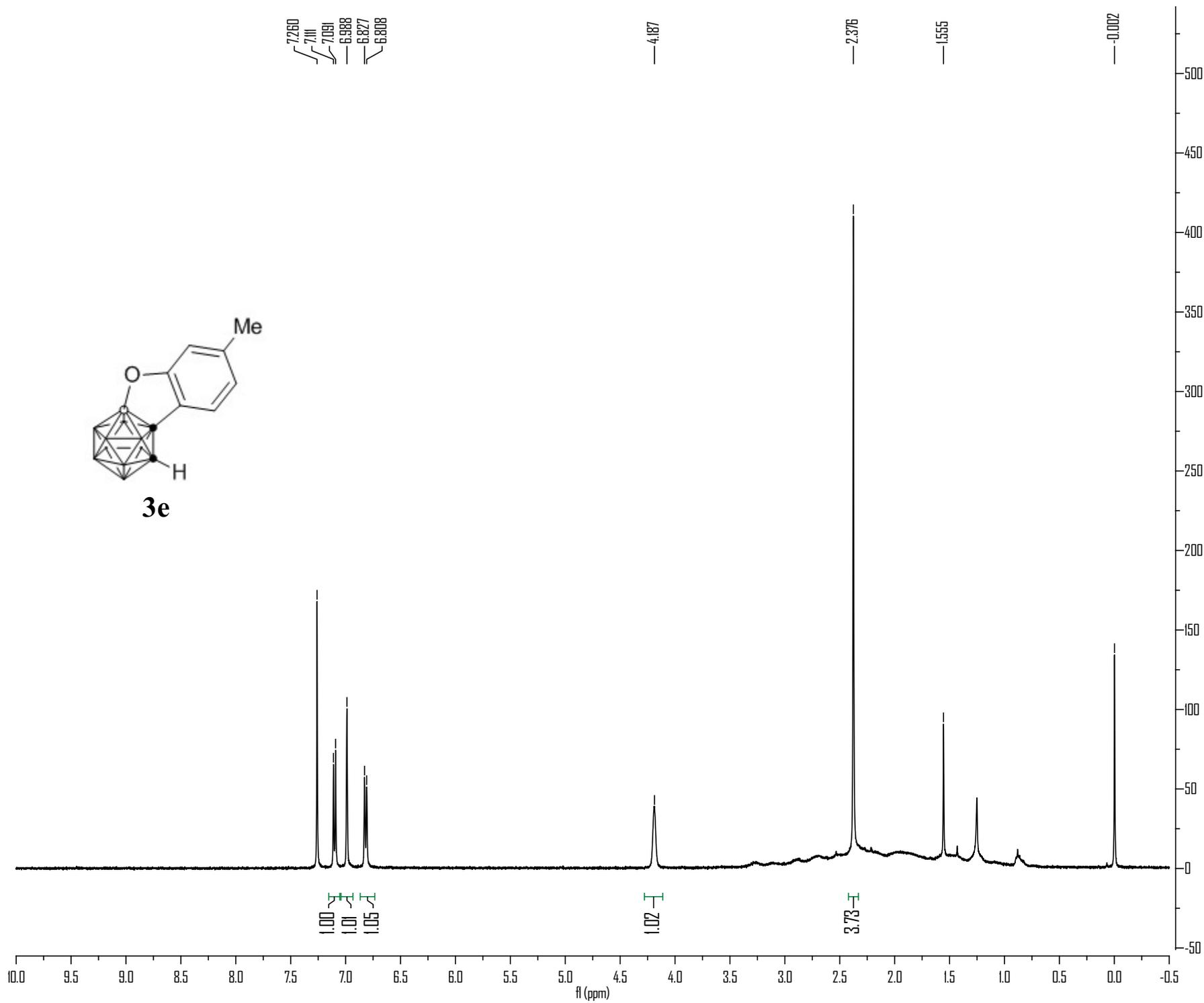


CCX-7-9-a 2015806 JS

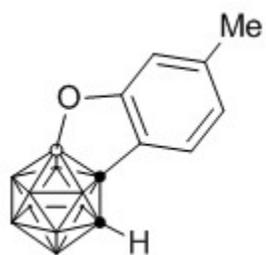


2e

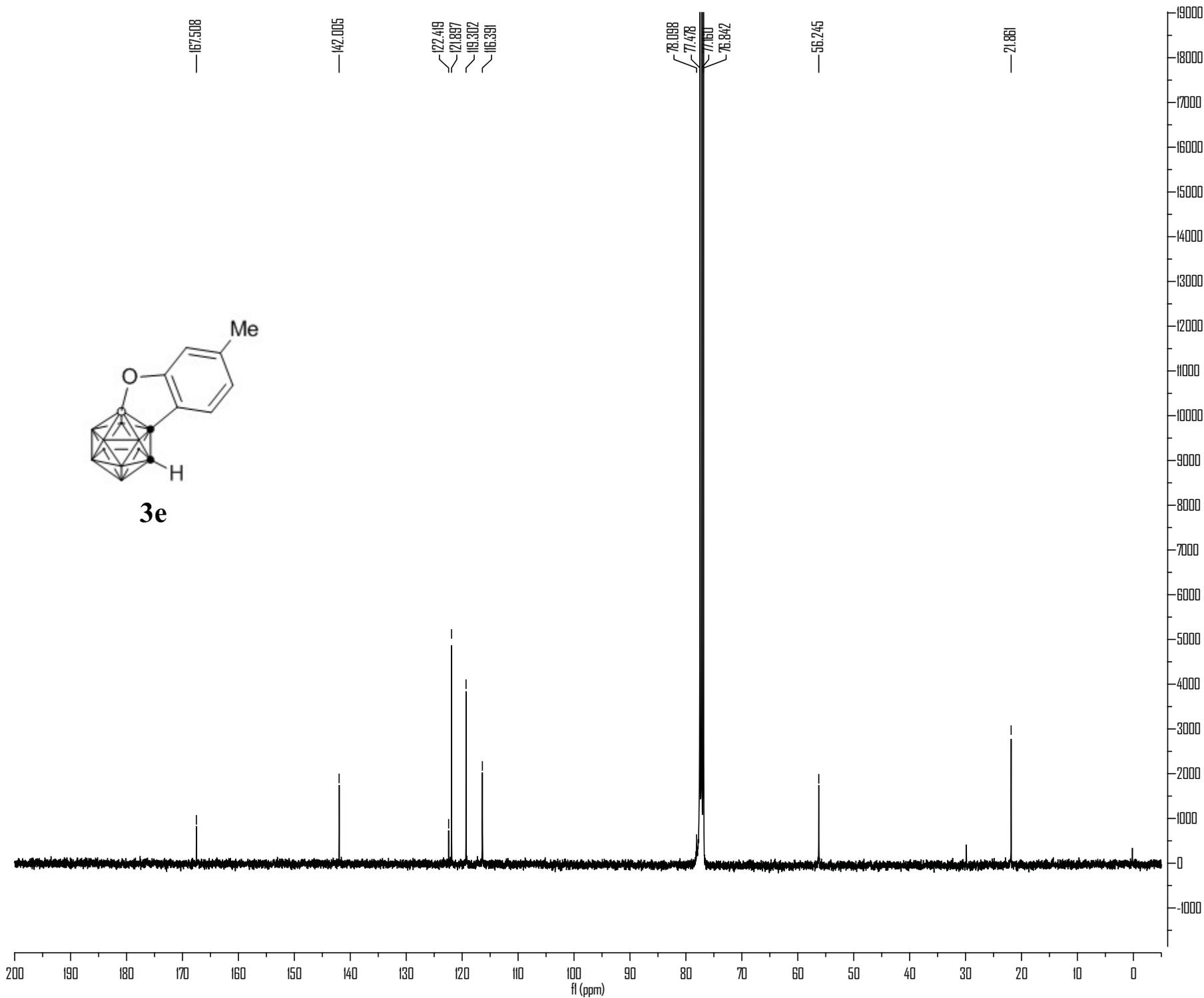
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-9-2/ccx-7-52-3.fid/fid
Title	ccx-7-52-3
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omcl
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	46
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-02-09T22:00:53
Modification Date	2017-02-09T14:01:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-793.8
Nucleus	1H
Acquired Size	21552
Spectral Size	65536

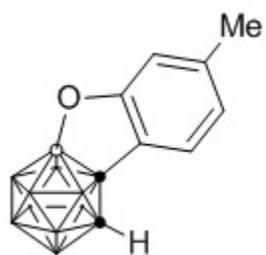


3e



S123

Parameter	Value
Data file Name	G:/Users/Administrator/Desktop/产物数据/7-9-2/ccx-7-52-b-c.fid/fid
Title	ccx-7-52-b-c
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	12944
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-02-13T22:23:59
Modification Date	2017-02-13T22:40:00
Spectrometer	100.60
Frequency	
Spectral Width	24509.8
Lowest Frequency	-1676.0
Nucleus	¹³ C
Acquired Size	31875
Spectral Size	65536



3e

8.377

4.239

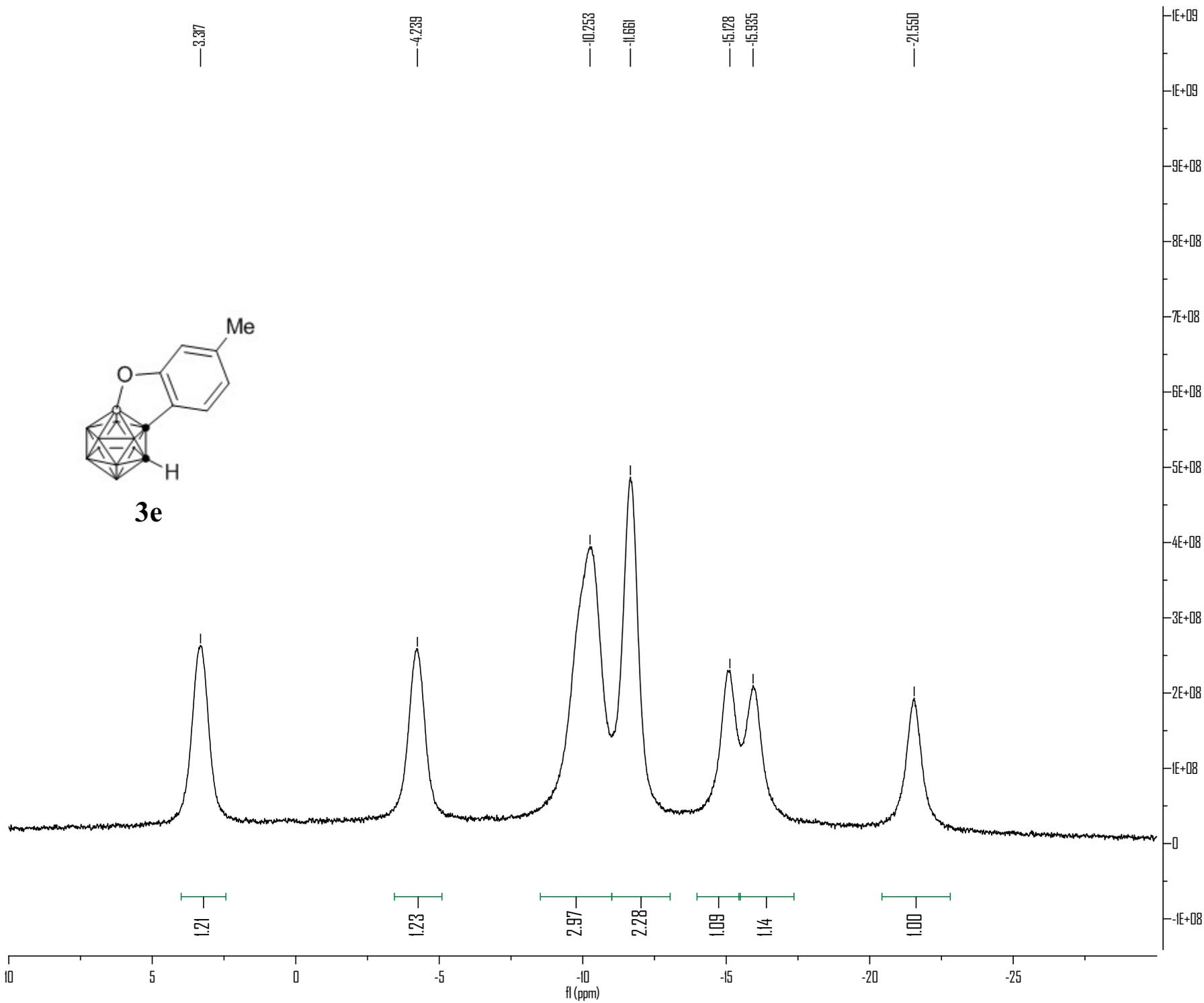
10.253

11.661

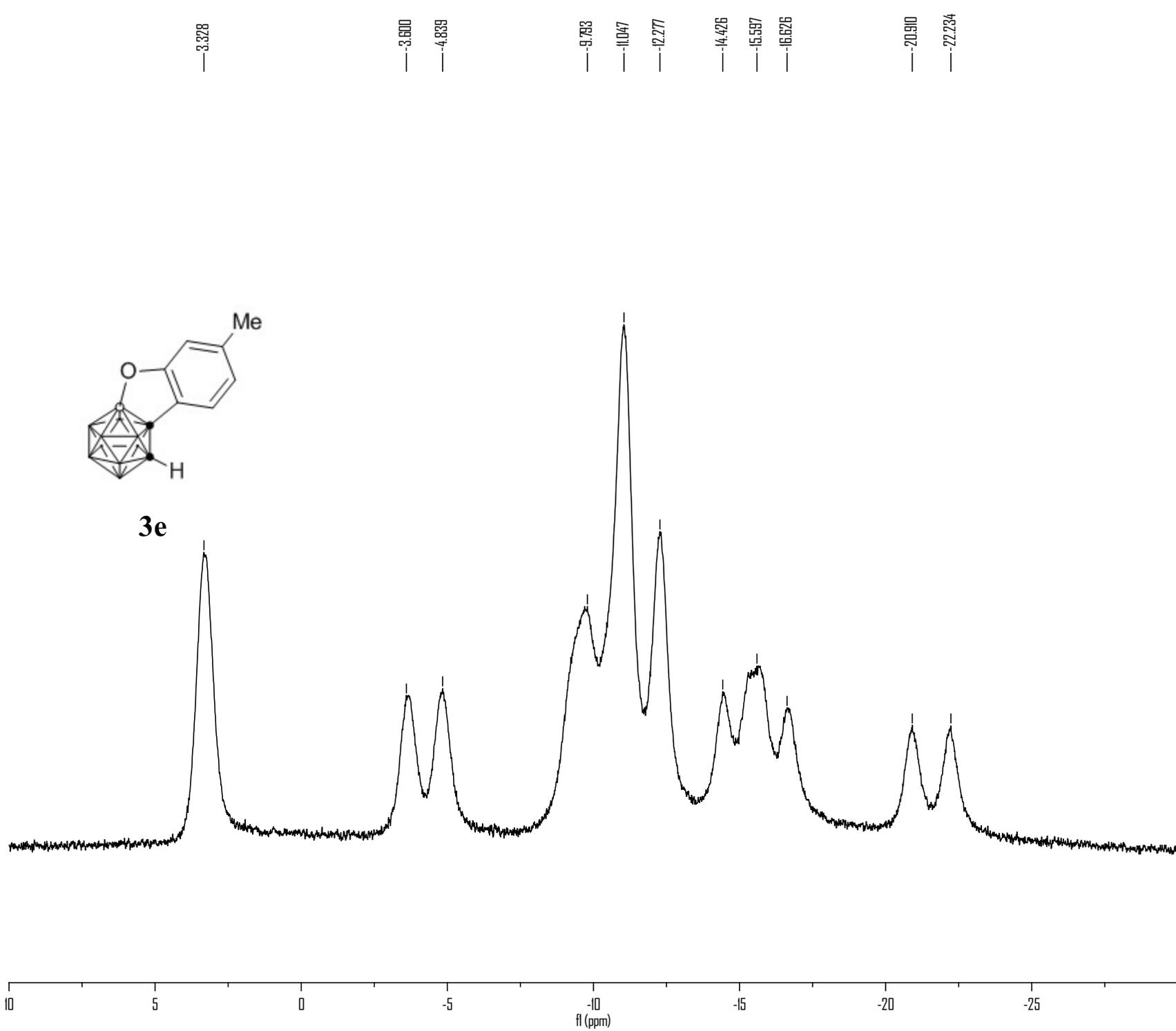
15.128

15.935

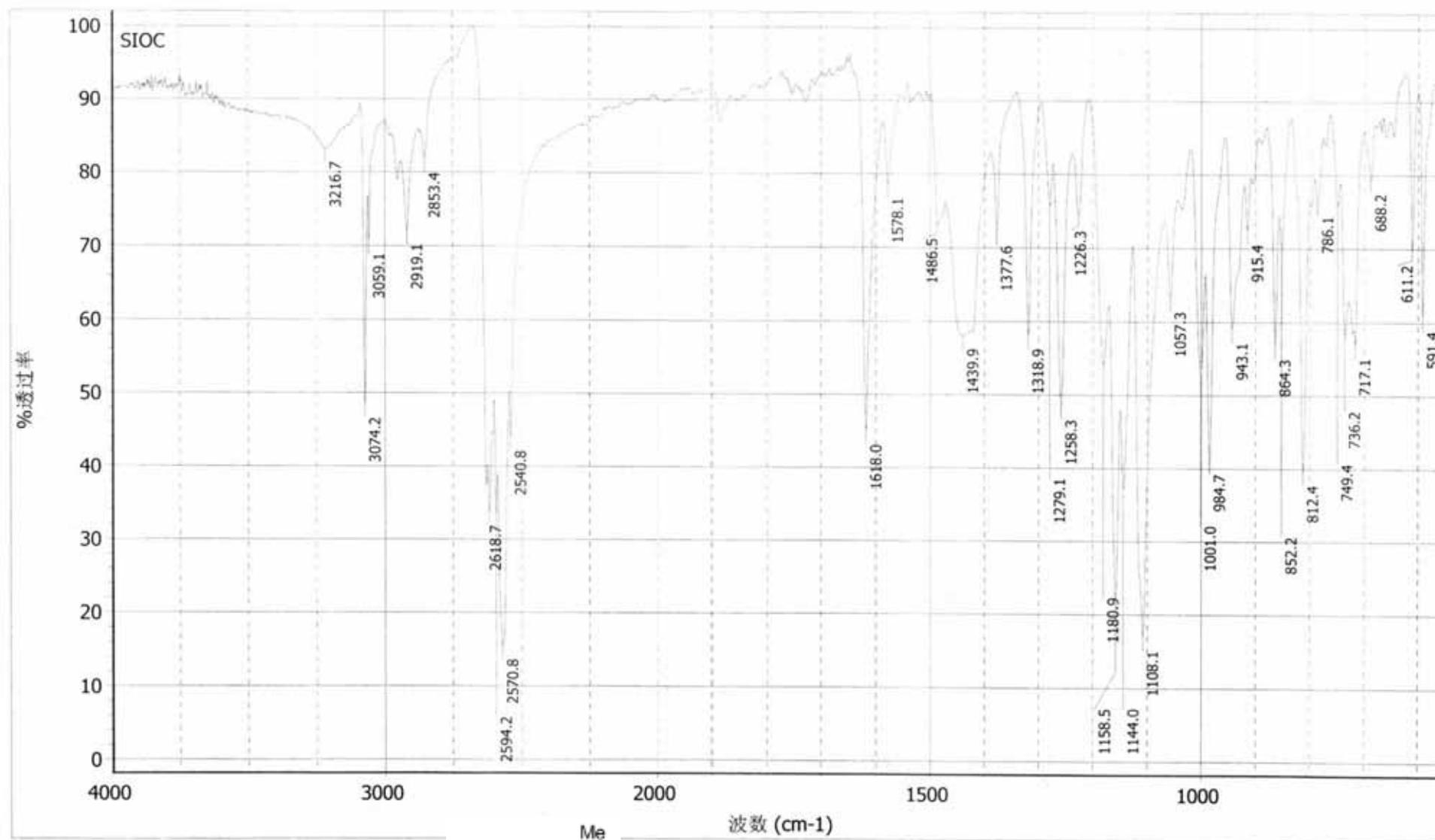
21.550



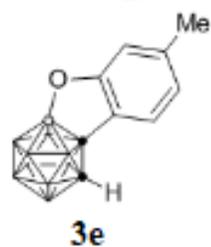
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-9-2/2012060b-ccx-7-52-b/1/pdata/1/1r
Title	2012060b-ccx-7-52-b
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	260
Receiver Gain	81.3
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-02-14T19:28:28
Modification Date	2017-02-14T15:05:14
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16416.9
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



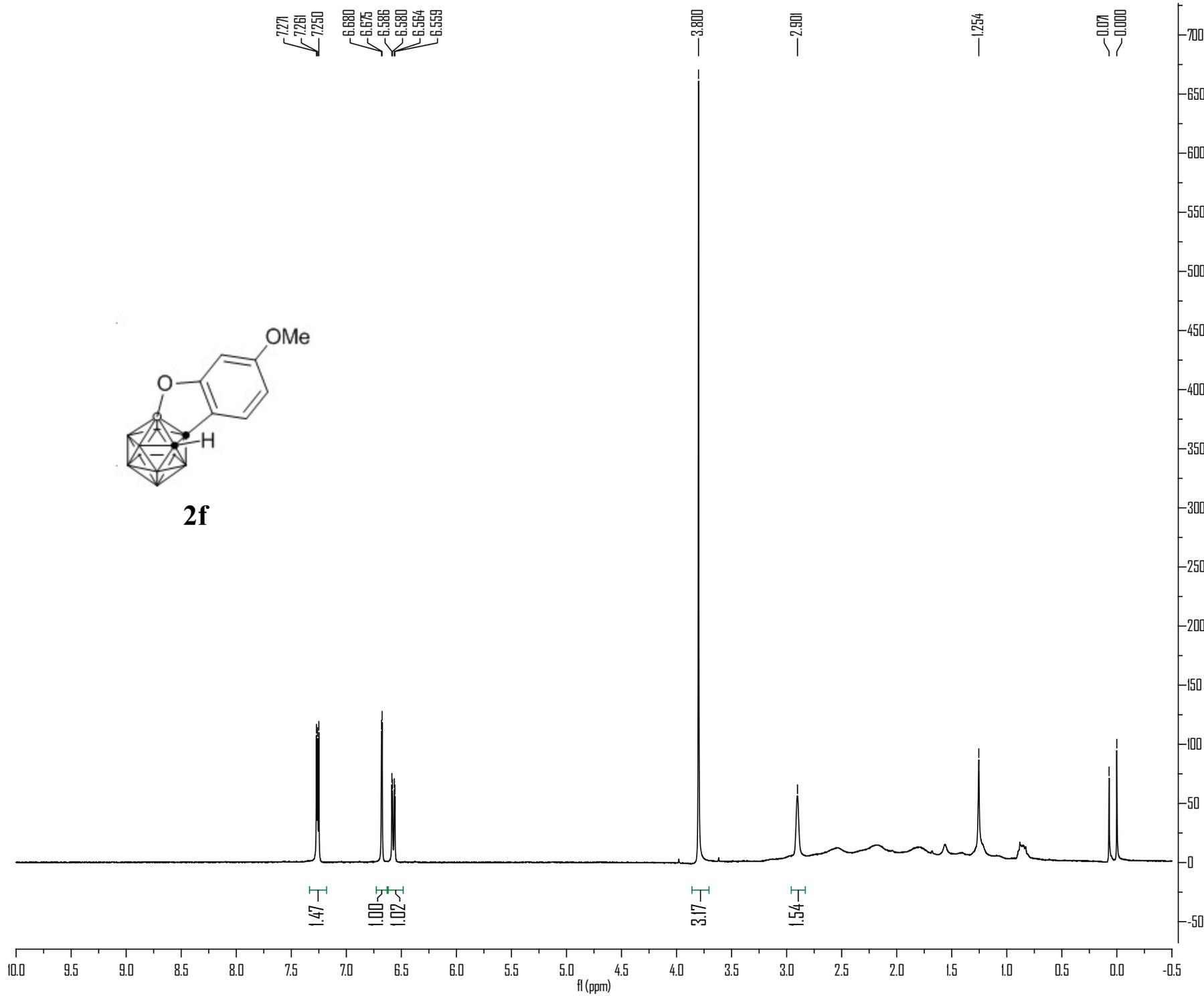
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-9-2/2012060b-ccx-7-52-b-coupling/1/pdata/1/1r
Title	2012060b-ccx-7-52-b-coupling
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	209
Receiver Gain	813
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-02-14T19:31:40
Modification Date	2017-02-14T15:05:06
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16416.9
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



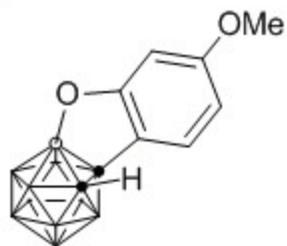
CCX-7-9-b 2015806 JS



样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



Parameter	Value
Data file Name	E:/Users/Administrator/Desktop/产物数据/7-22-a/ccx-7-22-1-1.fid/fid
Title	ccx-7-22-1-1
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	nmrns
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	40
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-11-12T08:54:15
Modification Date	2016-11-12T00:55:00
Spectrometer Frequency	400.03
Spectral Width	7267.4
Lowest Frequency	-845.5
Nucleus	1H
Acquired Size	21802
Spectral Size	65536



2f

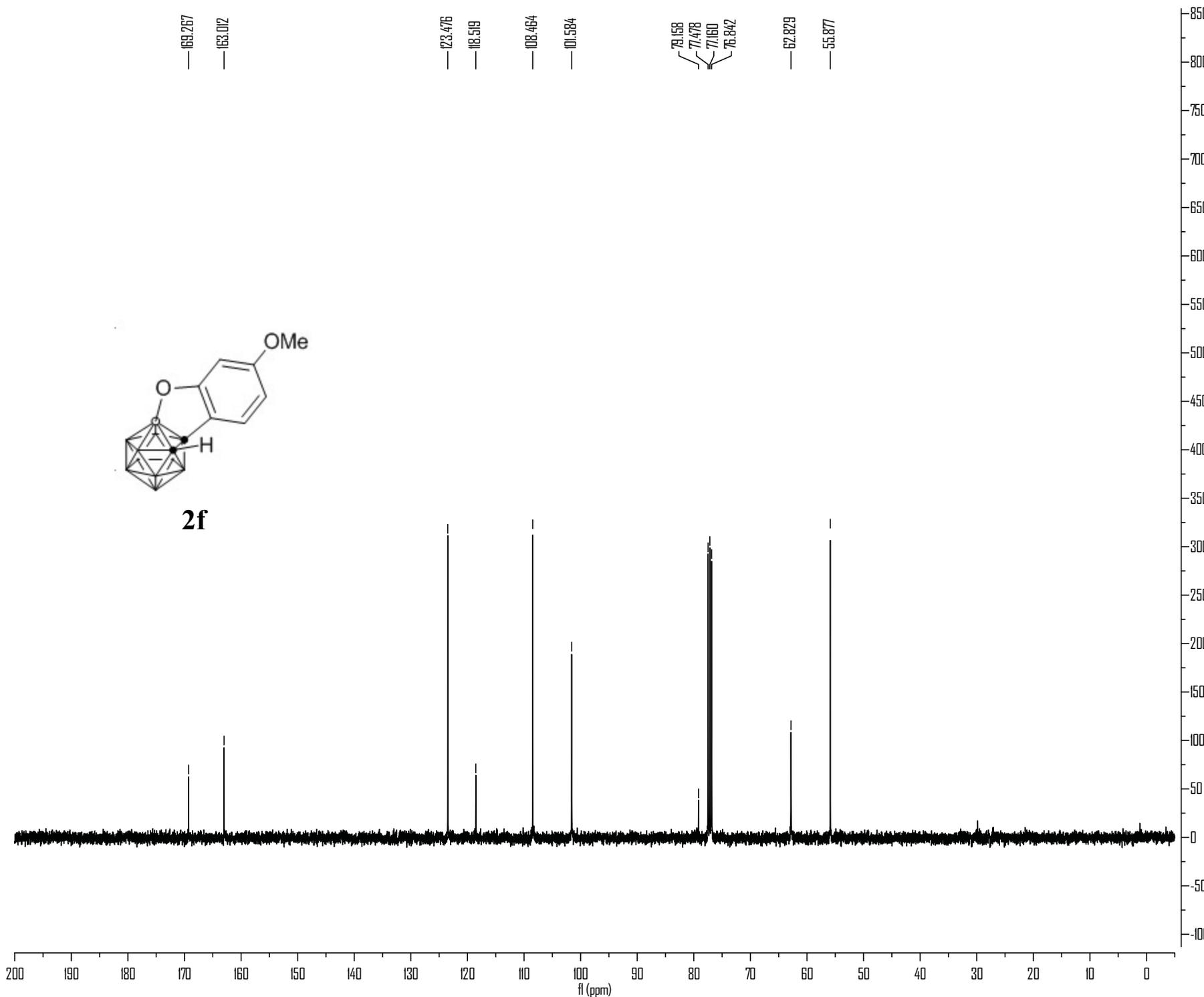
169.267
163.012

123.476
118.519

108.464
101.584

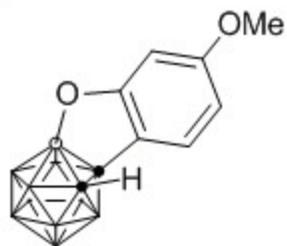
79.158
77.478
77.160
76.842

62.829
55.877

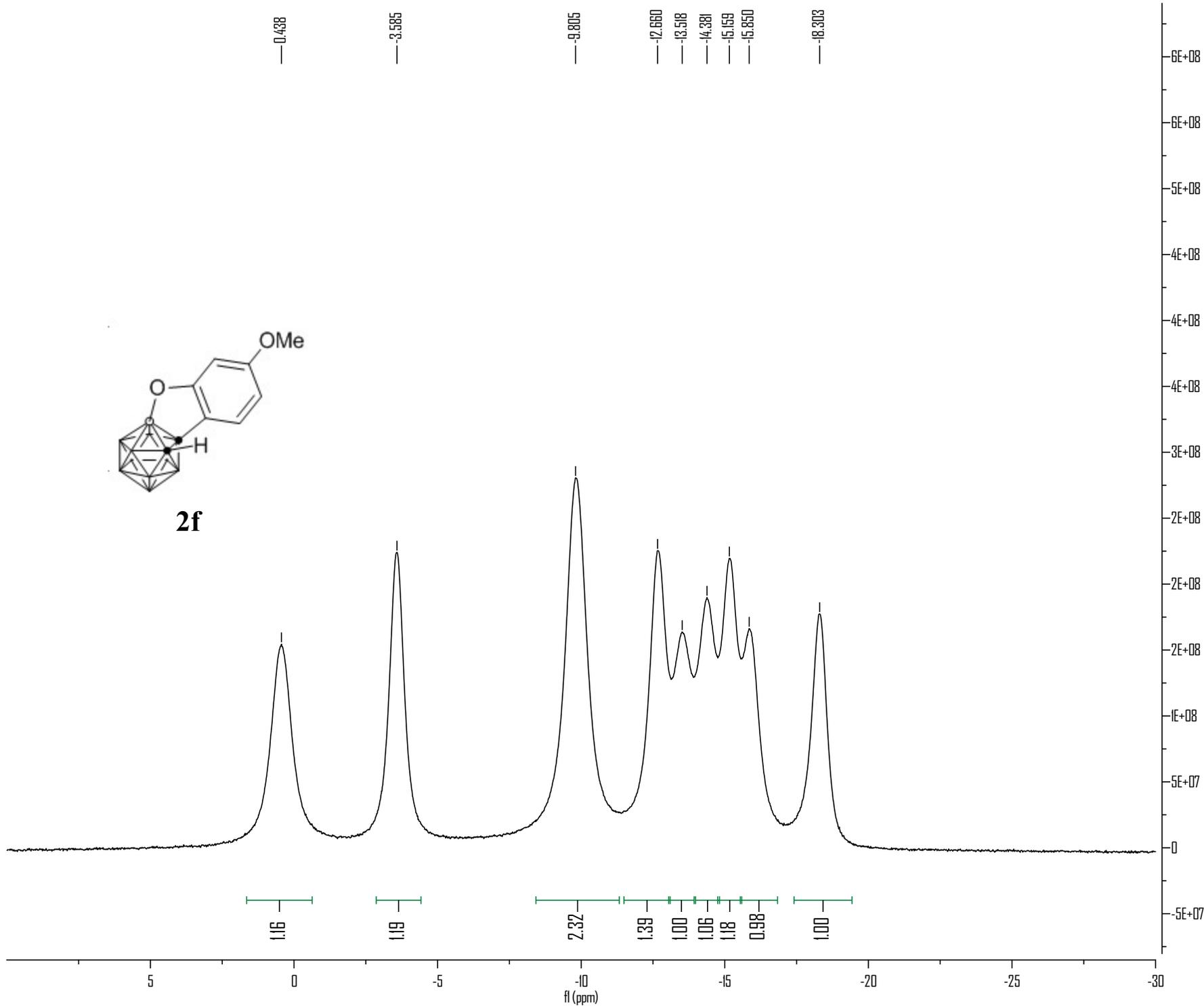


S128

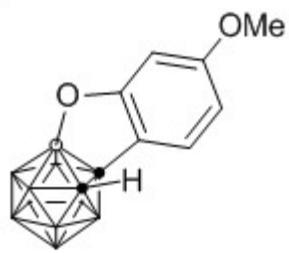
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-22-a/-CCX-7-22-1C.fid/fid
Title	-CCX-7-22-1C
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	stu
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	76
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-11-16T10:10:28
Modification Date	2016-11-16T10:14:00
Spectrometer Frequency	100.51
Spectral Width	25510.2
Lowest Frequency	-1681.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



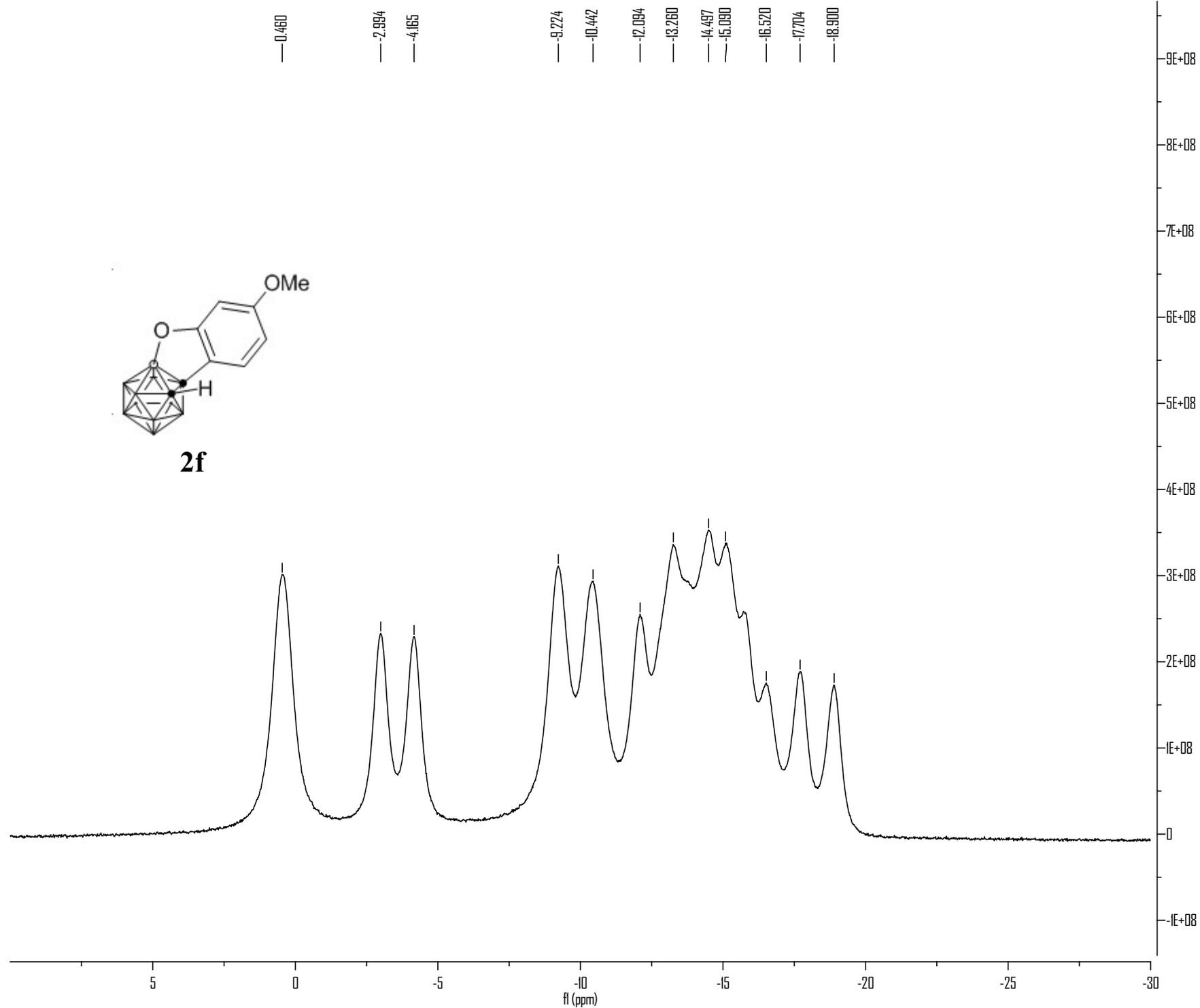
2f



Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/7-22-a/20120606-ccx-7-22-1/1/pdata/1/1r
Title	20120606-ccx-7-22-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	54
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2016-11-15T20:35:05
Modification Date	2016-11-15T14:20:22
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16419.8
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

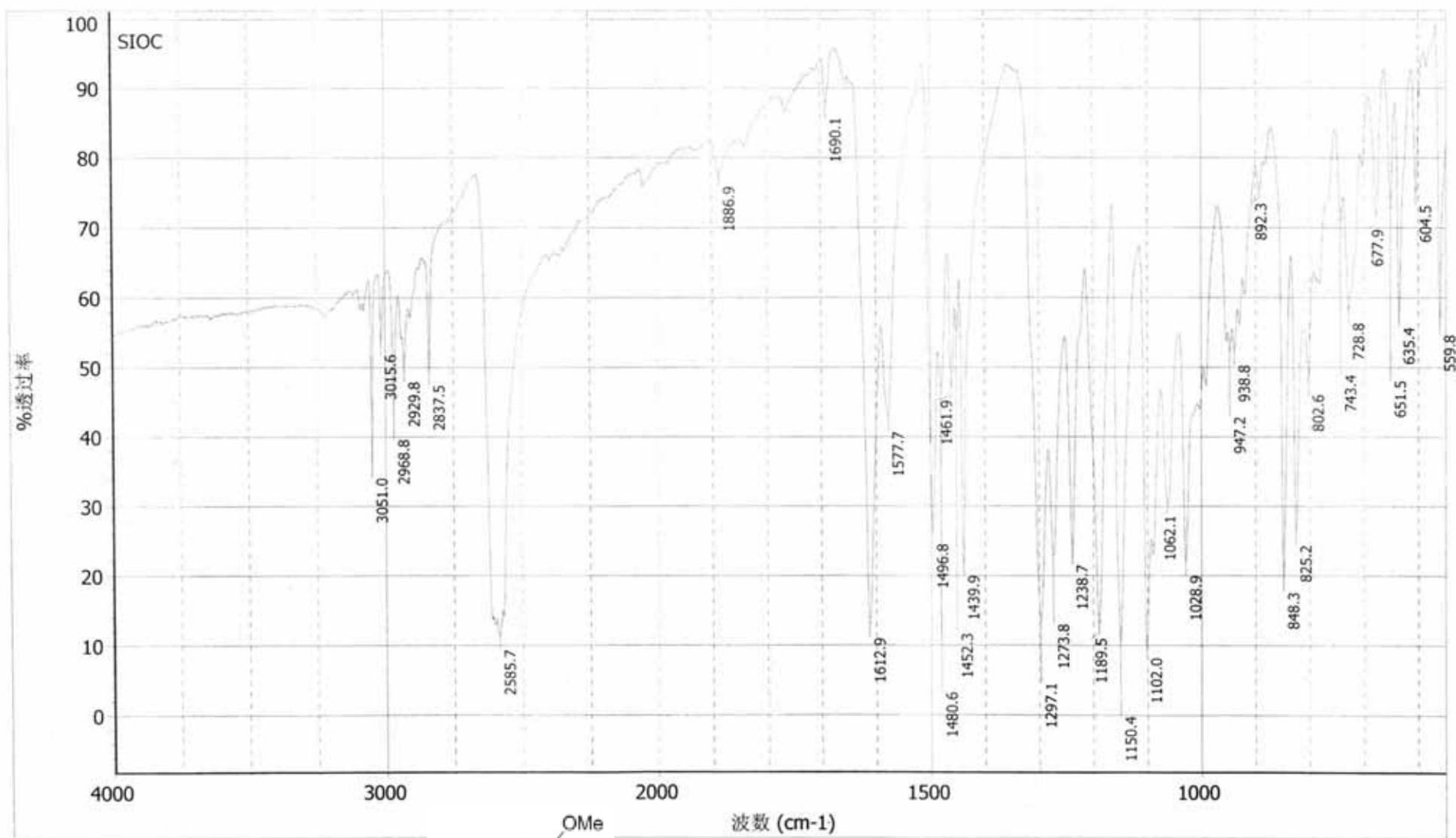


2f

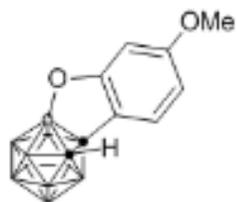


S130

Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-22-a/2012060b-ccx-7-22-1-coupling/1/pdata/1/1r
Title	2012060b-ccx-7-22-1-coupling
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring1gy
Number of Scans	54
Receiver Gain	128
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2016-11-15T20:38:26
Modification Date	2016-11-15T14:20:14
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16419.8
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

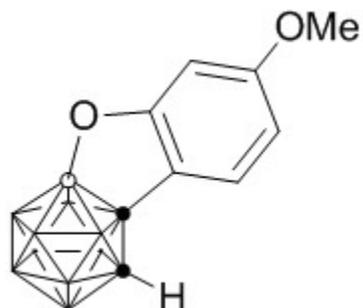


CCX-7-22-a 2015806 JS

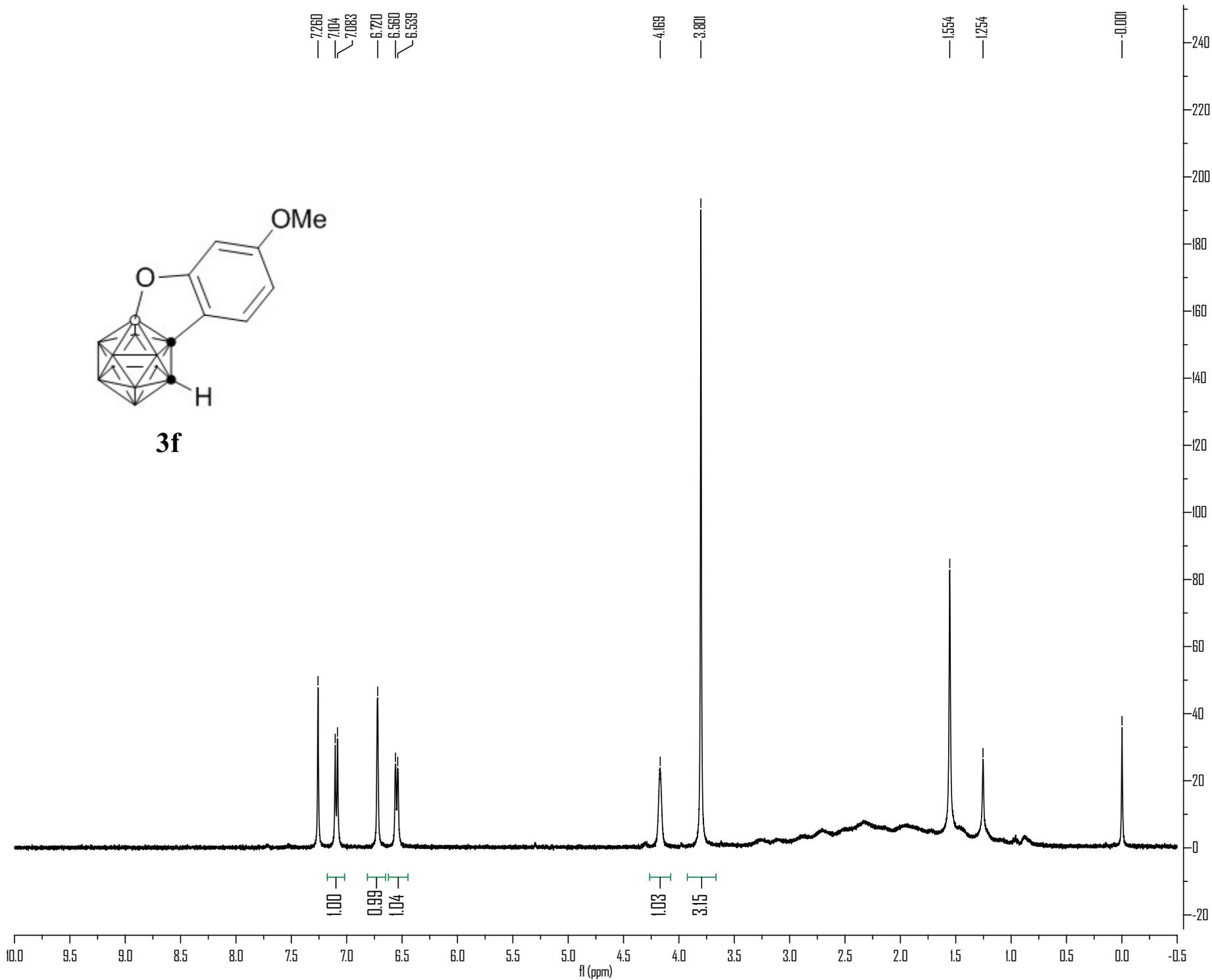


2f

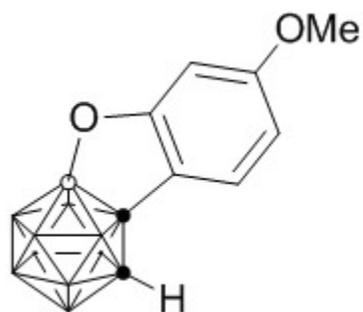
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



3f



Parameter	Value
Data File Name	// 10.0.16.23/ nmr/ HuGang/ CCX/ CCX-7/ ccx-7-22-b-b.fid/ fid
Title	ccx-7-22-b-b
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	omcl
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	44
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2018-10-08T12:10:21
Modification Date	2018-10-08T04:11:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-795.9
Nucleus	1H
Acquired Size	21552
Spectral Size	65536



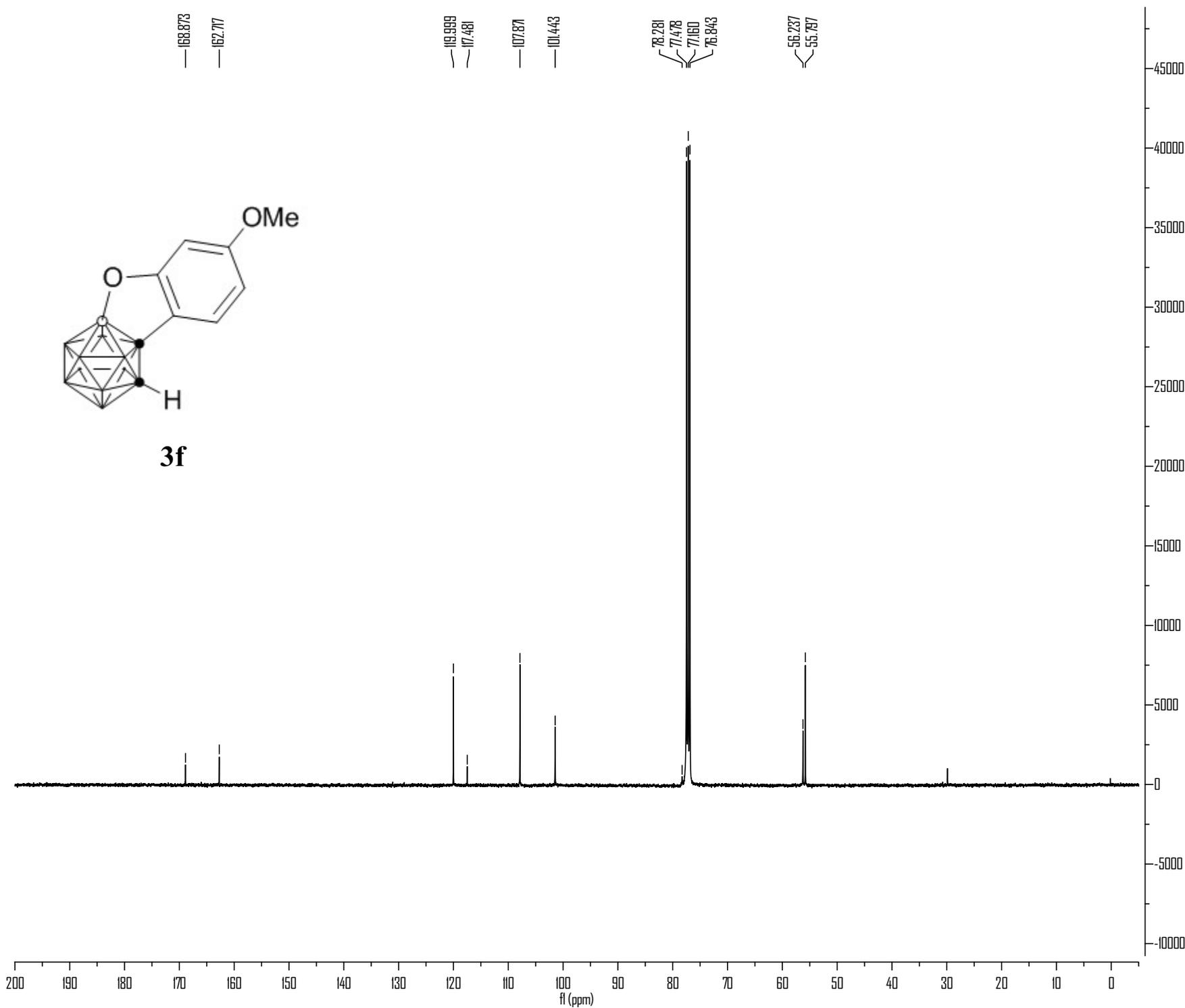
3f

168.873
162.777

119.999
117.481
107.871
101.443

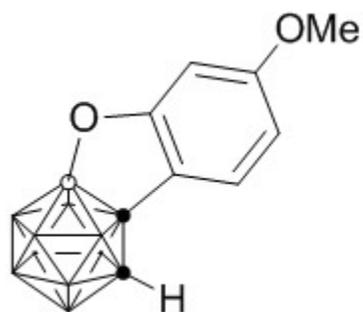
78.281
77.478
77.160
76.843

56.237
55.797

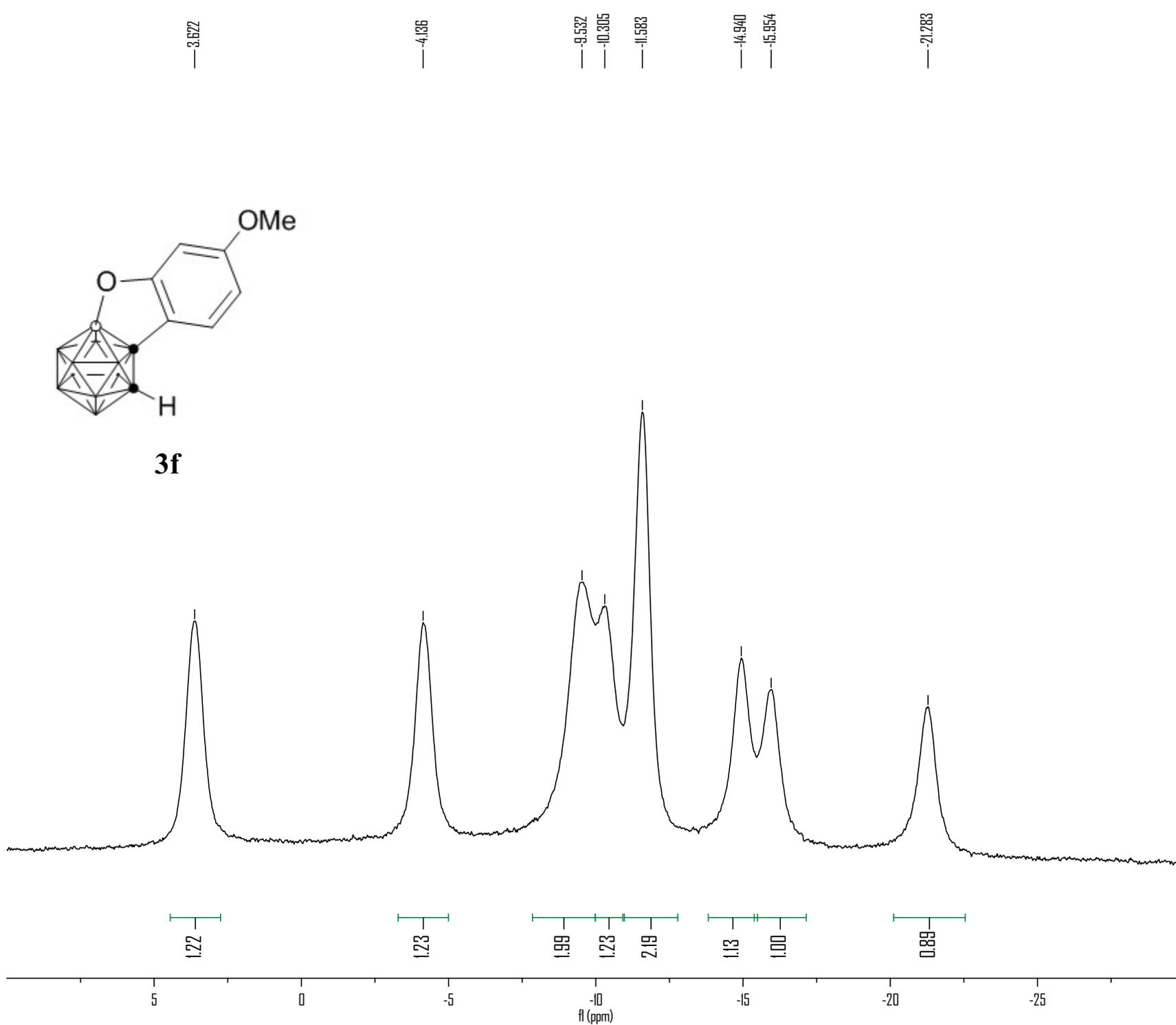


S133

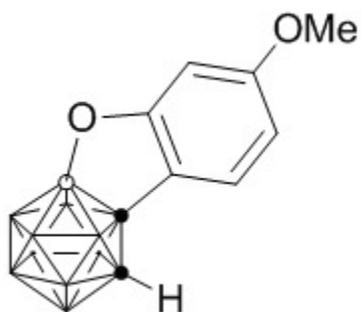
Parameter	Value
Data File Name	C:/Users/Administrator/Downloads/cccc-cx-7-22-b-b.fid/fid
Title	cccc-cx-7-22-b-b
Comment	ntnew experiment
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	16848
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2058
Acquisition Date	2018-10-09T15:07:27
Modification Date	2018-10-10T06:08:00
Spectrometer Frequency	100.51
Spectral Width	27173.9
Lowest Frequency	-3171.7
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



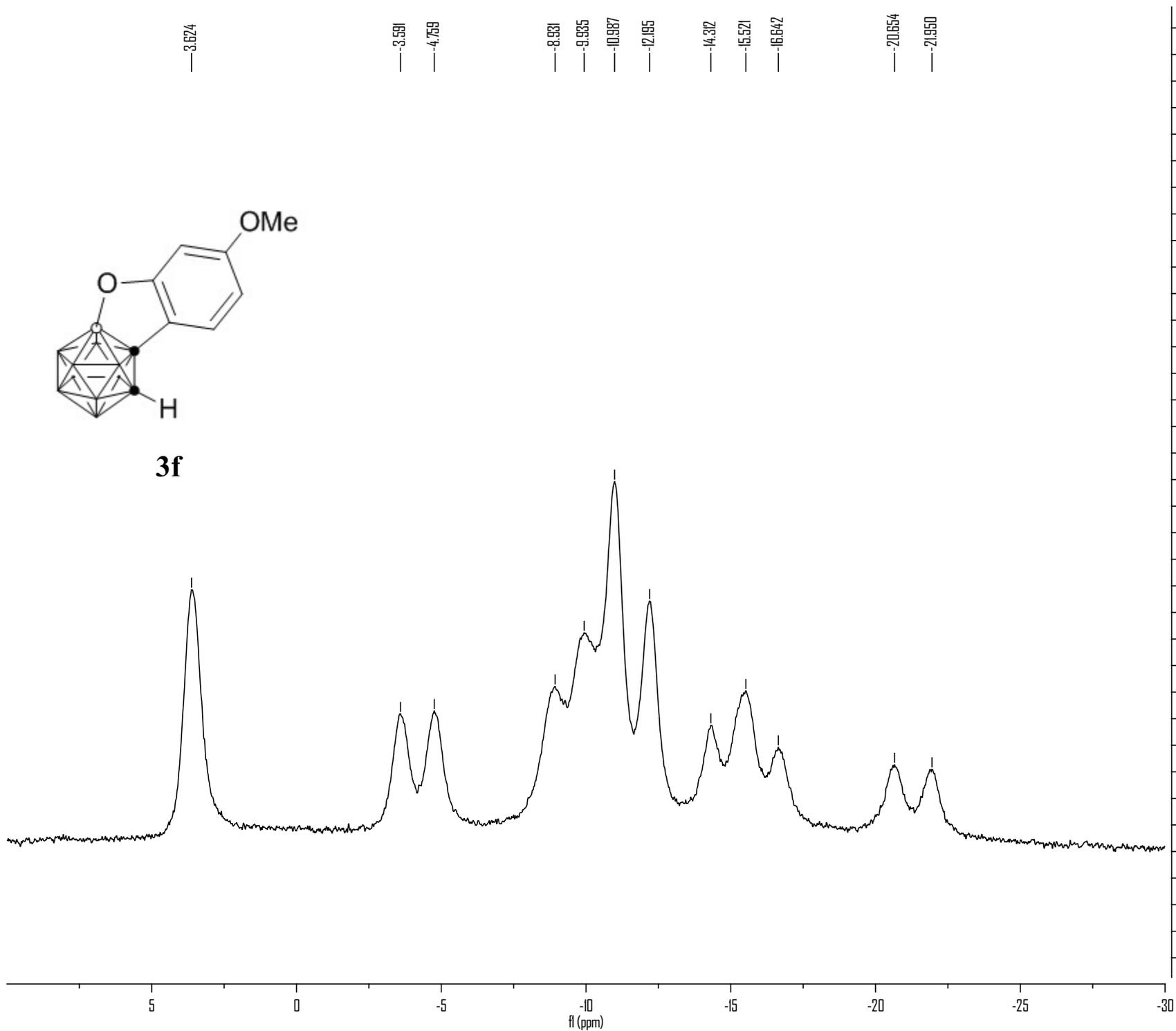
3f



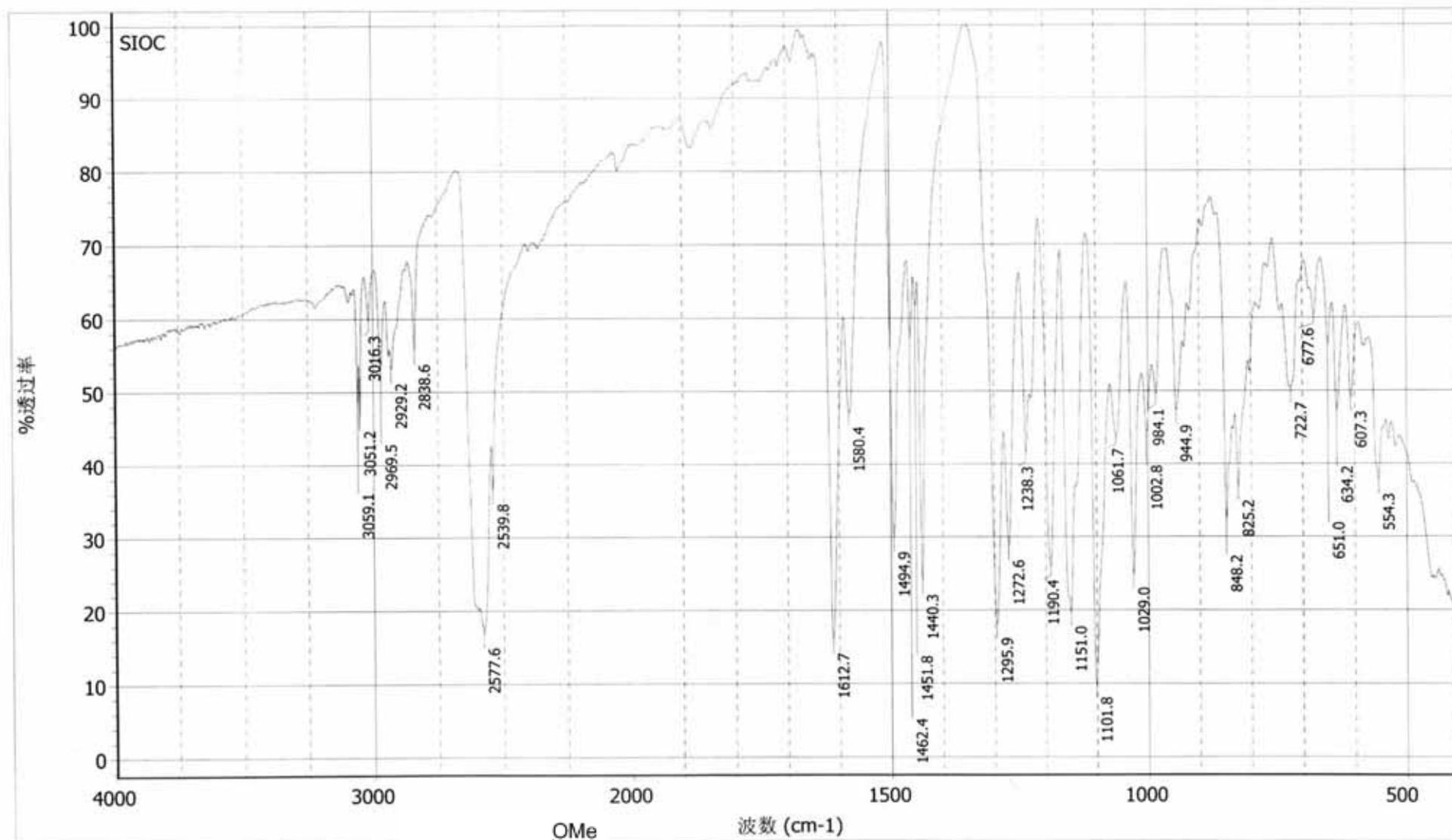
Parameter	Value
Data File Name	G:\Users\Administrator\Desktop\产物数据\7-22-b\2012060b-ccx-7-22-21-0105\1\pdata\1\1r
Title	2012060b-ccx-7-22-21-0105
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	97
Receiver Gain	256
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-01-05T20:44:52
Modification Date	2017-01-06T07:57:08
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16336.1
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



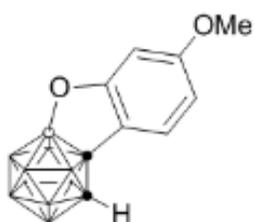
3f



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-22-b/2012060b-ccx-7-22-2-1-0105-coupling/1/pdata/1/1r
Title	2012060b-ccx-7-22-2-1-0105-coupling
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	108
Receiver Gain	256
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-01-05T20:43:25
Modification Date	2017-01-06T07:57:16
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-12696.1
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

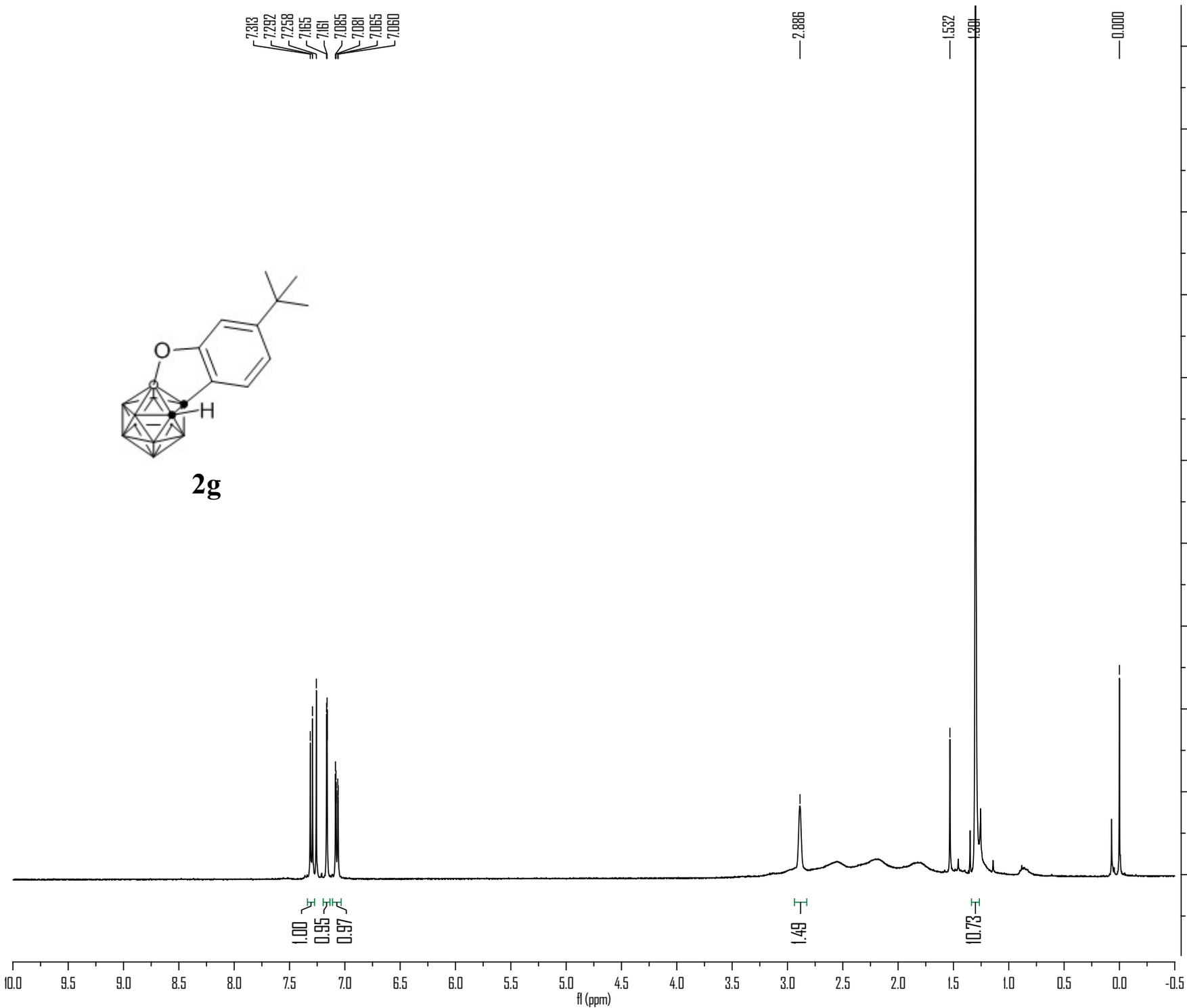


CCX-7-22-4 2015806 JS

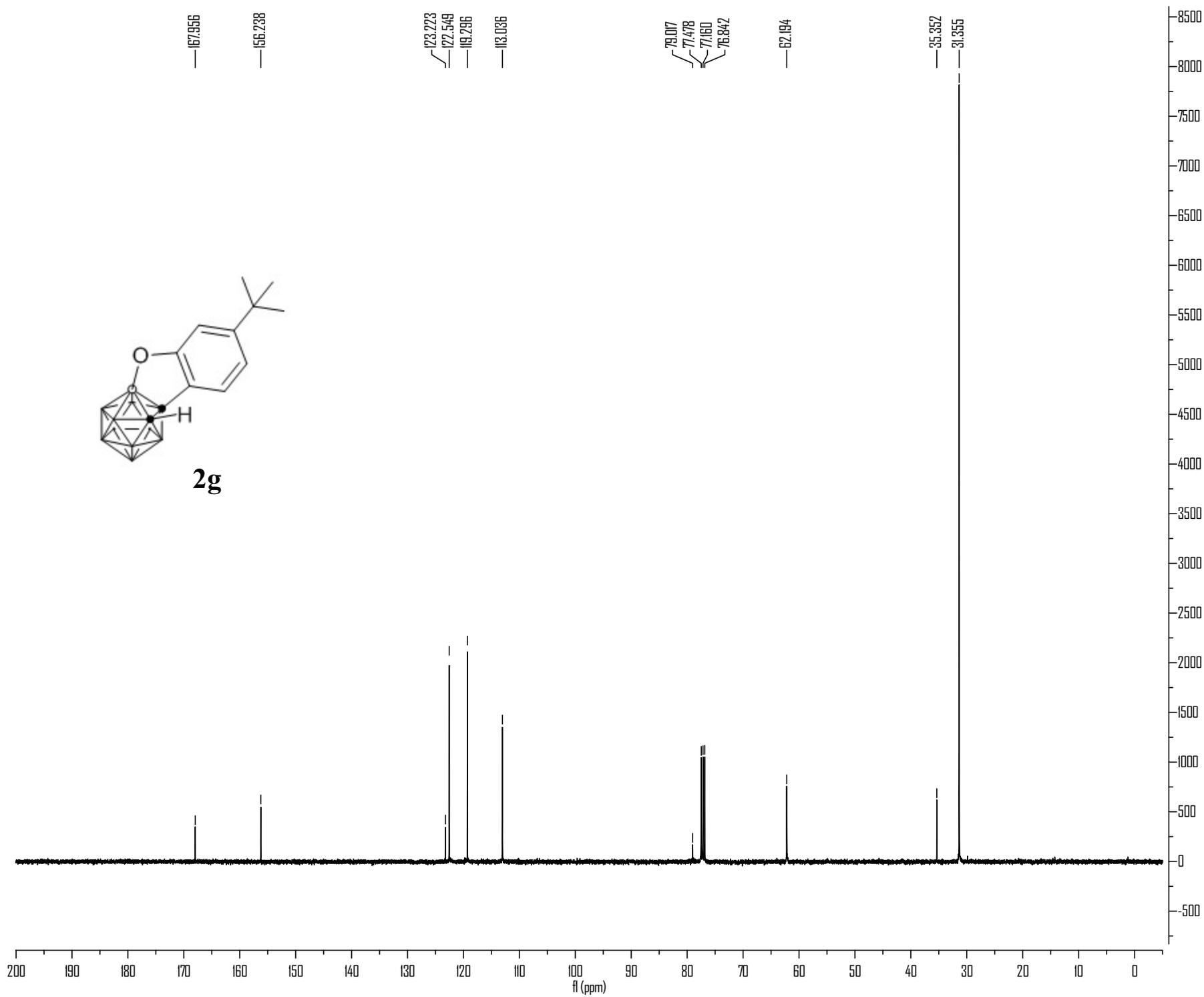


3f

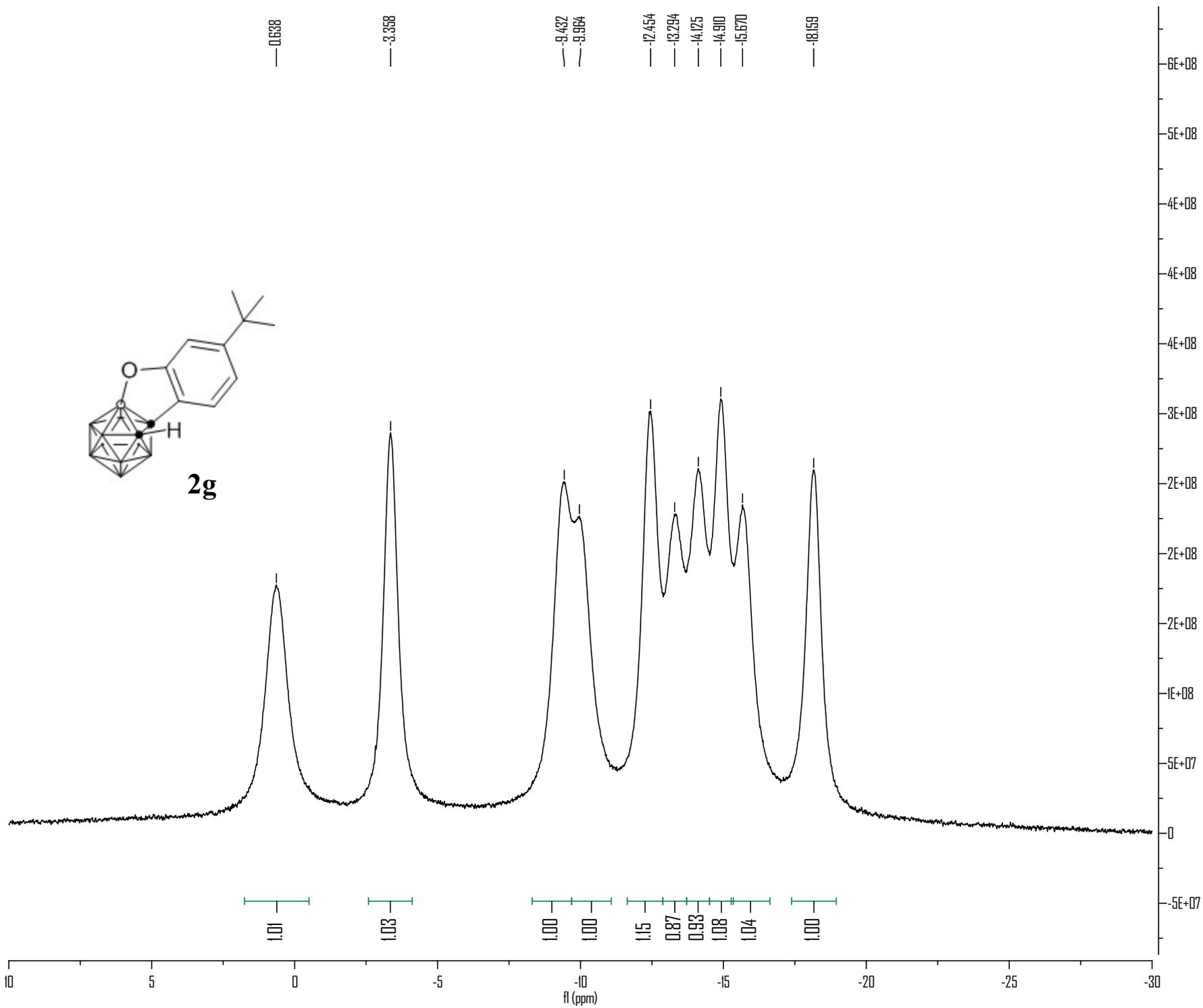
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.4747



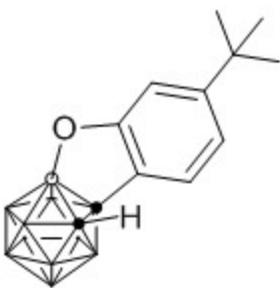
Parameter	Value
Data file Name	C:\Users\Administrator\Desktop\产物数据\6-63-1/h-cx6-63-1/pdata/1/1r
Title	6-63-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zg
Number of Scans	8
Receiver Gain	64
Relaxation Delay	2.0000
Pulse Width	5.0000
Acquisition Time	2.7263
Acquisition Date	2016-05-30T23:27:10
Modification Date	2016-05-30T17:27:00
Spectrometer Frequency	400.13
Spectral Width	12019.2
Lowest Frequency	-4565.0
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/6-63-1/C-CCX-6-63-1.fid/fid
Title	C-CCX-6-63-1
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	576
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-08-09T08:53:04
Modification Date	2016-08-09T01:17:00
Spectrometer	100.51
Frequency	
Spectral Width	25510.2
Lowest Frequency	-1682.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

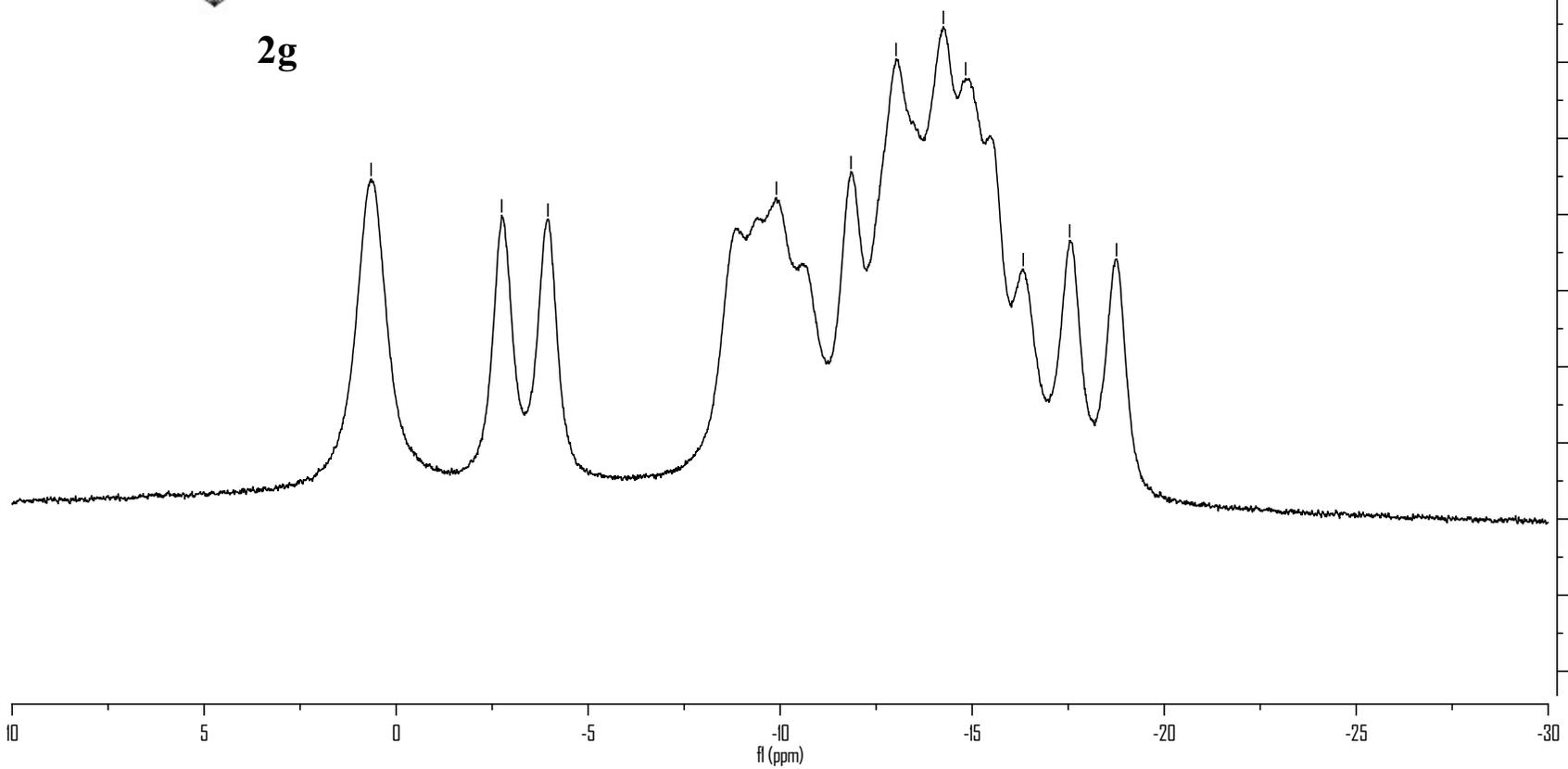


Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/G-63-1/b-cex-G-63-1/pdata/1/1r
Title	G-63-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring1gy
Number of Scans	212
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	8.5000
Acquisition Time	0.512
Acquisition Date	2016-05-30T23:29:04
Modification Date	2016-05-30T17:32:00
Spectrometer	128.38
Frequency	
Spectral Width	32051.3
Lowest Frequency	-16391.5
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



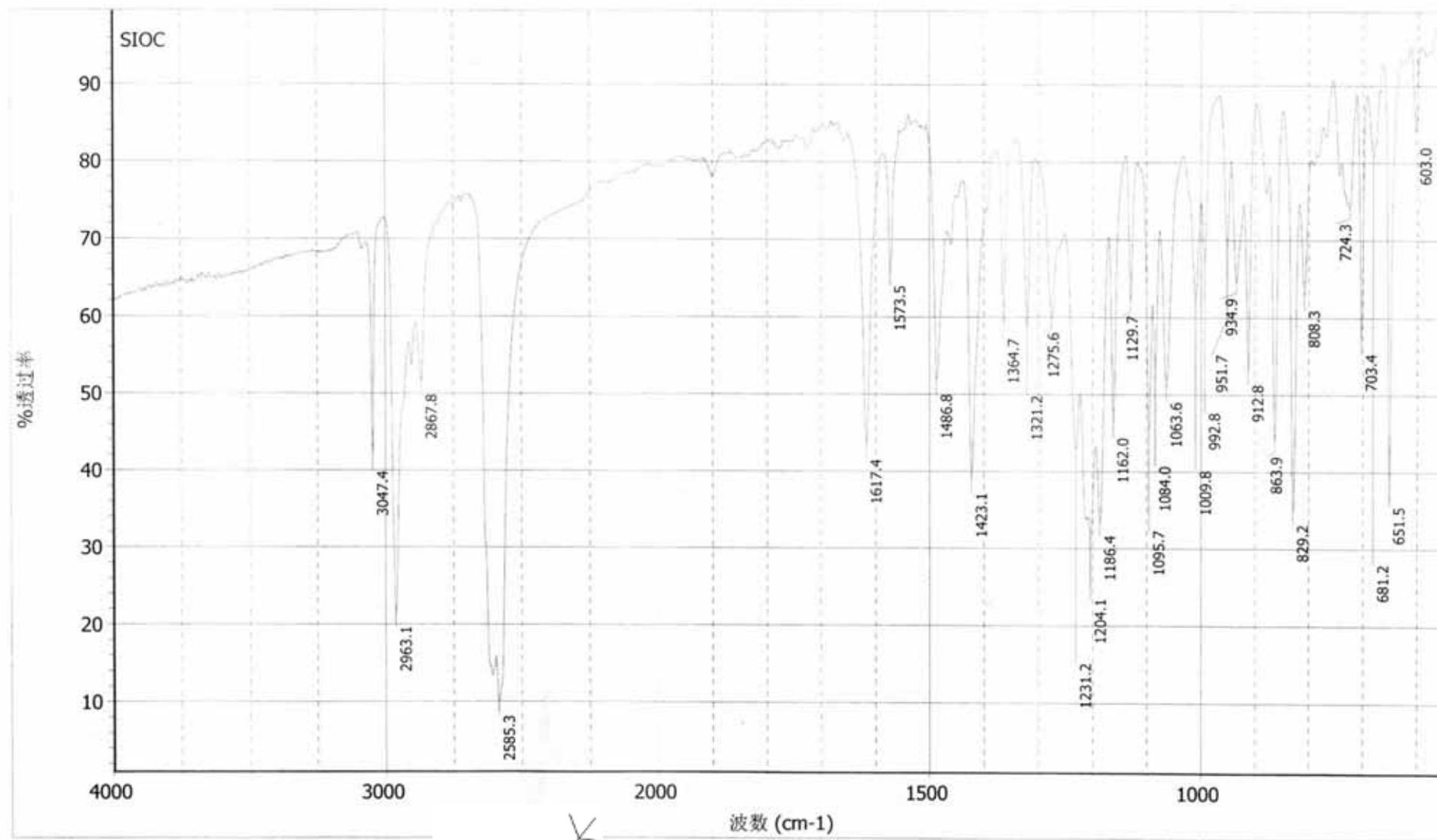
2g

0.653
-2.749
-3.953
-9.903
-11.844
-13.018
-14.251
-14.830
-16.330
-17.538
-18.759

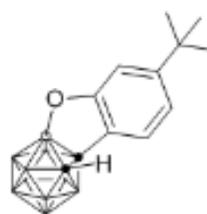


S140

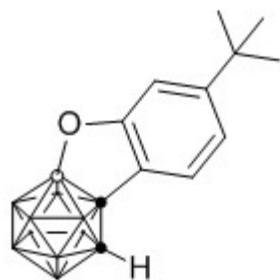
Parameter	Value
Data file Name	G:/Users/Administrator/Desktop/产物数据/6-63-1/b-cxx-6-63-1-coupling/pdata/1/1r
Title	6-63-1
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	256
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	8.5000
Acquisition Time	0.5112
Acquisition Date	2016-05-30T23:34:52
Modification Date	2016-05-30T17:40:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16391.5
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



CCX-6-63-1 2015806 JS

**2g**

样品扫描次数: 32
背景扫描次数: 32
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.6329



3g

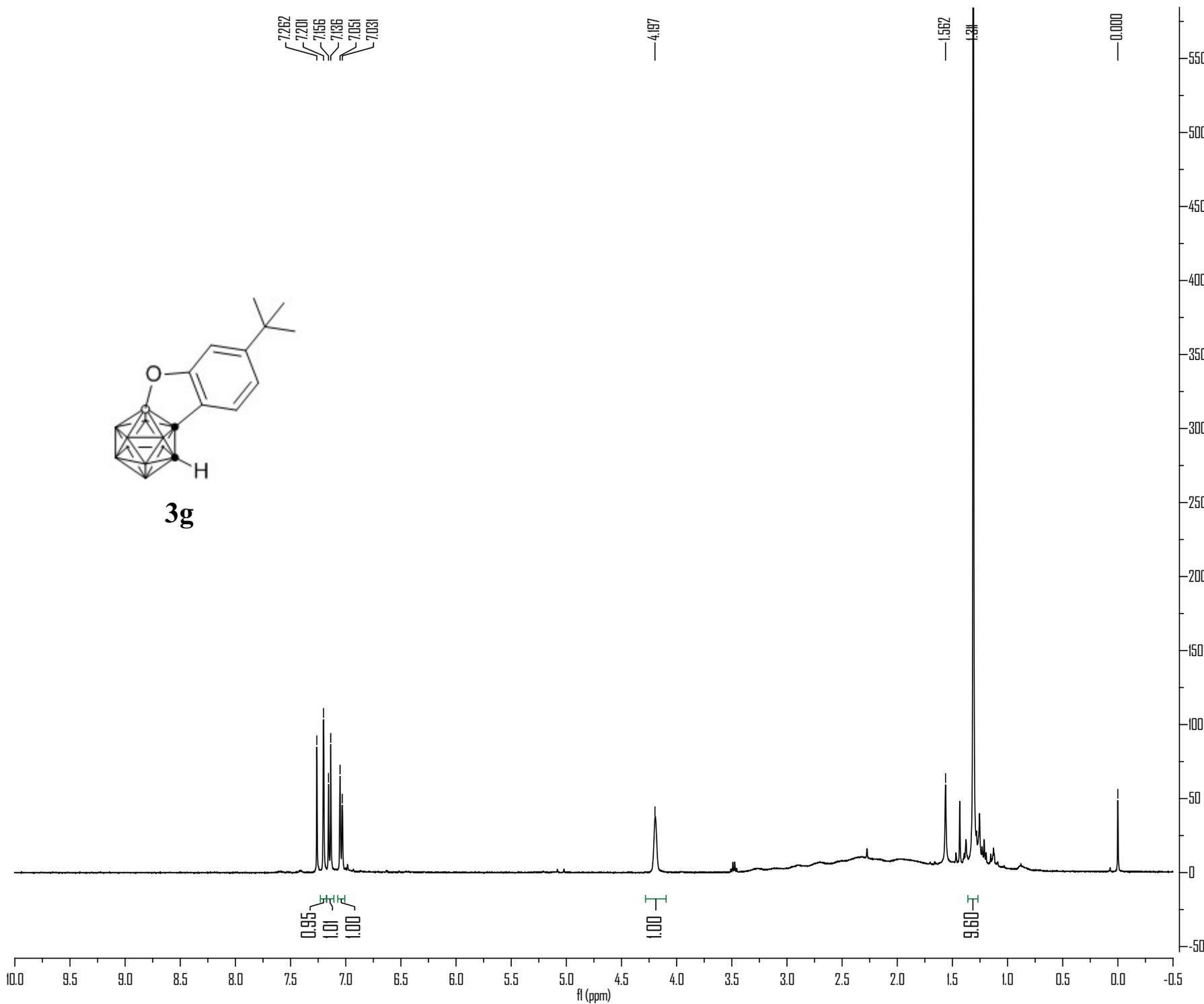
7.262
7.201
7.156
7.136
7.051
7.031

4.197

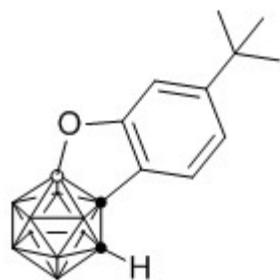
1.562

1.398

0.000



Parameter	Value
Data file Name	E:/Users/Administrator/Desktop/产物数据/7-83-2/ccx-7-83-2-1.fid/ fid
Title	ccx-7-83-2-1
Comment	xcc-Sci2
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-04-03T19:11:15
Modification Date	2017-04-03T11:12:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-793.1
Nucleus	1H
Acquired Size	21552
Spectral Size	65536



3g

167.536

155.440

122.210

118.822

113.055

78.170

77.478

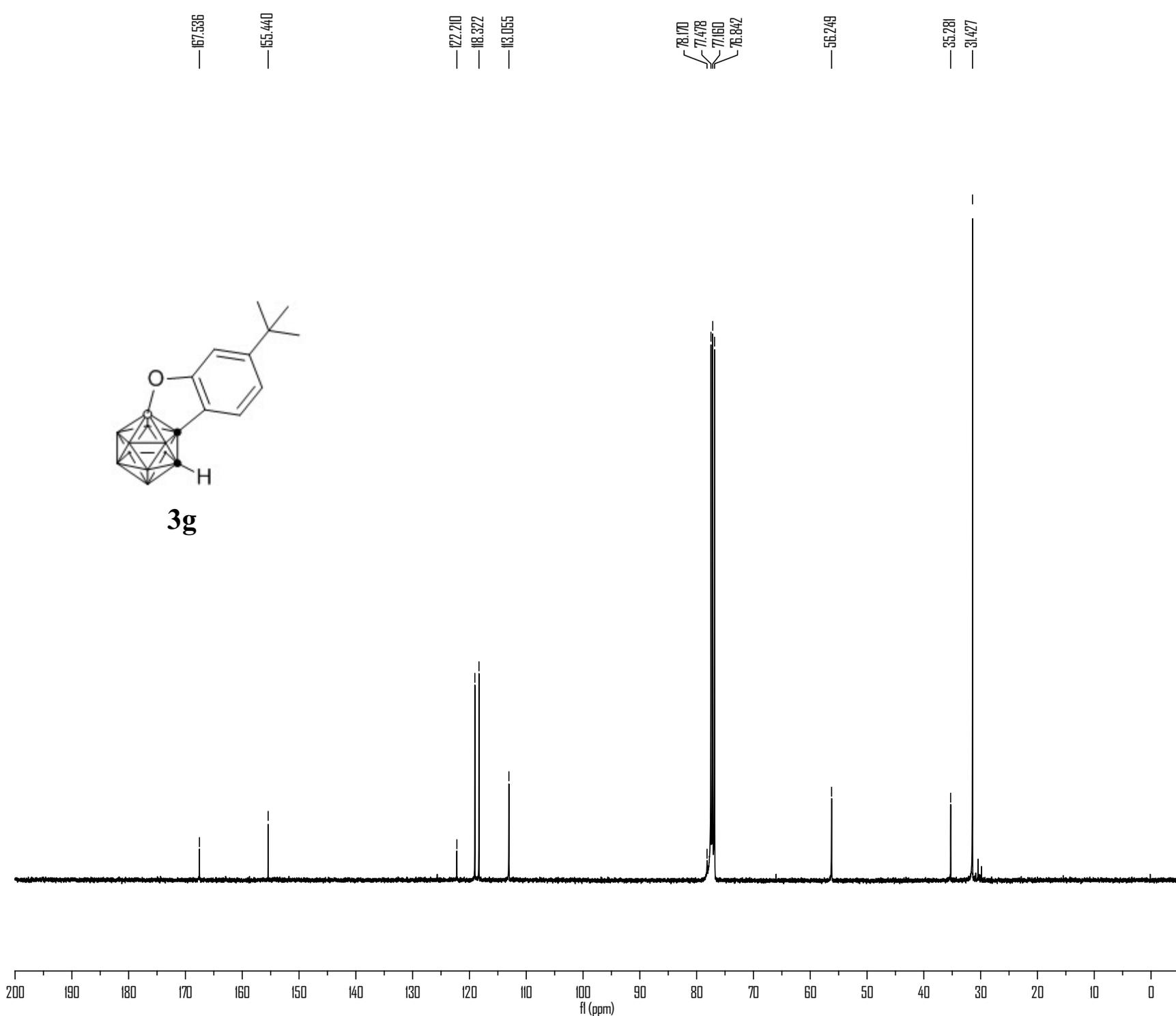
77.160

76.842

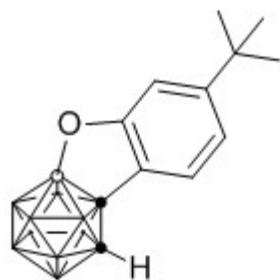
56.249

35.281

31.427



Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/7-83-2/-C-CX-7-83-2-1C.fid/ fid
Title	-C-CX-7-83-2-1C
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	27192
Receiver Gain	56
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.1272
Acquisition Date	2017-04-05 15:40:27
Modification Date	2017-04-06 07:45:00
Spectrometer	100.51
Frequency	
Spectral Width	29069.8
Lowest Frequency	-4040.0
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



3g

3.660

3.917

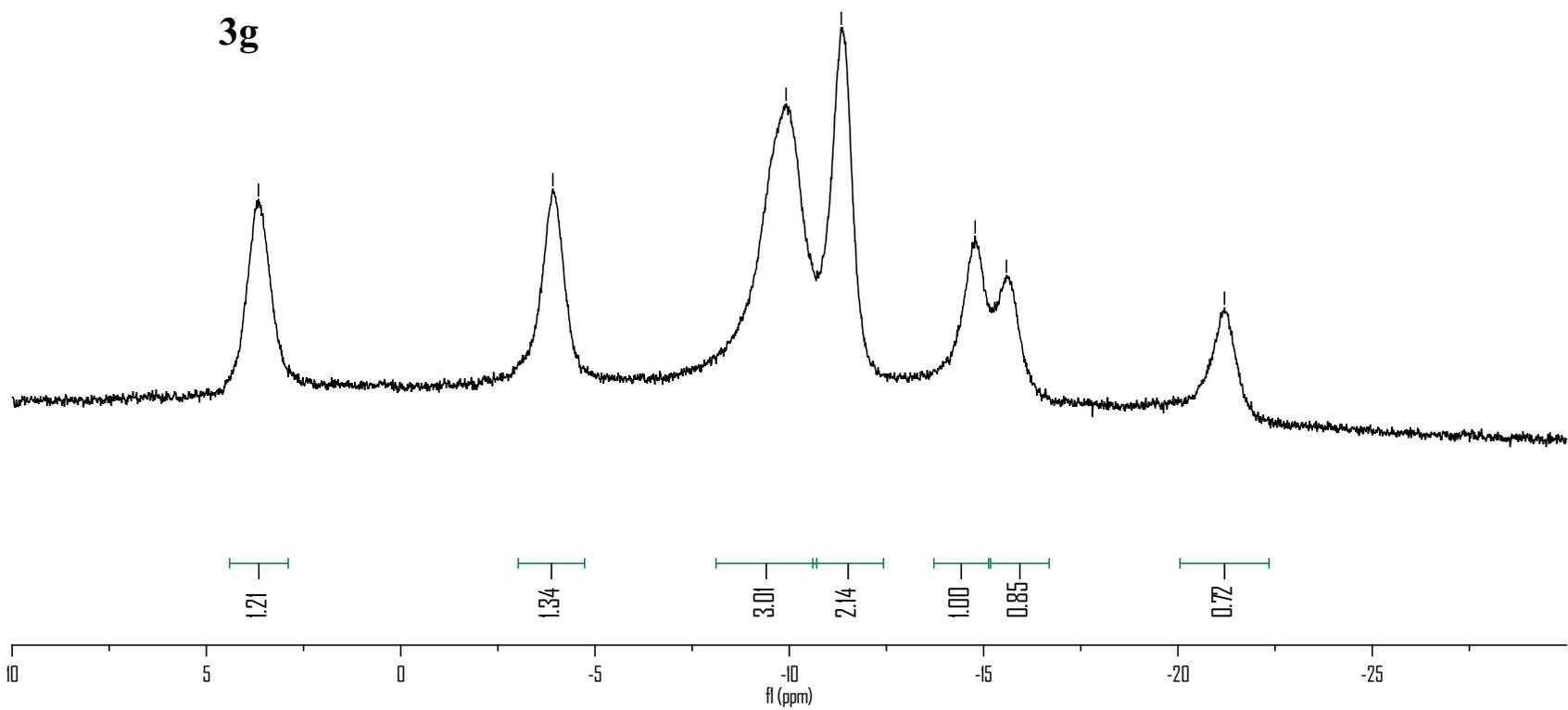
9.916

11.339

14.783

15.587

21.198



1.21

1.34

3.01

2.14

1.00

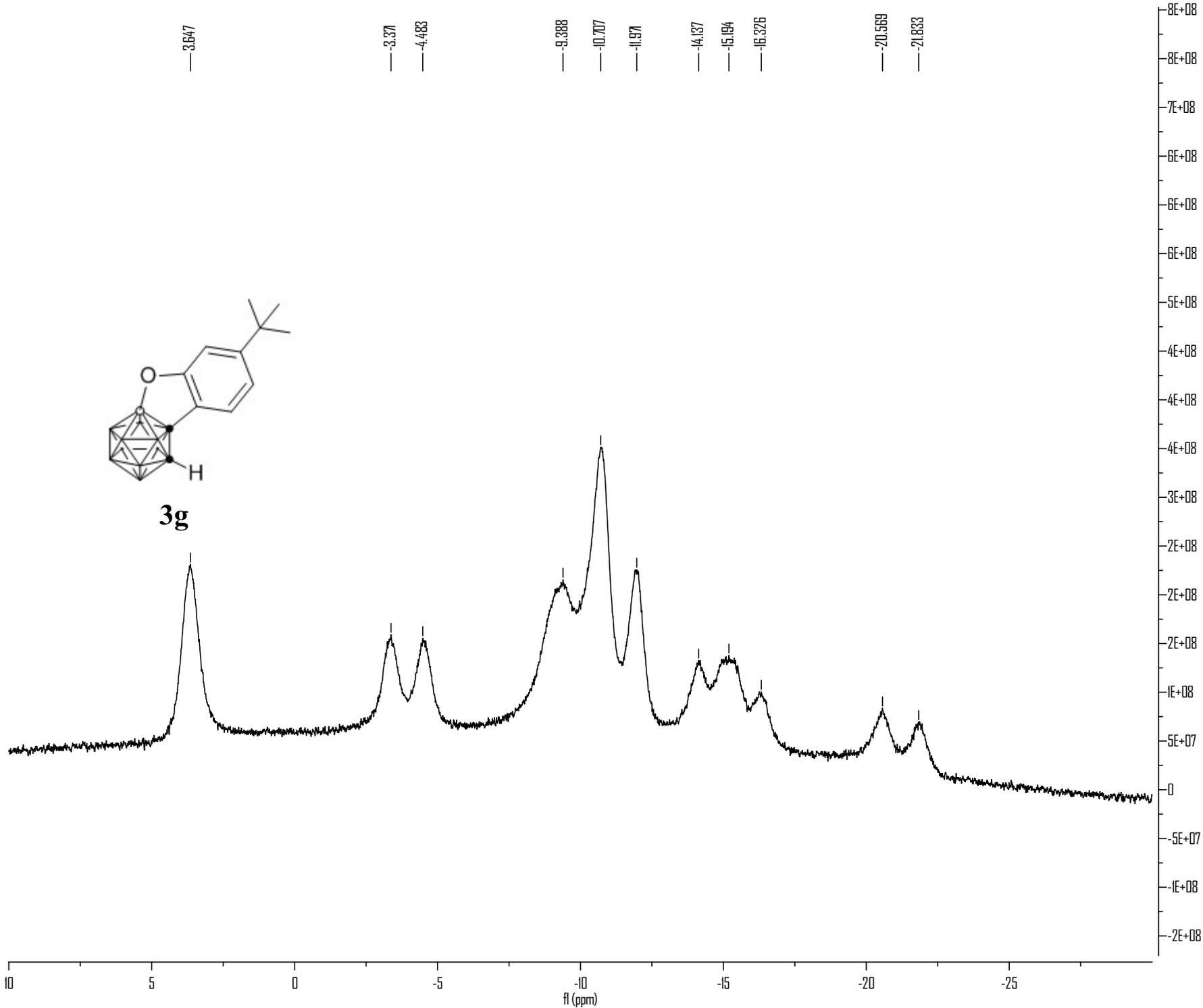
0.85

0.72

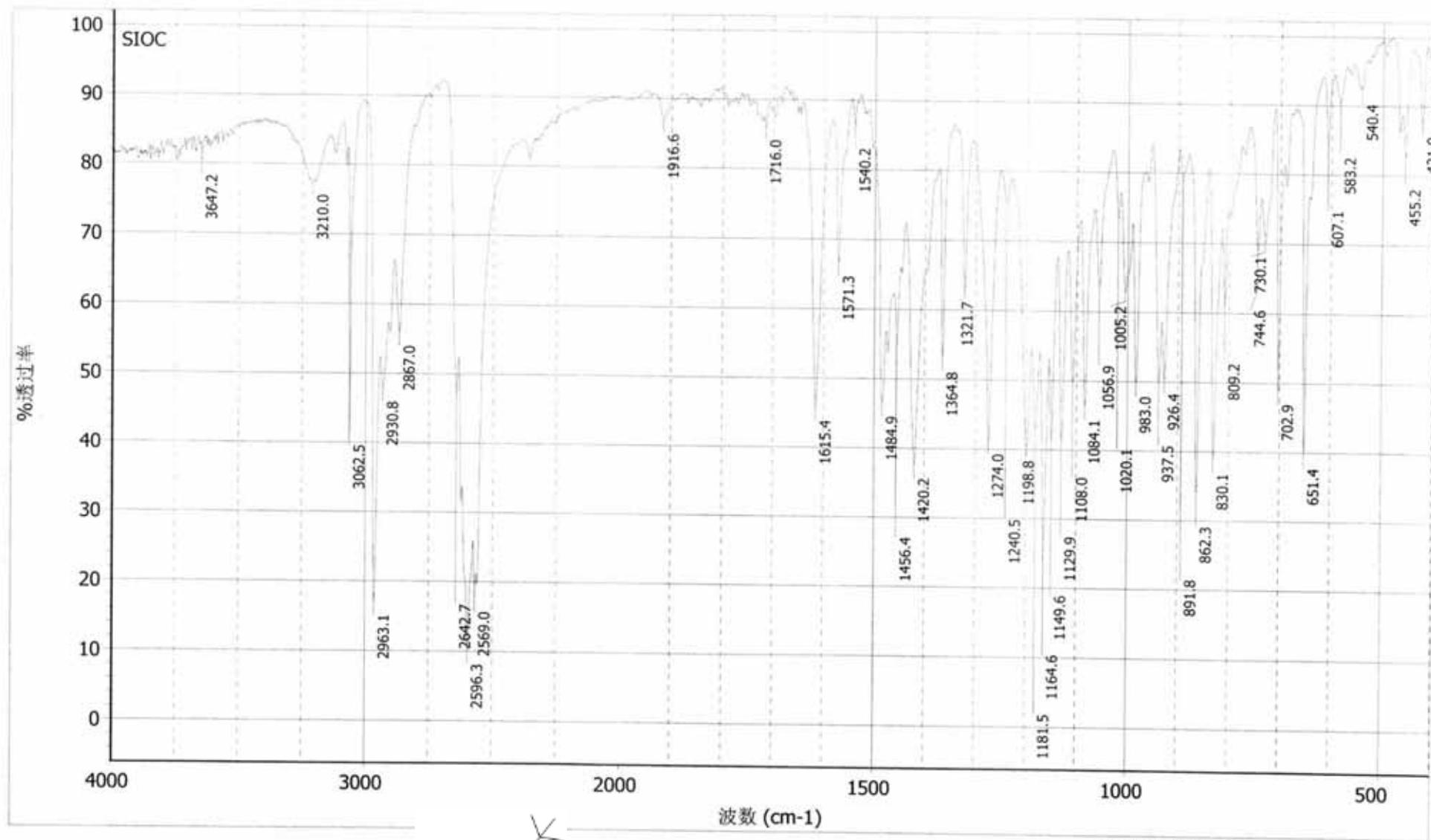
f1 (ppm)

S144

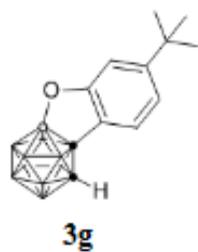
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-83-2/2012060b-ccx-7-83-2-1/pdata/1/1r
Title	2012060b-ccx-7-83-2-1
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	260
Receiver Gain	575
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-04-05T22:43:21
Modification Date	2017-04-05T16:06:06
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16379.7
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-83-2/2012060b-ccx-7-83-2-1-coupling/1/pdata/1/1r
Title	2012060b-ccx-7-83-2-1-coupling
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring, lgy
Number of Scans	355
Receiver Gain	575
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	1.0224
Acquisition Date	2017-04-05T22:46:44
Modification Date	2017-04-05T16:06:02
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16379.7
Nucleus	11B
Acquired Size	32768
Spectral Size	32768



CCX-7-83-2 2015806 JS

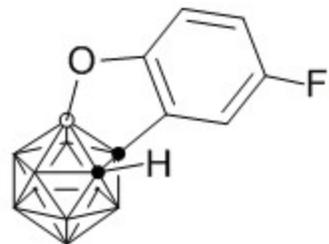


样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329

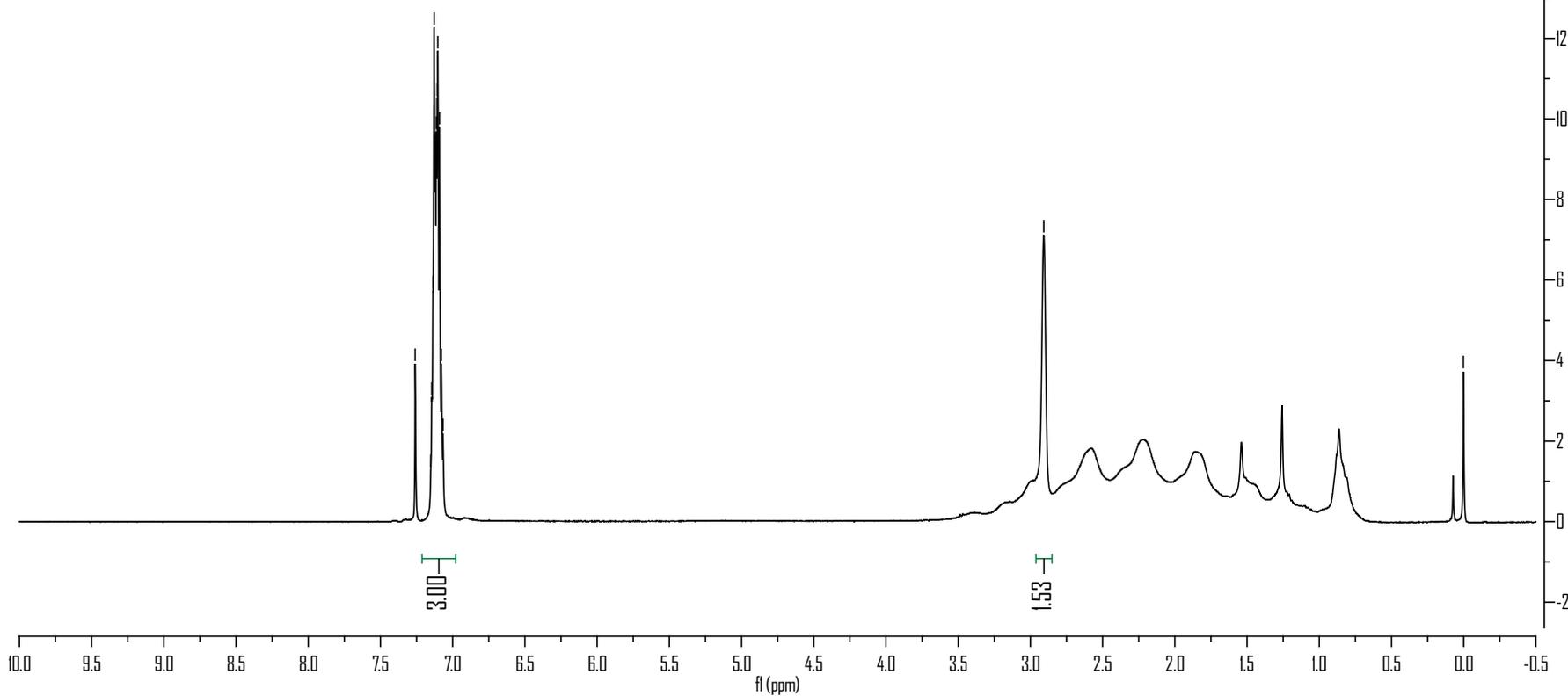
7.260
7.152
7.145
7.137
7.128
7.120
7.113
7.107
7.103
7.092
7.078
7.067

2.907

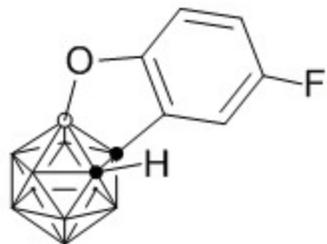
0.002



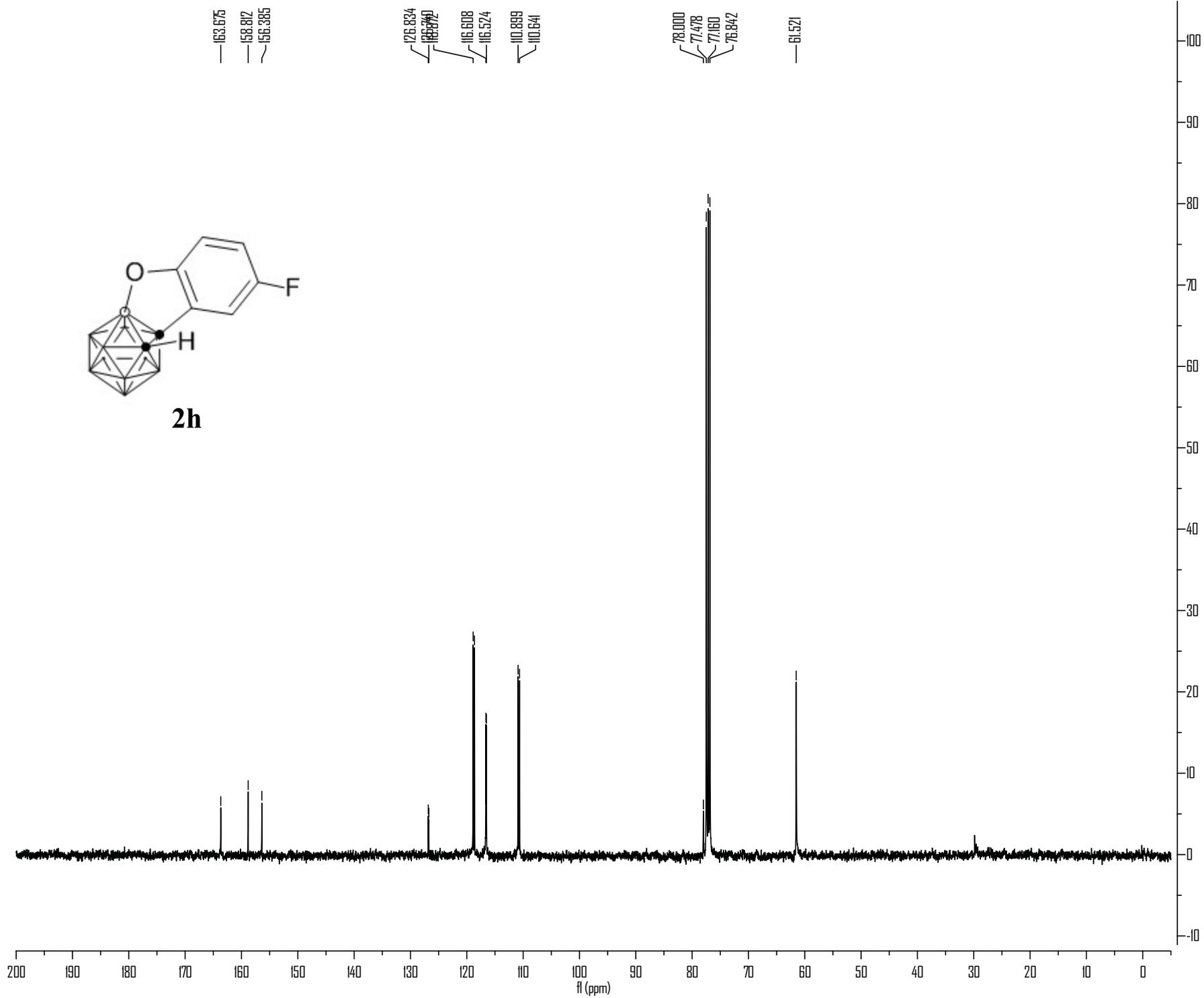
2h



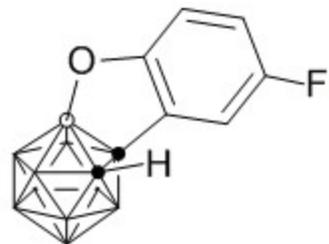
Parameter	Value
Title	h-cxx-6-38-1-a-h
Comment	ga STA NDA RD PROTON PA R A M E T E R S ga
Origin	Varian
Owner	
Site	
Spectrometer	vnmr's
Author	vnmr1
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	10
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.7224
Acquisition Date	2016-04-13T07:54:41
Modification Date	2016-04-13T01:04:00
Spectrometer Frequency	399.67
Spectral Width	8802.8
Lowest Frequency	-804.3
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



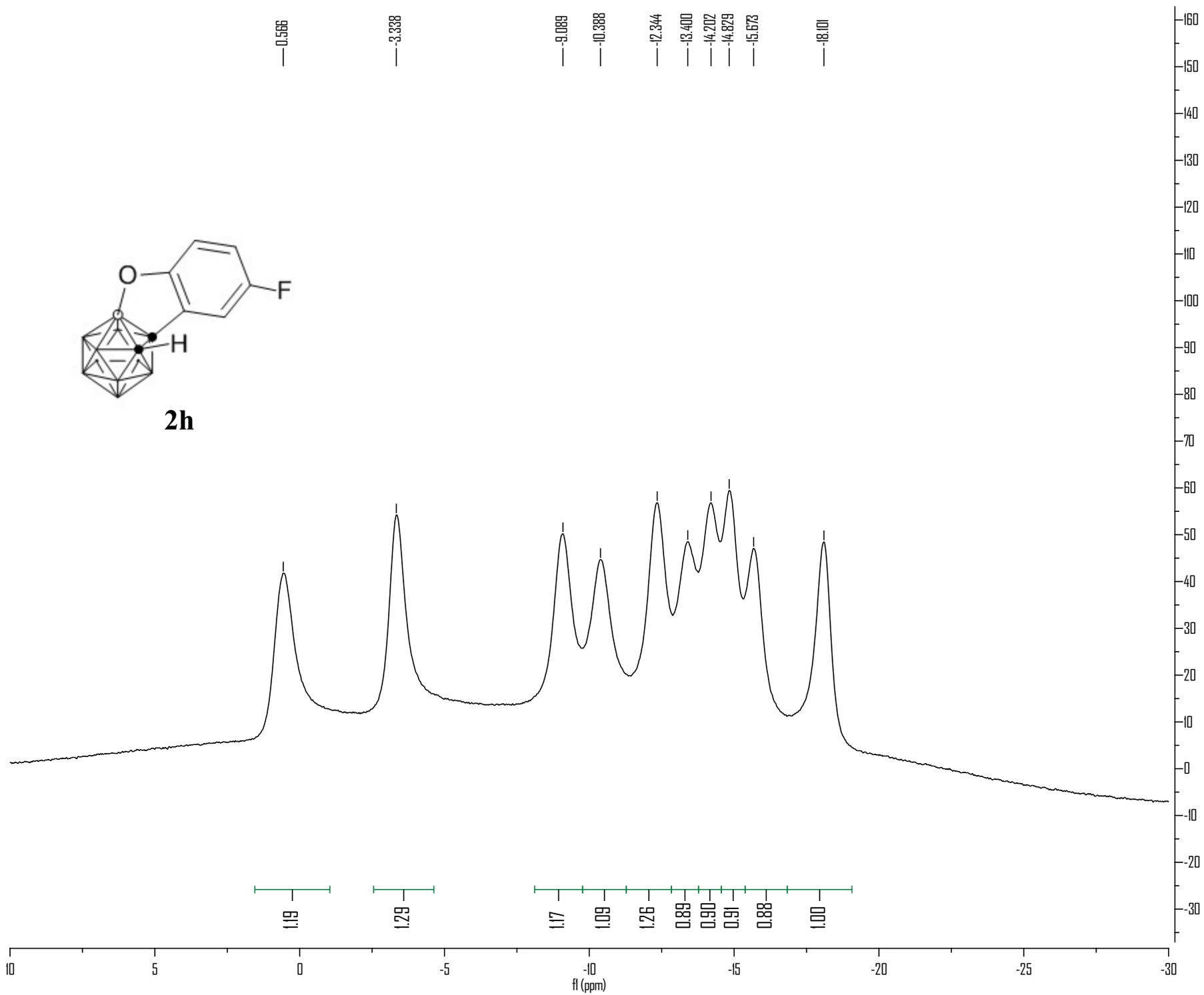
2h



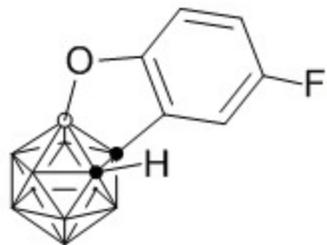
Parameter	Value
Title	cc-cx-6-33-1-acc
Comment	ga STANDARD PROTON PARAMETERSga
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	vnmr1
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	1208
Receiver Gain	30
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-04-13T07:53:25
Modification Date	2016-04-13T01:03:00
Spectrometer Frequency	100.51
Spectral Width	25510.2
Lowest Frequency	-1683.4
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



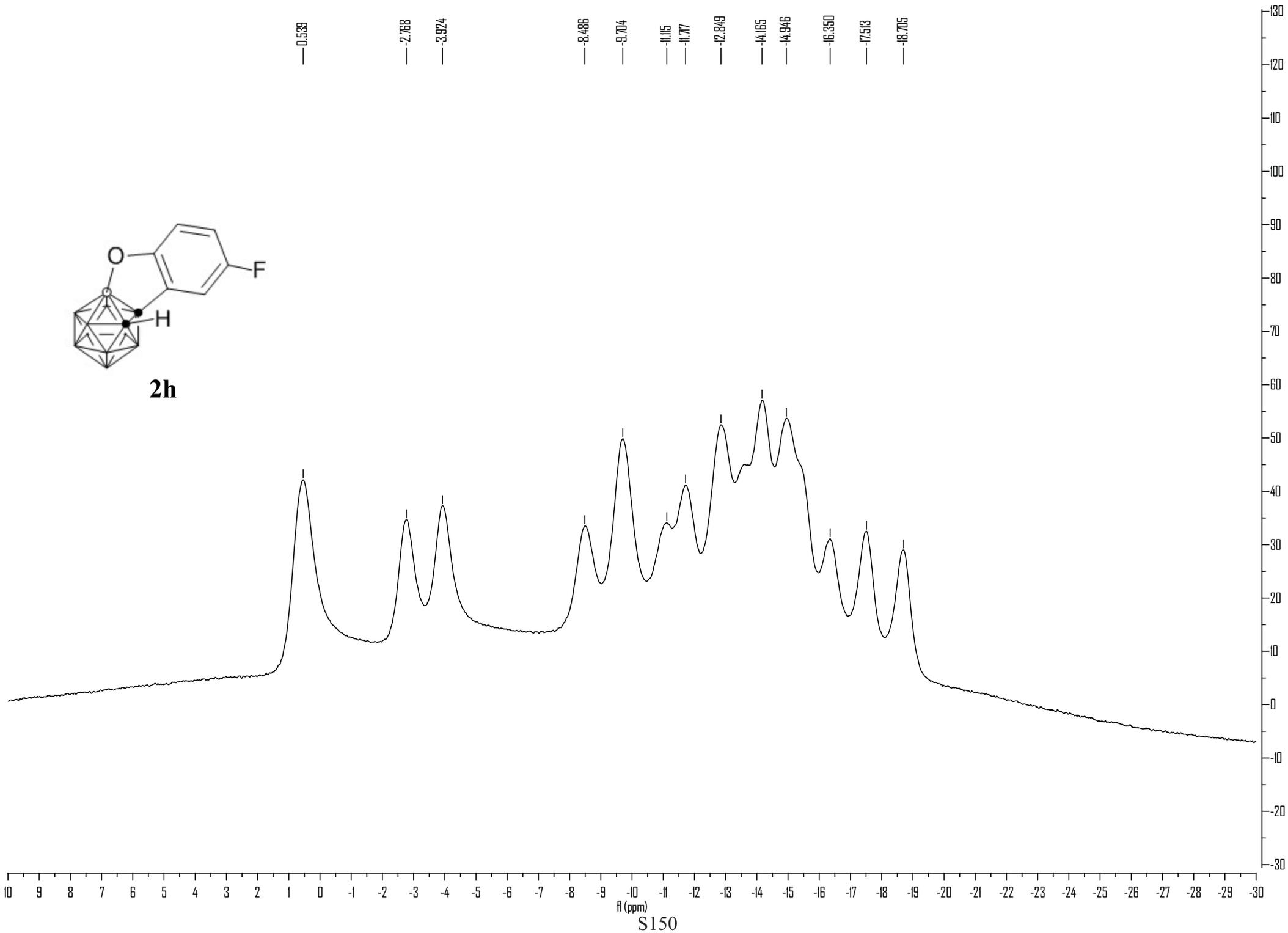
2h

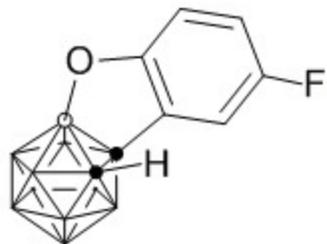


Parameter	Value
Title	b-ccx-6-38-1a
Comment	STANDARD CARBON PARAMETERS
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	cdcl3
Temperature	19.0
Pulse Sequence	s2pul
Number of Scans	256
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2533
Acquisition Date	2016-04-14T10:15:02
Modification Date	2016-04-14T02:17:00
Spectrometer	128.23
Frequency	
Spectral Width	26041.7
Lowest Frequency	-13541.5
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



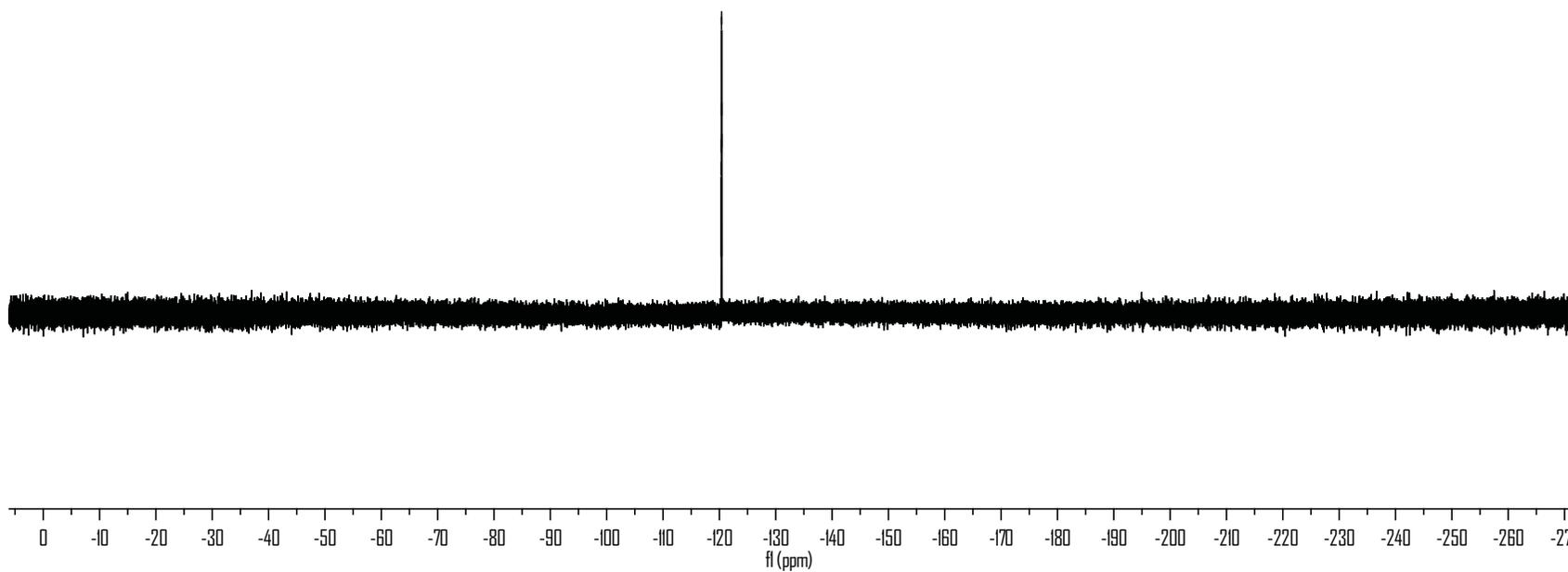
2h





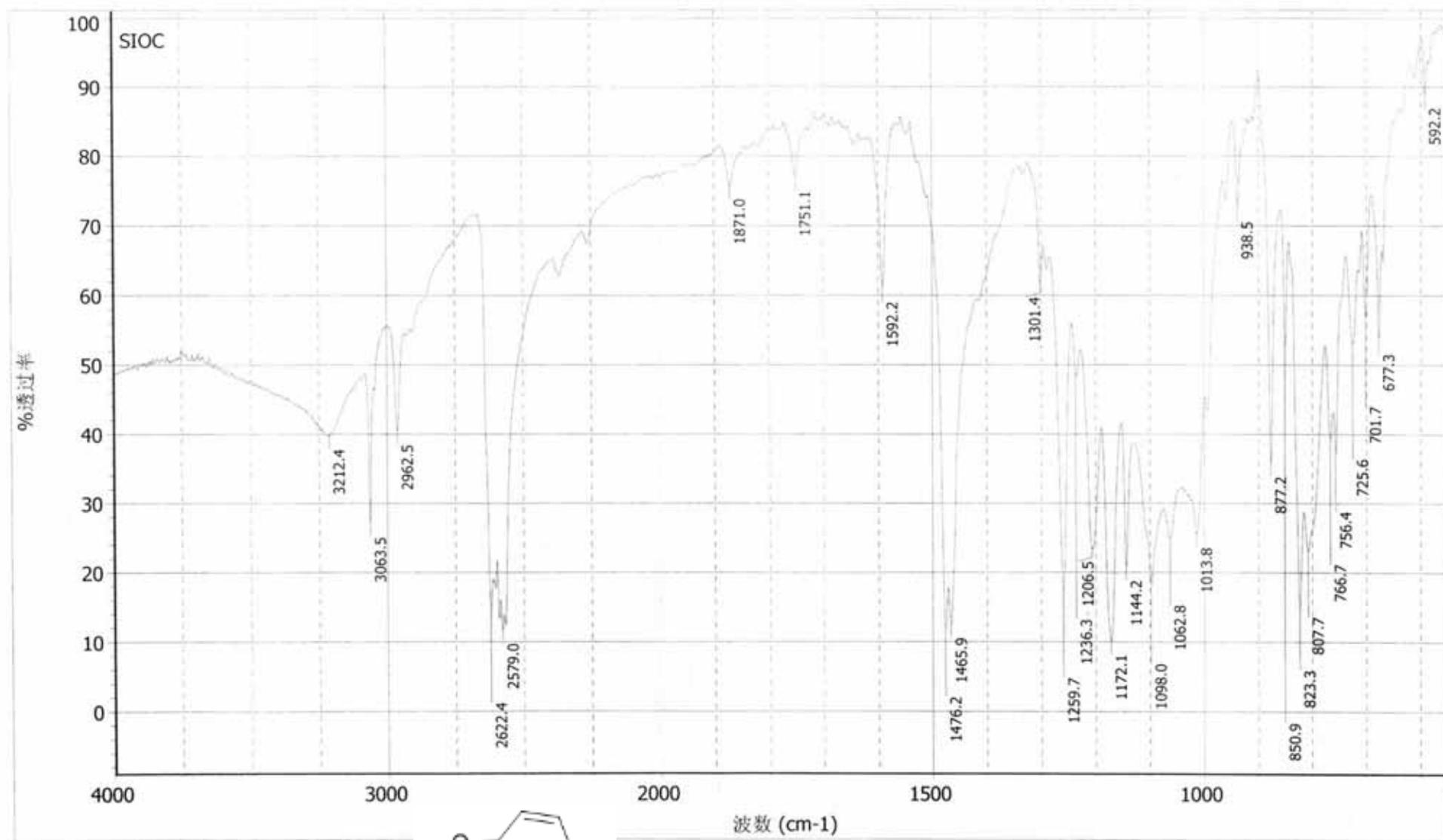
2h

120.356
120.373
120.383
120.399
120.408
120.426

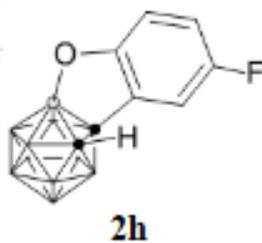


S151

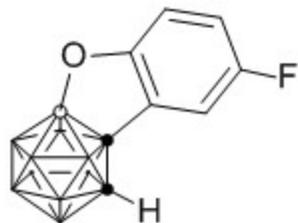
Parameter	Value
Title	ccx-6-41-a-F
Comment	19F OBSERVE STANDARD PARAMETERS
Origin	Varian
Owner	
Site	
Spectrometer	mercury
Author	omc
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Number of Scans	76
Receiver Gain	39
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	0.8192
Acquisition Date	2016-04-19T09:14:19
Modification Date	2016-04-19T09:16:00
Spectrometer	282.27
Frequency	
Spectral Width	78125.0
Lowest Frequency	-76429.6
Nucleus	19F
Acquired Size	64000
Spectral Size	131072



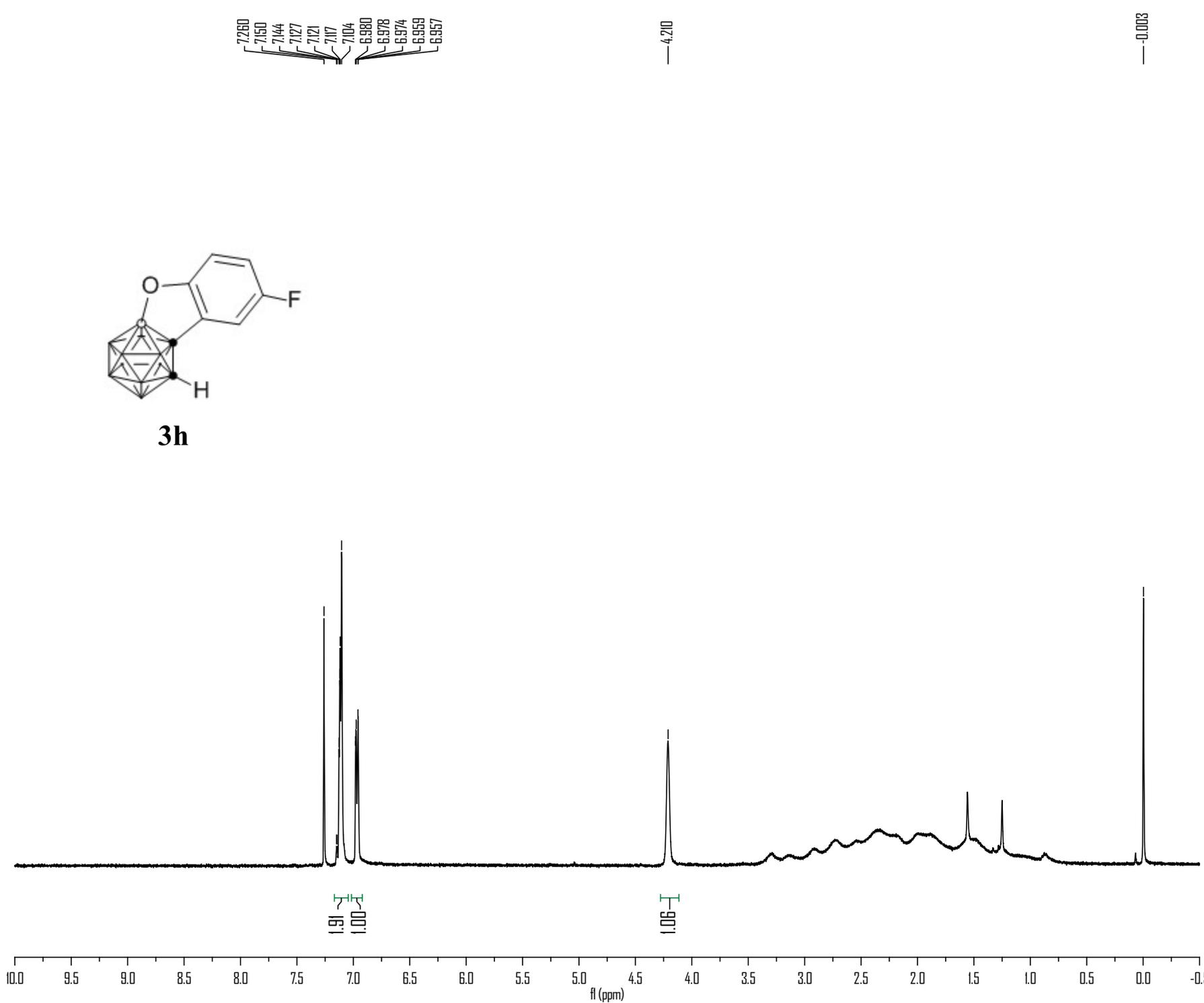
CCX-6-38-a 2015806 JS



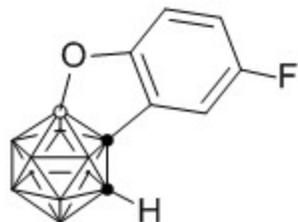
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



3h



Parameter	Value
Title	ccx-6-41-b-H
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omel
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	50
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-02-07T21:21:24
Modification Date	2017-02-07T13:22:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-793.8
Nucleus	¹ H
Acquired Size	21552
Spectral Size	65536



3h

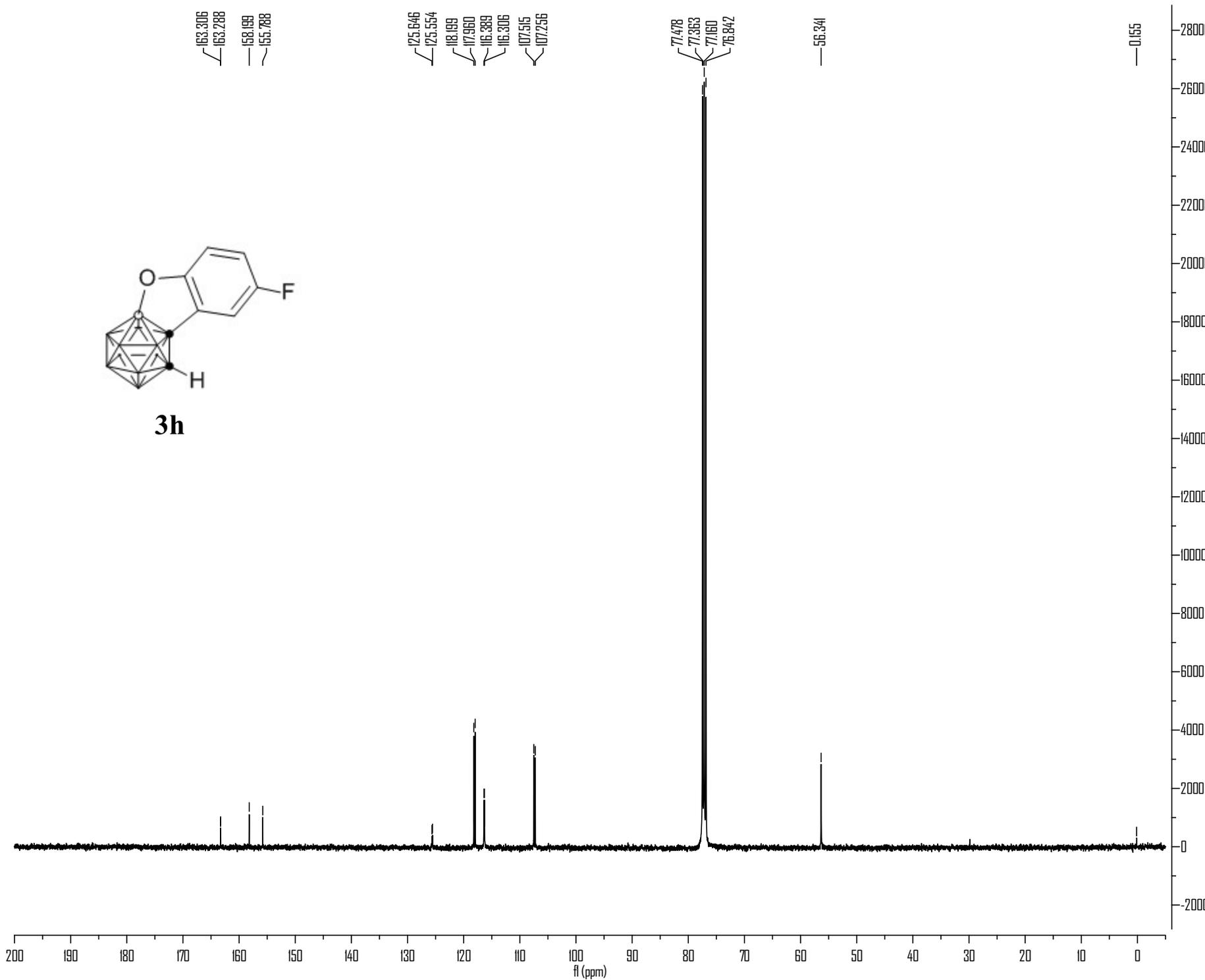
163.306
163.288
158.199
155.788

125.646
125.554
118.199
117.960
116.389
116.306
107.515
107.256

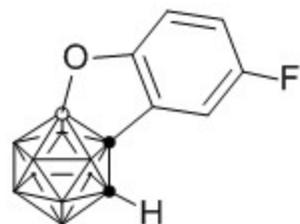
77.478
77.363
77.160
76.842

56.341

0.155

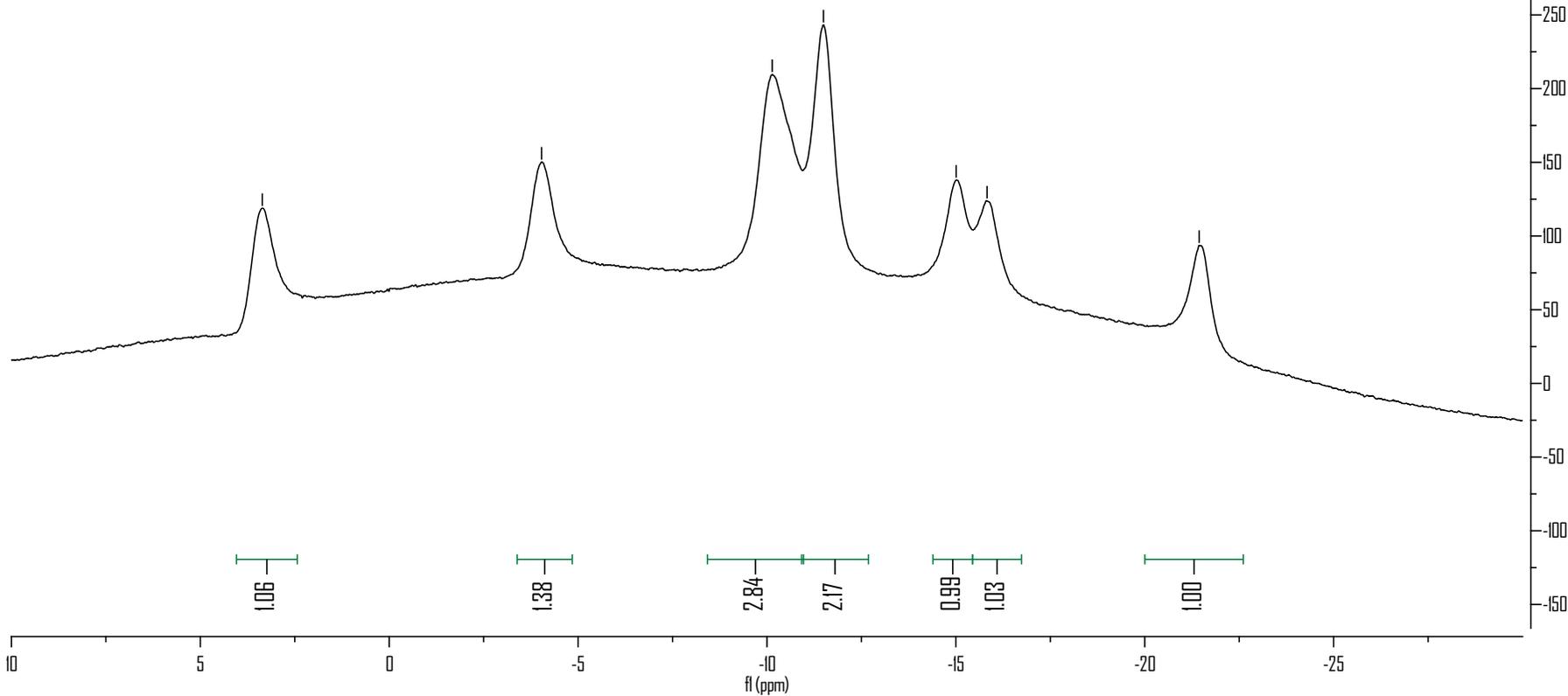


Parameter	Value
Title	ccx-6-41-b-000
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	11640
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Acquisition Date	2017-11-20T22:50:53
Modification Date	2017-11-20T22:19:00
Spectrometer	100.52
Frequency	
Spectral Width	25000.0
Lowest Frequency	-1428.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



3h

8.360
-4.033
-10.139
-11.495
-15.007
-15.825
-21.441



1.06

1.38

2.84

2.17

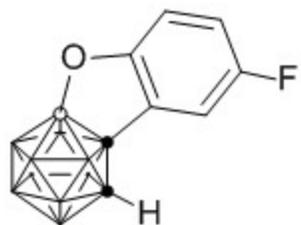
0.99

1.03

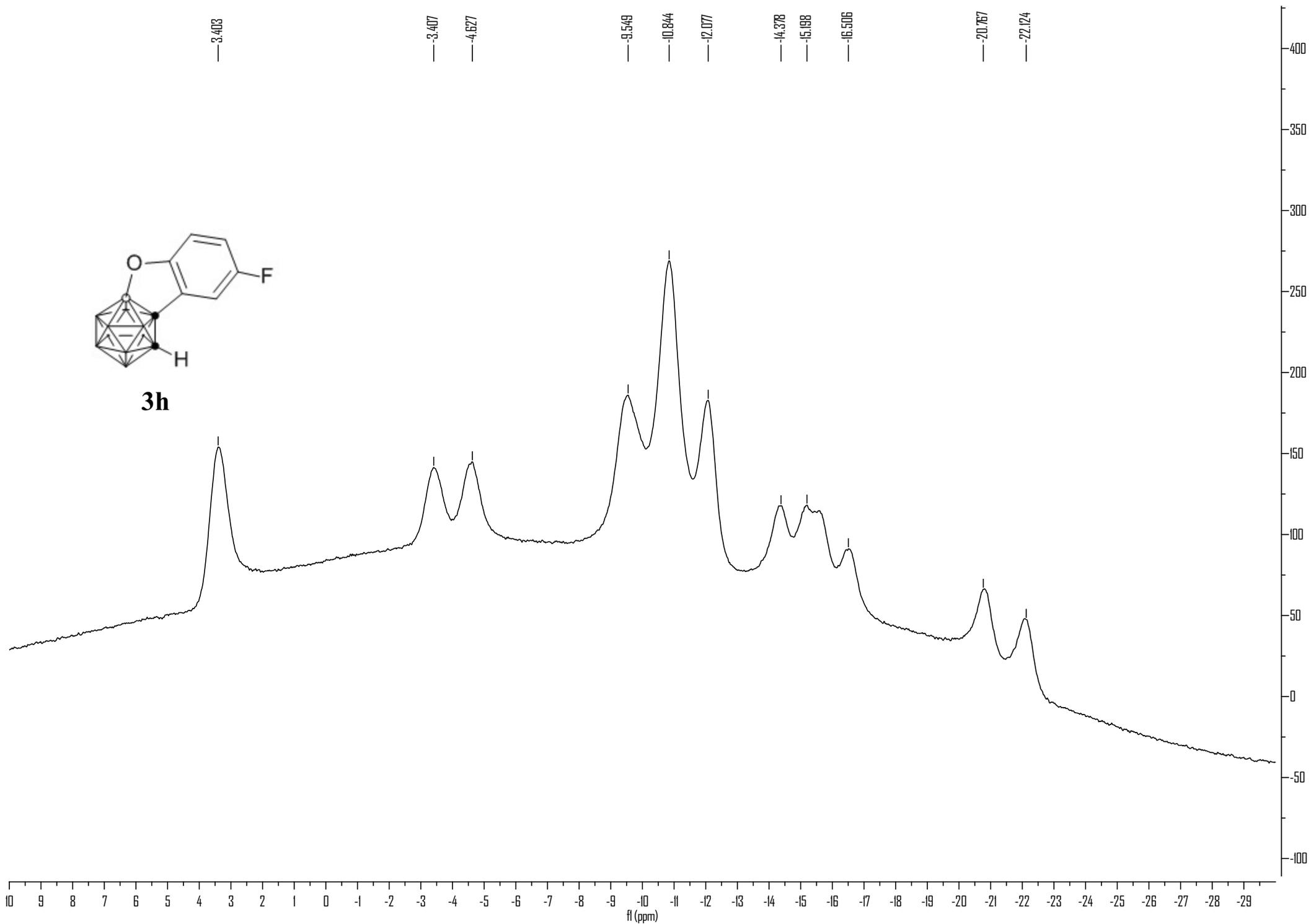
1.00

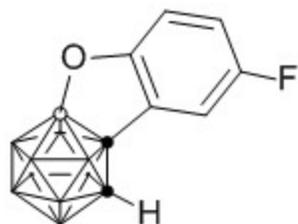
S155

Parameter	Value
Title	b-cxx-6-41-b-1
Comment	STANDARD CARBON PARAMETERS
Origin	Varian
Owner	
Site	
Spectrometer	nmrns
Author	nmr1
Solvent	cdcl3
Temperature	24.0
Pulse Sequence	s2pul
Number of Scans	546
Receiver Gain	30
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	0.5000
Acquisition Date	2016-04-22T06:25:04
Modification Date	2016-04-21T22:34:00
Spectrometer	128.23
Frequency	
Spectral Width	26041.7
Lowest Frequency	-13020.9
Nucleus	11B
Acquired Size	13021
Spectral Size	32768



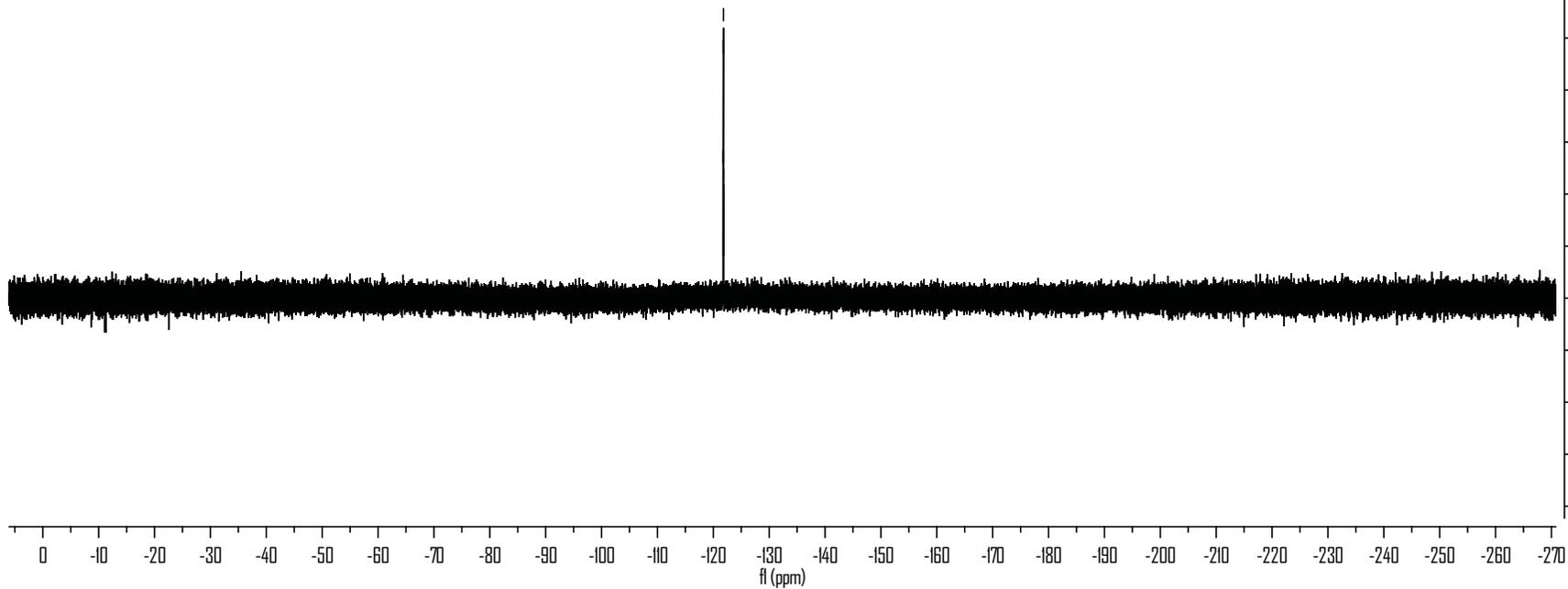
3h



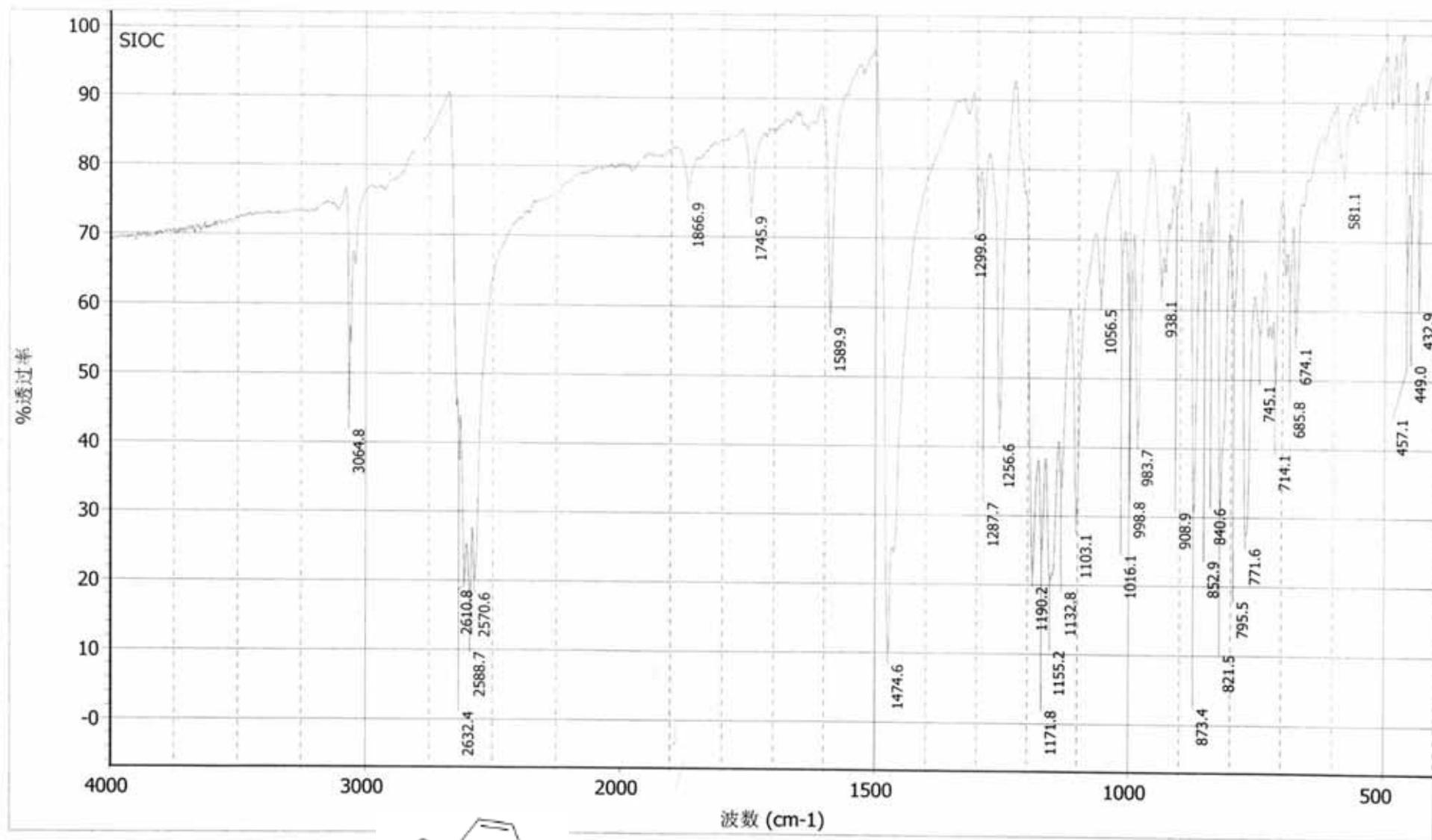


3h

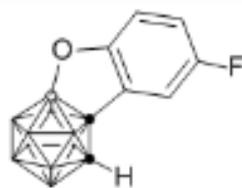
121.767
121.763
121.814
121.838



Parameter	Value
Title	ccx-6-41-b-2F
Comment	19FOBSERVE STANDARD PARAMETERS
Origin	Varian
Owner	
Site	
Spectrometer	mercury
Author	omc
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Number of Scans	100
Receiver Gain	39
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	0.8192
Acquisition Date	1999-11-13T16:22:48
Modification Date	2016-04-19T09:24:00
Spectrometer Frequency	282.27
Spectral Width	78125.0
Lowest Frequency	-76429.6
Nucleus	19F
Acquired Size	64000
Spectral Size	131072

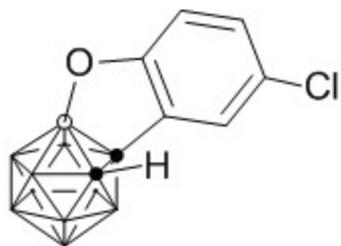


CCX-6-38-B 2015806 JS



3h

样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329

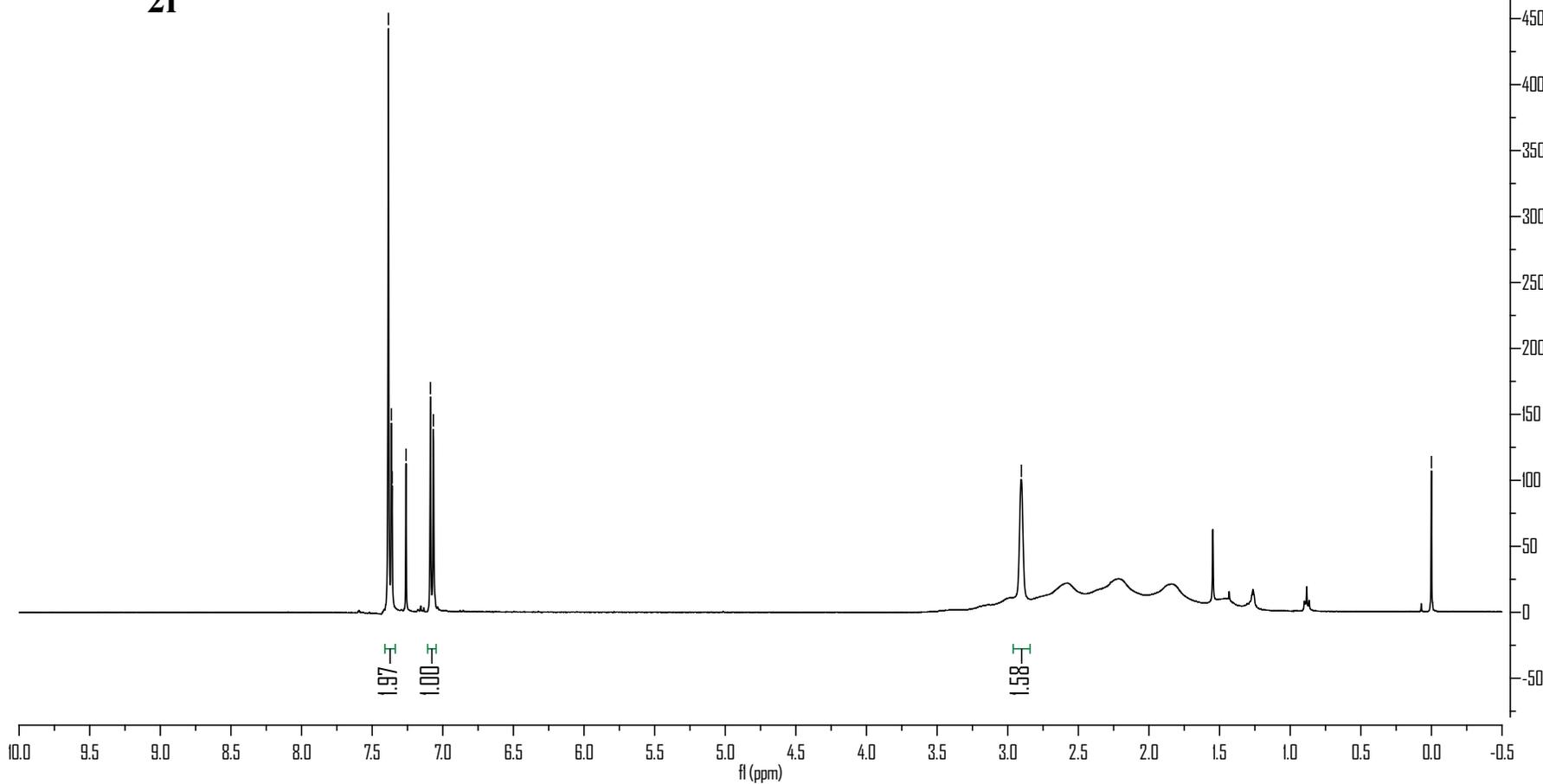


2i

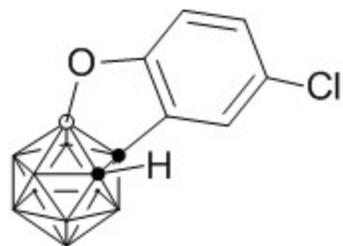
7.385
7.364
7.358
7.260
7.088
7.067

2.903

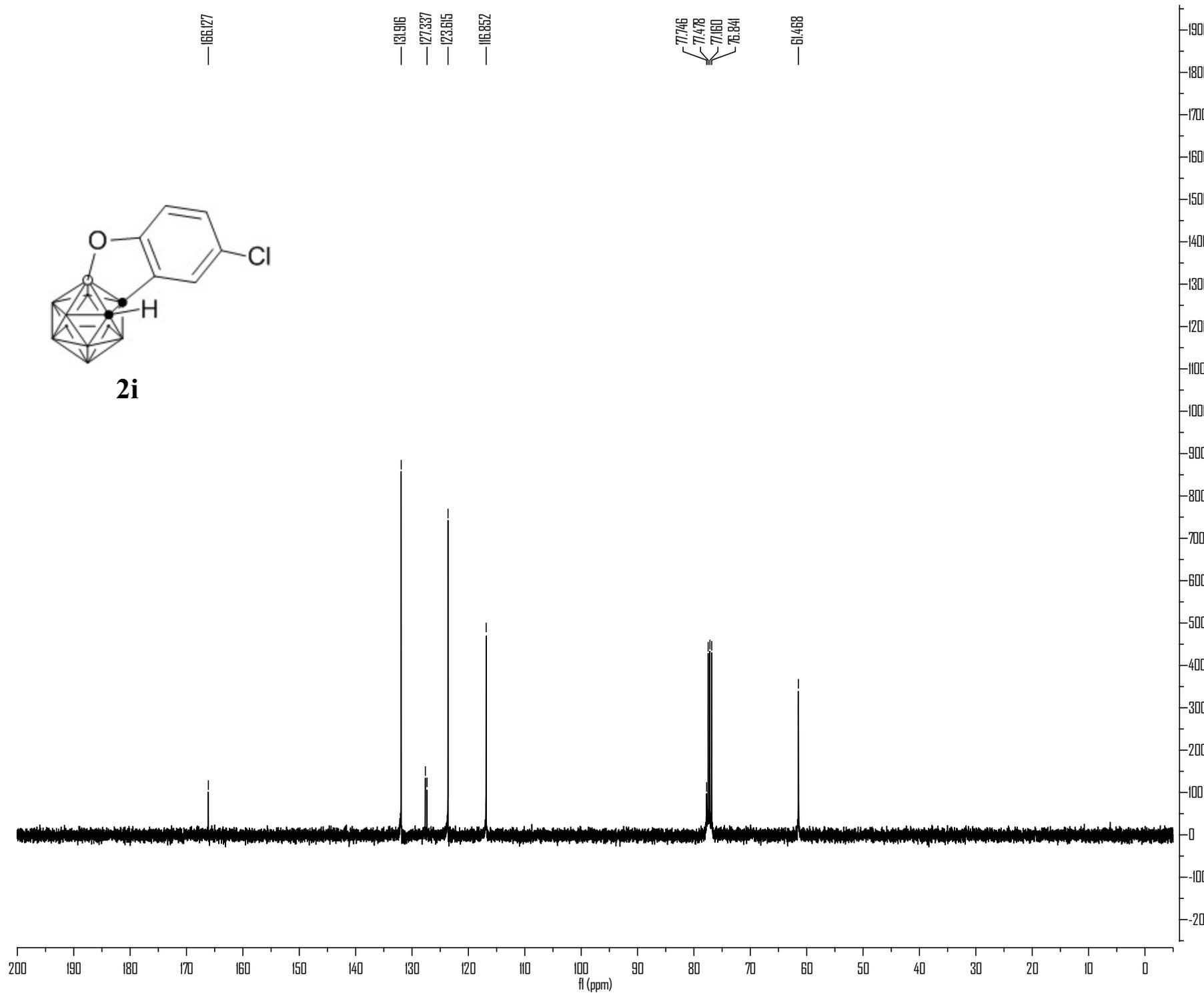
0.000



Parameter	Value
Title	ccx-7-61-1-1
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	40
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-02-19T17:46:58
Modification Date	2017-02-19T09:47:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-793.4
Nucleus	1H
Acquired Size	21552
Spectral Size	65536



2i



166.127

131.916

127.337

123.615

116.852

77.746

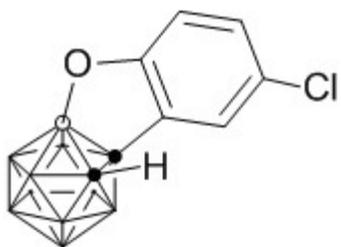
77.478

77.160

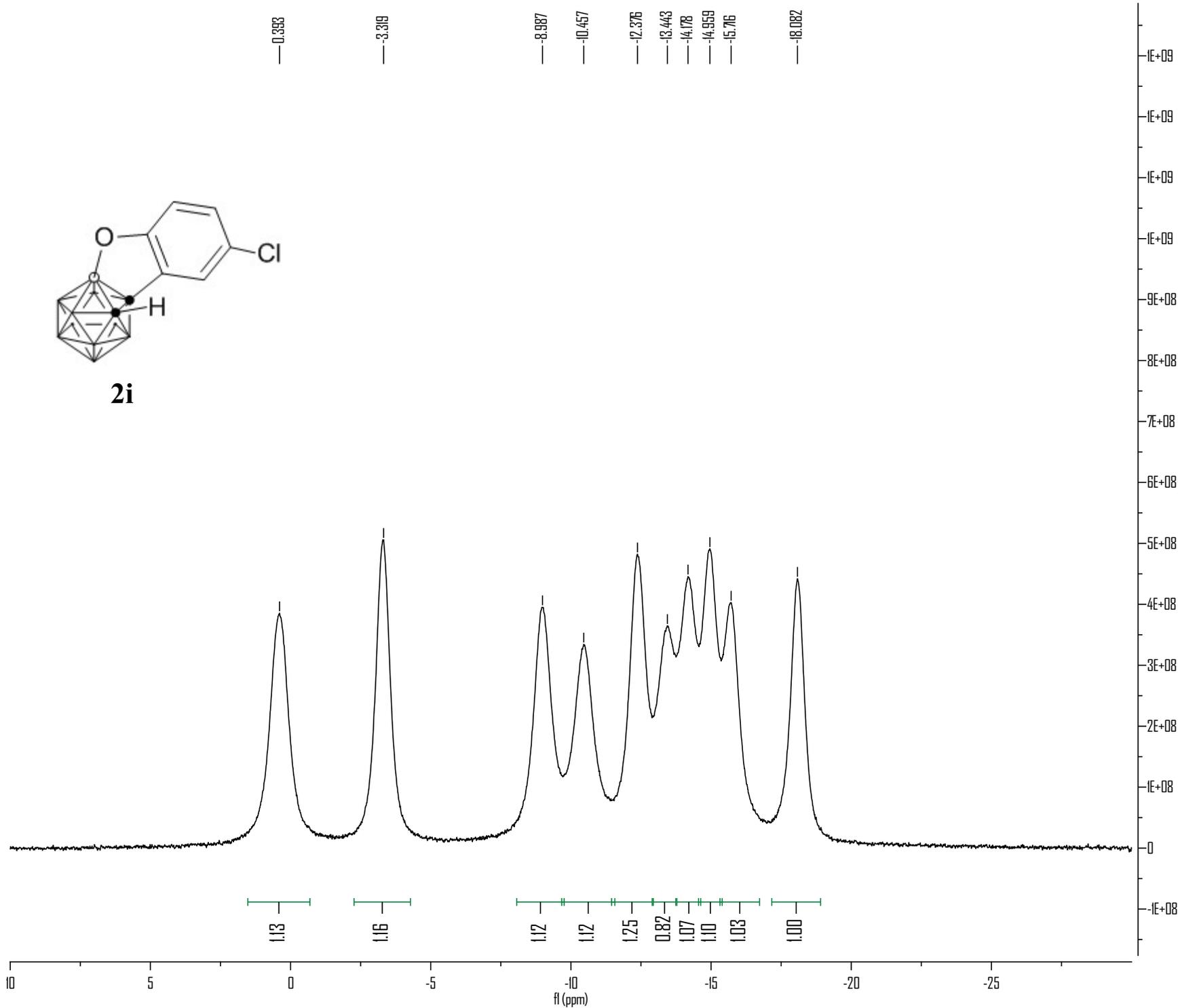
76.841

61.468

Parameter	Value
Title	-CCX-7-GI-1-1C
Comment	shimileneu experiment
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	420
Receiver Gain	56
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.1272
Acquisition Date	2017-02-21T12:55:37
Modification Date	2017-02-21T13:10:00
Spectrometer Frequency	100.51
Spectral Width	29069.8
Lowest Frequency	-4040.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

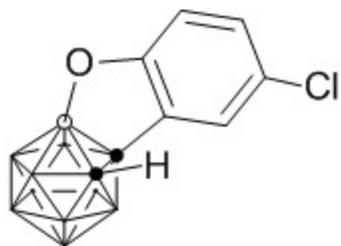


2i

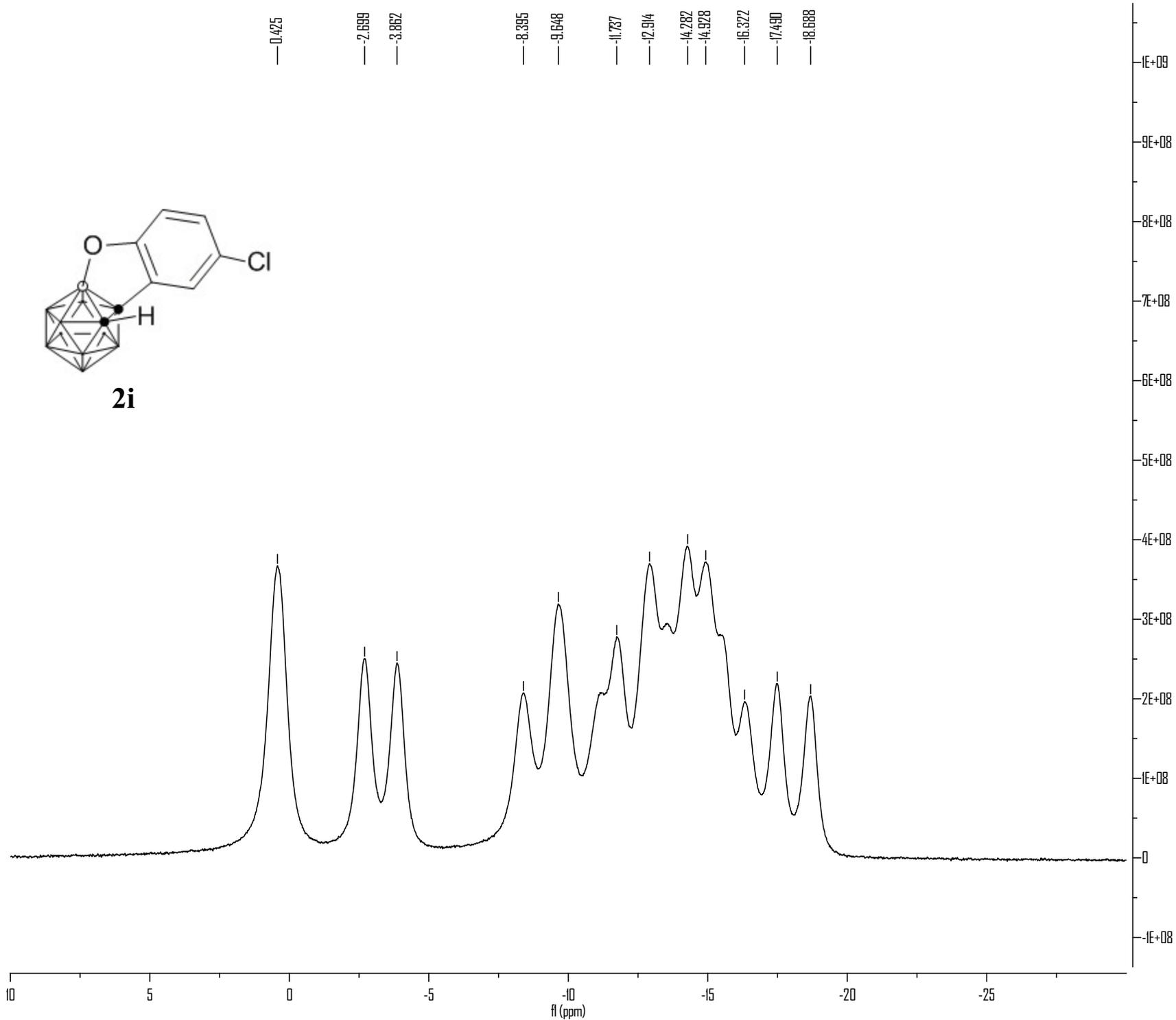


S161

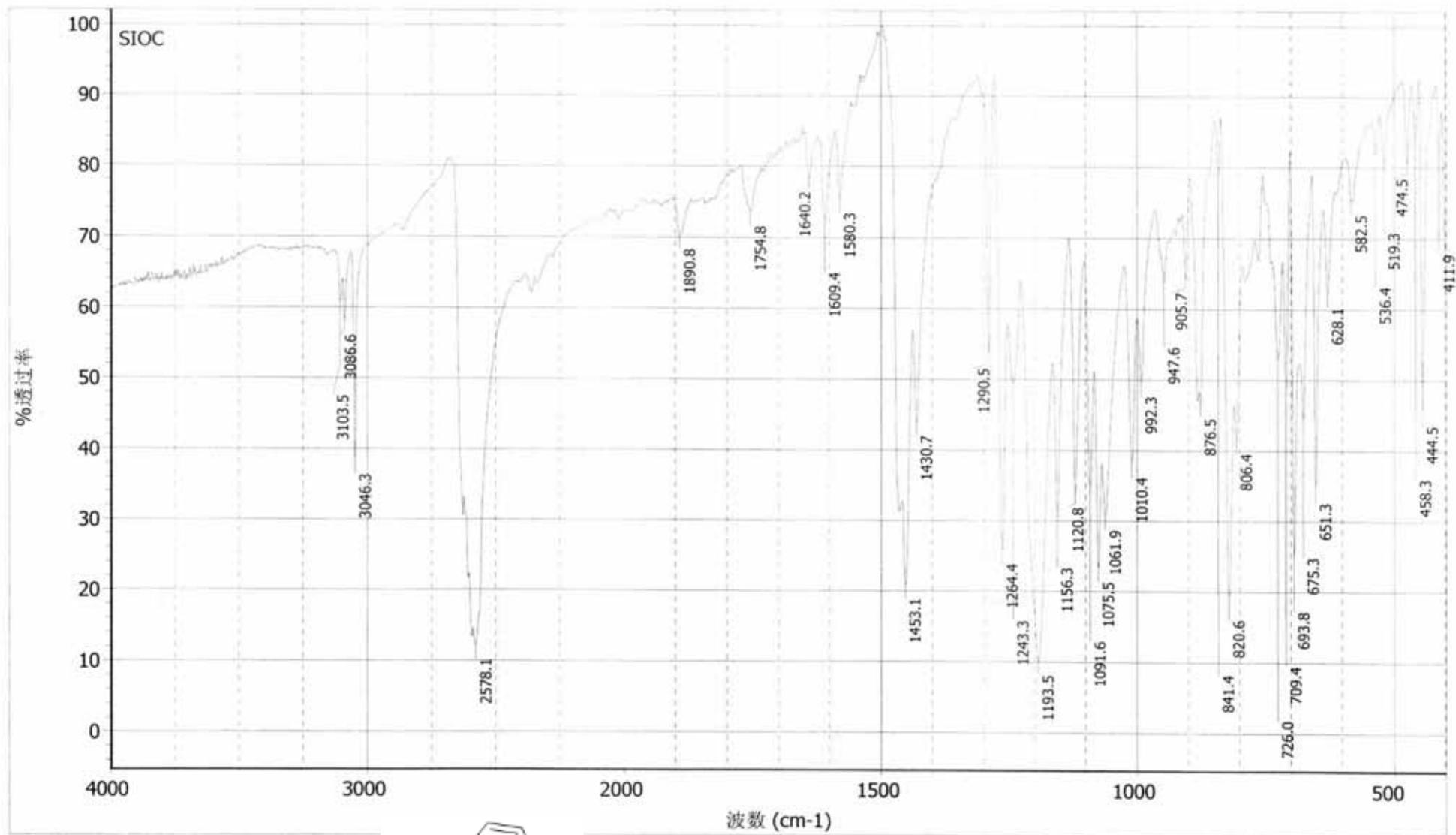
Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/产物数据/7-59-1/b-cx-7-61-1-1/pdata/1/1r
Title	7-59-1
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	79
Receiver Gain	181
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-02-21T19:21:38
Modification Date	2017-02-21T12:22:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16416.9
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



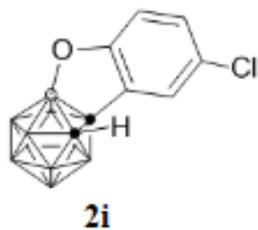
2i



Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-59-1/b-cx-7-61-1-1-coupling/pdata/1/1r
Title	7-59-1
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	101
Receiver Gain	181
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-02-21T19:23:51
Modification Date	2017-02-21T12:24:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16416.9
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



CCX-7-59-1 2015806 JS



样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329

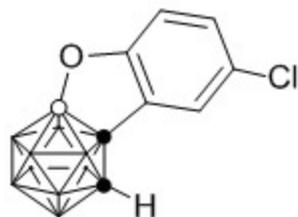
7.373
7.351
7.263
7.235
7.108
7.086

4.214

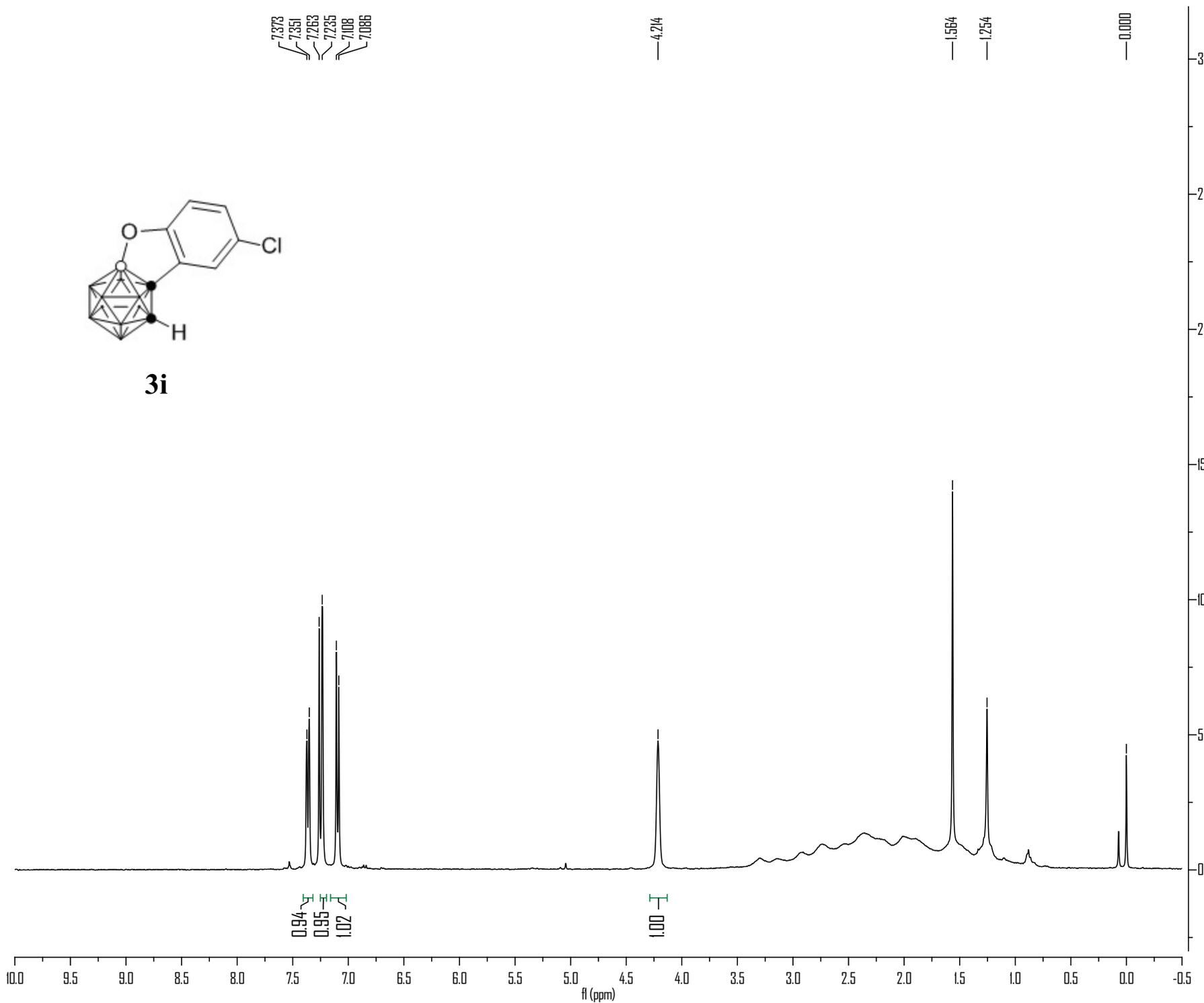
1.564

1.254

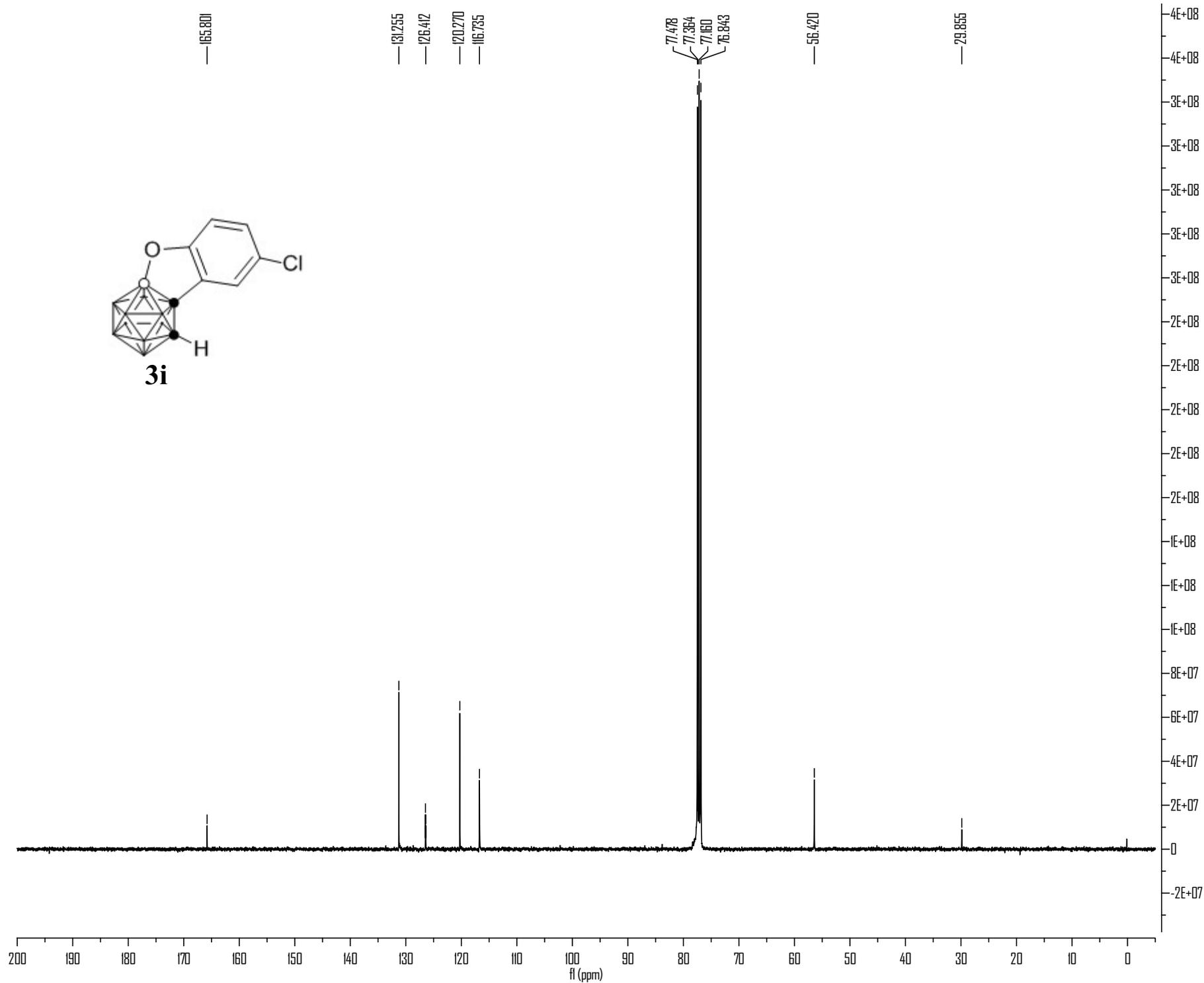
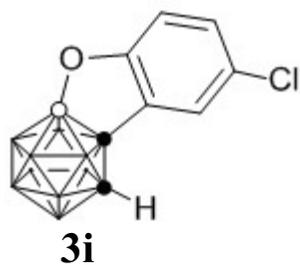
0.000



3i

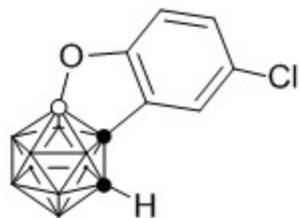


Parameter	Value
Data file Name	7-58-2/ ccx-7-6l-b-H.fid/ fid
Title	ccx-7-6l-b-H
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omel
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	46
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2018-12-07T13:58:02
Modification Date	2018-12-07T05:58:00
Spectrometer Frequency	399.72
Spectral Width	7575.8
Lowest Frequency	-1190.1
Nucleus	1H
Acquired Size	22727
Spectral Size	65536



S165

Parameter	Value
Data file Name	2012060cccc-cx-7-Gl-b/ 3/ pdata/ 1/ 1r
Title	2012060cccc-cx-7-Gl-b
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgdc
Number of Scans	21843
Receiver Gain	32768
Relaxation Delay	2.0000
Pulse Width	4.0000
Acquisition Time	0.9306
Acquisition Date	2018-12-05T22:47:41
Modification Date	2018-12-06T08:38:00
Spectrometer	100.61
Frequency	
Spectral Width	35211.3
Lowest Frequency	-6858.5
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



3i

3.523

3.743

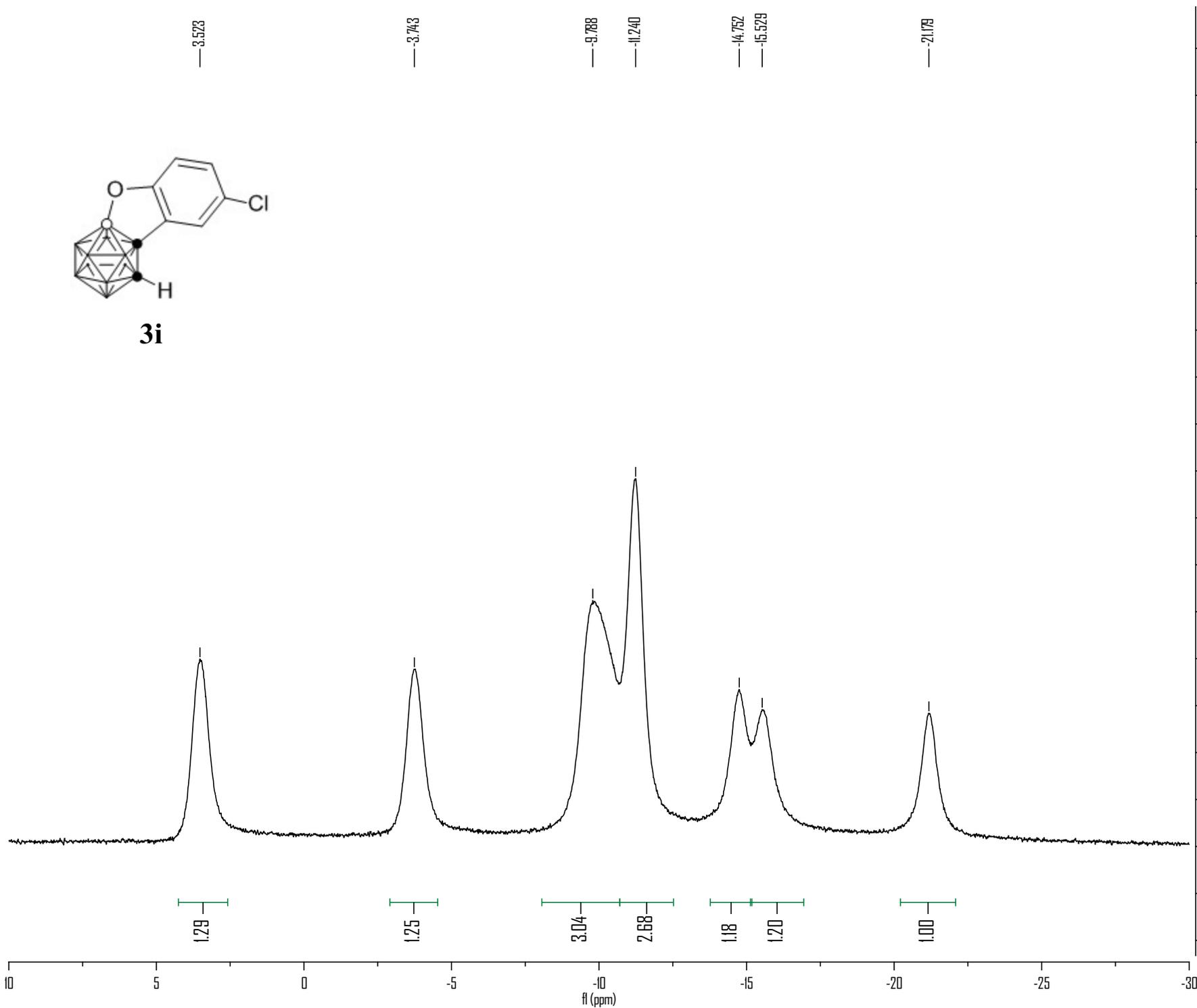
9.788

11.240

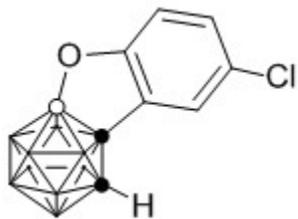
14.752

15.529

21.179



Parameter	Value
Data file Name	2012060b-ccx-7-G-b/ 1/pdata/1/1r
Title	2012060b-ccx-7-G-b
Comment	
Origin	UXMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	256
Receiver Gain	512
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.4260
Acquisition Date	2018-12-05T21:36:36
Modification Date	2018-12-06T08:38:14
Spectrometer	128.38
Frequency	
Spectral Width	38461.5
Lowest Frequency	-19594.6
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



3i

3.514

3.159

4.286

9.235

10.596

11.810

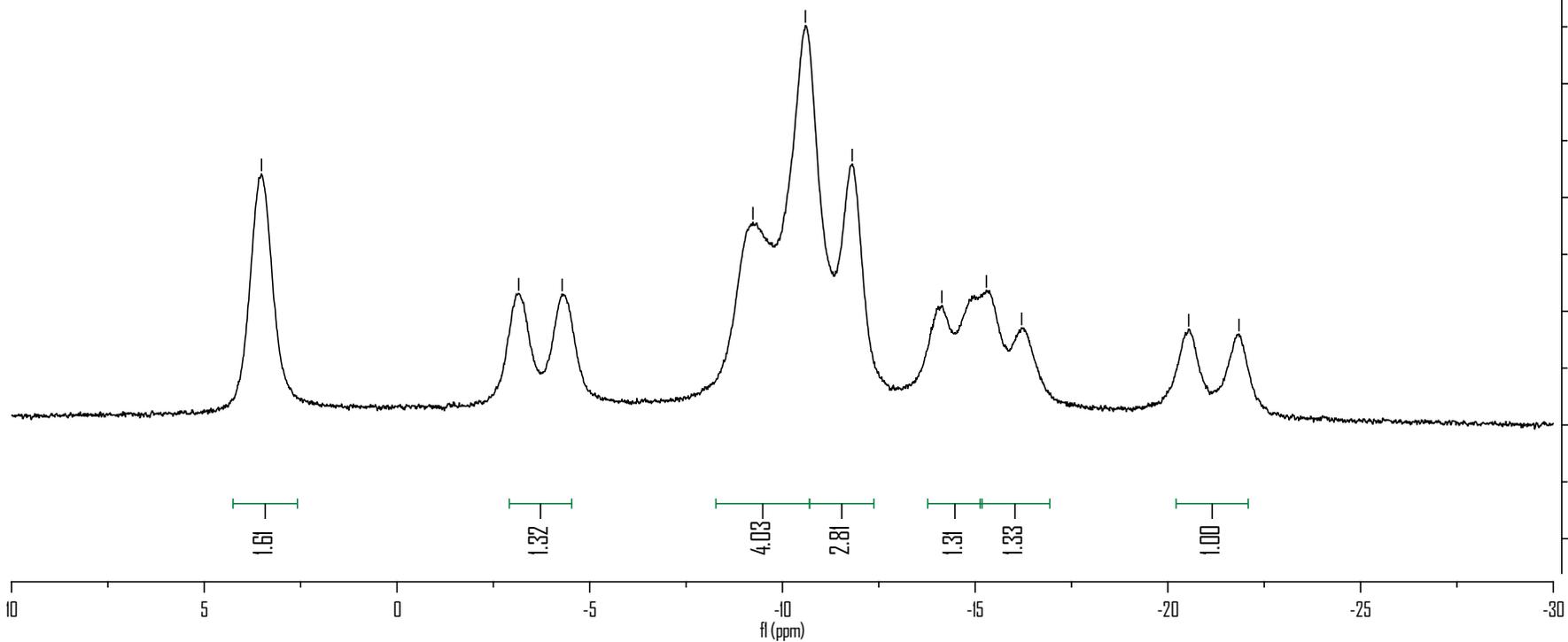
14.136

15.292

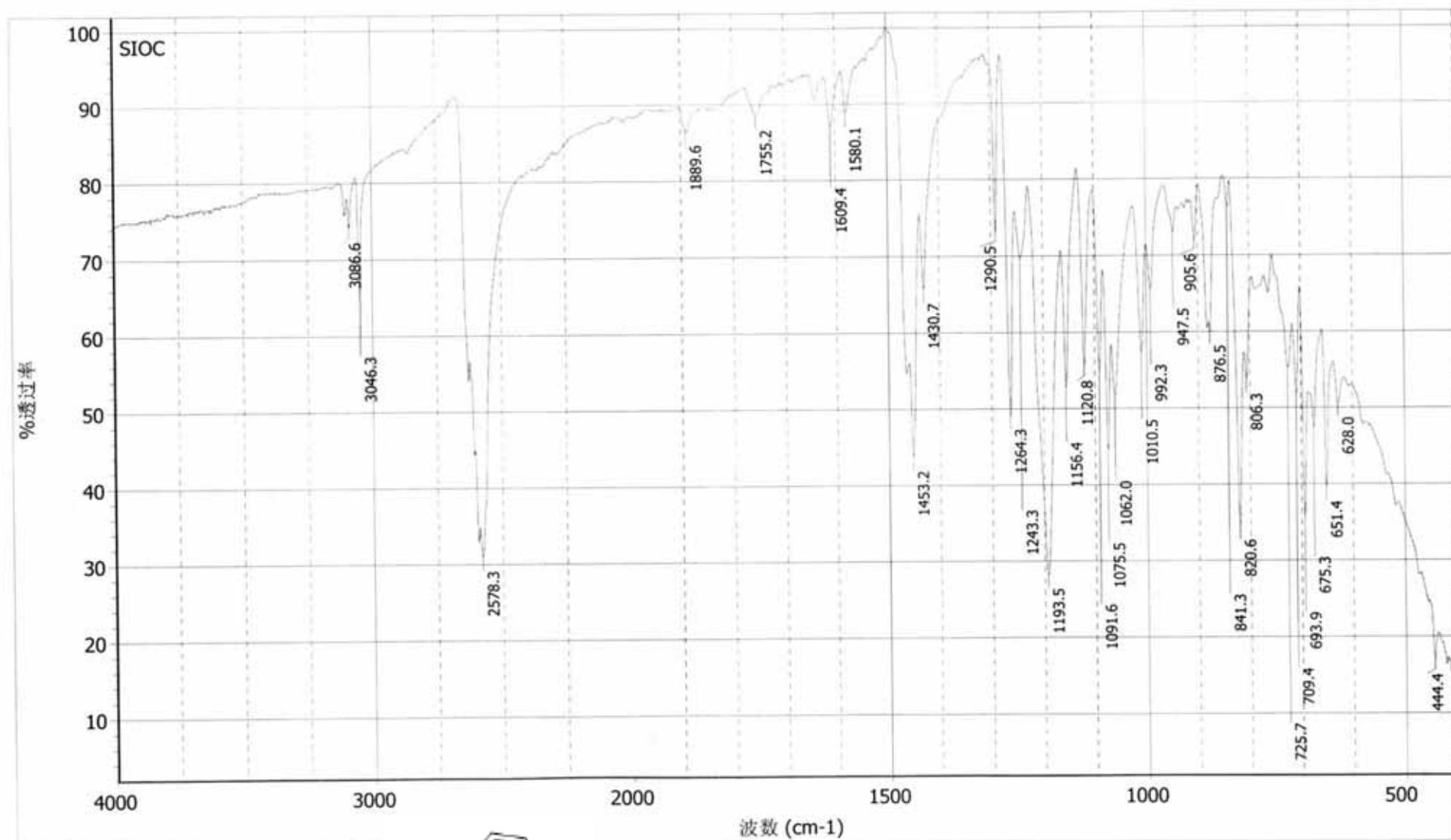
16.206

20.540

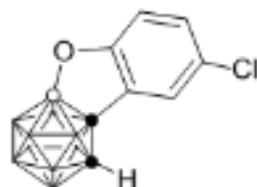
21.846



Parameter	Value
Data file Name	2012060b-ccx-7-6l-b-coupling/1/pdata/1/1r
Title	2012060b-ccx-7-6l-b-coupling
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.lgy
Number of Scans	256
Receiver Gain	512
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.4260
Acquisition Date	2018-12-05T21:38:53
Modification Date	2018-12-06T08:38:08
Spectrometer	128.38
Frequency	
Spectral Width	38461.5
Lowest Frequency	-19594.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

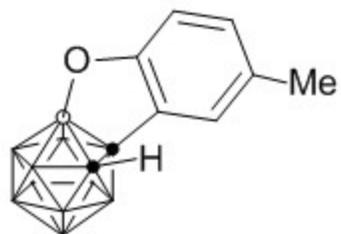


CCX-7-59-4 2015806 JS

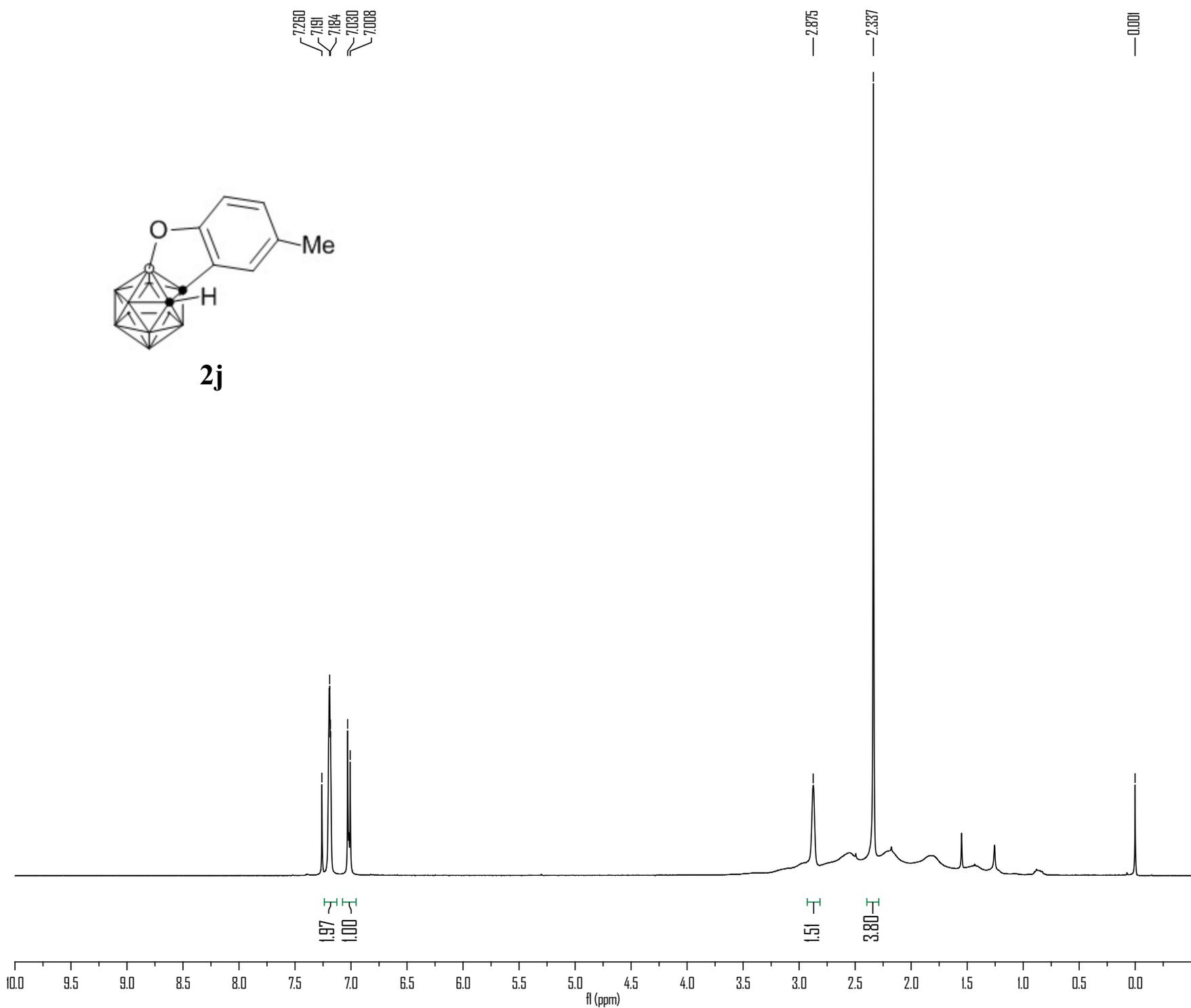


3i

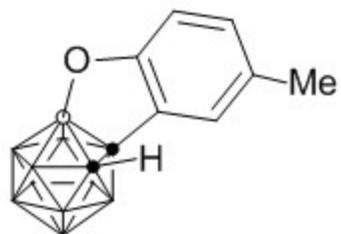
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.4747



2j



Parameter	Value
Title	ccx-7-72-1
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-03-08T20:07:41
Modification Date	2017-03-08T12:09:00
Spectrometer Frequency	400.03
Spectral Width	7225.4
Lowest Frequency	-804.9
Nucleus	¹ H
Acquired Size	21676
Spectral Size	65536



2j

165.598

132.384

131.943

125.953

123.641

115.374

78.926

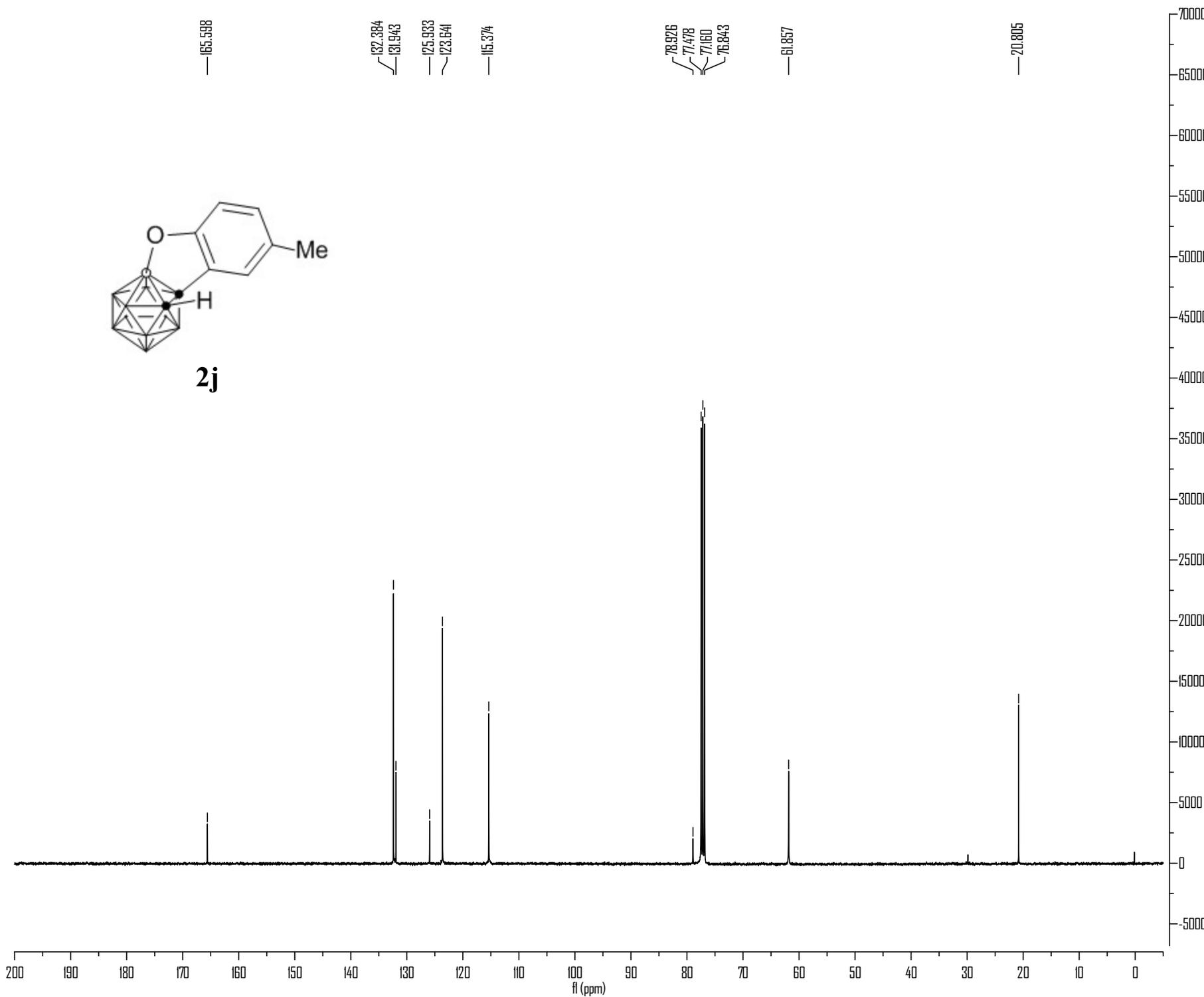
77.478

77.160

76.843

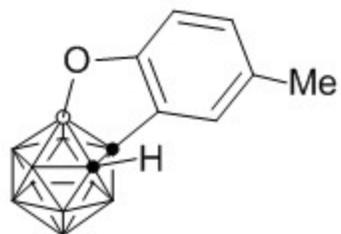
61.857

20.805

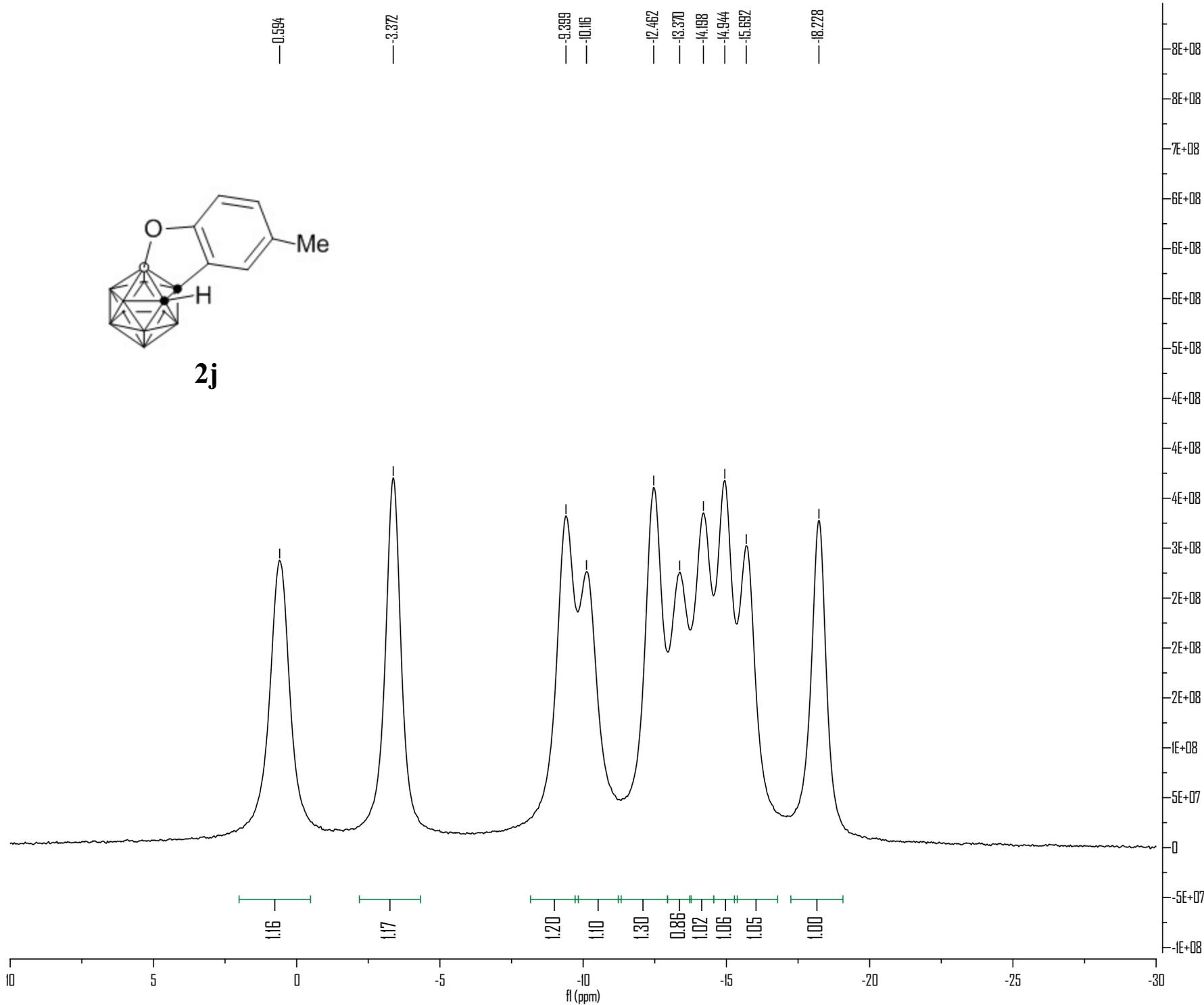


S170

Parameter	Value
Title	ccx-7-72-1-c
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	13408
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0486
Acquisition Date	2017-03-08T23:38:03
Modification Date	2017-03-08T23:16:00
Spectrometer Frequency	100.52
Spectral Width	31250.0
Lowest Frequency	-1151.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

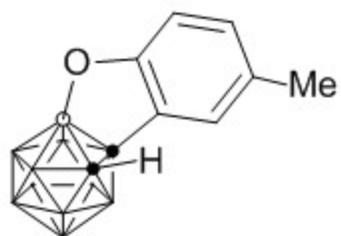


2j

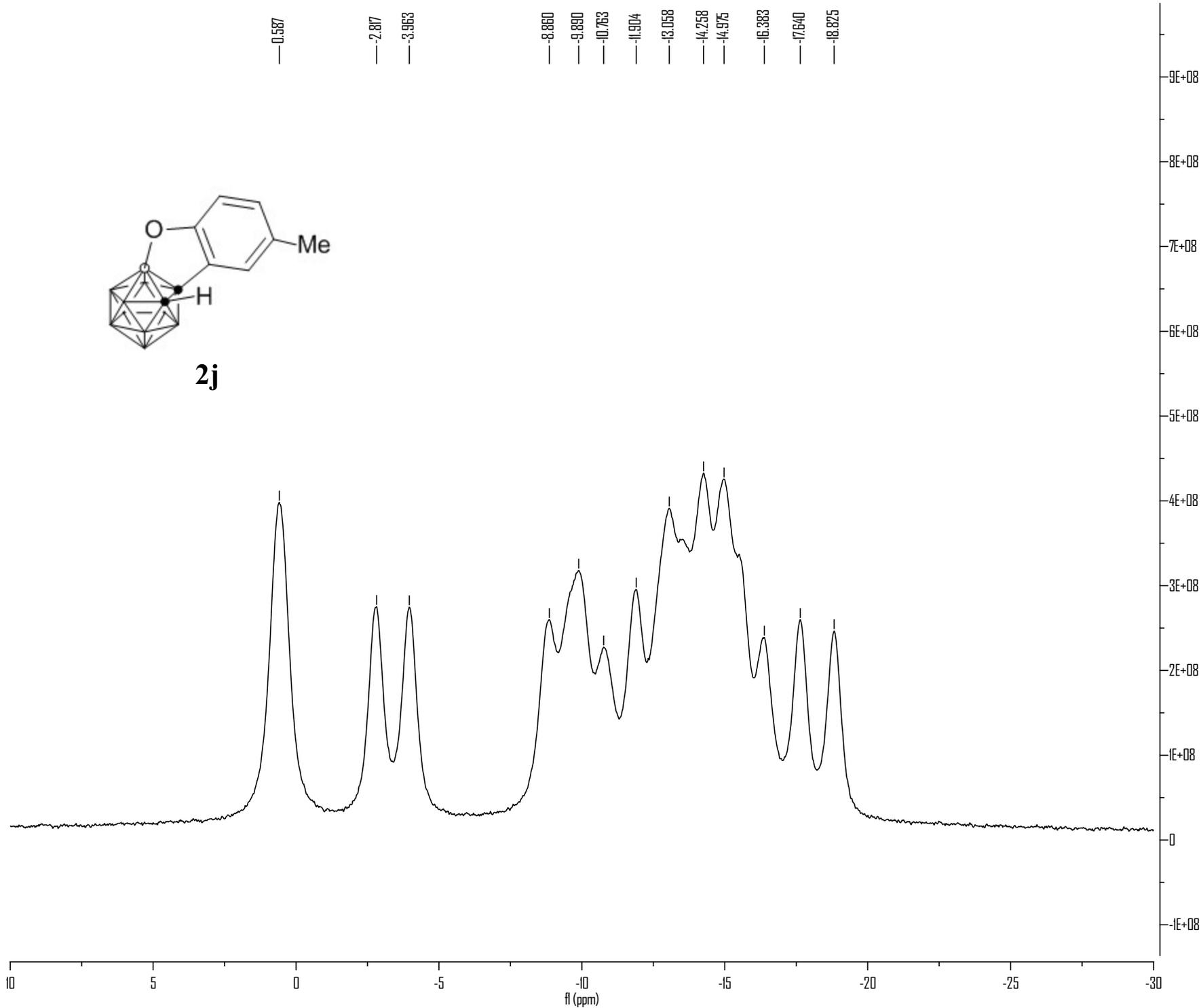


S171

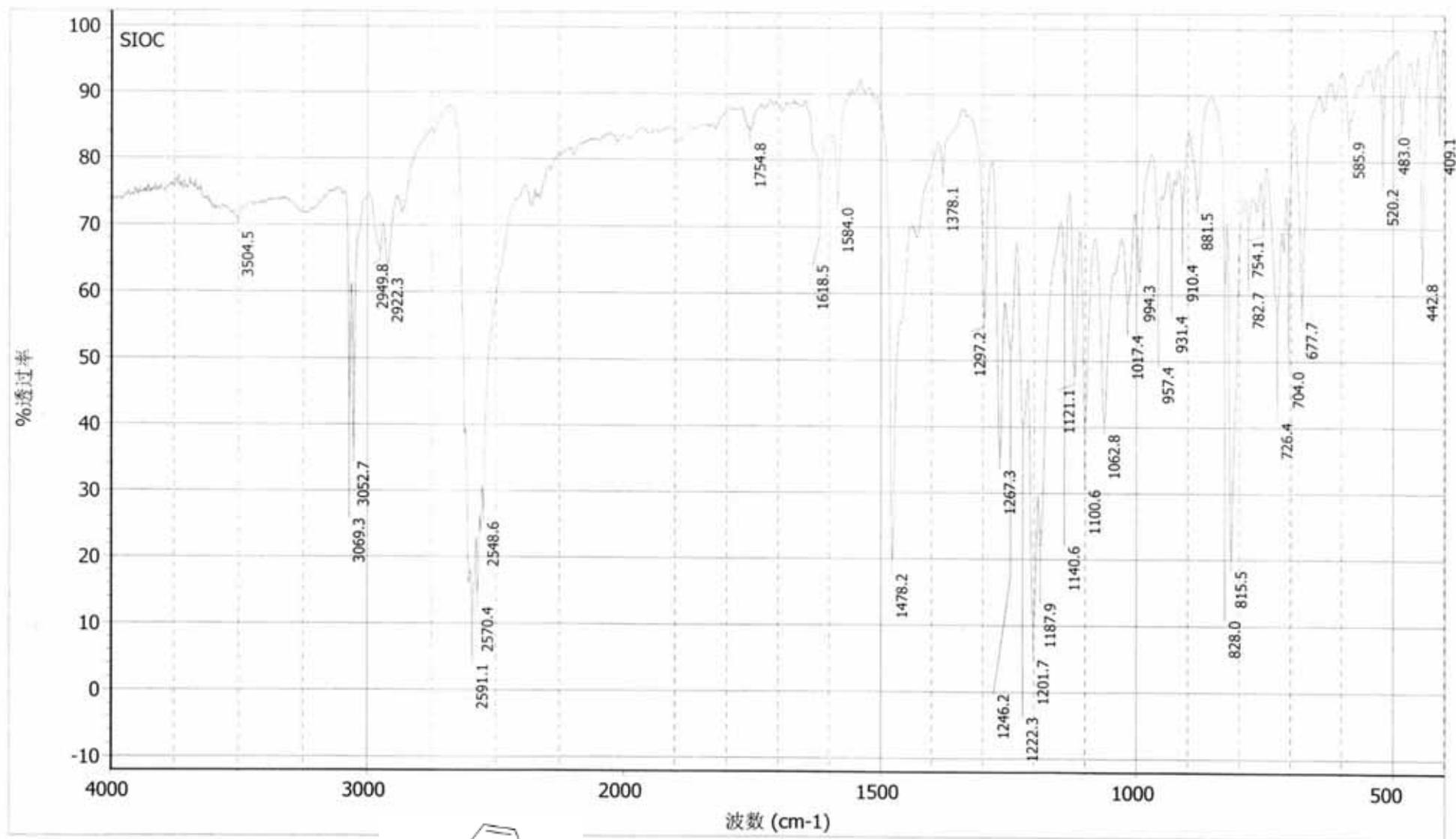
Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-72-1/b-ccx-7-72-1/pdata/1/1r
Title	7-72-1
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring1gy
Number of Scans	162
Receiver Gain	322
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-03-28T20:13:49
Modification Date	2017-03-28T13:13:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16396.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



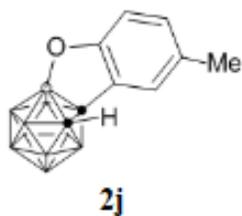
2j



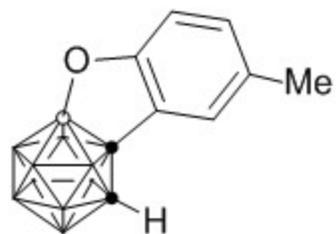
Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-72-1/b-cx-7-72-1-coupling/pdata/1/1r
Title	7-72-1
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.lgy
Number of Scans	80
Receiver Gain	228
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-03-28T20:11:54
Modification Date	2017-03-28T13:11:00
Spectrometer	128.38
Frequency	
Spectral Width	32051.3
Lowest Frequency	-16396.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



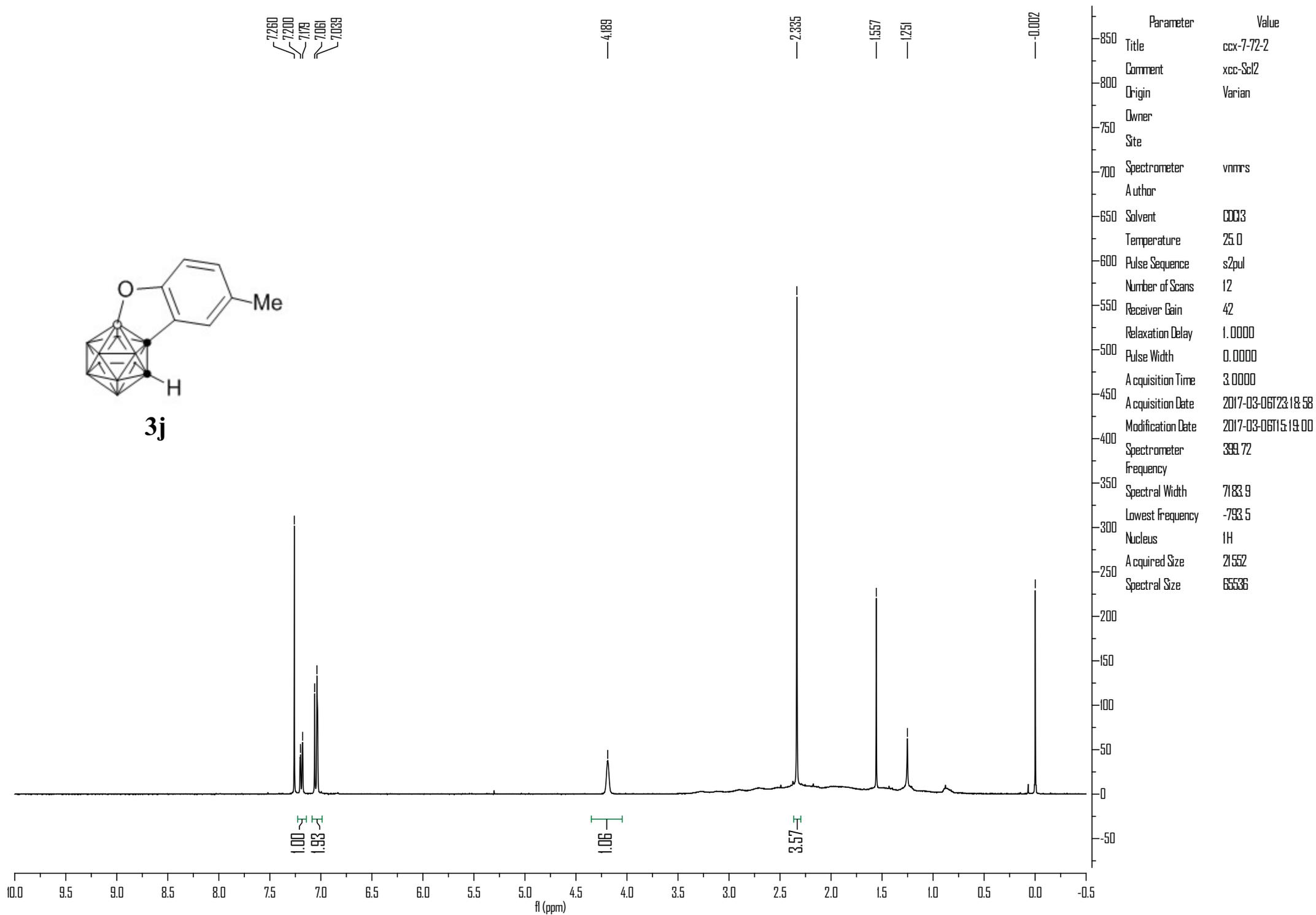
CCX-7-72-1 2015806 JS



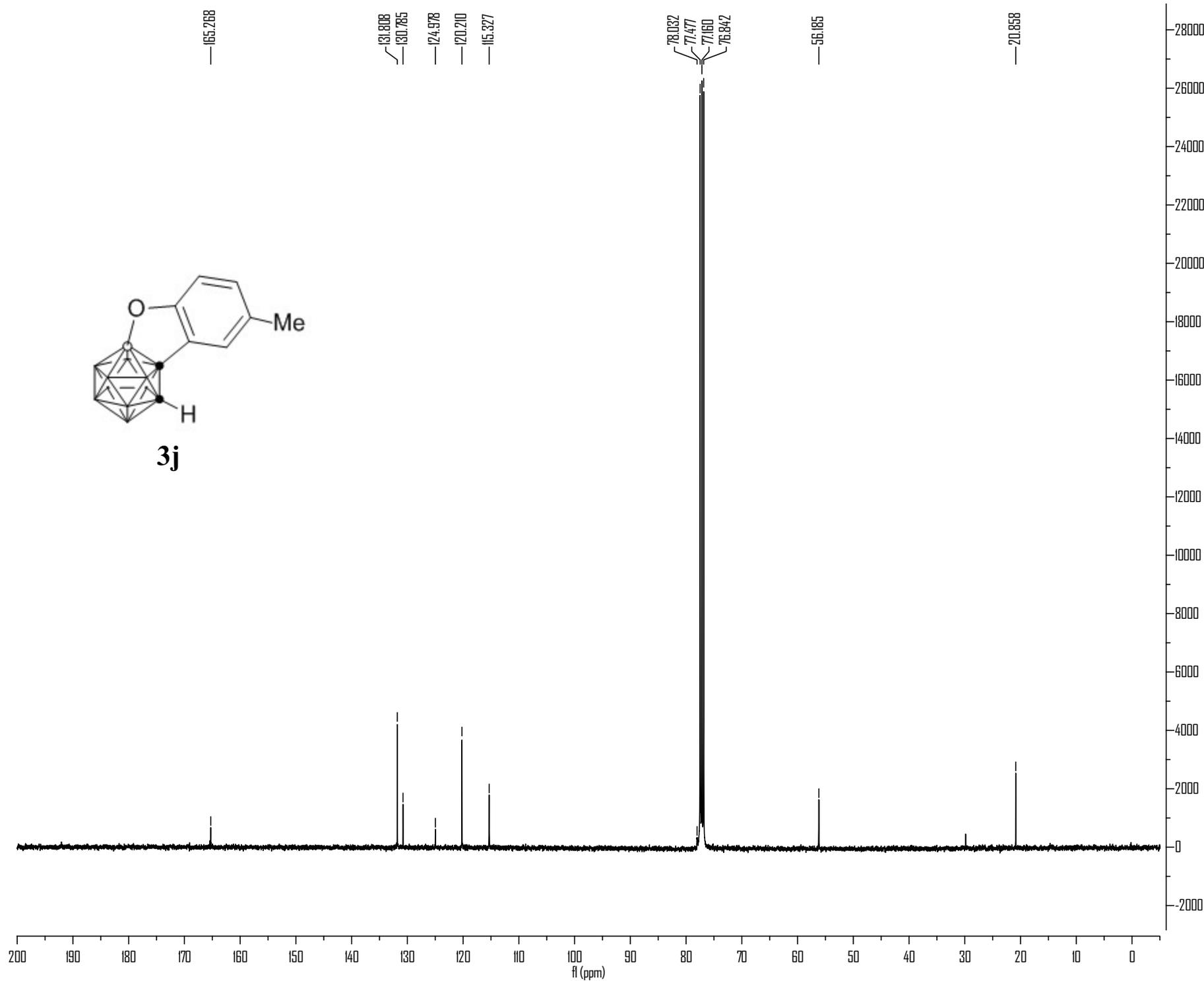
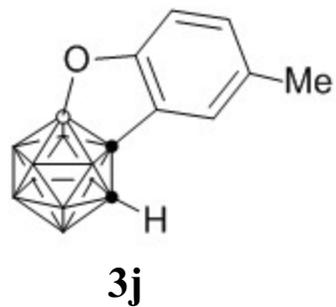
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



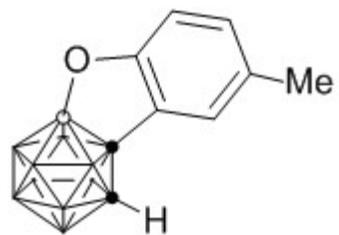
3j



Parameter	Value
Title	ccx-7-72-2
Comment	xcc-Sc12
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-03-06T23:18:58
Modification Date	2017-03-06T15:19:00
Spectrometer	399.72
Frequency	
Spectral Width	7183.9
Lowest Frequency	-793.5
Nucleus	1H
Acquired Size	21552
Spectral Size	65536



Parameter	Value
Title	ccx-7-72-b-c
Comment	lxj-2-54-C-H
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	10200
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3369
Acquisition Date	2017-03-30T00:02:18
Modification Date	2017-03-29T22:39:00
Spectrometer	100.52
Frequency	
Spectral Width	24509.8
Lowest Frequency	-1319.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



3j

3.498

-4.006

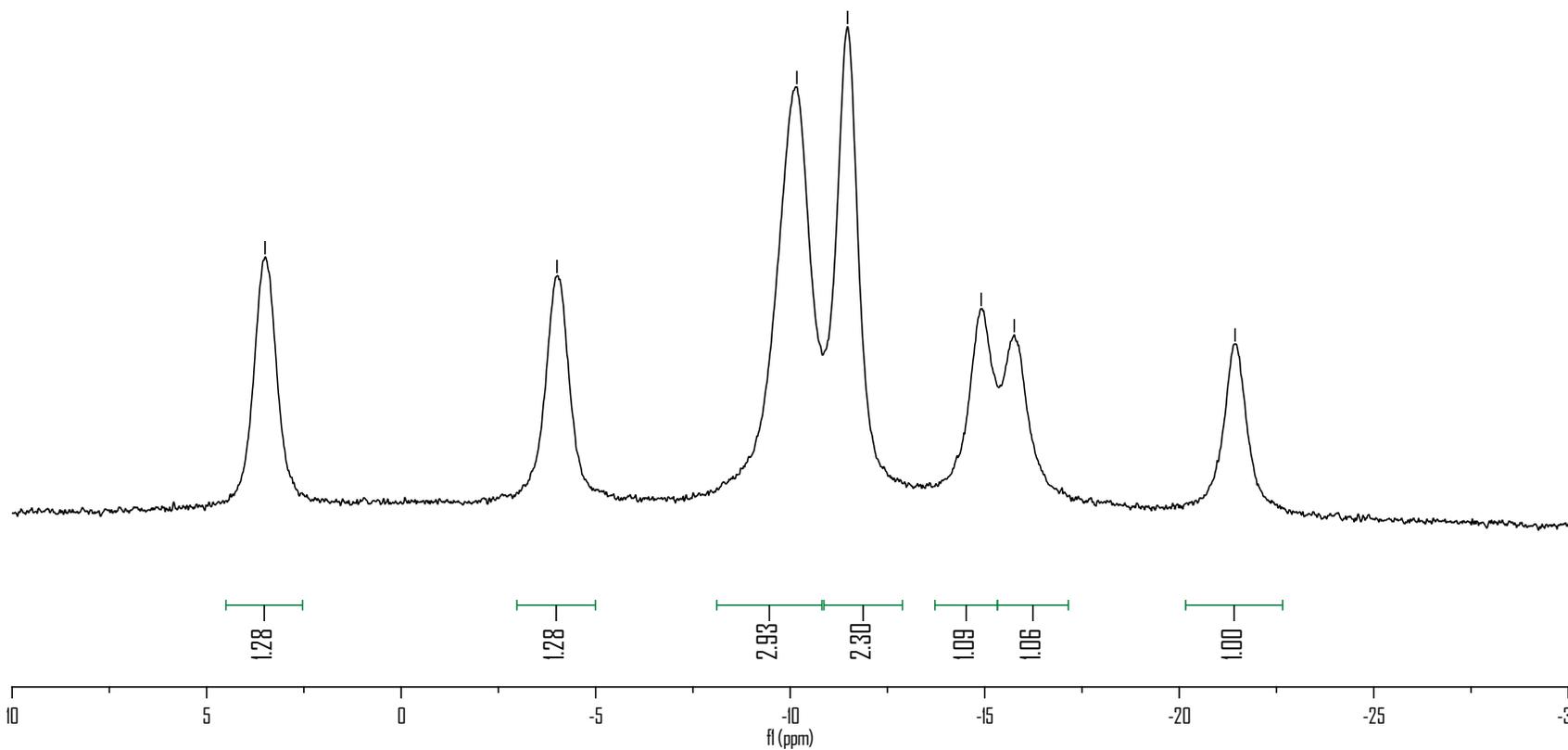
-10.172

-11.476

-14.909

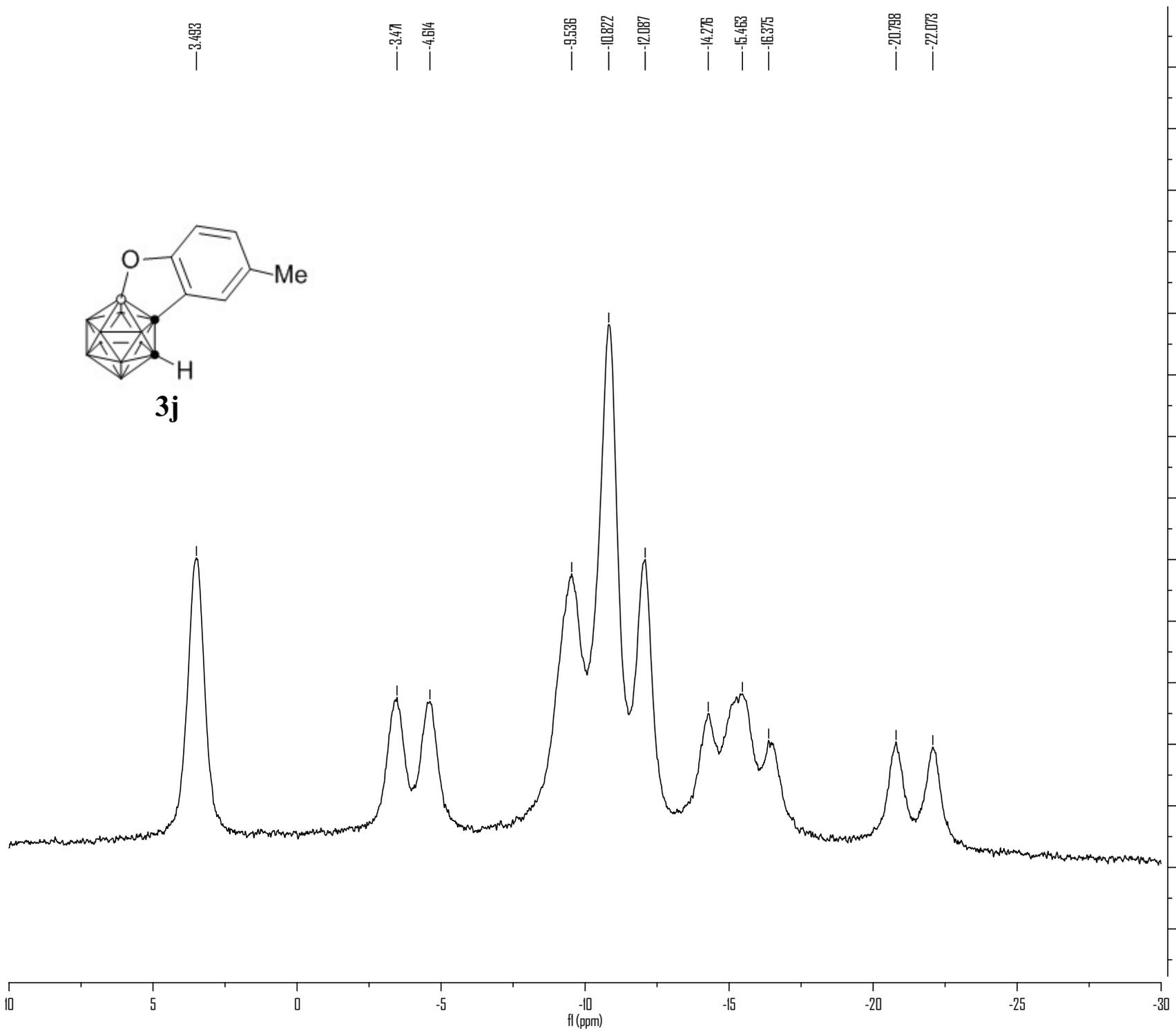
-15.759

-21.436

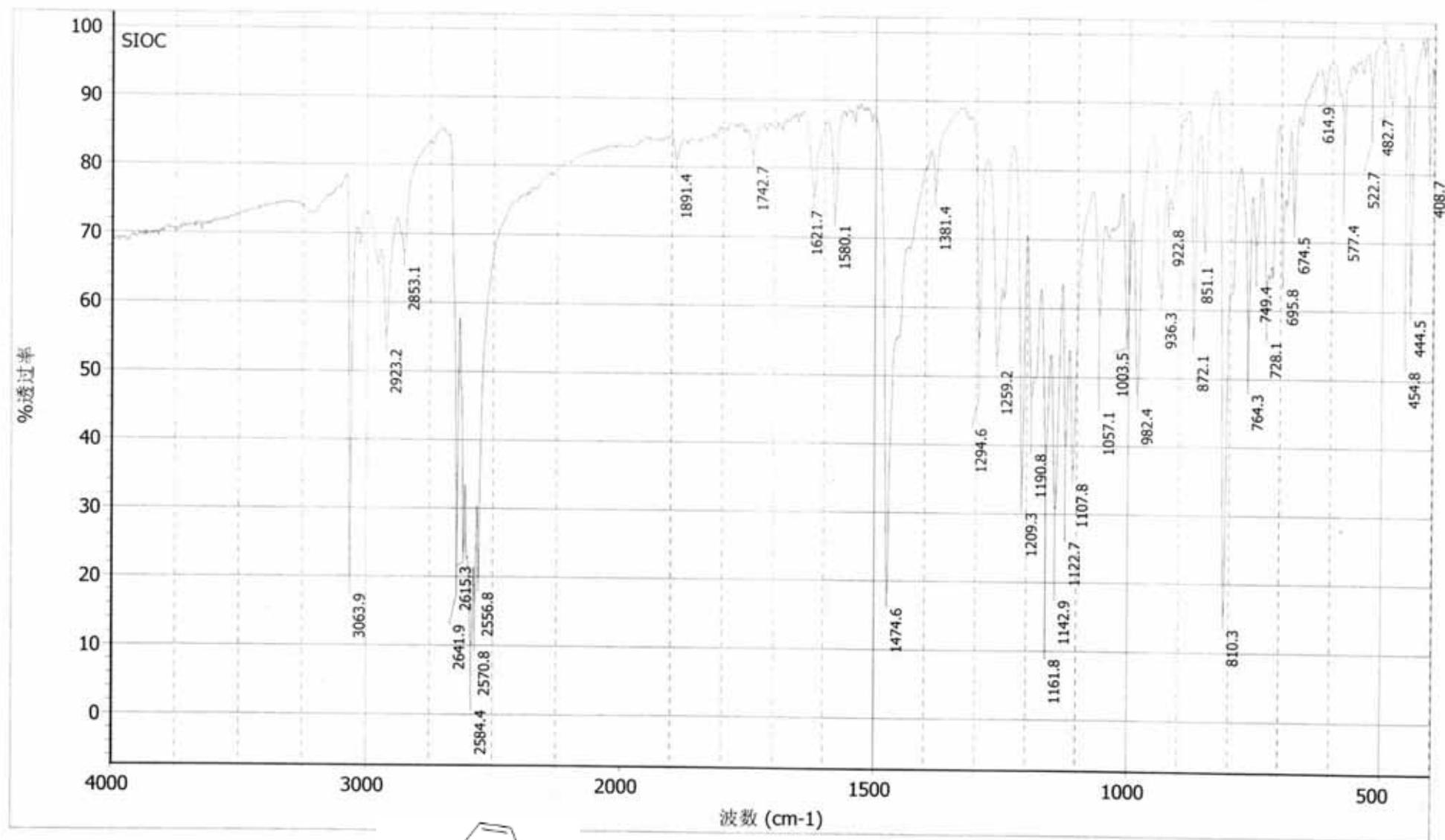


S176

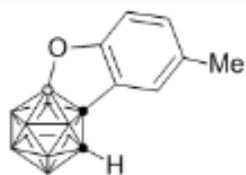
Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-72-2/b-cck-7-72-2/pdata/1/1r
Title	7-72-2
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	99
Receiver Gain	575
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-03-28T20:06:27
Modification Date	2017-03-28T13:07:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16396.3
Nucleus	1H
Acquired Size	16394
Spectral Size	32768



Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-72-2/b-ccx-7-72-2-coupling/pdata/1/1r
Title	7-72-2
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	98
Receiver Gain	645
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-03-28T20:08:03
Modification Date	2017-03-28T13:08:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16396.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

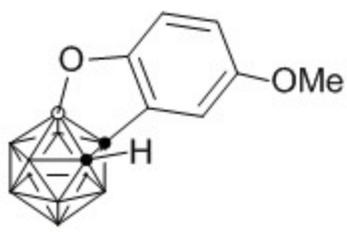


CCX-7-72-B 2015806 JS

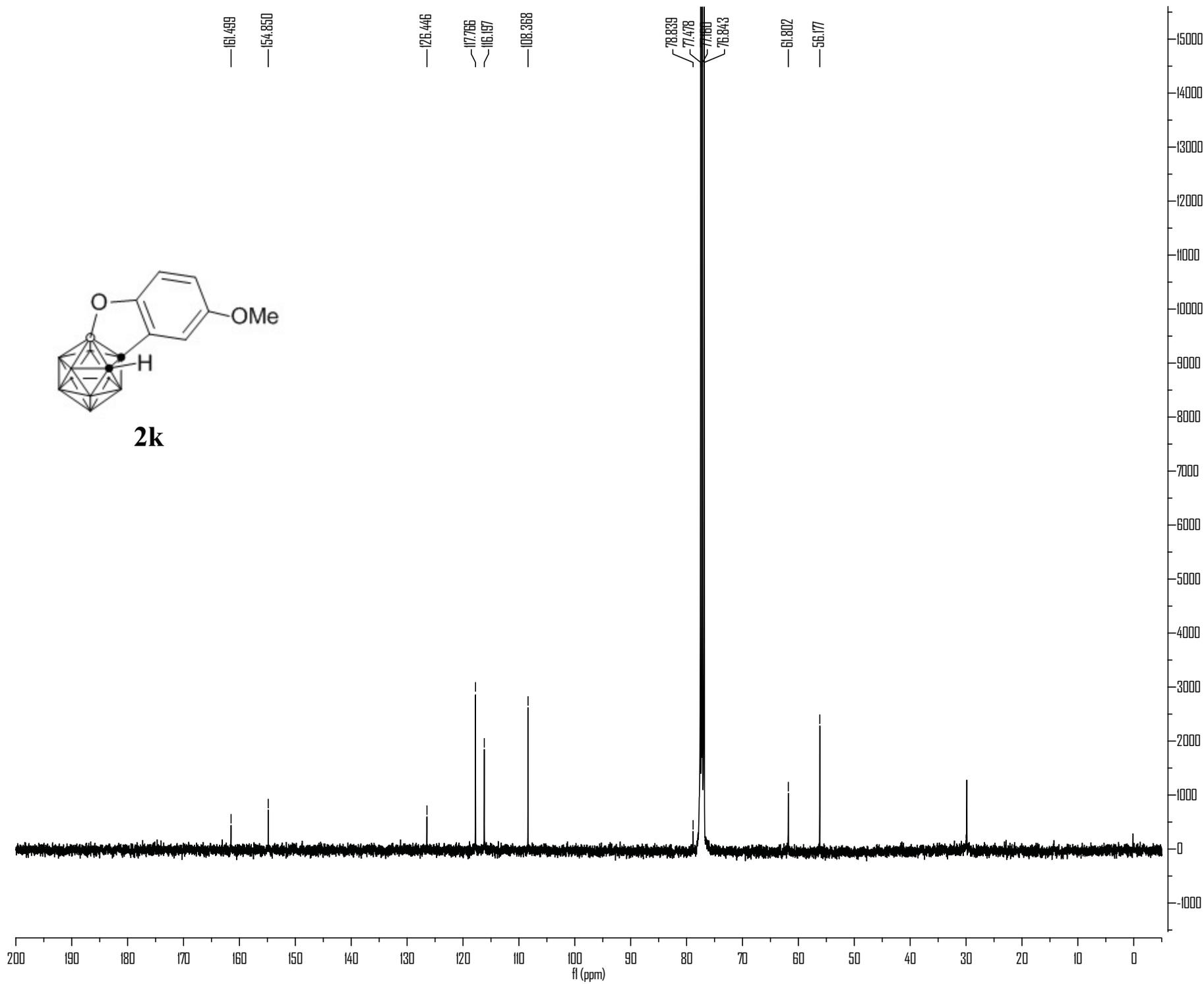


3j

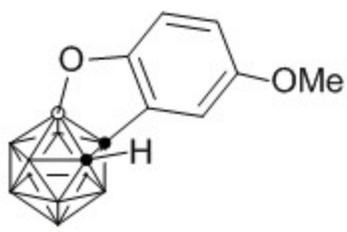
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



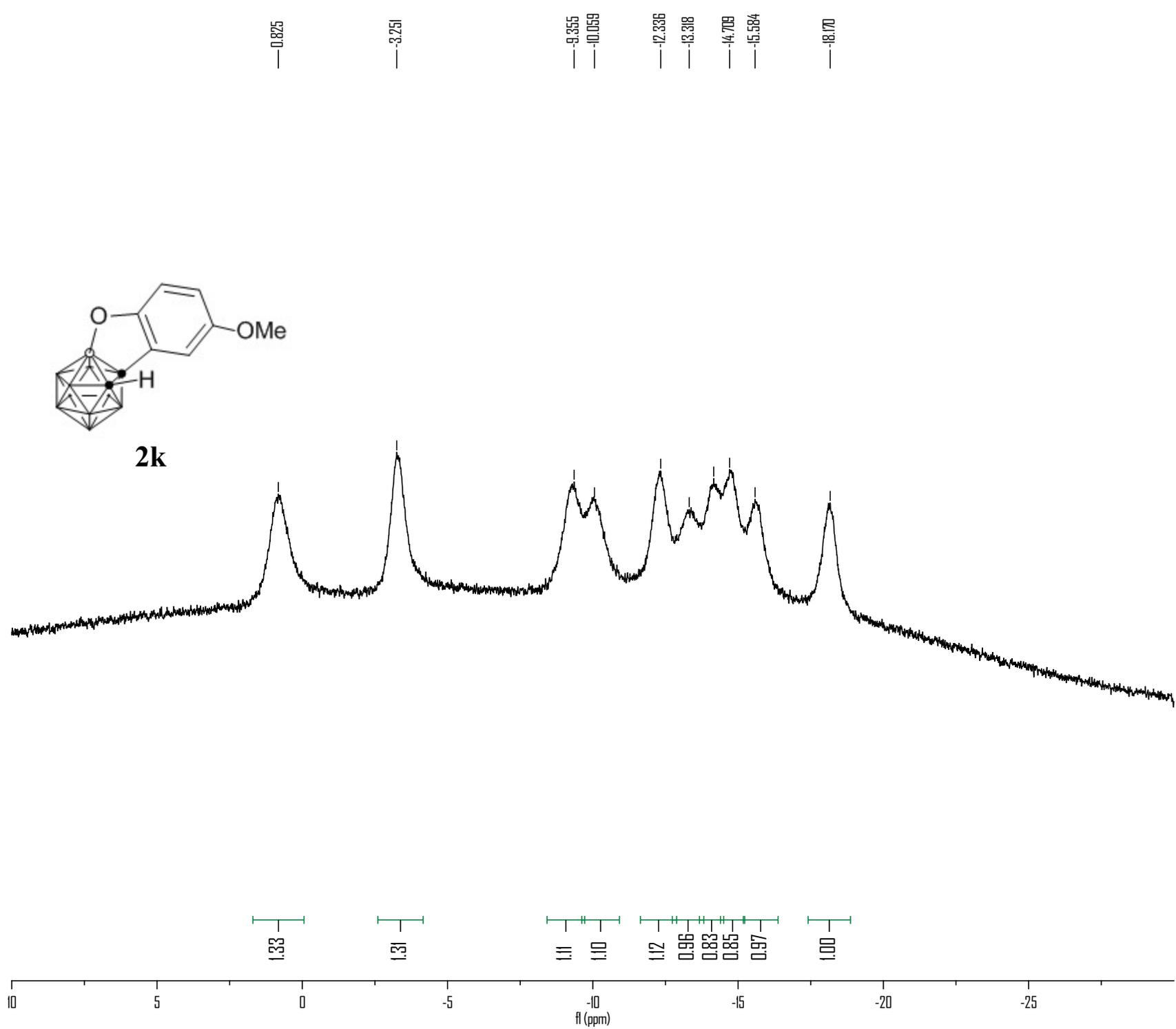
2k



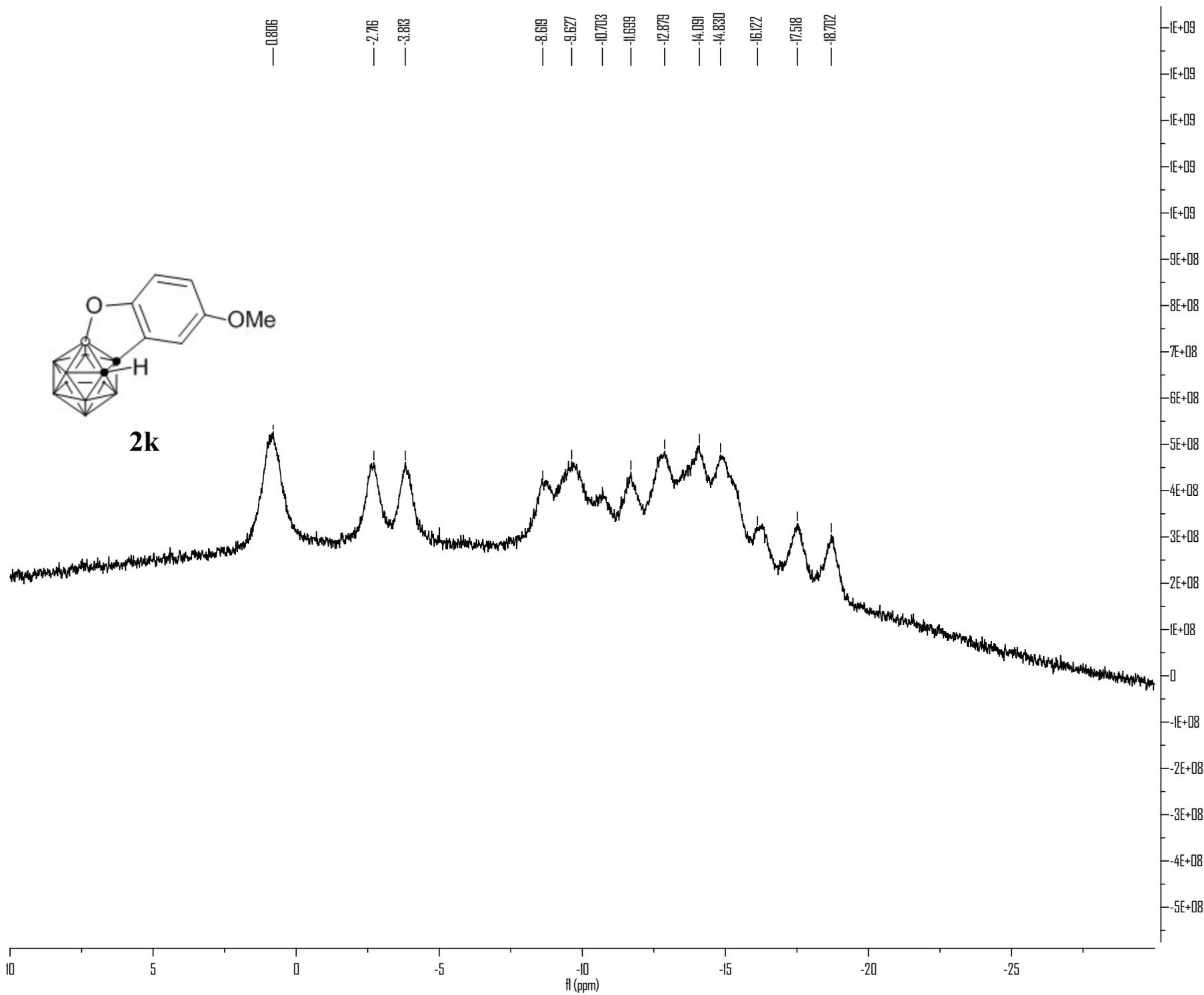
Parameter	Value
Title	ccx-7-79-a-1-1c
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	13368
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-04-08T23:16:31
Modification Date	2017-04-08T23:49:00
Spectrometer Frequency	100.60
Spectral Width	26041.7
Lowest Frequency	-1687.9
Nucleus	13C
Acquired Size	33867
Spectral Size	131072



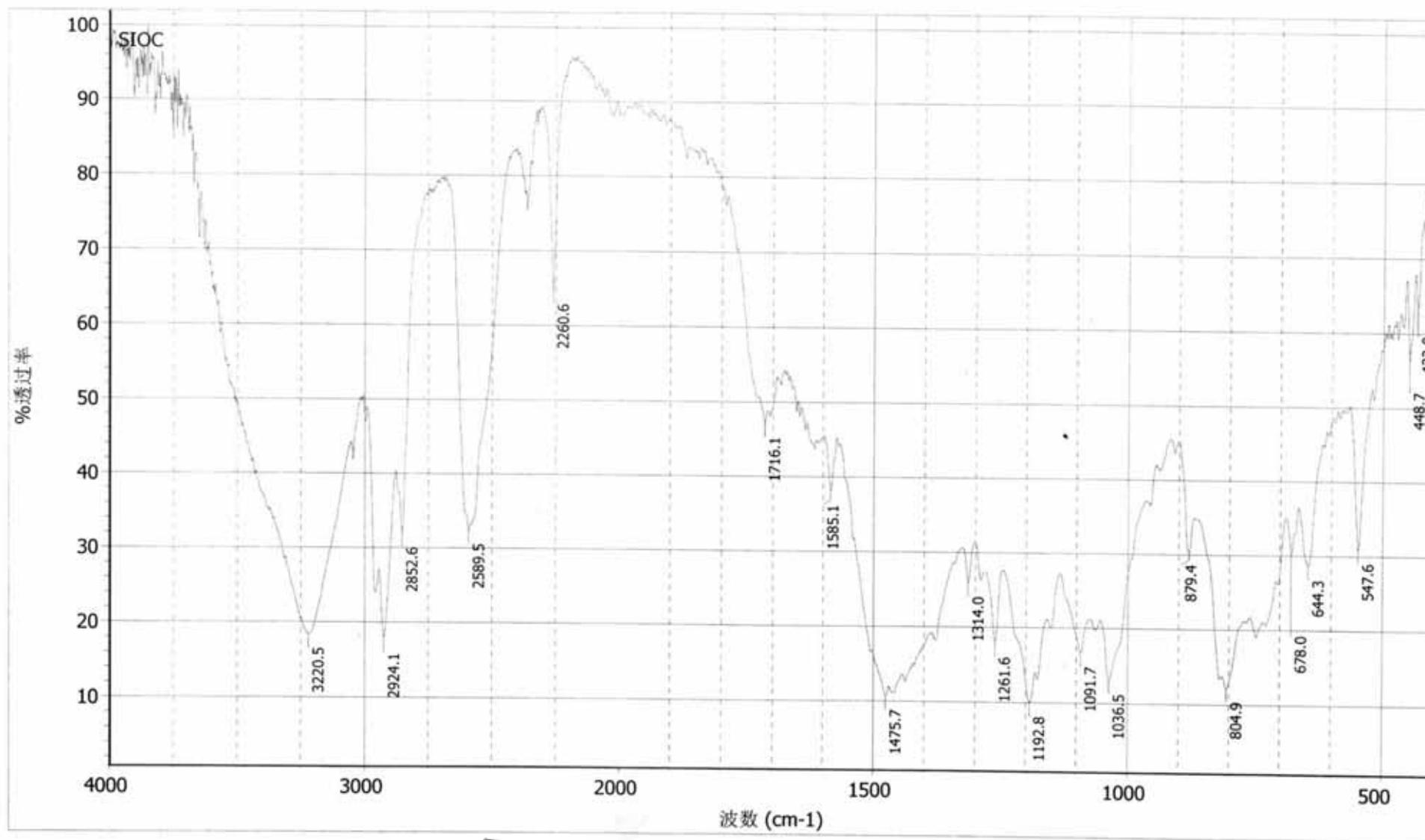
2k



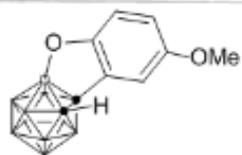
Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-79-1/2012060b-ccx-7-79-a-1/1/pdata/1/1r
Title	2012060b-ccx-7-79-a-1
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring_1gy
Number of Scans	1047
Receiver Gain	575
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	1.0224
Acquisition Date	2017-04-05T22:23:32
Modification Date	2017-04-05T16:06:16
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16379.7
Nucleus	1H
Acquired Size	32768
Spectral Size	32768



Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/产物数据/7-79-1/2012060b-ccx-7-79-a-1-coupling/1/ pdata/1/1r
Title	2012060b-ccx-7-79-a-1-coupling
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	835
Receiver Gain	575
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	1.0224
Acquisition Date	2017-04-05T22:29:42
Modification Date	2017-04-05T16:06:10
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16379.7
Nucleus	1H
Acquired Size	32768
Spectral Size	32768

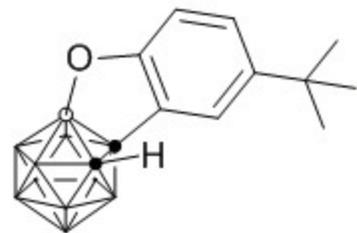


CCX-7-79-a 2015806 JS



2k

样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



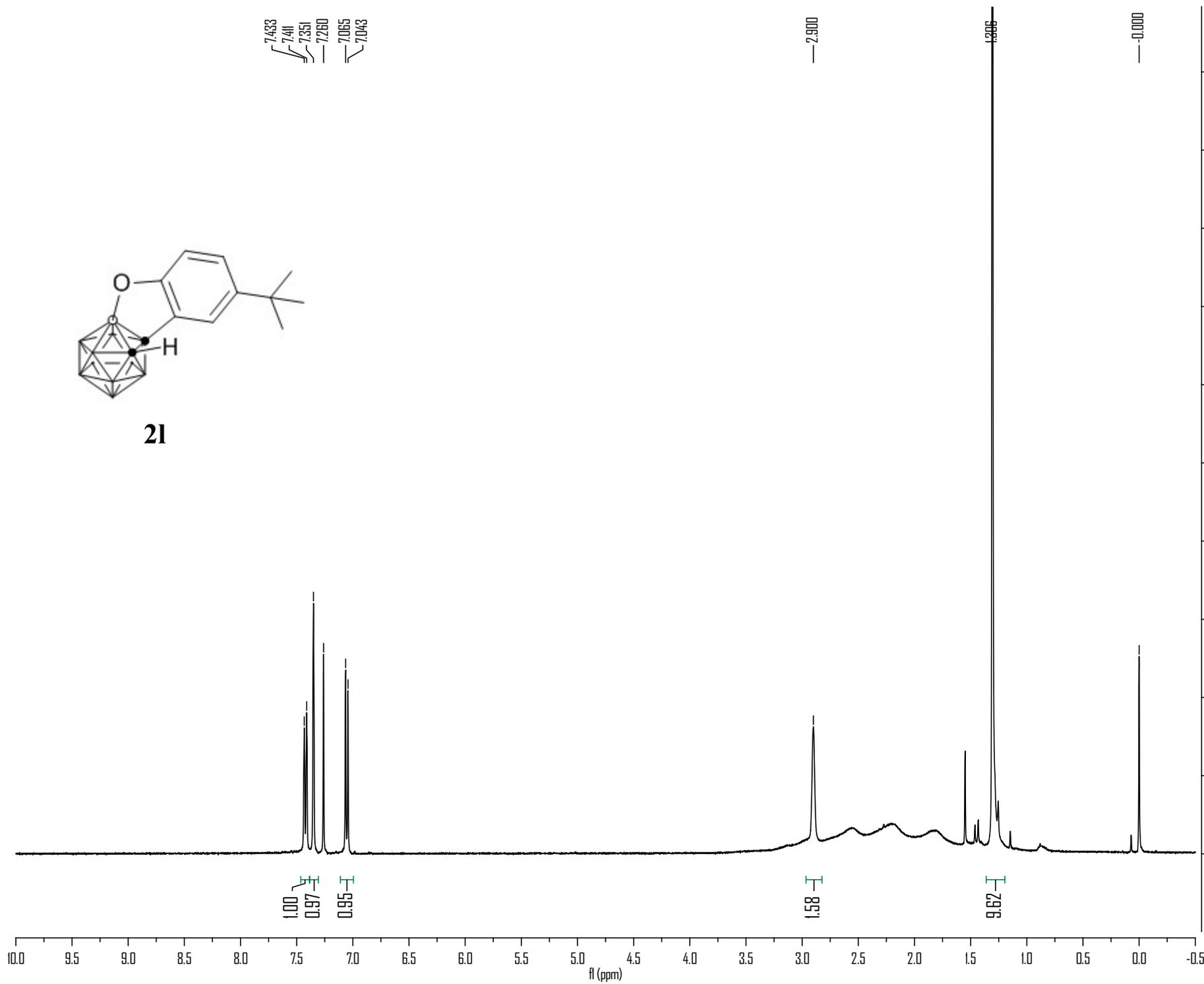
21

7.433
7.411
7.351
7.260
7.055
7.043

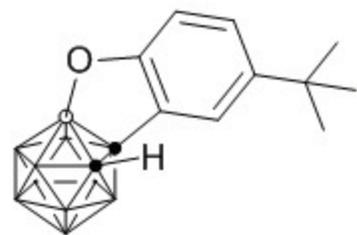
2.900

1.206

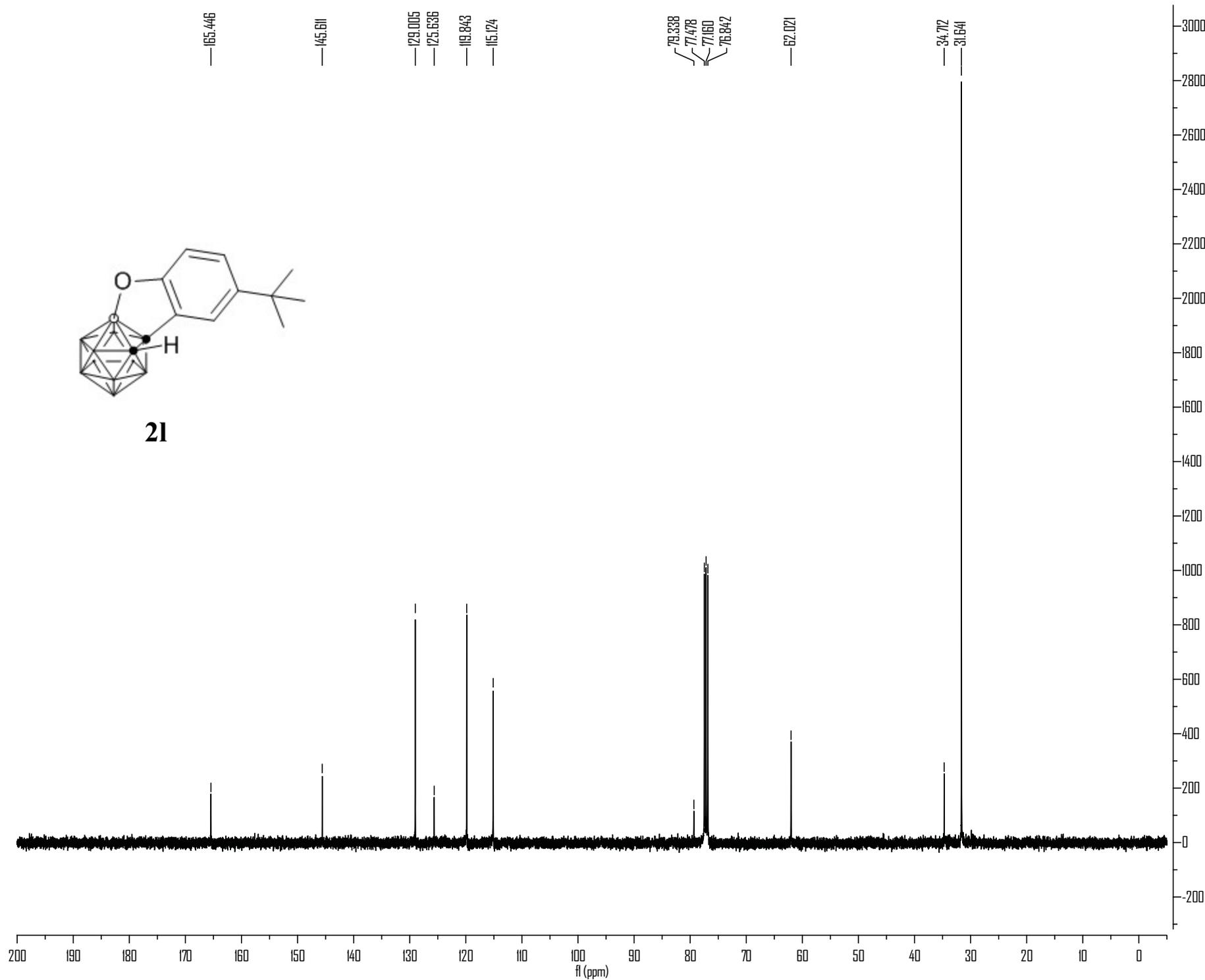
-0.000



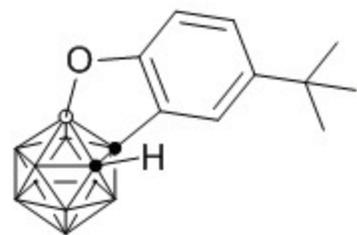
Parameter	Value
Title	ccx-7-65-1
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse	s2pul
Sequence	
Number of Scans	12
Receiver Gain	36
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-02-21 10:51:54
Modification Date	2017-02-20 12:53:00
Spectrometer Frequency	400.03
Spectral Width	7309.9
Lowest Frequency	-846.8
Nucleus	¹ H
Acquired Size	21330
Spectral Size	65536



21



Parameter	Value
Title	C-COX-6-67-1
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	stu
Solvent	pyridine
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	408
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-08-10T10:06:08
Modification Date	2016-08-10T02:28:00
Spectrometer	100.51
Frequency	
Spectral Width	25510.2
Lowest Frequency	-1713.6
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



21

0.595

-3.422

-9.485

-10.082

-12.540

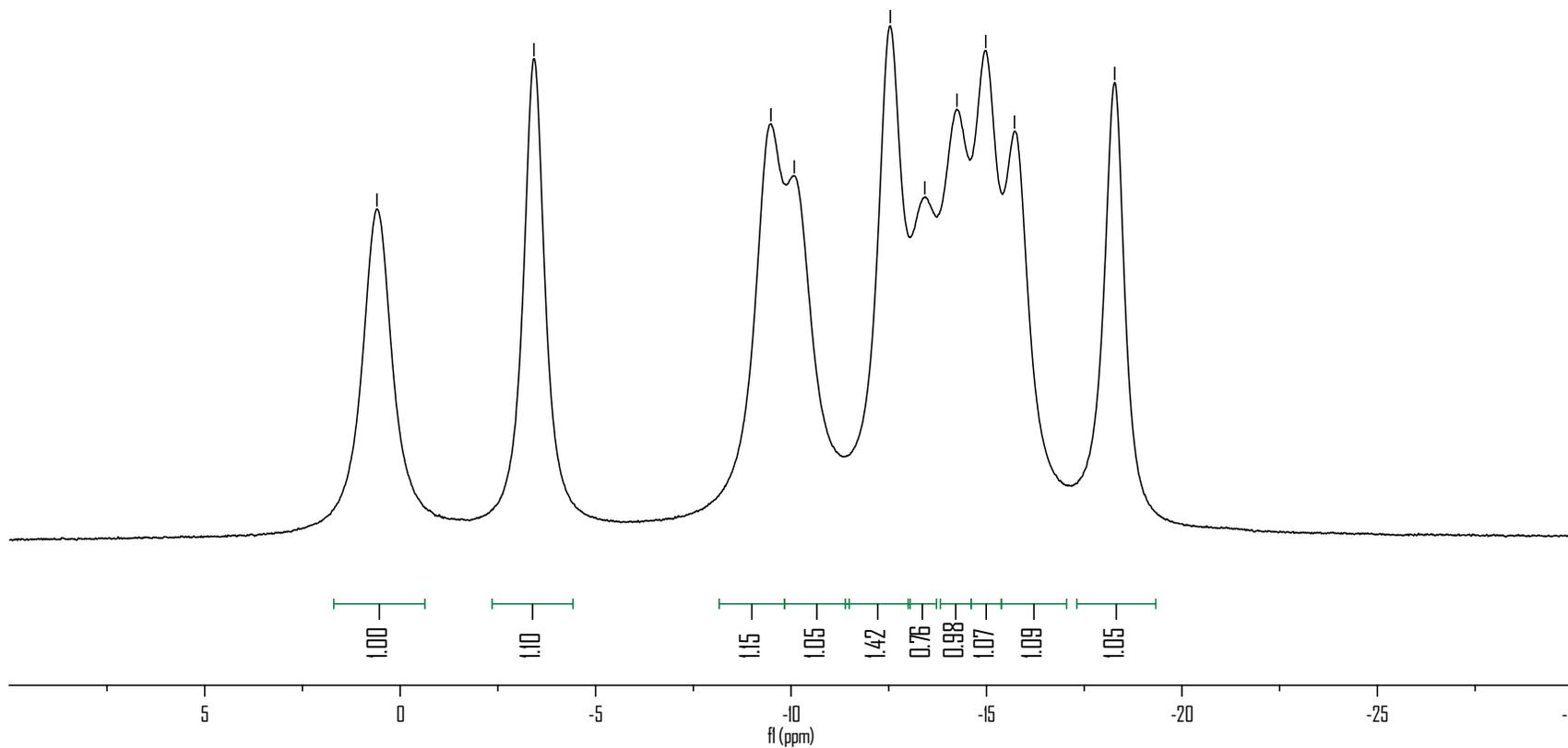
-13.422

-14.245

-14.981

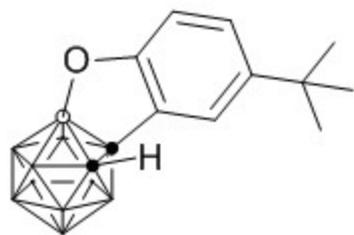
-15.716

-18.279

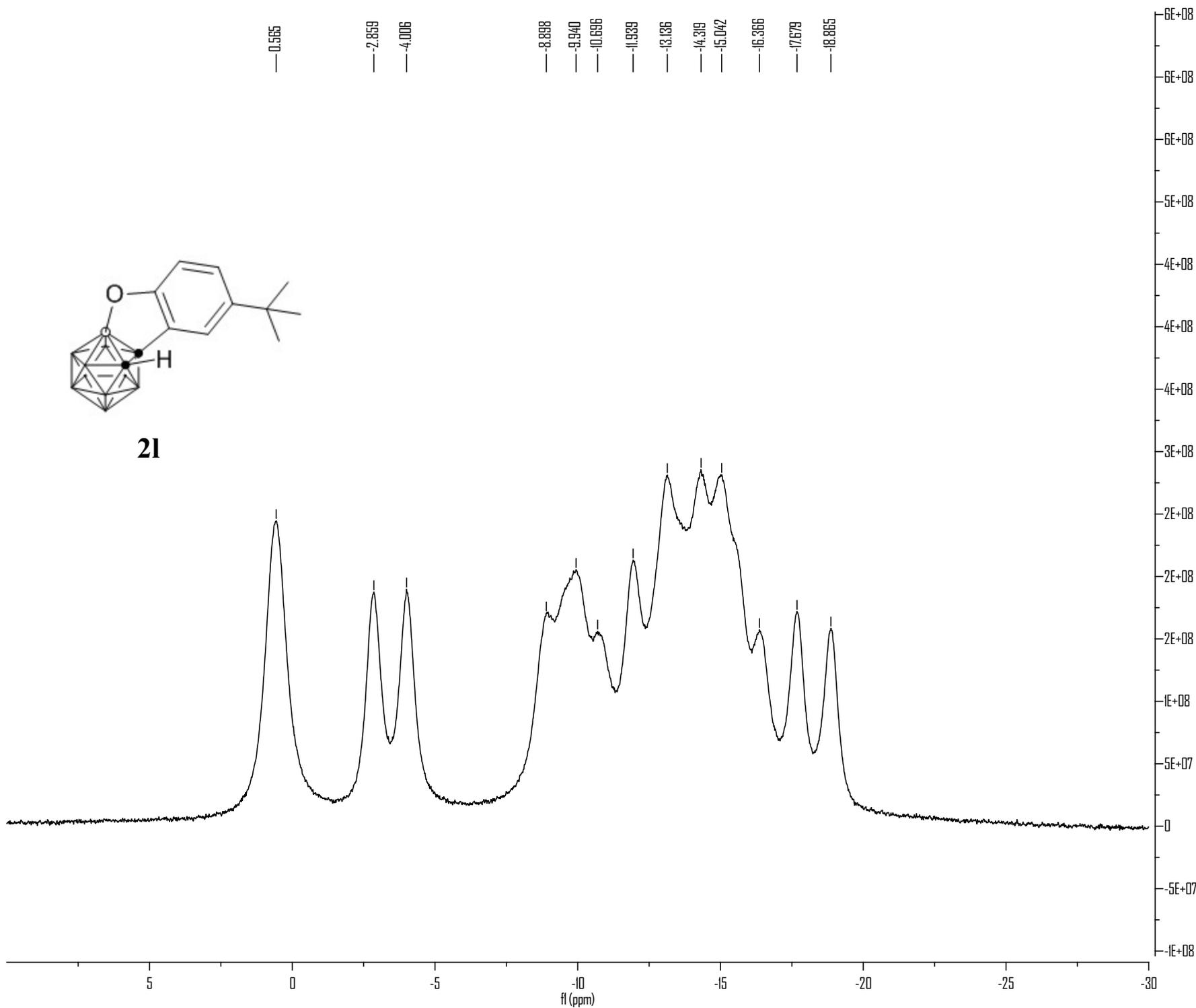


S186

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/6-67-1/b-cx-6-67-1(1)/pdata/1/1r
Title	6-67-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	256
Receiver Gain	203
Relaxation Delay	0.0000
Pulse Width	8.5000
Acquisition Time	0.3195
Acquisition Date	2016-08-10T19:32:44
Modification Date	2016-08-10T19:32:00
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-26020.4
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



21



0.565

-2.859

-4.006

-8.898

-9.940

-10.696

-11.939

-13.136

-14.319

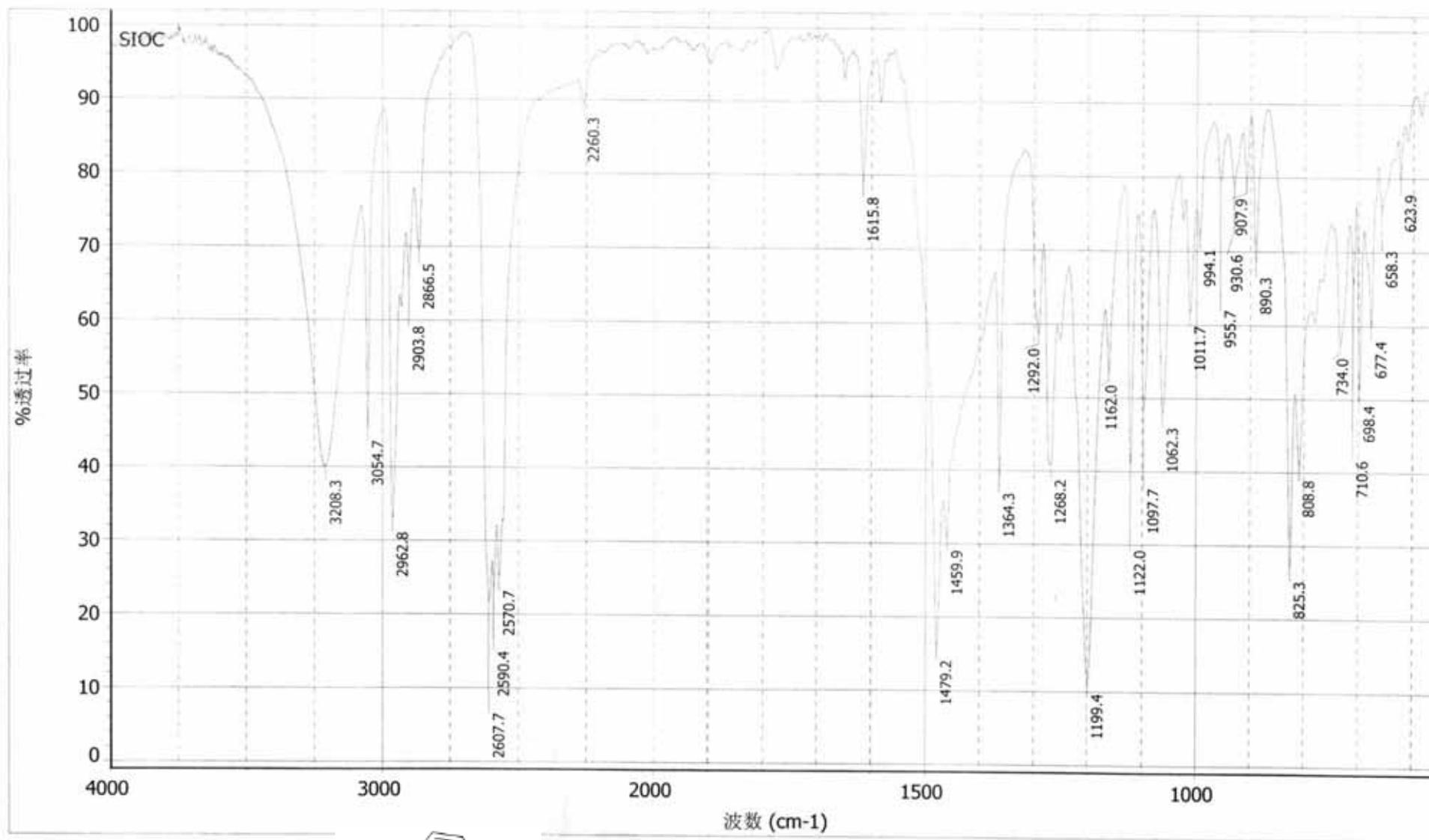
-15.042

-16.366

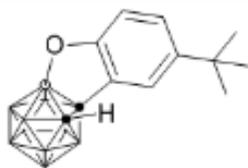
-17.679

-18.865

Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/产物数据/6-67-1/b-cx-6-67-1-coupling (1)/pdata/1/1r
Title	6-67-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	512
Receiver Gain	256
Relaxation Delay	0.0000
Pulse Width	4.0000
Acquisition Time	0.3195
Acquisition Date	2016-08-10T19:37:19
Modification Date	2016-08-10T13:37:00
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-27479.9
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

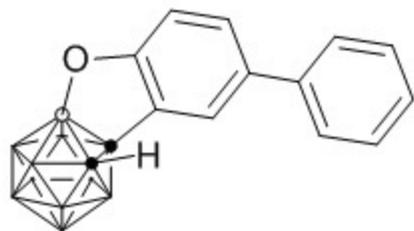


CCX-6-67a 2015806 JS



21

样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



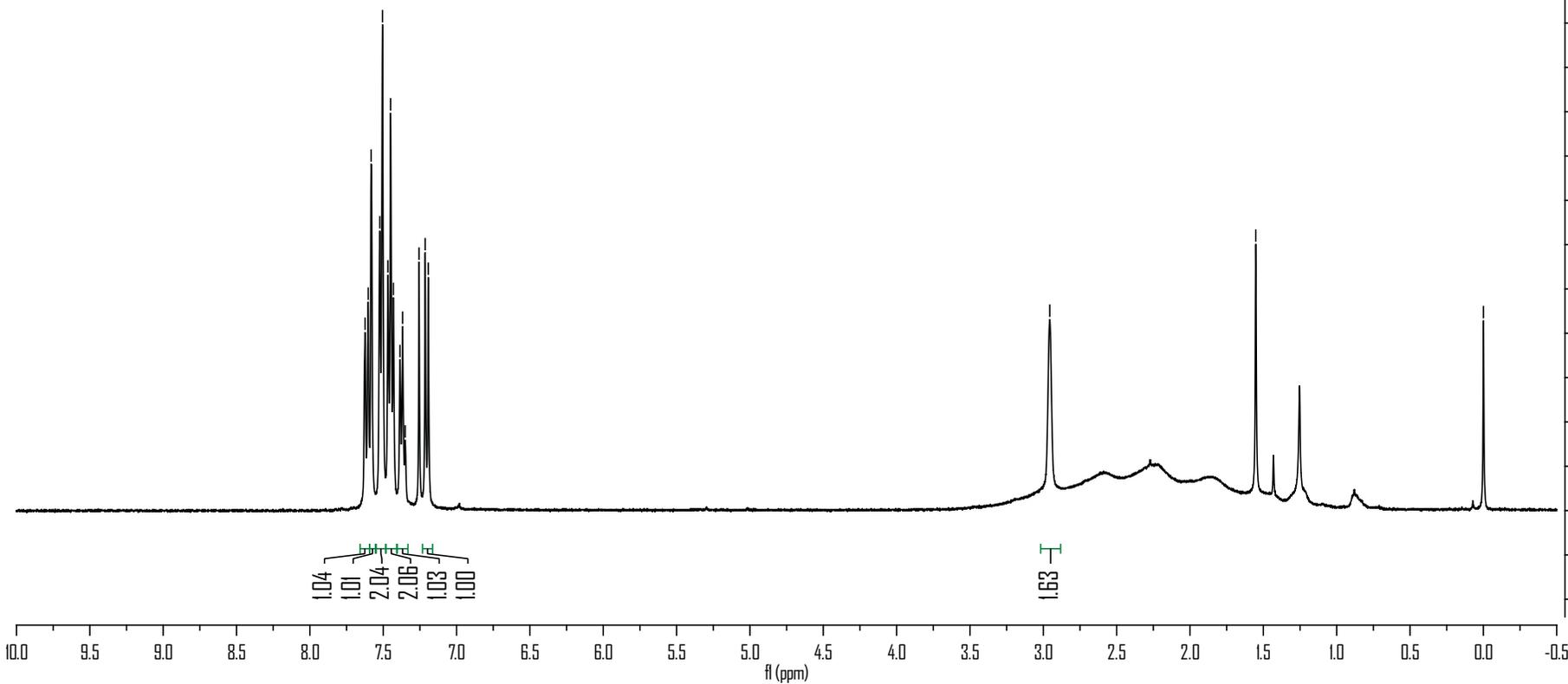
2m

7.674
7.602
7.583
7.524
7.505
7.468
7.450
7.431
7.386
7.368
7.350
7.256
7.214
7.193

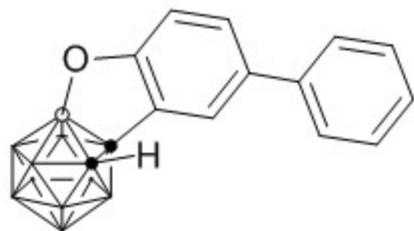
2.956

1.552

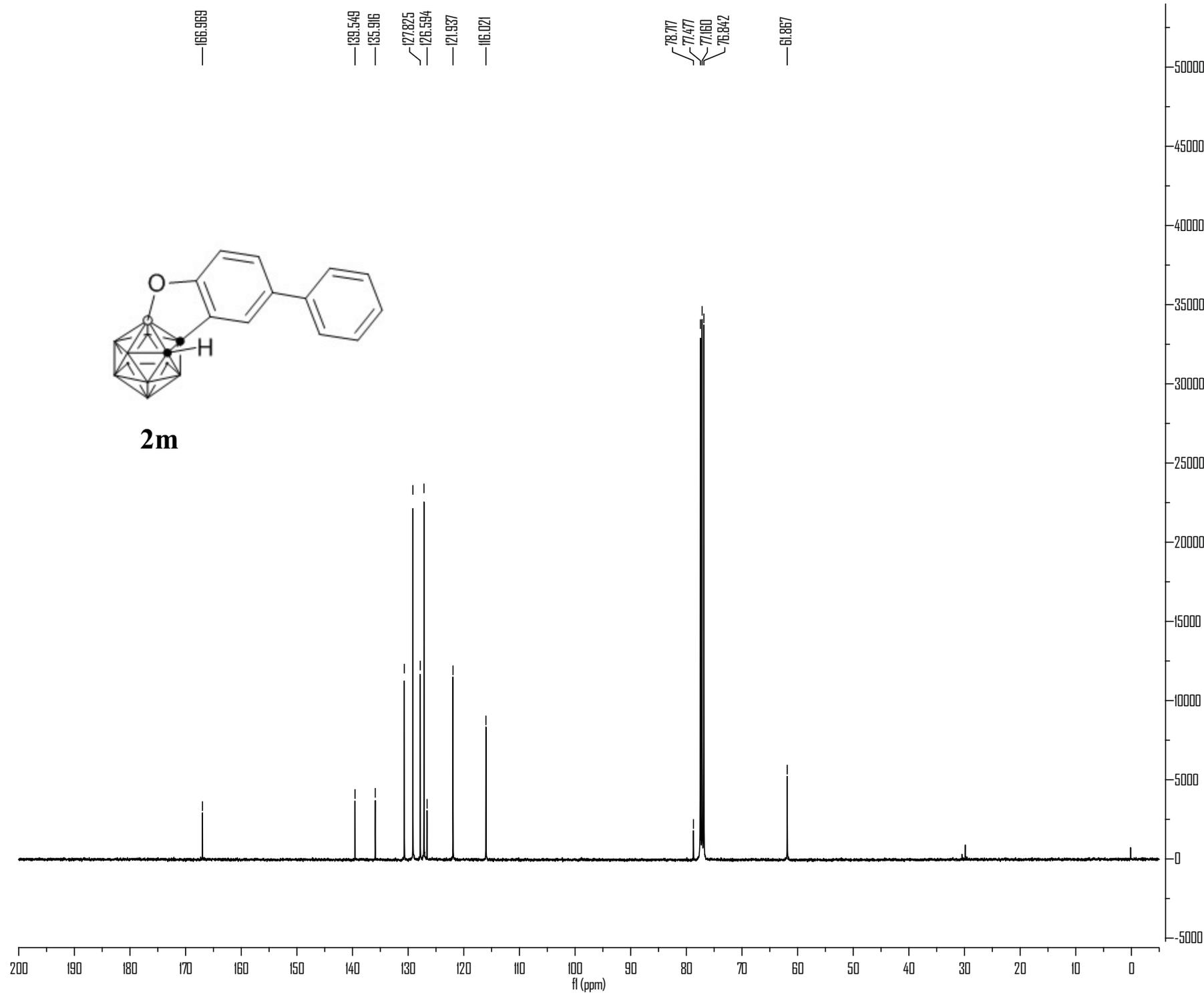
0.000



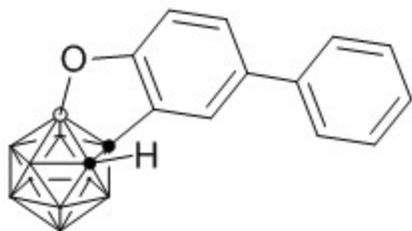
Parameter	Value
Title	ccx-7-73-1
Comment	xcc-Sc12
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	38
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-03-10T22:06:17
Modification Date	2017-03-10T14:07:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-795.5
Nucleus	1H
Acquired Size	21552
Spectral Size	65536



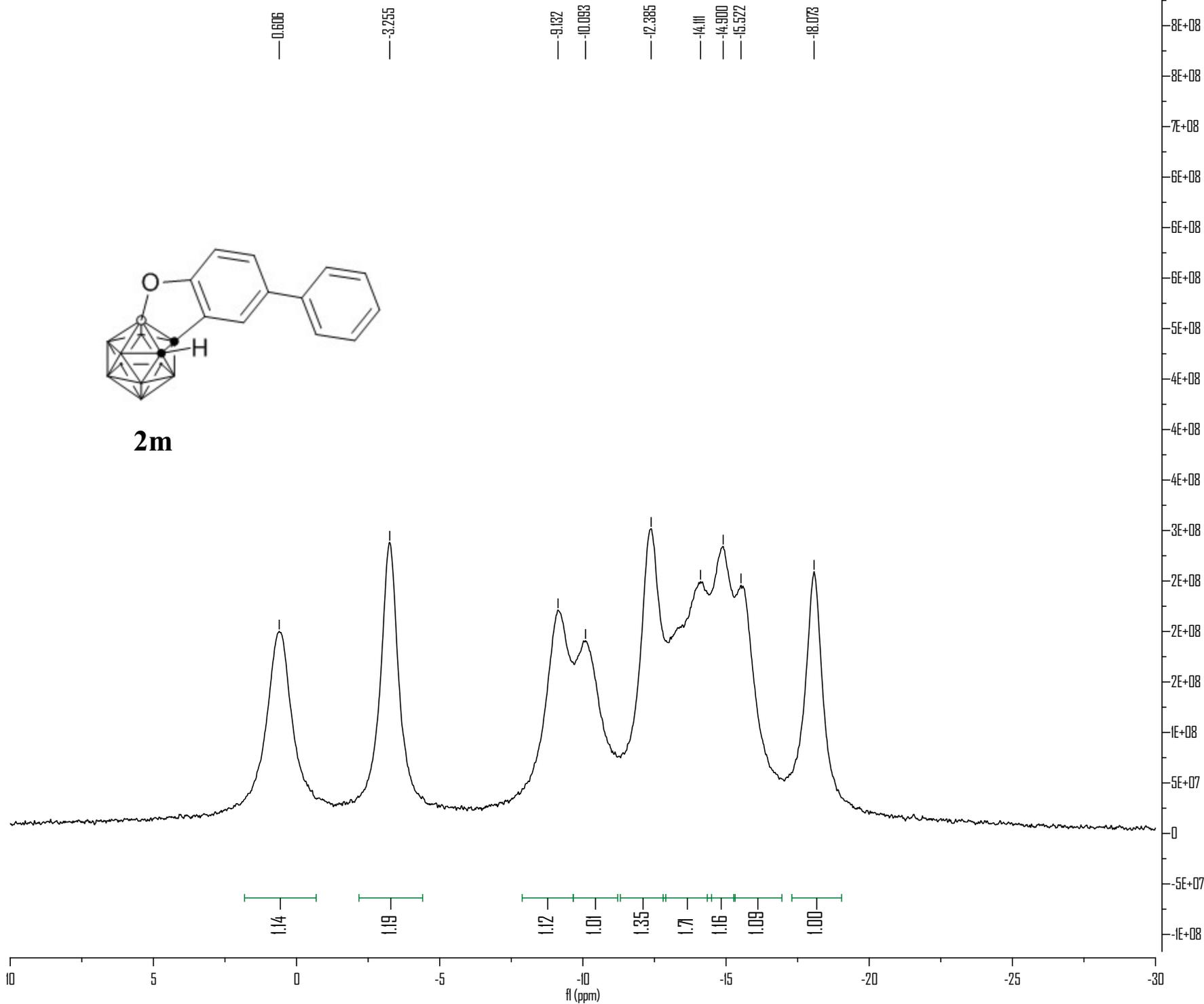
2m



Parameter	Value
Title	ccx-7-73-1-c
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	omcl
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	13320
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Acquisition Date	2017-03-10T22:15:40
Modification Date	2017-03-10T23:12:00
Spectrometer Frequency	100.62
Spectral Width	25000.0
Lowest Frequency	-1429.3
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

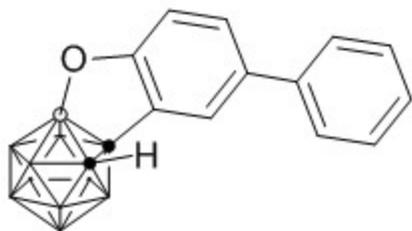


2m

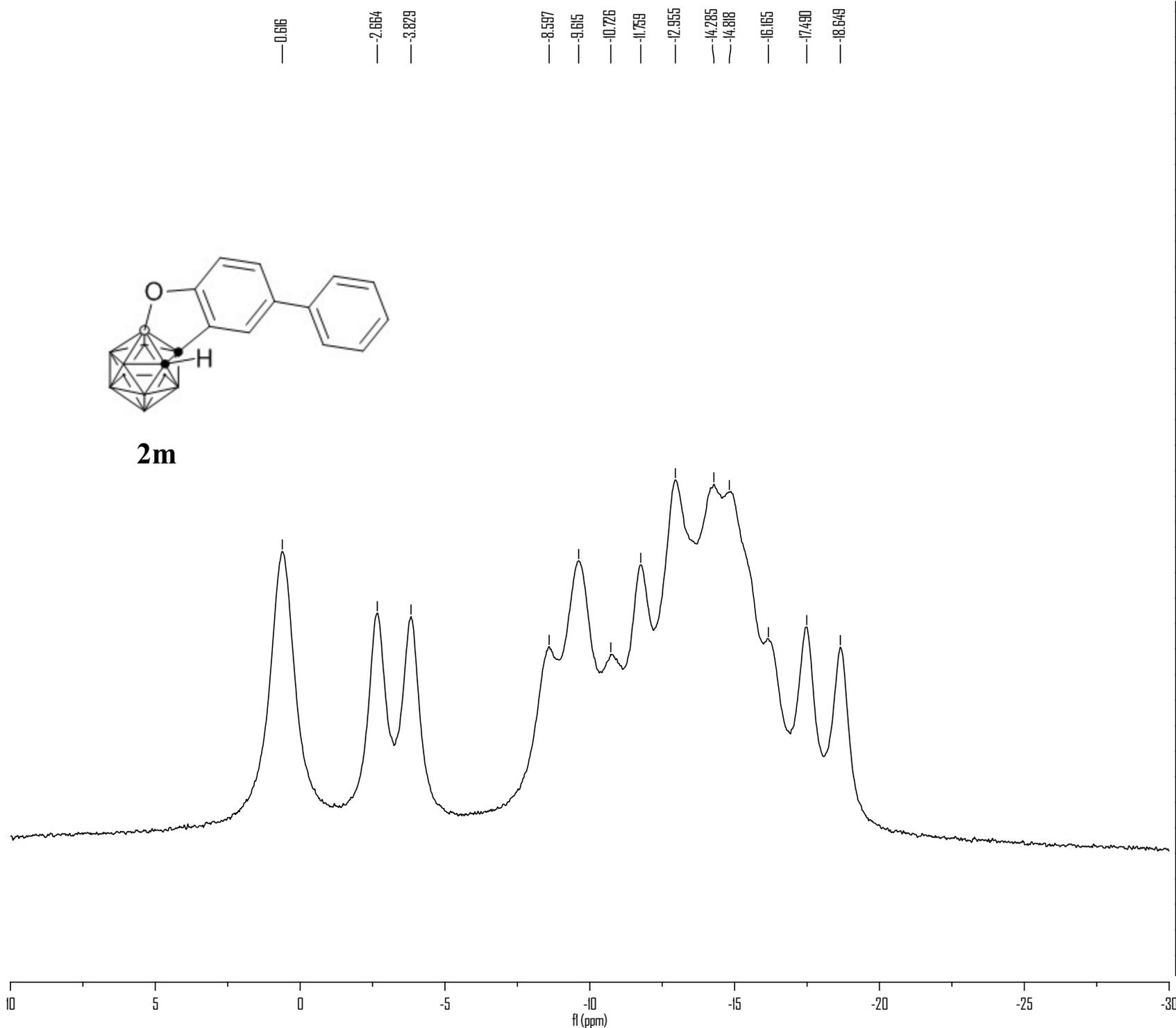


S191

Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/产物数据/7-73-1/b-cx-7-73-1/pdata/1/1r
Title	7-73-1
Comment	
Origin	UXMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	89
Receiver Gain	228
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-03-28T19:47:00
Modification Date	2017-03-28T12:47:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16396.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

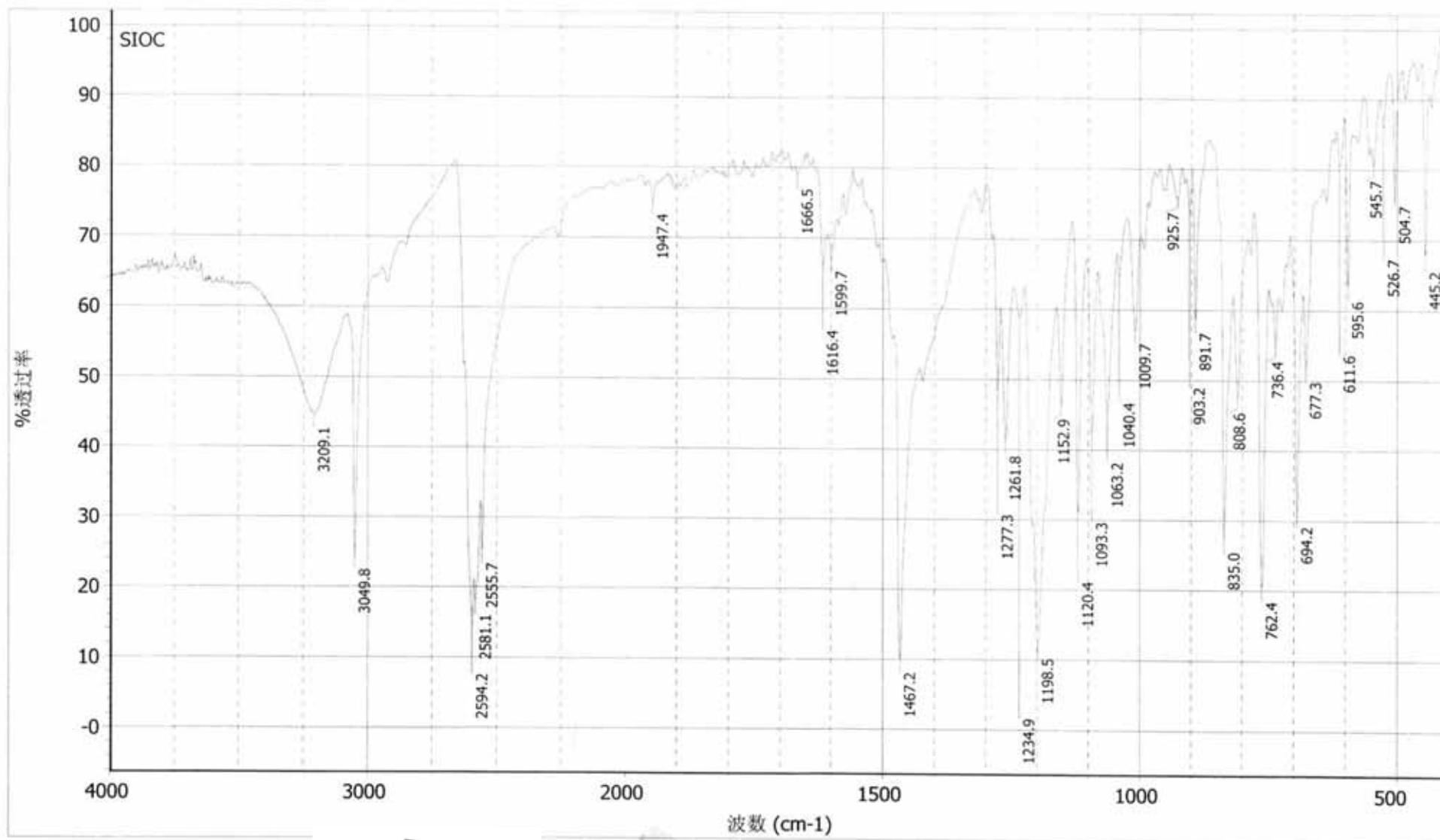


2m

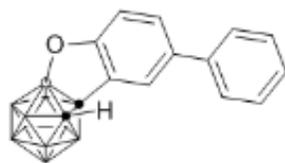


S192

Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-73-1/b-cx-7-73-1-coupling/pdata/1/1r
Title	7-73-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	259
Receiver Gain	228
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-03-28T19:47:57
Modification Date	2017-03-28T12:49:00
Spectrometer	128.38
Frequency	
Spectral Width	32051.3
Lowest Frequency	-16396.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



CCX-7-73A 2015806 JS



2m

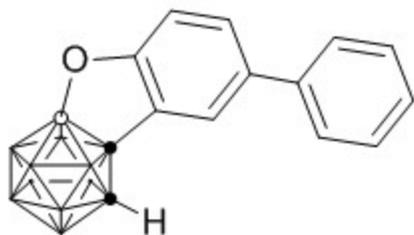
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329

7.633
7.628
7.61
7.606
7.525
7.504
7.461
7.442
7.427
7.423
7.375
7.356
7.338
7.261
7.242
7.220

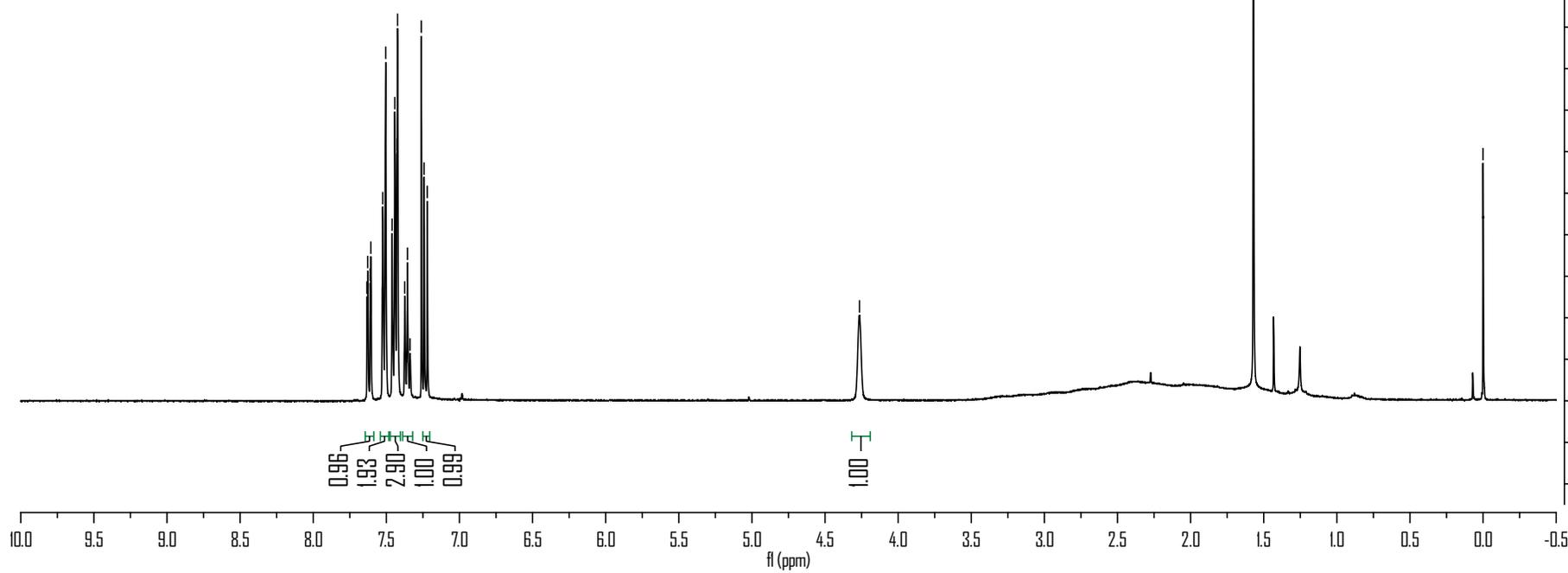
4.265

1.57

0.000



3m



Parameter	Value
Title	ccx-7-81-b-H
Comment	xcc-Sci2
Origin	Varian
Owner	
Site	
Spectrometer	nmrns
Author	
Solvent	CDCl3
Temperature	25.0
Pulse	s2pul
Sequence	
Number of Scans	16
Receiver Gain	52
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-04-09T12:13:19
Modification Date	2017-04-09T04:20:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-793.9
Nucleus	1H
Acquired Size	21552
Spectral Size	65536

166.645

139.872

134.823

129.099

127.118

125.667

118.512

115.944

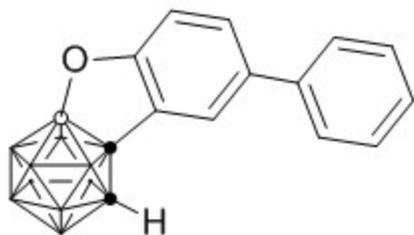
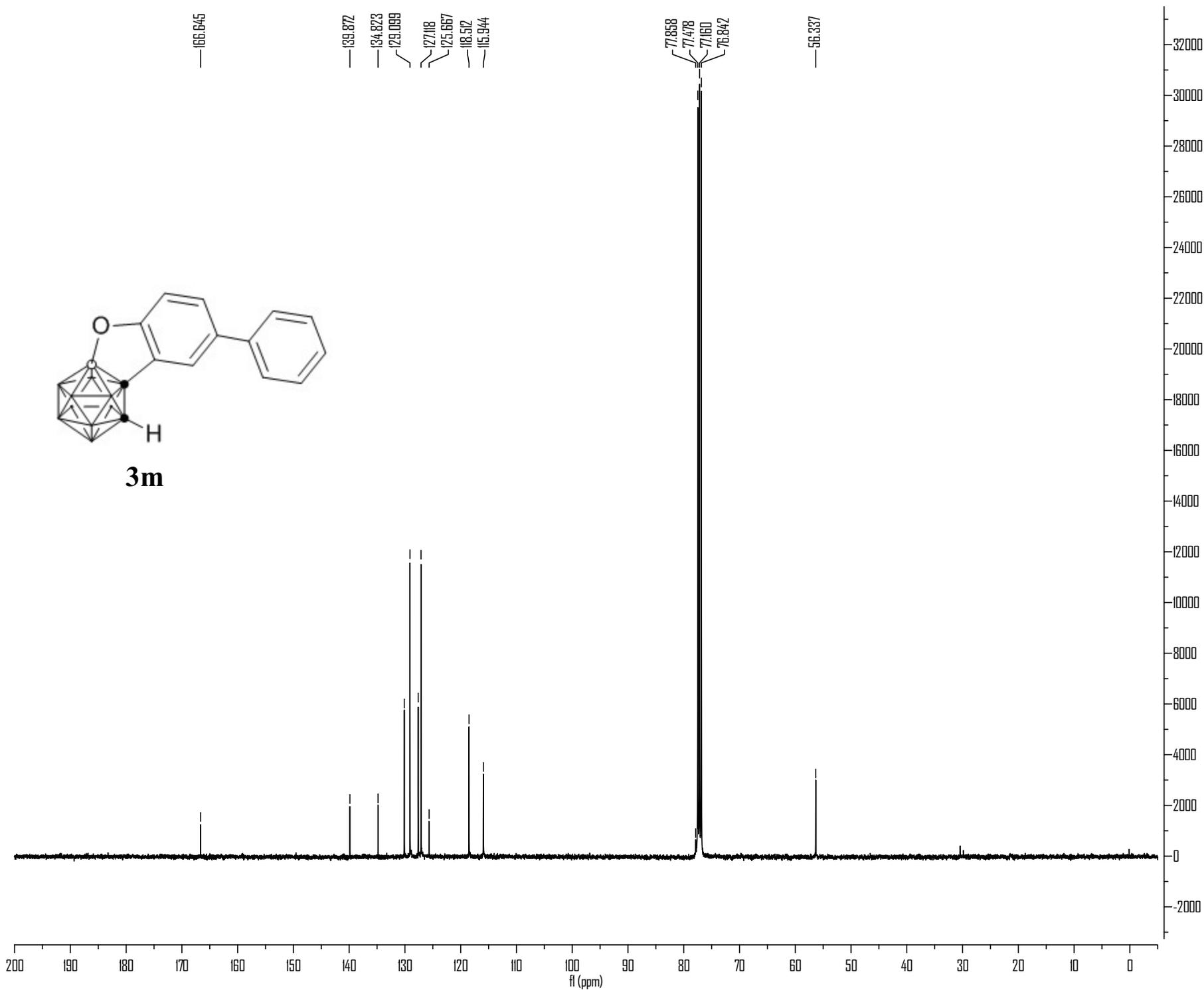
77.858

77.478

77.160

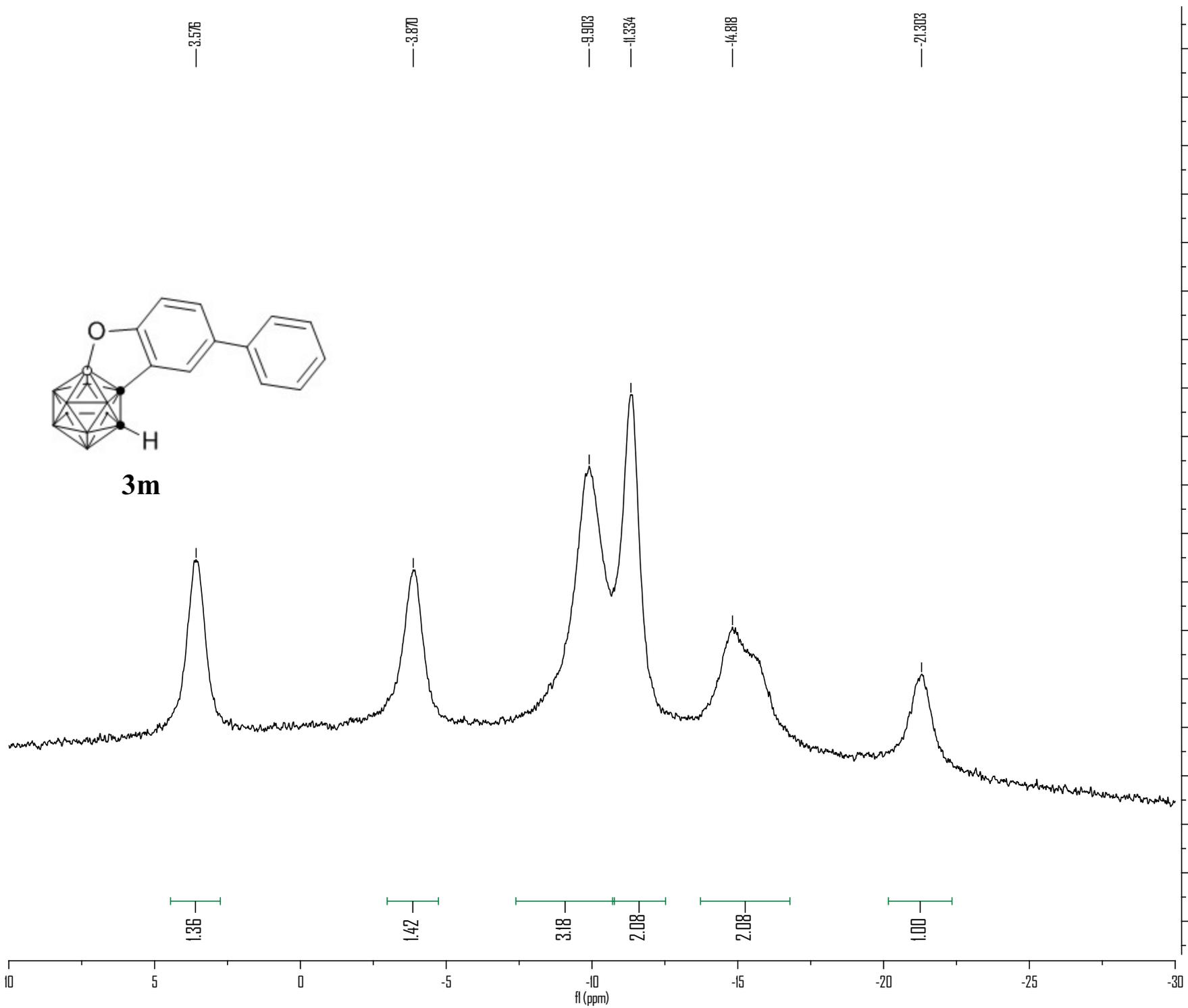
76.842

56.837

**3m**

S195

Parameter	Value
Title	ccx-7-81-b-2c
Comment	lxj-2-54-C-H
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	11236
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2017-04-11T23:30:16
Modification Date	2017-04-11T22:38:00
Spectrometer Frequency	100.52
Spectral Width	25510.2
Lowest Frequency	-1272.0
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-73-2/b-cx-7-73-2/pdata/1/1r
Title	7-73-2
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	533
Receiver Gain	724
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-03-28T20:00:58
Modification Date	2017-03-28T13:04:00
Spectrometer frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16396.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

3.673

3.300

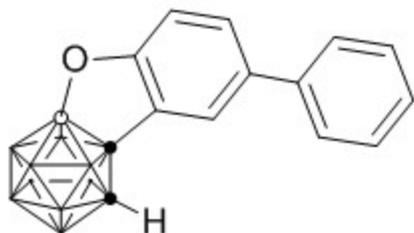
4.480

8.305

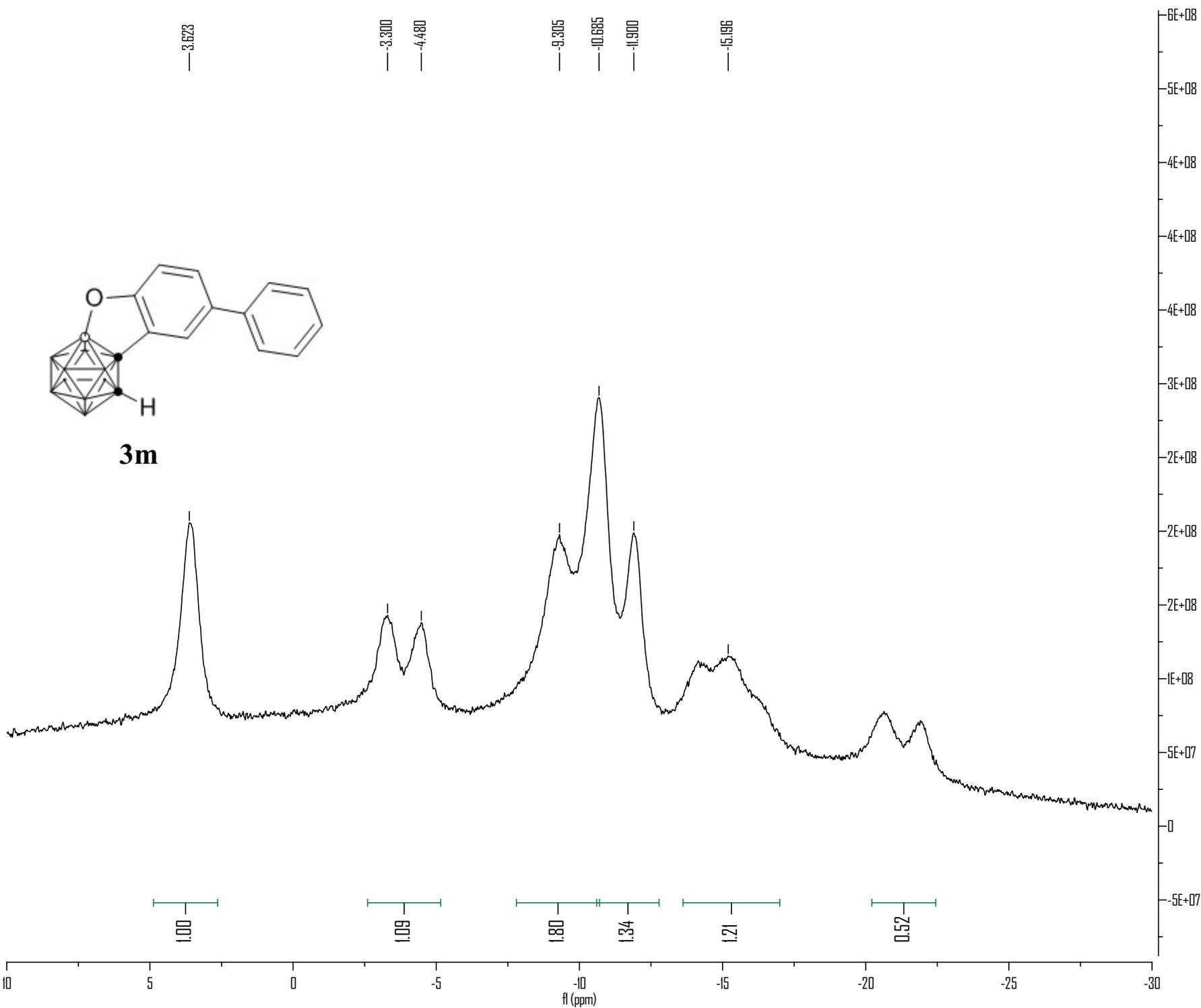
10.685

11.900

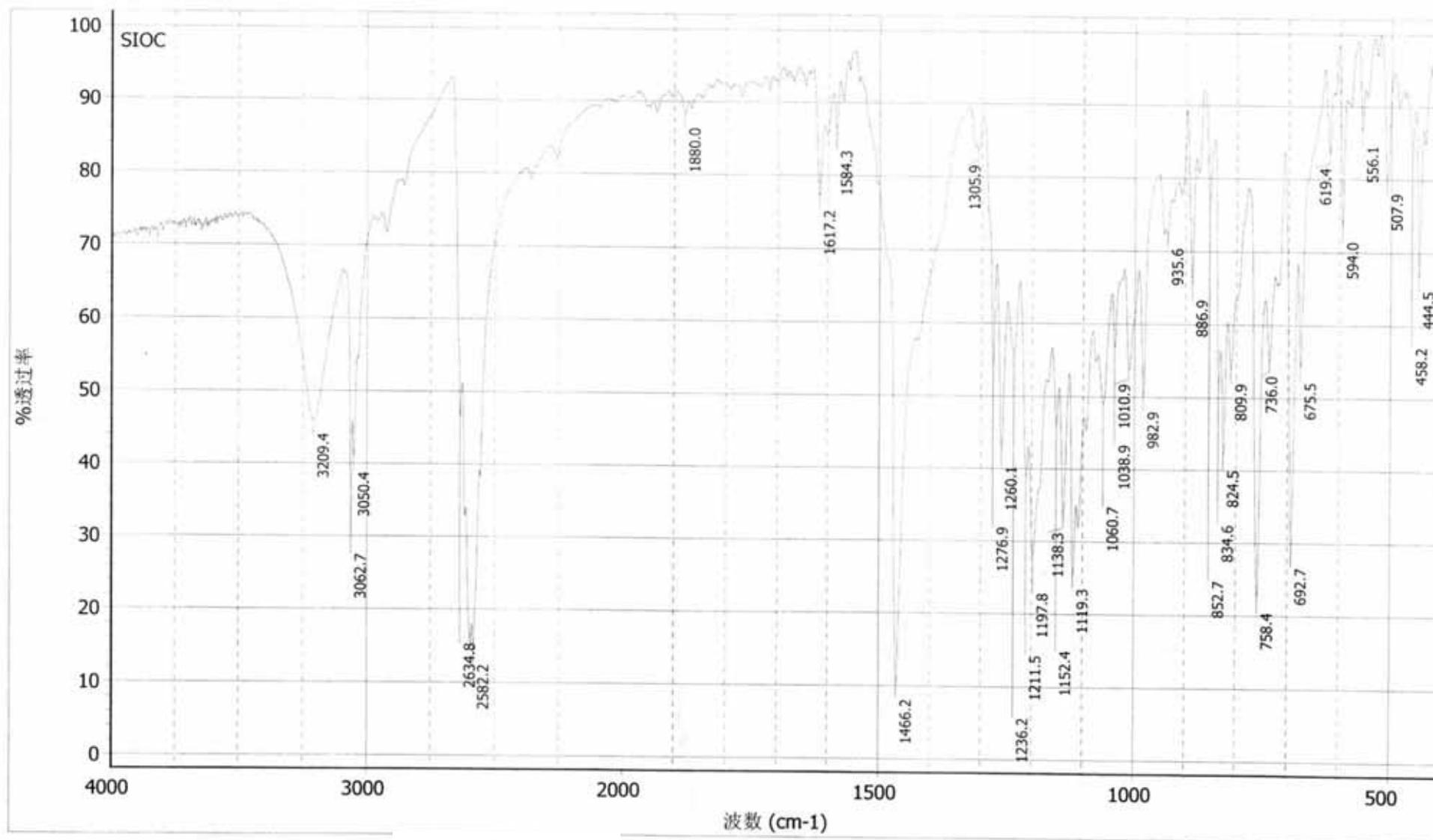
15.196



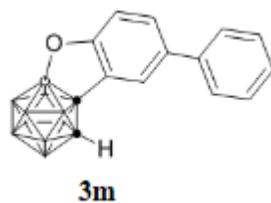
3m



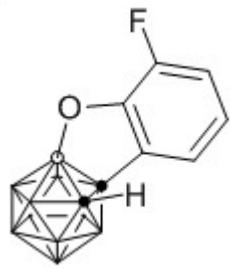
Parameter	Value
Data file Name	C:/Users/cuichunxiao/Desktop/产物数据/7-73-2/b-csx-7-73-2-coupling/pdata/1/1r
Title	7-73-2
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	848
Receiver Gain	1149
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-03-28T19:52:39
Modification Date	2017-03-28T12:59:00
Spectrometer	128.38
Frequency	
Spectral Width	32051.3
Lowest Frequency	-16396.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



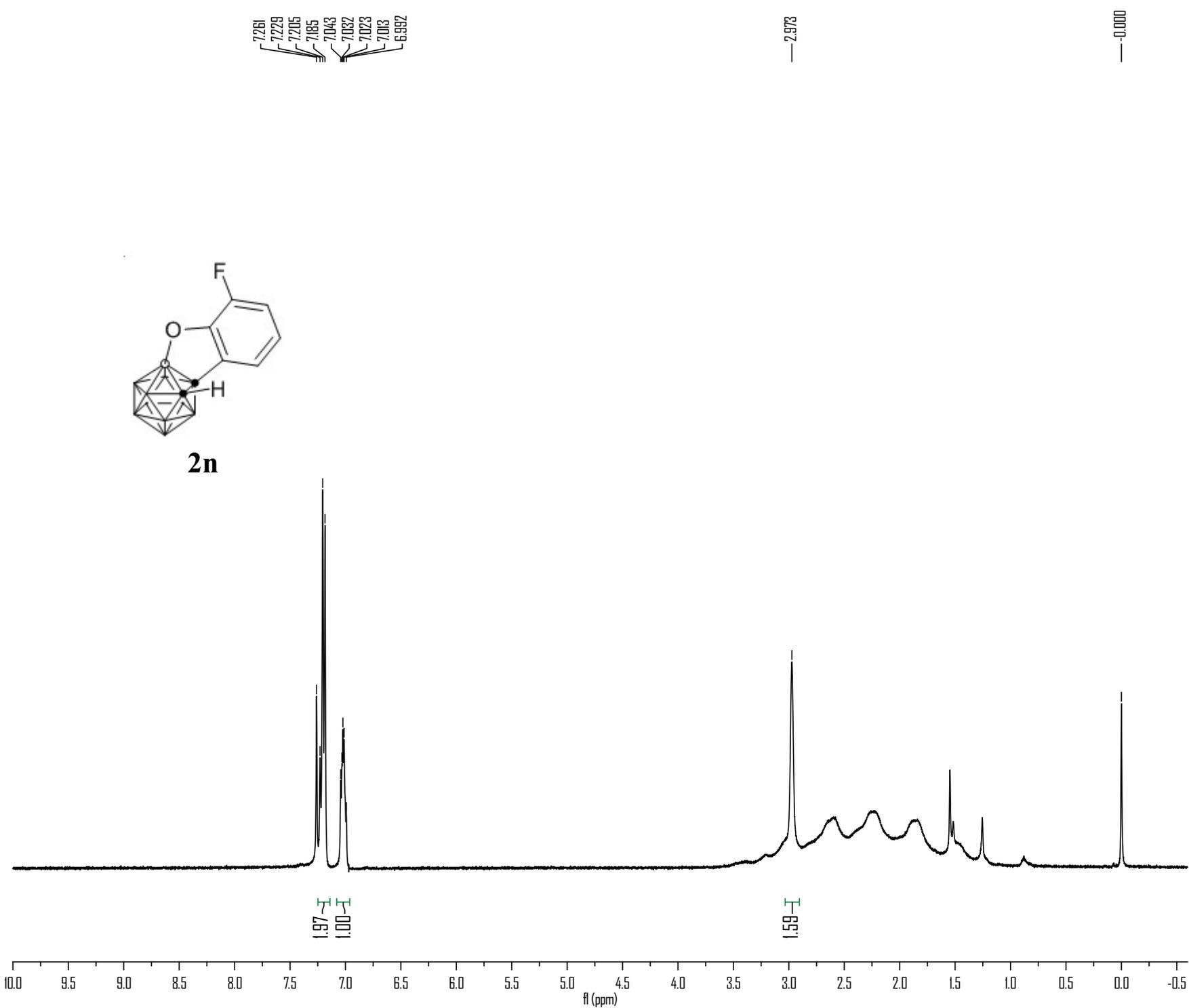
CCX-7-81-B 2015806 JS



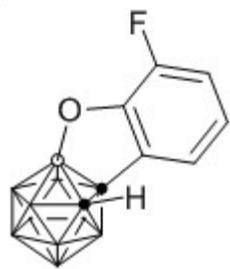
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



2n



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-24-a/ccx-7-24-1-1.fid/ fid
Title	ccx-7-24-1-1
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	38
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-11-14T17:19:45
Modification Date	2016-11-14T09:20:00
Spectrometer Frequency	400.03
Spectral Width	7267.4
Lowest Frequency	-845.5
Nucleus	¹ H
Acquired Size	21802
Spectral Size	65536



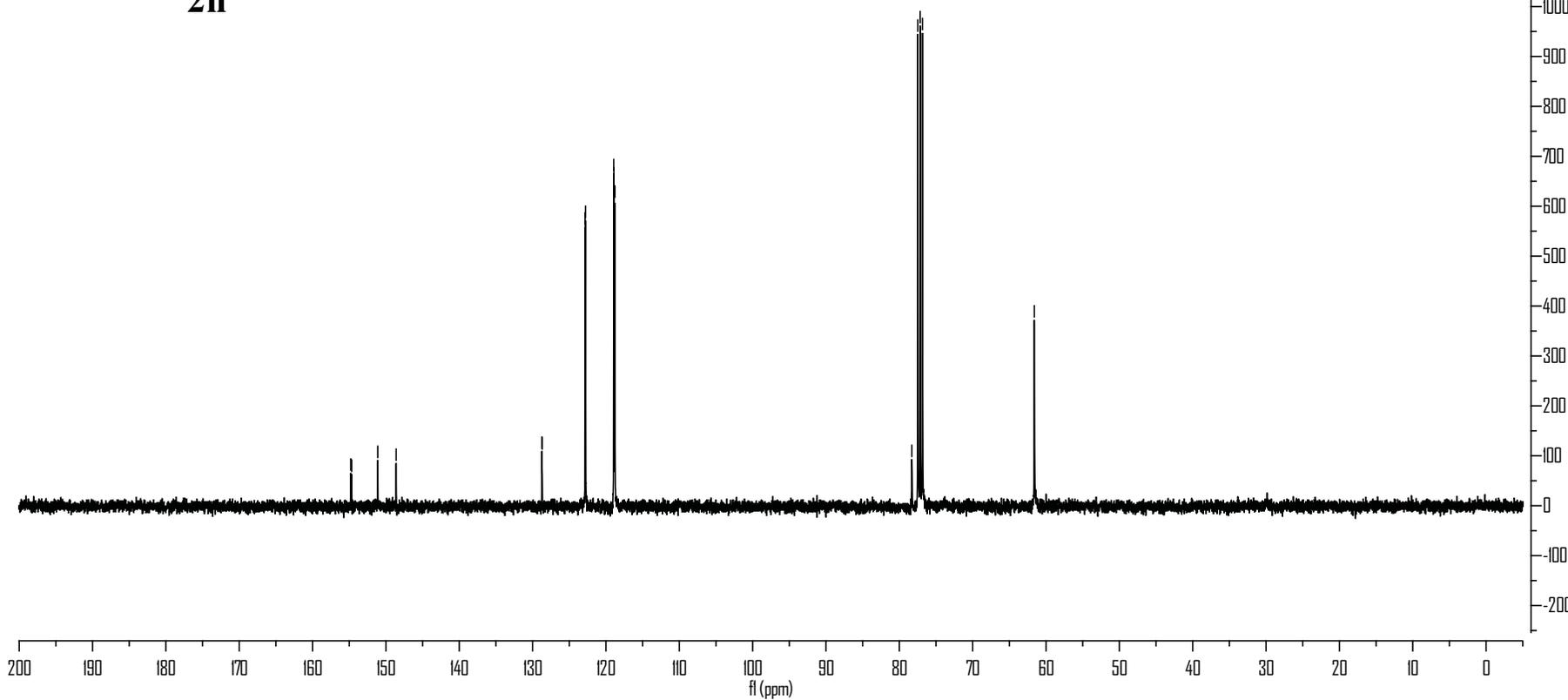
2n

154.797
154.674
151.114
148.603

128.720
128.692
122.784
118.942
118.919
118.879
118.774

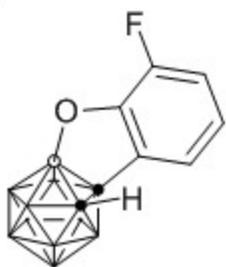
78.291
77.478
77.160
76.843

61.591

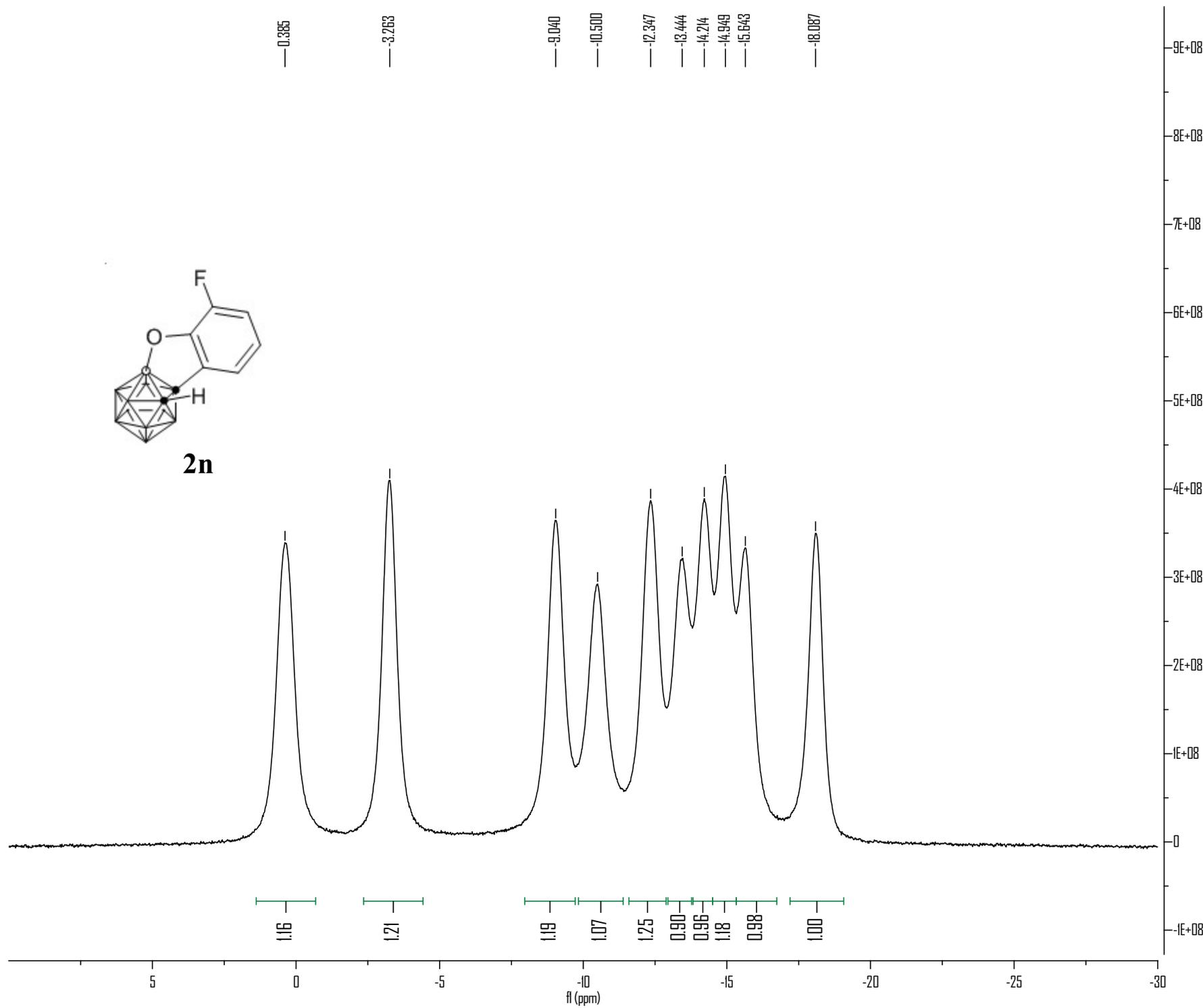


S200

Parameter	Value
Data file Name	E:/Users/Administrator/Desktop/产物数据/7-24-a/-CCX-7-24-1C.fid/ fid
Title	-CCX-7-24-1C
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	stu
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	292
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2016-11-16T09:46:43
Modification Date	2016-11-16T10:03:00
Spectrometer	100.51
Frequency	
Spectral Width	25510.2
Lowest Frequency	-1681.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

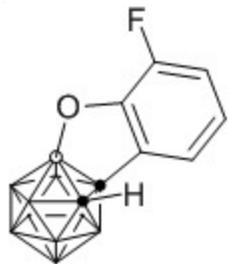


2n

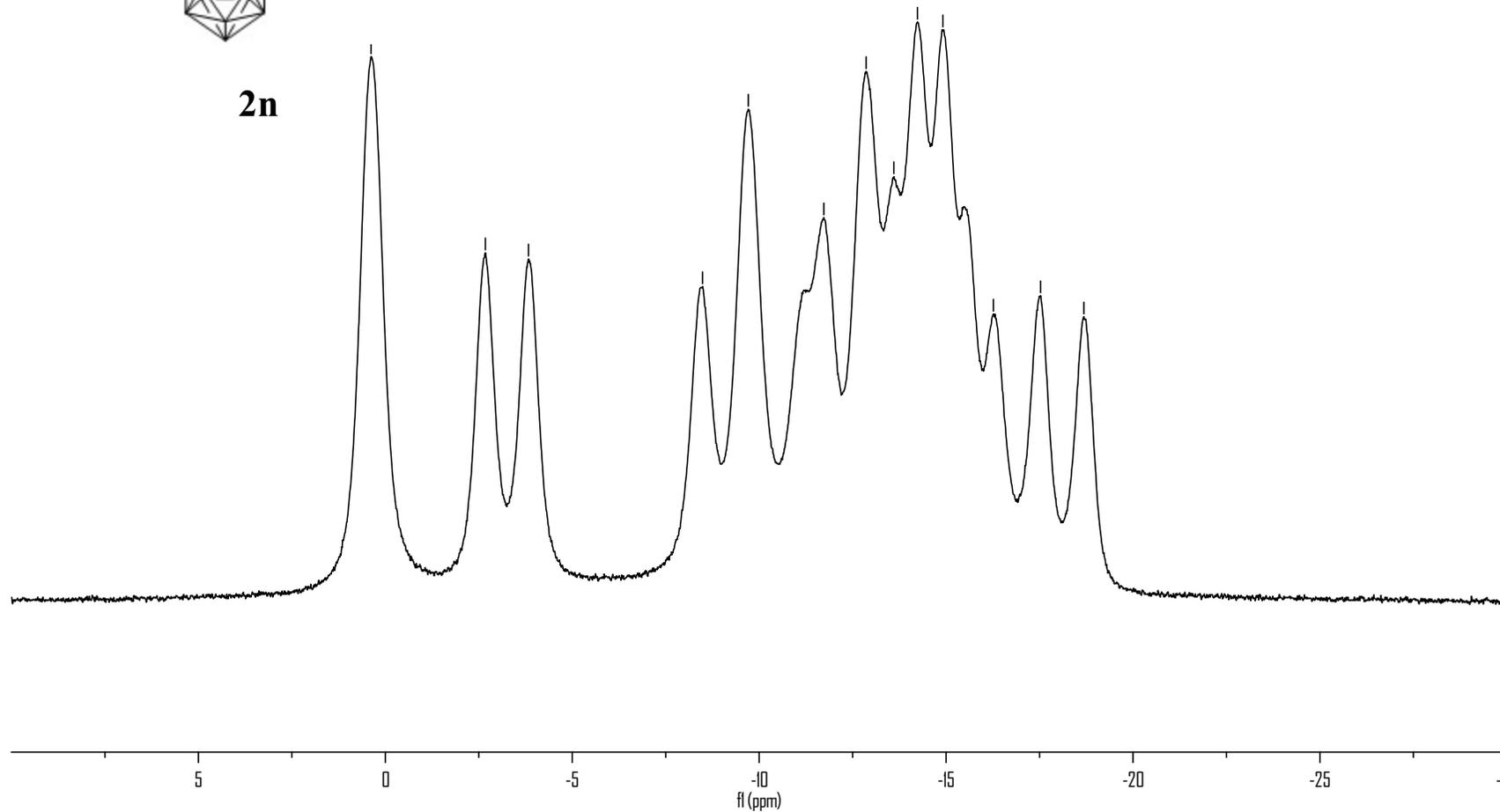


S201

Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-24-a/2012060b-ccx-7-24-1/pdata/1/1r
Title	2012060b-ccx-7-24-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	48
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-11-15T20:29:19
Modification Date	2016-11-15T14:20:44
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-1649.8
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

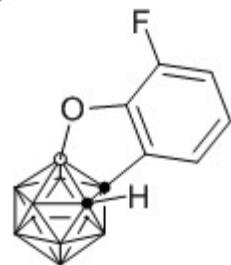


2n



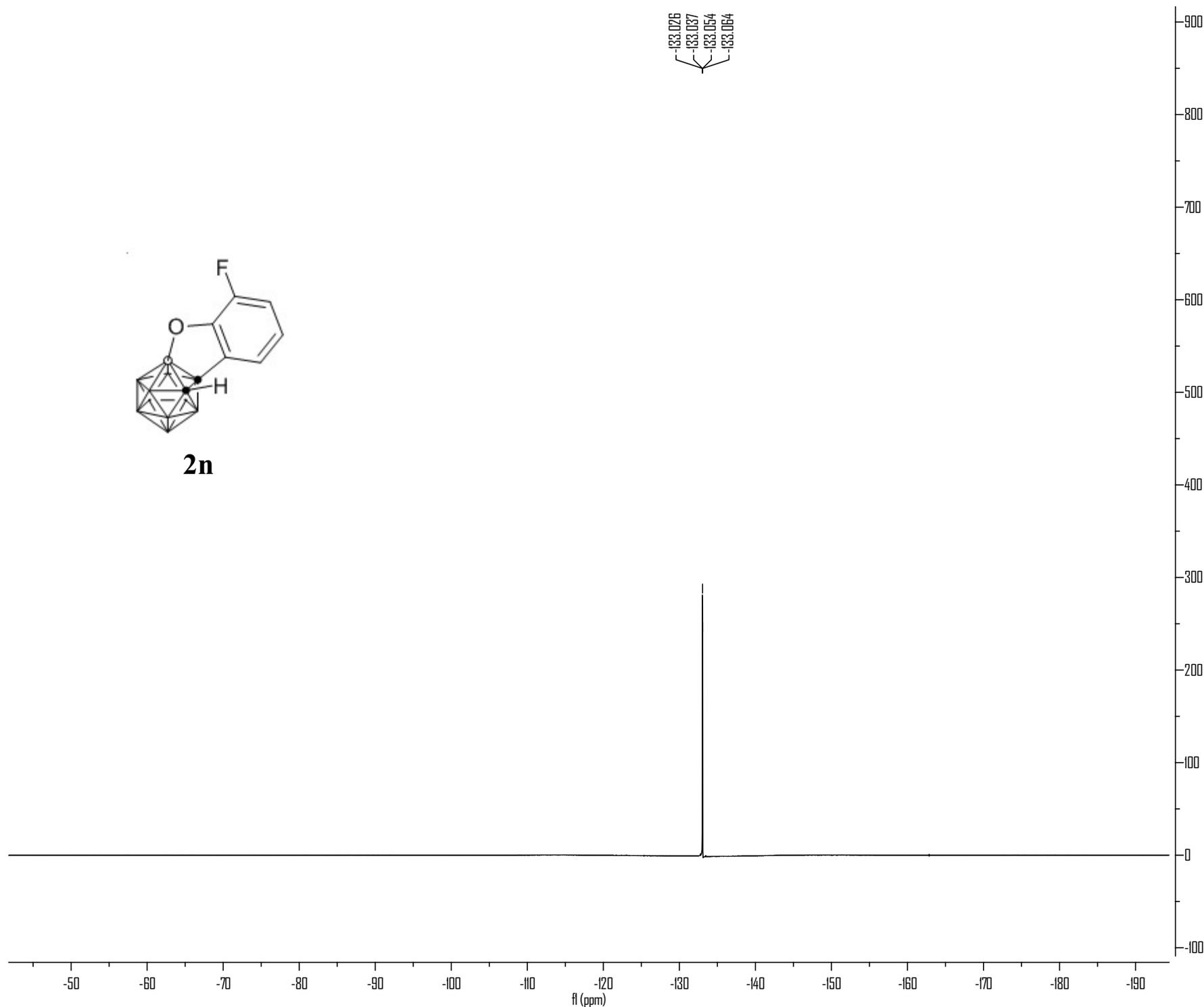
S202

Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-24-a/2012060b-cxx-7-24-1-coupling/1/pdata/1/1r
Title	2012060b-cxx-7-24-1-coupling
Comment	
Origin	LNMNR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	40
Receiver Gain	128
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-11-15T20:31:12
Modification Date	2016-11-15T14:20:34
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16419.8
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



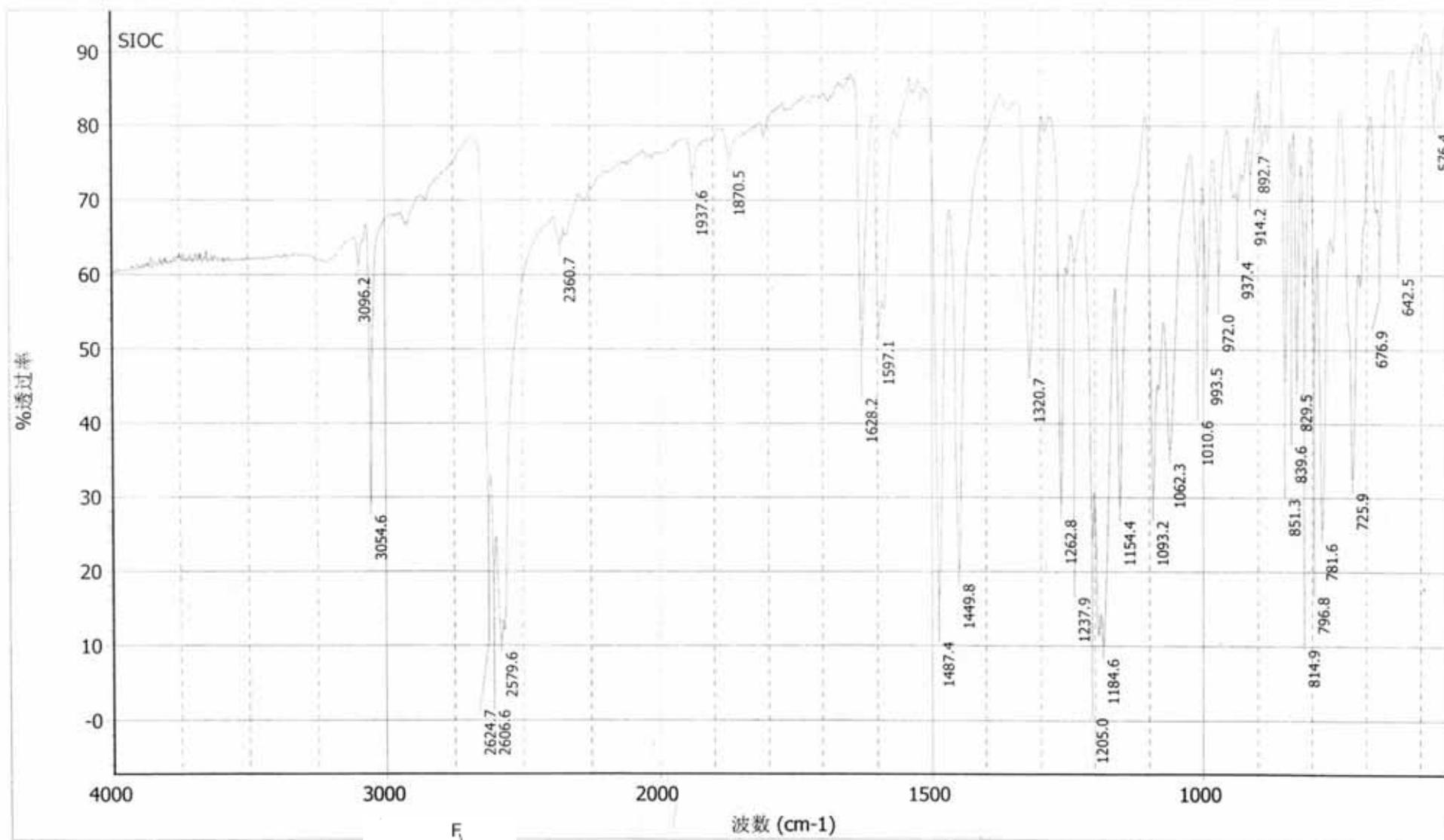
2n

133.026
133.037
133.054
133.064

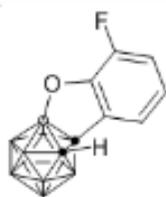


S203

Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/7-24-a/-CCX-7-24-1F.fid/ fid
Title	-CCX-7-24-1F
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	stu
Solvent	cdcl3
Temperature	26.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	44
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.0972
Acquisition Date	2016-11-16T10:04:30
Modification Date	2016-11-16T10:05:00
Spectrometer Frequency	376.01
Spectral Width	125000.0
Lowest Frequency	-116352.9
Nucleus	13C
Acquired Size	262144
Spectral Size	262144

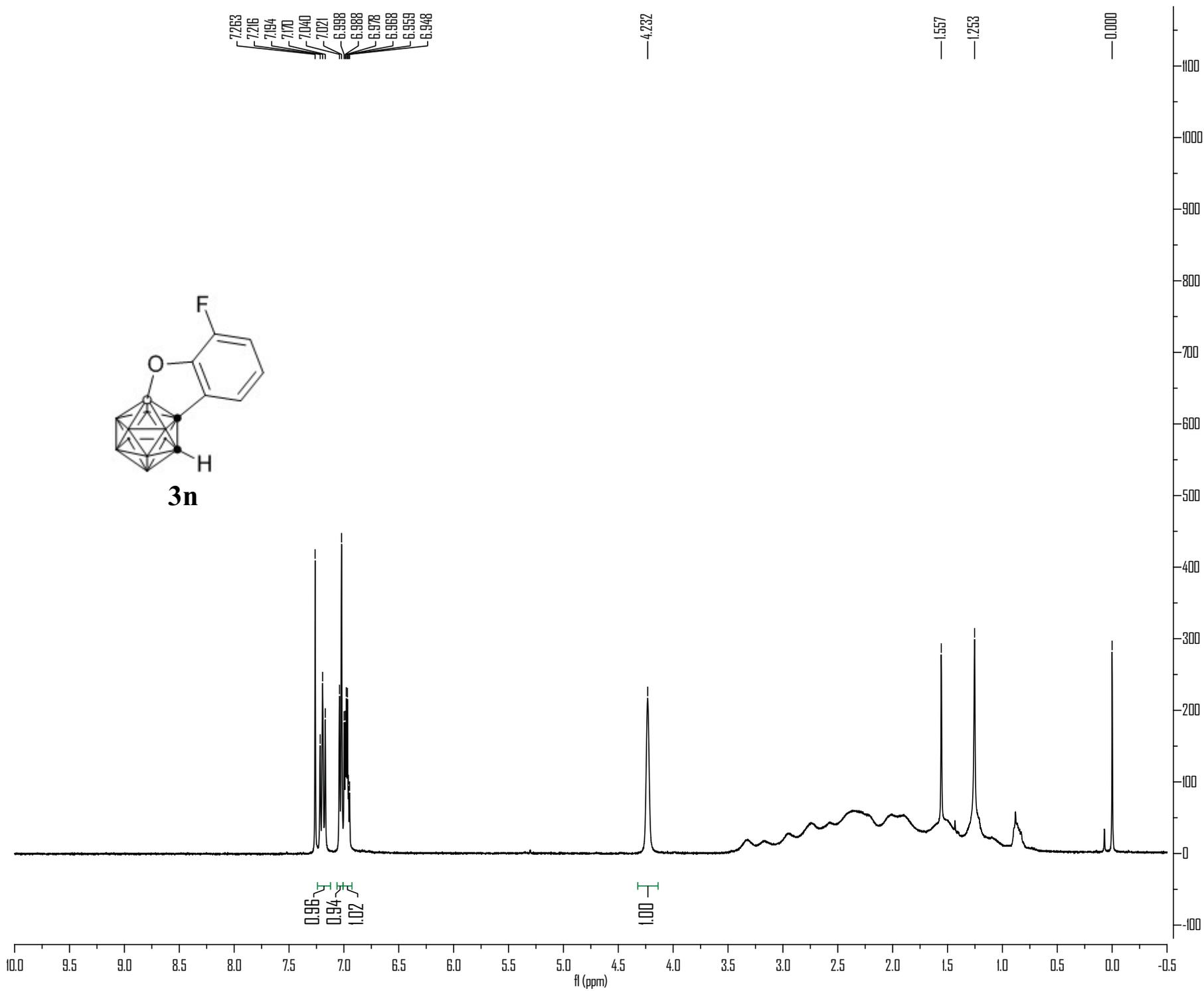


CCX-7-24-A 2015806 JS

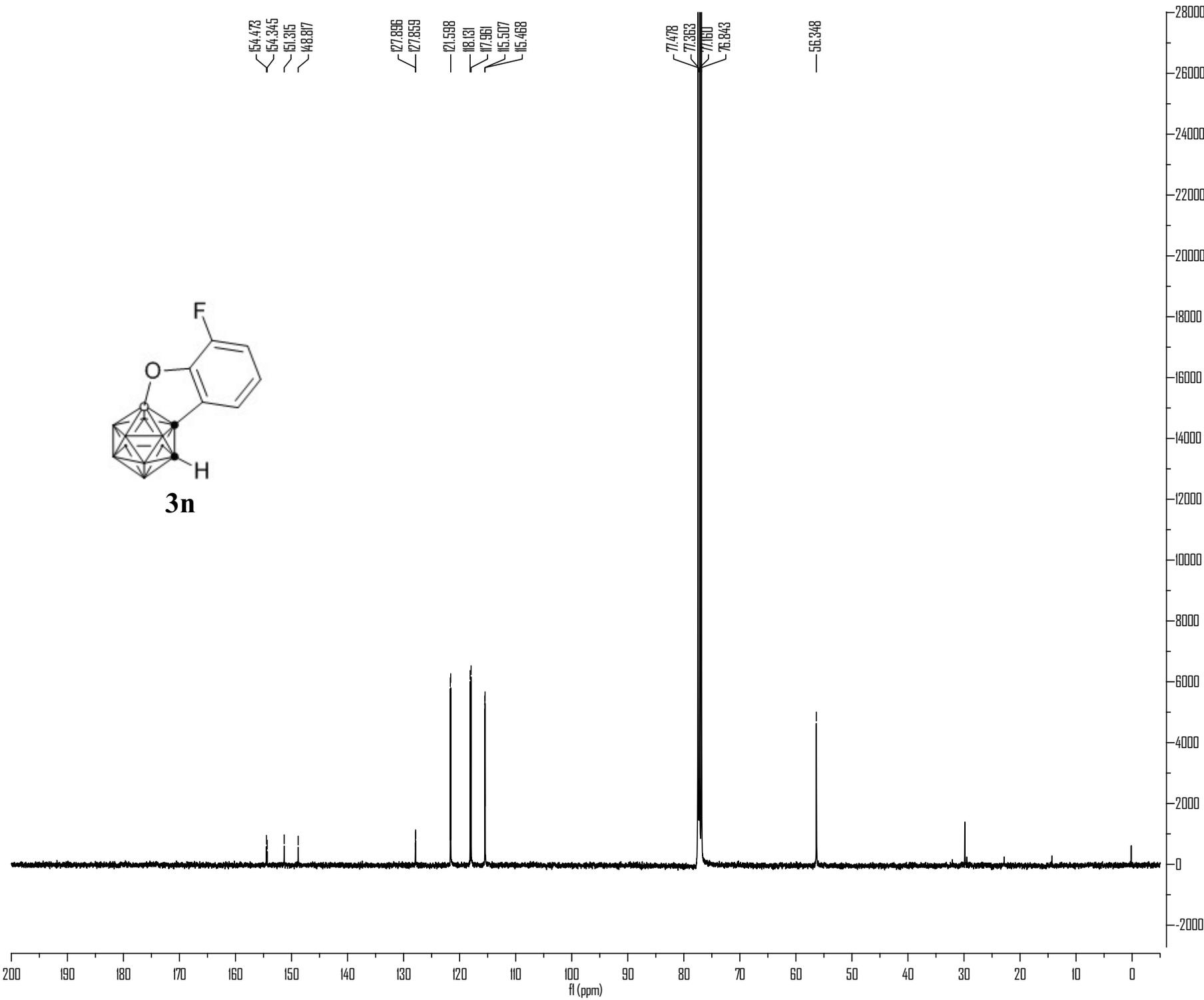


2n

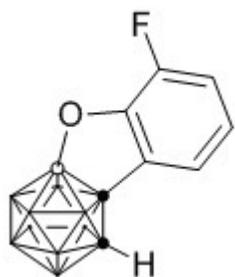
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



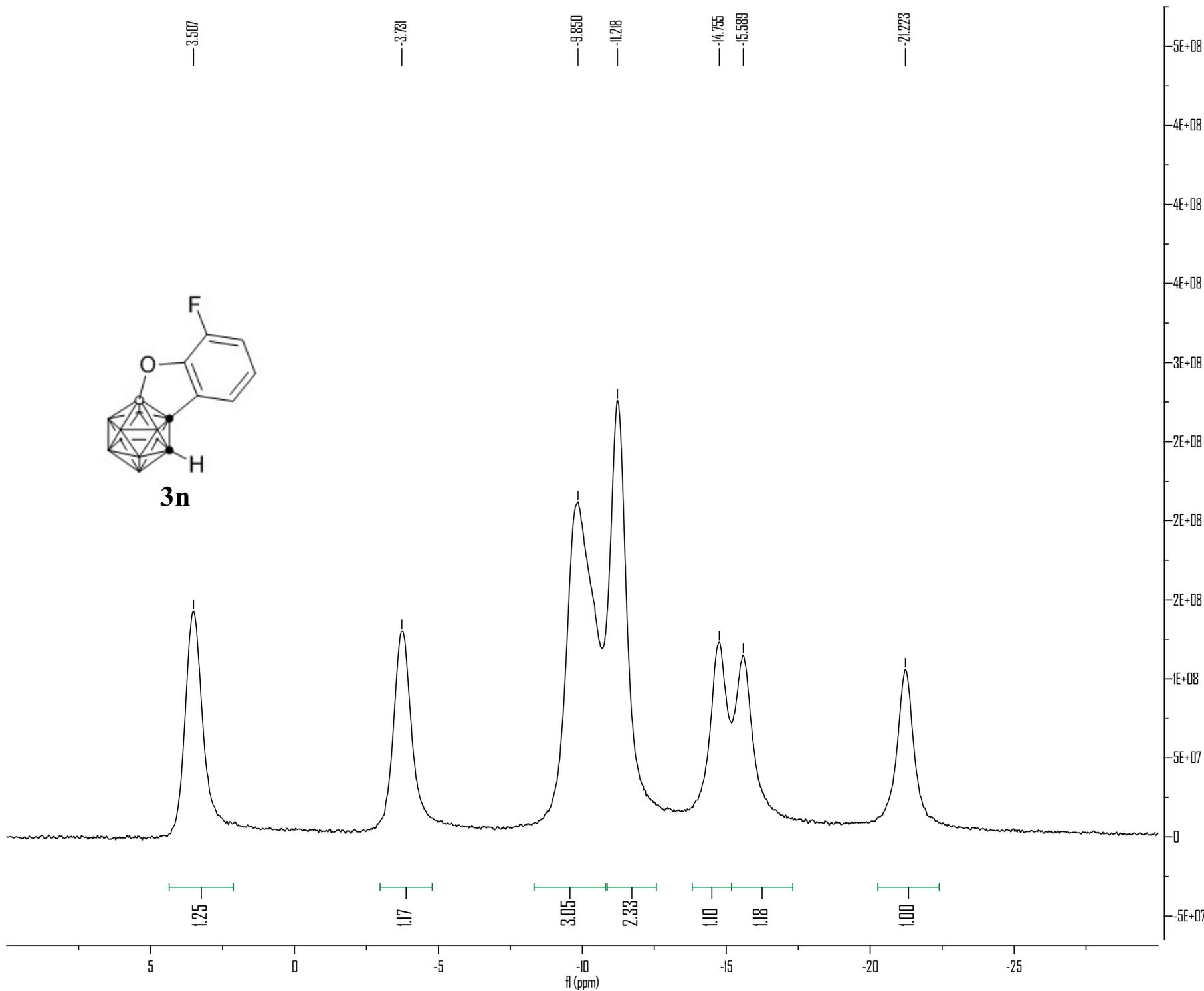
Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/7-24-b/ccx-7-24-b-H fid/ fid
Title	ccx-7-24-b-H
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	48
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-02-27T21:44:02
Modification Date	2017-02-27T13:45:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-793.0
Nucleus	¹ H
Acquired Size	21552
Spectral Size	65536



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-24-b/ccx-7-24-b-c.fid/ fid
Title	ccx-7-24-b-c
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	omcl
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	14496
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Acquisition Date	2017-02-27T21:47:28
Modification Date	2017-02-27T23:06:00
Spectrometer Frequency	100.52
Spectral Width	25000.0
Lowest Frequency	-1428.9
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

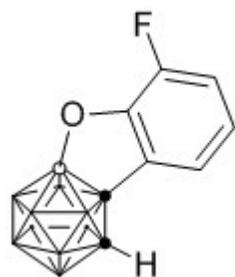


3n

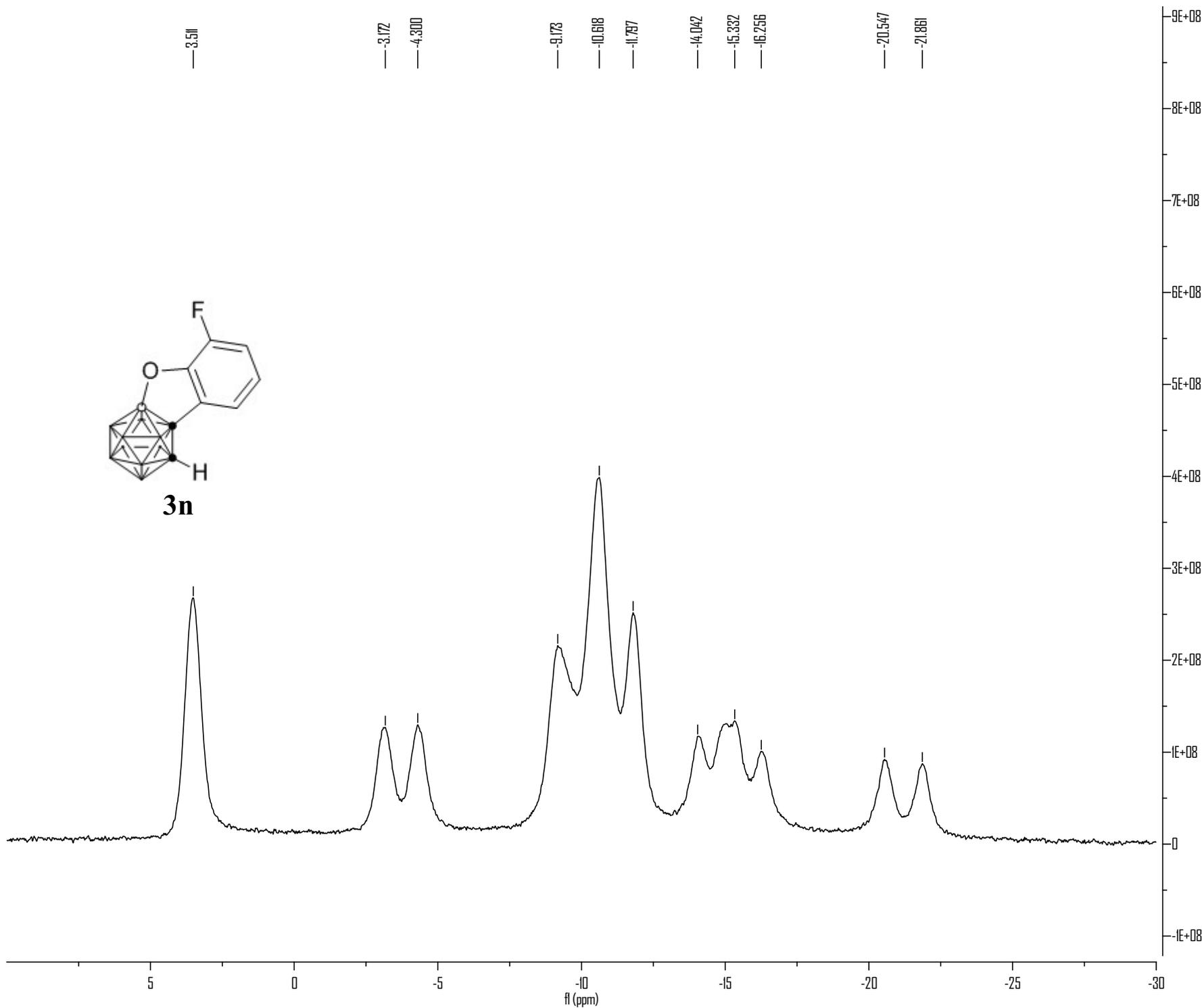


S207

Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-24-b/2012060b-ccx-7-24-2-1-0105/1/pdata/1/1r
Title	2012060b-ccx-7-24-2-1-0105
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	63
Receiver Gain	256
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-01-05T20:39:14
Modification Date	2017-01-06T07:57:38
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16396.1
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

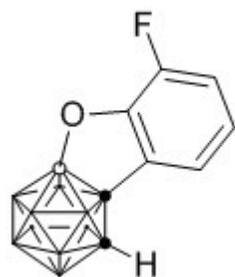


3n



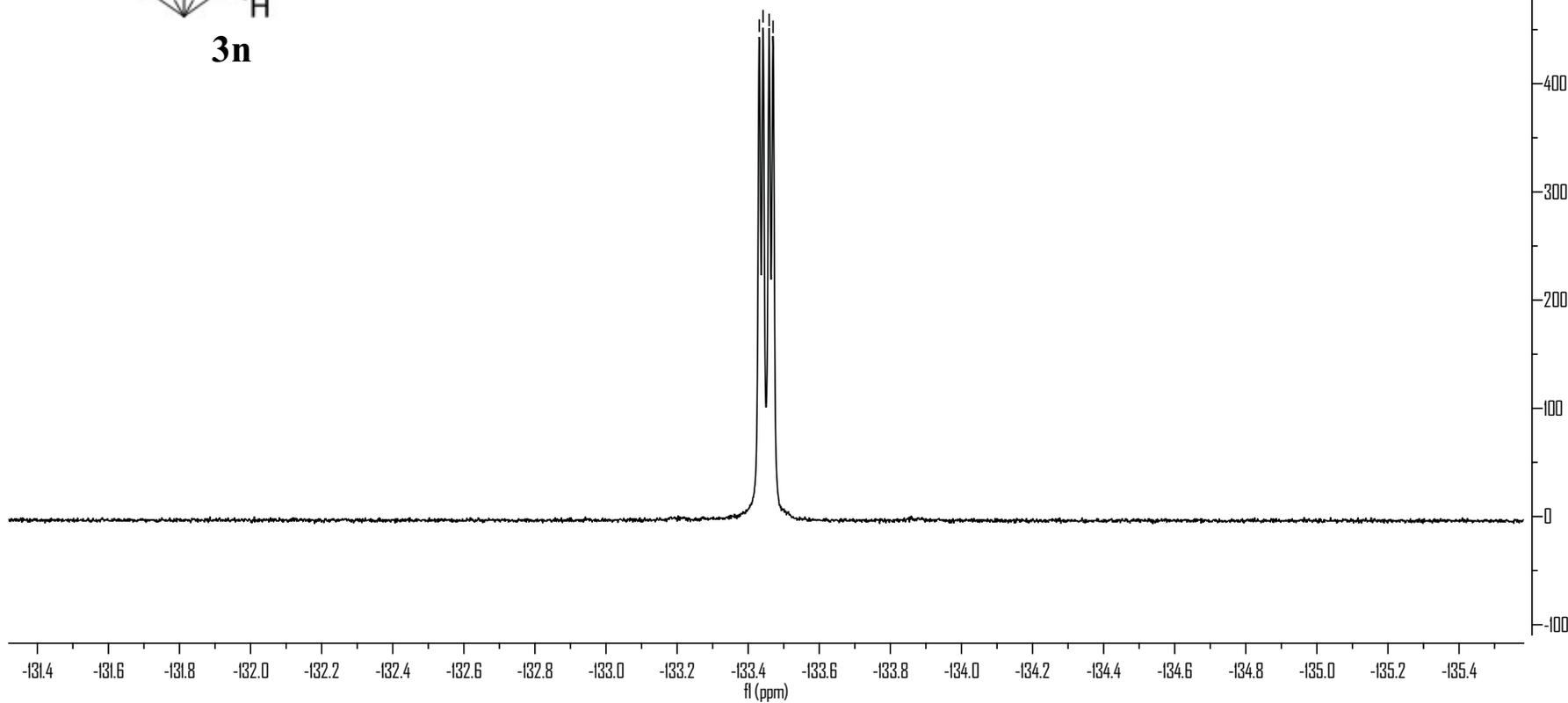
S208

Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-24-b/2012060b-ccx-7-24-2-1-0105-coupling/1/pdata/1/1r
Title	2012060b-ccx-7-24-2-1-0105-coupling
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	77
Receiver Gain	256
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-01-05T20:40:18
Modification Date	2017-01-06T07:57:30
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-12696.1
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



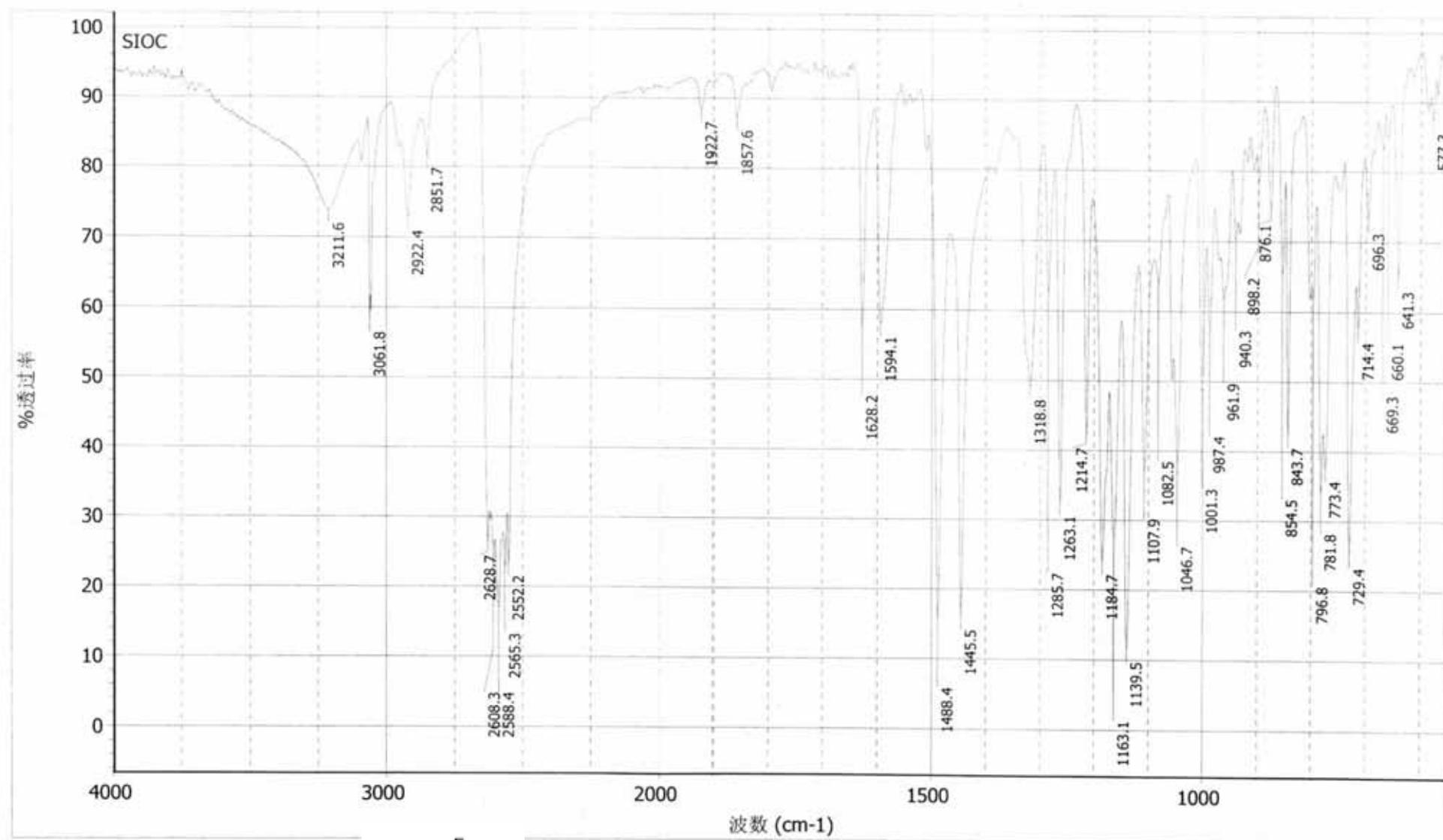
3n

-133.431
 -133.442
 -133.459
 -133.470

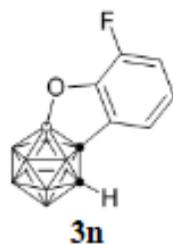


S209

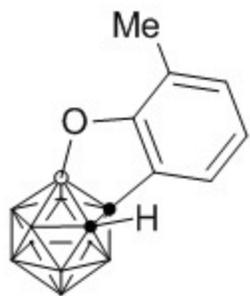
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-24-b/ccx-7-24-b-fid/fid
Title	ccx-7-24-b-F
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	omcl
Solvent	CDCl ₃
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	20
Receiver Gain	48
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	1.3631
Acquisition Date	2017-02-27T21:45:37
Modification Date	2017-02-27T13:47:00
Spectrometer	376.08
Frequency	
Spectral Width	96153.8
Lowest Frequency	-77752.2
Nucleus	13C
Acquired Size	131072
Spectral Size	262144



CCX-7-24-b 2015806 JS



样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



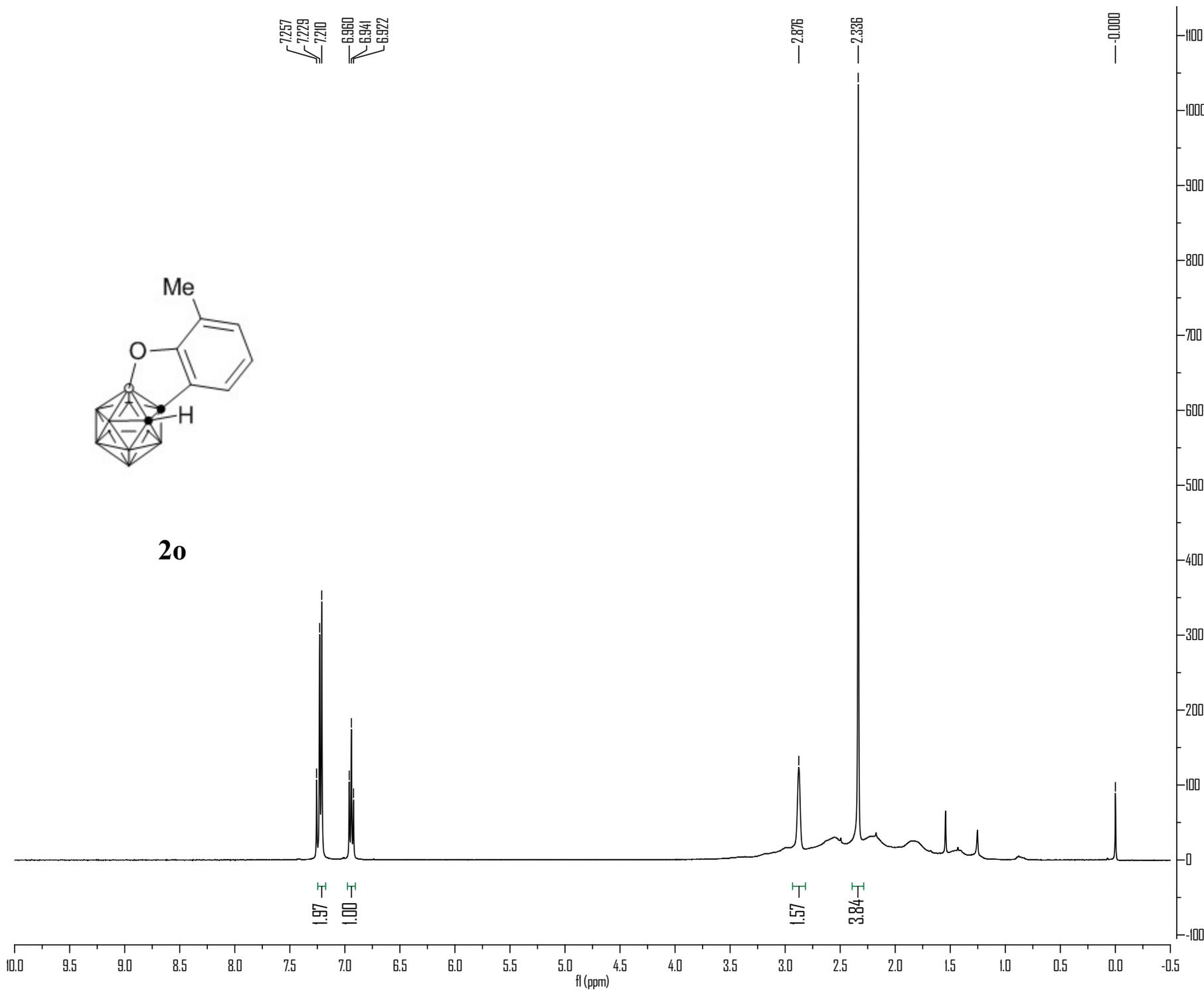
2o

7.257
7.229
7.210
6.960
6.941
6.922

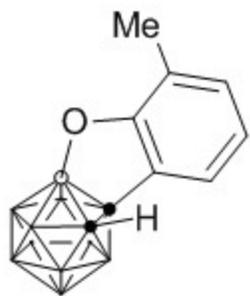
2.876

2.386

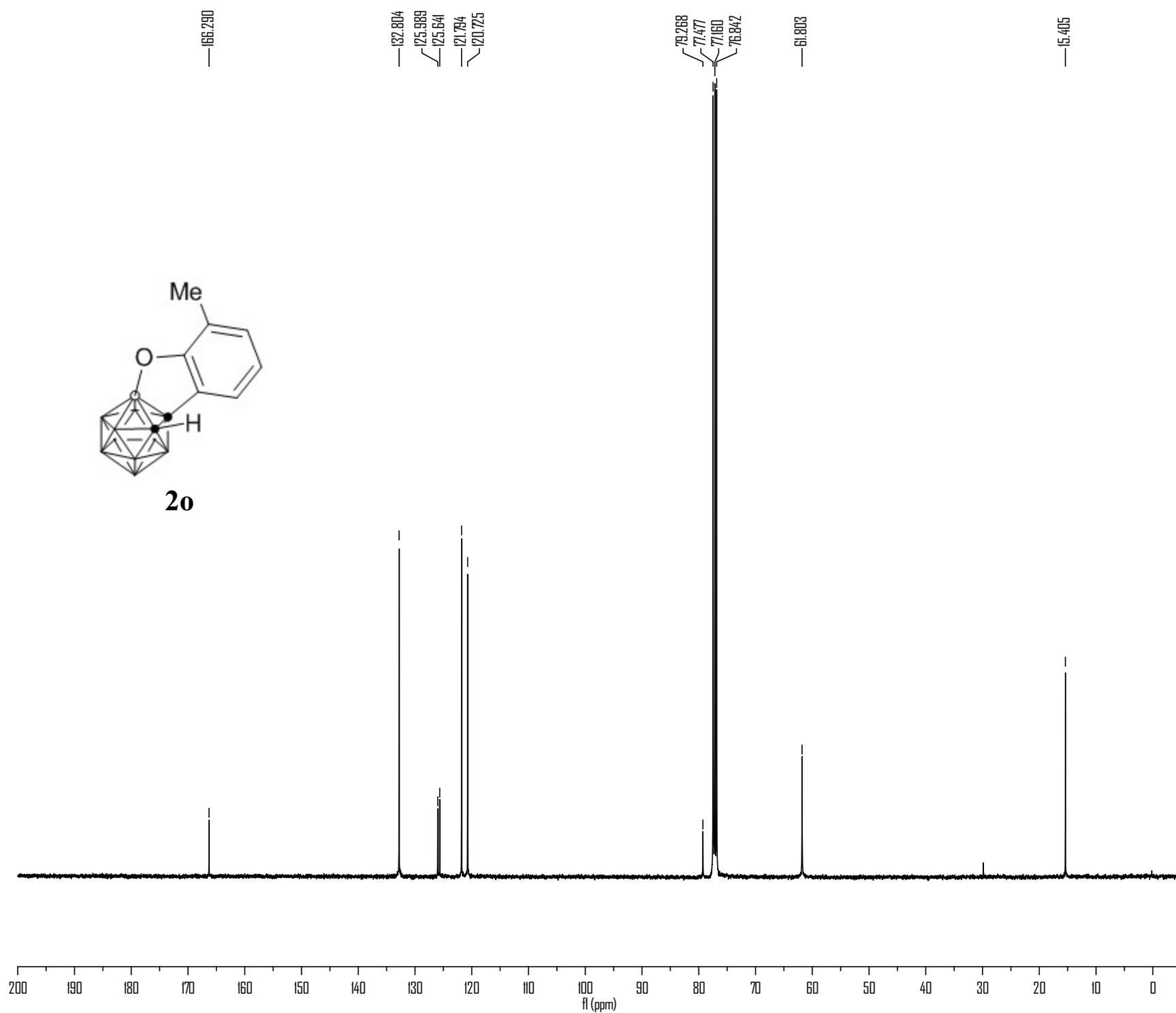
0.000



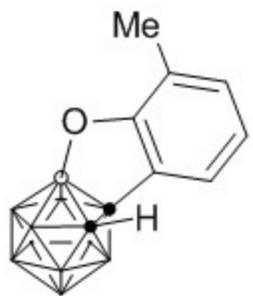
Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/7-42-a/ccx-7-42-a.fid/fid
Title	ccx-7-42-a
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-01-13T21:47:17
Modification Date	2017-01-13T13:48:00
Spectrometer Frequency	400.03
Spectral Width	7225.4
Lowest Frequency	-806.1
Nucleus	1H
Acquired Size	21676
Spectral Size	65536



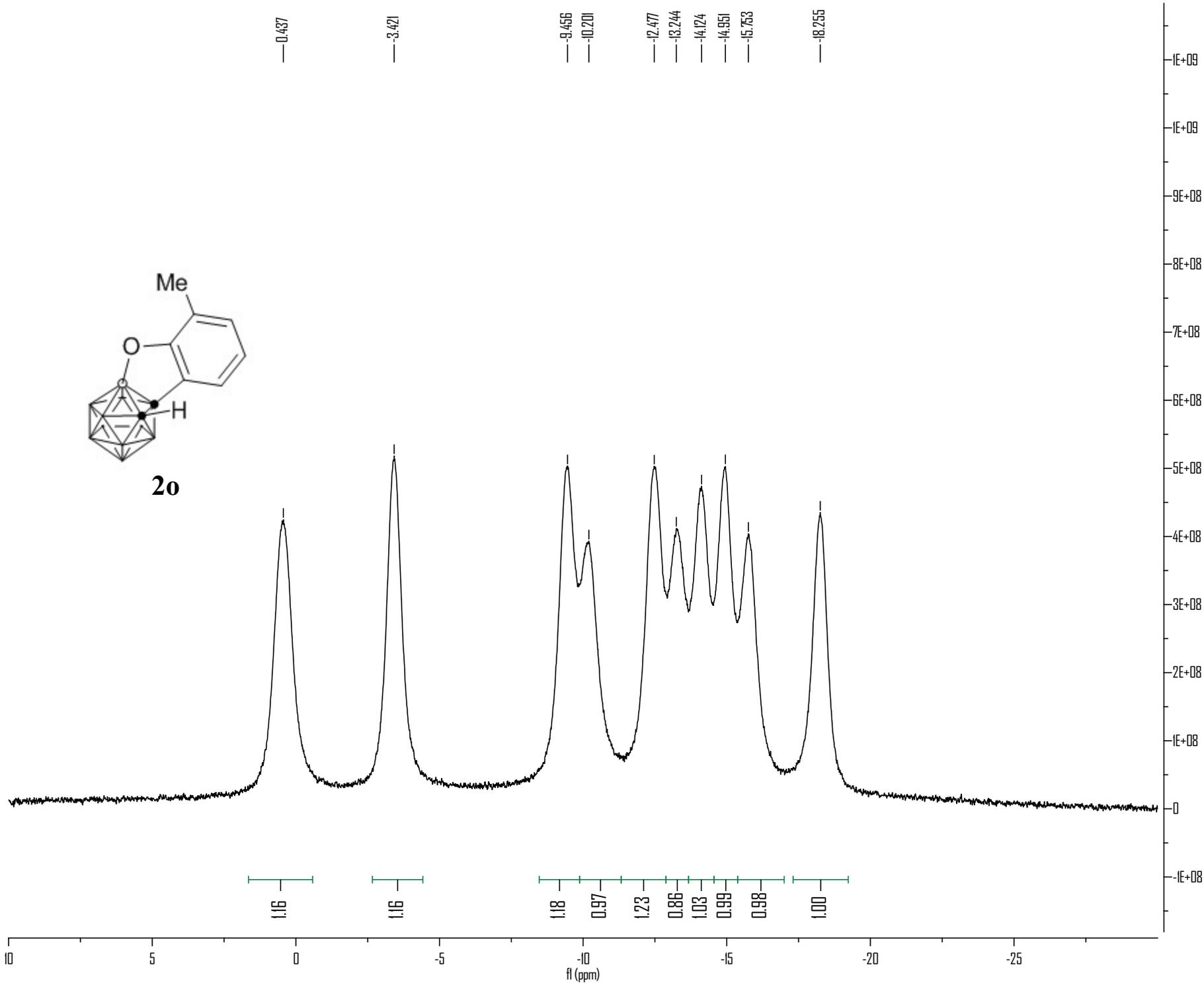
20



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-42-a/ccx-7-42-a-C.fid/fid
Title	ccx-7-42-a-C
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	12268
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-01-16T23:30:27
Modification Date	2017-01-16T23:21:00
Spectrometer Frequency	100.60
Spectral Width	24509.8
Lowest Frequency	-1676.2
Nucleus	¹³ C
Acquired Size	31875
Spectral Size	65536

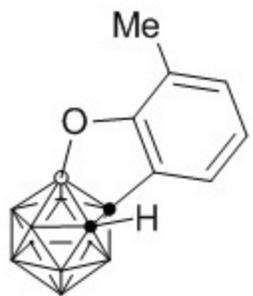


20

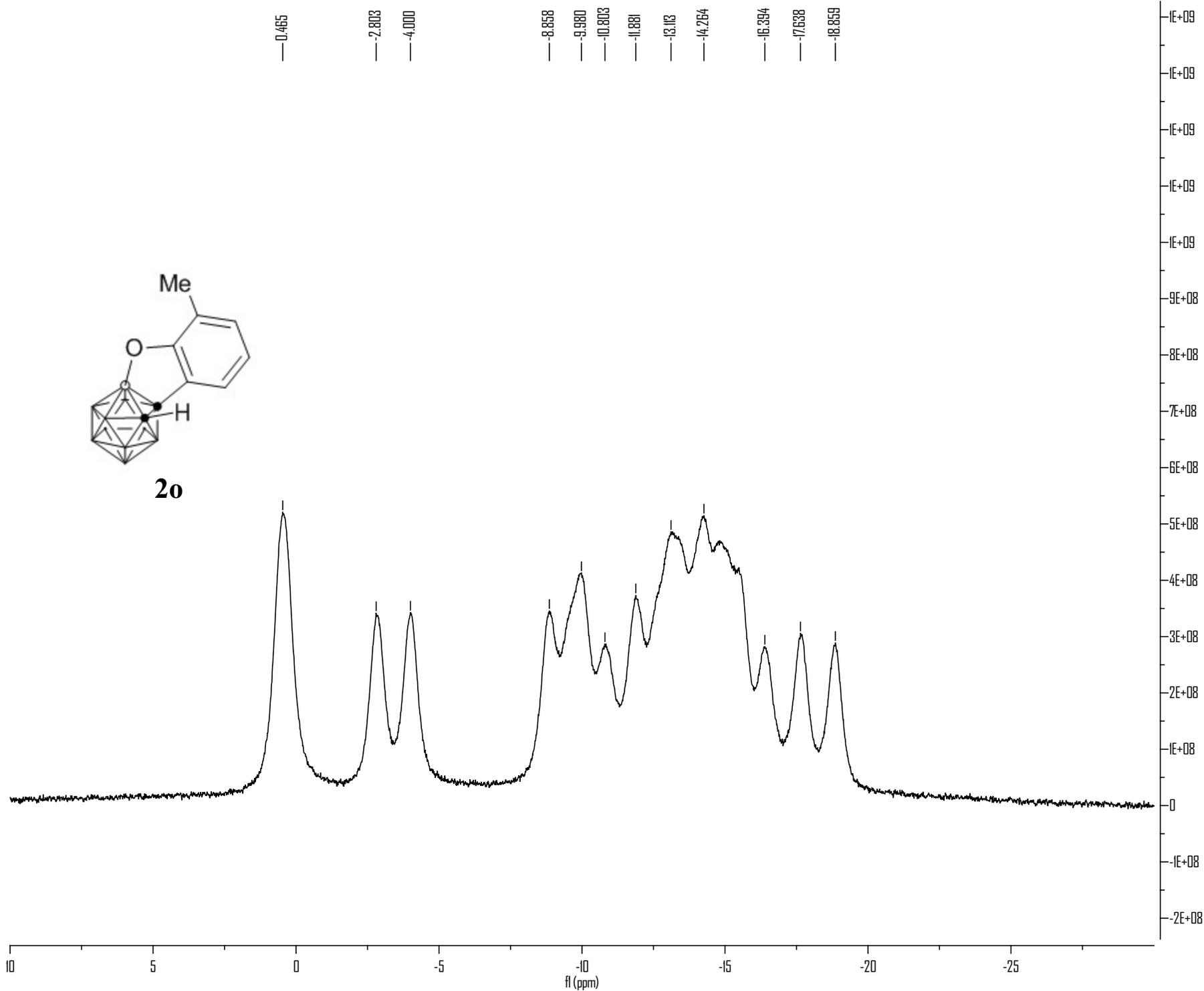


S213

Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/7-42-a/2012060b-ccx-7-42-a/1/pdata/1/1r
Title	2012060b-ccx-7-42-a
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	52
Receiver Gain	181
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-01-16T19:43:22
Modification Date	2017-01-16T13:53:56
Spectrometer	128.38
Frequency	
Spectral Width	32051.3
Lowest Frequency	-16399.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

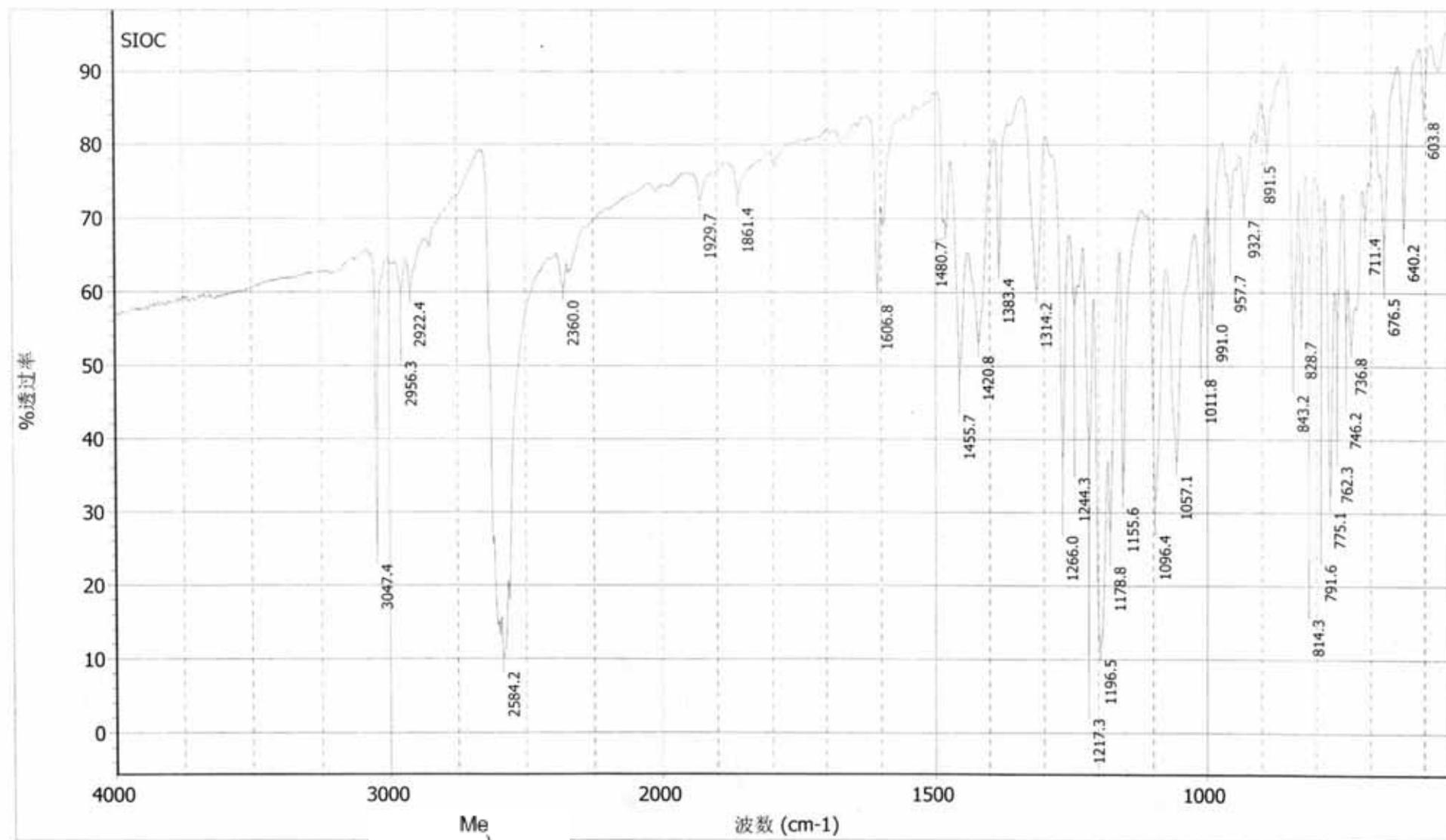


20

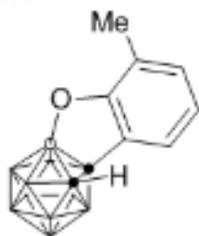


S214

Parameter	Value
Data file Name	C:\Users\Administrator\Desktop/产物数据/7-42-a/2012060b-ccx-7-42-a-coupling/1/pdata/1/1r
Title	2012060b-ccx-7-42-a-coupling
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	58
Receiver Gain	362
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-01-16 11:46:33
Modification Date	2017-01-16 11:53:52
Spectrometer	128.38
Frequency	
Spectral Width	32051.3
Lowest Frequency	-16399.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

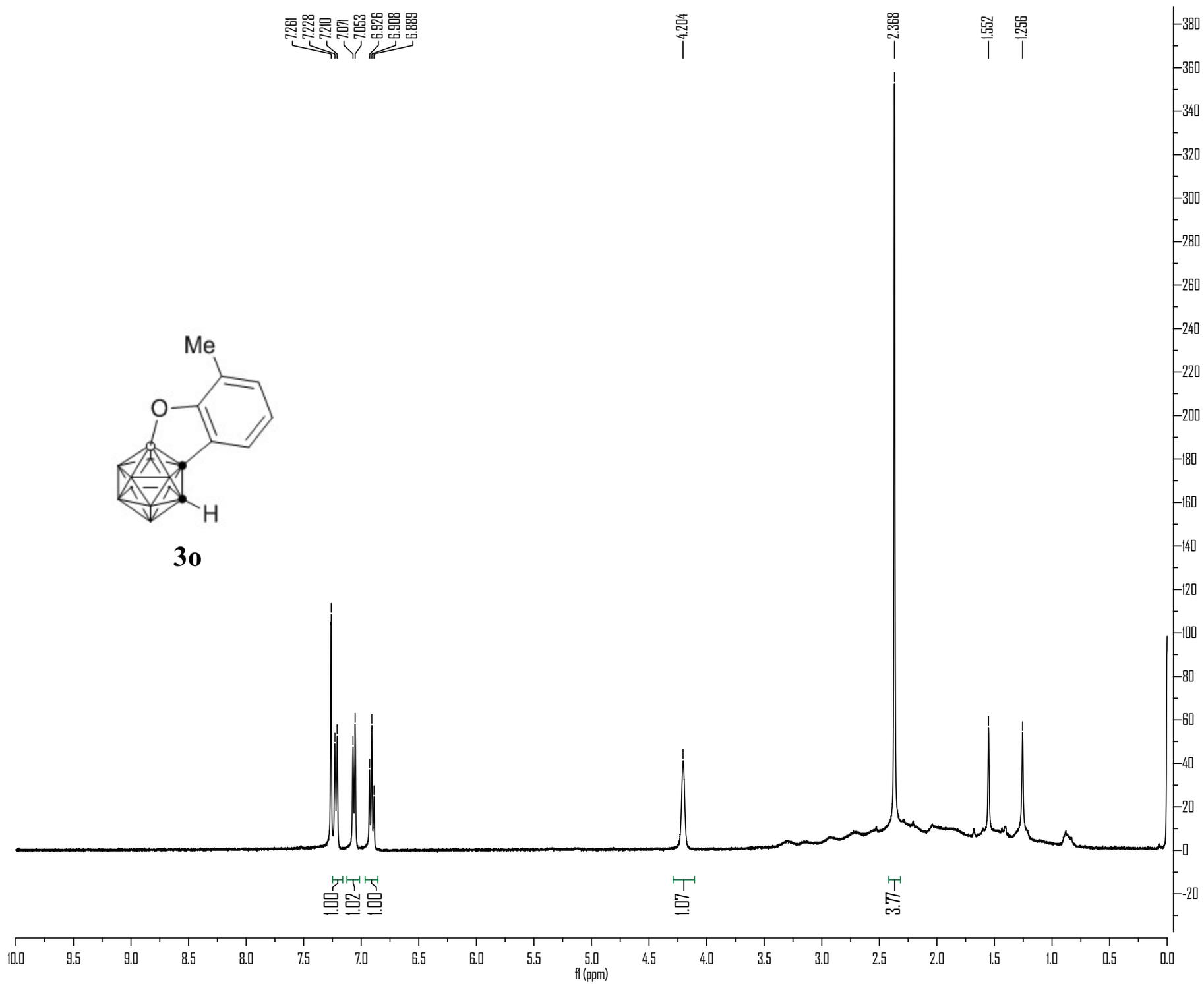


CCX-7-42-a 2015806 JS



2o

样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-42-b/ccx-7-42-b.fid/ fid
Title	ccx-7-42-b
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-01-13T21:49:37
Modification Date	2017-01-13T13:50:00
Spectrometer Frequency	400.03
Spectral Width	7225.4
Lowest Frequency	-803.7
Nucleus	1H
Acquired Size	21676
Spectral Size	65536

165.915

132.115

125.884

124.586

120.723

117.219

78.398

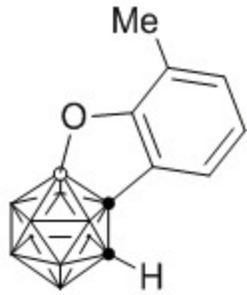
77.478

77.160

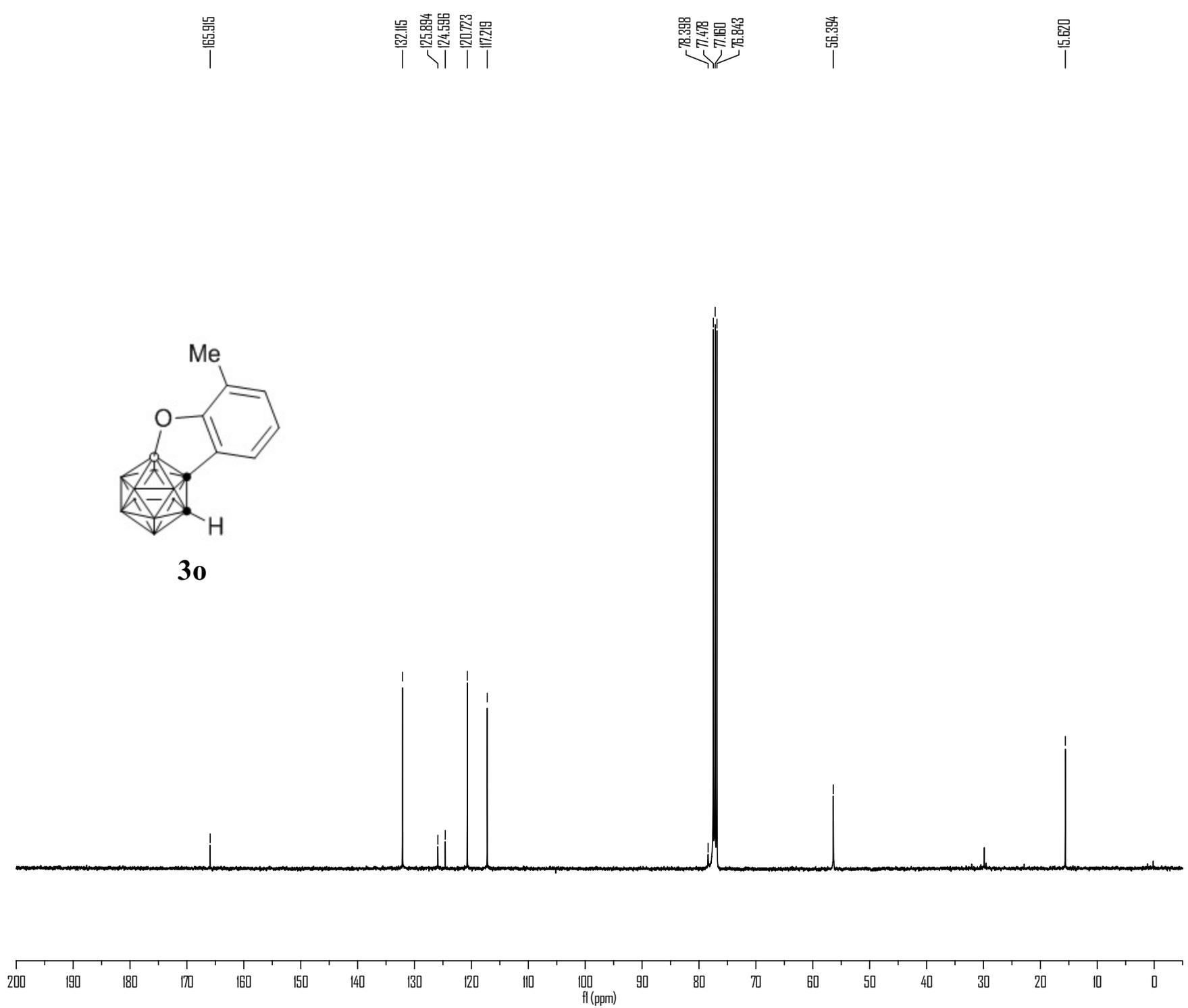
76.843

56.394

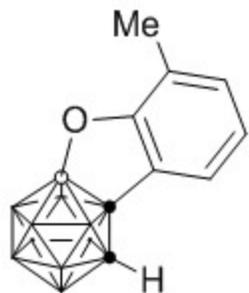
15.620



3o



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-42-b/ccx-7-49-b-c.fid/fid
Title	ccx-7-49-b-c
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	13520
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-02-16T21:48:47
Modification Date	2017-02-16T22:28:00
Spectrometer Frequency	100.60
Spectral Width	24509.8
Lowest Frequency	-1676.6
Nucleus	¹³ C
Acquired Size	31875
Spectral Size	65536



30

3.382

-3.983

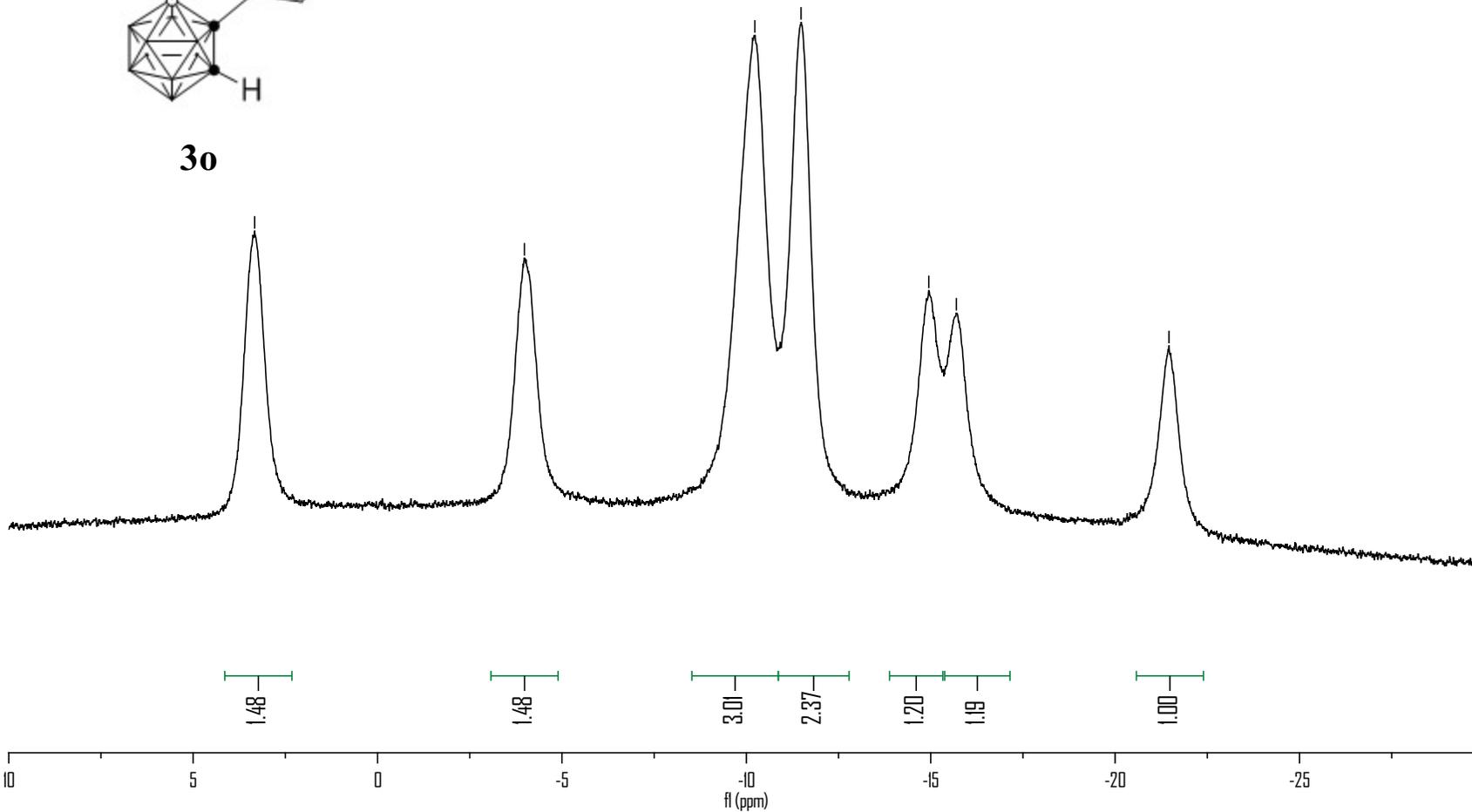
-10.230

-11.483

-14.947

-15.695

-21.460



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-42-b/2012060b-ccx-7-42-b/1/pdata/1/1r
Title	2012060b-ccx-7-42-b
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	1000
Receiver Gain	724
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-01-16T20:17:44
Modification Date	2017-01-16T13:53:40
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16399.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

3.346

3.406

4.644

9.627

10.873

12.074

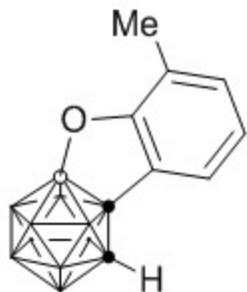
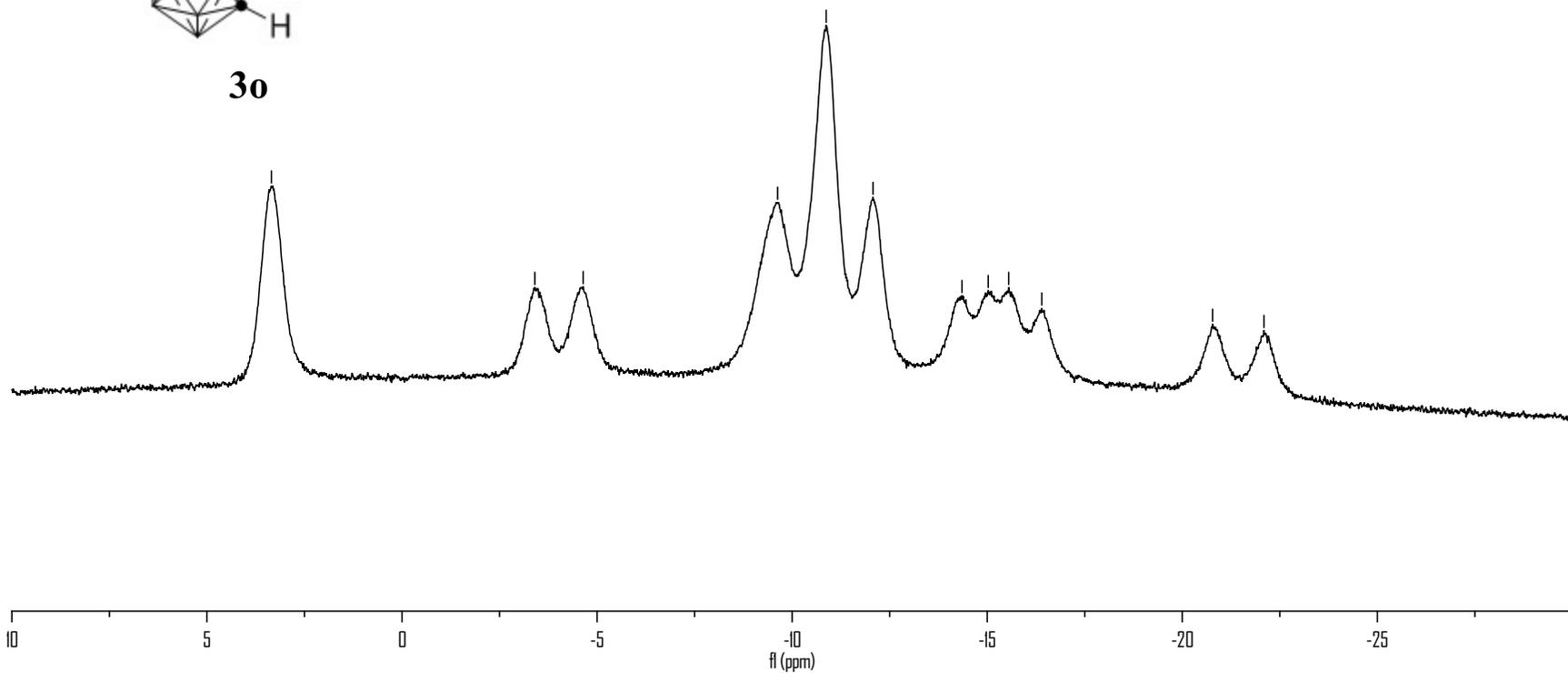
14.354

15.550

16.399

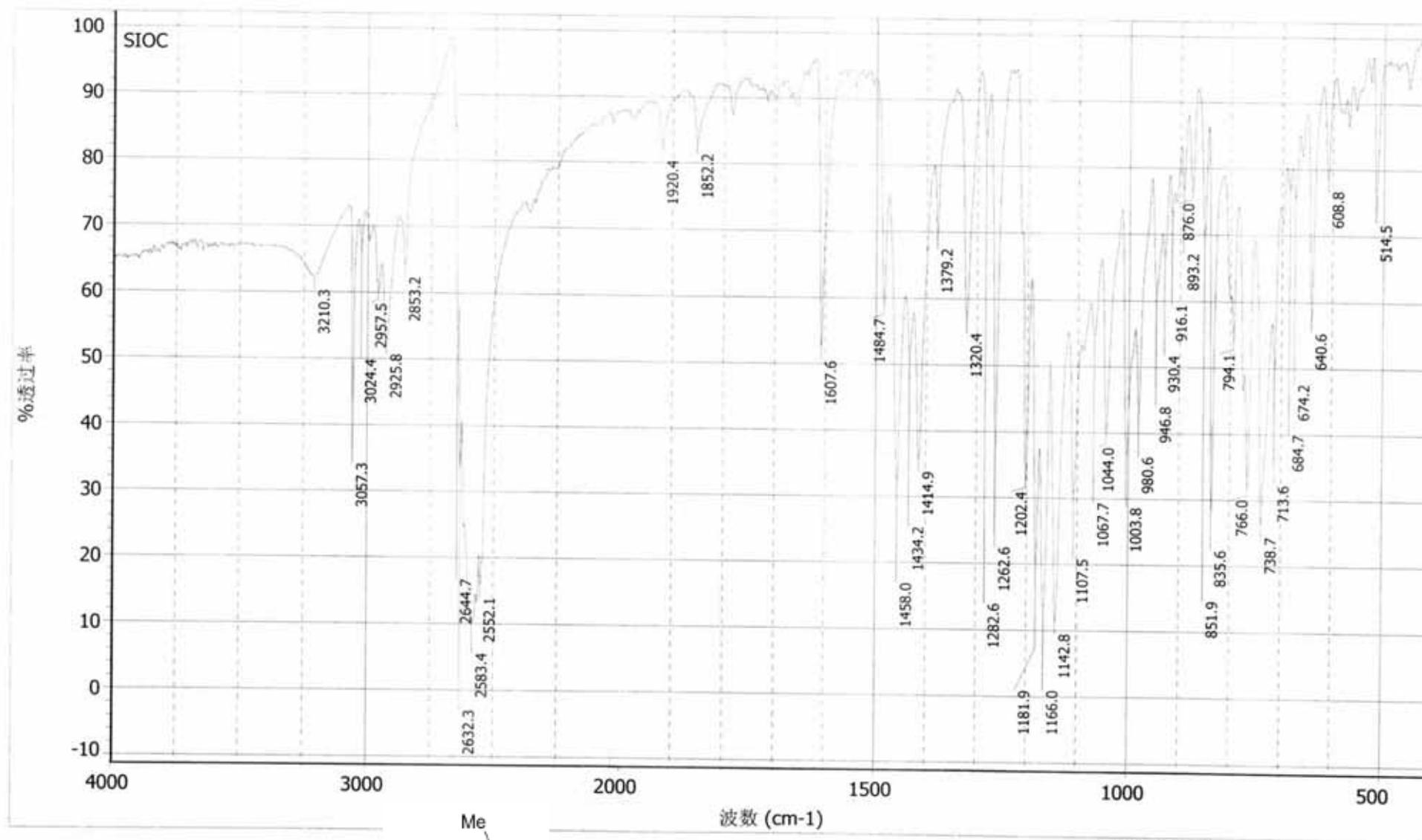
20.777

22.095

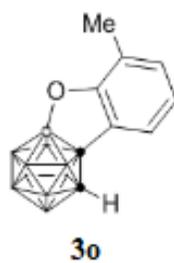
**3o**

S219

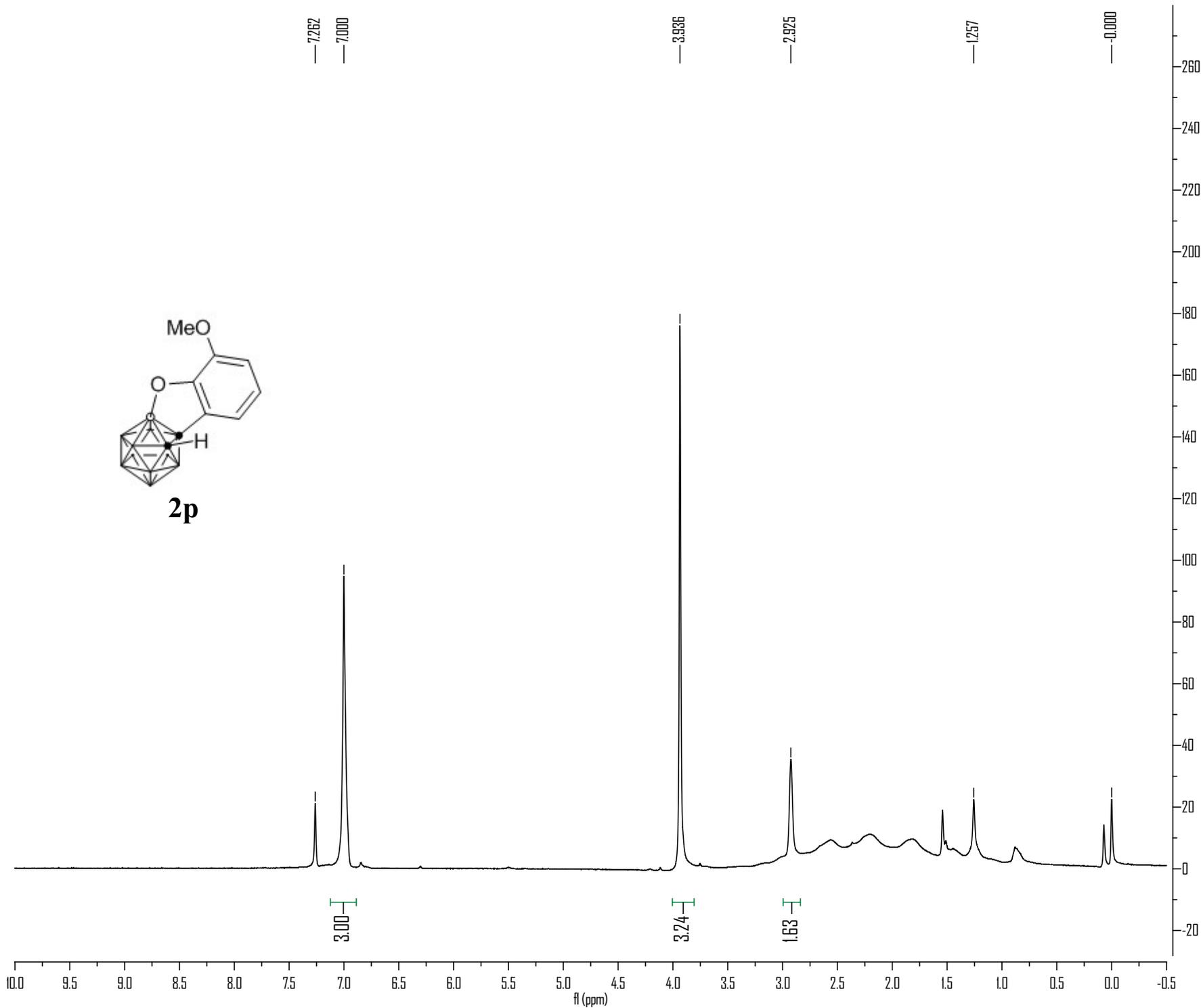
Parameter	Value
Data file Name	G:/Users/Administrator/Desktop/产物数据/7-42-b/2012060b-ccx-7-42-b-coupling/1/pdata/1/1r
Title	2012060b-ccx-7-42-b-coupling
Comment	
Origin	UXNMR Bruker
	Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	629
Receiver Gain	362
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-01-16T20:23:50
Modification Date	2017-01-16T13:53:46
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16399.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



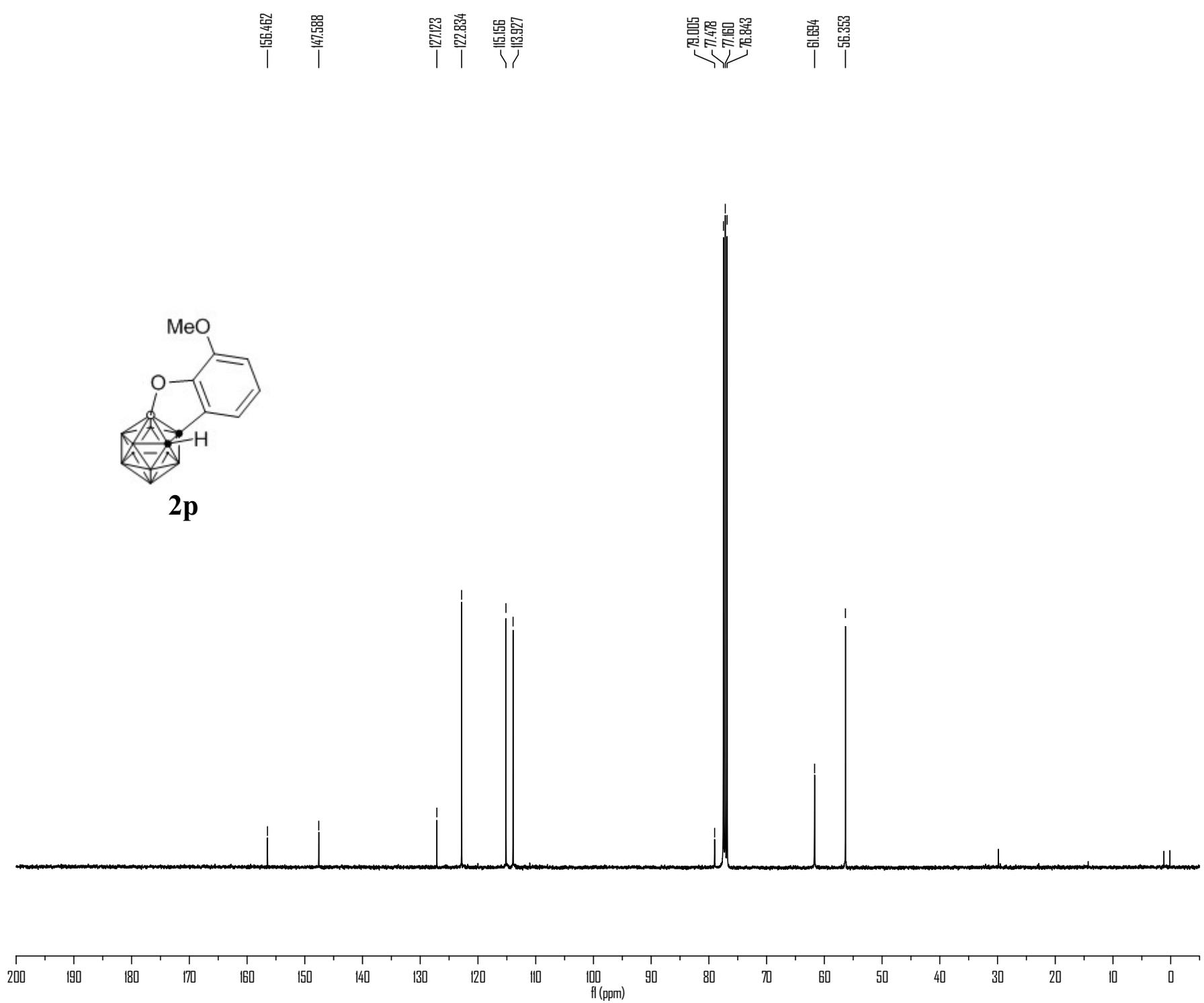
CCX-7-42-B 2015806 JS



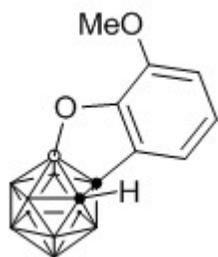
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



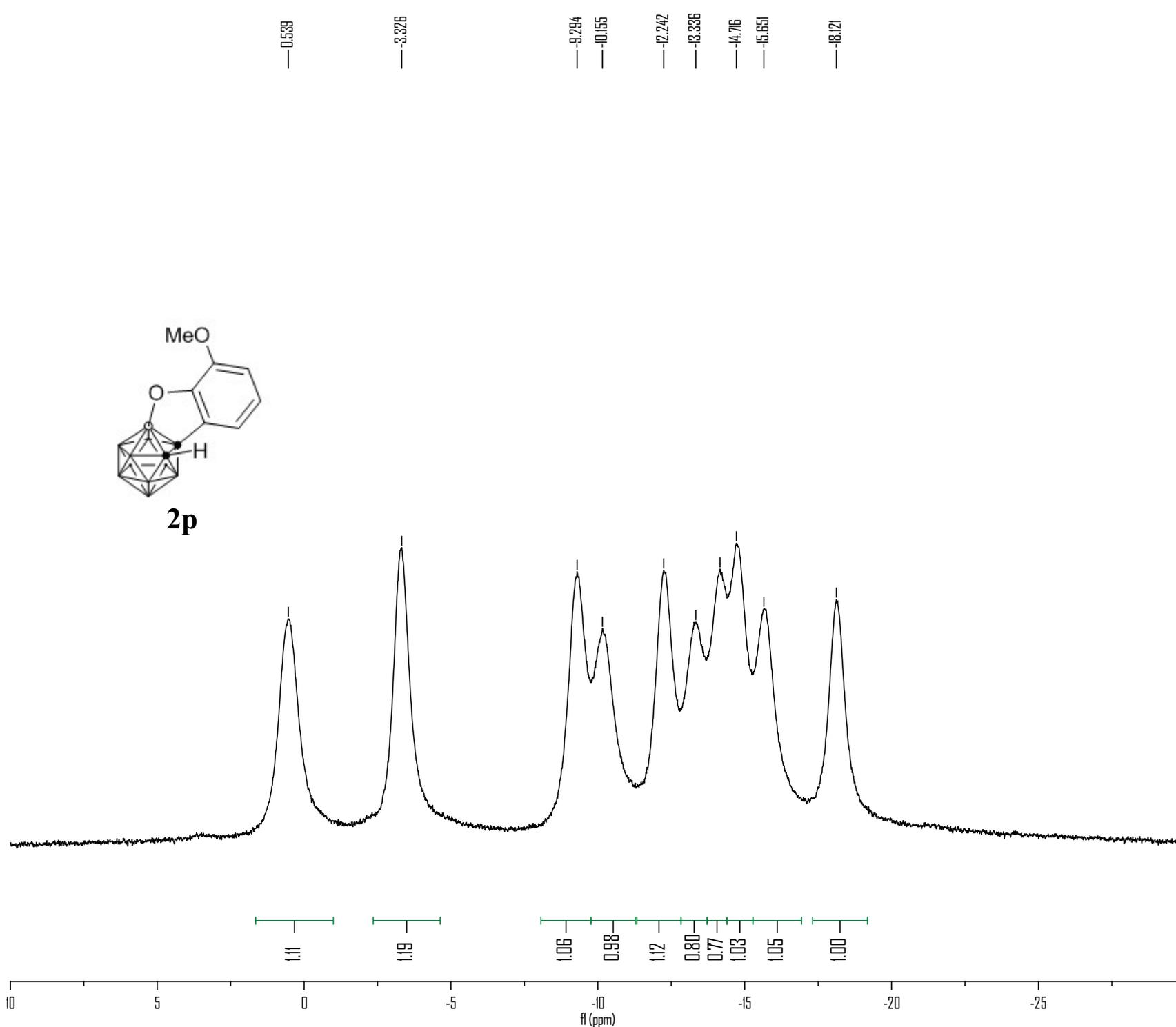
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-36-1/-CCX-7-36-1.fid/fid
Title	-CCX-7-36-1
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	stu
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.2768
Acquisition Date	2016-12-09T09:16:46
Modification Date	2016-12-09T09:17:00
Spectrometer Frequency	399.68
Spectral Width	10000.0
Lowest Frequency	-2002.4
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-36-1/ccx-7-36-1-C.fid/ fid
Title	ccx-7-36-1-C
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	cdcl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	12768
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3000
Acquisition Date	2016-12-12 23:18:15
Modification Date	2016-12-12 23:28:00
Spectrometer Frequency	100.62
Spectral Width	24509.8
Lowest Frequency	-1404.4
Nucleus	¹³ C
Acquired Size	31863
Spectral Size	65536

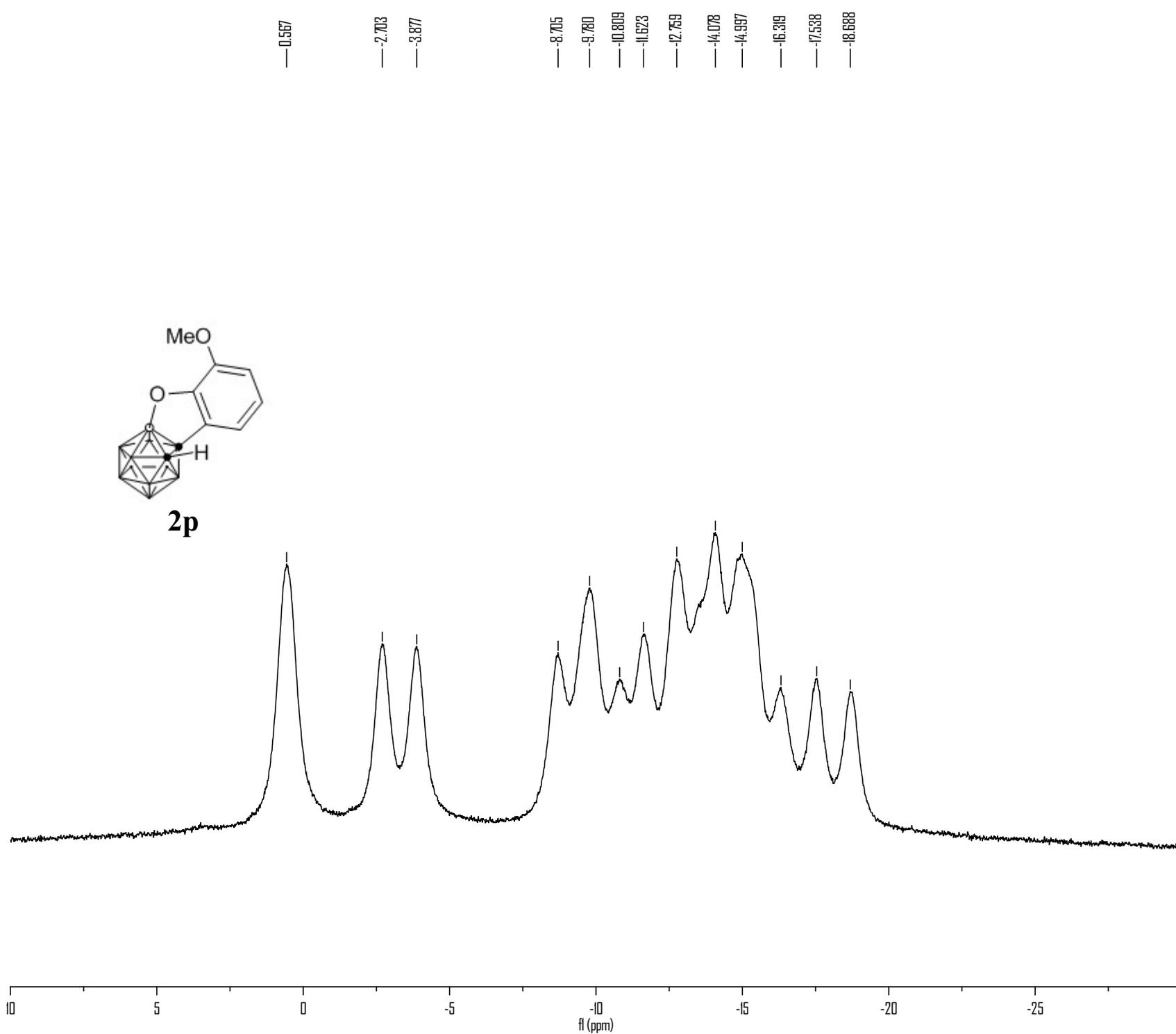


2p

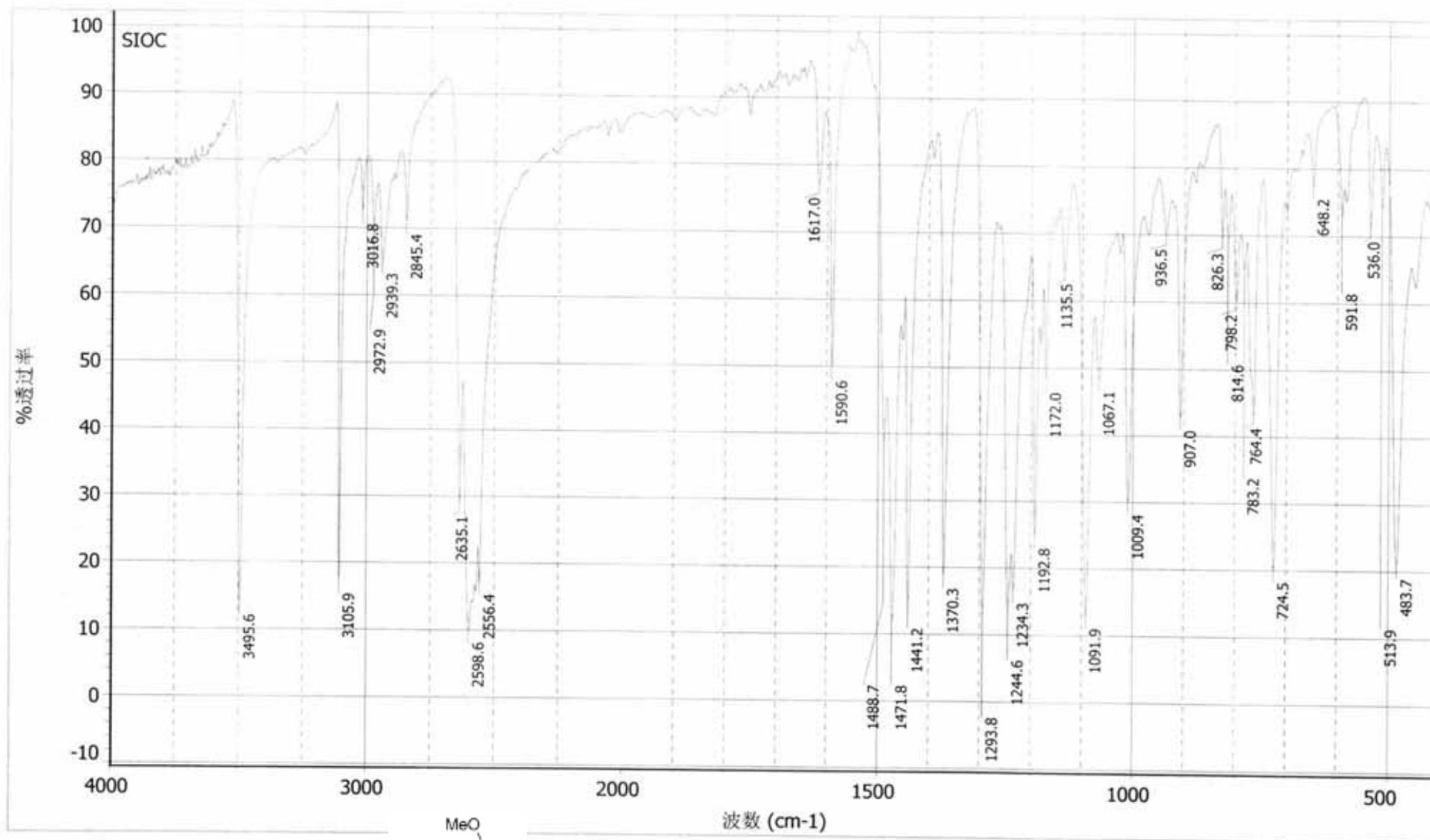


S223

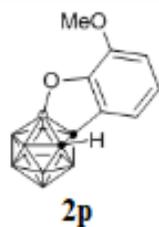
Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/7-36-1/bccx-7-36-1/pdata/1/1r
Title	7-36-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	166
Receiver Gain	228
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2016-12-09T20:59:47
Modification Date	2016-12-09T14:00:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16391.5
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



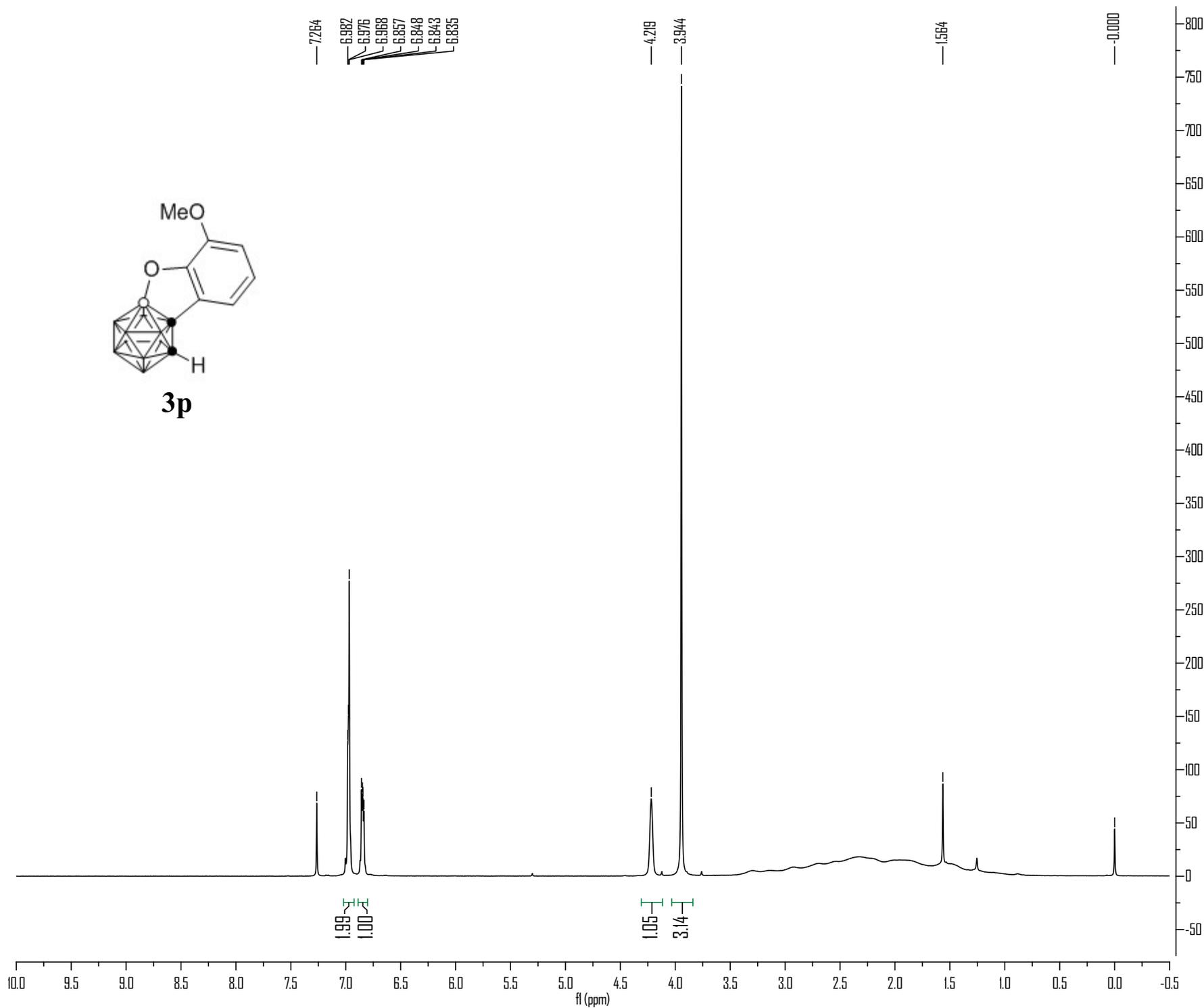
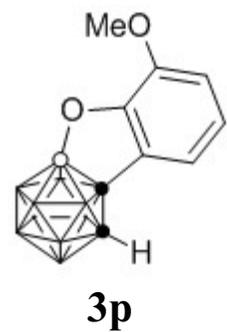
Parameter	Value
Data File Name	E:/Users/Administrator/Desktop/产物数据/7-36-1/b-cx-7-36-1-coupling/pdata/1/1r
Title	7-36-1
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	Acetone
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	256
Receiver Gain	256
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2016-12-09T21:03:25
Modification Date	2016-12-09T14:03:00
Spectrometer	128.38
Frequency	
Spectral Width	32051.3
Lowest Frequency	-16391.5
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



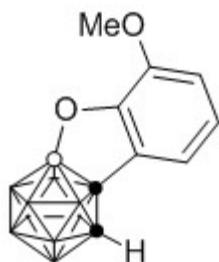
CCX-7-36-1 2015806 JS



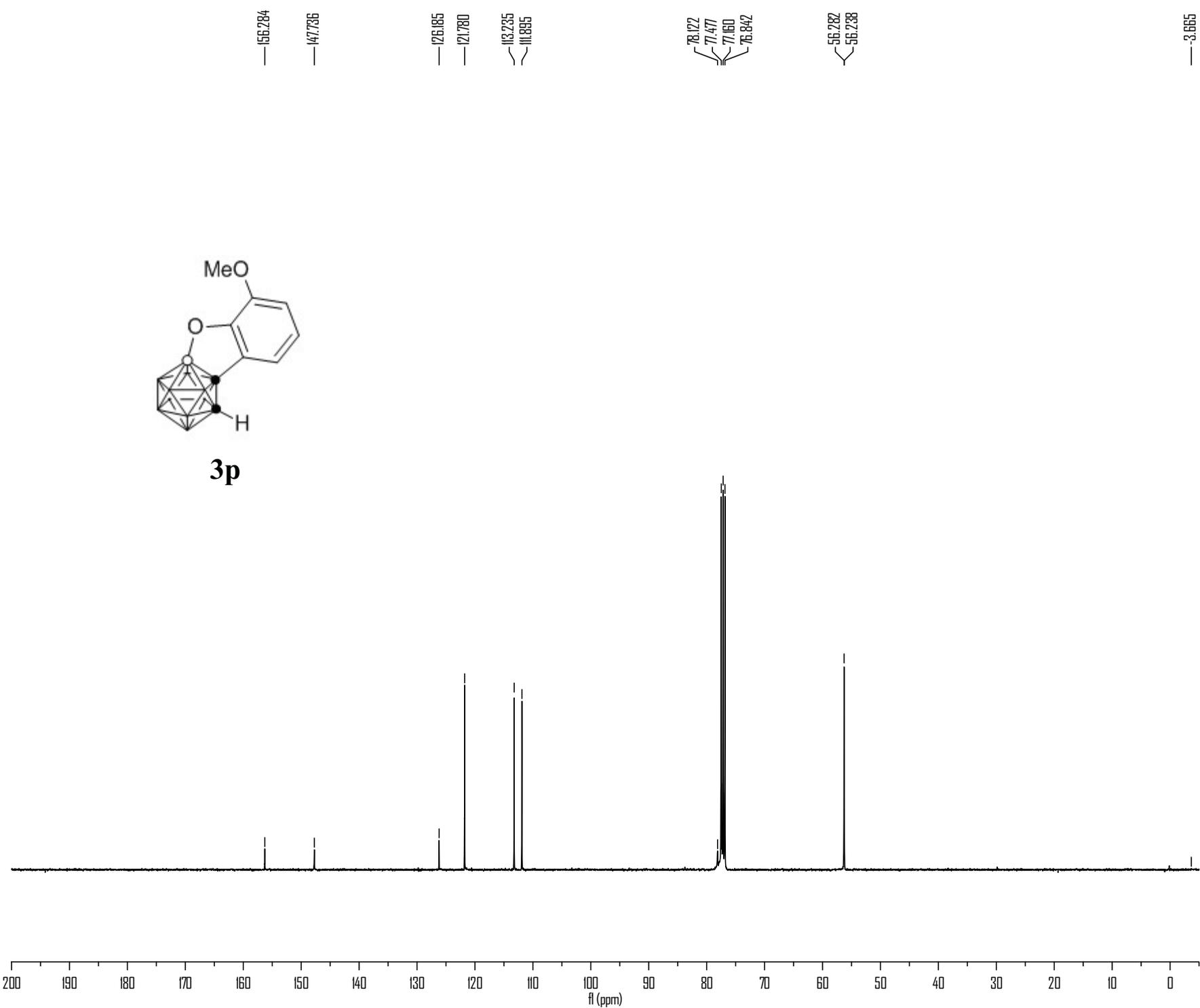
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



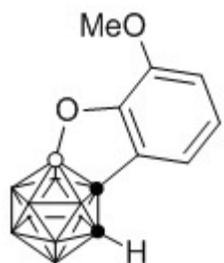
Parameter	Value
Data file Name	ccx-7-45-3-2.fid/ fid
Title	ccx-7-45-3-2
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
A uthor	omcl
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	40
Relaxation Delay	1.0000
Pulse Width	0.0000
A cquisition Time	3.0000
A cquisition Date	2018-12-17T10:15:35
Modification Date	2018-12-17T02:17:00
Spectrometer	399.72
Frequency	
Spectral Width	7575.8
Lowest Frequency	-1188.9
Nucleus	1H
A cquired Size	22727
Spectral Size	65536



3p

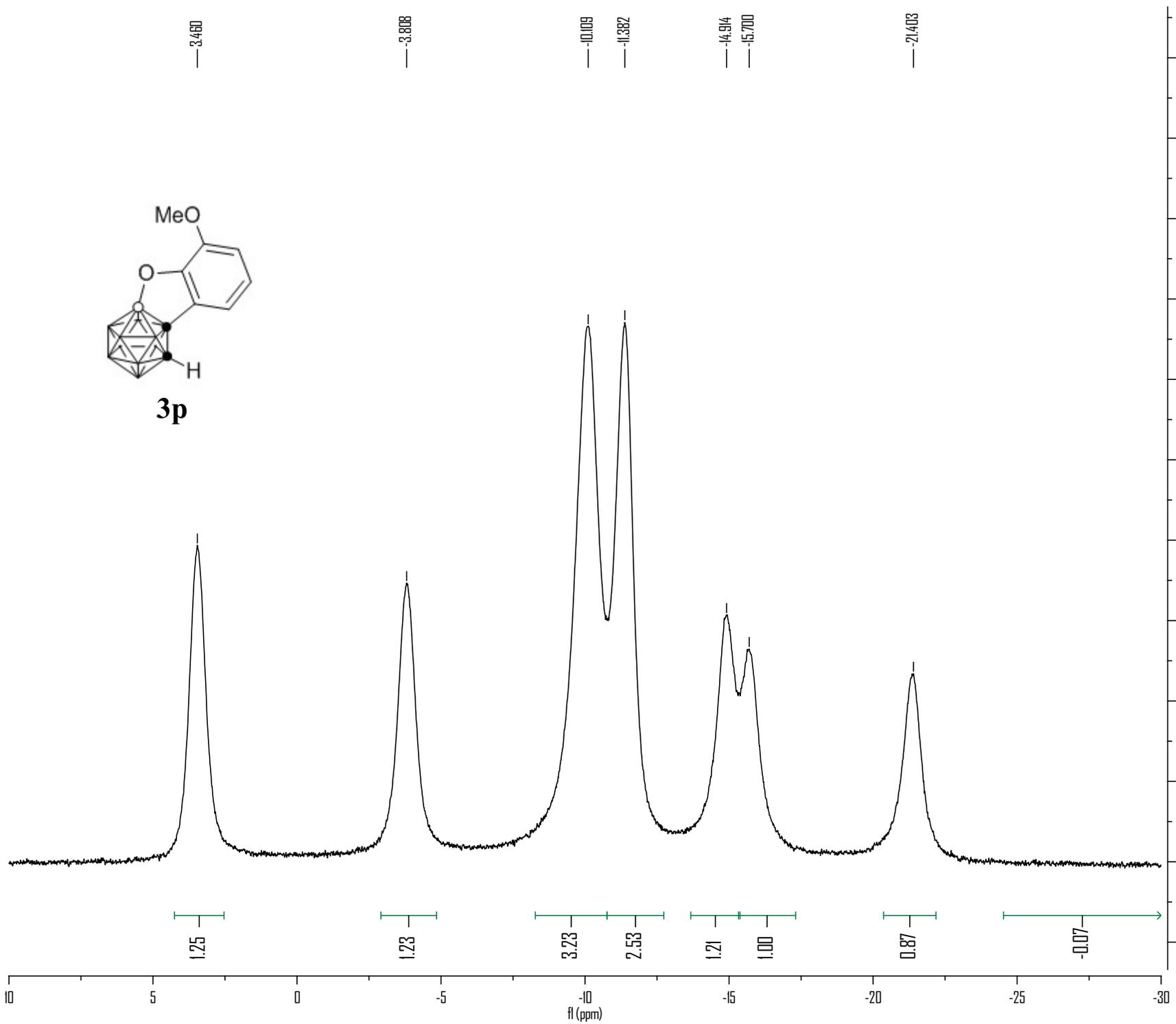


Parameter	Value
Data file Name	2012060cccc-cx-7-45-3-2/ 3/ pdata/ 1/ 1r
Title	2012060cccc-cx-7-45-3-2
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zgdc
Number of Scans	21802
Receiver Gain	32768
Relaxation Delay	2.0000
Pulse Width	4.0000
Acquisition Time	0.9306
Acquisition Date	2018-12-17T23:38:05
Modification Date	2018-12-18T13:34:16
Spectrometer Frequency	100.61
Spectral Width	35211.3
Lowest Frequency	-68663.5
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

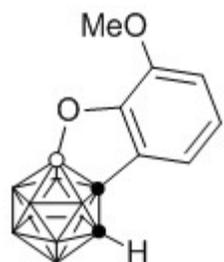


3p

3.460 3.808 10.109 11.882 14.914 15.700 21.408



Parameter	Value
Data File Name	2012060b-ccx-7-45-3-2/1/pdata/1/1r
Title	2012060b-ccx-7-45-3-2
Comment	
Origin	LXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	THF
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	65
Receiver Gain	362
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.4260
Acquisition Date	2018-12-17T21:20:54
Modification Date	2018-12-17T14:23:18
Spectrometer Frequency	128.38
Spectral Width	3848.5
Lowest Frequency	-19606.4
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



3p

3.443

3.266

4.377

9.495

10.750

11.963

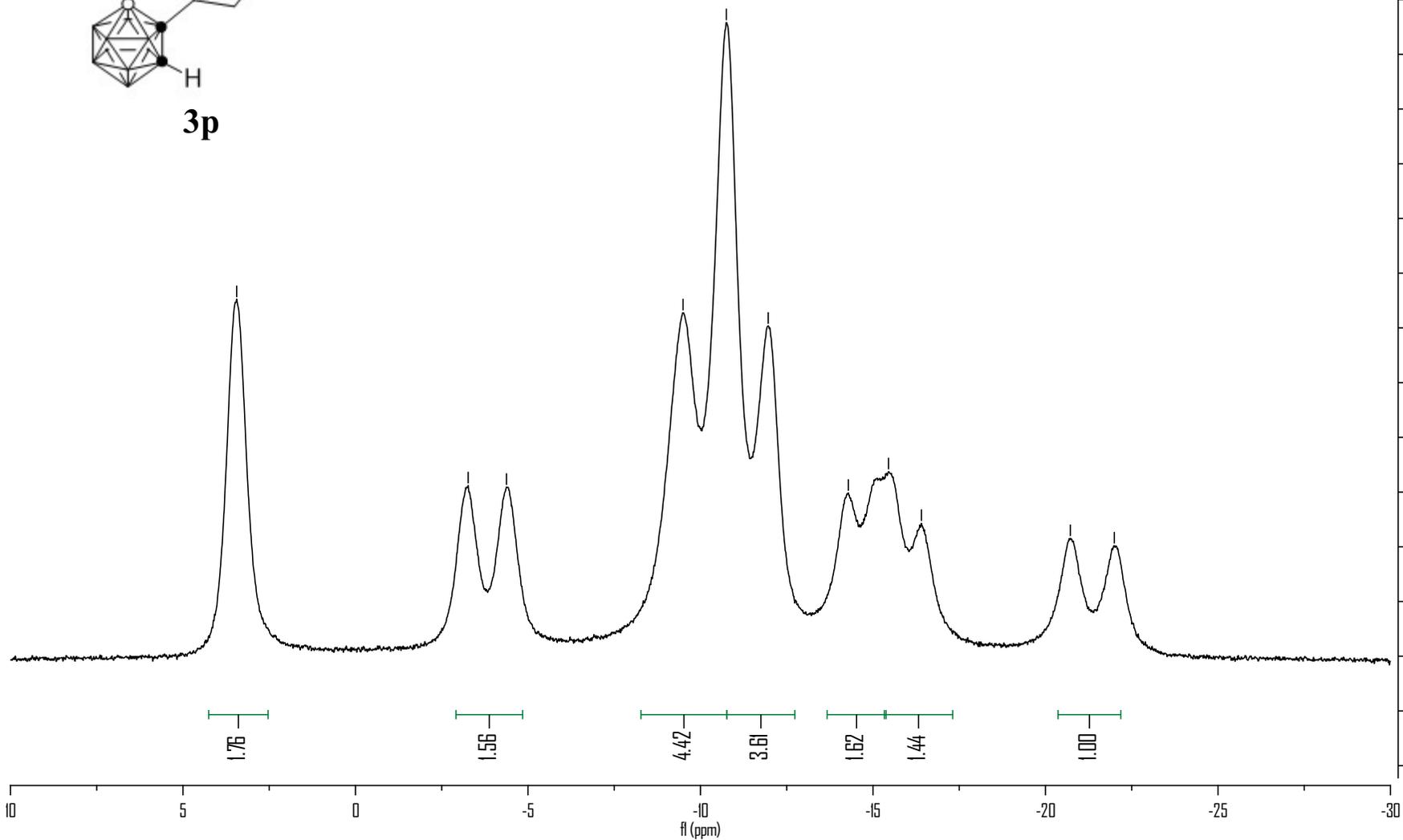
14.286

15.451

16.405

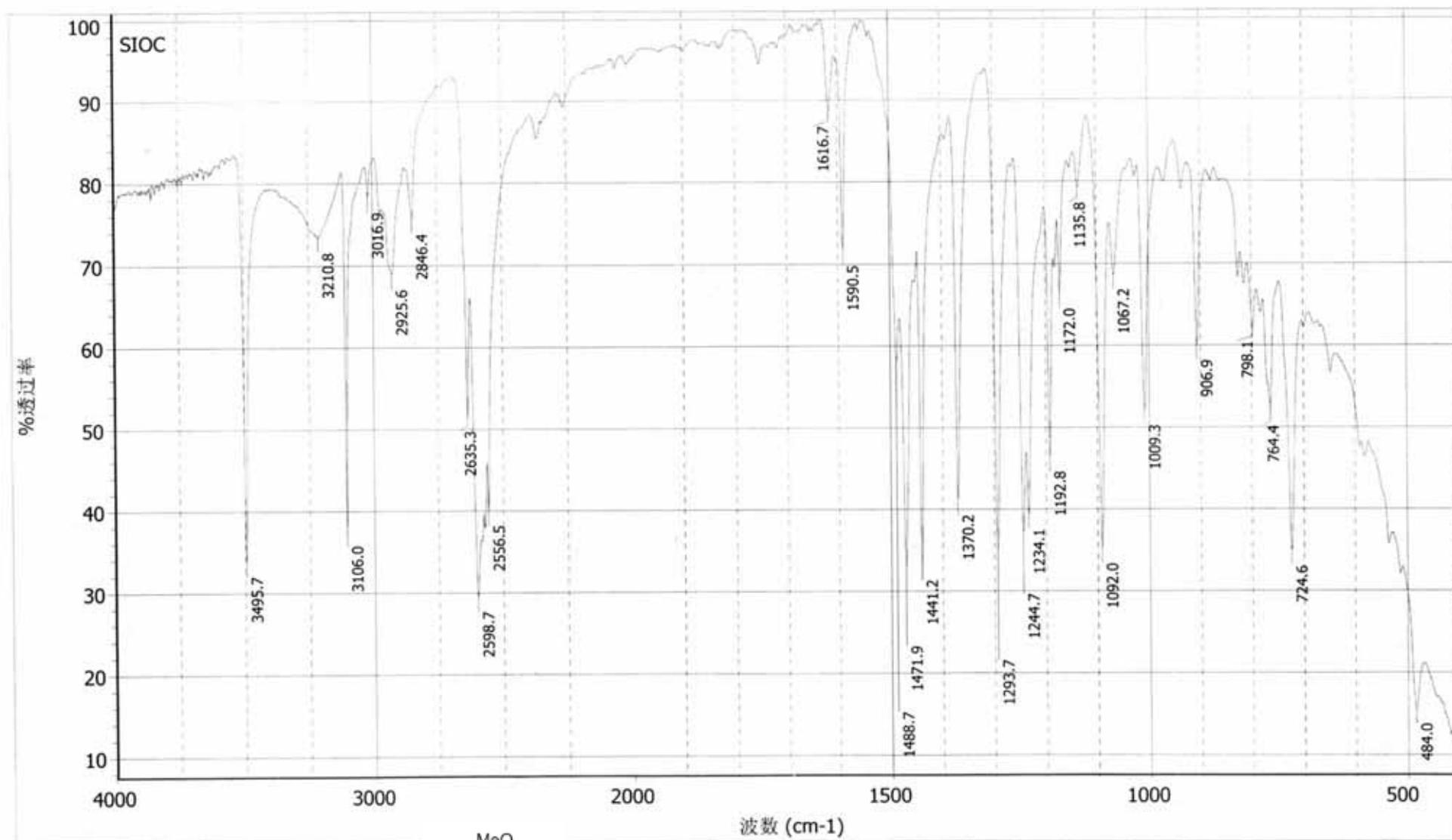
20.772

21.995

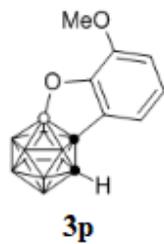


S229

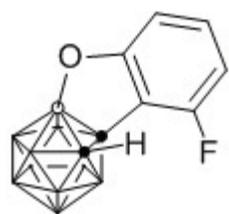
Parameter	Value
Data File Name	2012060b-ccx-7-45-3-2-coupling/1/ pdata/1/1r
Title	2012060b-ccx-7-45-3-2-coupling
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	THF
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	121
Receiver Gain	203
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.4260
Acquisition Date	2018-12-17T21:22:12
Modification Date	2018-12-17T14:23:17
Spectrometer Frequency	128.38
Spectral Width	38461.5
Lowest Frequency	-19606.4
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



CCX-7-36-4 2015806 JS



样品扫描次数: 32
背景扫描次数: 32
分辨率: 4.000
采样增益: 1.0
动镜速度: 0.4747



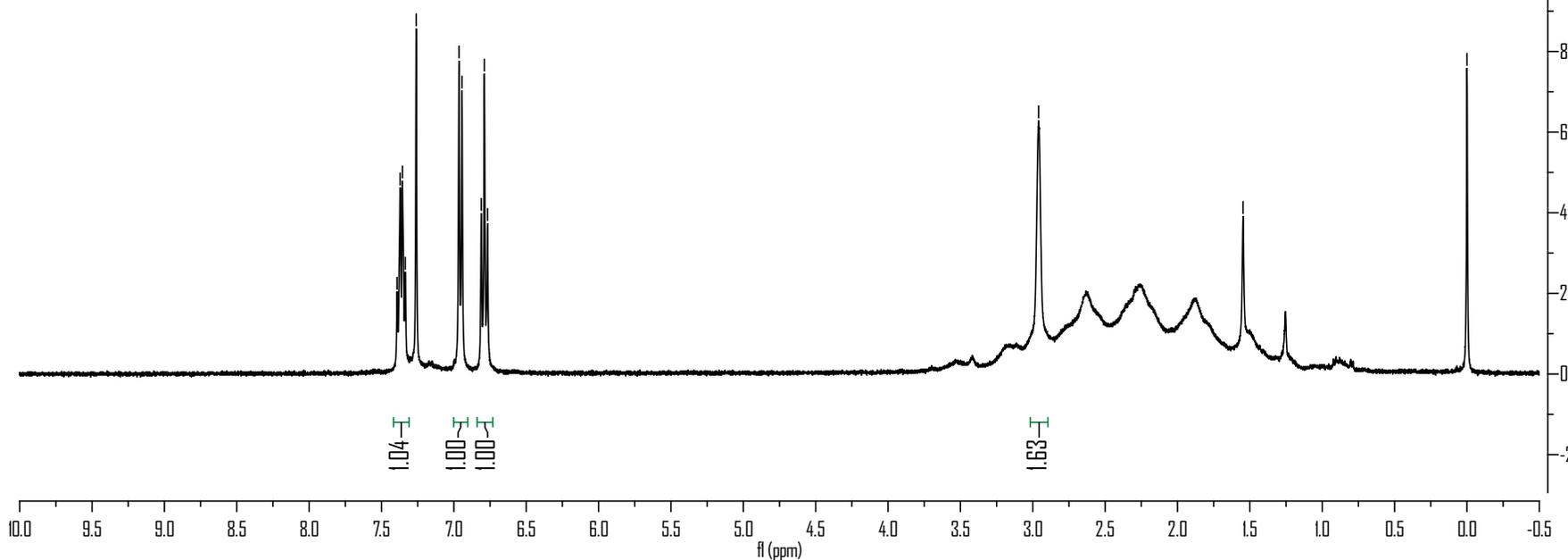
2q

7.393
7.372
7.355
7.336
7.260
6.965
6.944
6.890
6.789
6.768

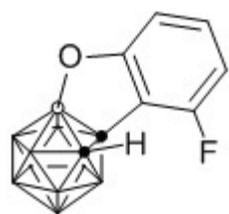
2.960

1.547

0.000



Parameter	Value
Data file Name	E:/Users/Administrator/Desktop/产物数据/7-13-1/ccx-7-13-1-2.fid/fid
Title	ccx-7-13-1-2
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-01-13T21:52:38
Modification Date	2017-01-13T13:53:00
Spectrometer Frequency	400.03
Spectral Width	7225.4
Lowest Frequency	-804.5
Nucleus	1H
Acquired Size	21676
Spectral Size	65536



2q

169.363
169.316

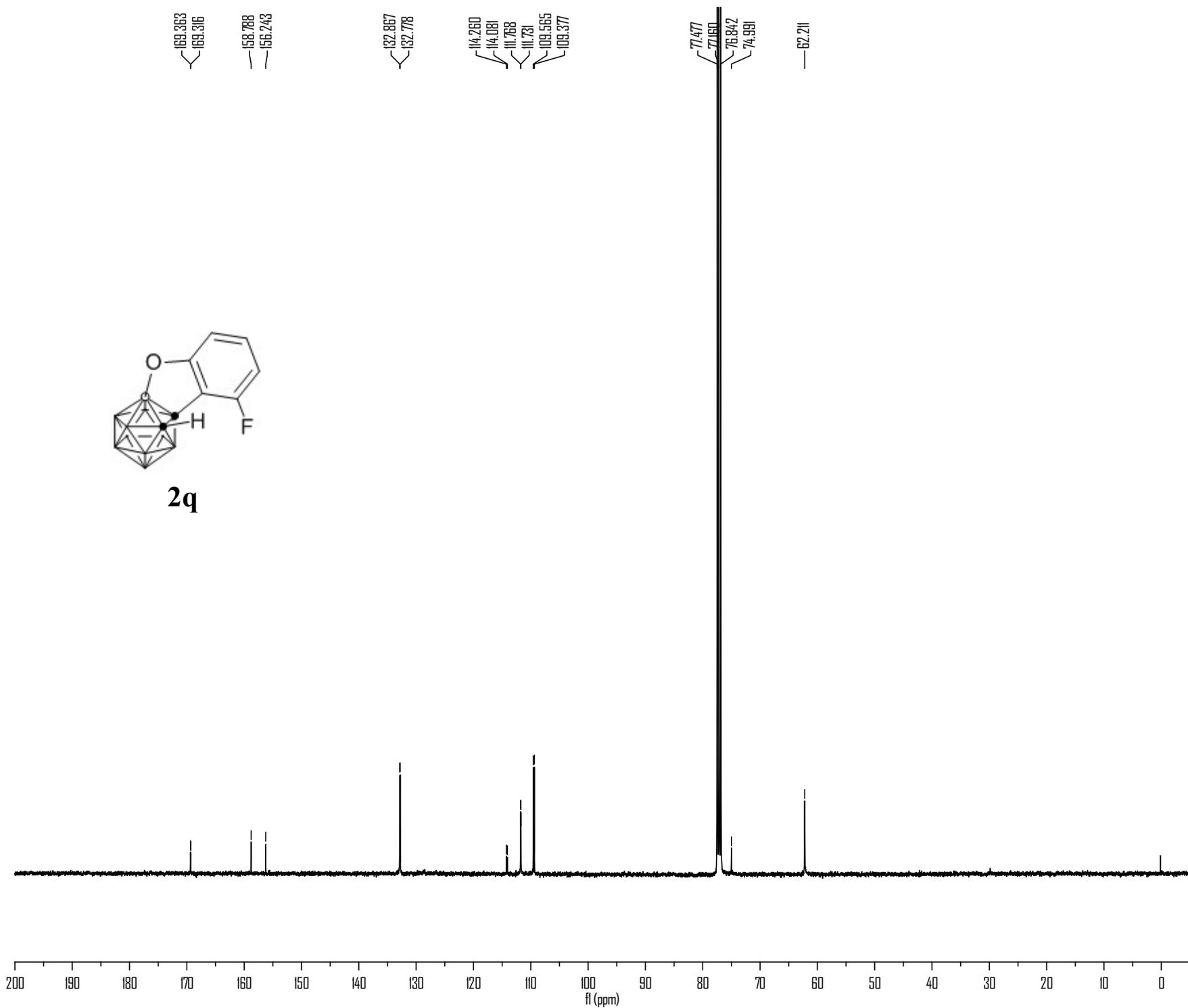
158.788
156.243

132.867
132.778

114.260
114.081
111.768
111.731
109.565
109.377

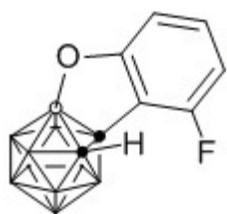
77.477
77.160
76.842
74.991

62.211

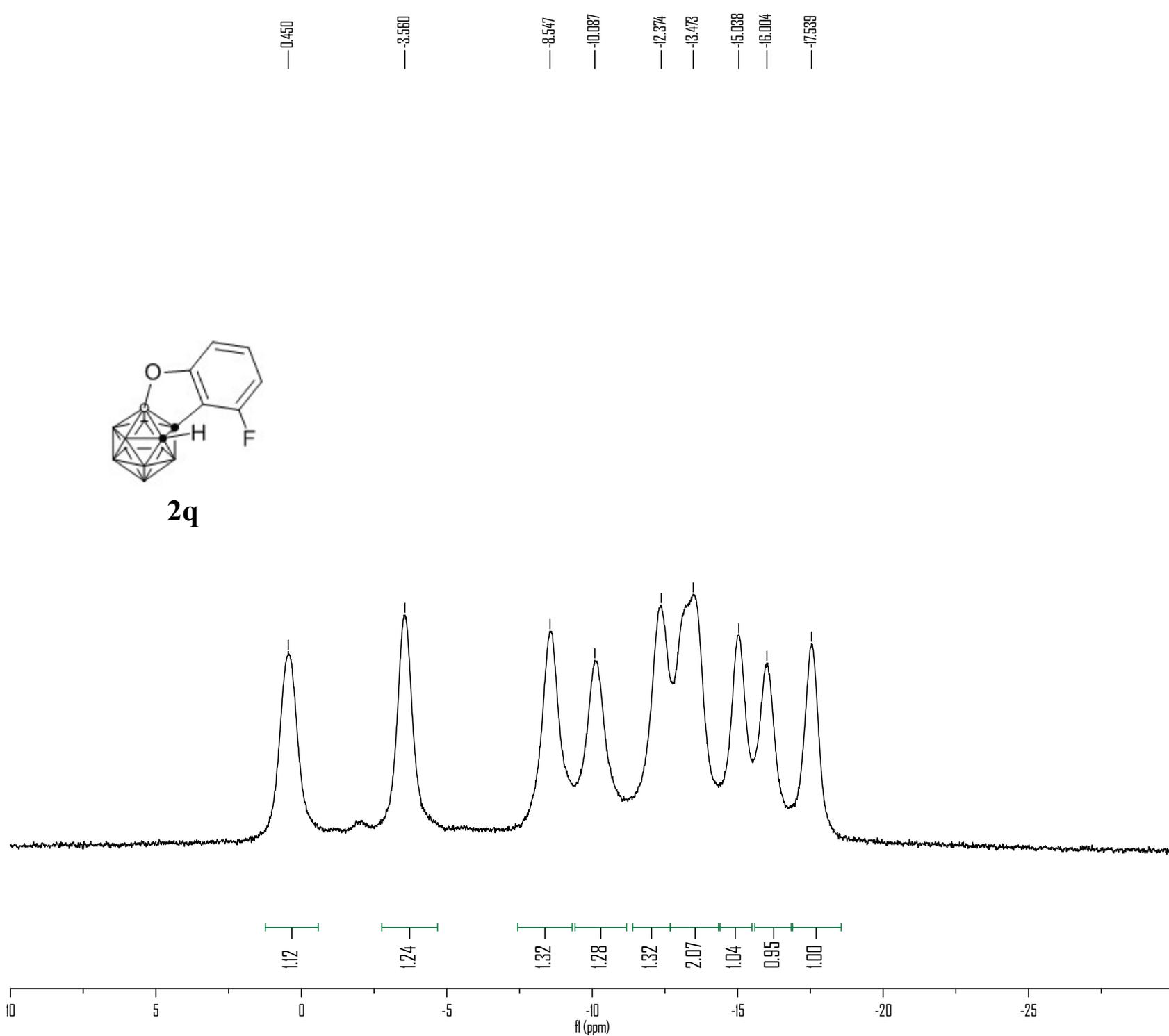


S232

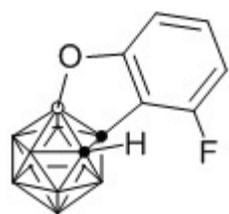
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-13-1/ccx-7-13-1-1-2C.fid/ fid
Title	ccx-7-13-1-1-2C
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	14412
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-01-13T22:04:00
Modification Date	2017-01-13T23:17:00
Spectrometer Frequency	100.60
Spectral Width	24509.8
Lowest Frequency	-1675.9
Nucleus	13C
Acquired Size	31875
Spectral Size	65536



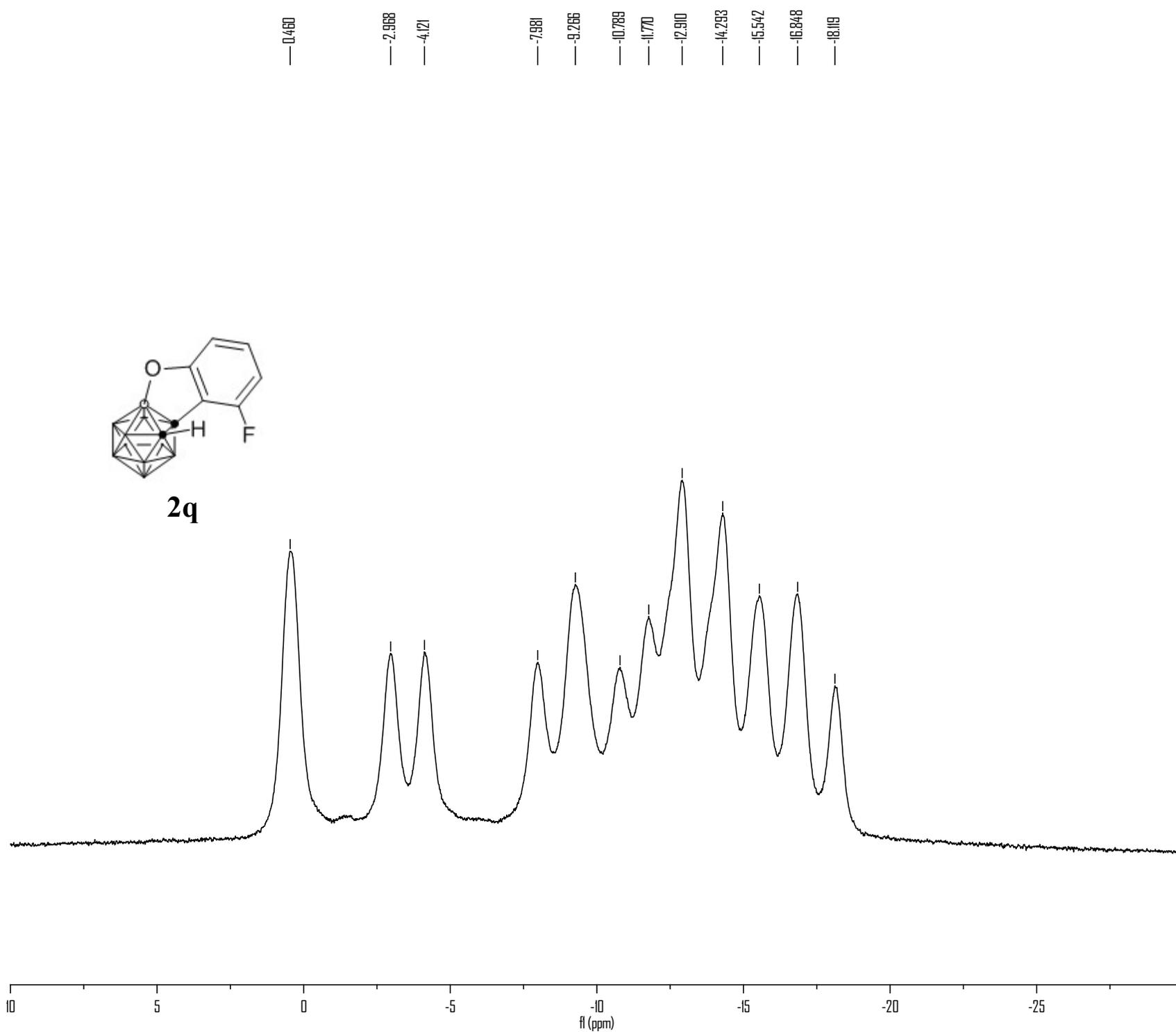
2q



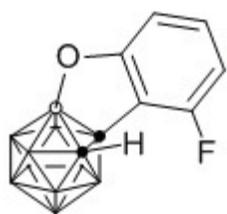
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-13-1/2012060b-ccx-7-13-1-2/1/pdata/1/1r
Title	2012060b-ccx-7-13-1-2
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	85
Receiver Gain	362
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-01-16T20:32:25
Modification Date	2017-01-16T13:53:28
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16399.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



2q

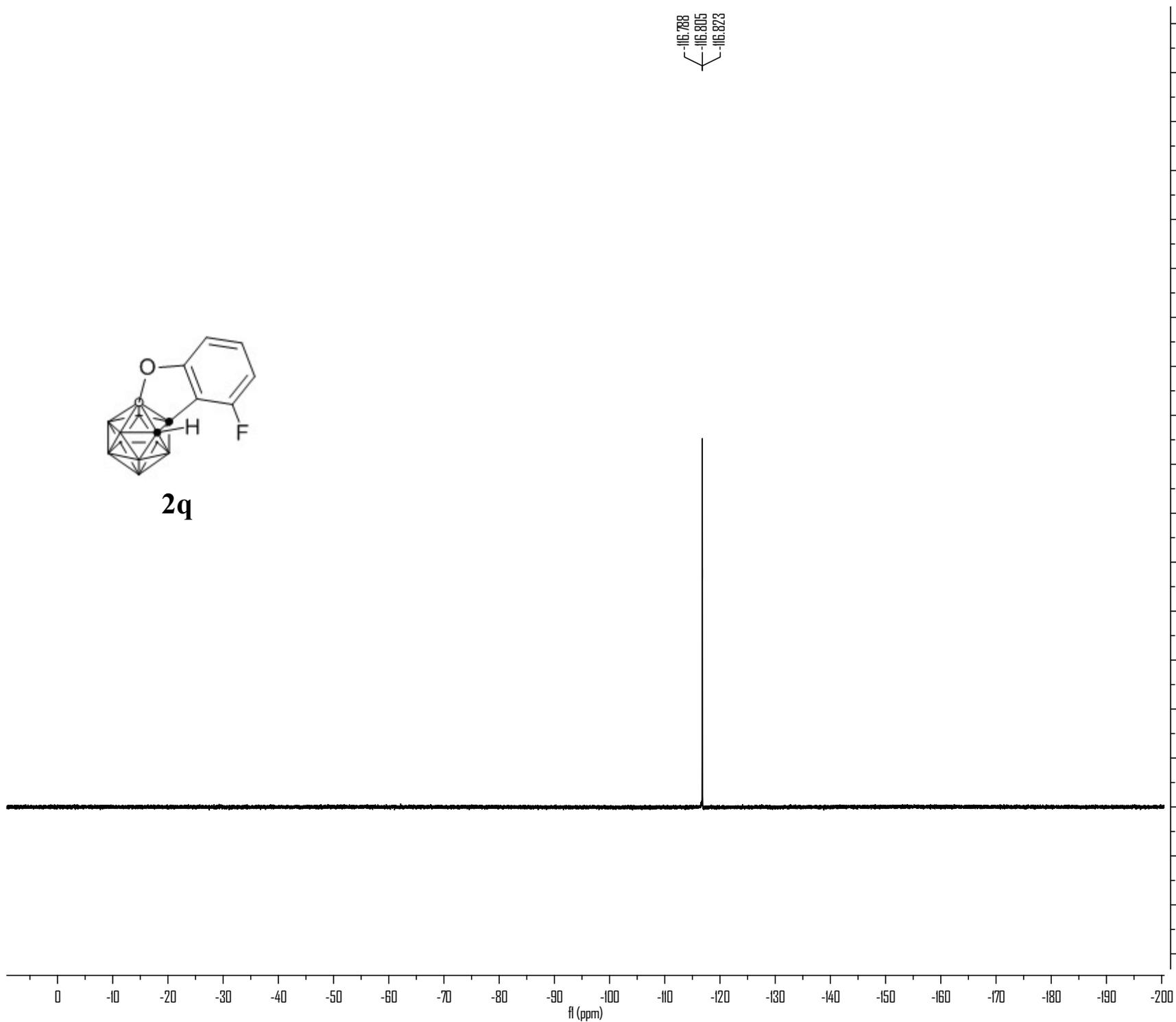


Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/7-13-1/2012060b-ccx-7-13-1-2-coupling/1/pdata/1/1r
Title	2012060b-ccx-7-13-1-2-coupling
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	415
Receiver Gain	362
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-01-16T20:26:44
Modification Date	2017-01-16T13:53:34
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16399.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

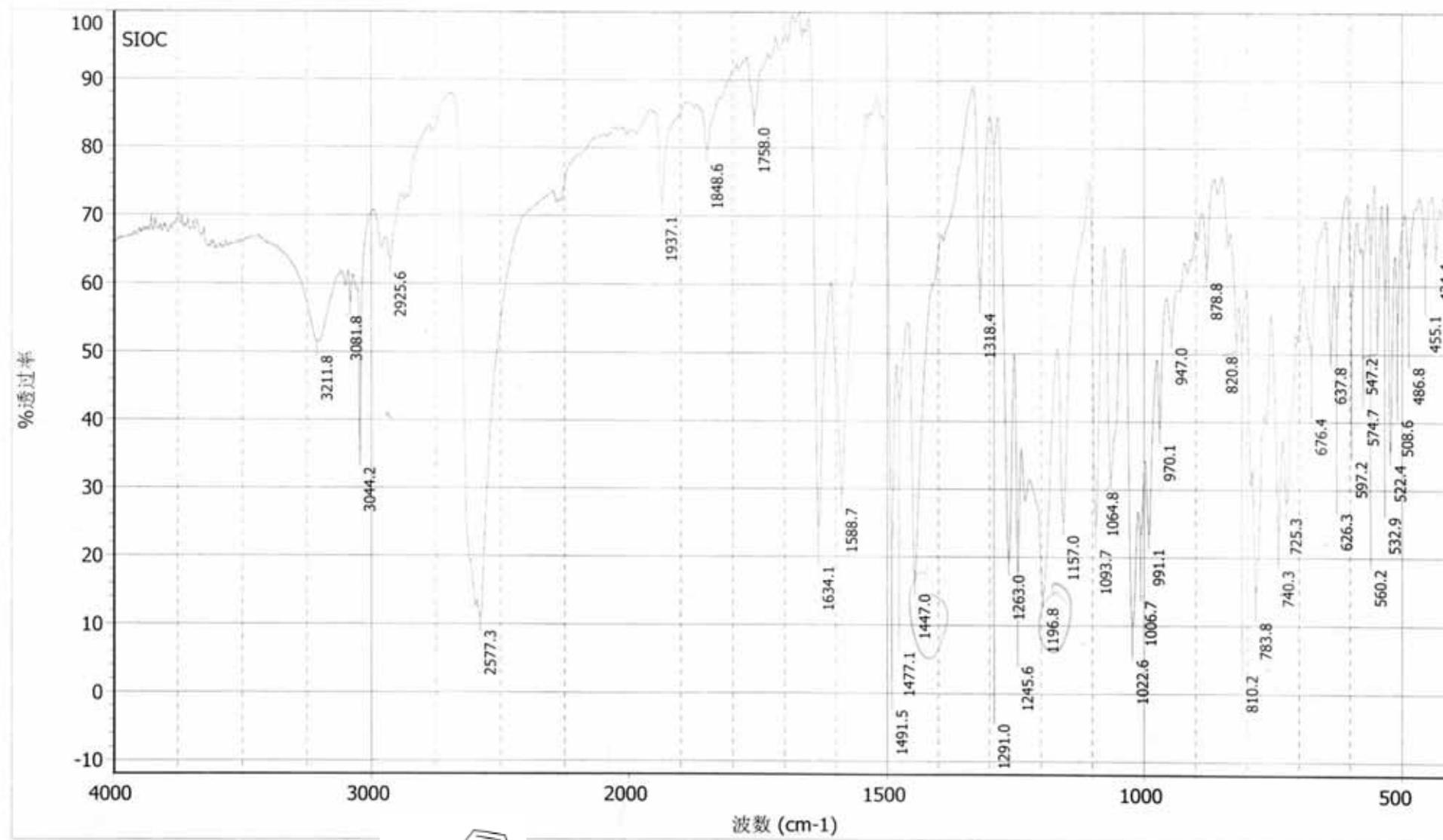


2q

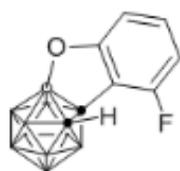
116.788
116.805
116.823



Parameter	Value
Data file Name	G:/Users/Administrator/Desktop/产物数据/7-13-1/ccx-7-13-1-1-2F.fid
Title	ccx-7-13-1-1-2F
Comment	Std fluorine
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	40
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0000
Acquisition Date	2017-01-13T22:01:58
Modification Date	2017-01-13T14:03:00
Spectrometer	376.38
Frequency	
Spectral Width	227272.7
Lowest Frequency	-123987.4
Nucleus	19F
Acquired Size	227273
Spectral Size	524288

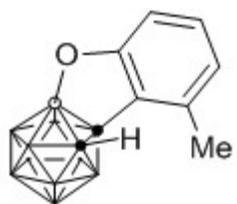


ccx-7-13-1 2015806 js



2q

样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



2r

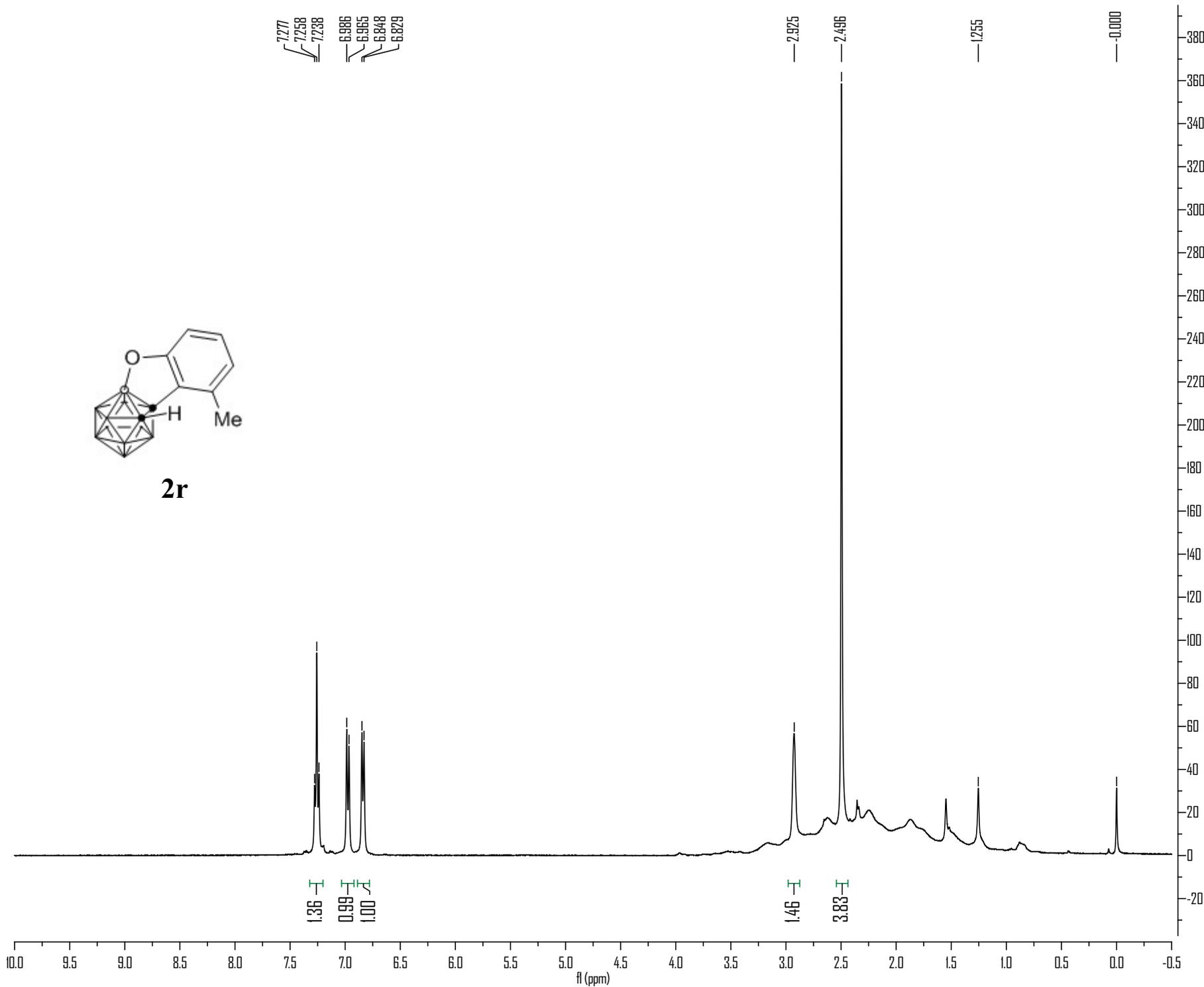
7.277
7.258
7.238
6.986
6.965
6.948
6.829

2.925

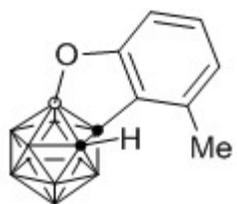
2.496

1.255

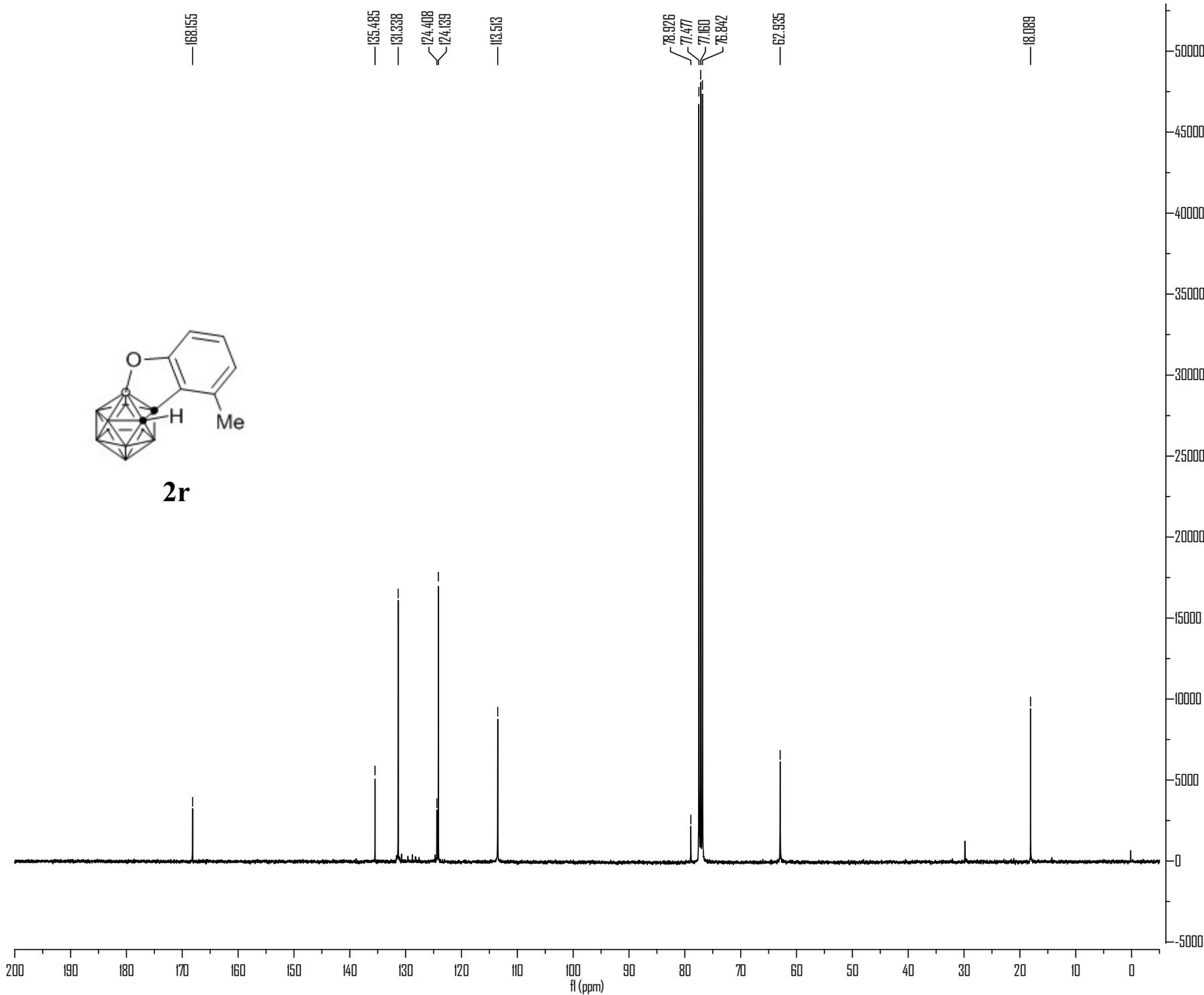
0.000



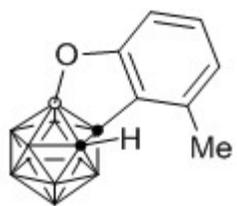
Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/7-35-1/ccx-7-35-3H.fid
Title	ccx-7-35-3H
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	36
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-12-22T22:06:37
Modification Date	2016-12-22T14:07:00
Spectrometer Frequency	400.03
Spectral Width	7225.4
Lowest Frequency	-805.3
Nucleus	1H
Acquired Size	21676
Spectral Size	65536



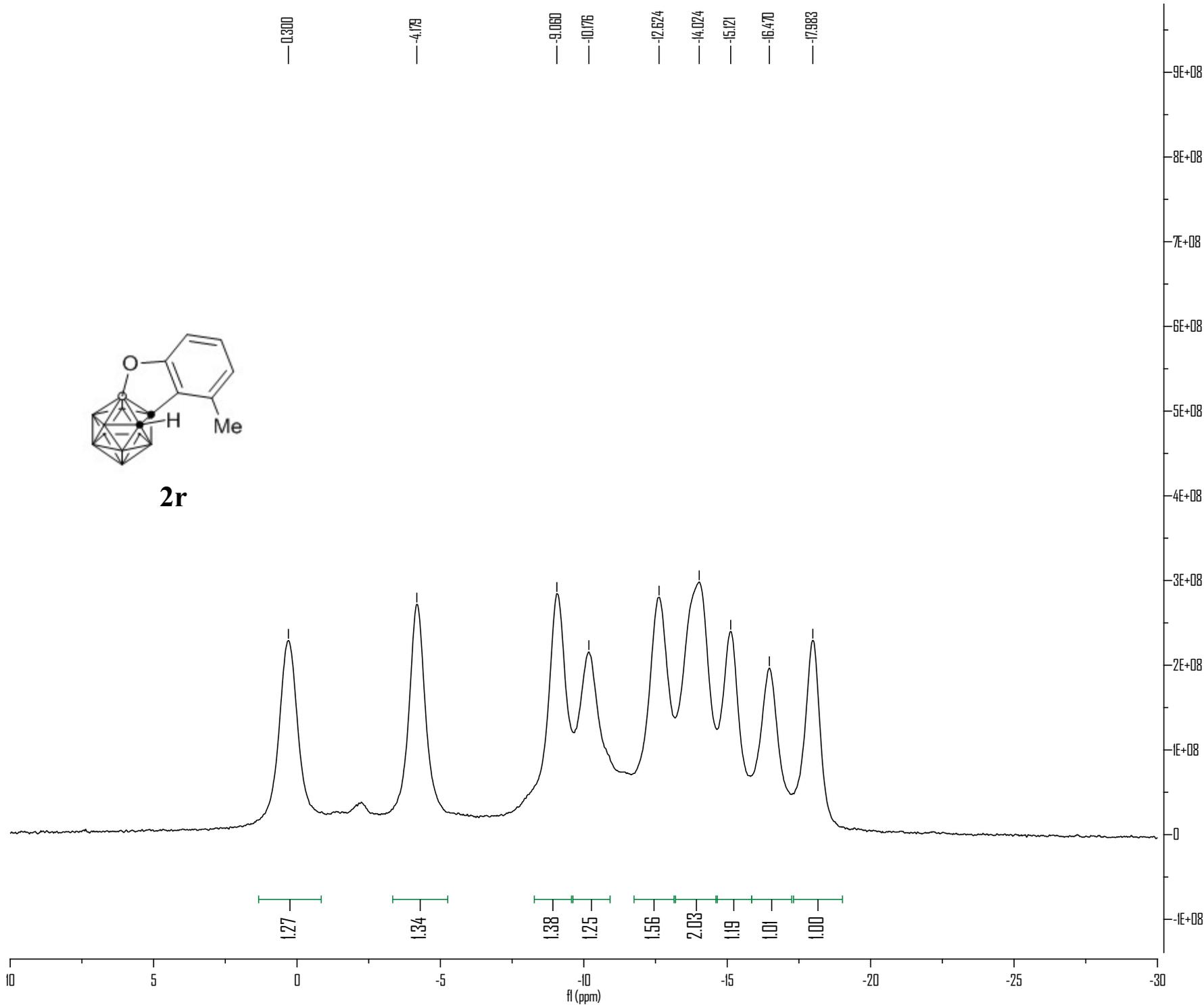
2r



Parameter	Value
Data file Name	C:\Users\Administrator\Desktop\产物数据\7-35-1\ccx-7-35-3C.fid
Title	ccx-7-35-3C
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	13848
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2016-12-22T22:07:58
Modification Date	2016-12-22T22:59:00
Spectrometer Frequency	100.60
Spectral Width	24509.8
Lowest Frequency	-1676.5
Nucleus	13C
Acquired Size	31875
Spectral Size	65536

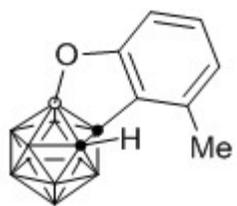


2r



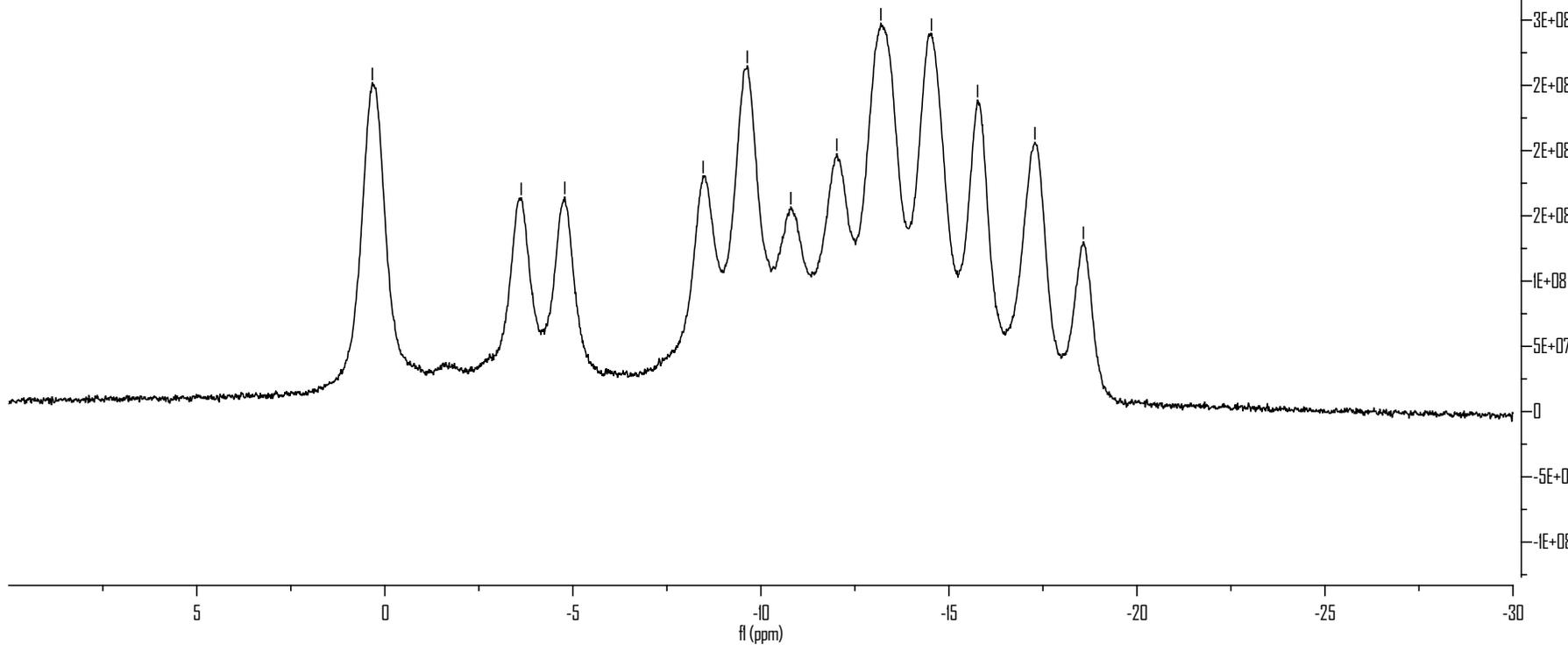
S239

Parameter	Value
Data file Name	C:\Users\Administrator\Desktop\产物数据\7-35-1\b-csx-7-35-3\pdata\1\1r
Title	7-35-1
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	99
Receiver Gain	256
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2016-12-23T21:14:59
Modification Date	2016-12-23T14:15:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16431.6
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



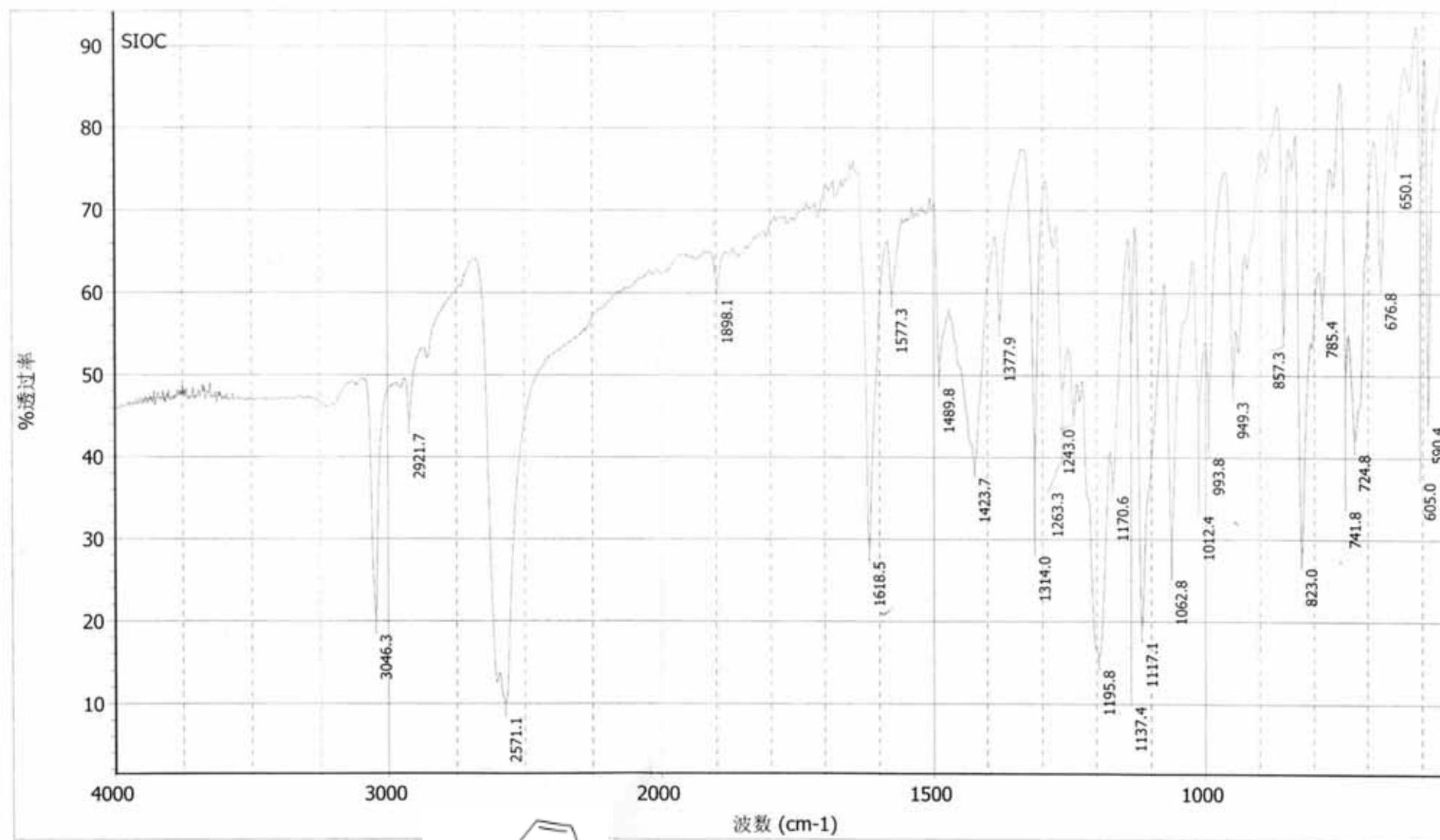
2r

0.333
 -3.627
 -4.786
 -8.464
 -9.638
 -10.796
 -12.020
 -13.191
 -14.535
 -15.762
 -17.287
 -18.576

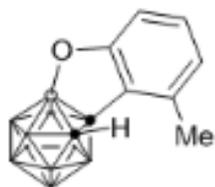


S240

Parameter	Value
Data file Name	C:\Users\Administrator\Desktop\产物数据\7-35-1\b-cx-7-35-3-coupling\data\1\1r
Title	7-35-1
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.lgy
Number of Scans	213
Receiver Gain	181
Relaxation Delay	0.0000
Pulse Width	4.0000
Acquisition Time	0.4260
Acquisition Date	2016-12-23T21:17:02
Modification Date	2016-12-23T14:17:00
Spectrometer Frequency	128.38
Spectral Width	38461.5
Lowest Frequency	-20641.9
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

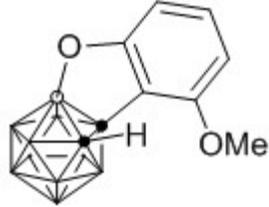


CCX-7-35-1 2015806 JS

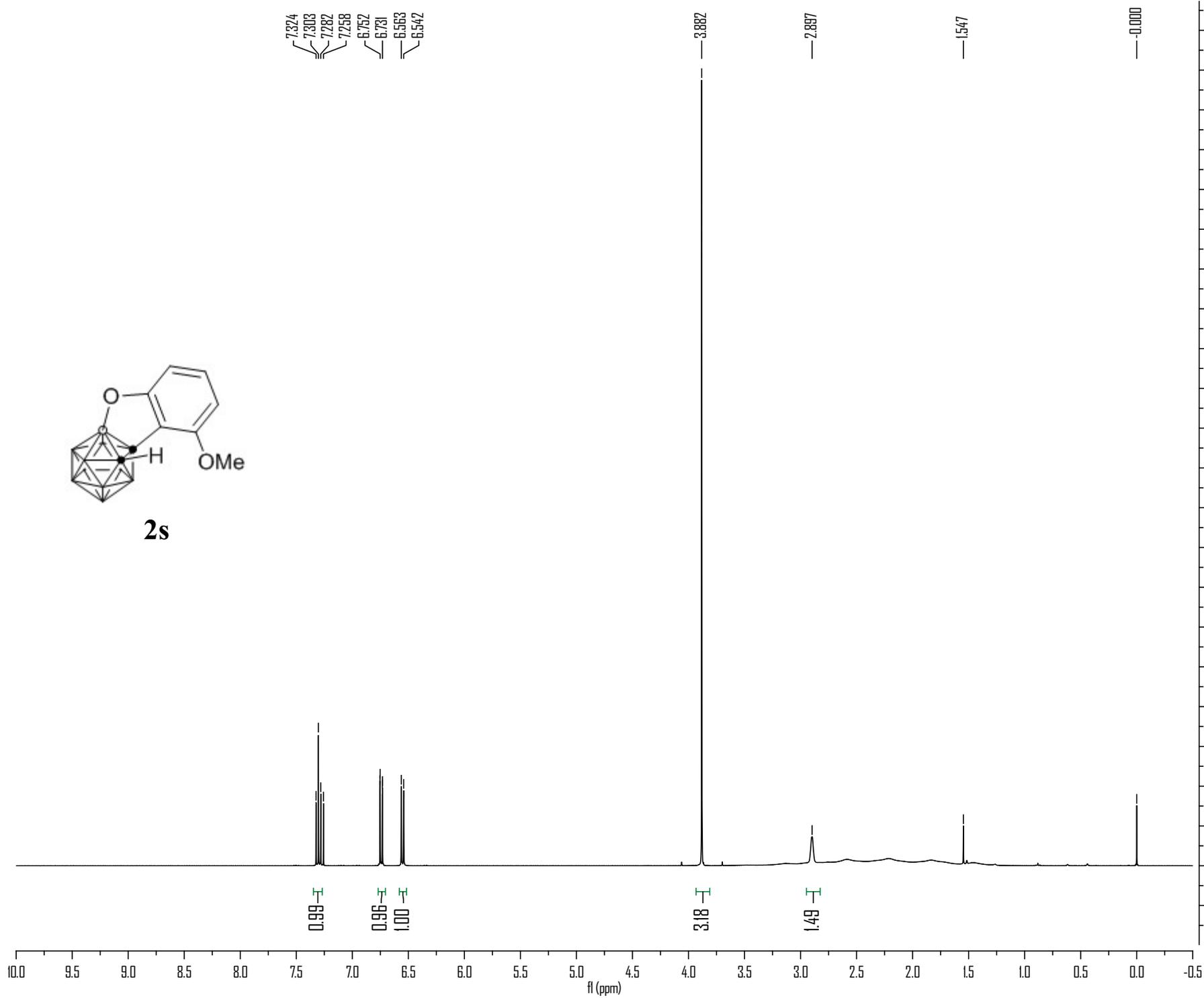


2r

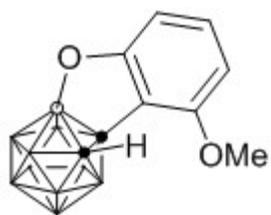
样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329



2s

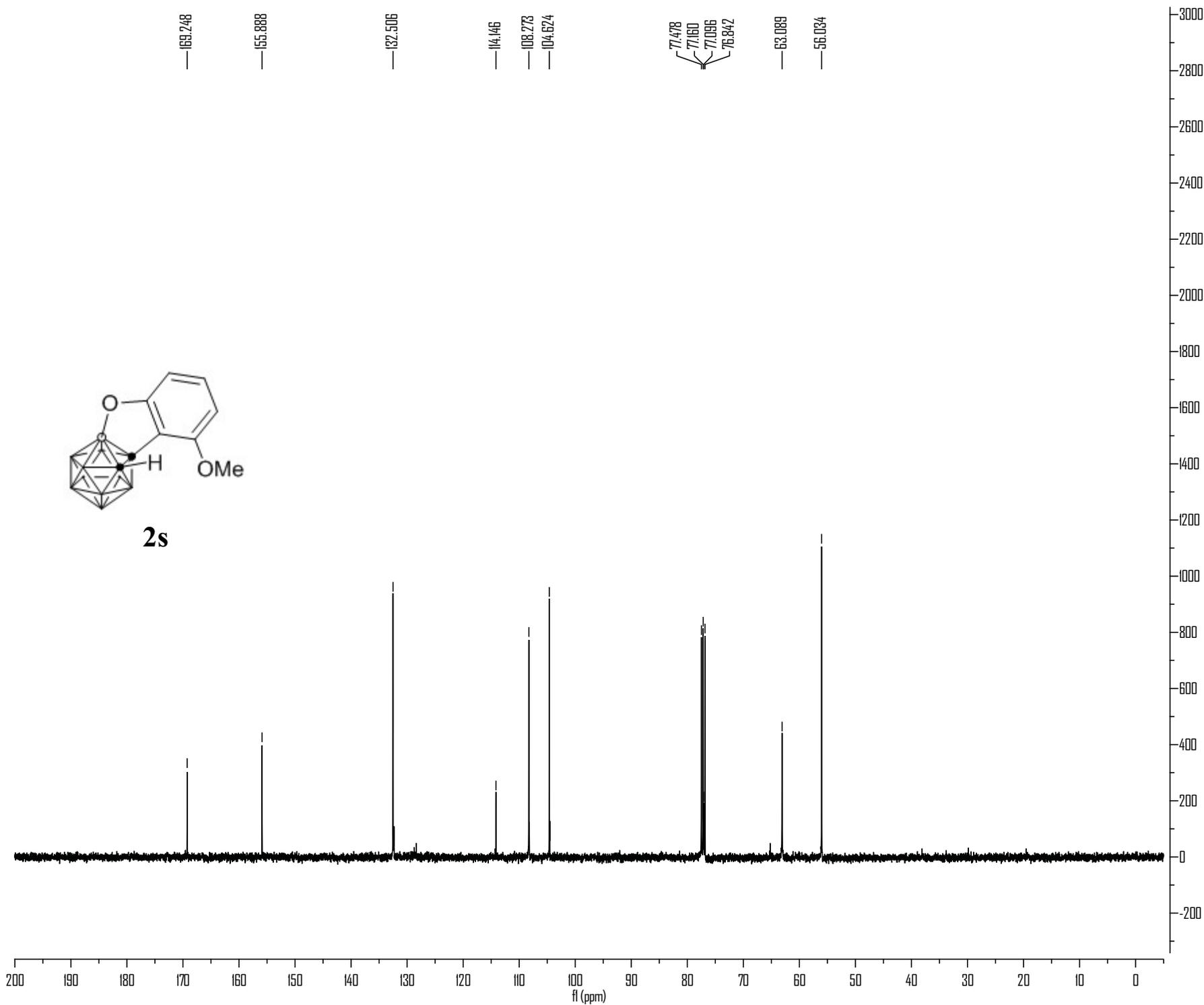


Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/6-93/ccx-6-93-2-1.fid/fid
Title	ccx-6-93-2-1
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmrns
Author	
Solvent	CDCl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	36
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2016-11-19T13:17:25
Modification Date	2016-11-19T05:18:00
Spectrometer	399.72
Frequency	
Spectral Width	7183.9
Lowest Frequency	-794.7
Nucleus	1H
Acquired Size	21552
Spectral Size	65536



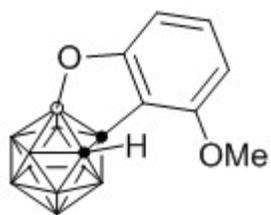
2s

169.248
155.888
132.506
114.146
108.273
104.624
77.478
77.160
77.096
76.842
63.089
56.034

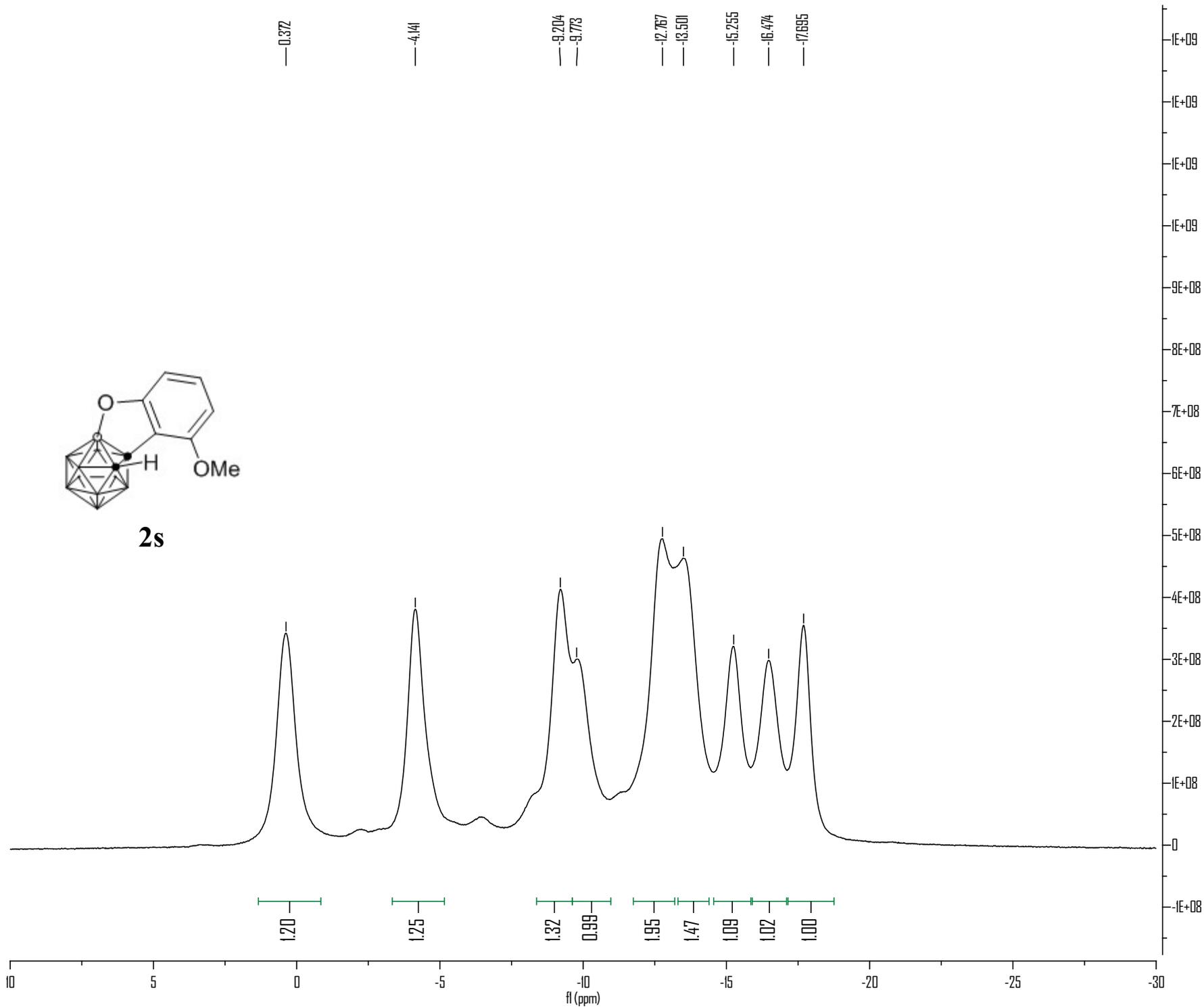


S243

Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/6-93/ccx-6-93-2-000.fid
Title	ccx-6-93-2-000
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmr-s
Author	omcl
Solvent	cdcl3
Temperature	21.0
Pulse Sequence	s2pul
Number of Scans	240
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3000
Acquisition Date	2016-10-07T18:44:35
Modification Date	2016-10-07T10:54:00
Spectrometer Frequency	100.62
Spectral Width	25000.0
Lowest Frequency	-1431.6
Nucleus	13C
Acquired Size	32500
Spectral Size	65536

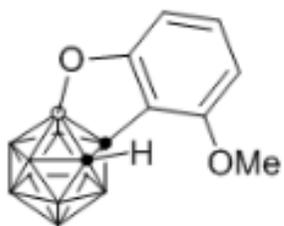


2s

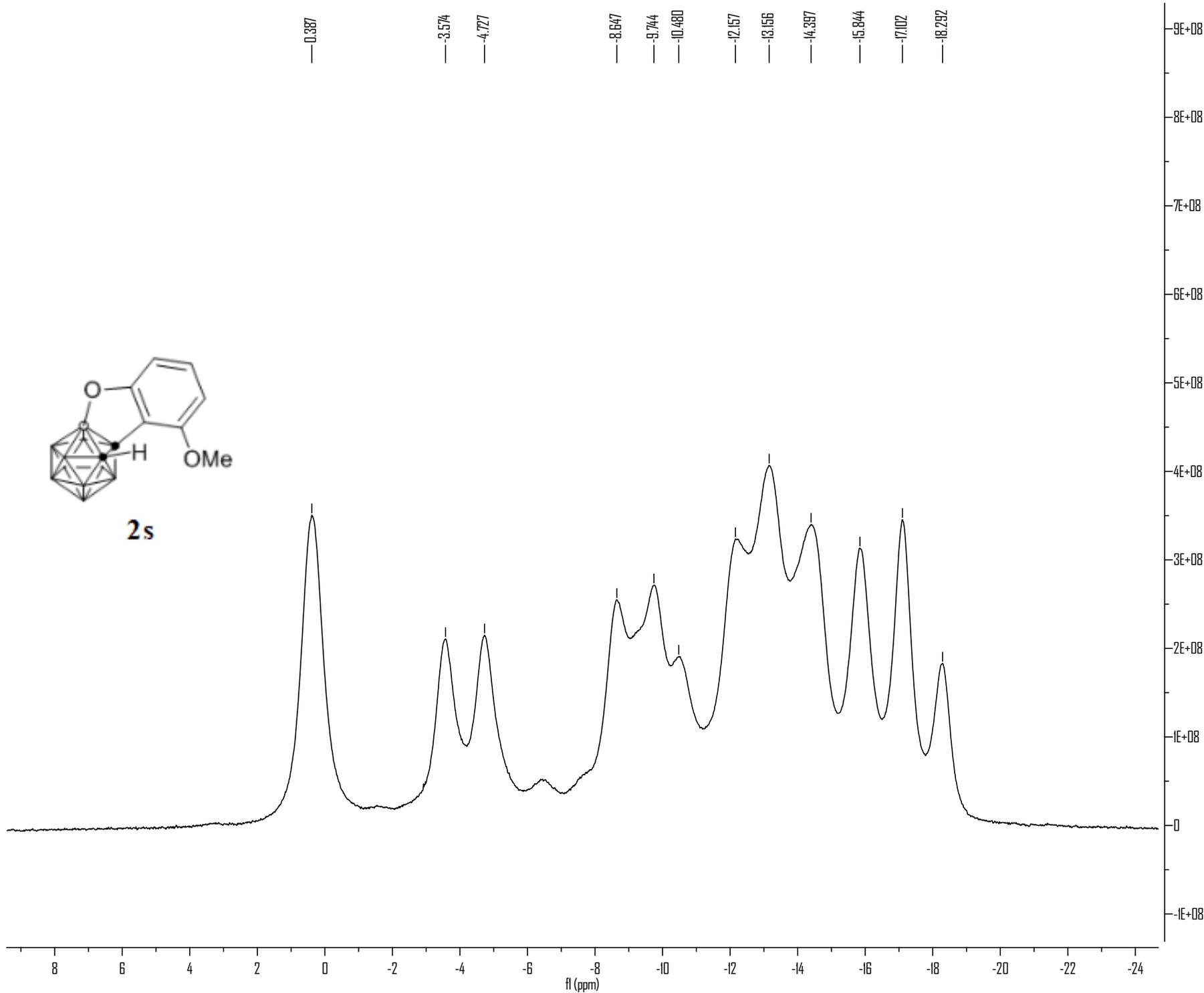


S244

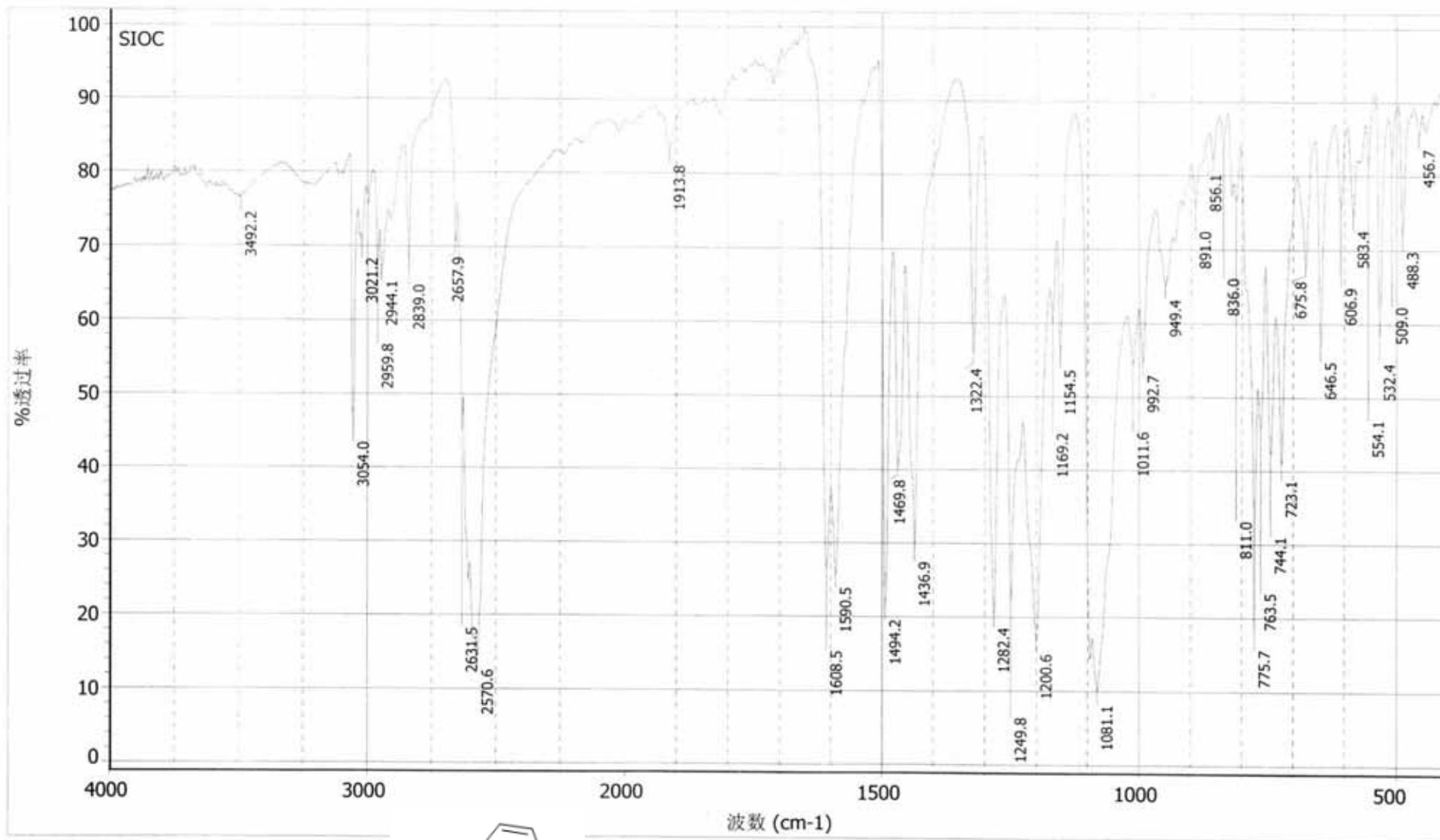
Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/6-93/2012060b-ccx-6-93-2/1/pdata/1/1r
Title	2012060b-ccx-6-93-2
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	256
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-09-08T20:00:30
Modification Date	2016-09-08T13:19:51
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16400.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



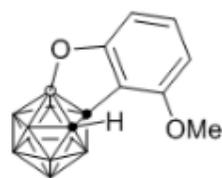
2s



Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/6-93/2012060b-ccx-6-93-2-coupling/1/pdata/1/1r
Title	2012060b-ccx-6-93-2-coupling
Comment	
Origin	LXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	256
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2016-09-08T20:10:41
Modification Date	2016-09-08T13:19:46
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16400.3
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



CCX-6-93-2 2015806 JS



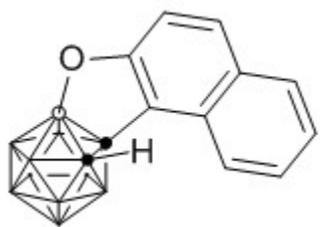
2s

样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329

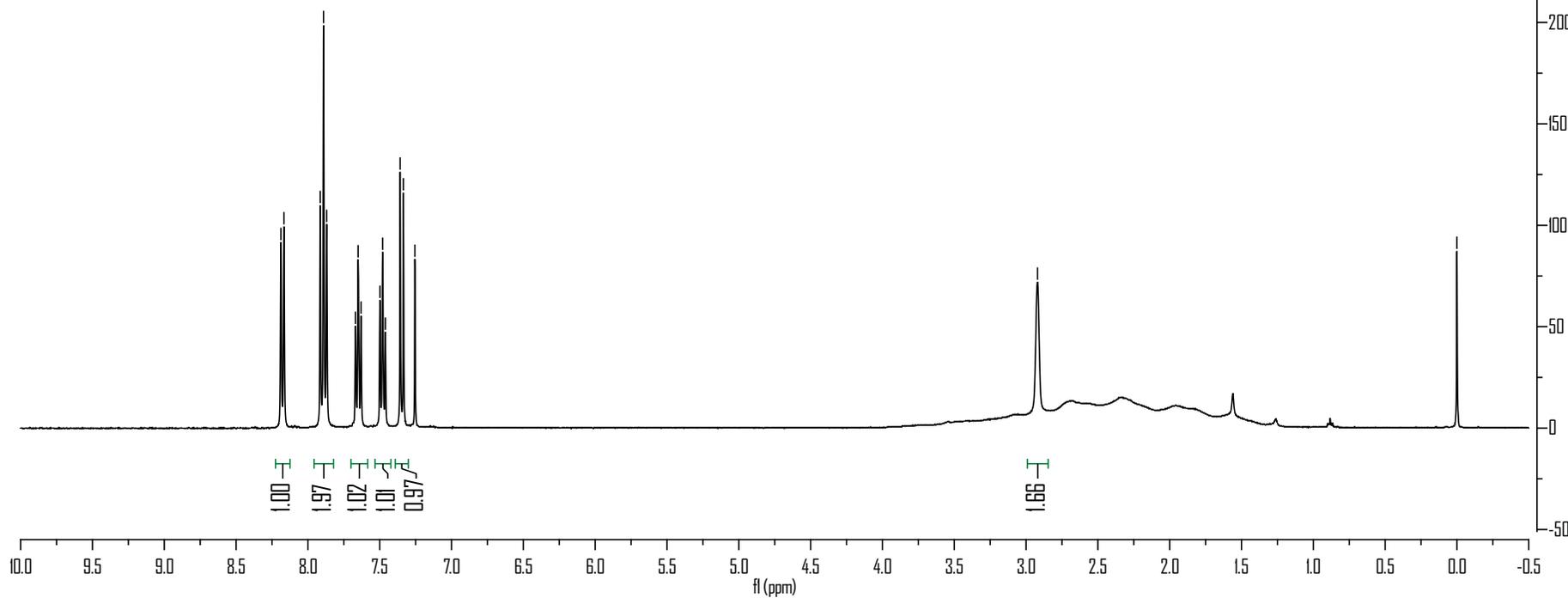
8.188
8.167
7.869
7.669
7.651
7.630
7.499
7.480
7.461
7.358
7.335
7.255

2.970

0.000



2t



Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/6-100/ccx-6-100-4-1H.fid/ fid
Title	ccx-6-100-4-1H
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	38
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-02-07T21:23:52
Modification Date	2017-02-07T13:24:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-735.8
Nucleus	1H
Acquired Size	21552
Spectral Size	65536

167.486

132.969

128.657

125.211

121.844

119.020

116.204

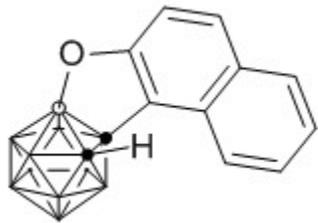
79.159

77.478

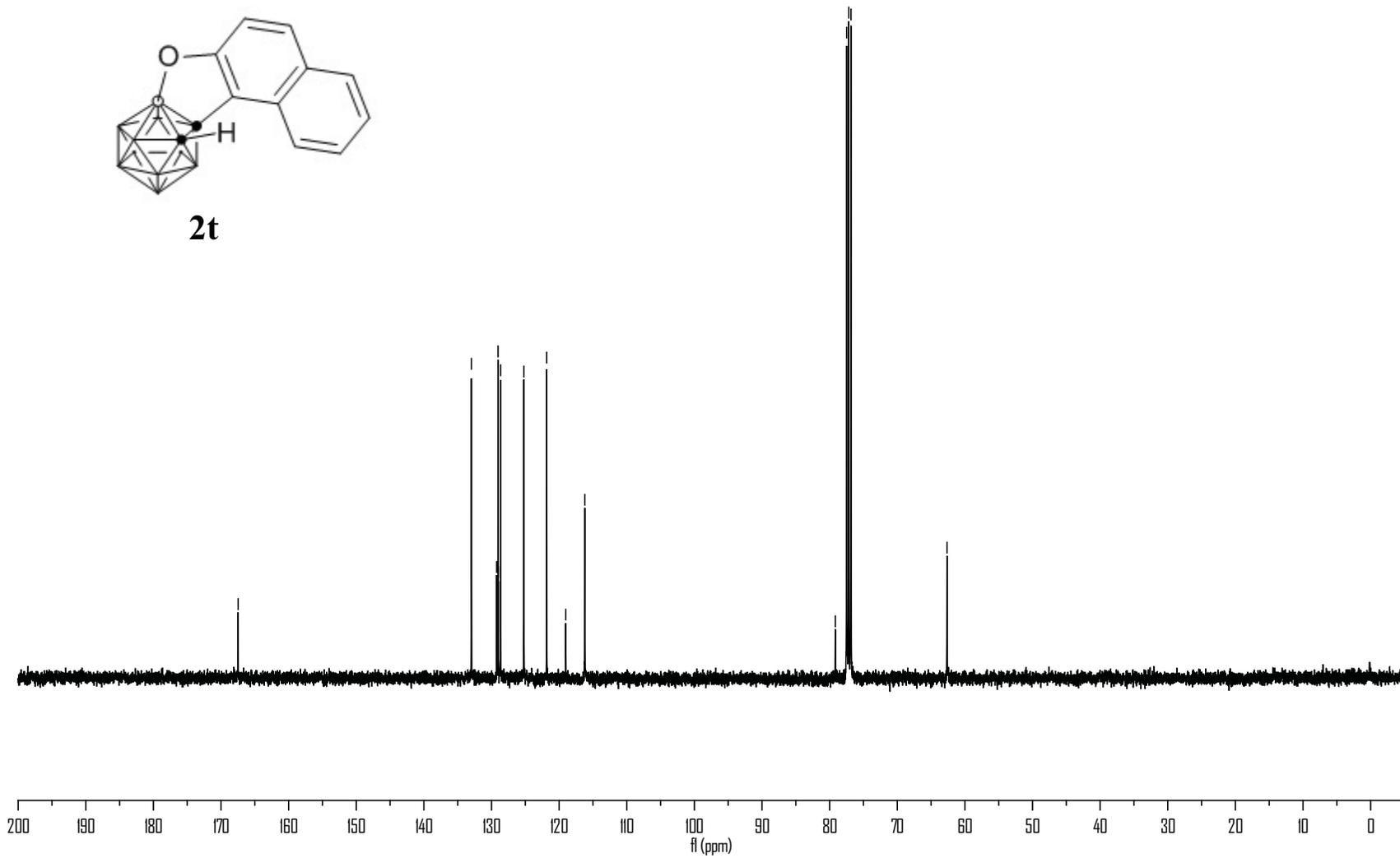
77.160

76.843

62.647

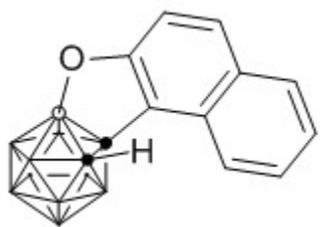


2t

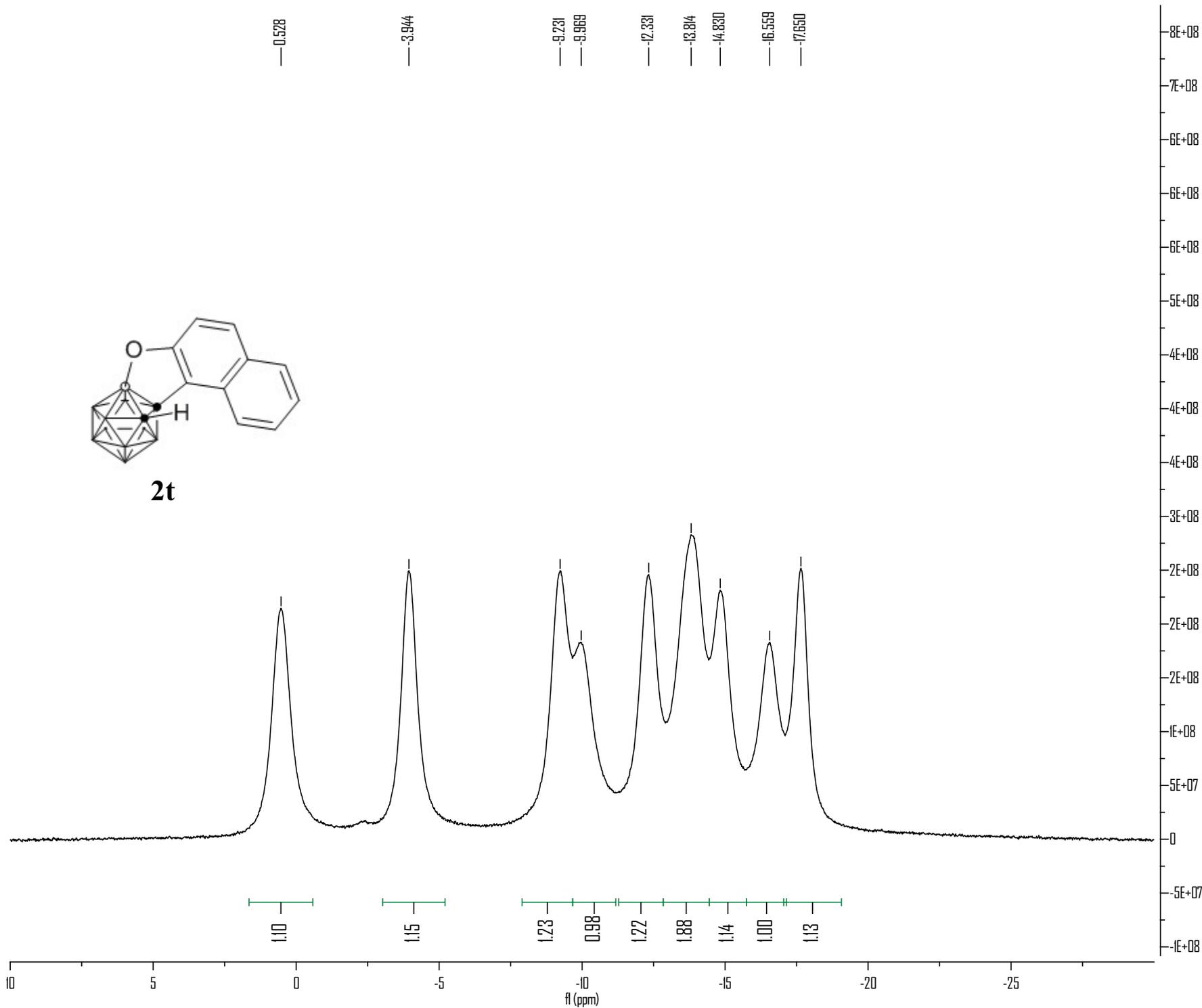


S248

Parameter	Value
Data File Name	C:/Users/Administrator/Desktop/产物数据/6-100/ccx-6-100-4-1C.fid/fid
Title	ccx-6-100-4-1C
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	800
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-02-07T21:26:06
Modification Date	2017-02-07T13:57:00
Spectrometer	100.60
Frequency	
Spectral Width	24509.8
Lowest Frequency	-1677.2
Nucleus	13C
Acquired Size	31875
Spectral Size	65536

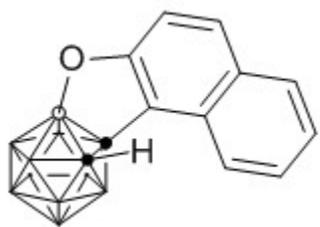


2t

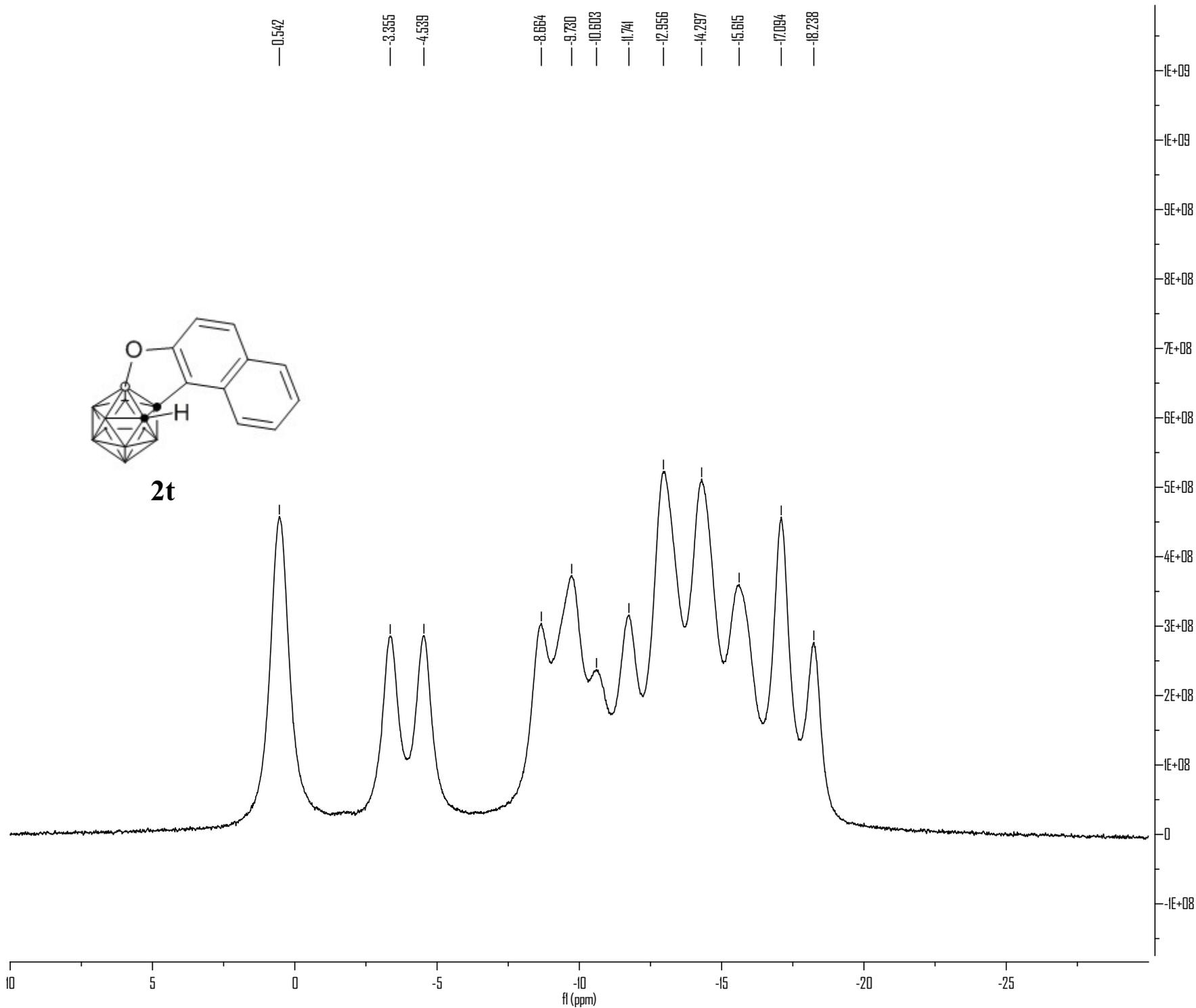


S249

Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/6-100/2012060b-ccx-6-100-4-1/1/pdata/1/1r
Title	2012060b-ccx-6-100-4-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.tgy
Number of Scans	259
Receiver Gain	203
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.512
Acquisition Date	2017-02-08T18:34:48
Modification Date	2017-02-08T11:50:30
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16416.9
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

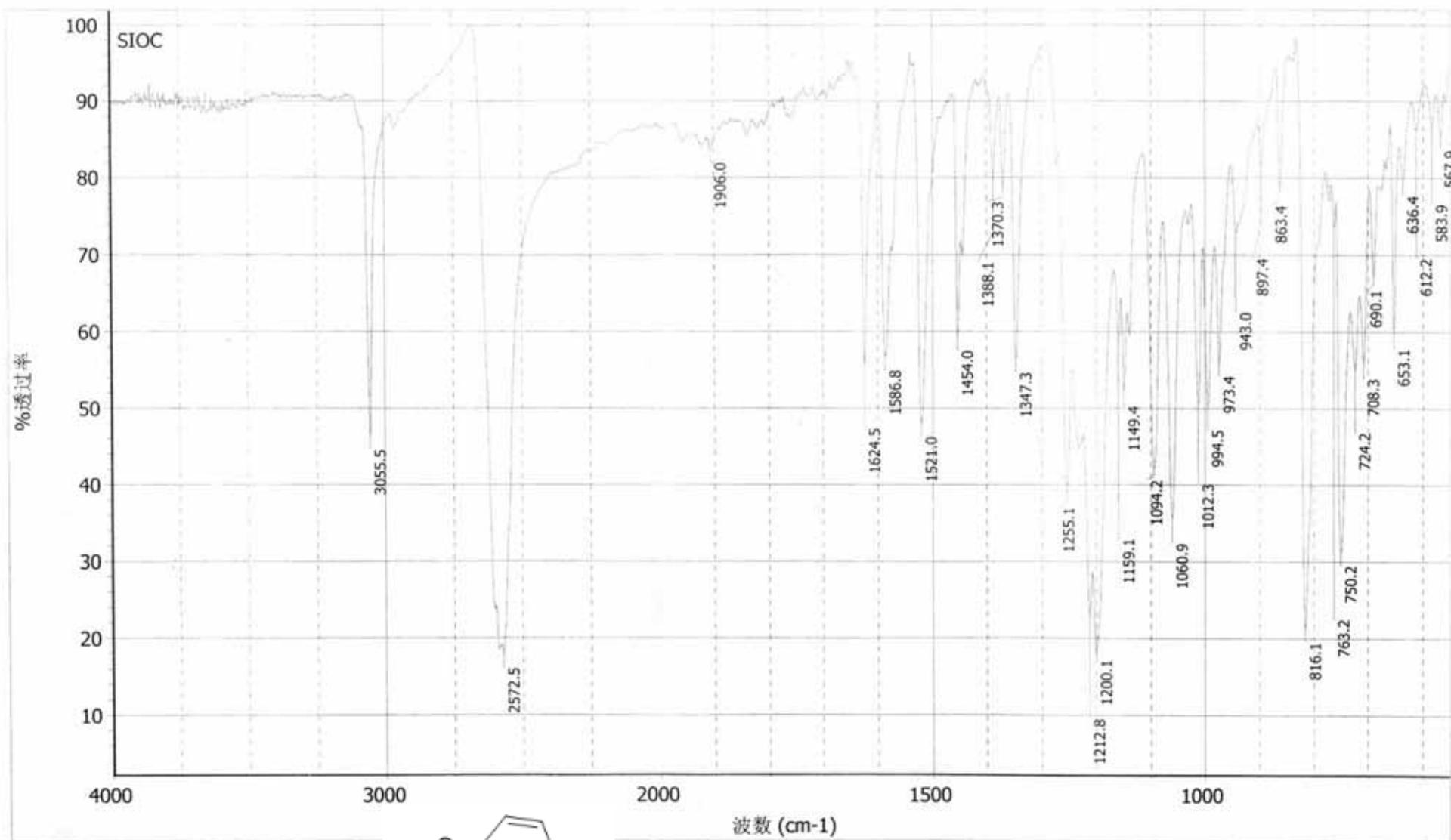


2t

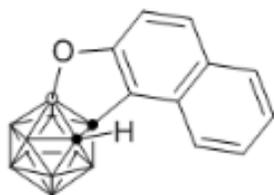


S250

Parameter	Value
Data file Name	C:/Users/Administrator/Desktop/产物数据/6-100/2012060b-ccx-6-100-4-1-coupling/1/pdata/1/1r
Title	2012060b-ccx-6-100-4-1-coupling
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	276
Receiver Gain	203
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-02-08T18:39:04
Modification Date	2017-02-08T11:50:24
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16416.9
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



CCX-6-100-4-1 2015806 JS



2t

样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.6329