

Electronic Supplementary Information

Light-enabled alkenylation of iodocarboranes with unactivated alkenes

Hangcheng Ni, Zhenpin Lu, and Zuowei Xie*

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

Email: zxie@cuhk.edu.hk

Table of Contents

| | |
|--|----|
| Crystal Data and Summary of Data Collection and Refinement | S2 |
| Setup of the photoreaction | S3 |
| NMR Spectra | S4 |

Table S1. Crystal Data and Summary of Data Collection and Refinement for **3Aa**, **3An**, **3Ap** and **3Fa**.

| Compound | 3Aa | 3An | 3Ap | 3Fa |
|--|---|---|---|--|
| formula | C ₁₁ H ₂₀ B ₁₀ | C ₁₂ H ₂₂ B ₁₀ | C ₁₇ H ₂₄ B ₁₀ | C ₁₃ H ₂₆ B ₁₀ Si |
| Cryst size(mm ³) | 0.40 x 0.30 x 0.20 | 0.50 x 0.40 x 0.30 | 0.40 x 0.30 x 0.20 | 0.50 x 0.40 x 0.30 |
| Fw | 260.37 | 274.39 | 336.46 | 318.53 |
| Cryst syst | orthorhombic | orthorhombic | orthorhombic | monoclinic |
| Space group | Pna2 ₁ | P2 ₁ 2 ₁ 2 ₁ | Pca2 ₁ | P2 ₁ /c |
| <i>a</i> , Å | 20.057(11) | 11.7028(5) | 21.065(8) | 17.950(15) |
| <i>b</i> , Å | 7.8629(4) | 11.9322(6) | 8.0636(4) | 7.2031(6) |
| <i>c</i> , Å | 19.9257(12) | 12.0721(6) | 11.902(6) | 17.2814(14) |
| α, deg | 90.00 | 90.00 | 90.00 | 90.00 |
| β, deg | 90.00 | 90.00 | 90.00 | 116.825(4) |
| γ, deg | 90.00 | 90.00 | 90.00 | 90.00 |
| <i>V</i> , Å ³ | 3142.4(3) | 1685.75(14) | 2021.69(16) | 1994.0(3) |
| <i>Z</i> | 8 | 4 | 4 | 4 |
| <i>D</i> _{calc} , Mg/m ³ | 1.101 | 1.081 | 1.105 | 1.061 |
| Radiation (λ), Å | 1.54178 | 0.71073 | 0.71073 | 0.71073 |
| 2θ range, deg | 8.82 to 137.42 | 4.82 to 50.50 | 5.05 to 50.49 | 2.54 to 50.50 |
| μ, mm ⁻¹ | 0.361 | 0.052 | 0.055 | 0.109 |
| <i>F</i> (000) | 1088 | 576 | 704 | 672 |
| no. of obsd reflns | 5743 | 3039 | 3650 | 3611 |
| no. of params refnd | 379 | 208 | 245 | 217 |
| Goodness of fit | 1.043 | 1.054 | 1.066 | 1.054 |
| R1 | 0.0737 | 0.0782 | 0.0570 | 0.0443 |
| wR2 | 0.1893 | 0.2140 | 0.1419 | 0.1234 |

Setup of the photoreaction

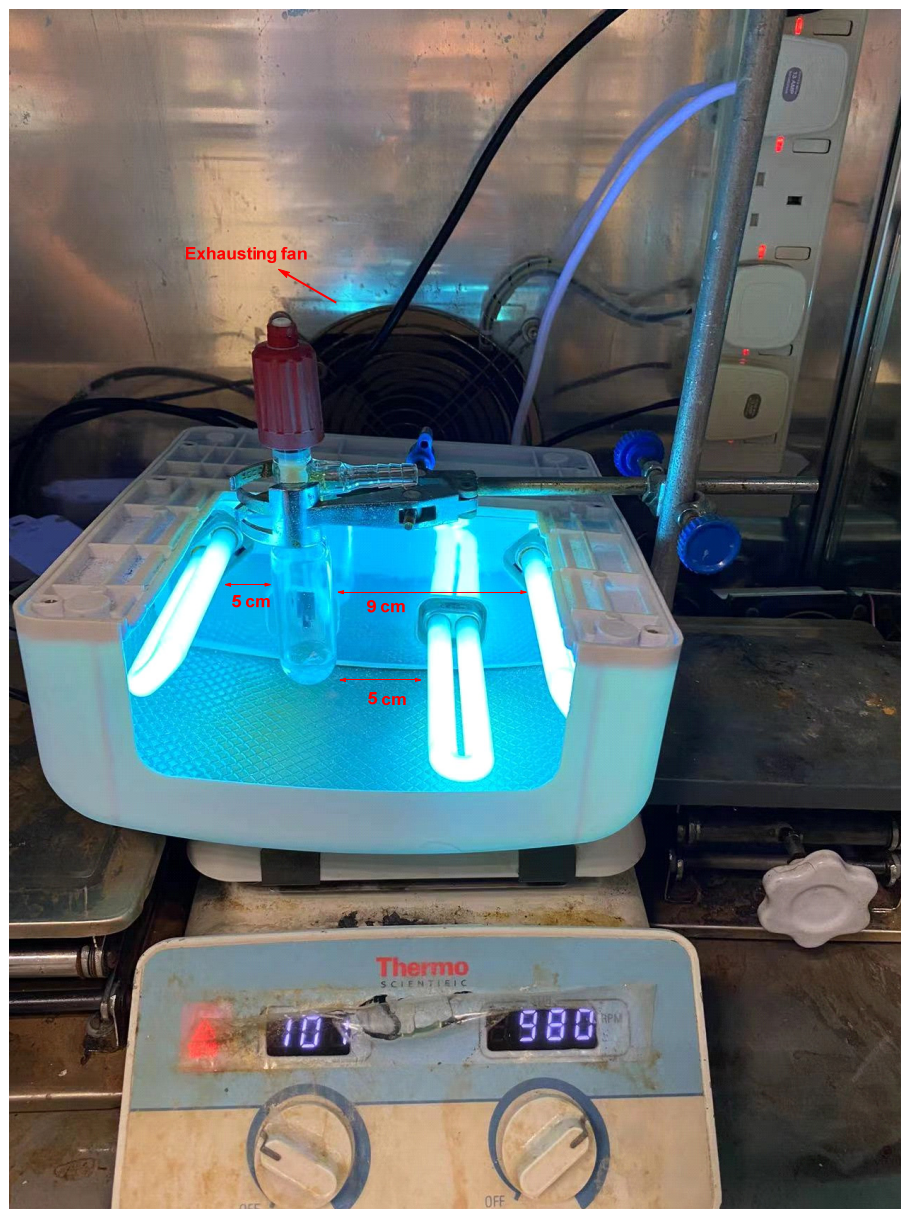
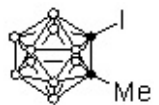
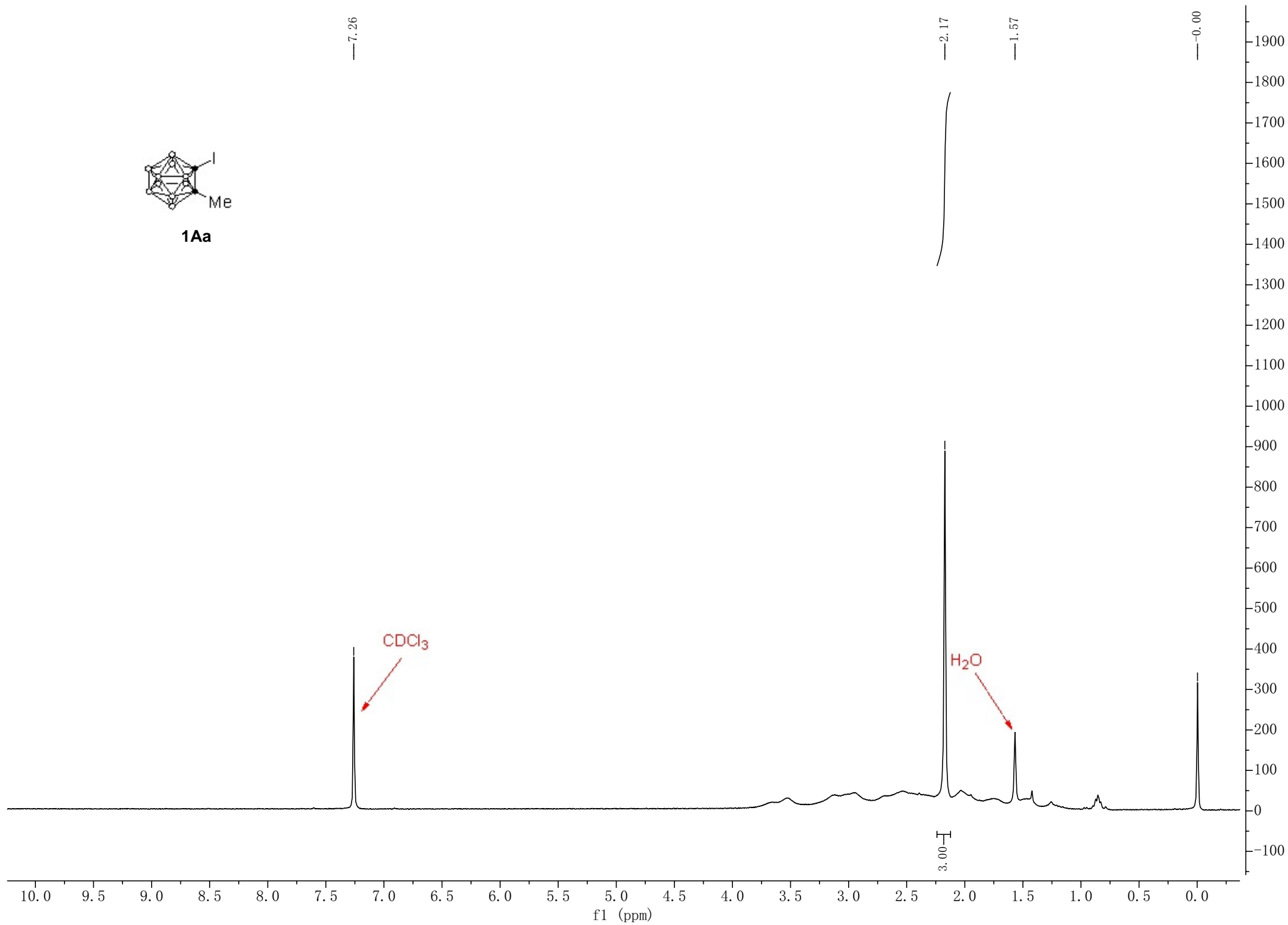
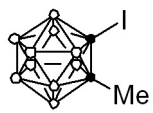


Figure S1. Standard setup of the photoreaction [3 x 9 W UV (365 nm) lamp]



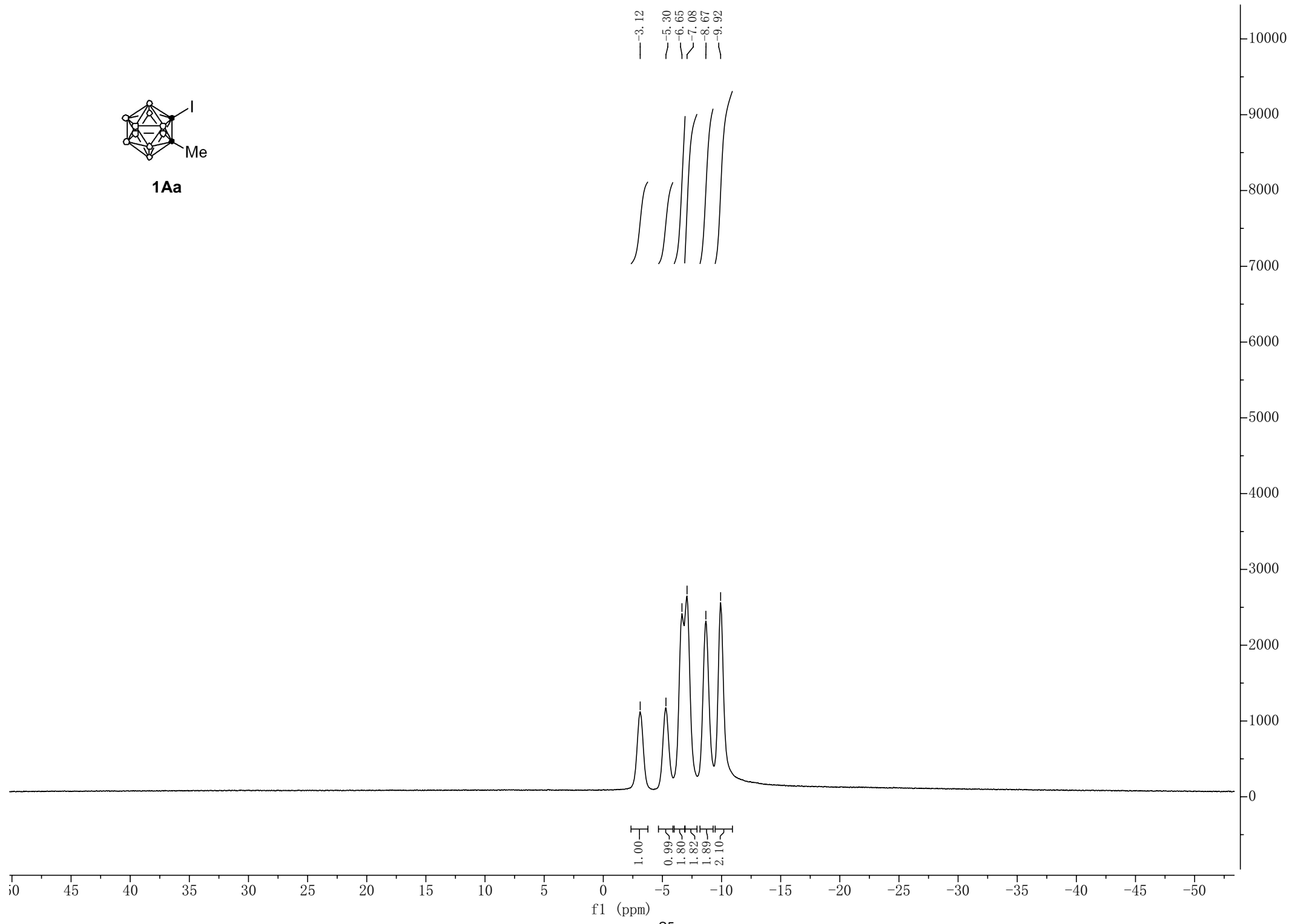
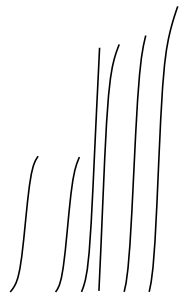
1Aa

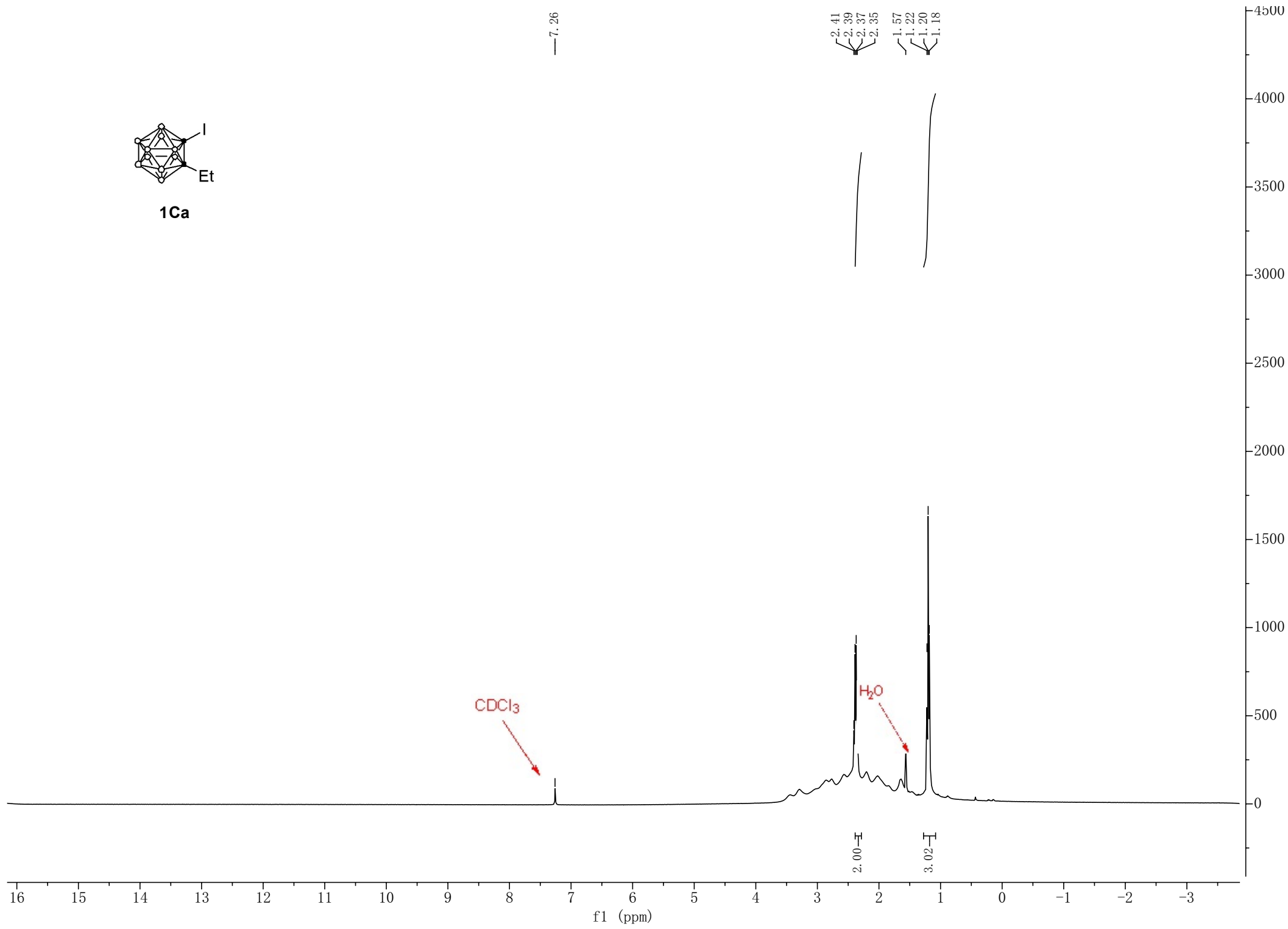
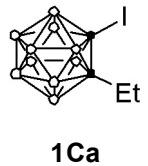


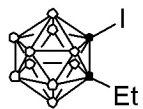


1Aa

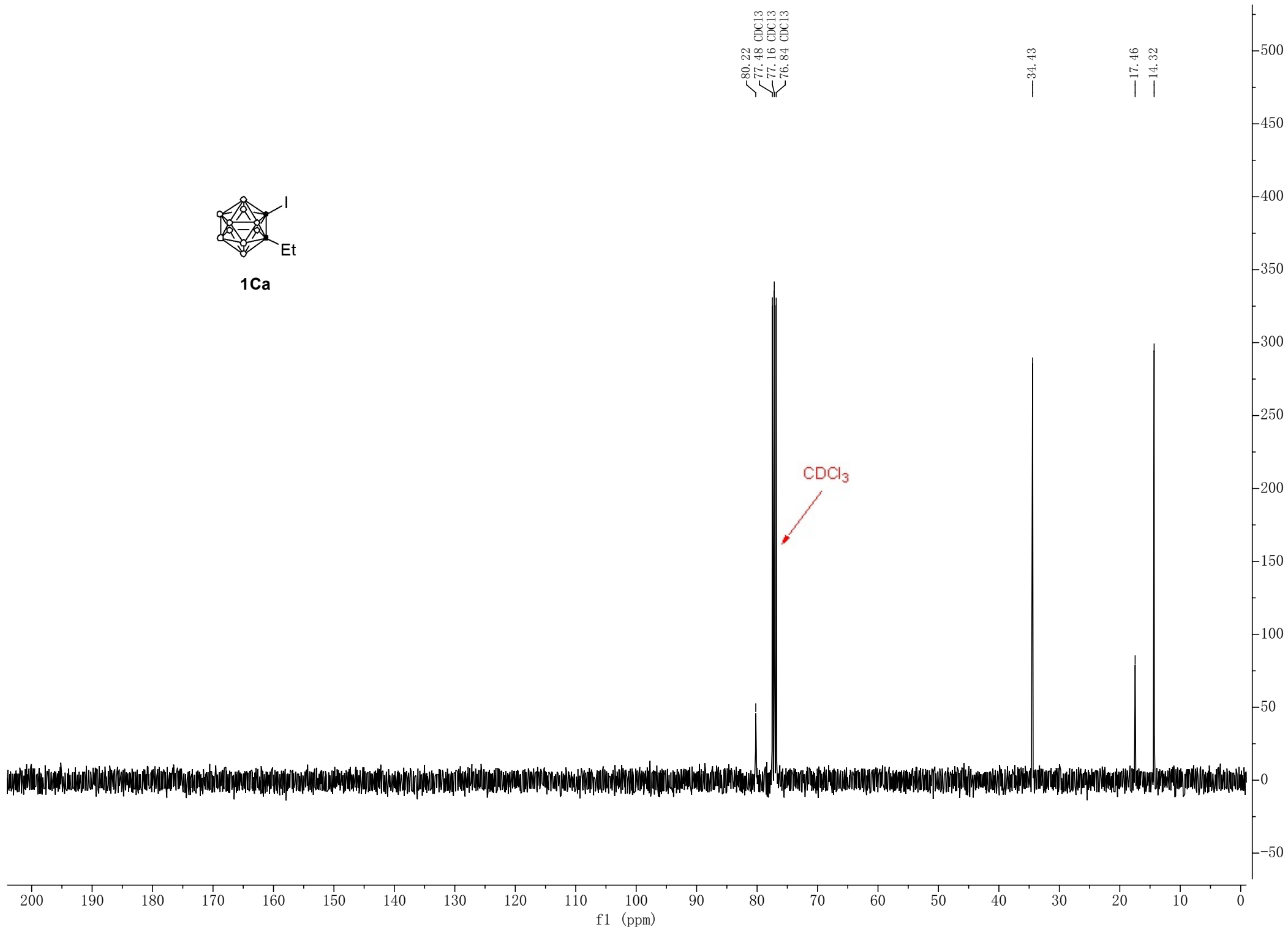
— -3.12
— -5.30
— -6.65
— -7.08
— -8.67
— -9.92

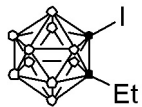




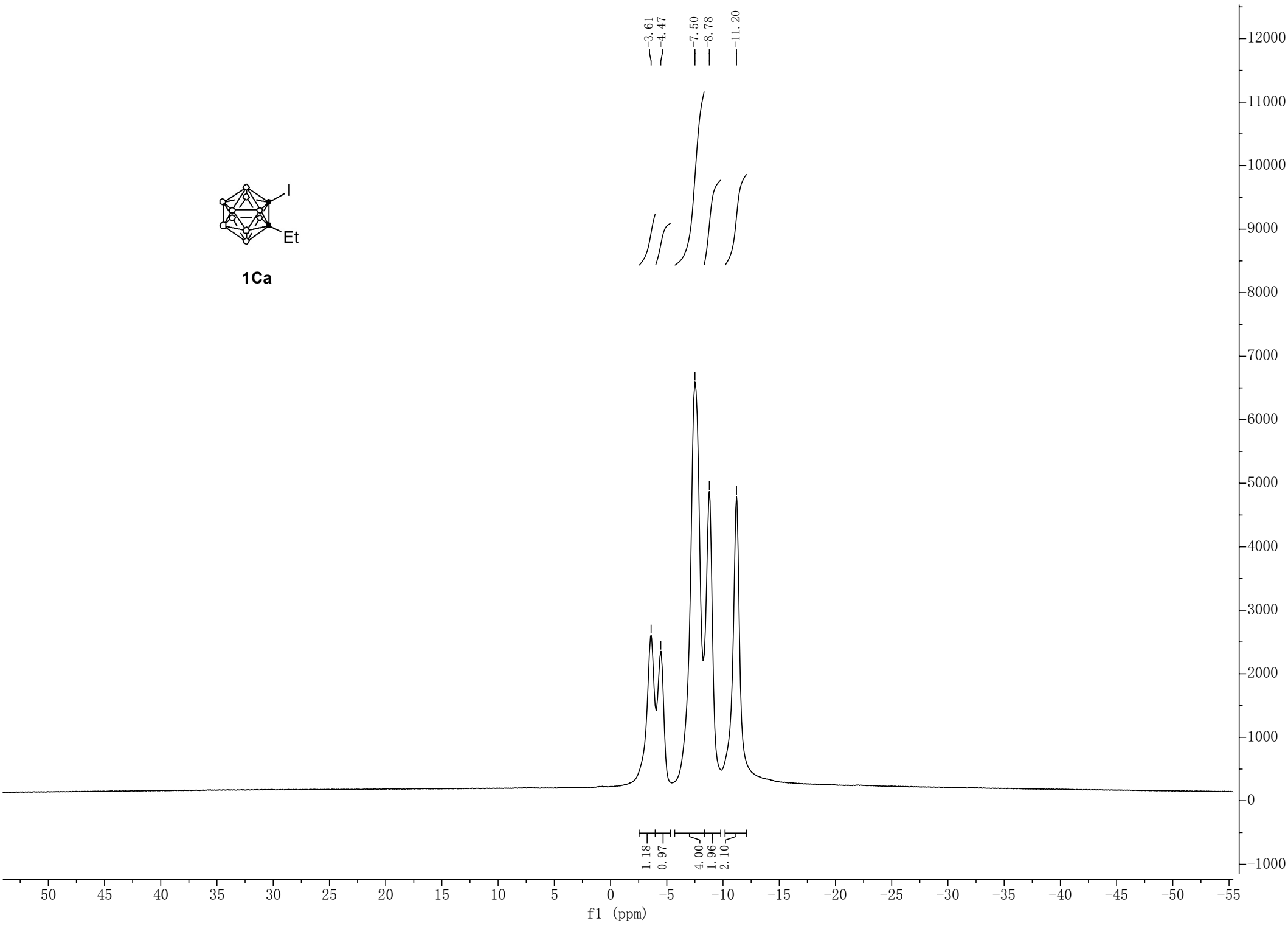


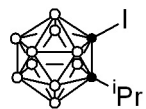
1Ca



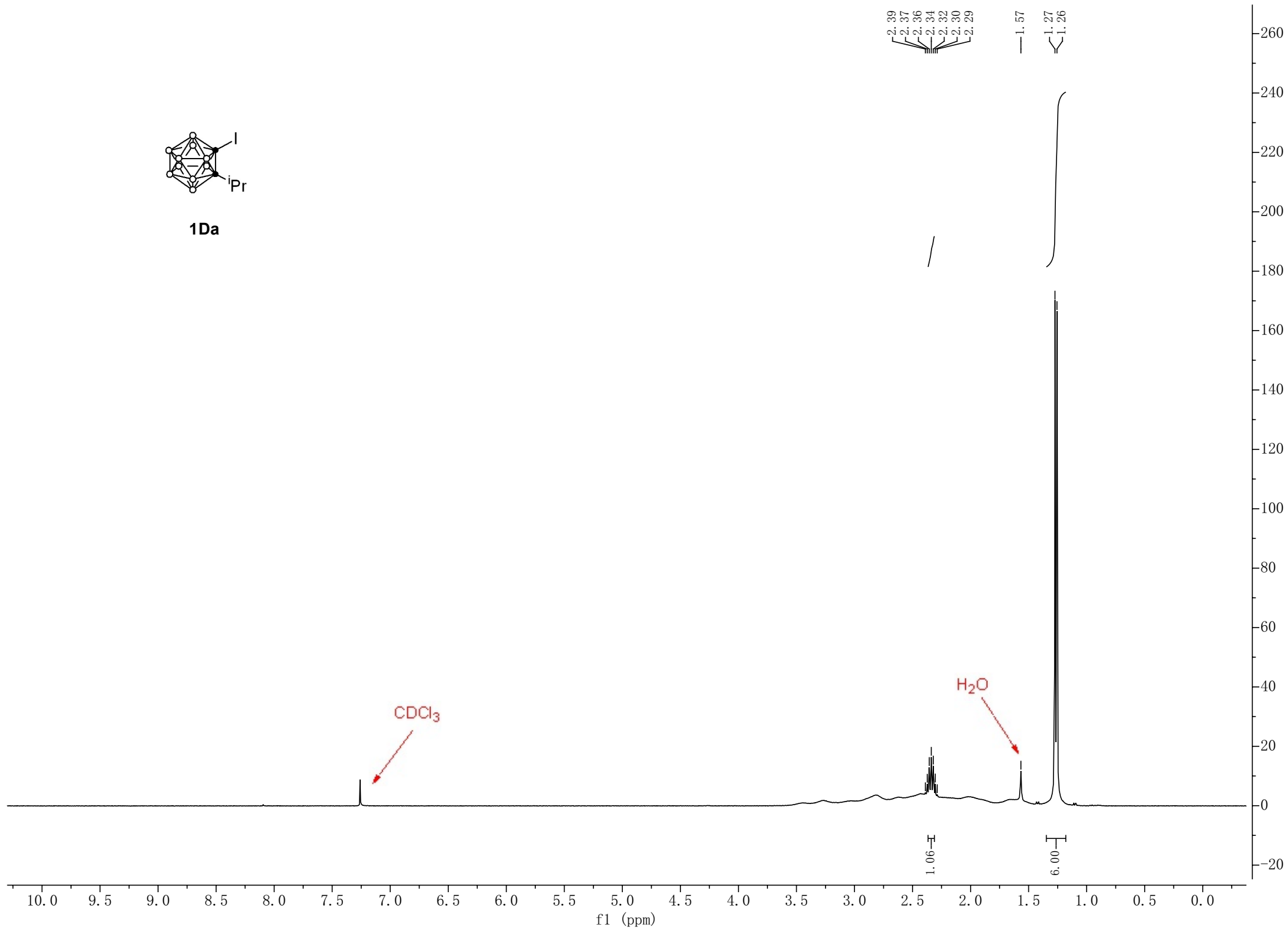


1Ca



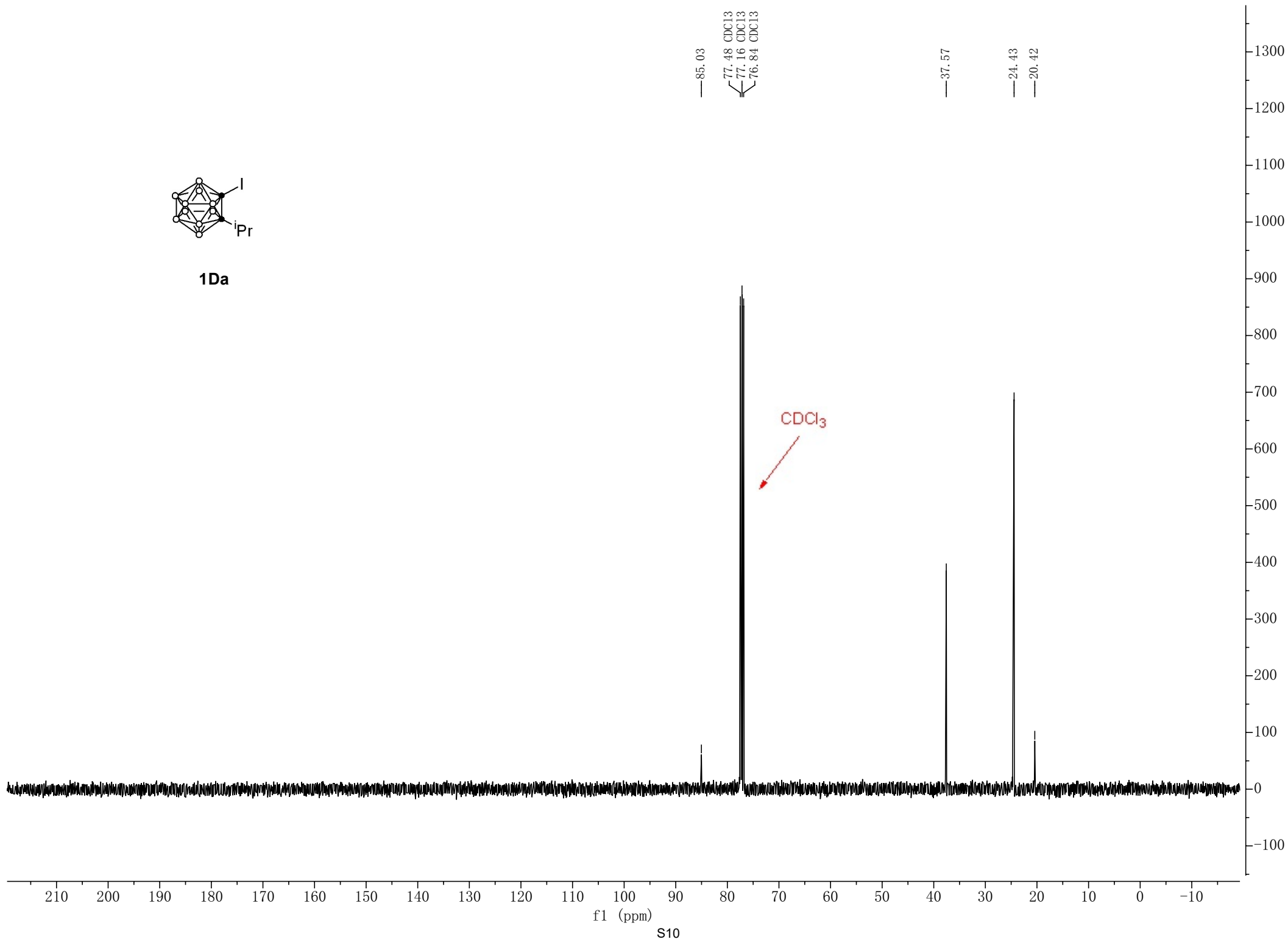


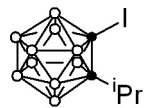
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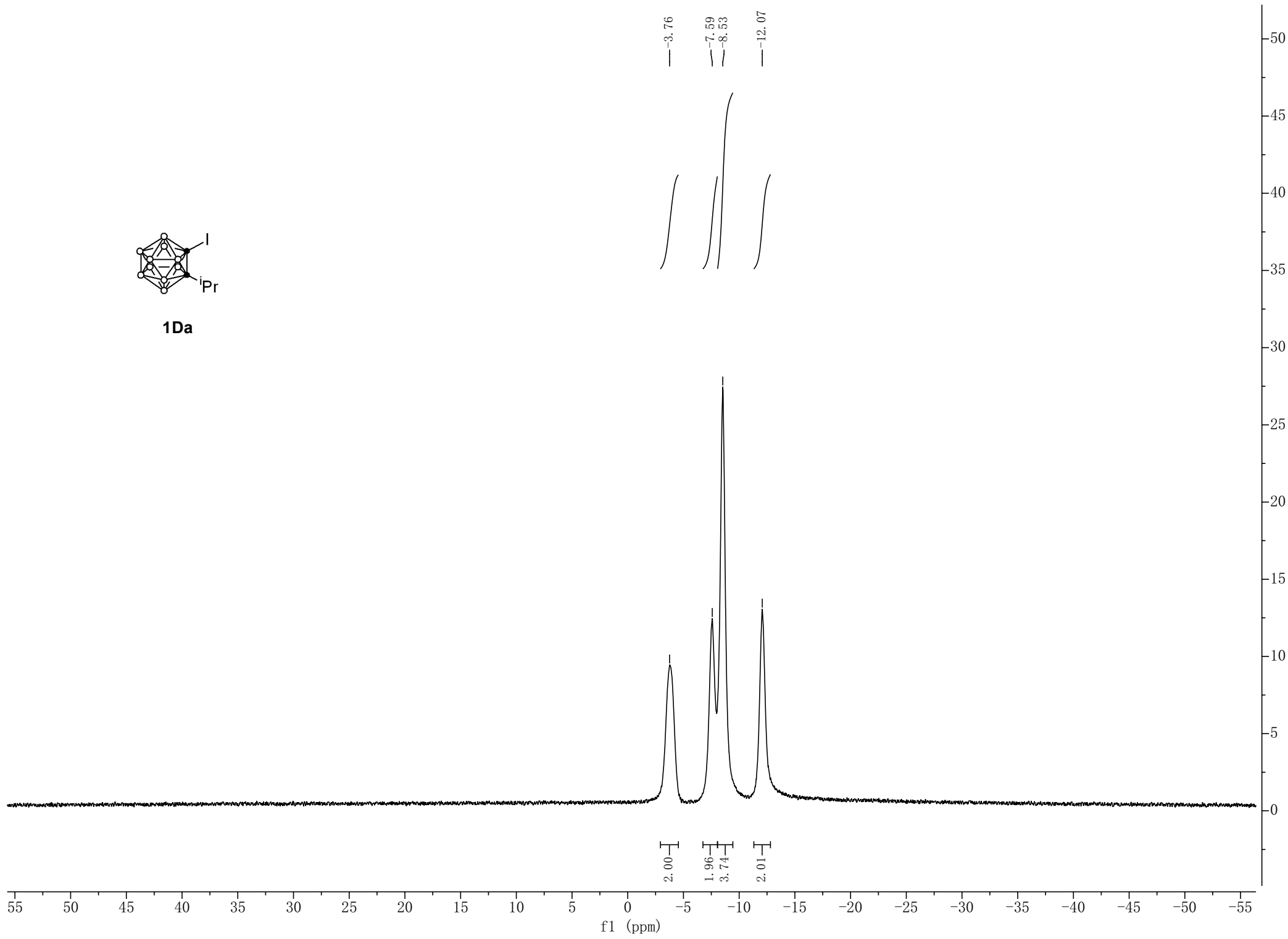


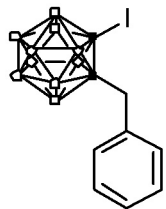
1Da





1Da



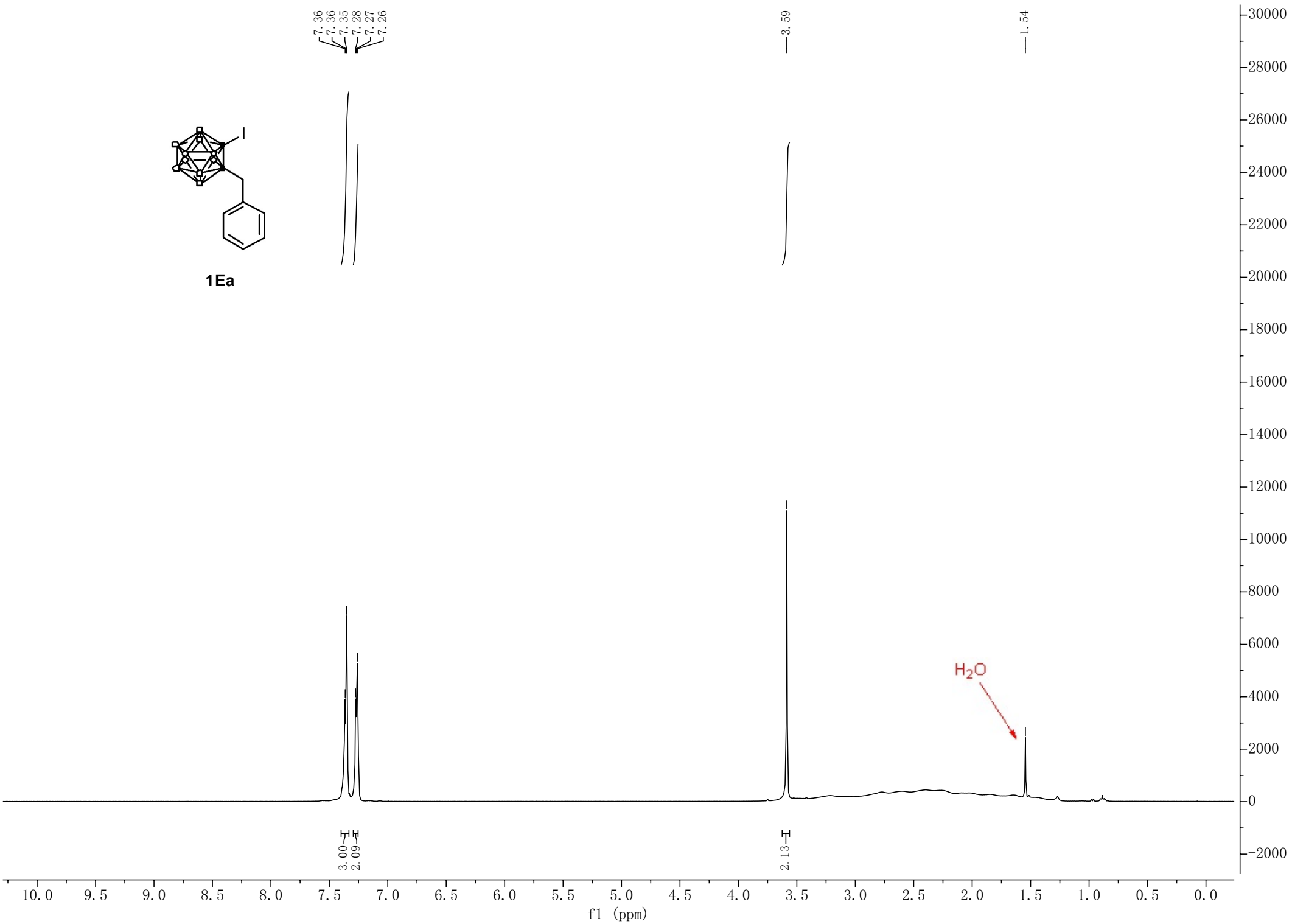


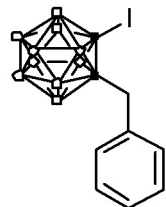
1Ea

7.36
7.36
7.35
7.28
7.27
7.26

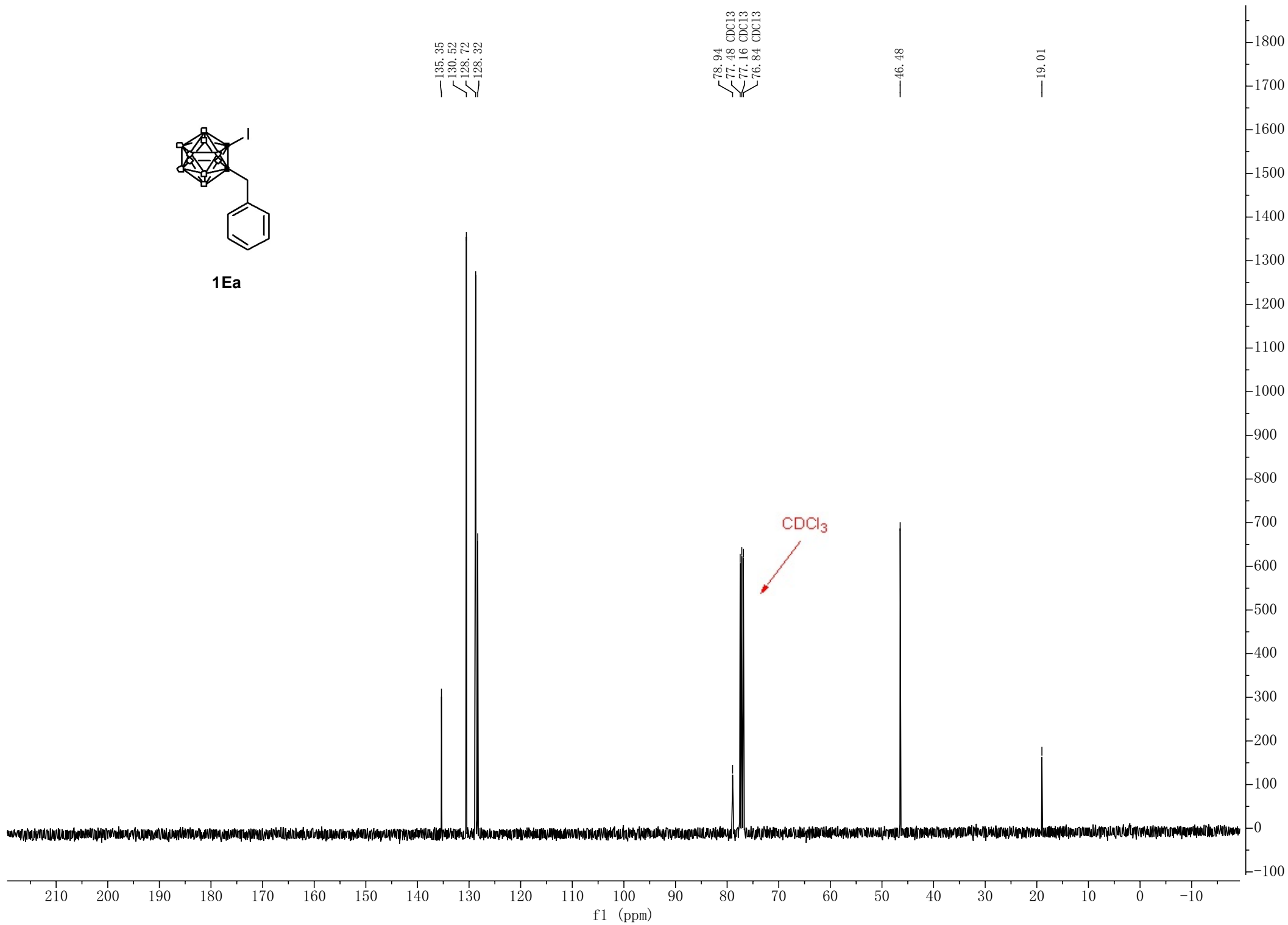
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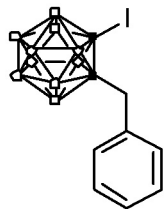
1.54





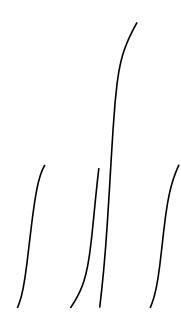
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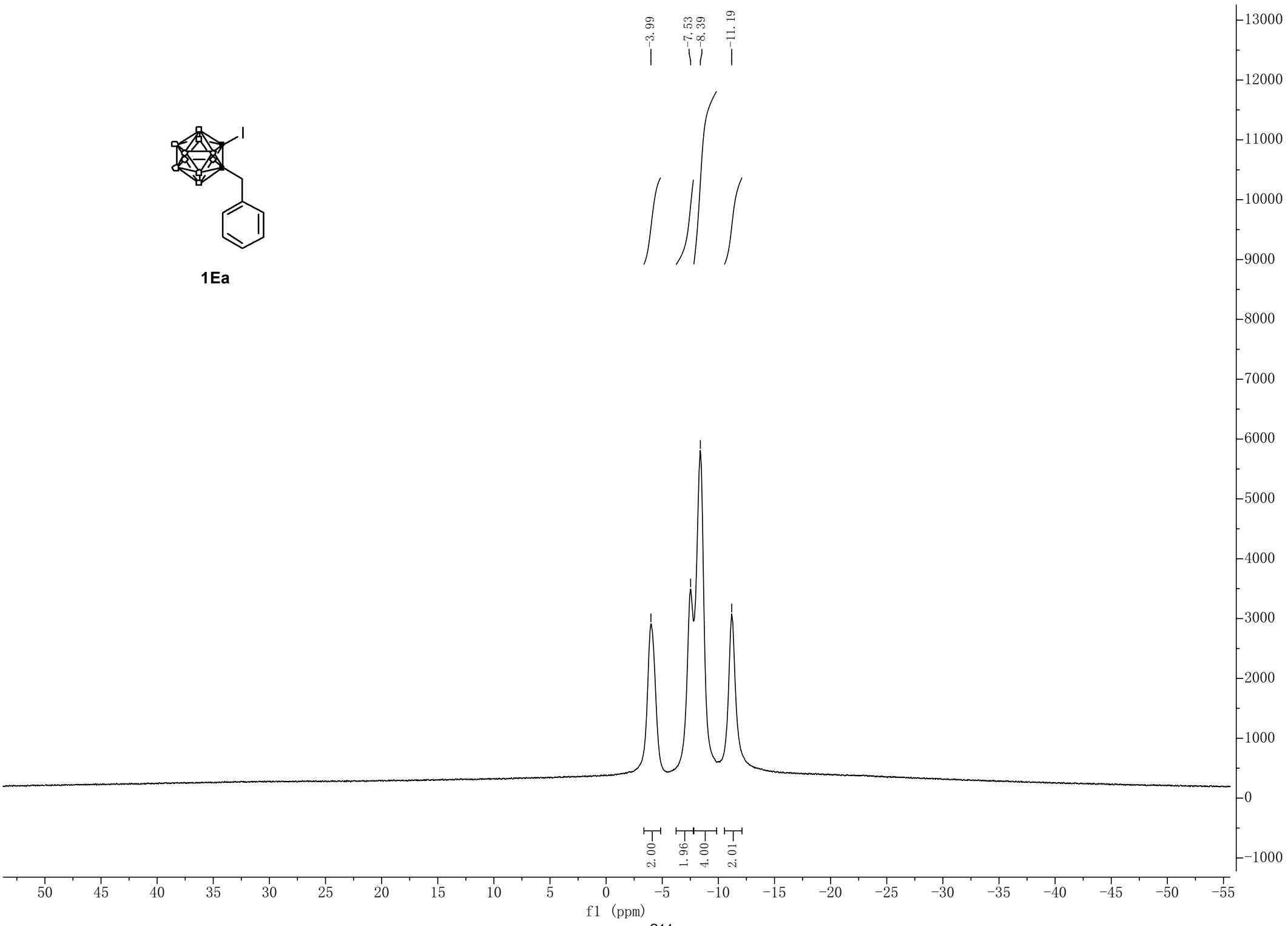


1Ea

— 3.99
— 7.53
— 8.39
— 11.19

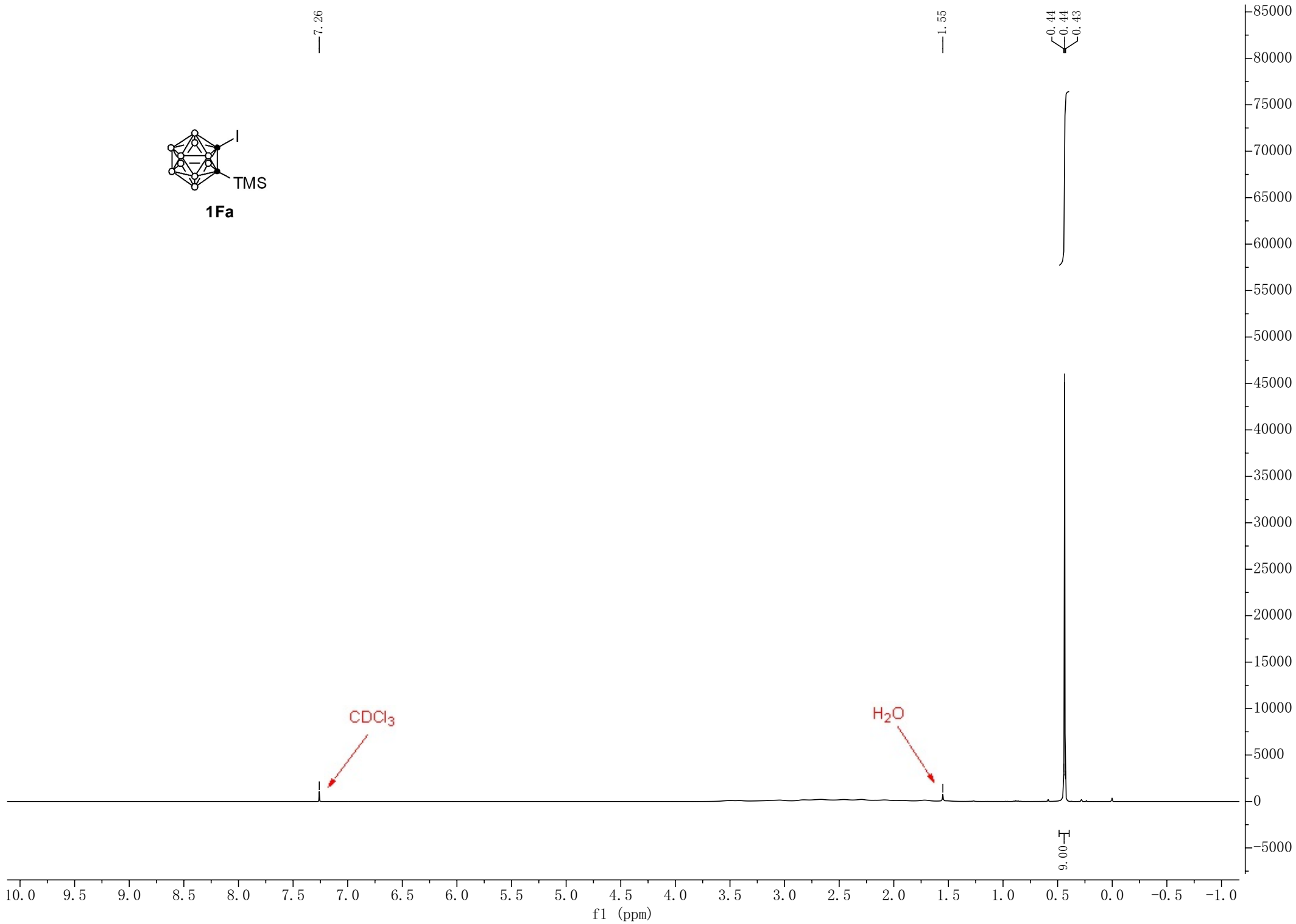
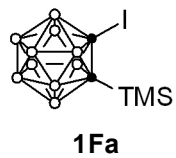


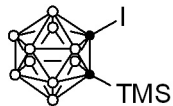
2.00
1.96
4.00
2.01



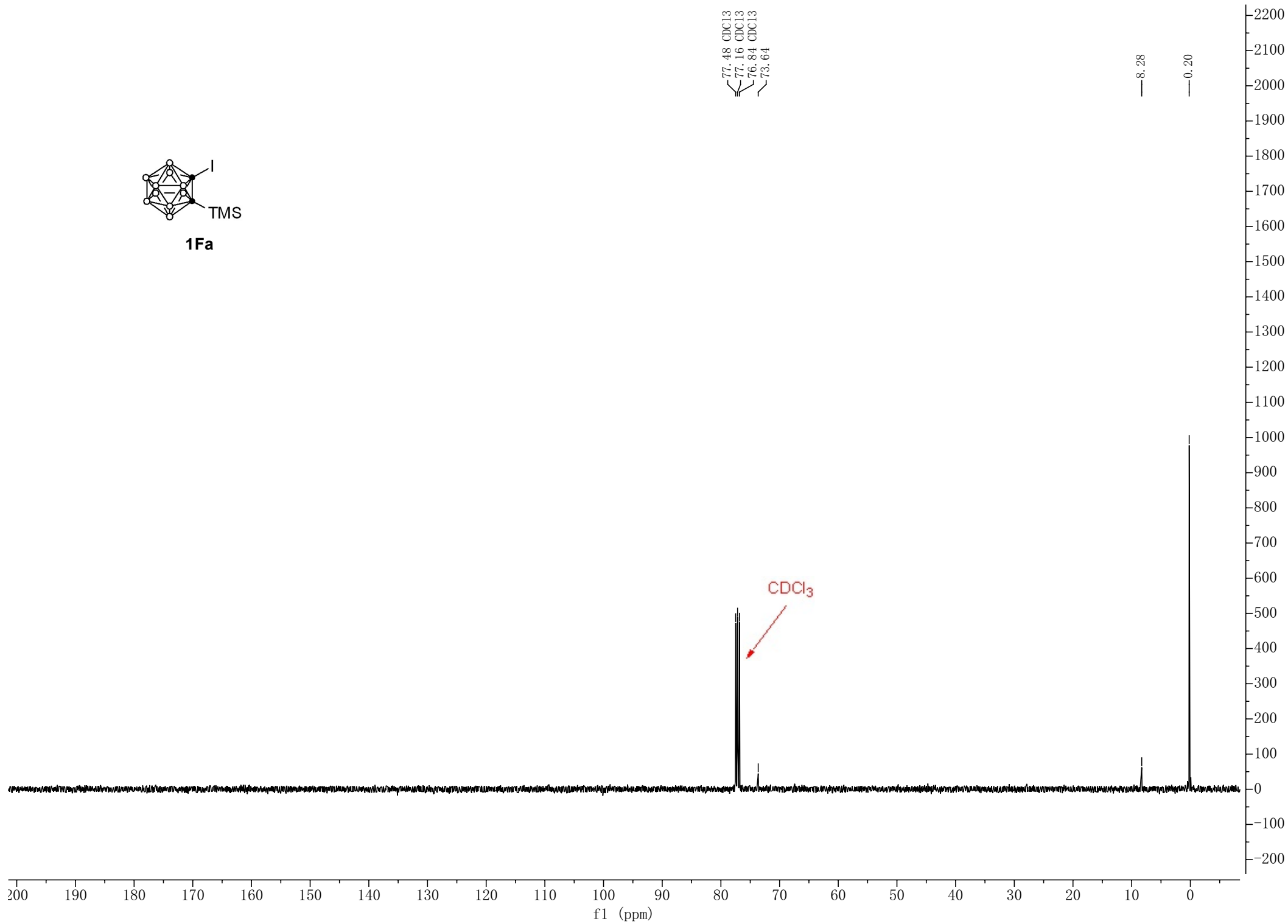
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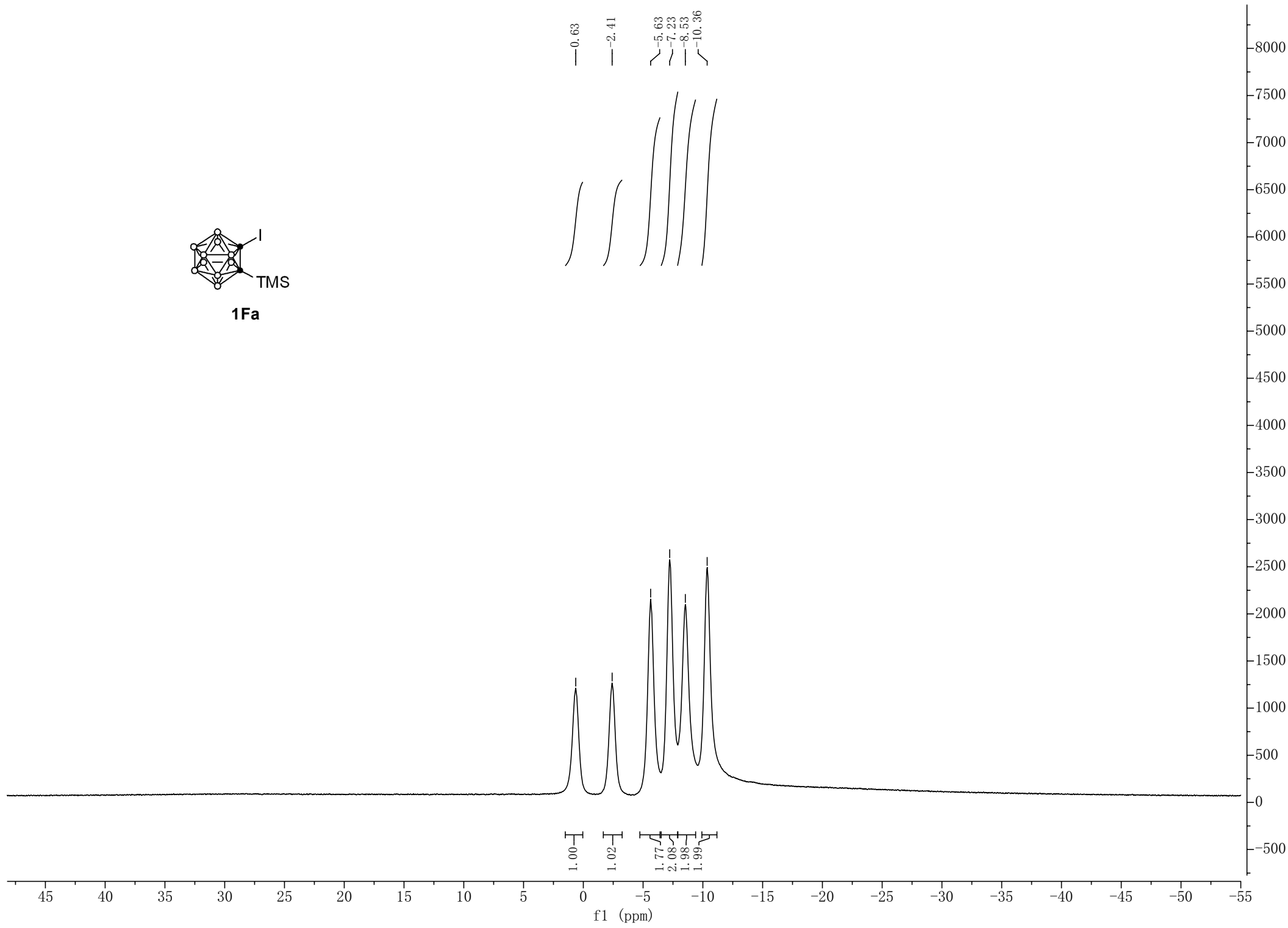
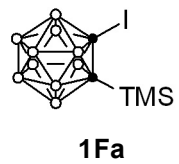
S14

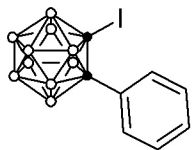




1Fa







1Ga

7.66
7.64
7.54
7.52
7.50
7.45
7.44
7.42
7.26



1.57

H₂O

CDCl₃

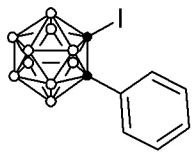
1.96
1.00
1.89

10.5 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

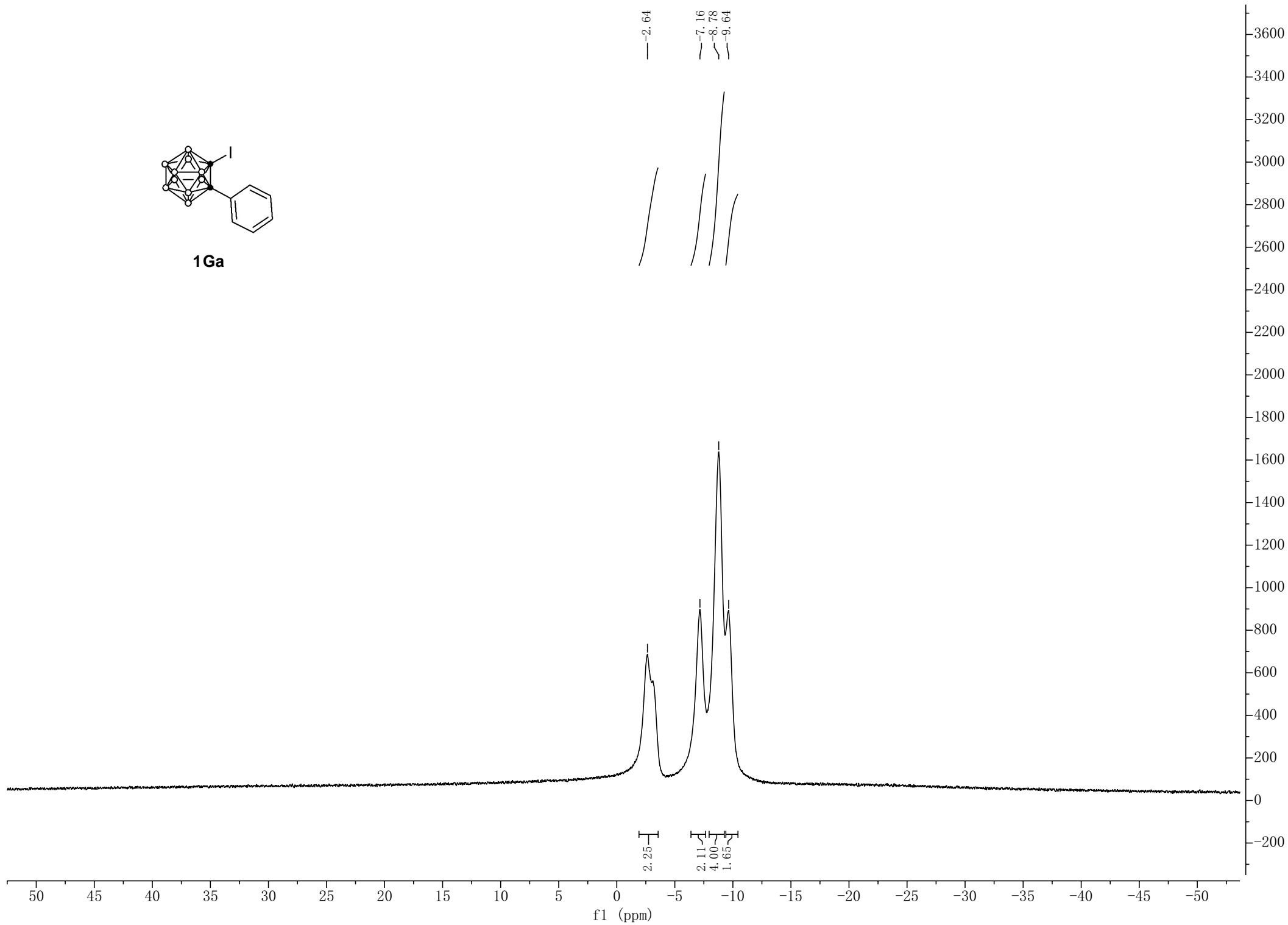
f1 (ppm)

S18

3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200

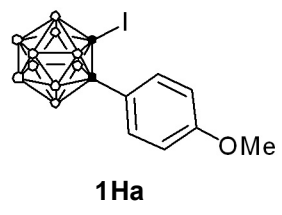


1Ga



-2.64
-7.16
-8.78
-9.64

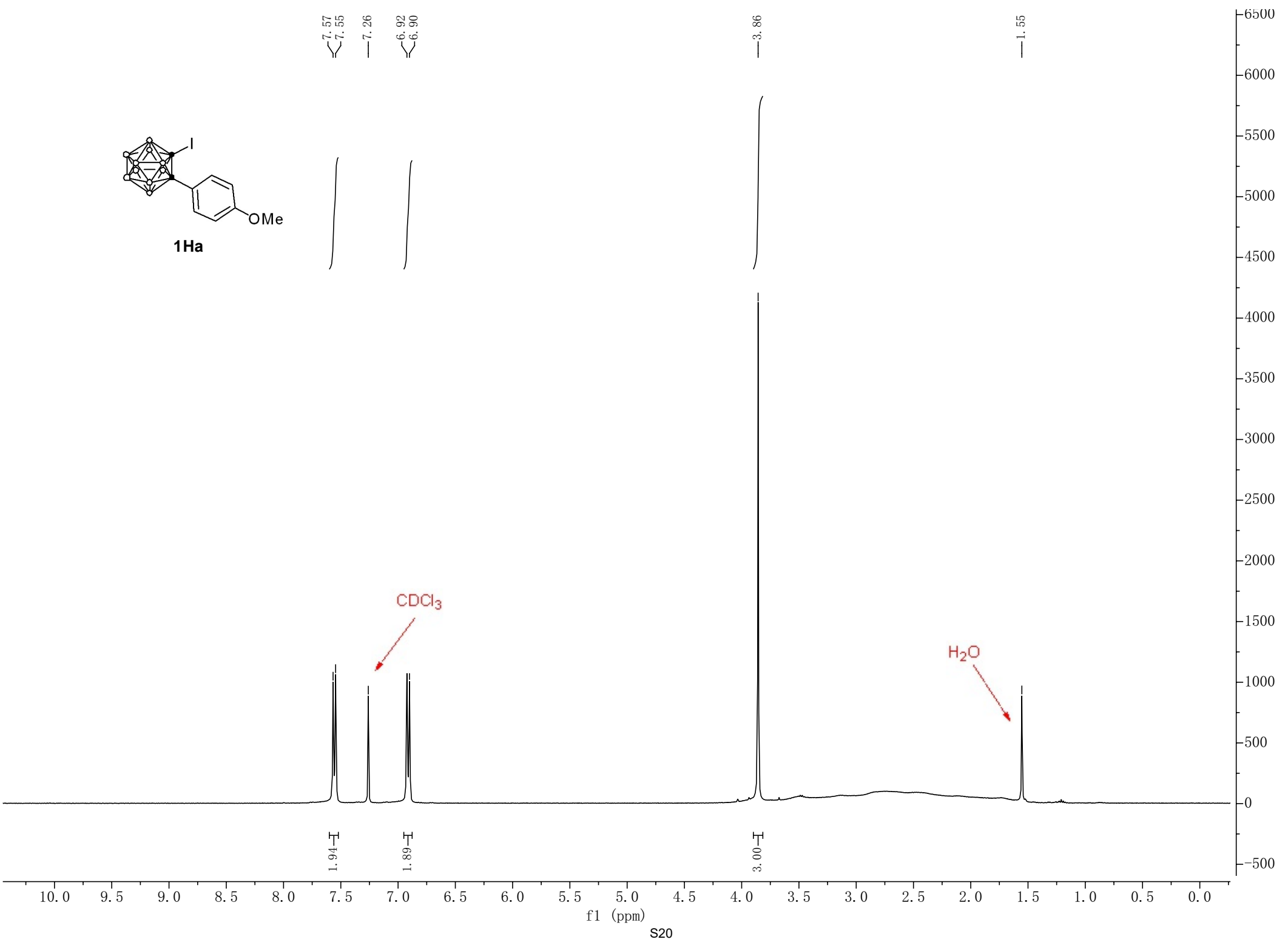
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2.11
4.00
1.65

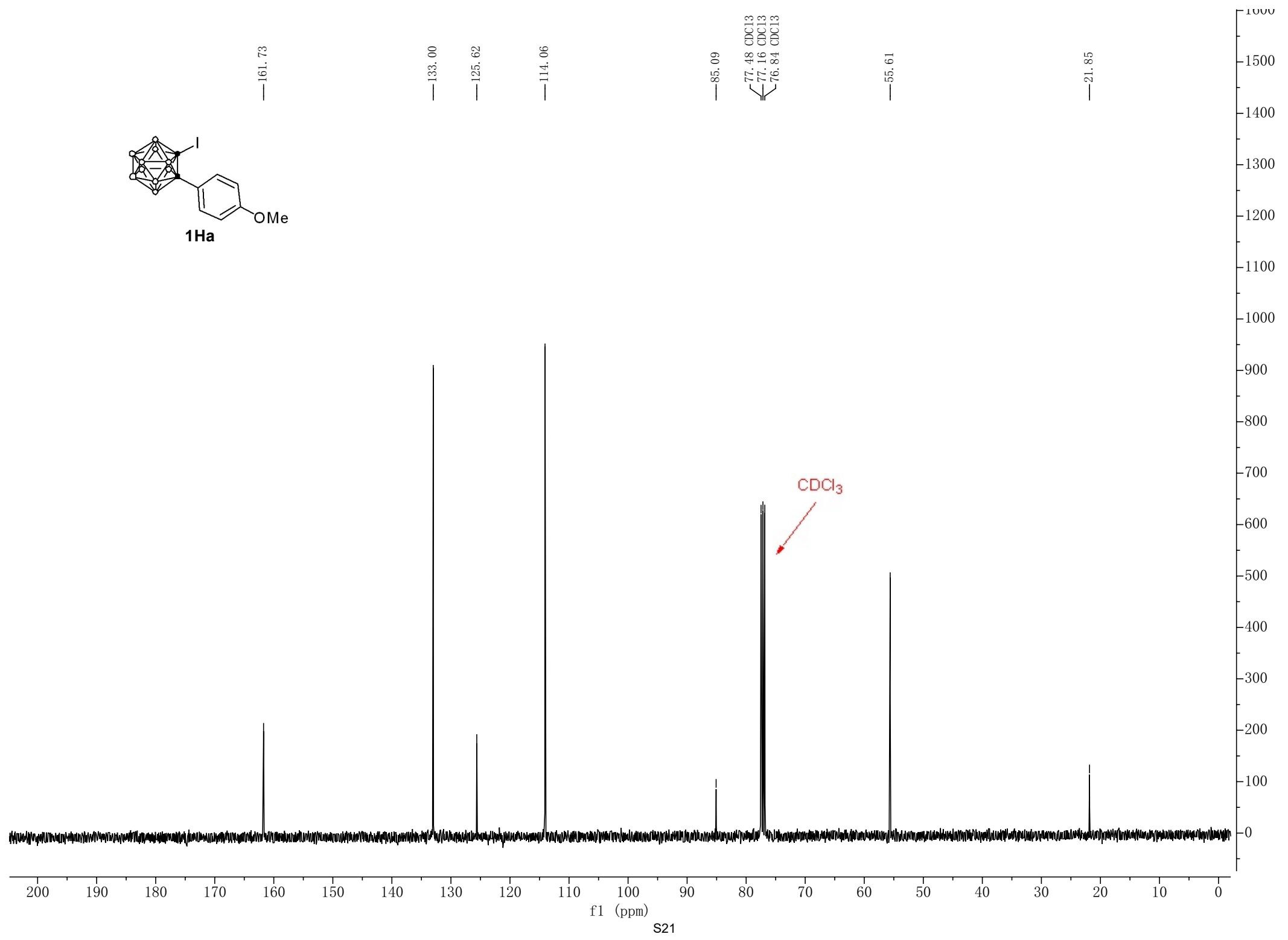
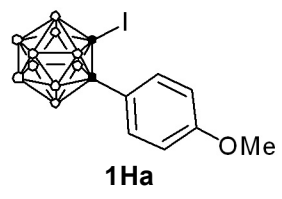


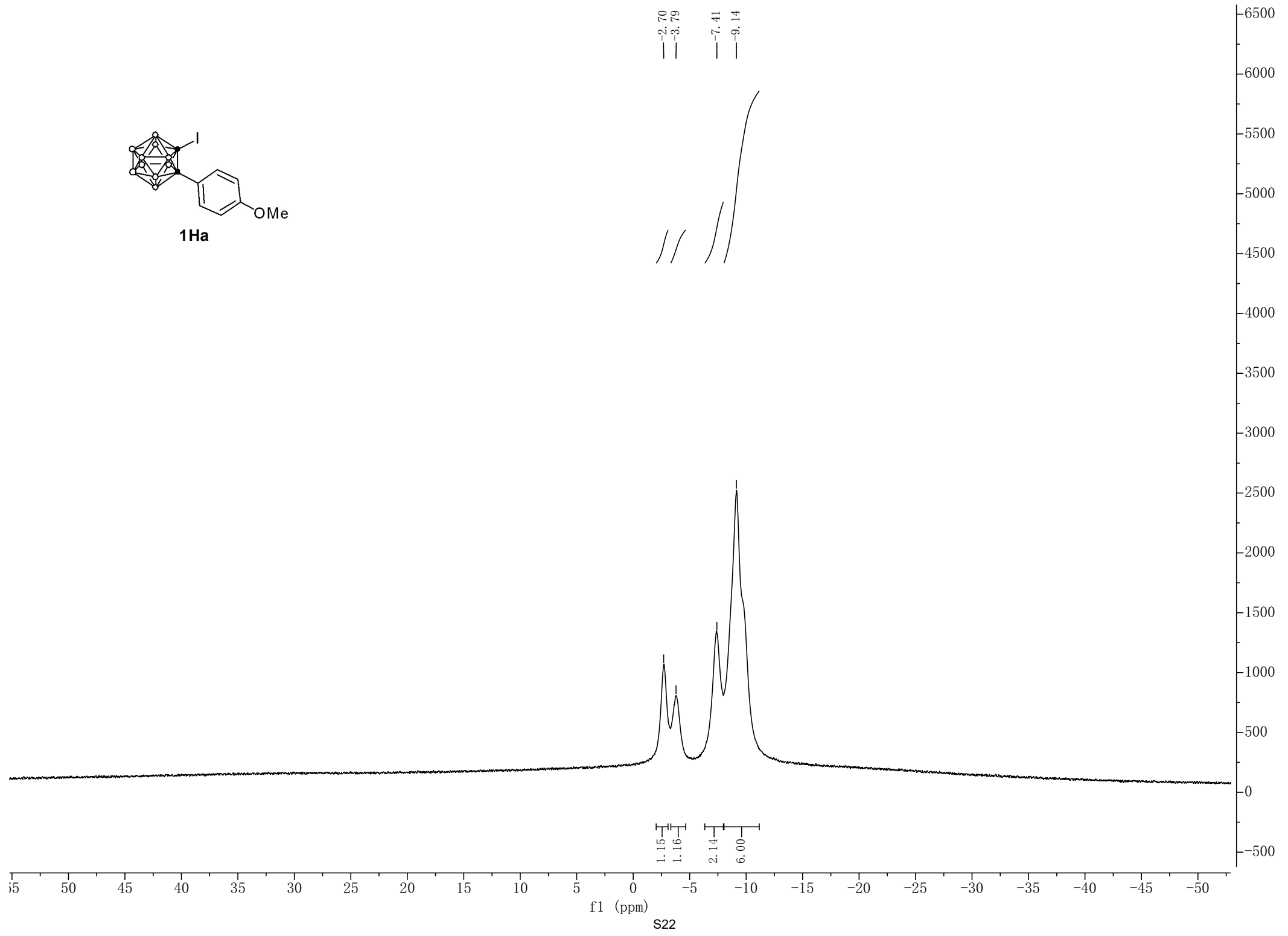
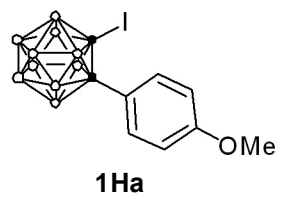
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7.55
7.26
6.92
6.90

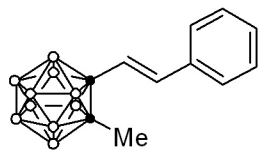
3.86

1.55

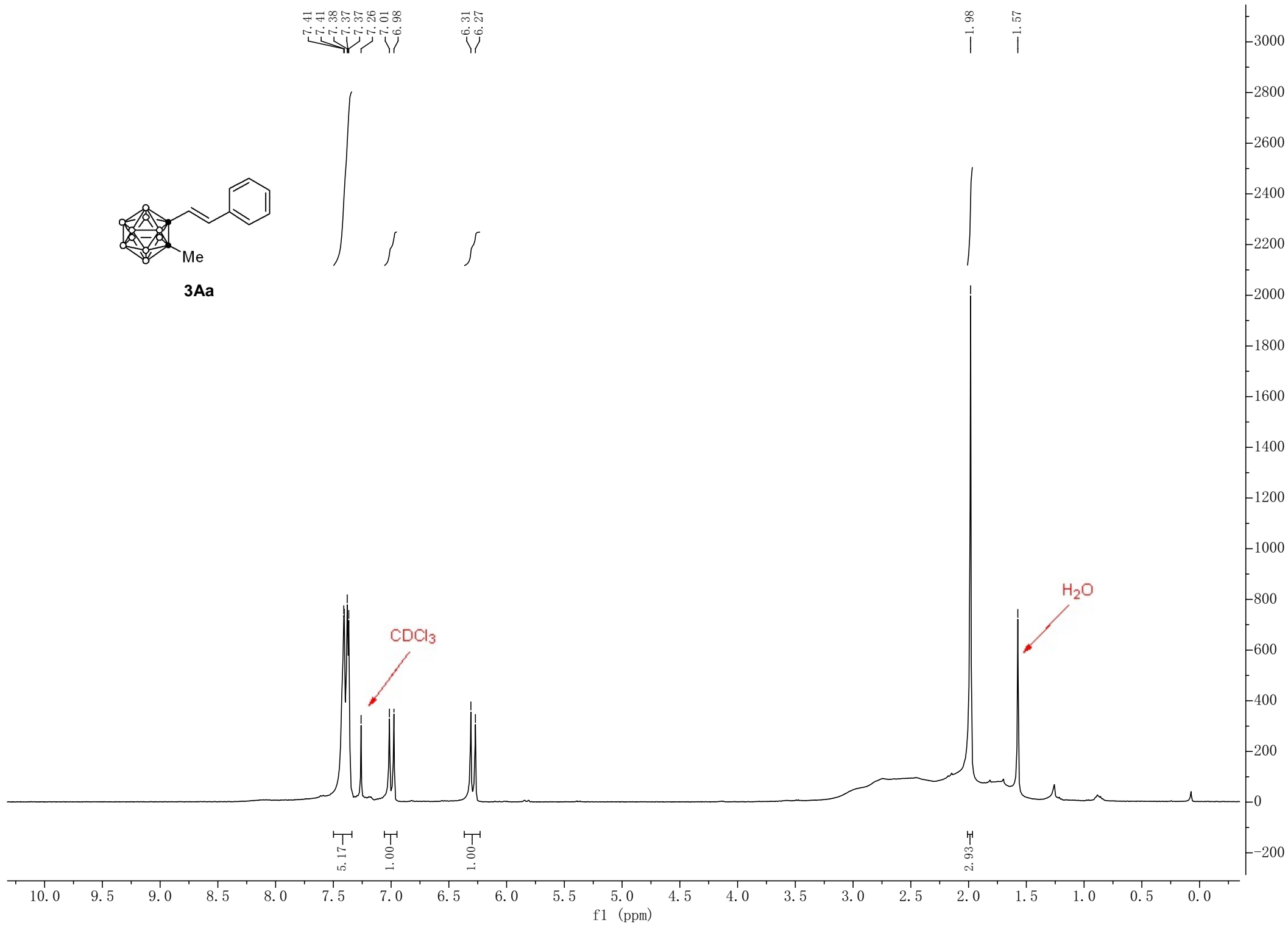


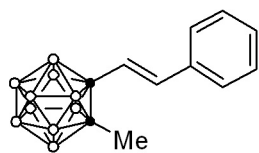




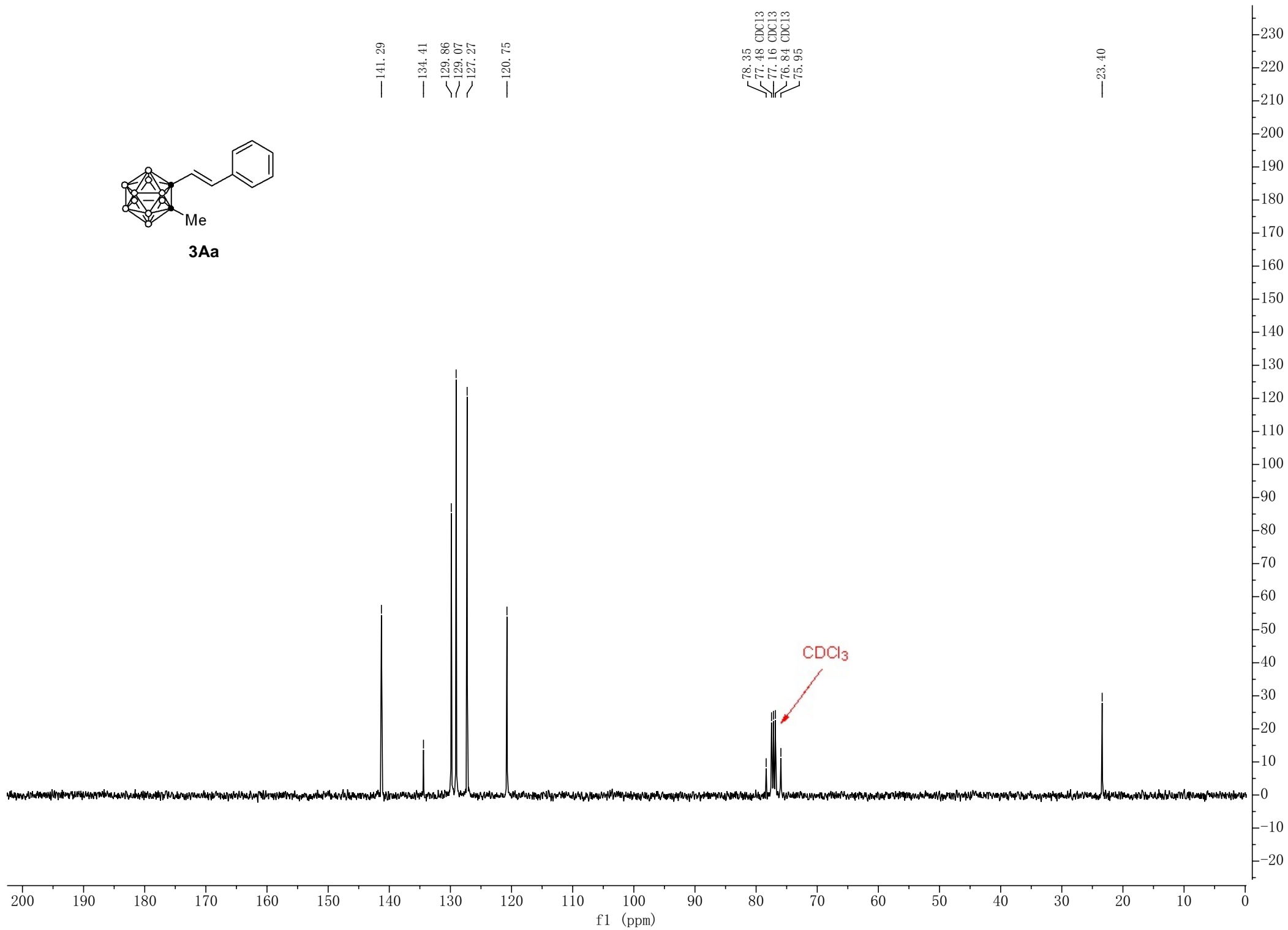


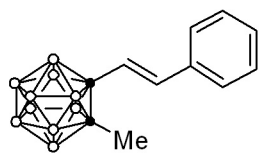
3Aa



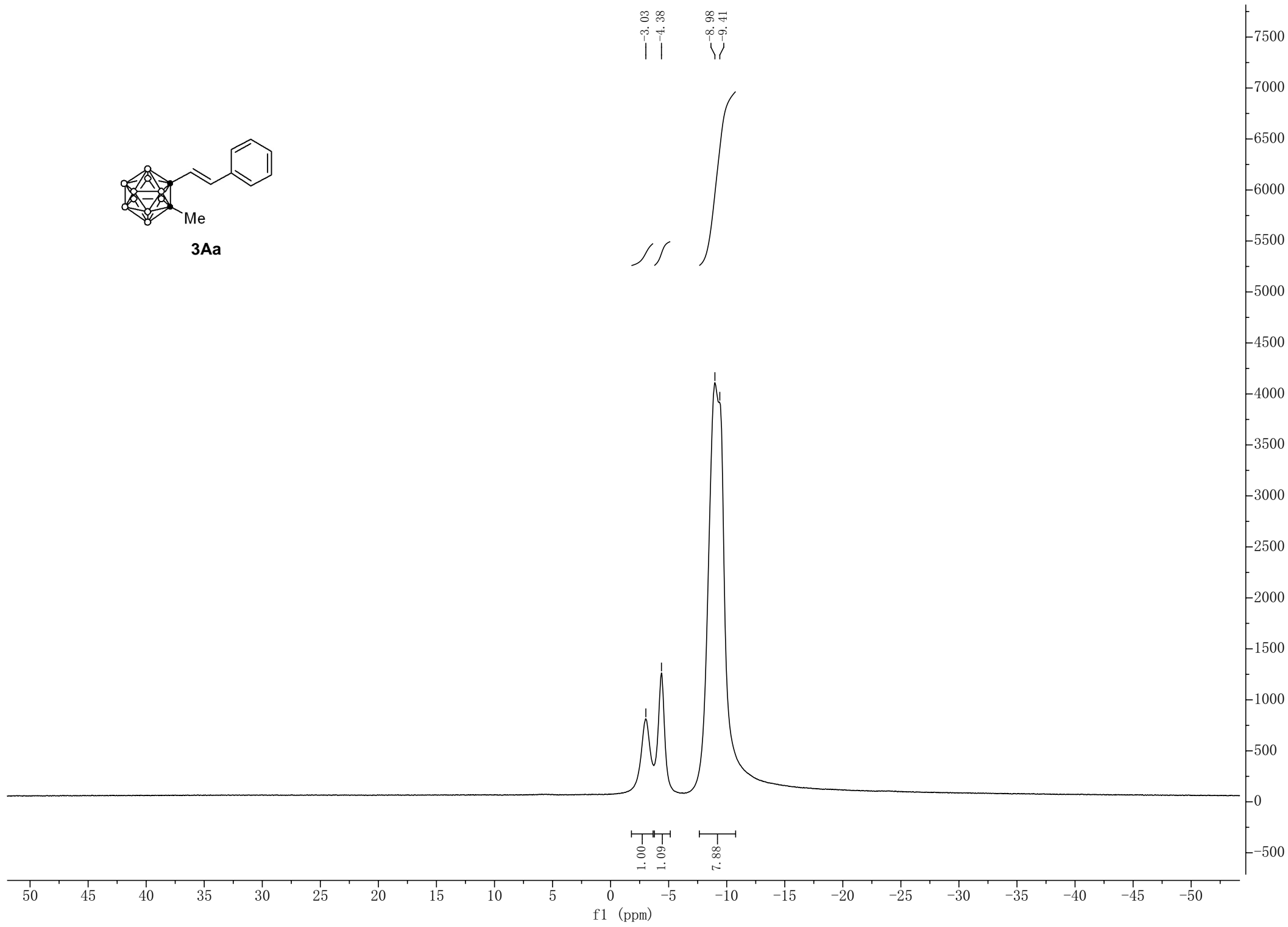


3Aa





3Aa

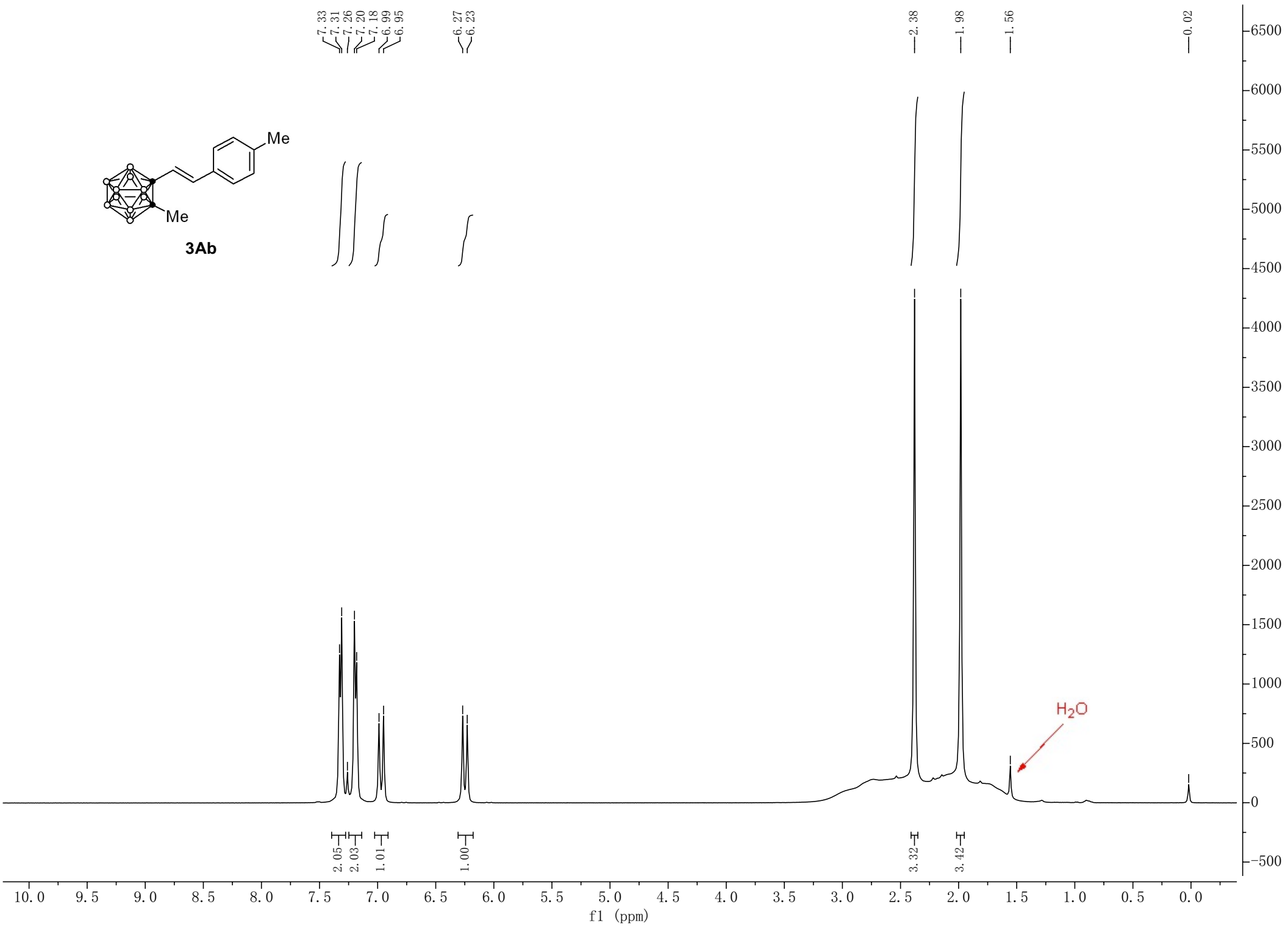
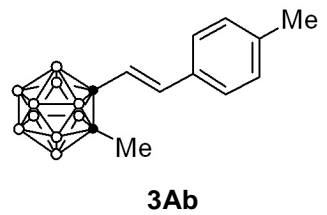


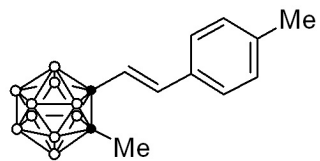
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— 4.38
— 8.98
— 9.41

1.00
1.09
7.88

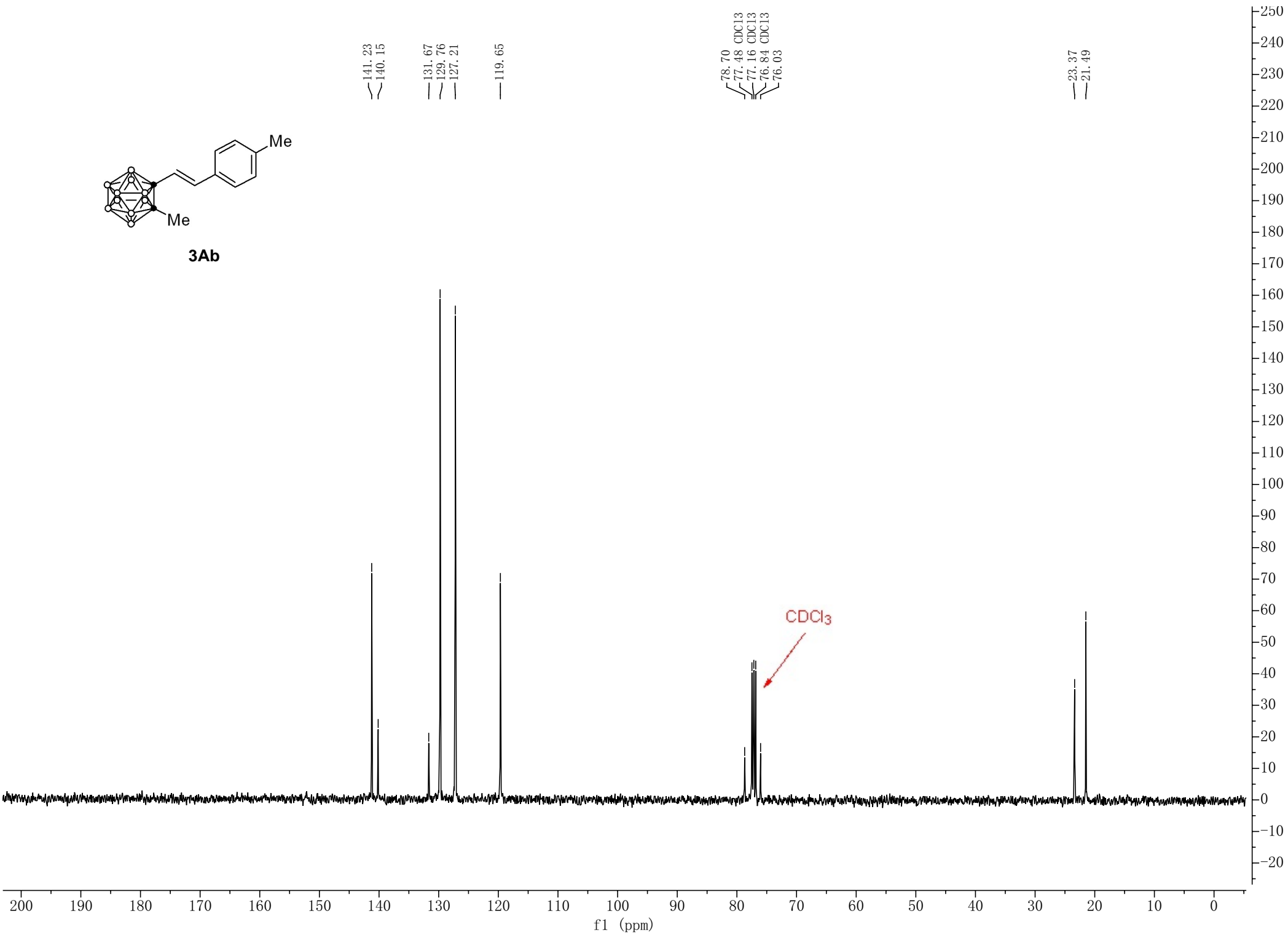
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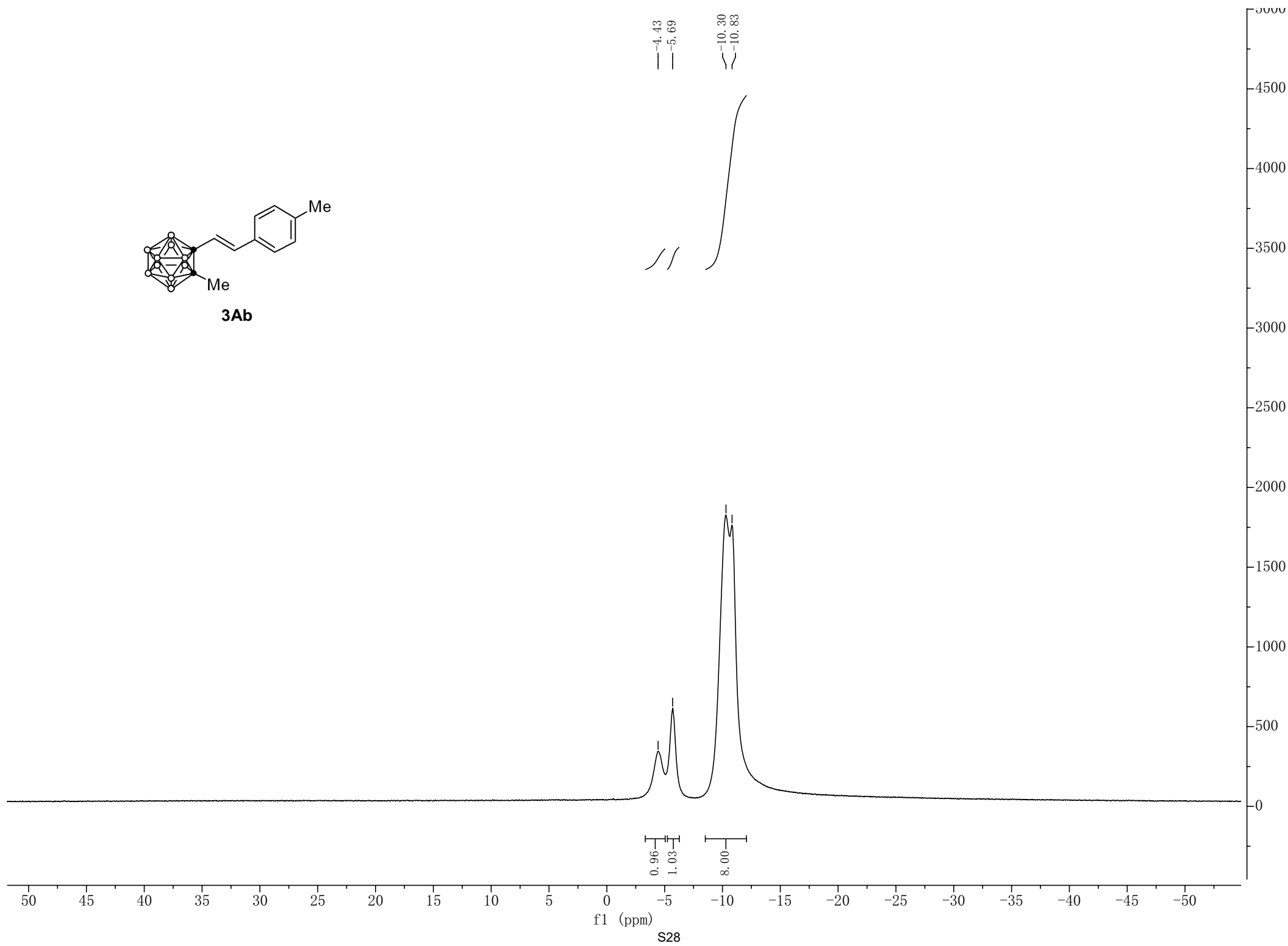
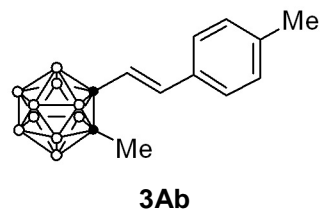
S25

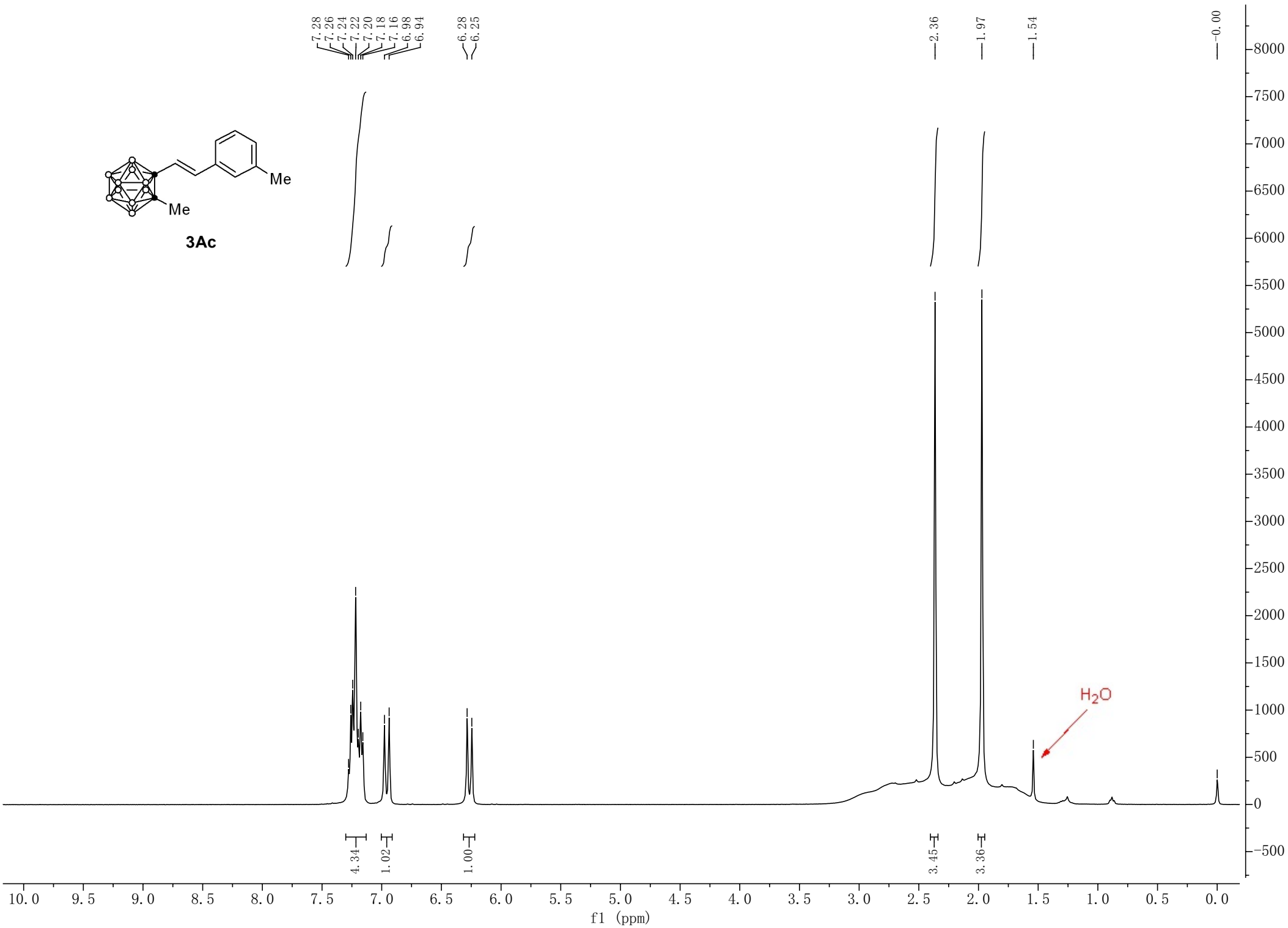
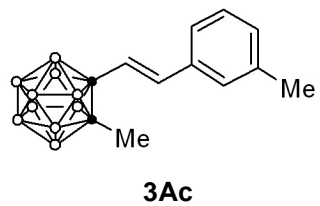


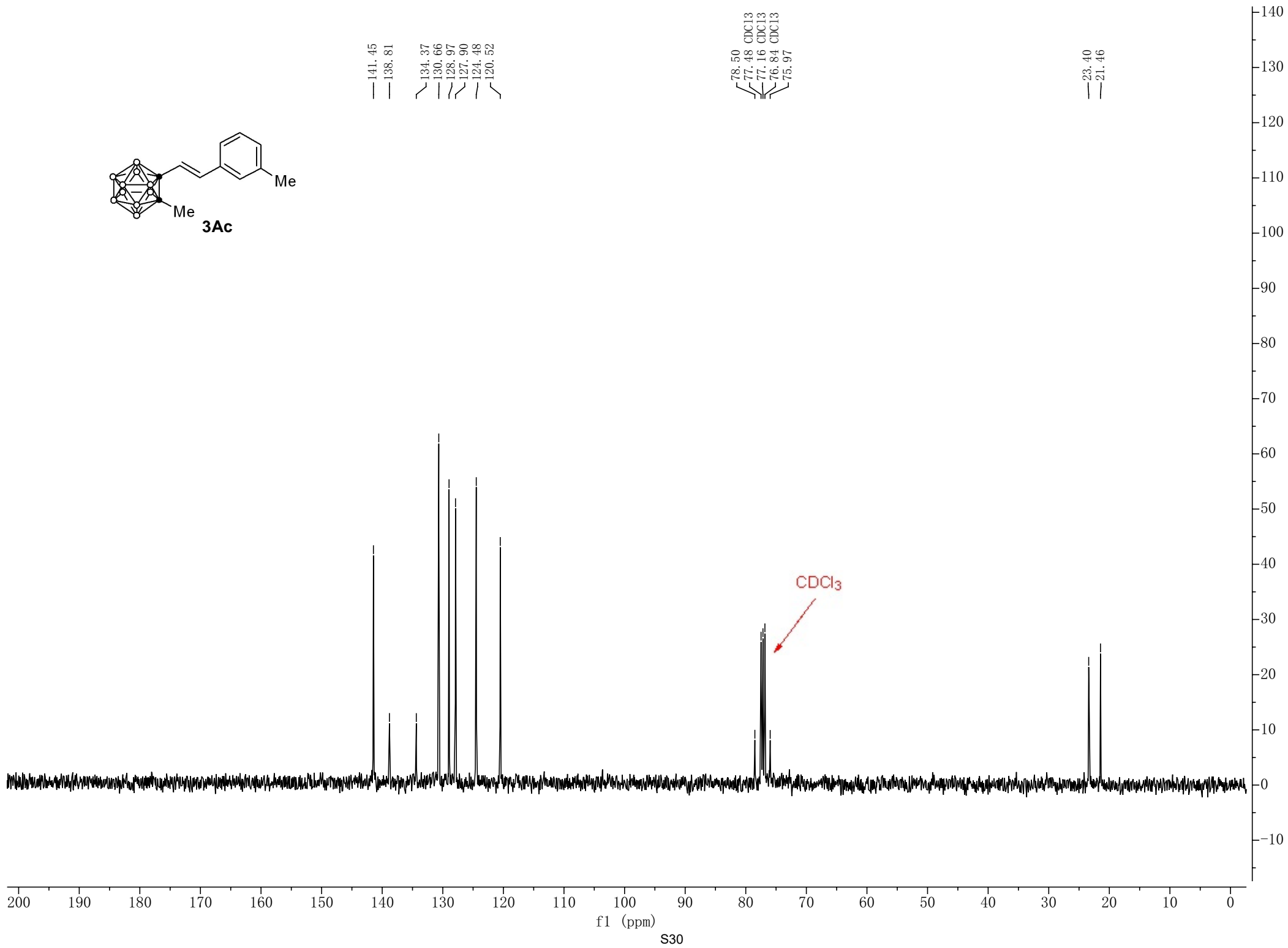
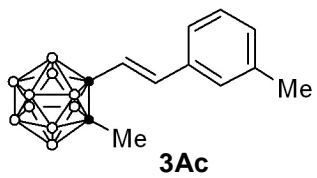


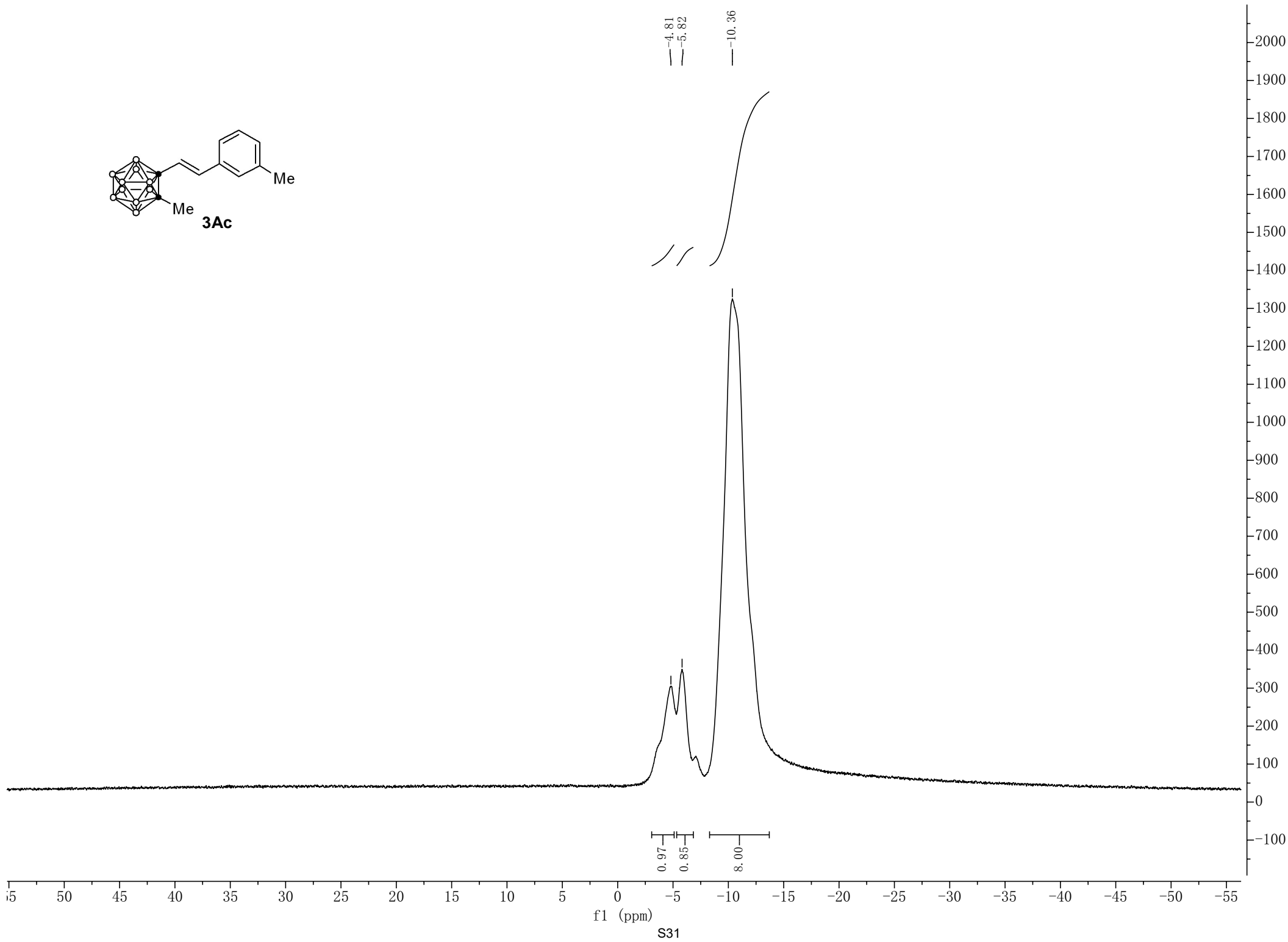
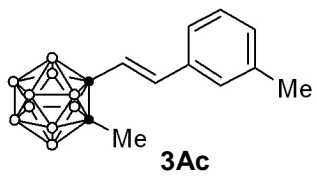
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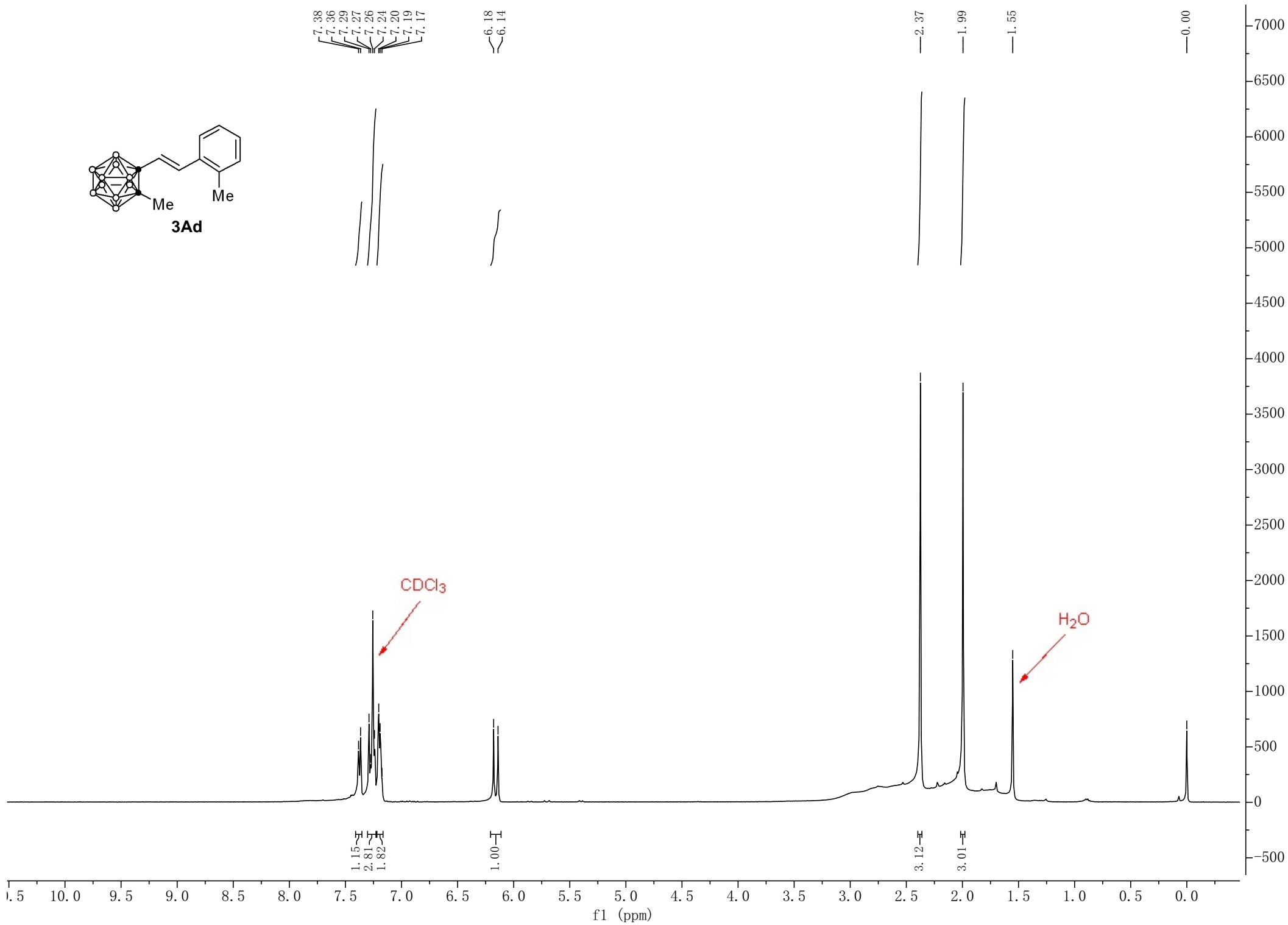
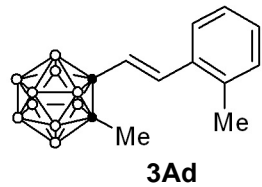


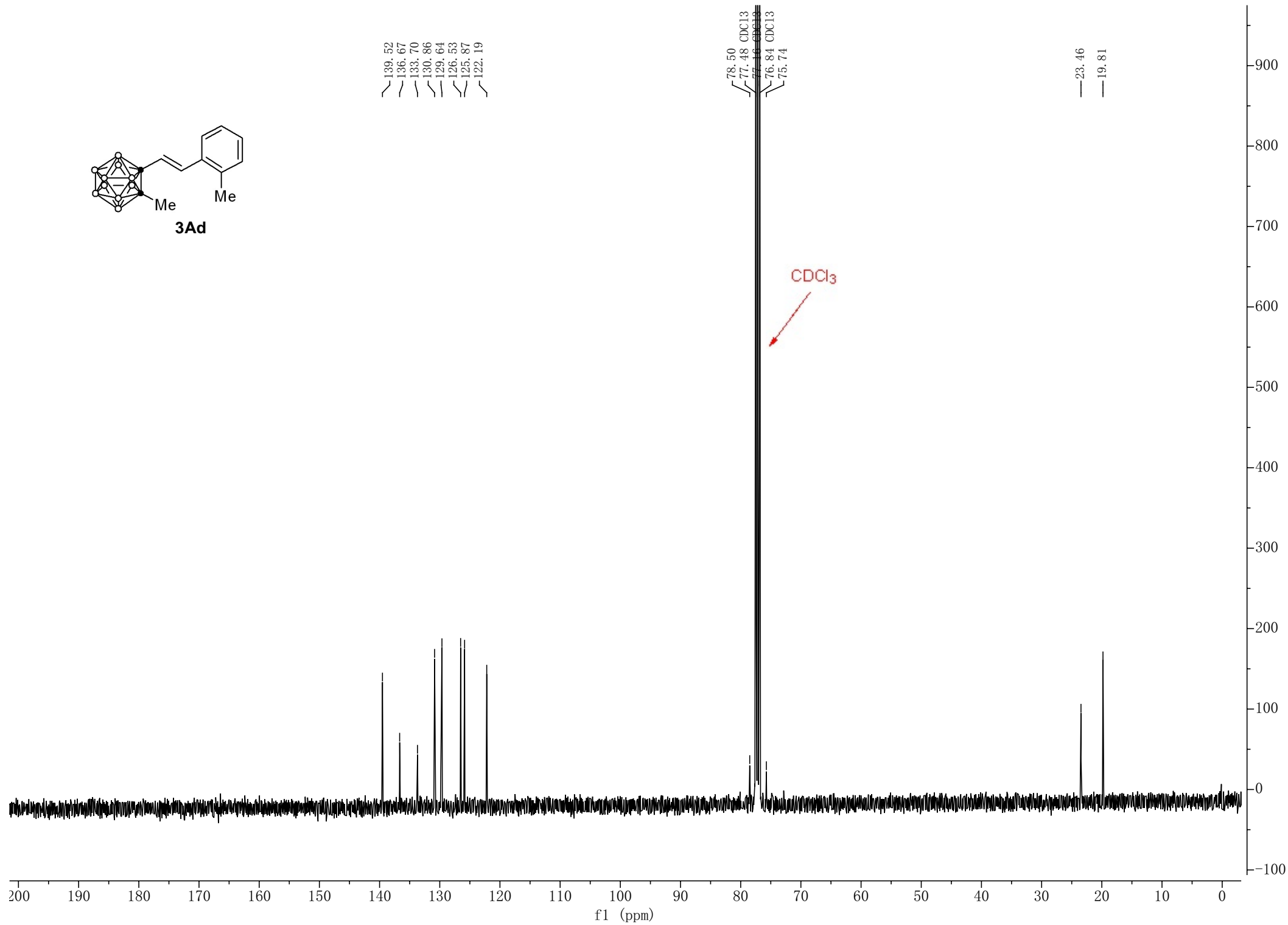
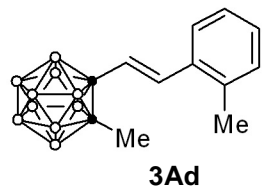


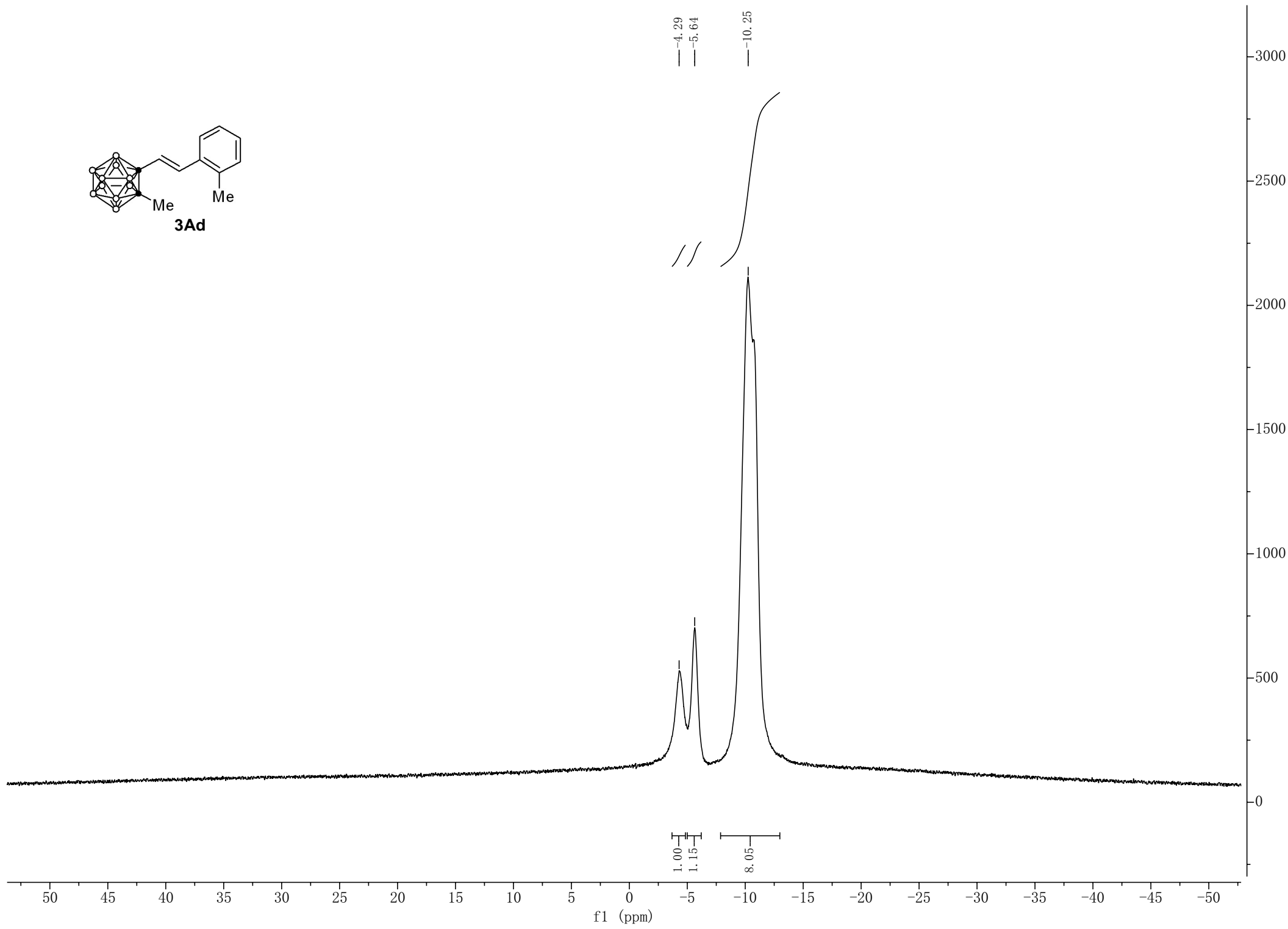
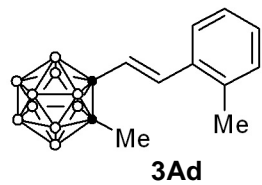


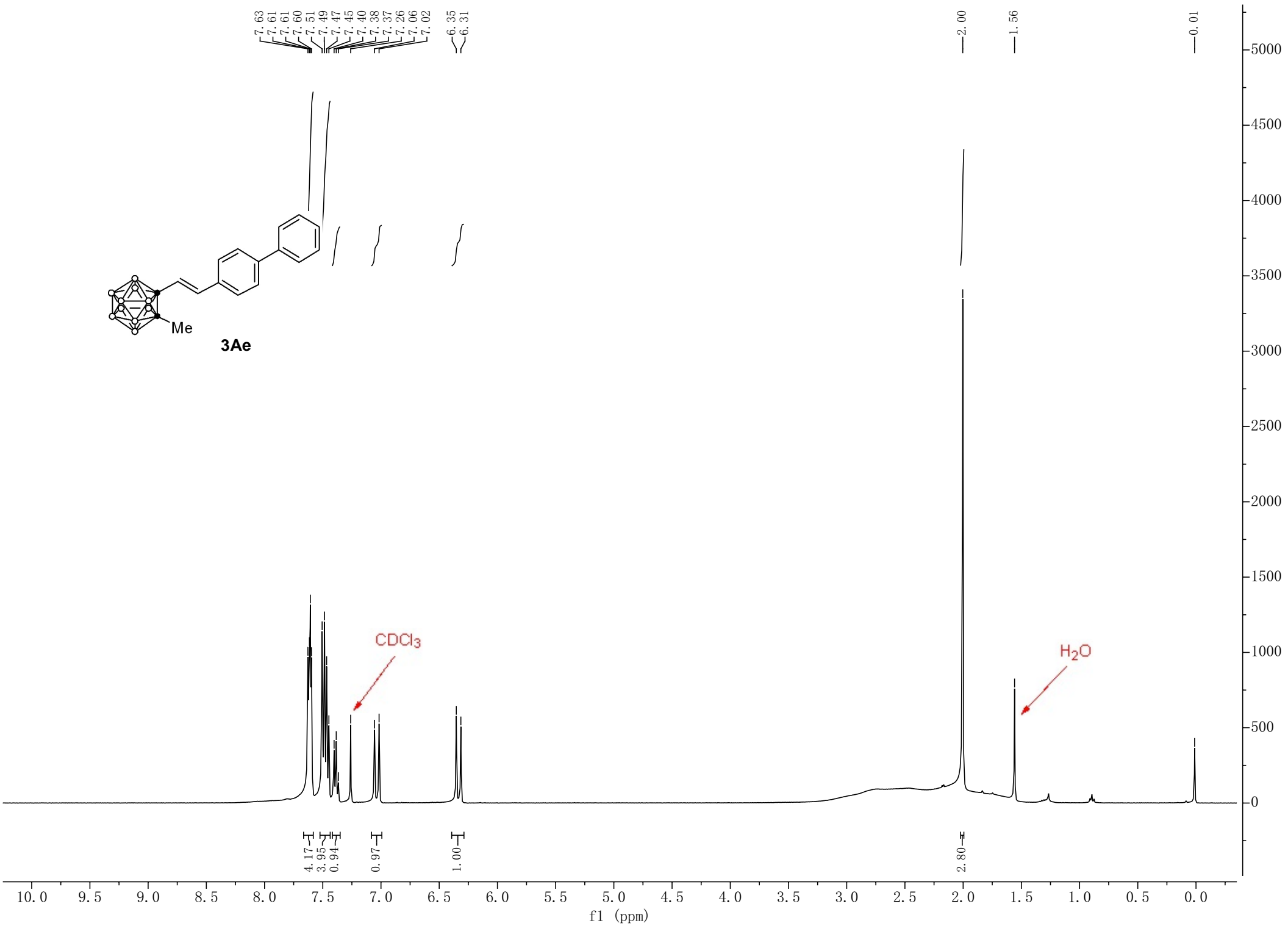


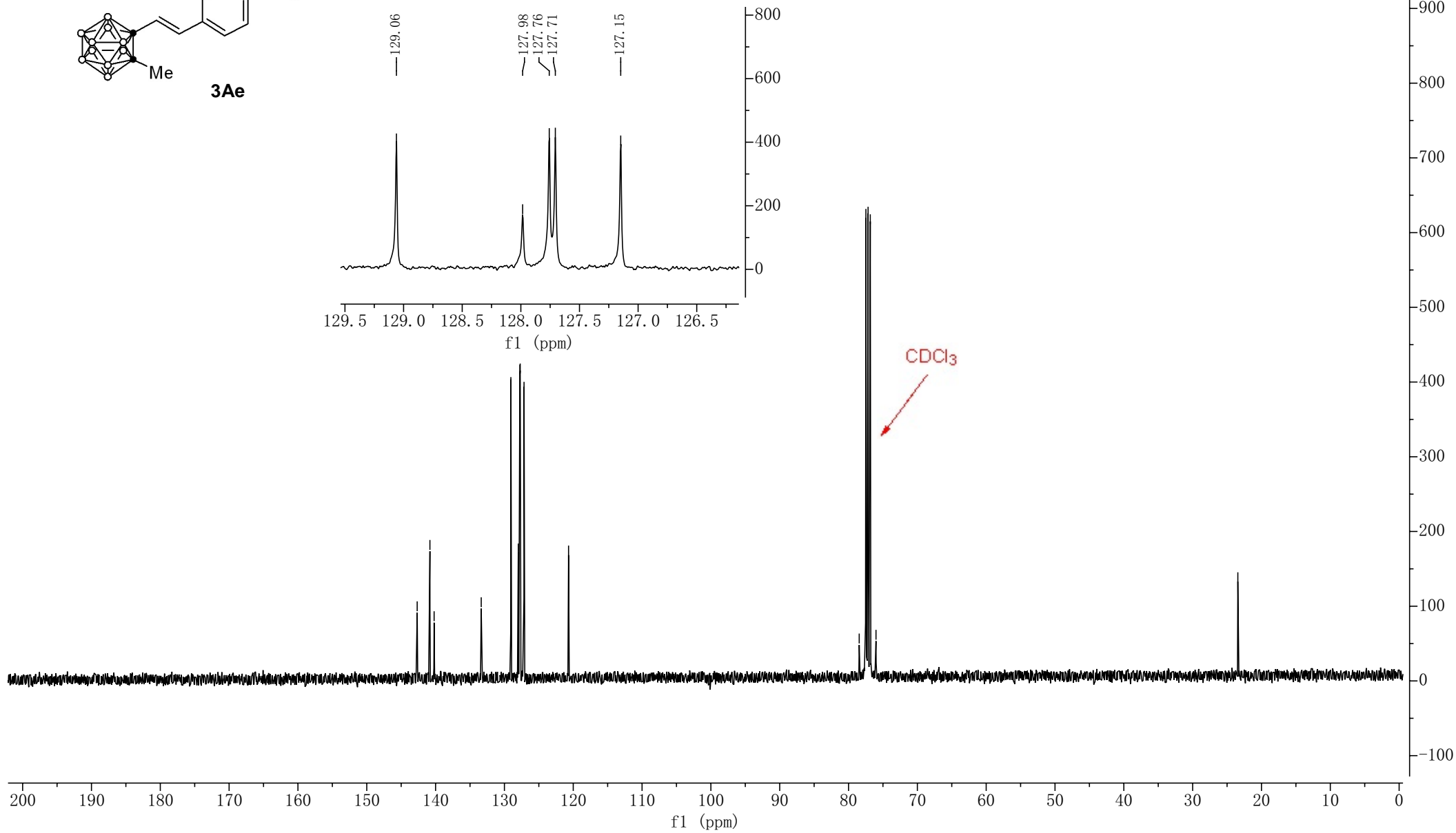
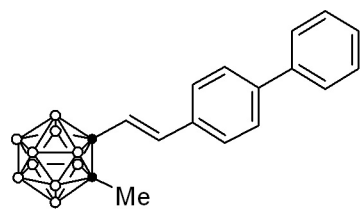


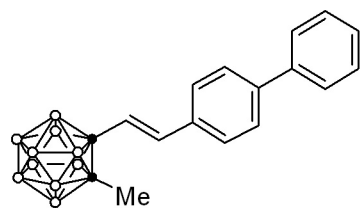




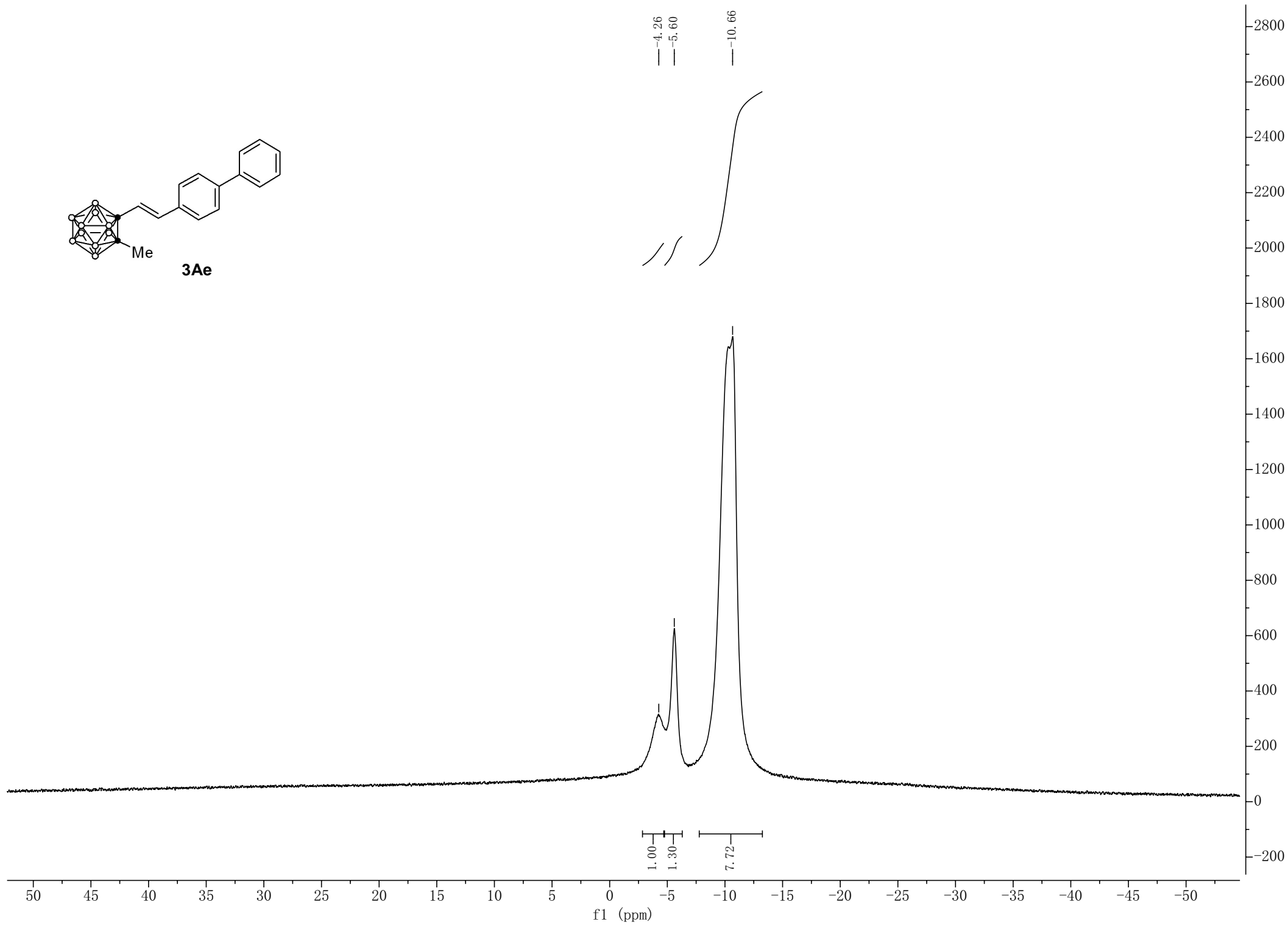






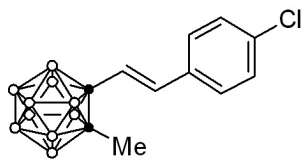


3Ae

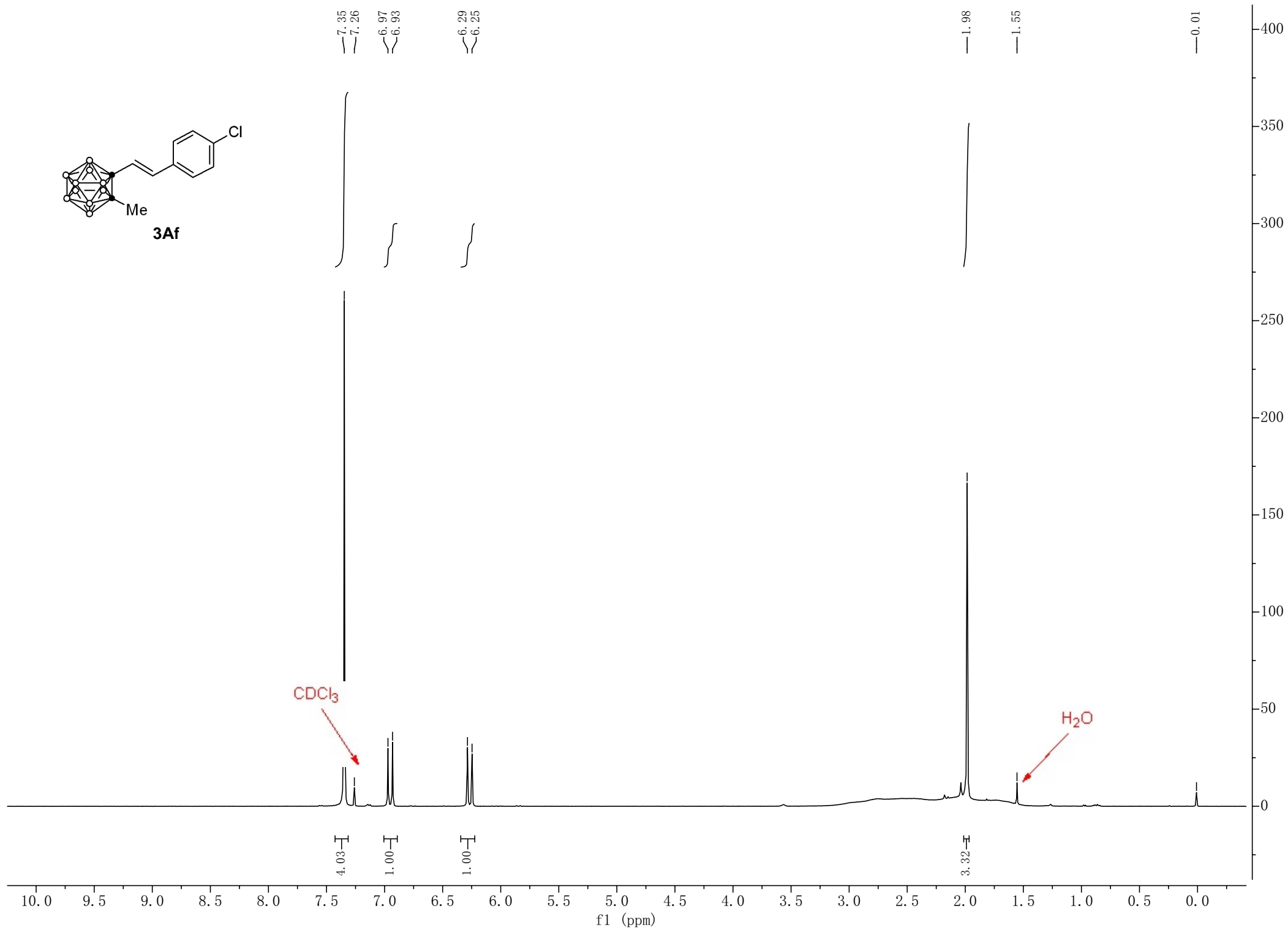


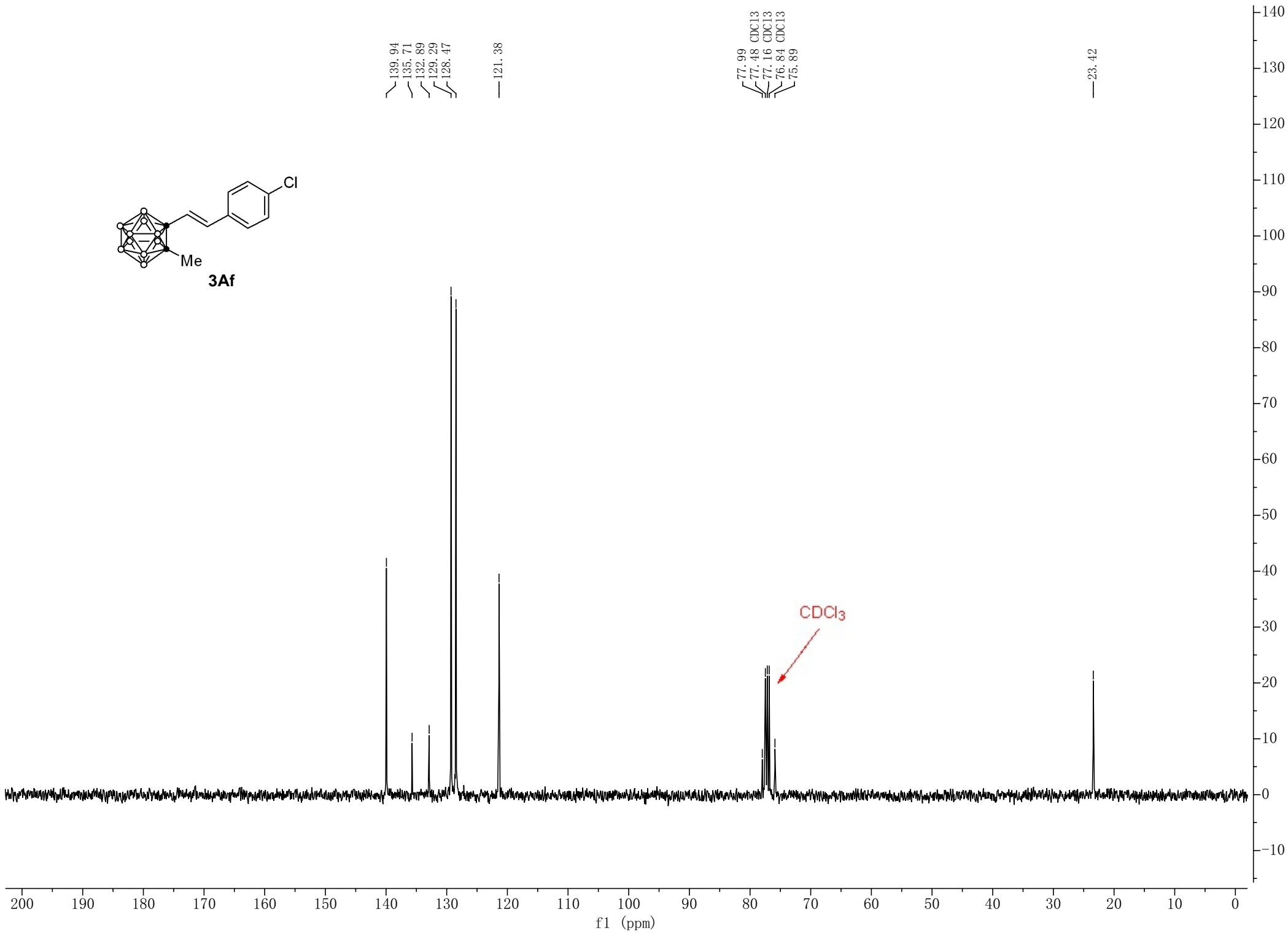
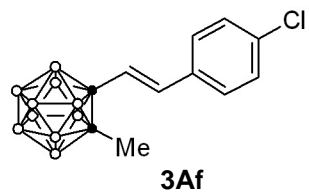
-4.26
-5.60
-10.66

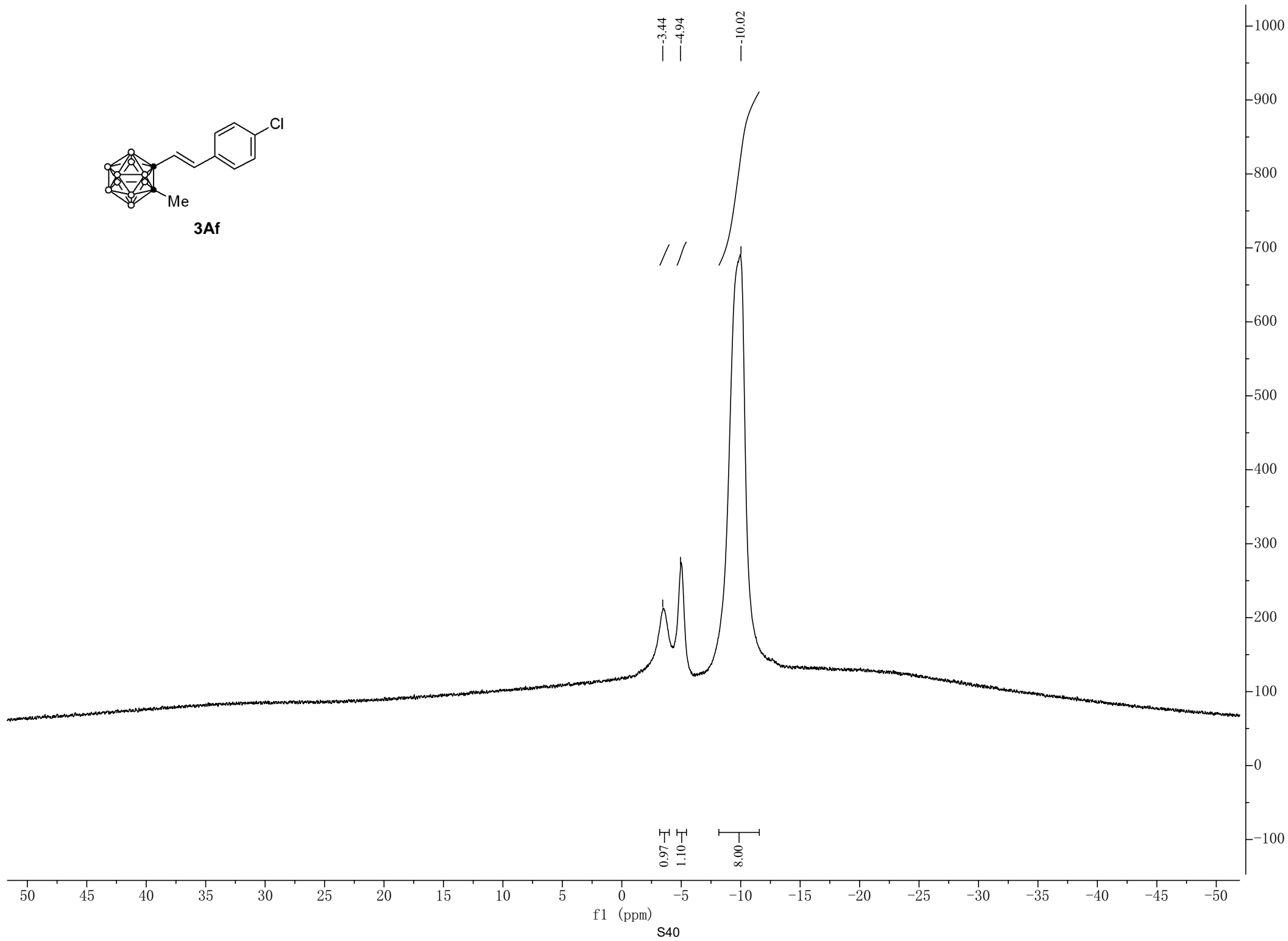
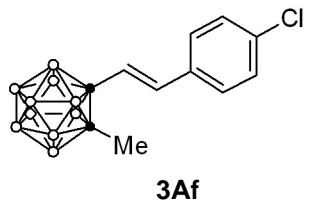
1.00
1.30
7.72

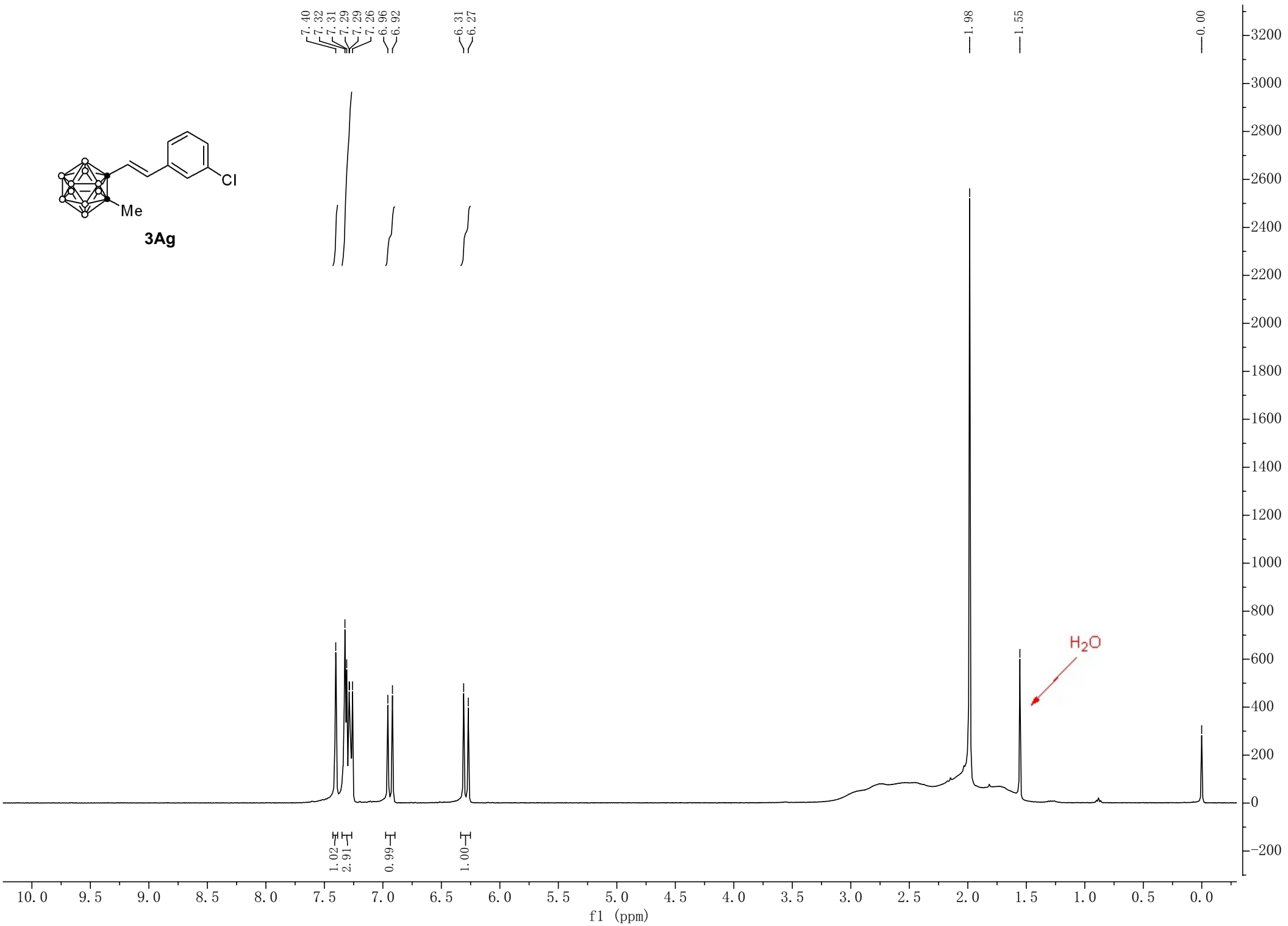
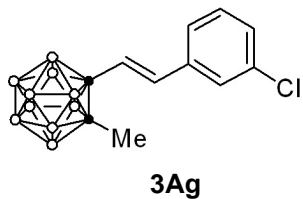


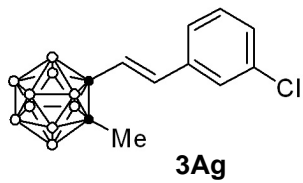
3Af







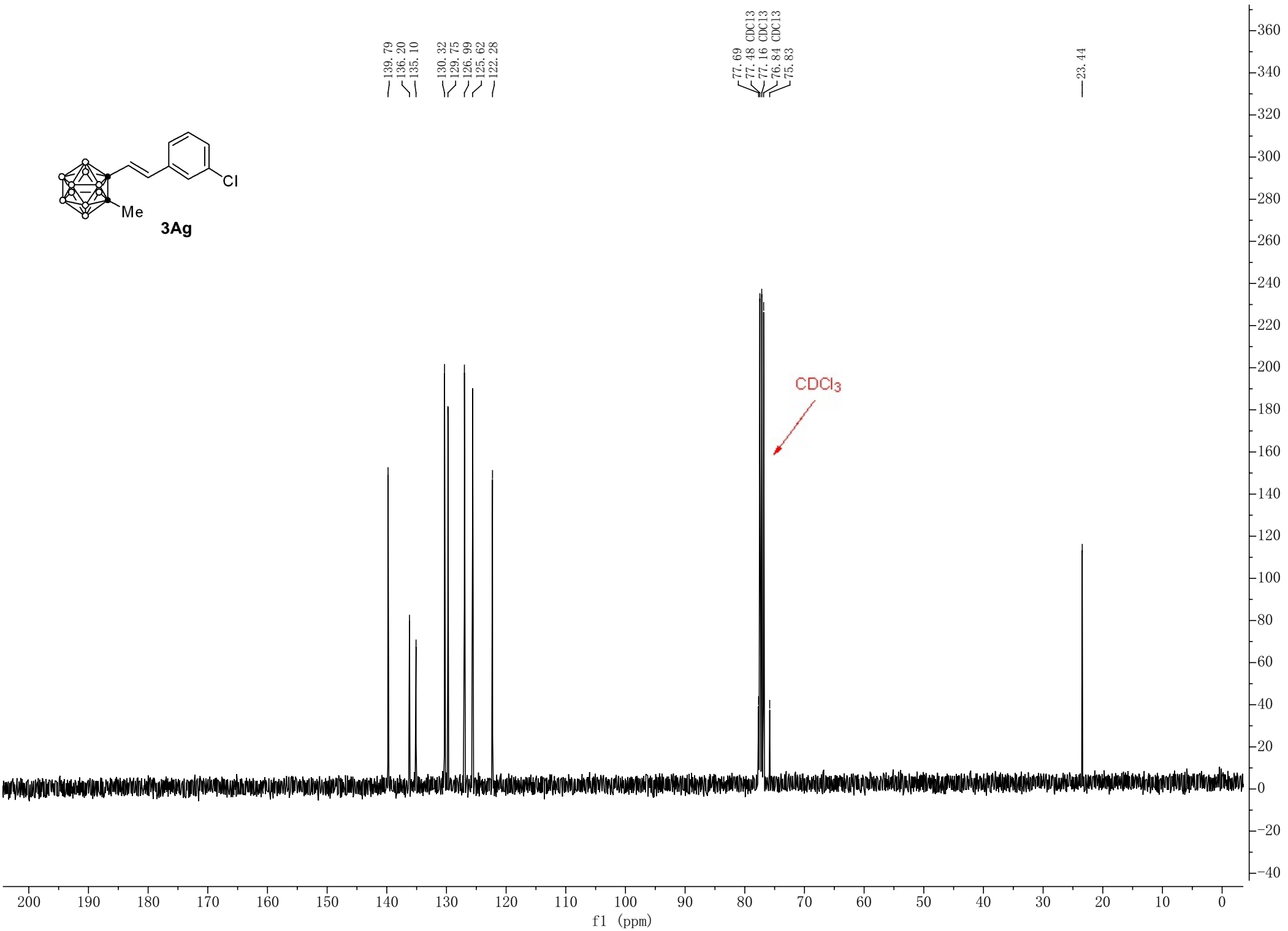


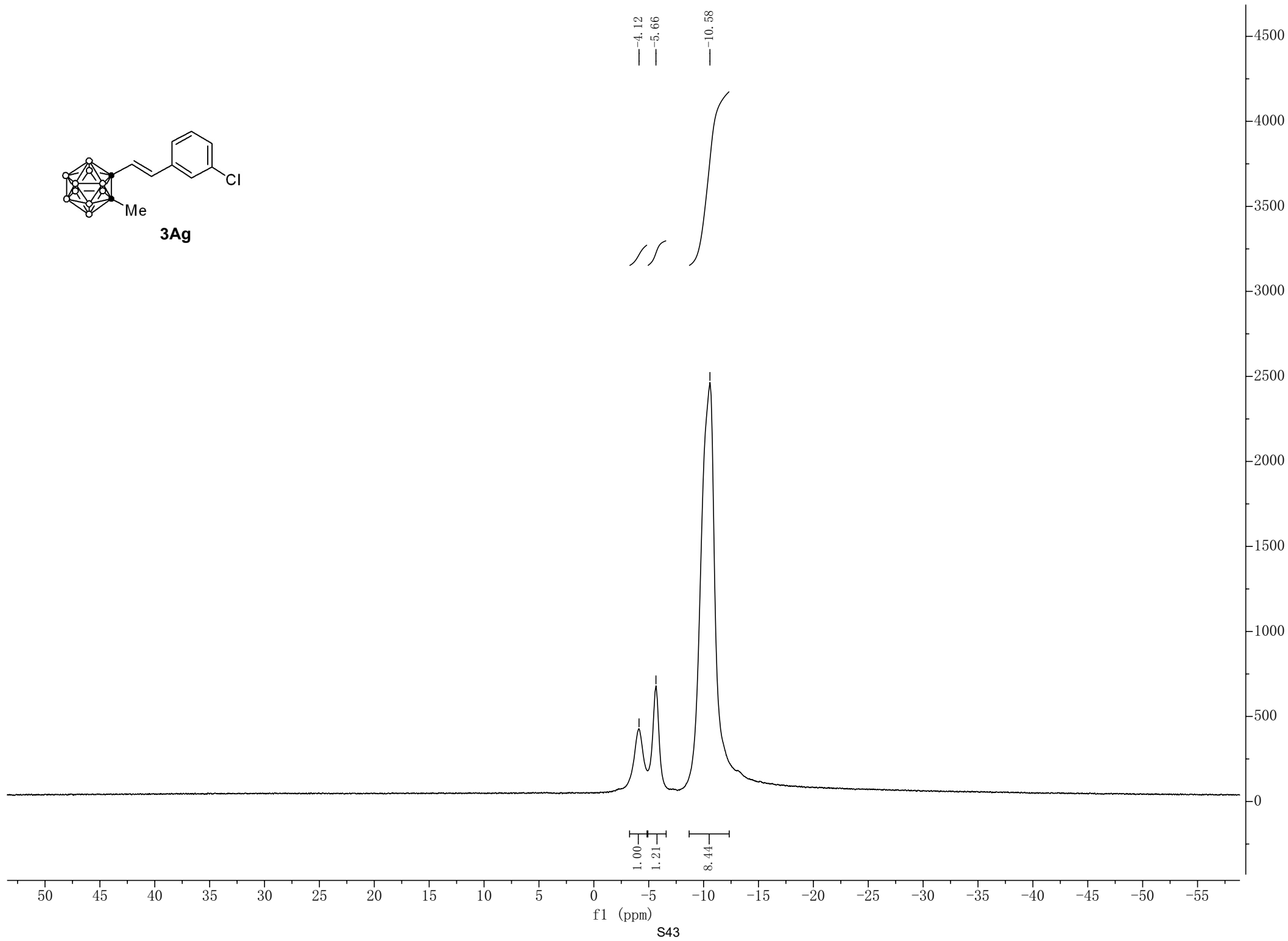
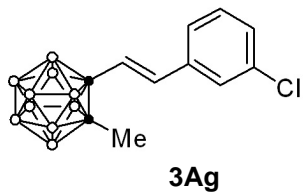


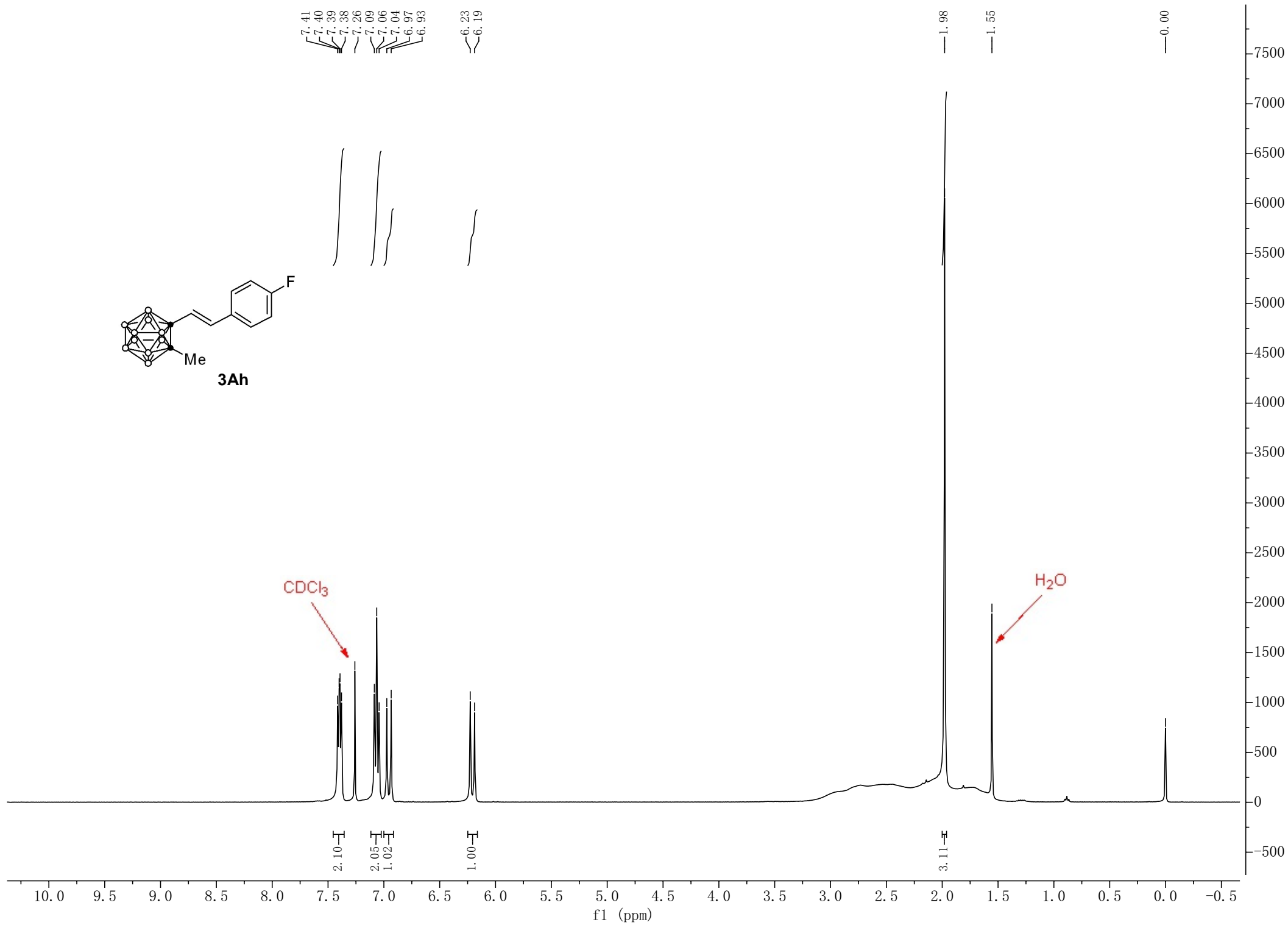
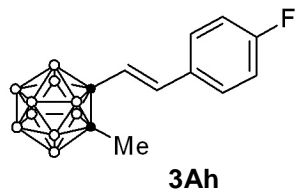
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136.20
135.10
130.32
129.75
126.99
125.62
122.28

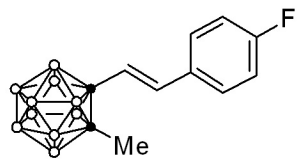
77.69
77.48
77.16
76.84
75.83

23.44

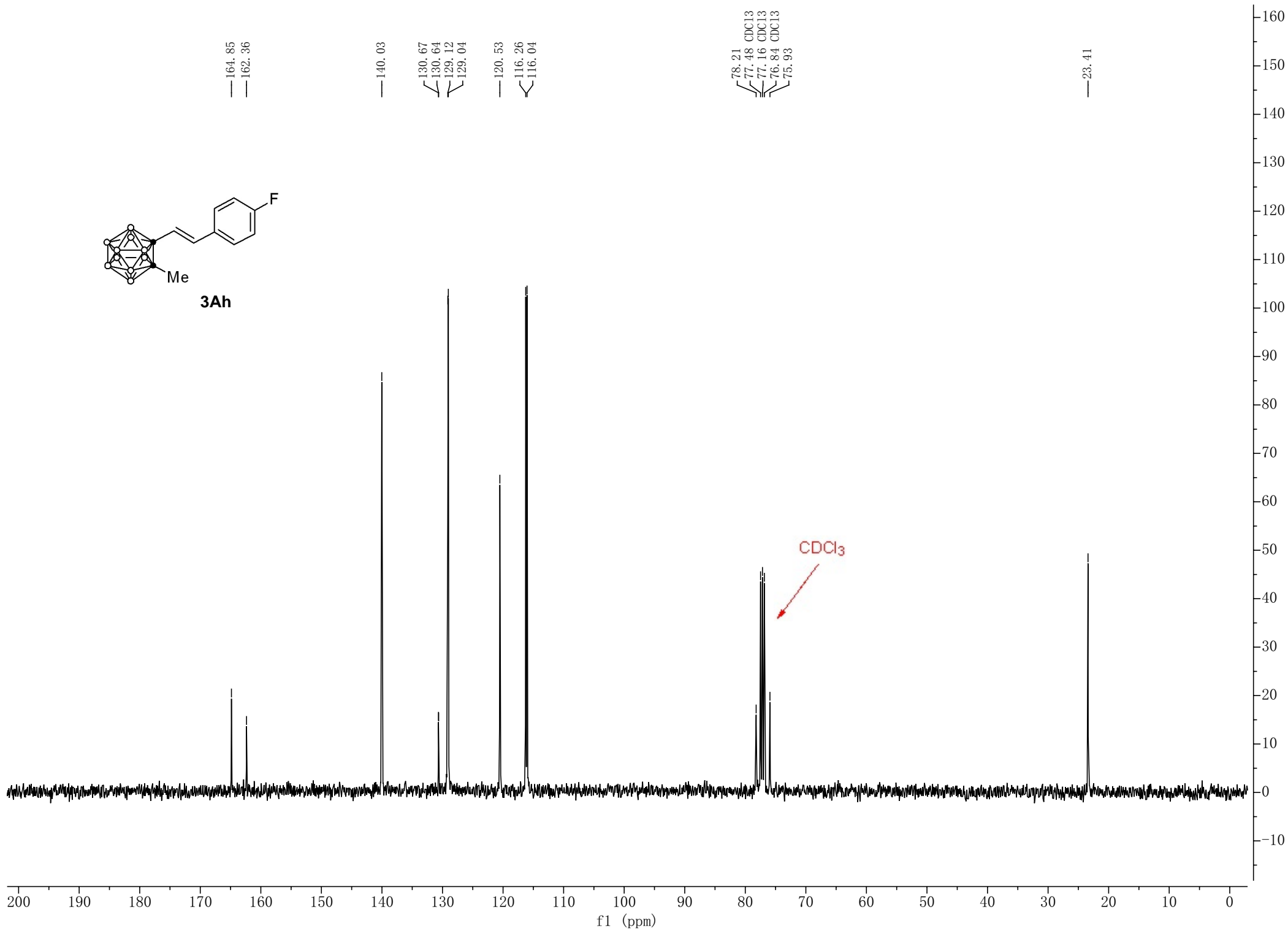


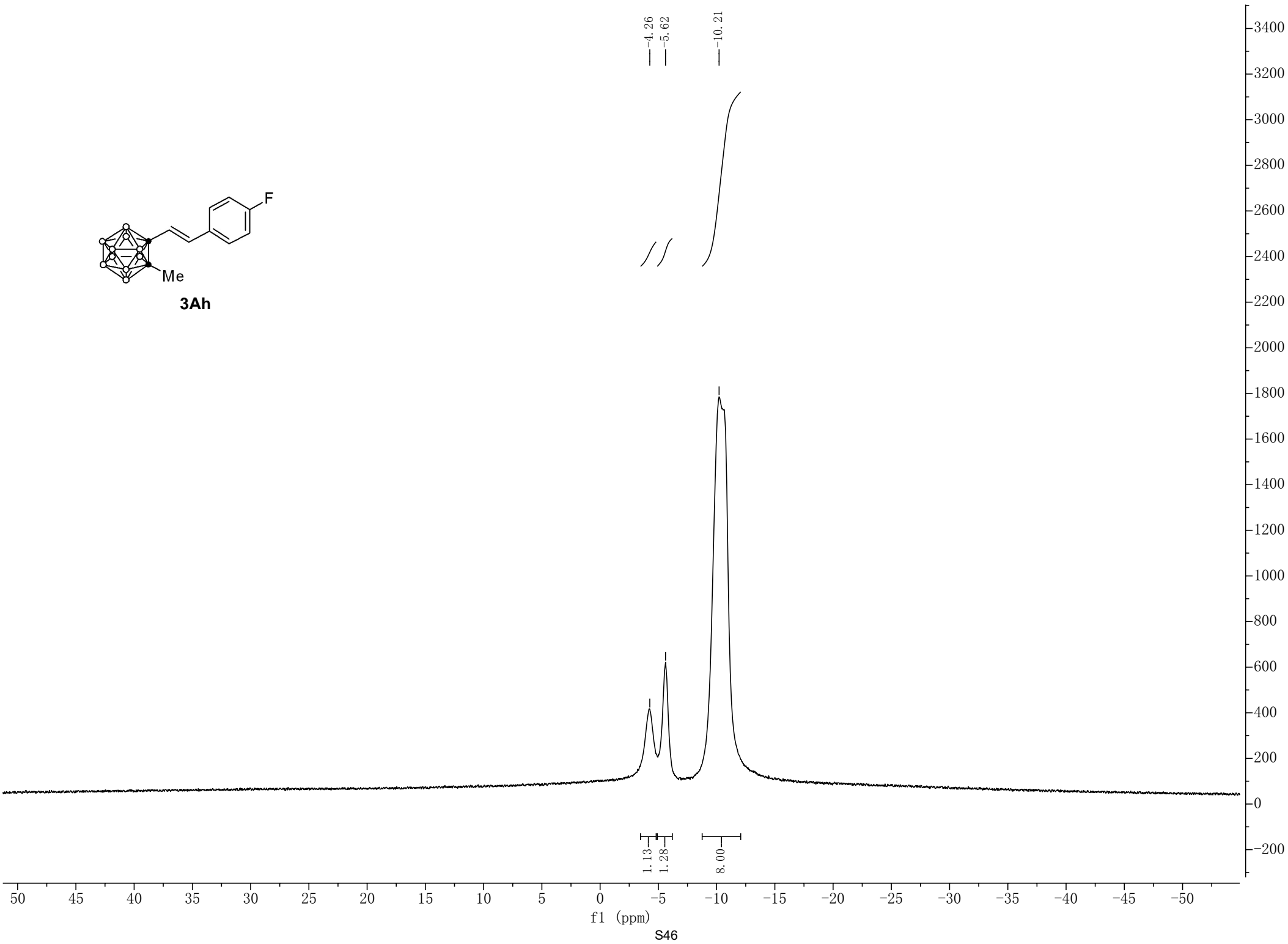
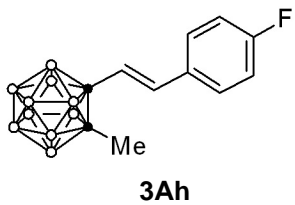


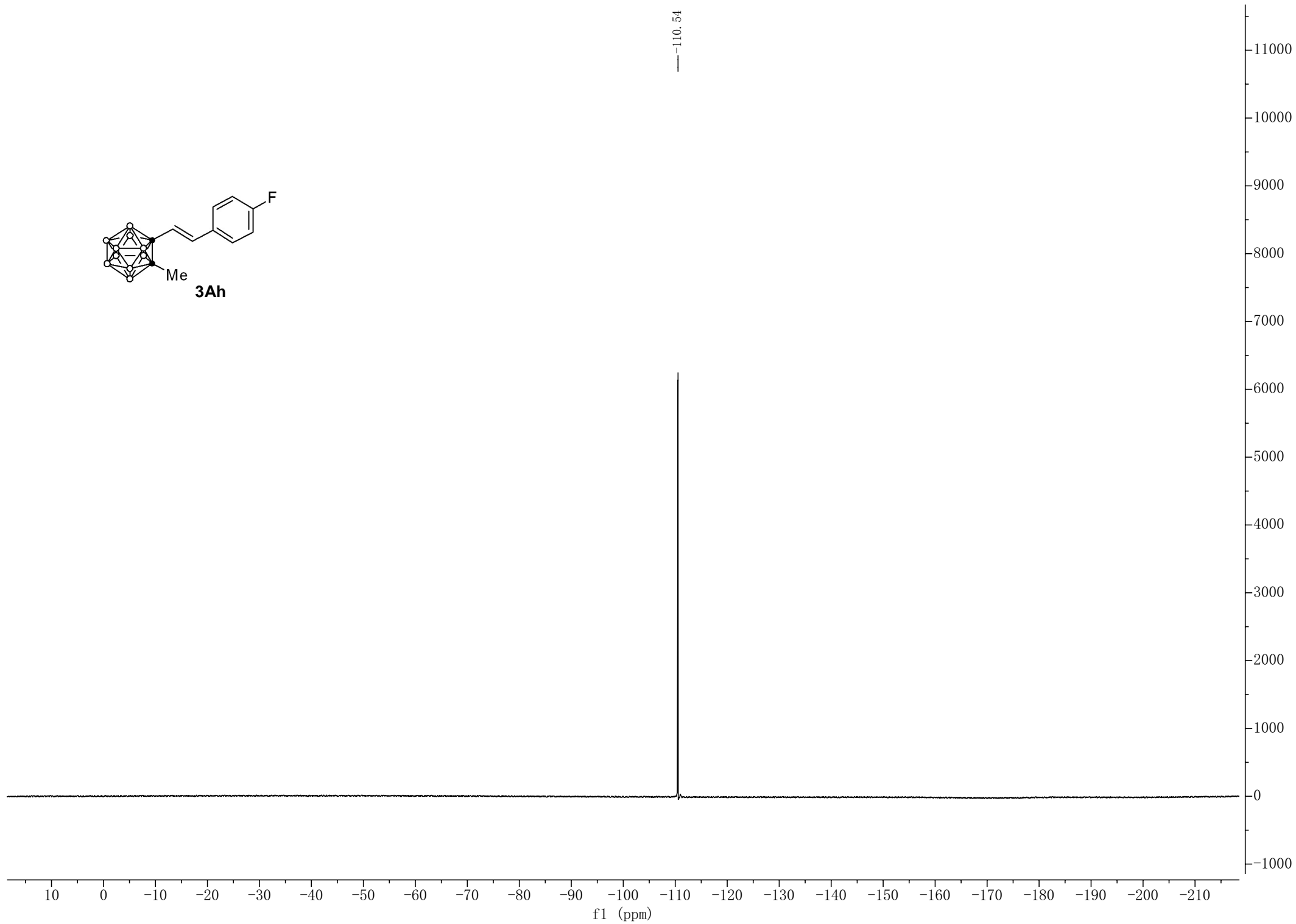
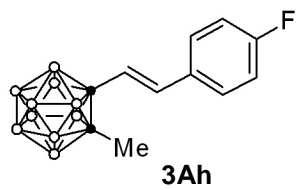


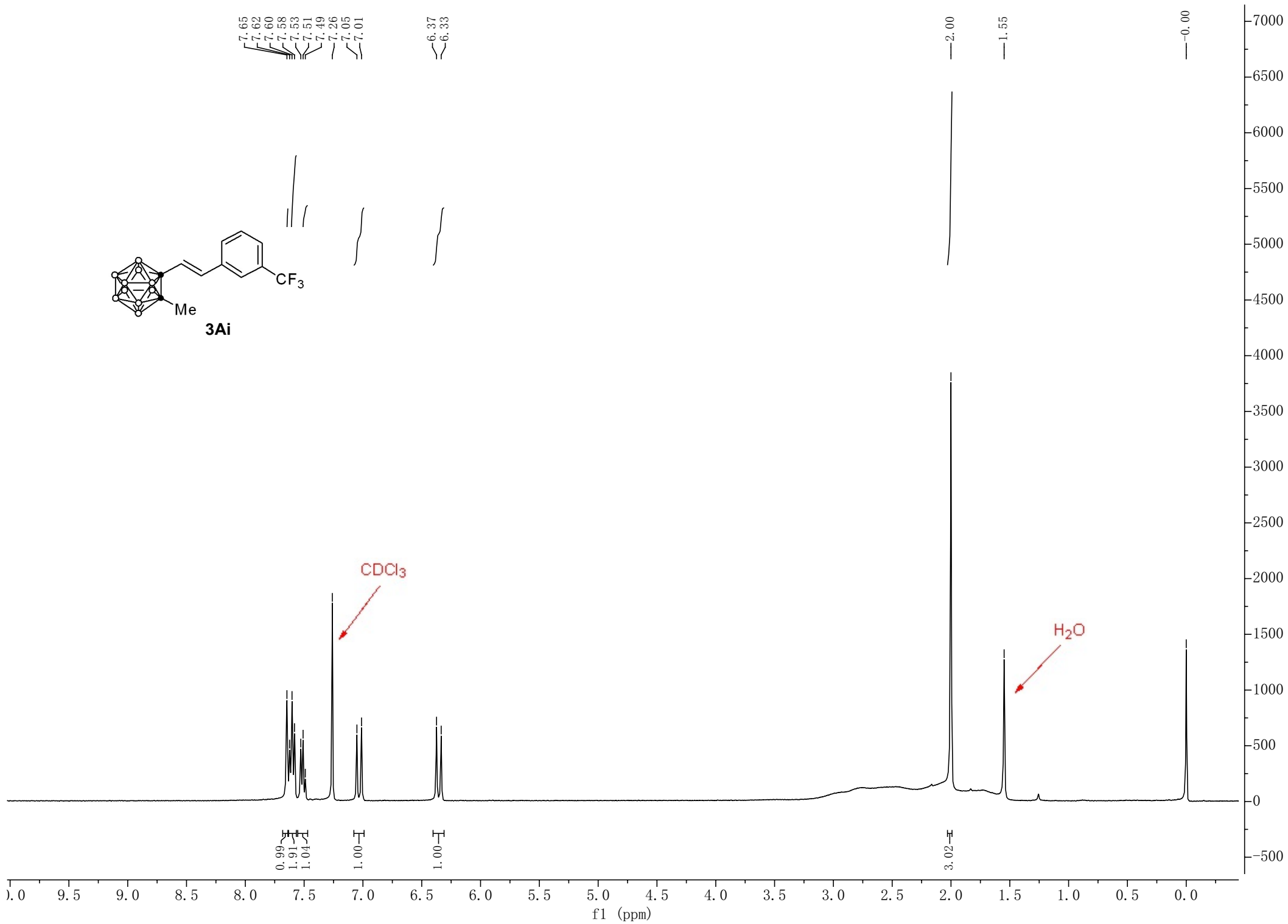


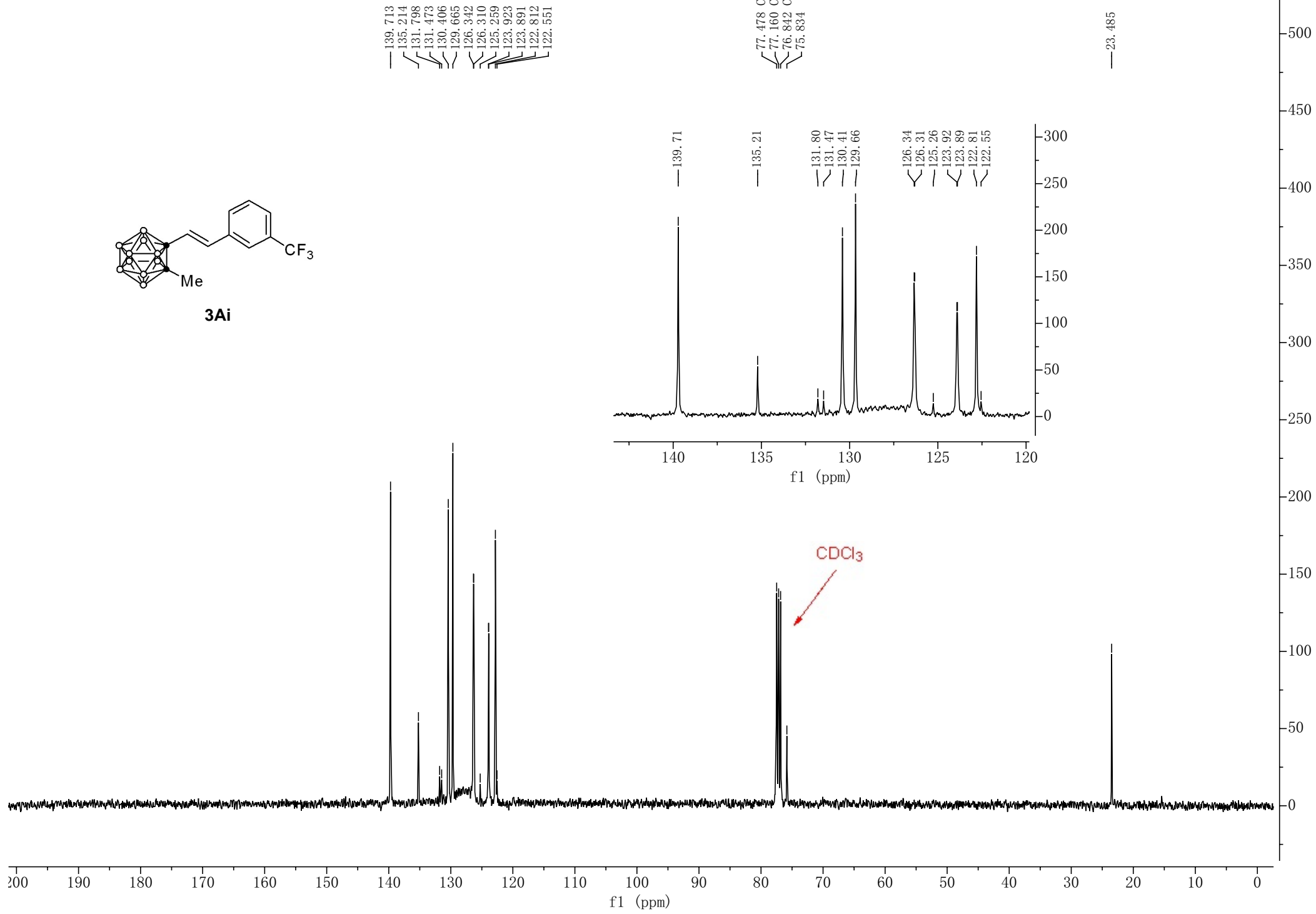
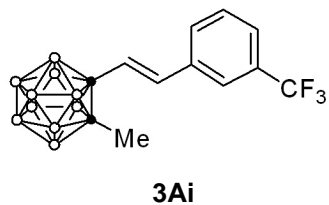
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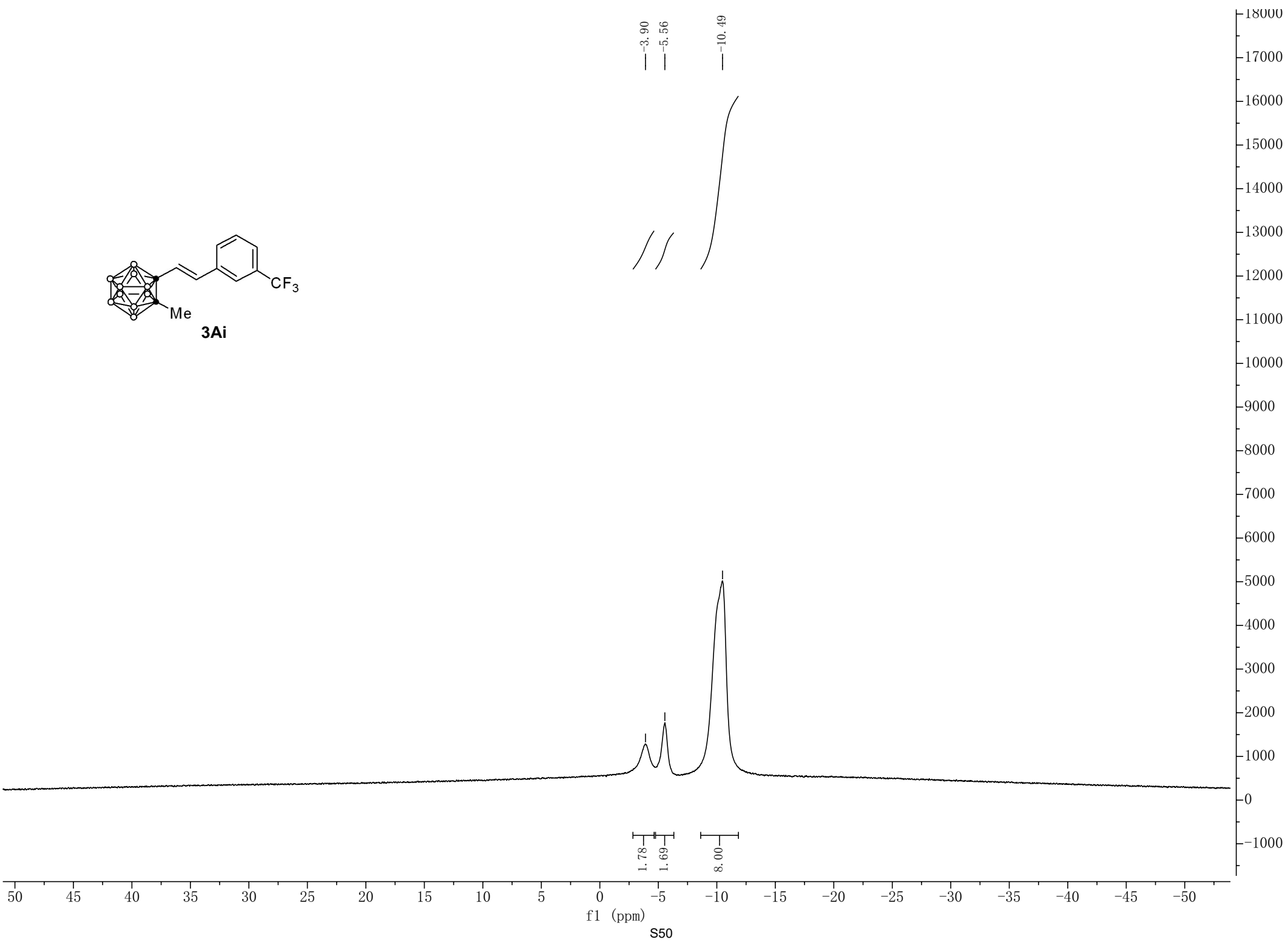
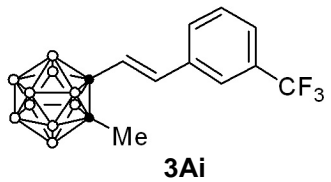


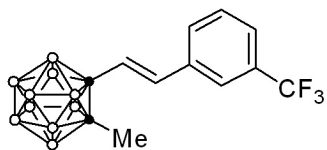




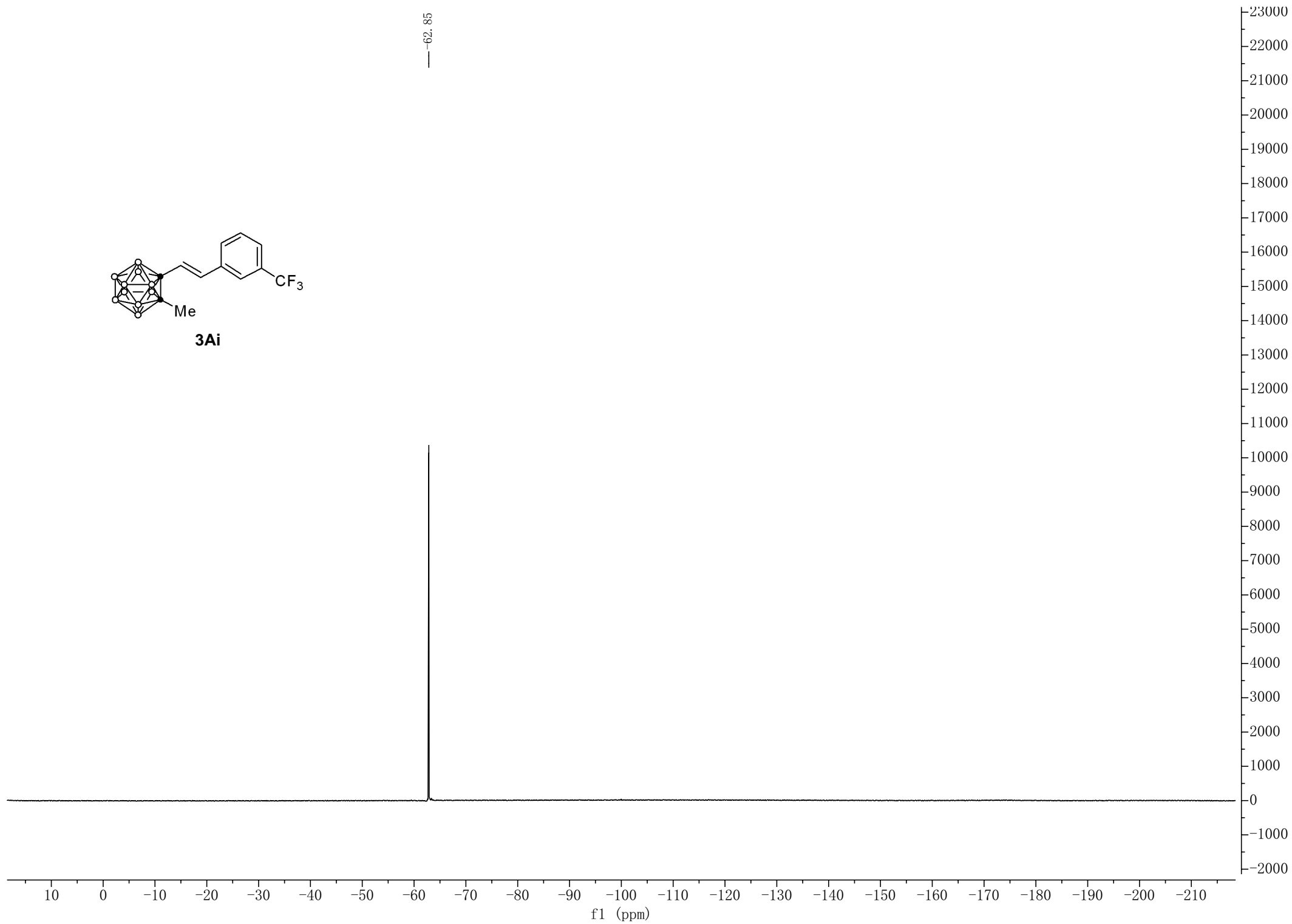


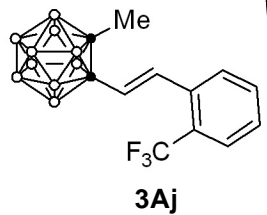






3Ai



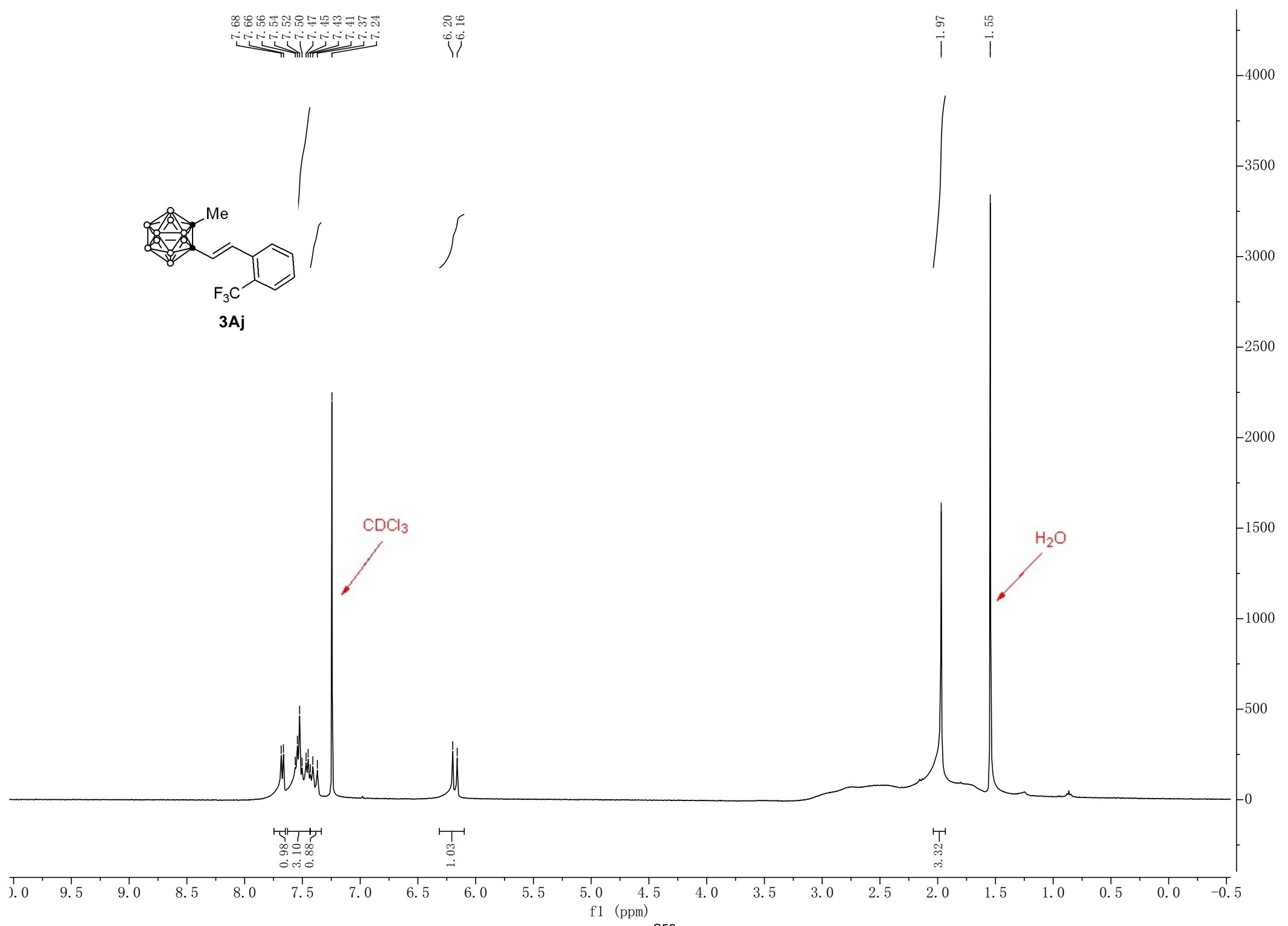


7.68
7.66
7.56
7.54
7.52
7.50
7.47
7.45
7.43
7.41
7.37
7.24

6.20
6.16

1.97

1.55

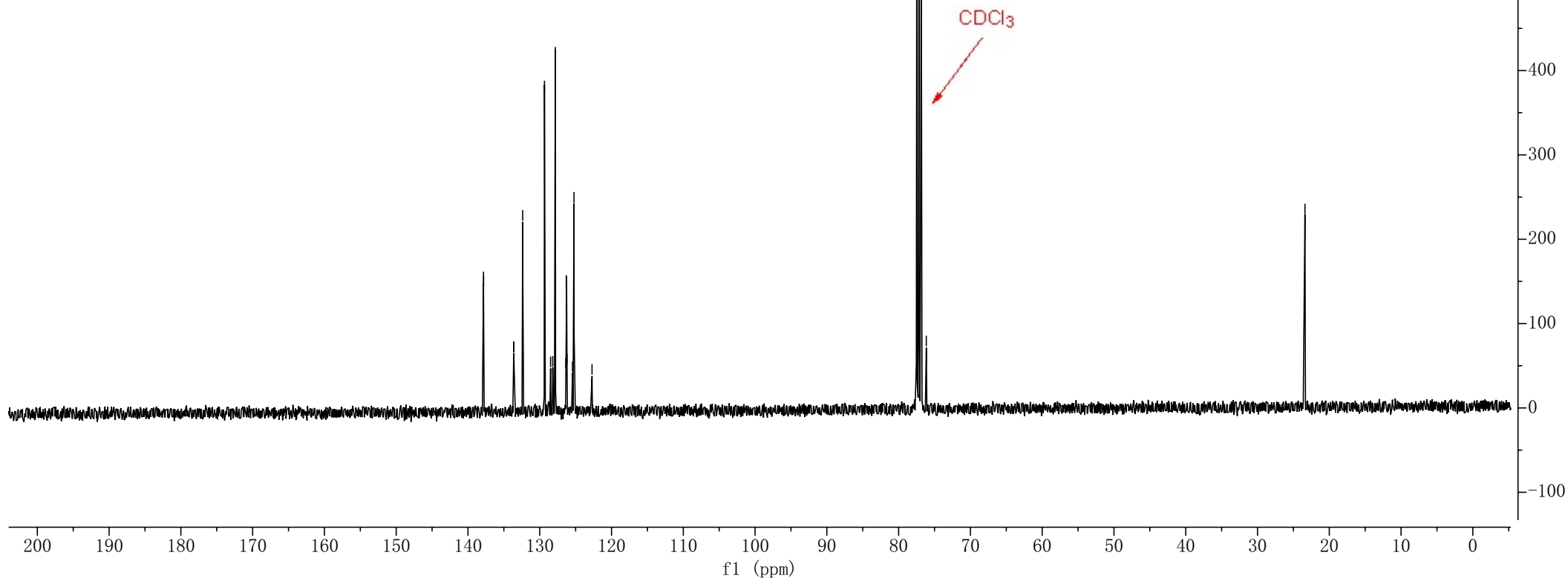
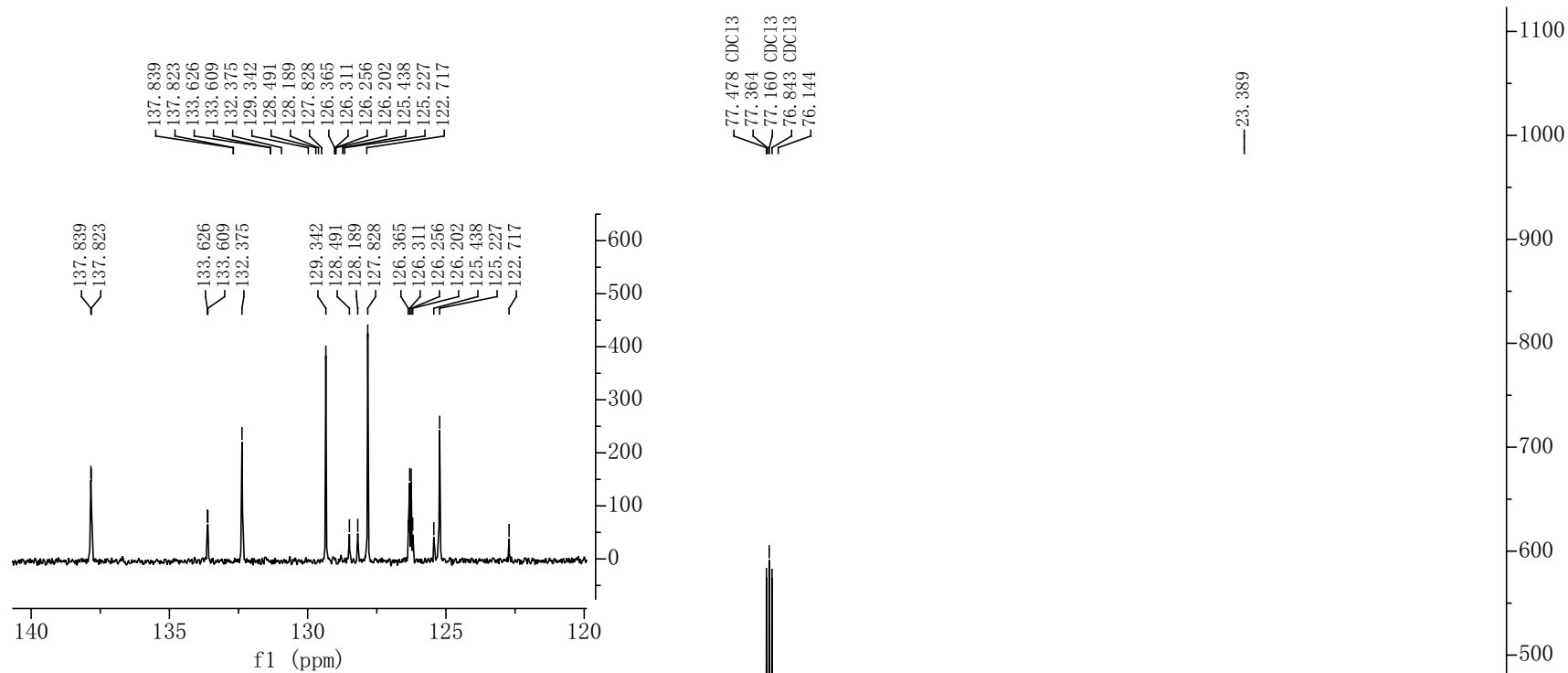
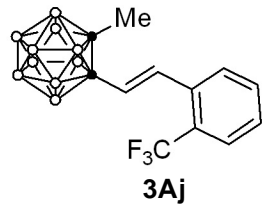


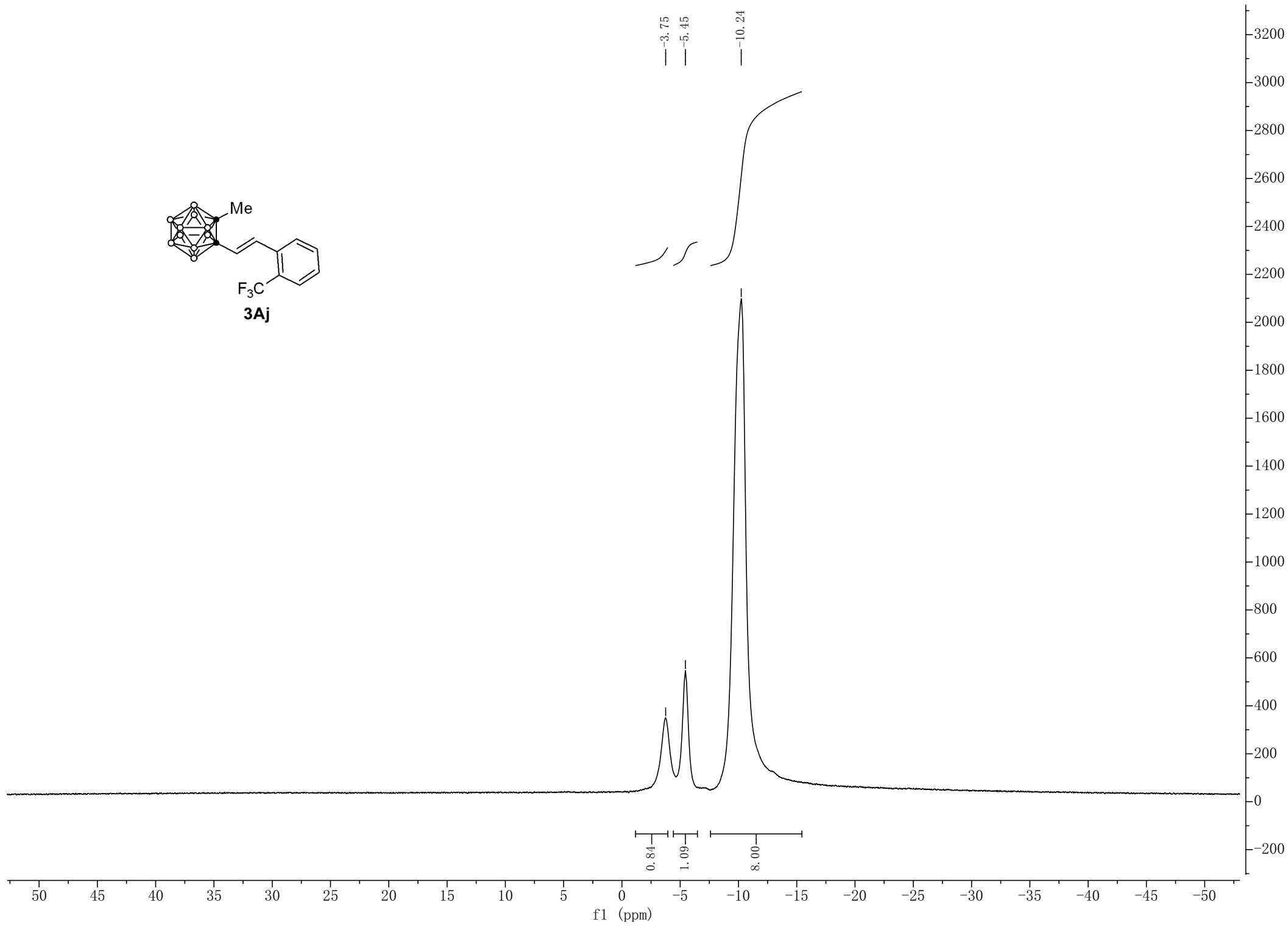
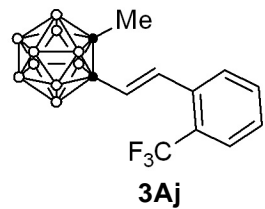
CDCl₃

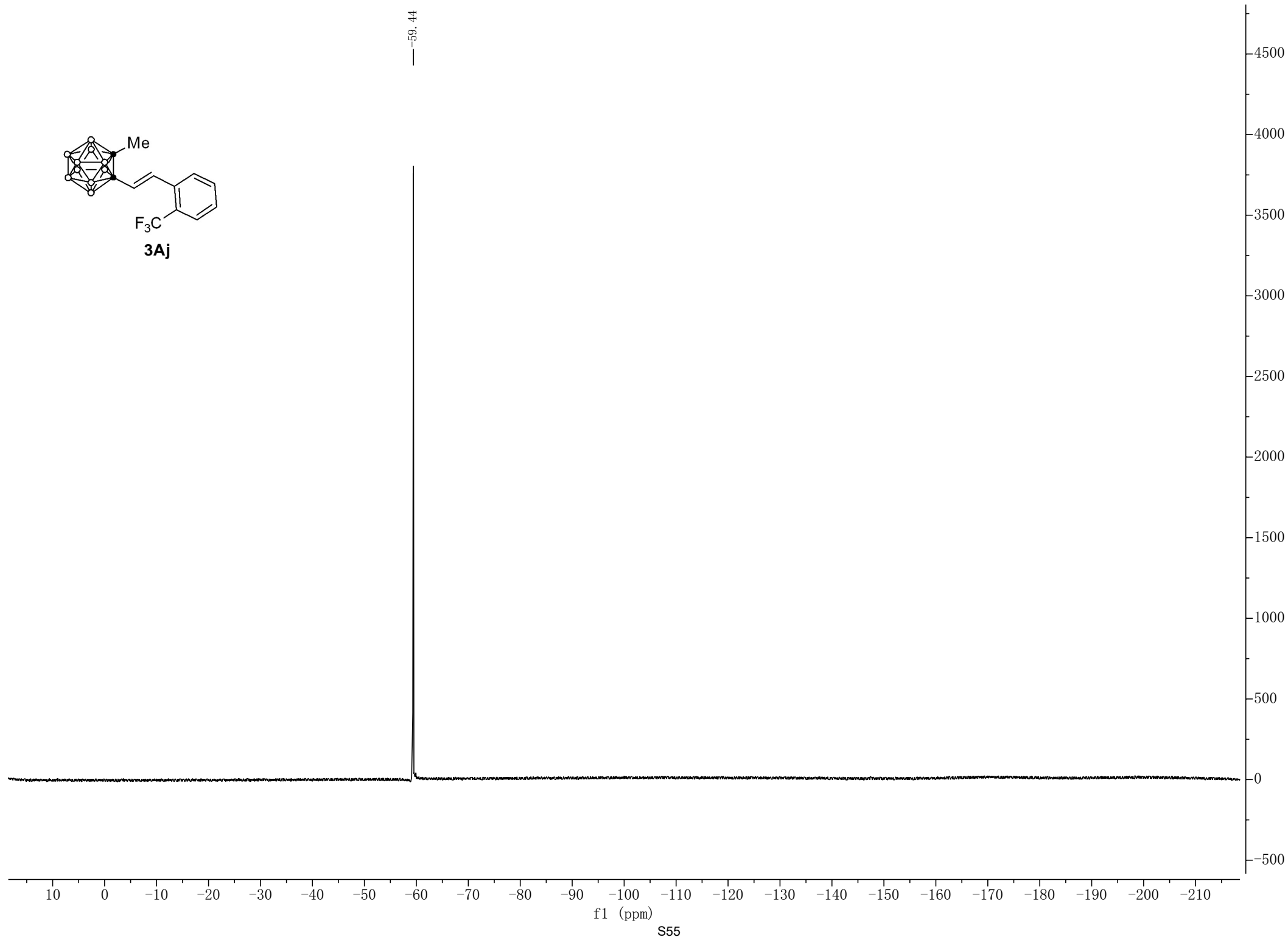
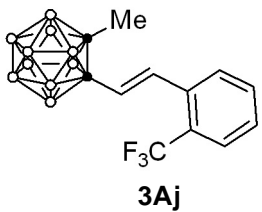
H₂O

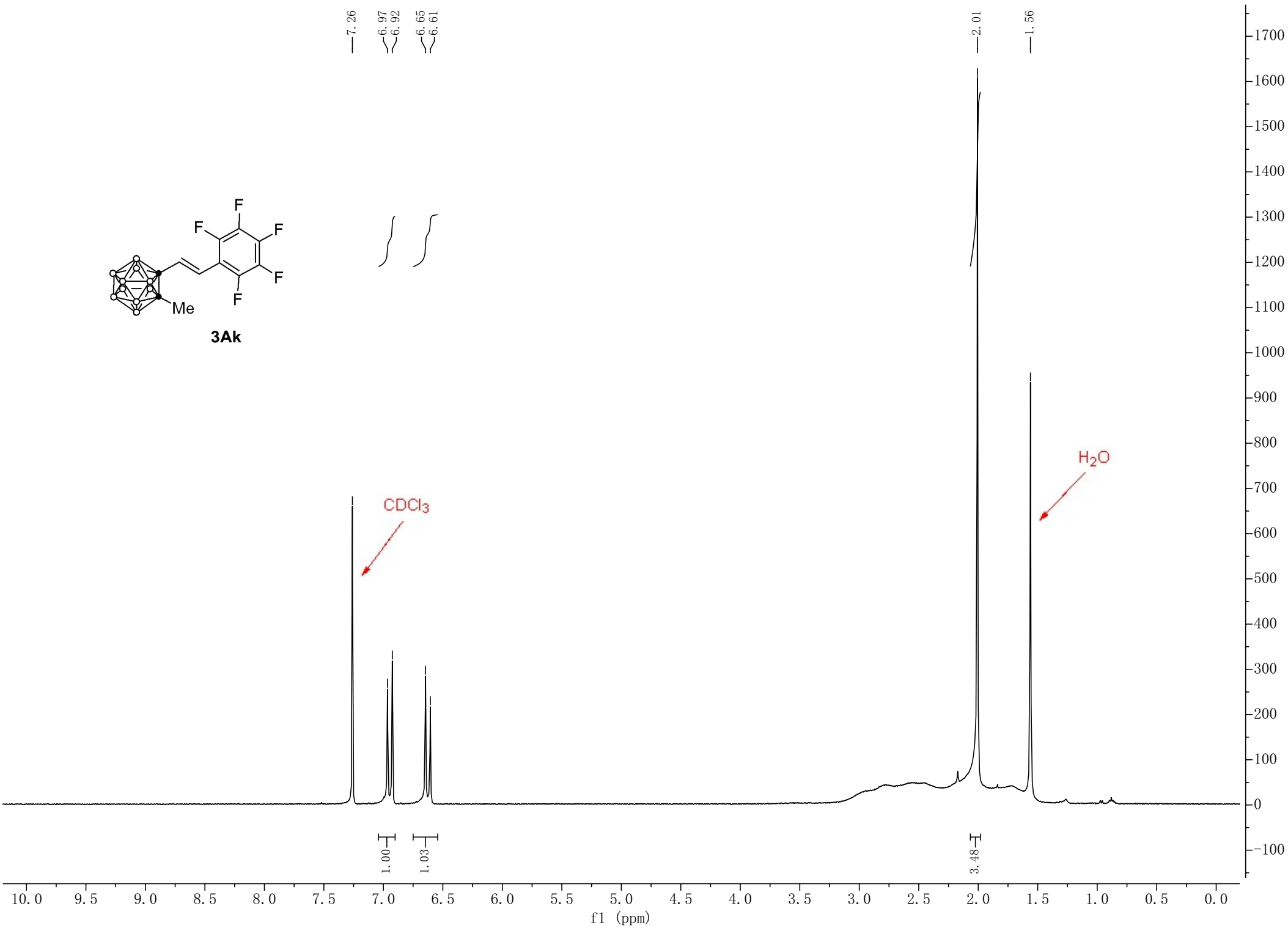
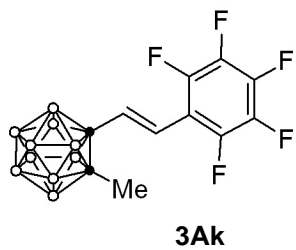
f1 (ppm)

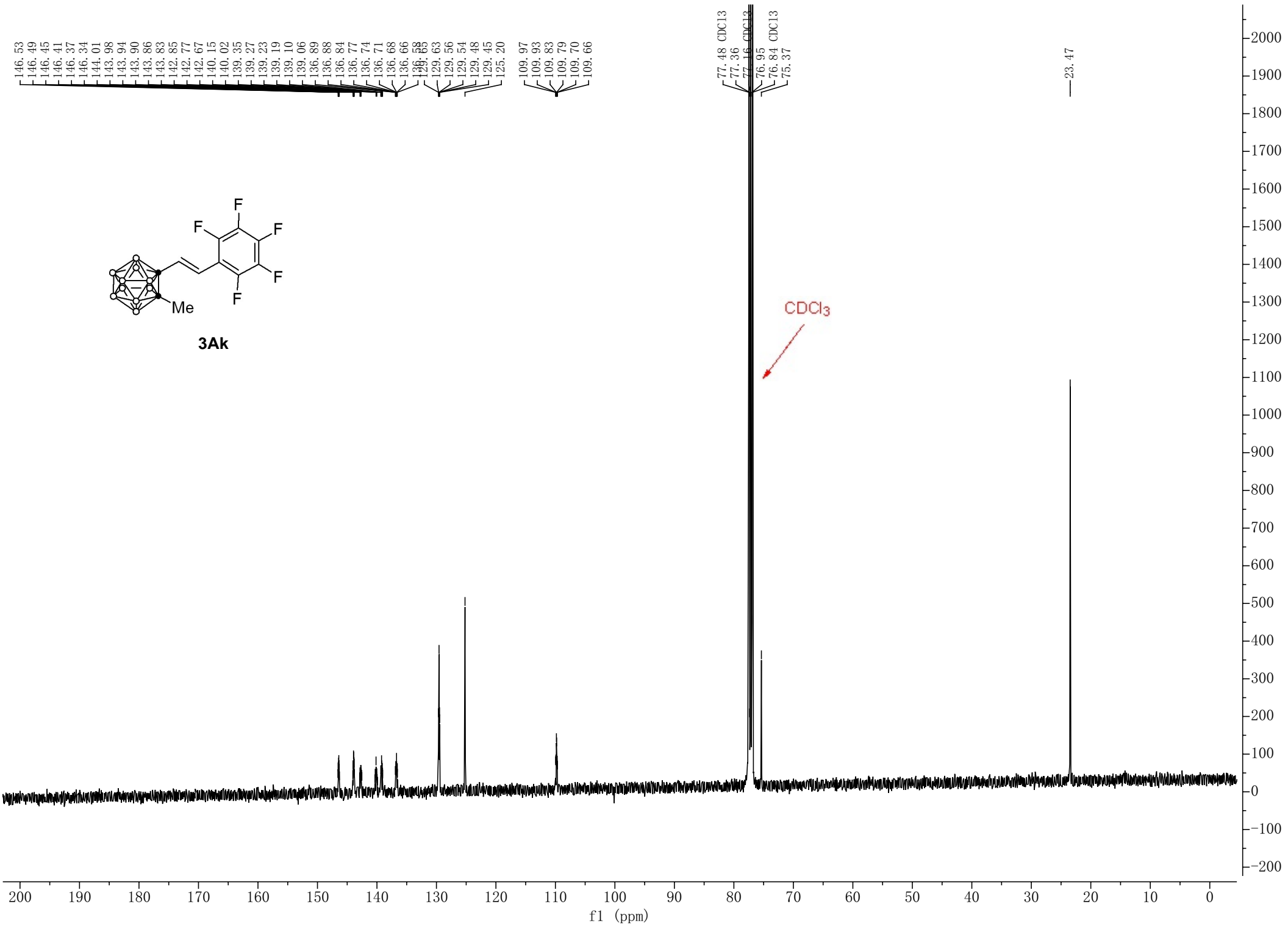
S52

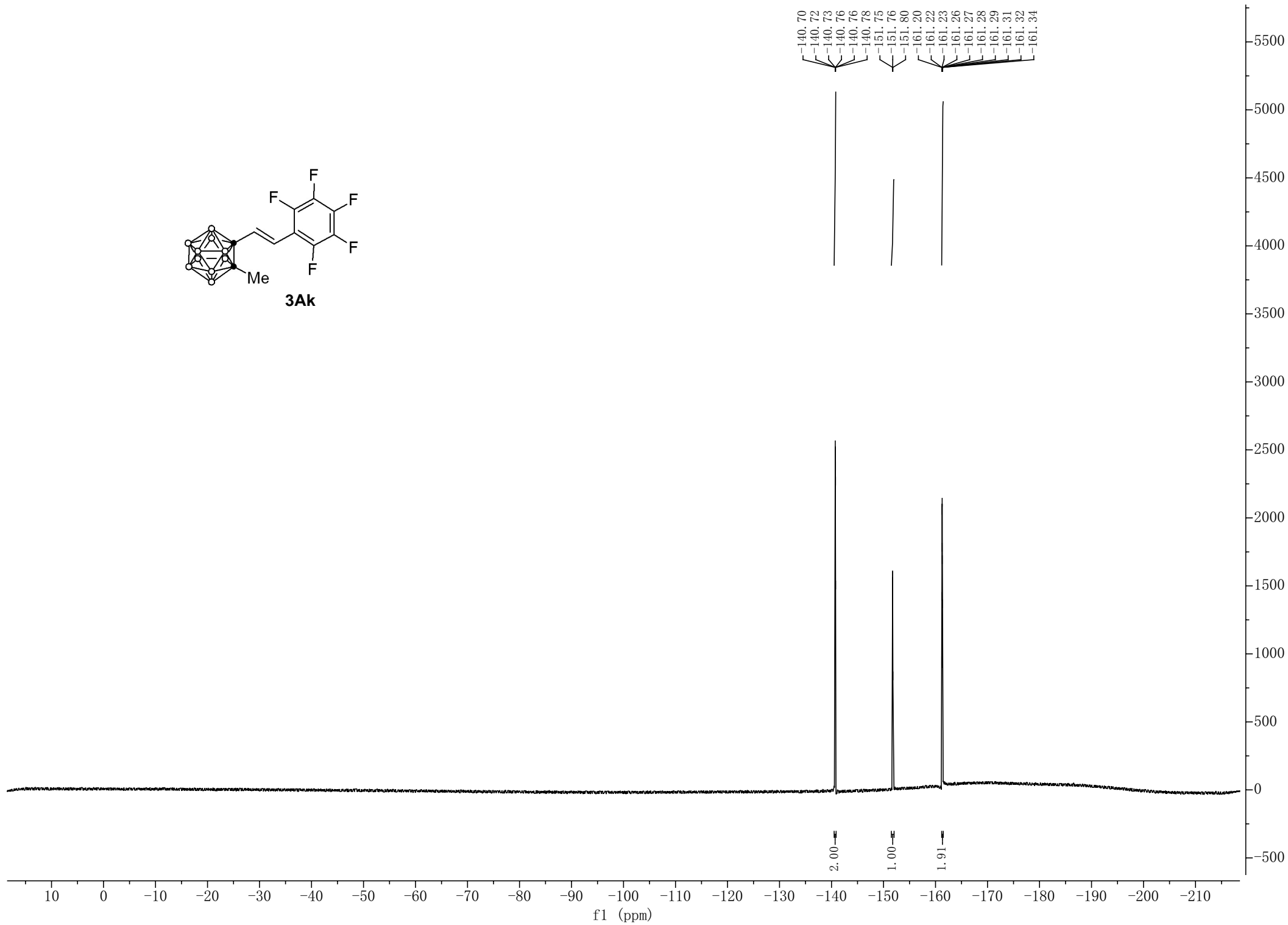
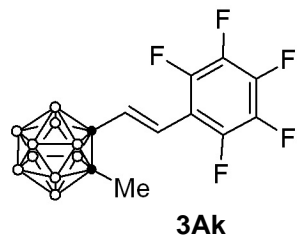


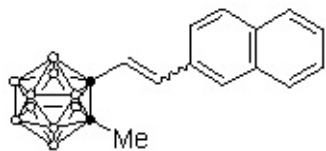








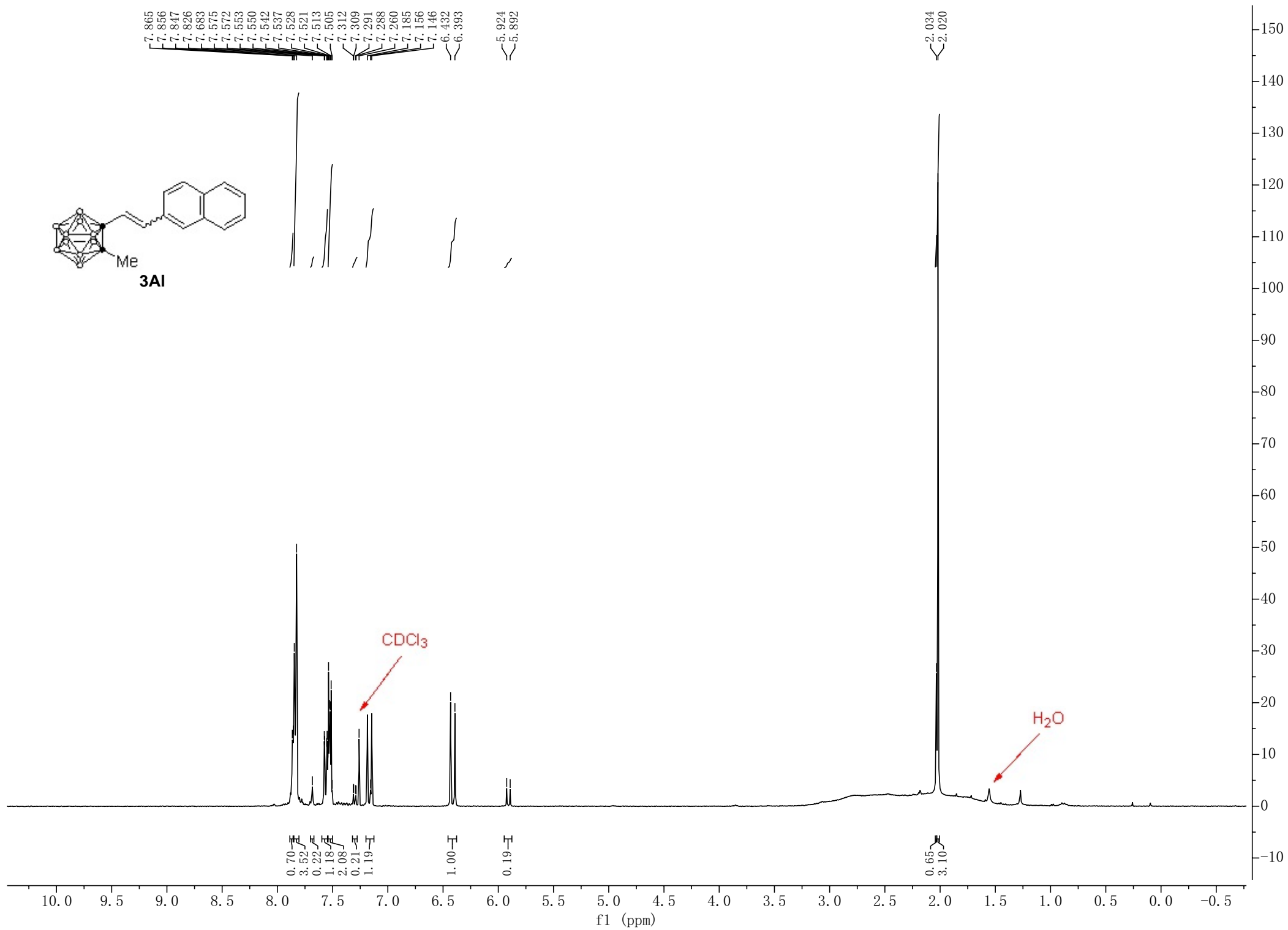


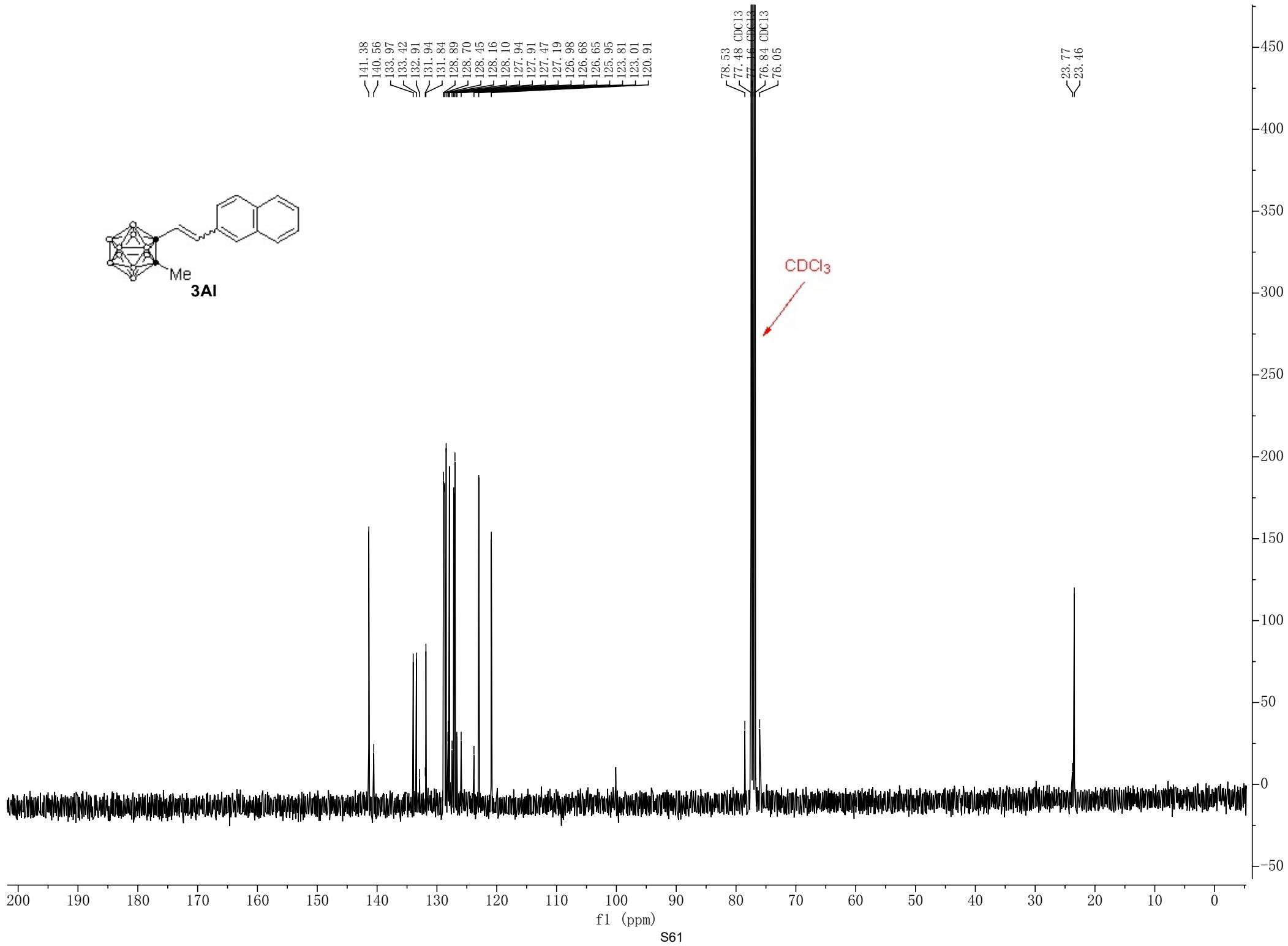
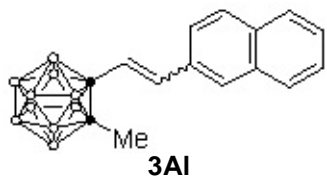


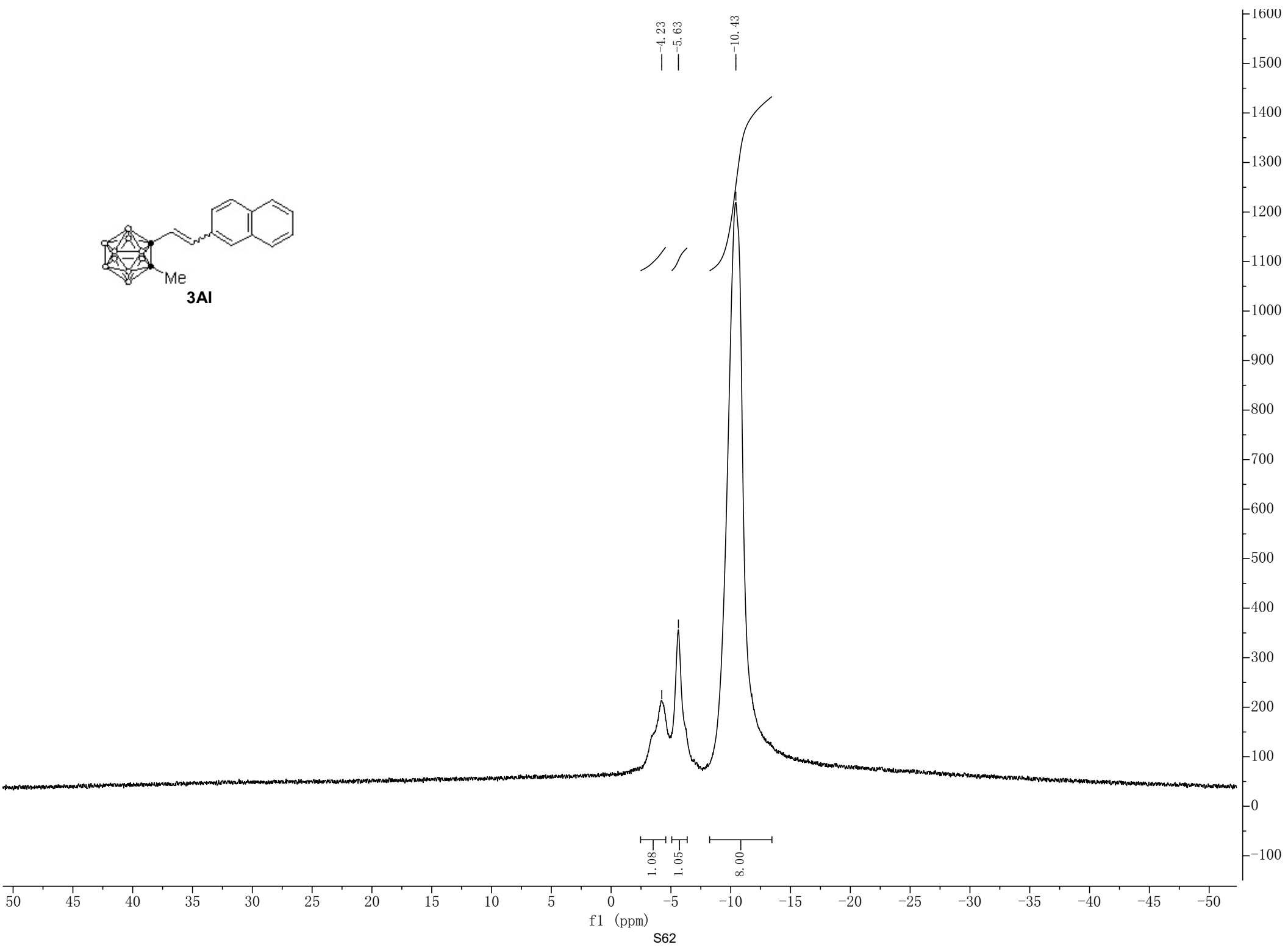
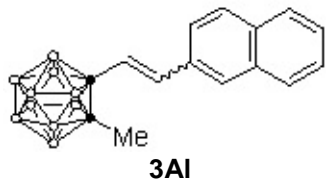
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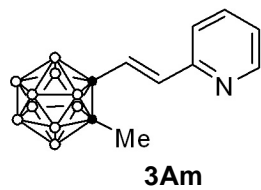
7.865
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7.826
7.683
7.575
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7.553
7.550
7.542
7.537
7.528
7.521
7.513
7.505
7.312
7.309
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7.288
7.260
7.185
7.156
7.146
6.432
6.393
5.924
5.892

2.034
2.020

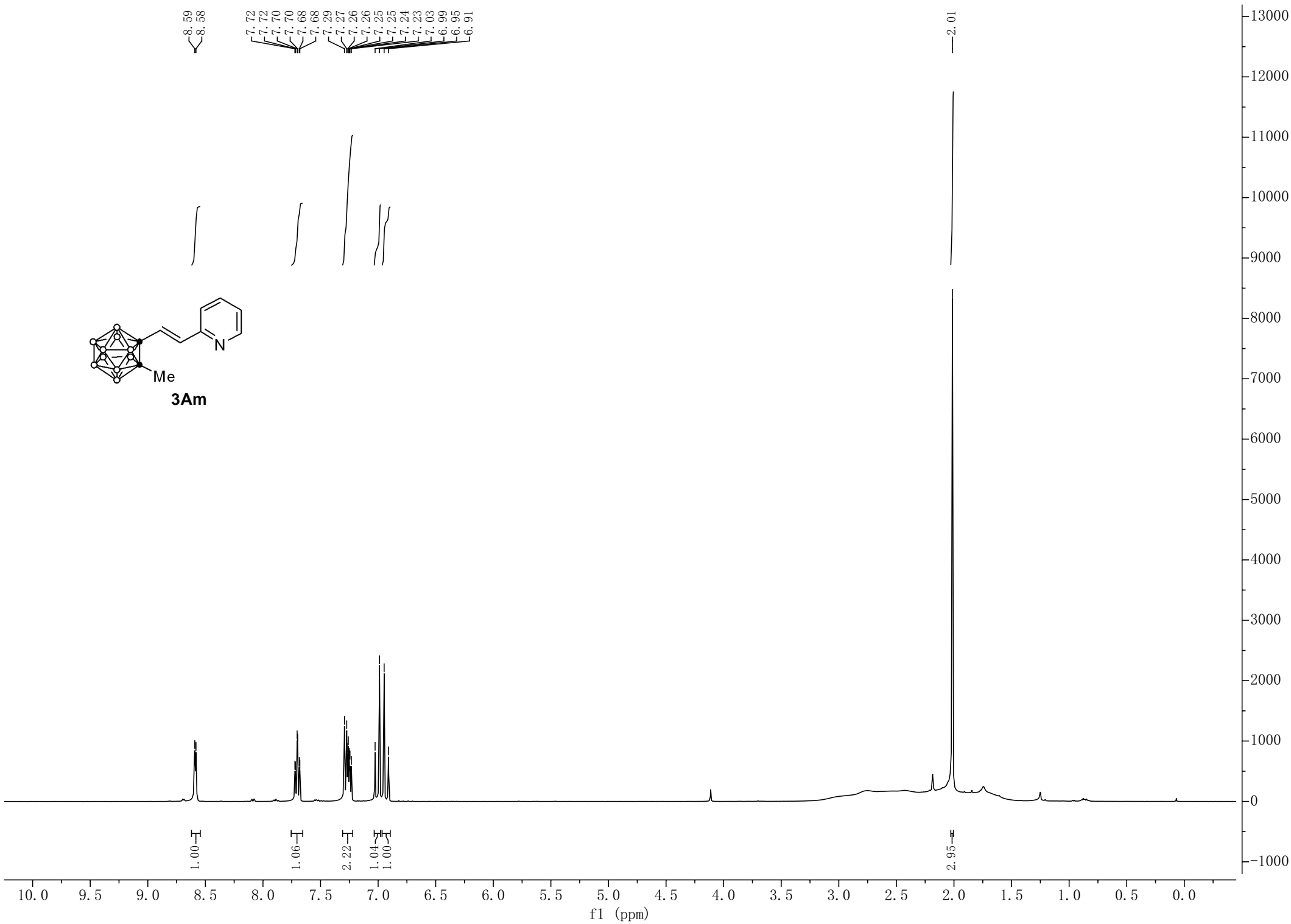


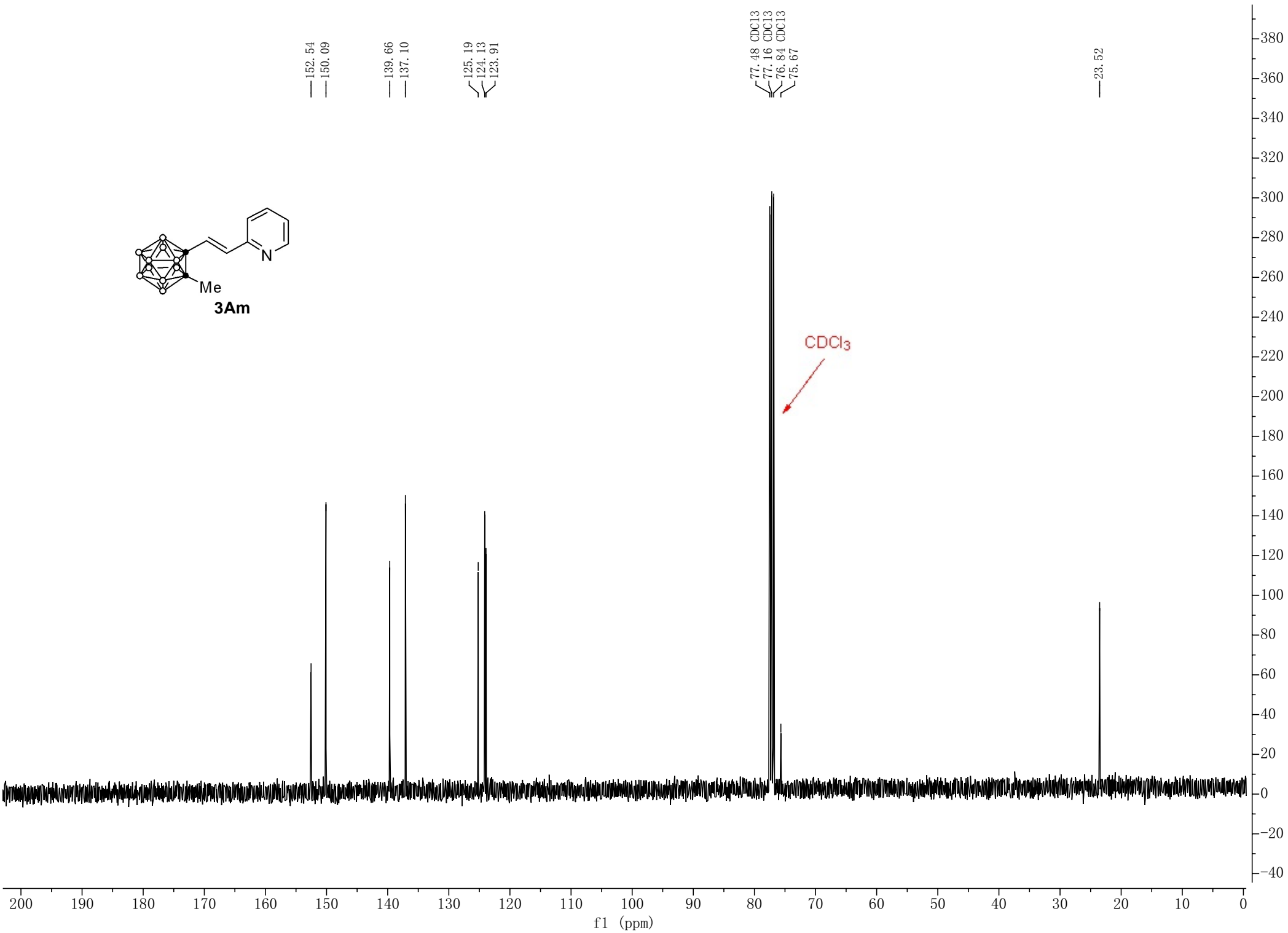
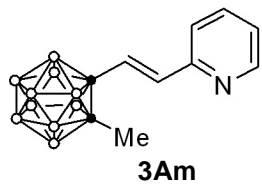


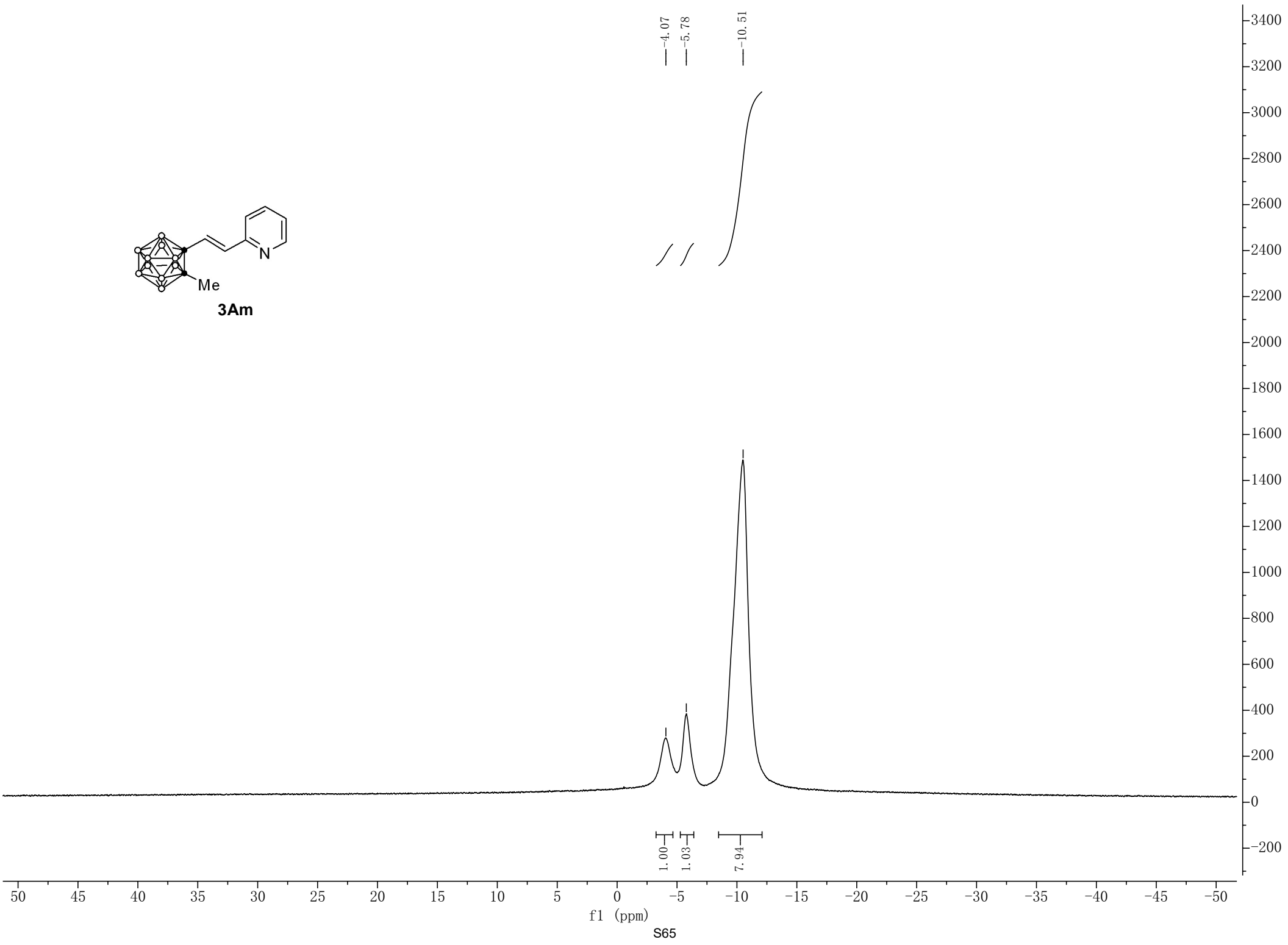
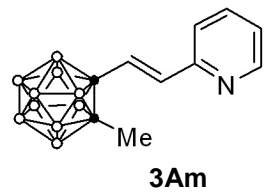


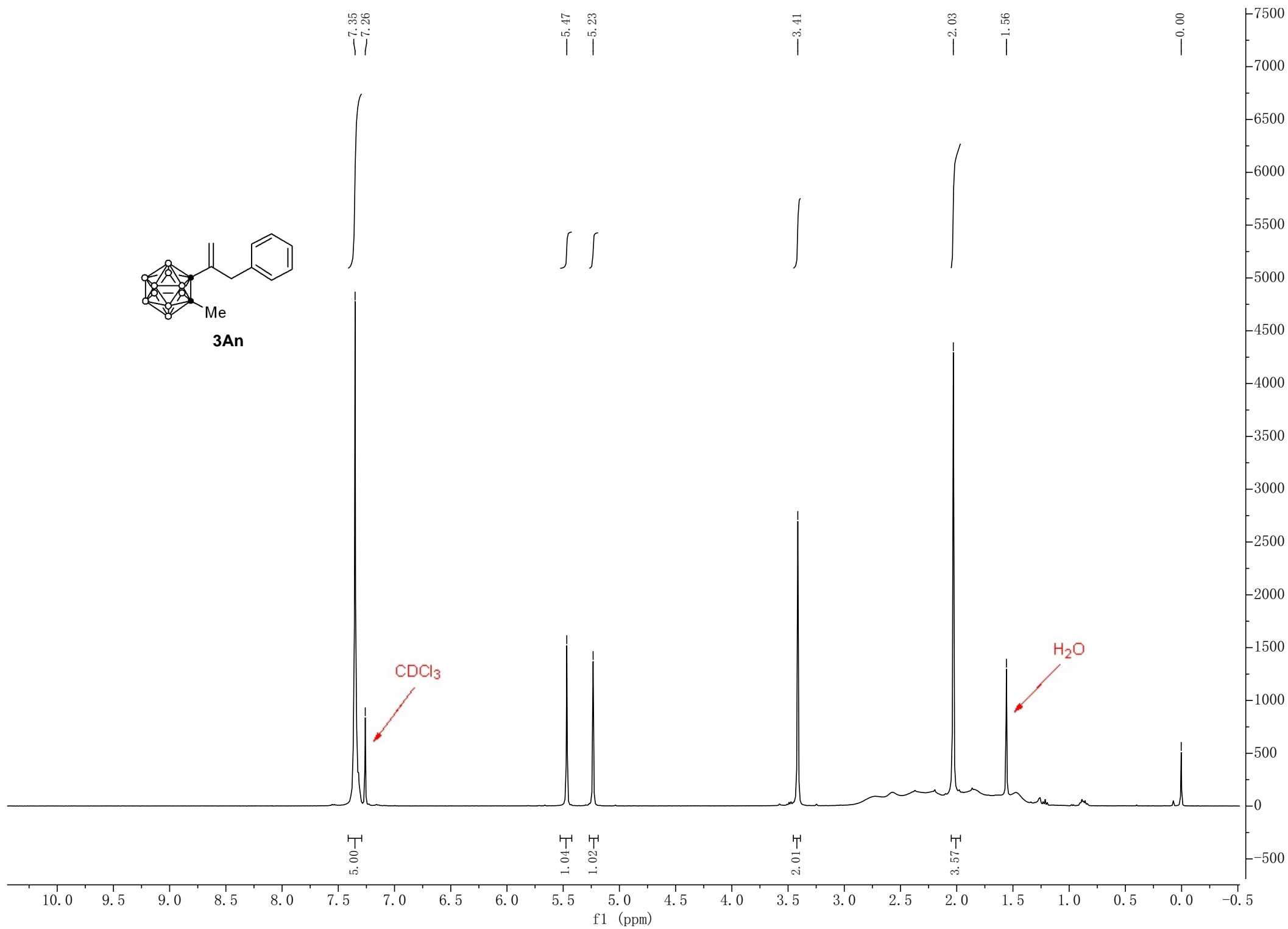
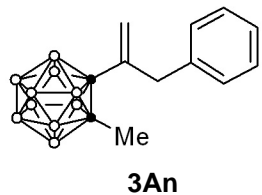


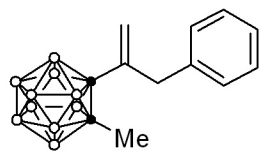
8.59
8.58
7.72
7.72
7.70
7.70
7.68
7.68
7.29
7.27
7.26
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7.25
7.25
7.24
7.23
7.03
6.99
6.95
6.91











3An

143.51
140.05

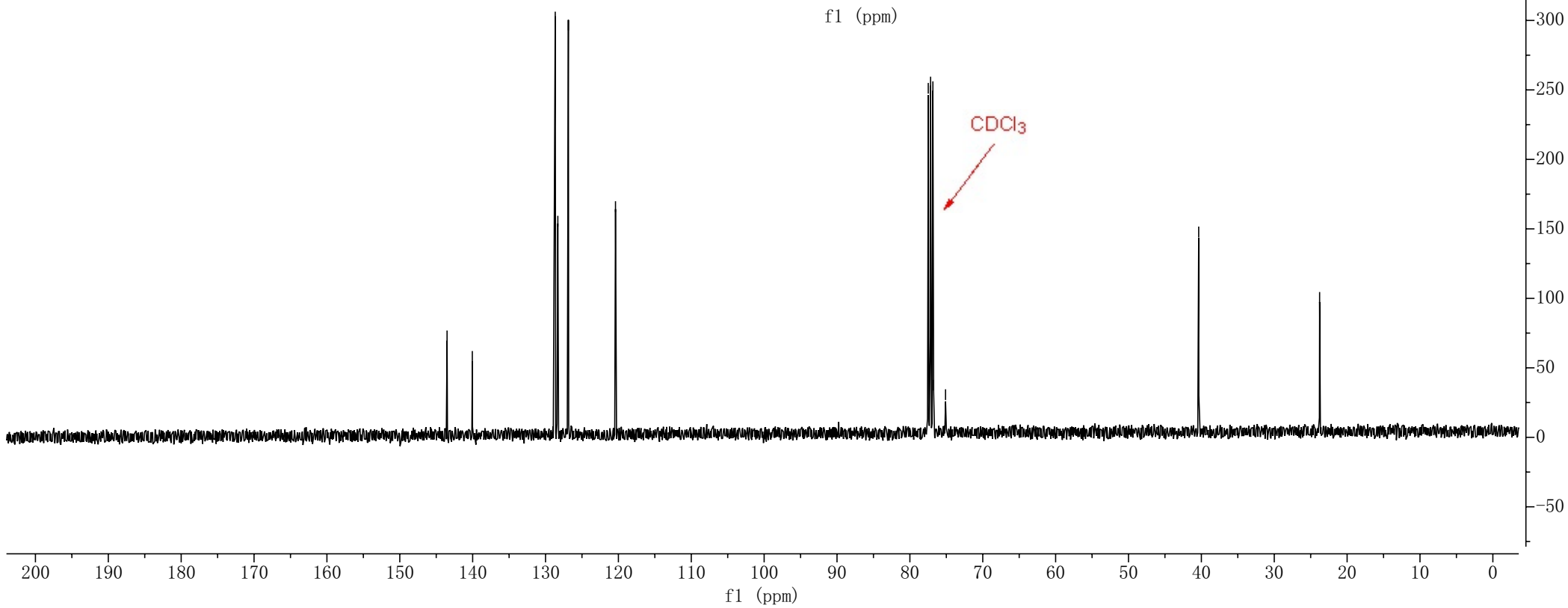
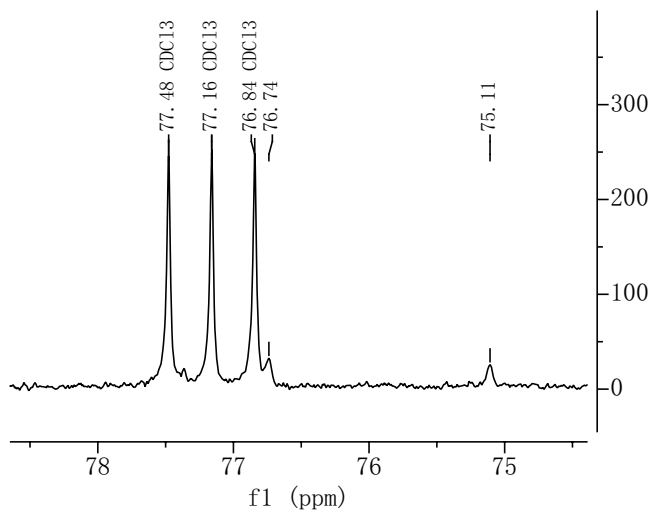
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128.31
126.87

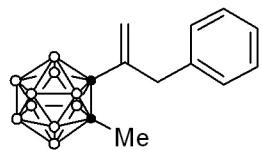
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77.48 CDCl₃
77.16 CDCl₃
76.84 CDCl₃
76.74
75.11

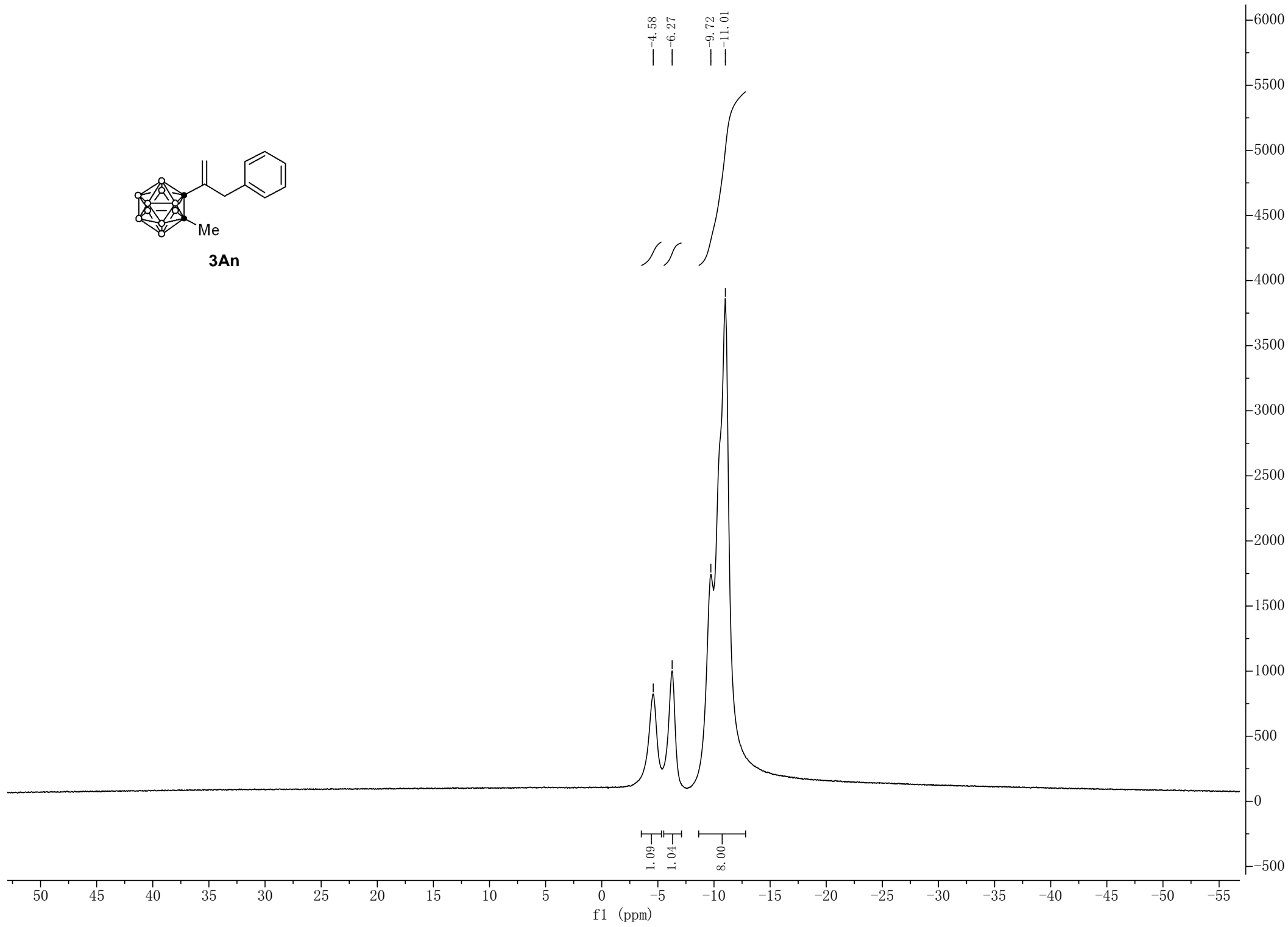
40.37

23.77



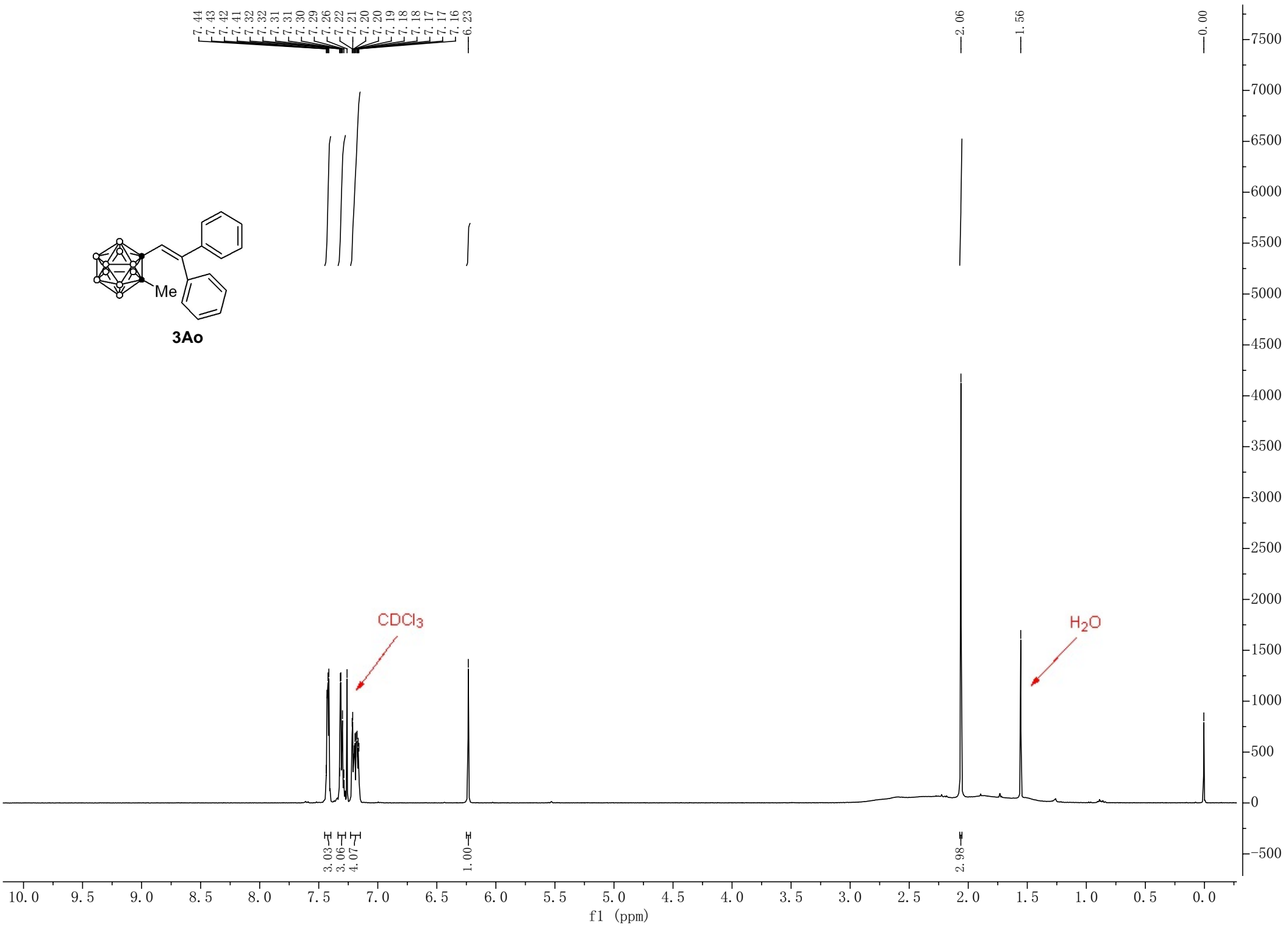


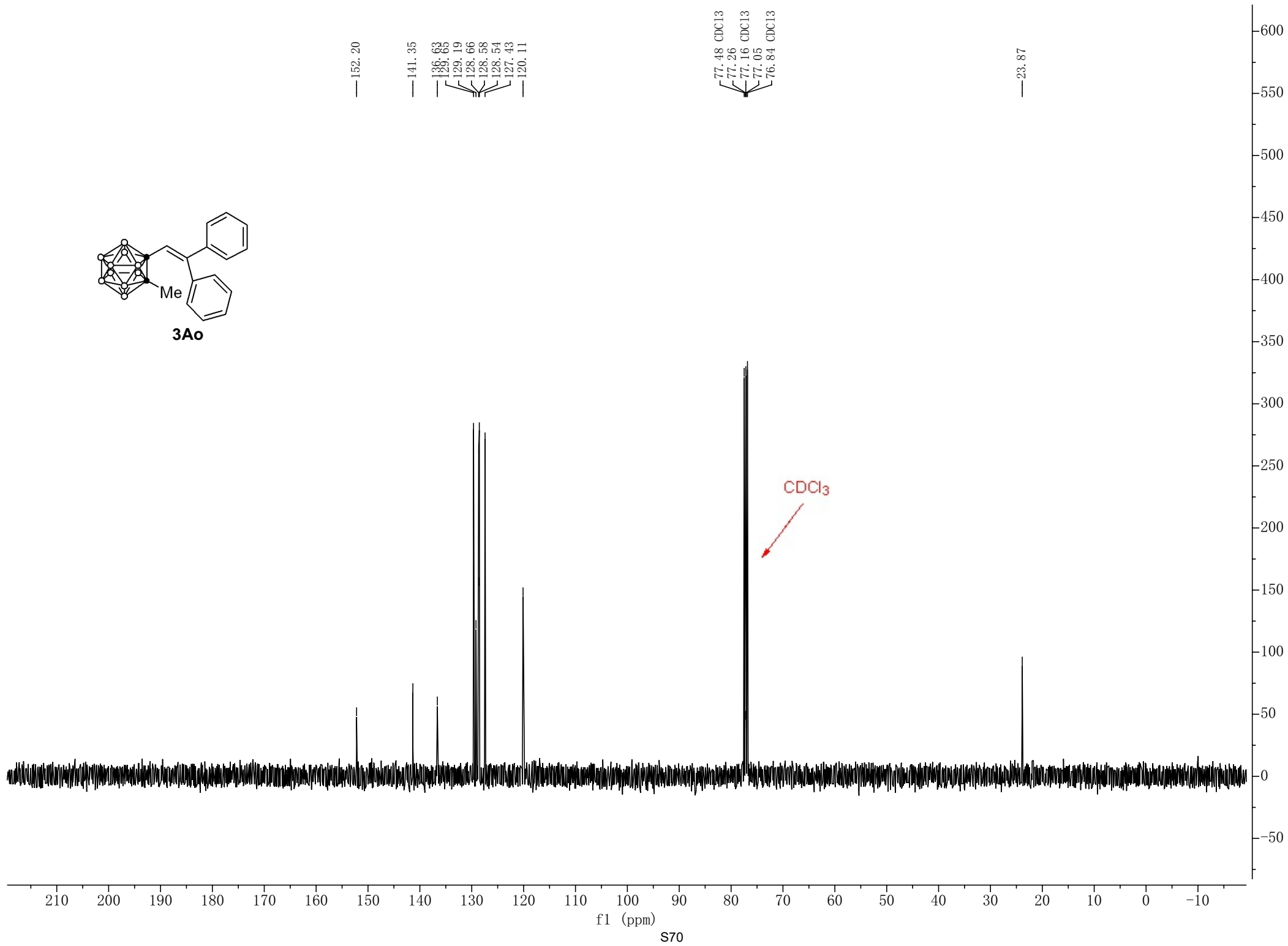
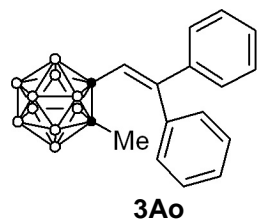
3An

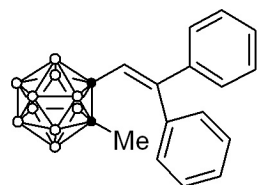


1.09
1.04
8.00

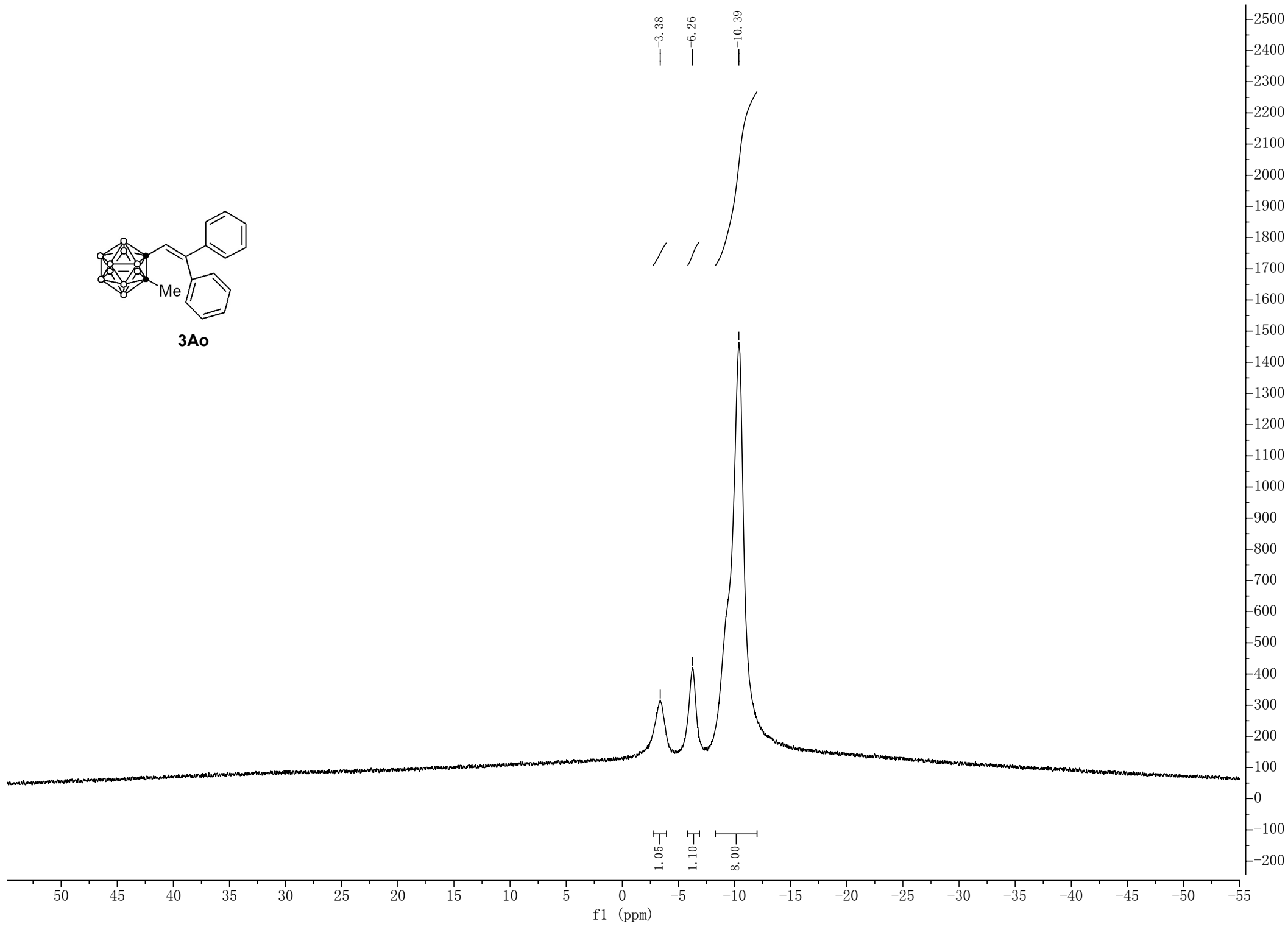
-4.58
-6.27
-9.72
-11.01

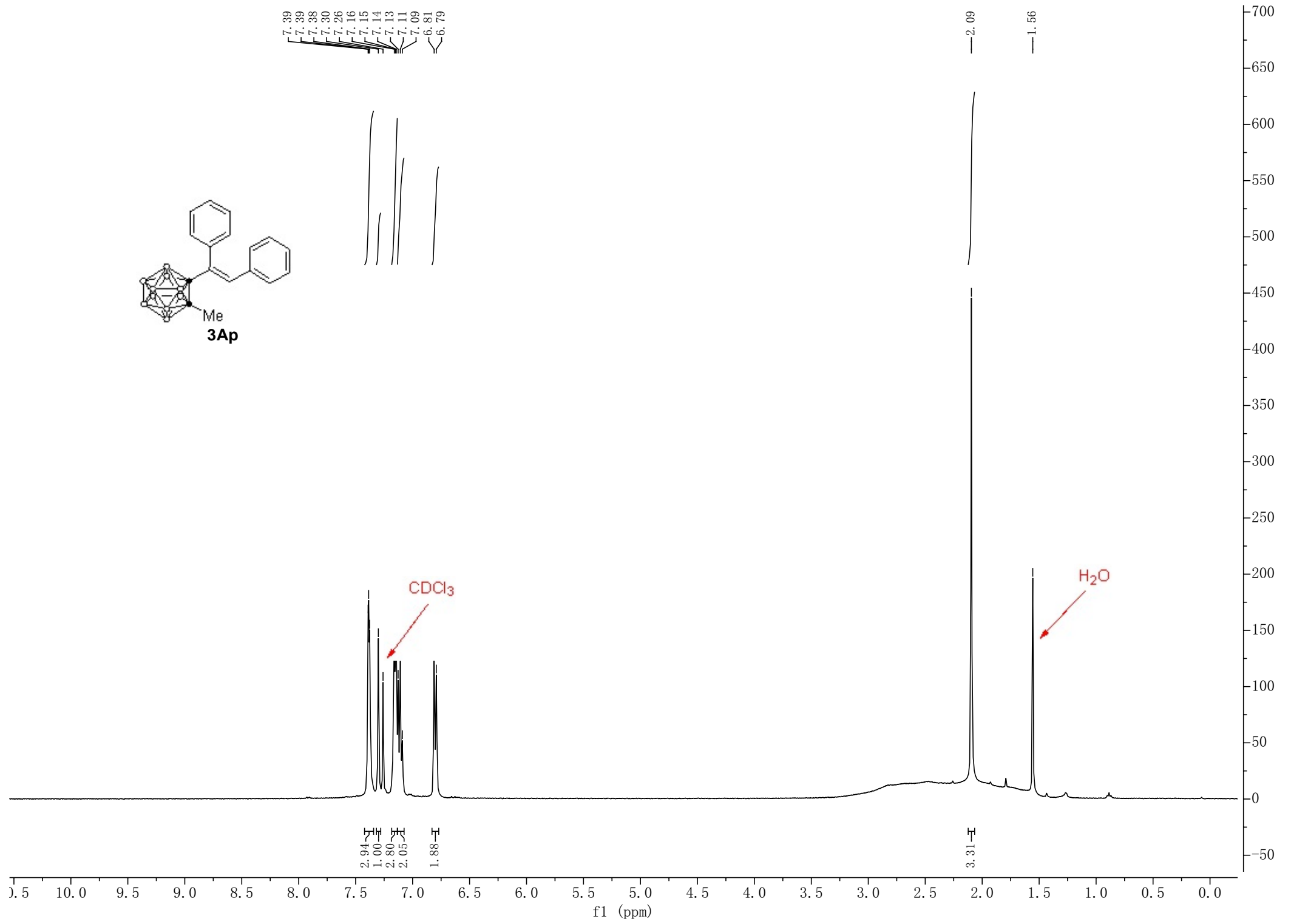


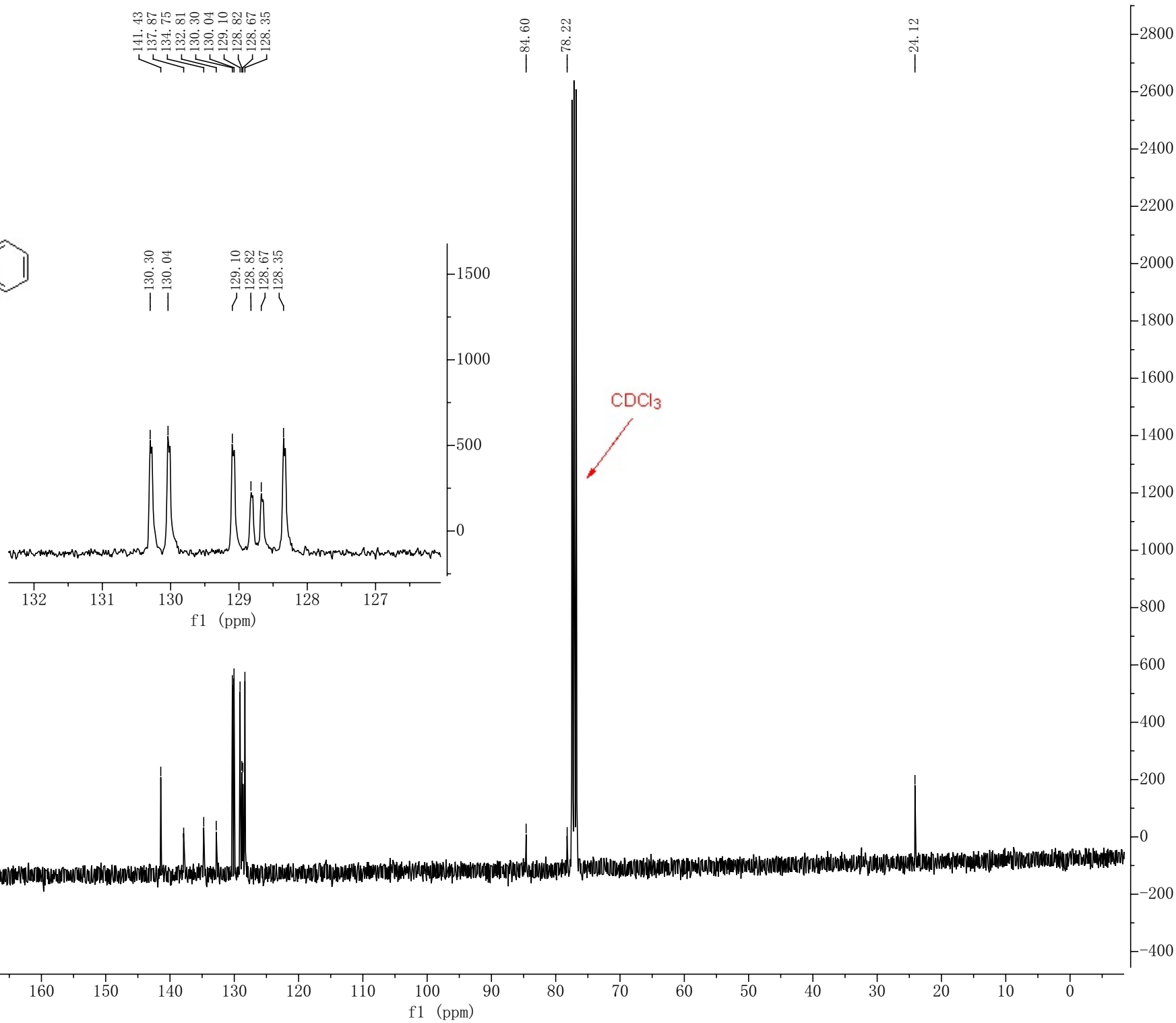
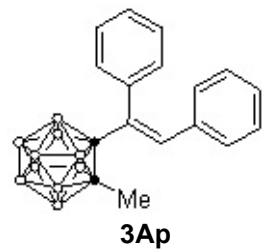


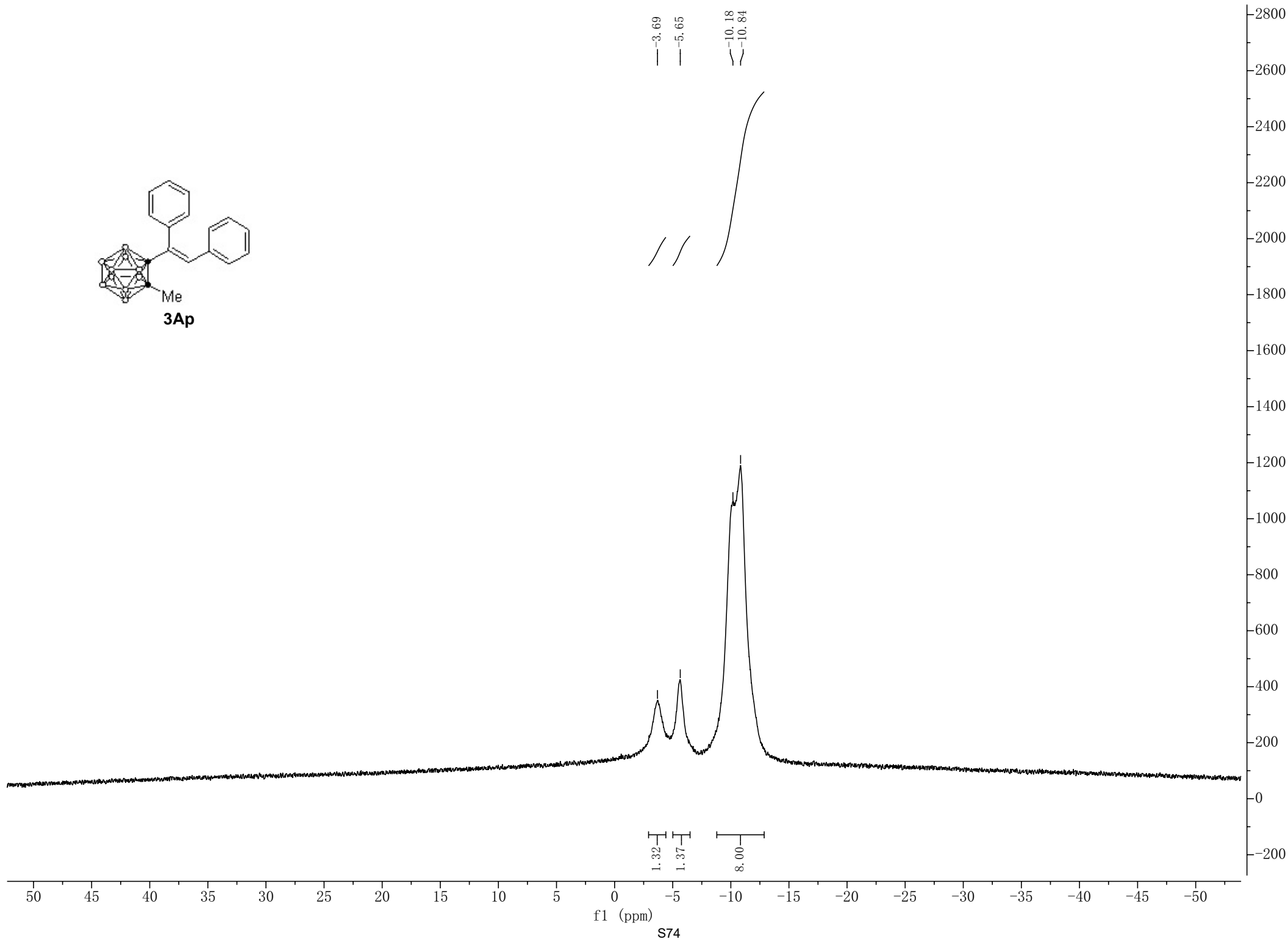
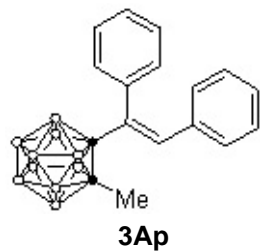


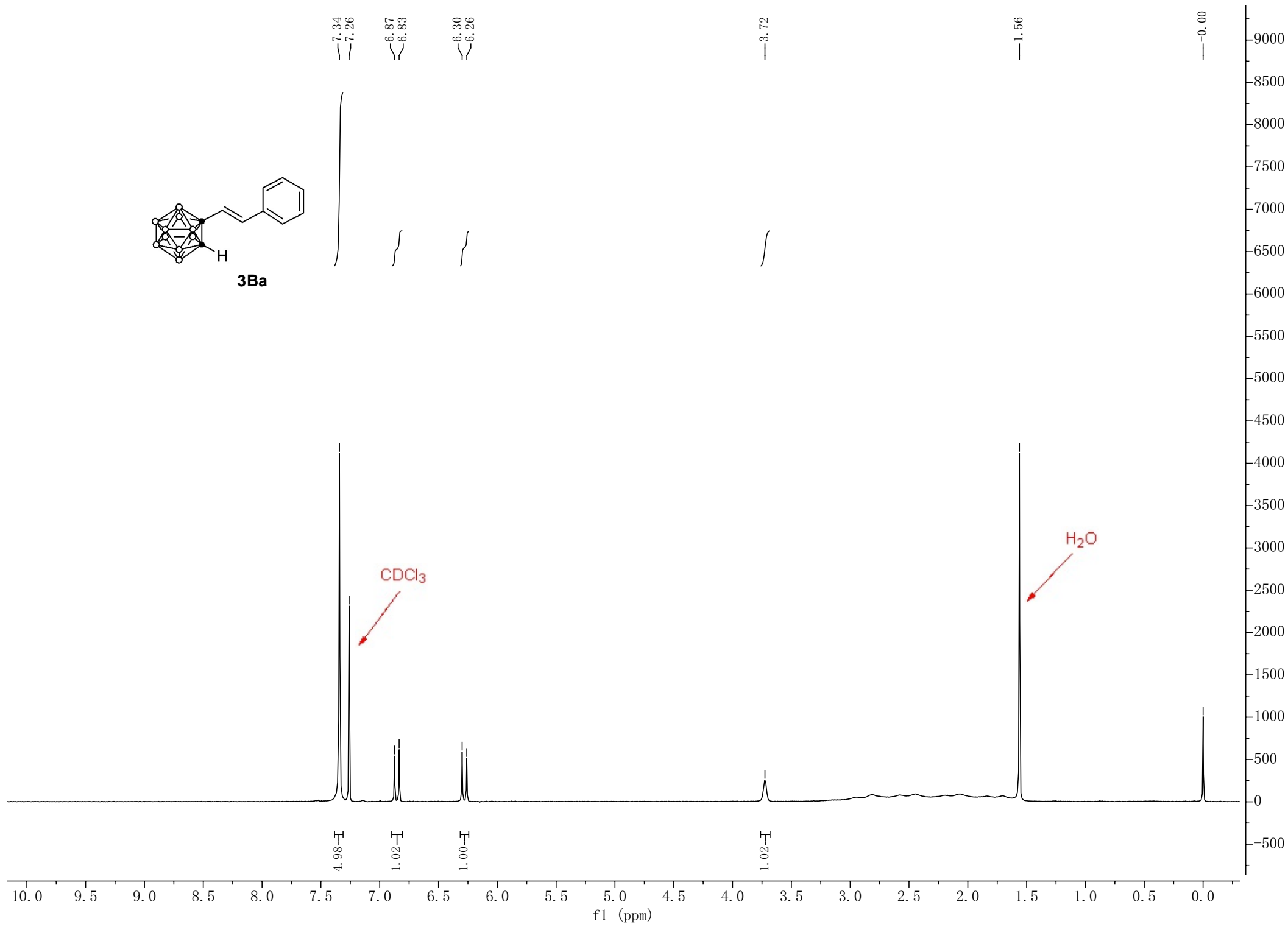
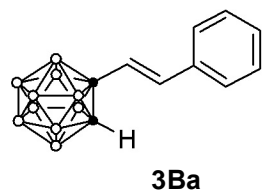
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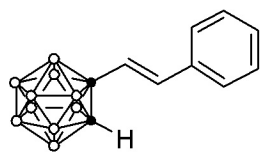






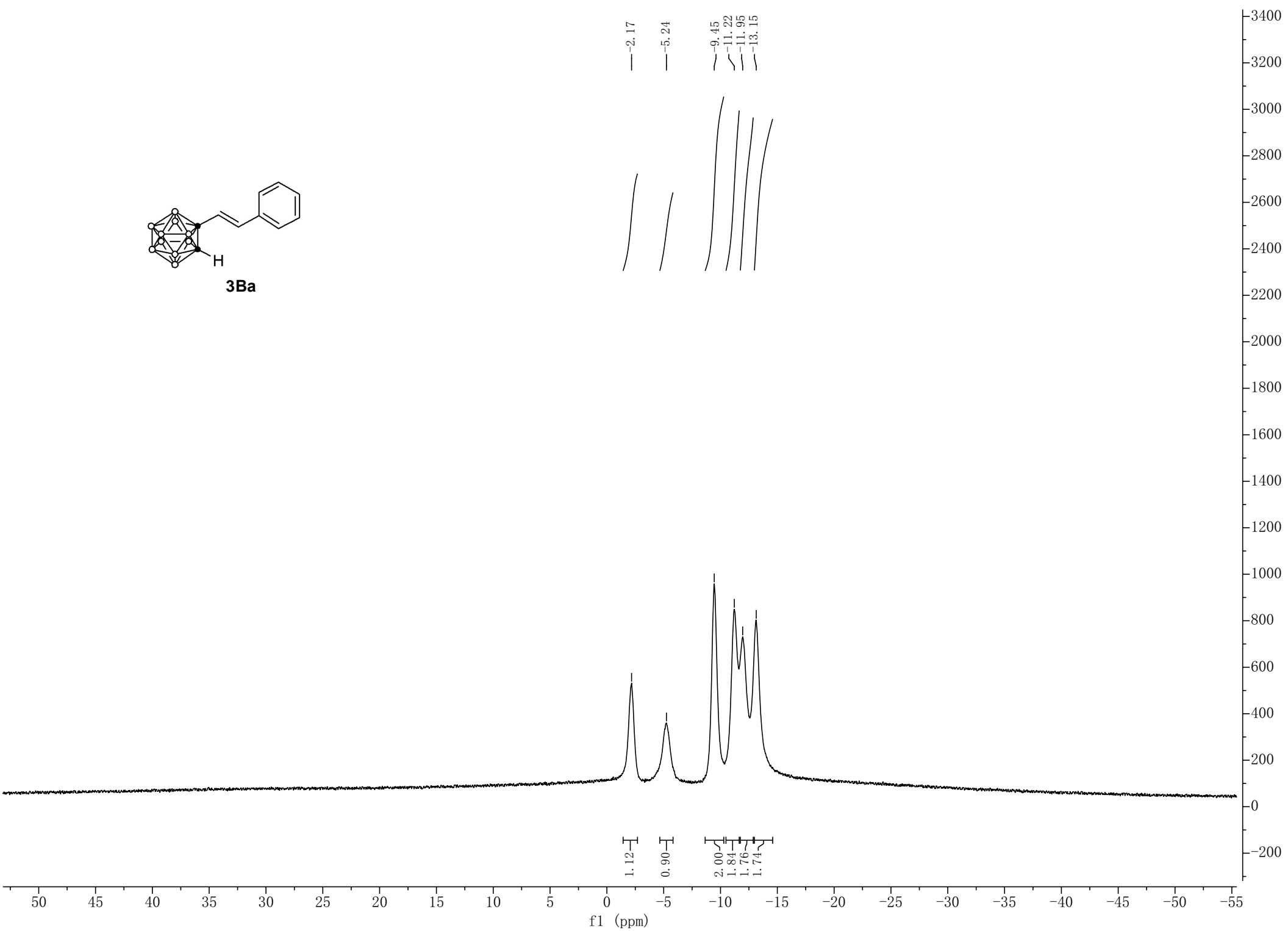


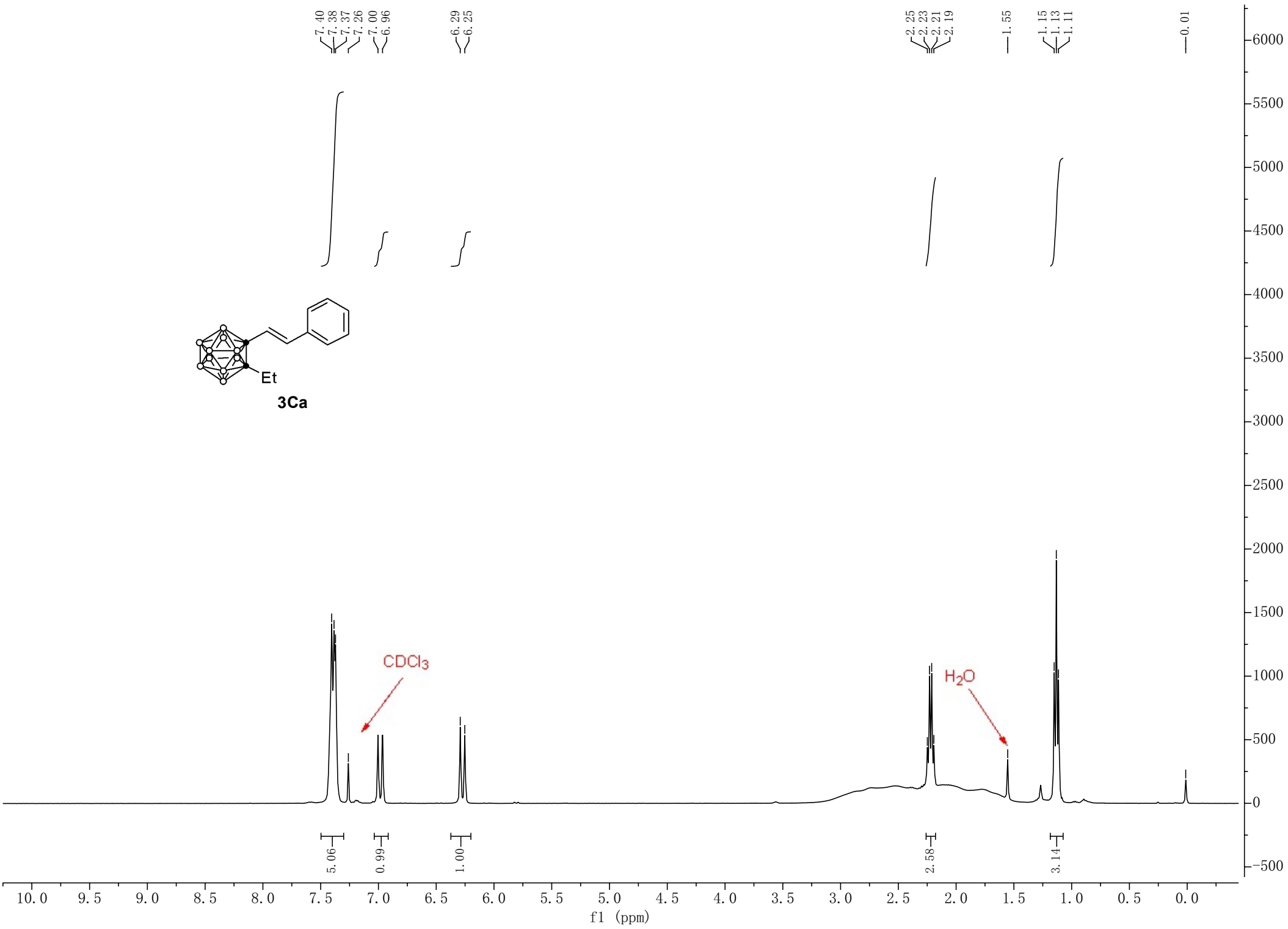


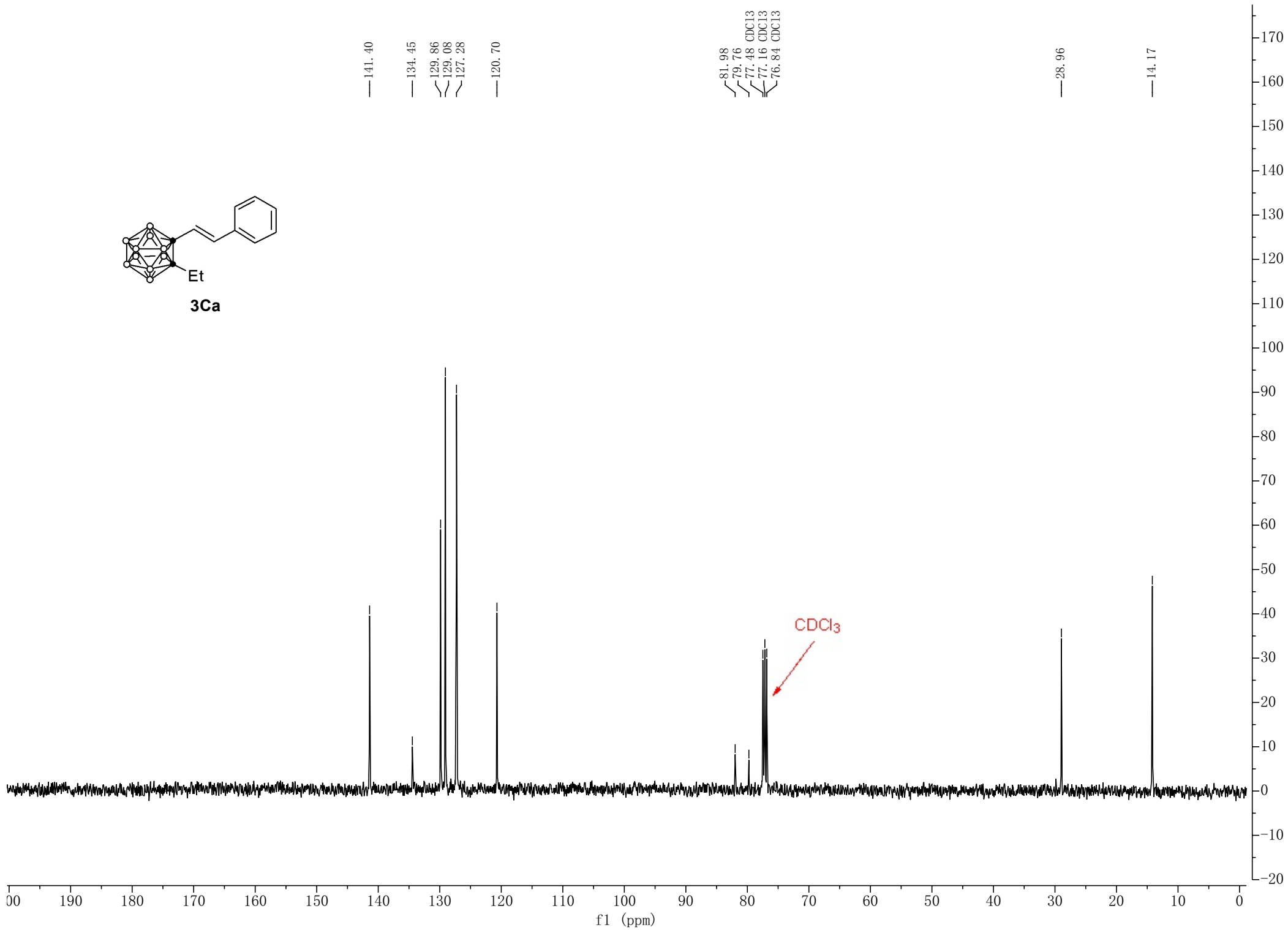
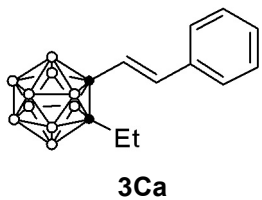


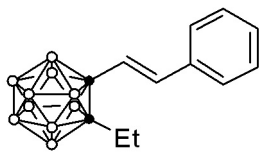
3Ba

— 2.17
— 5.24
— 9.45
— 11.22
— 11.95
— 13.15

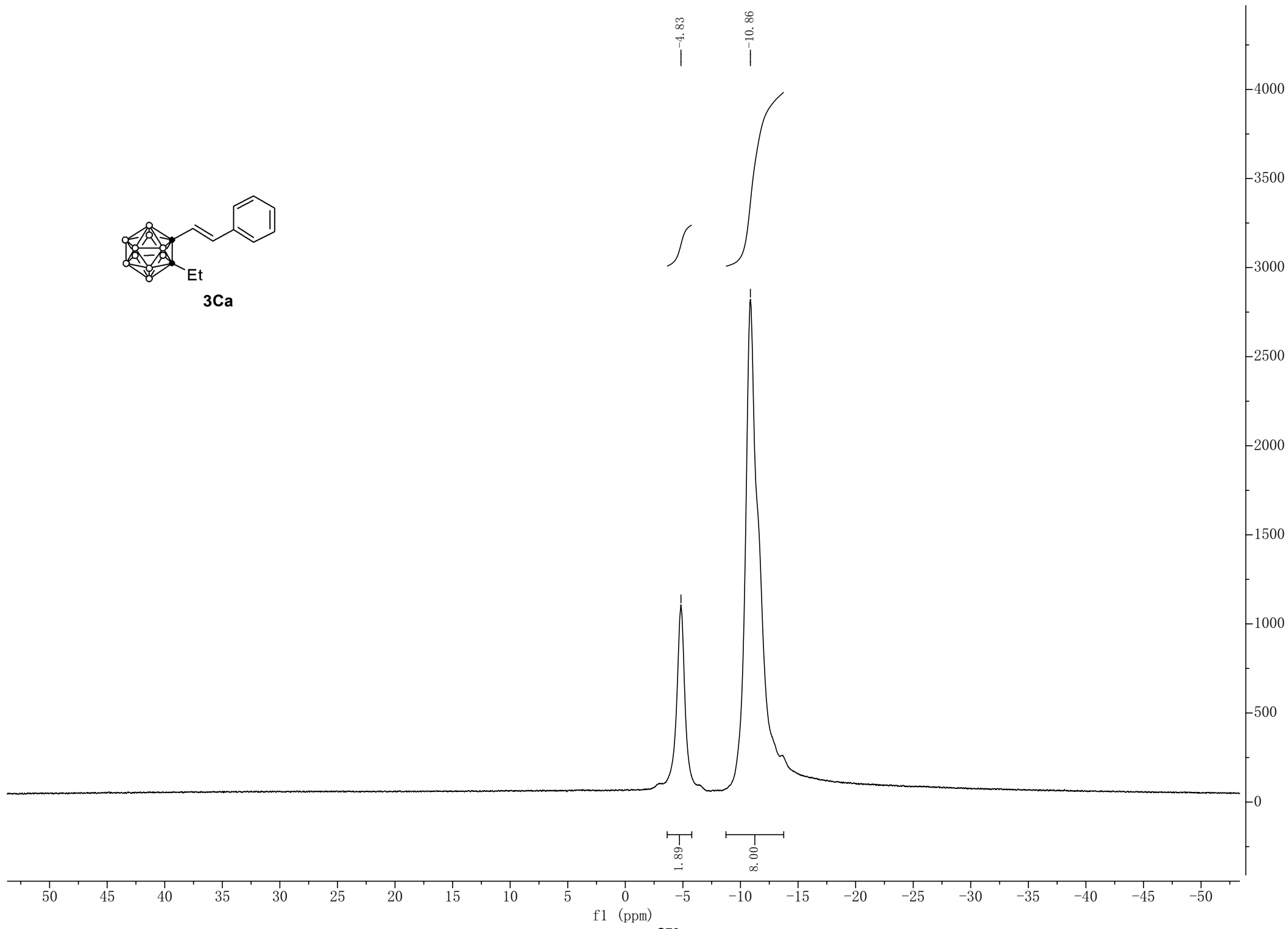


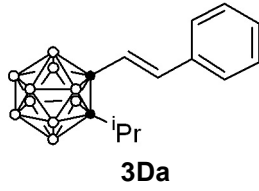






3Ca





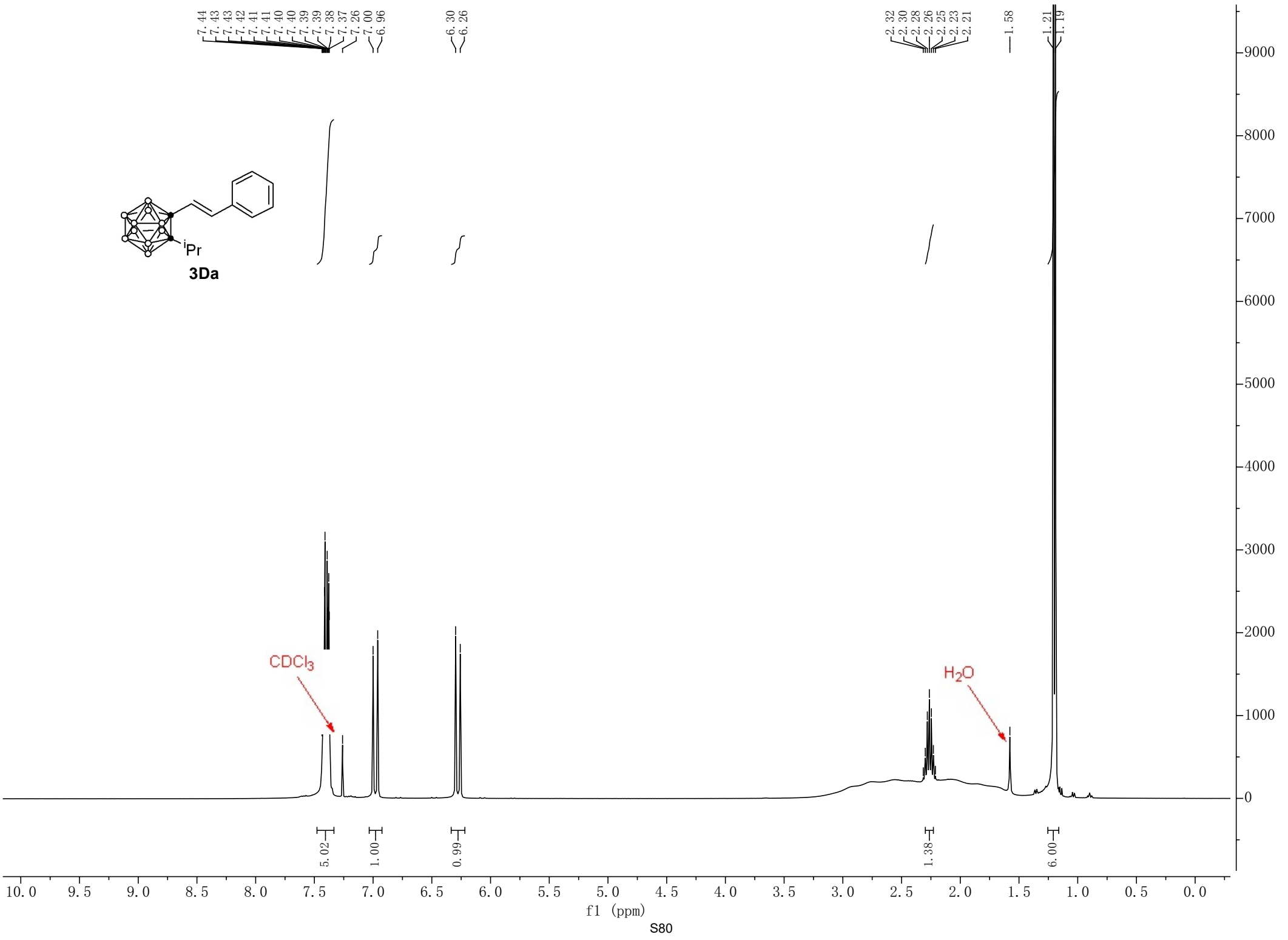
7.44
7.43
7.43
7.42
7.41
7.41
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7.39
7.39
7.38
7.37
7.26
7.00
6.96

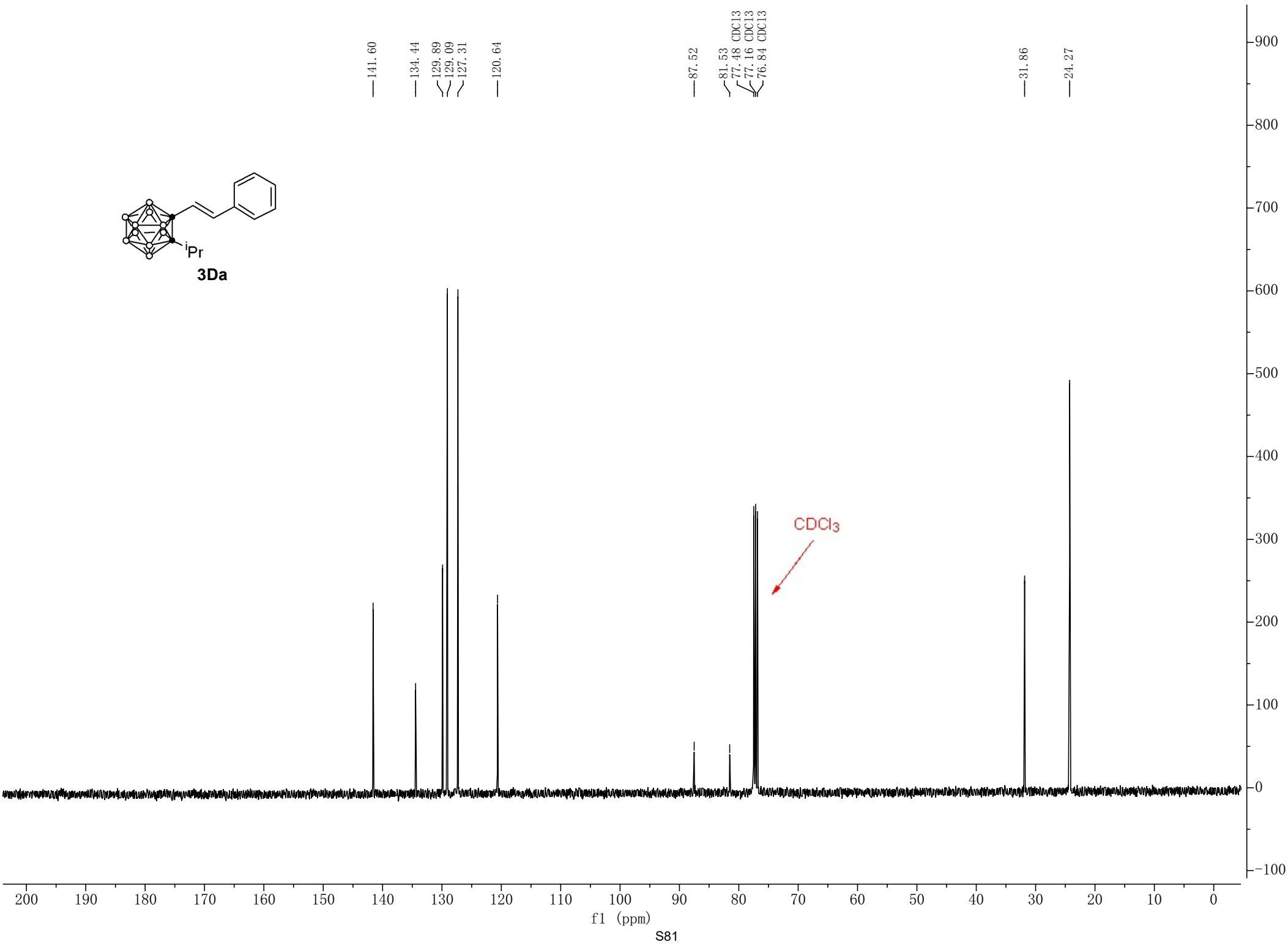
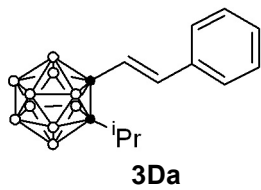
6.30
6.26

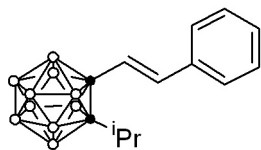
2.32
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2.25
2.23
2.21

1.58

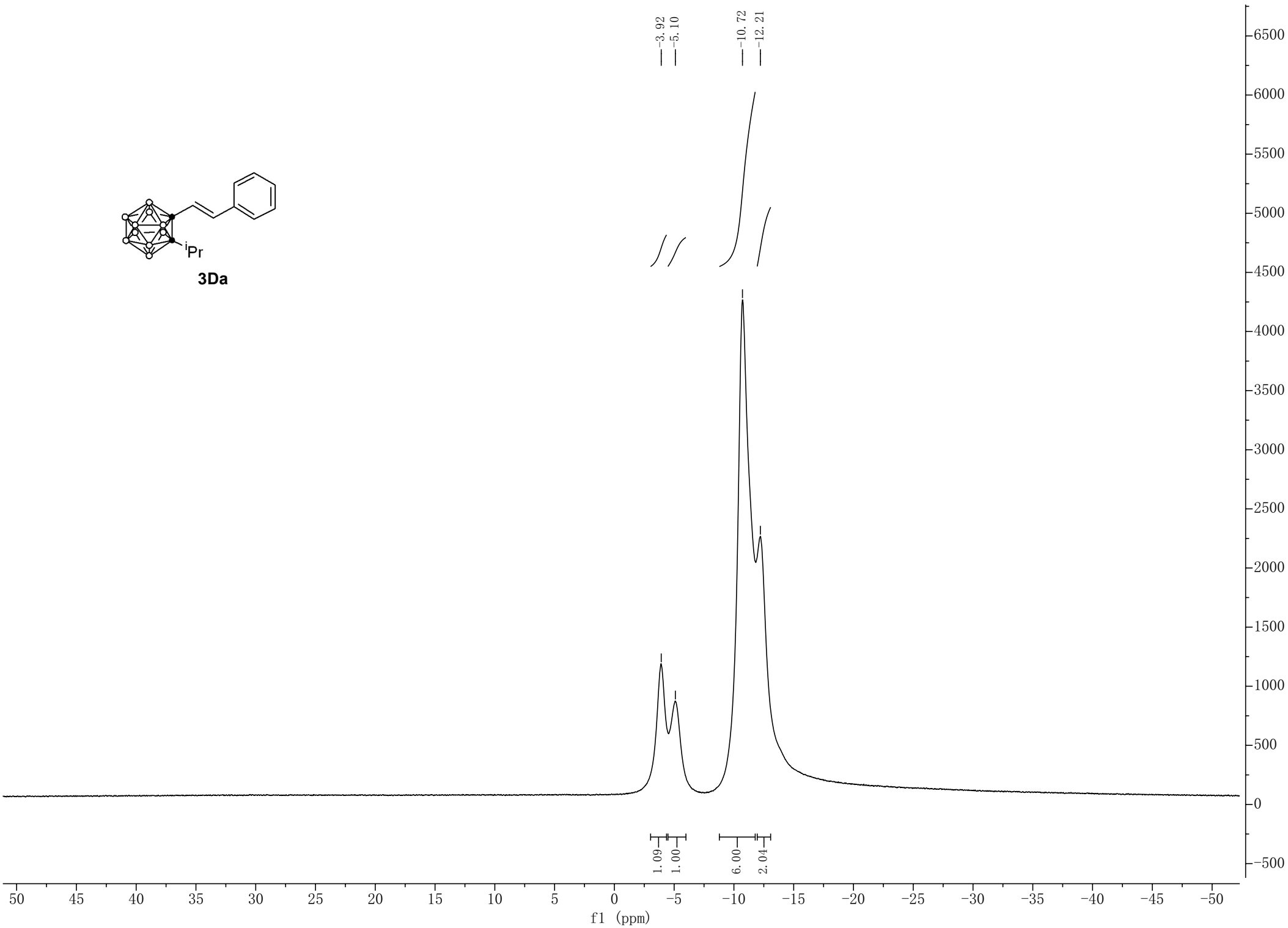
1.21
1.19

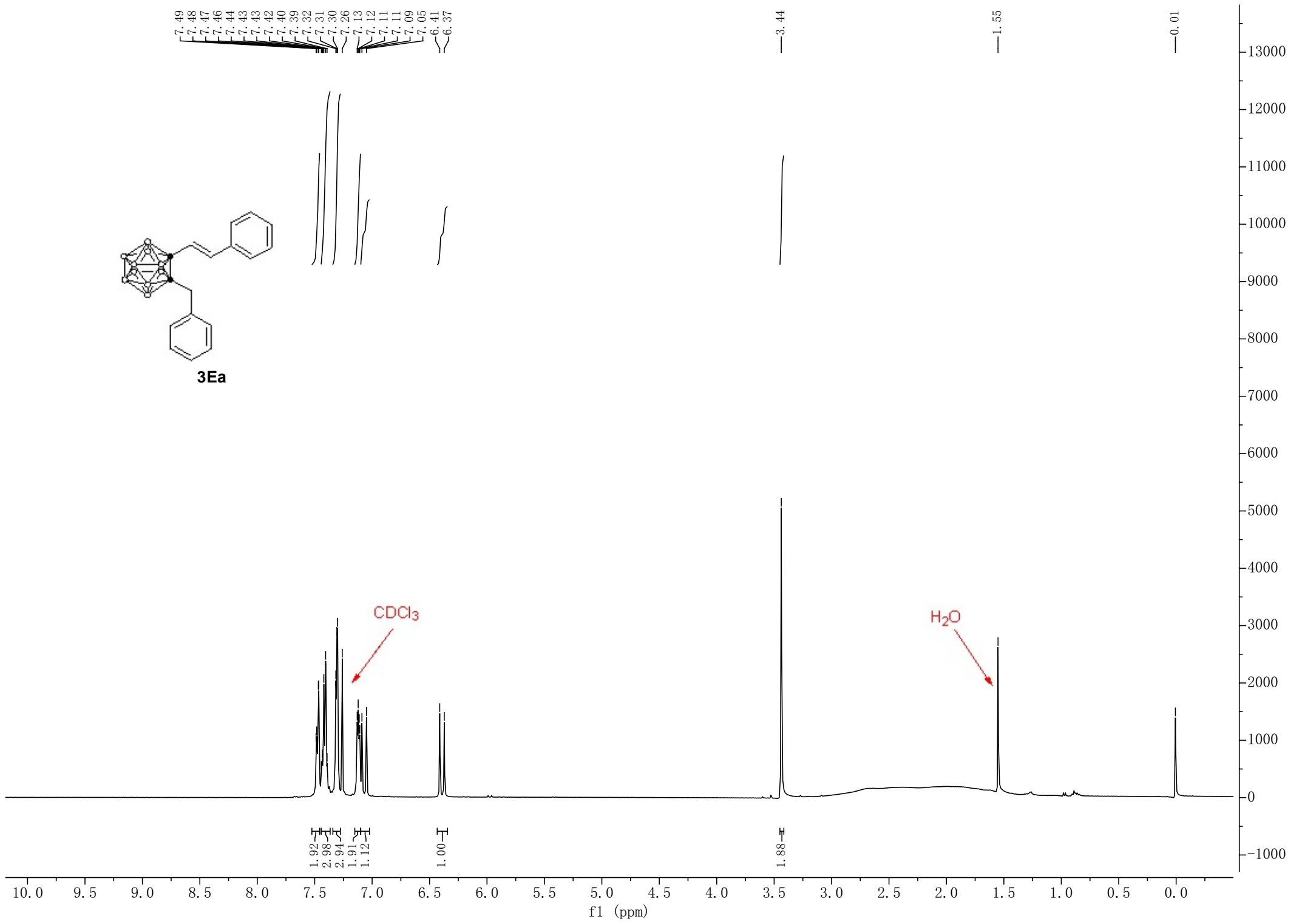


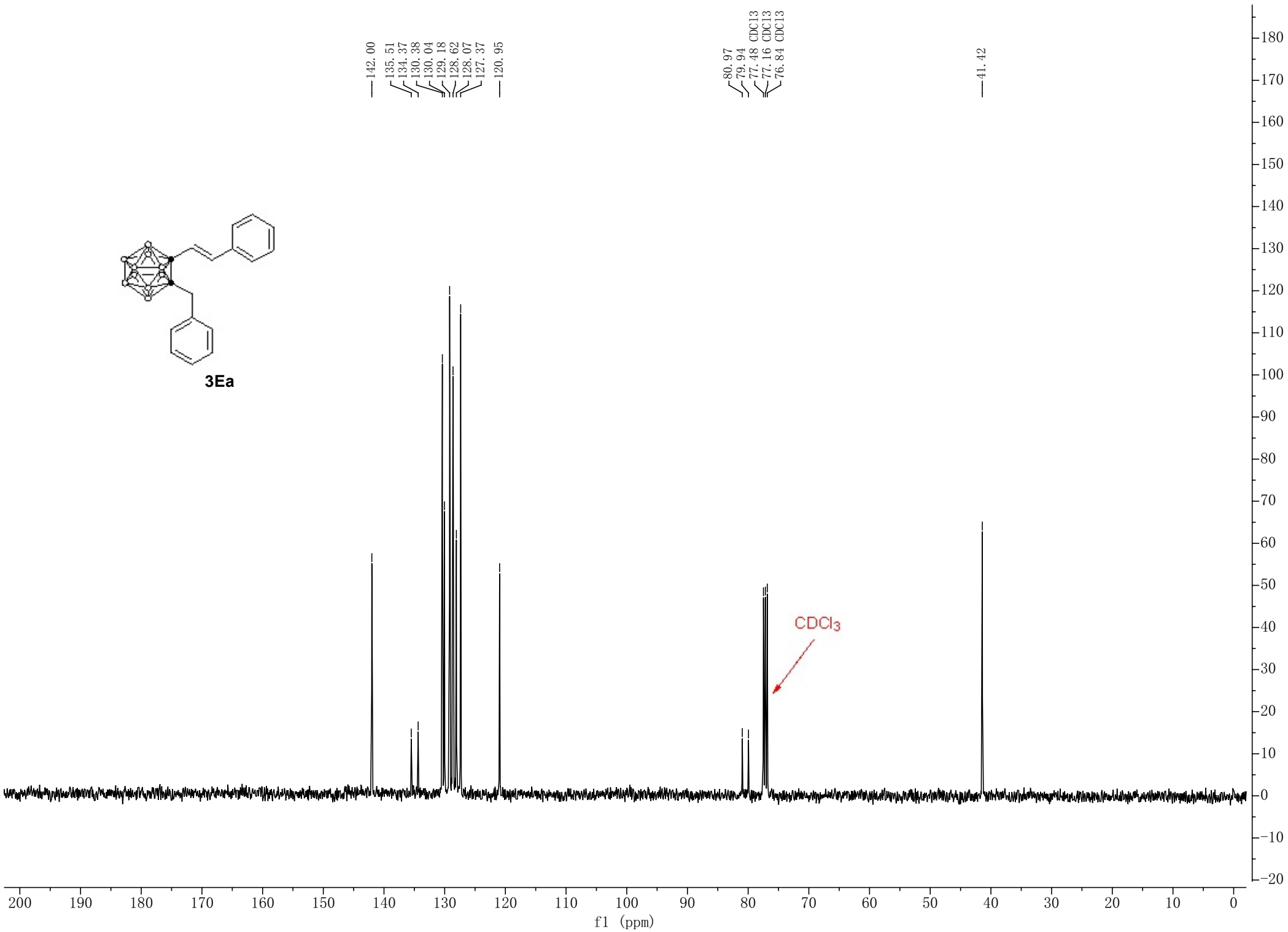
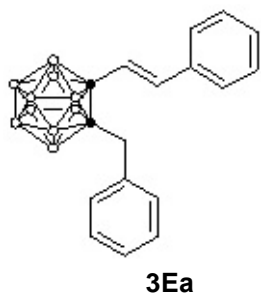


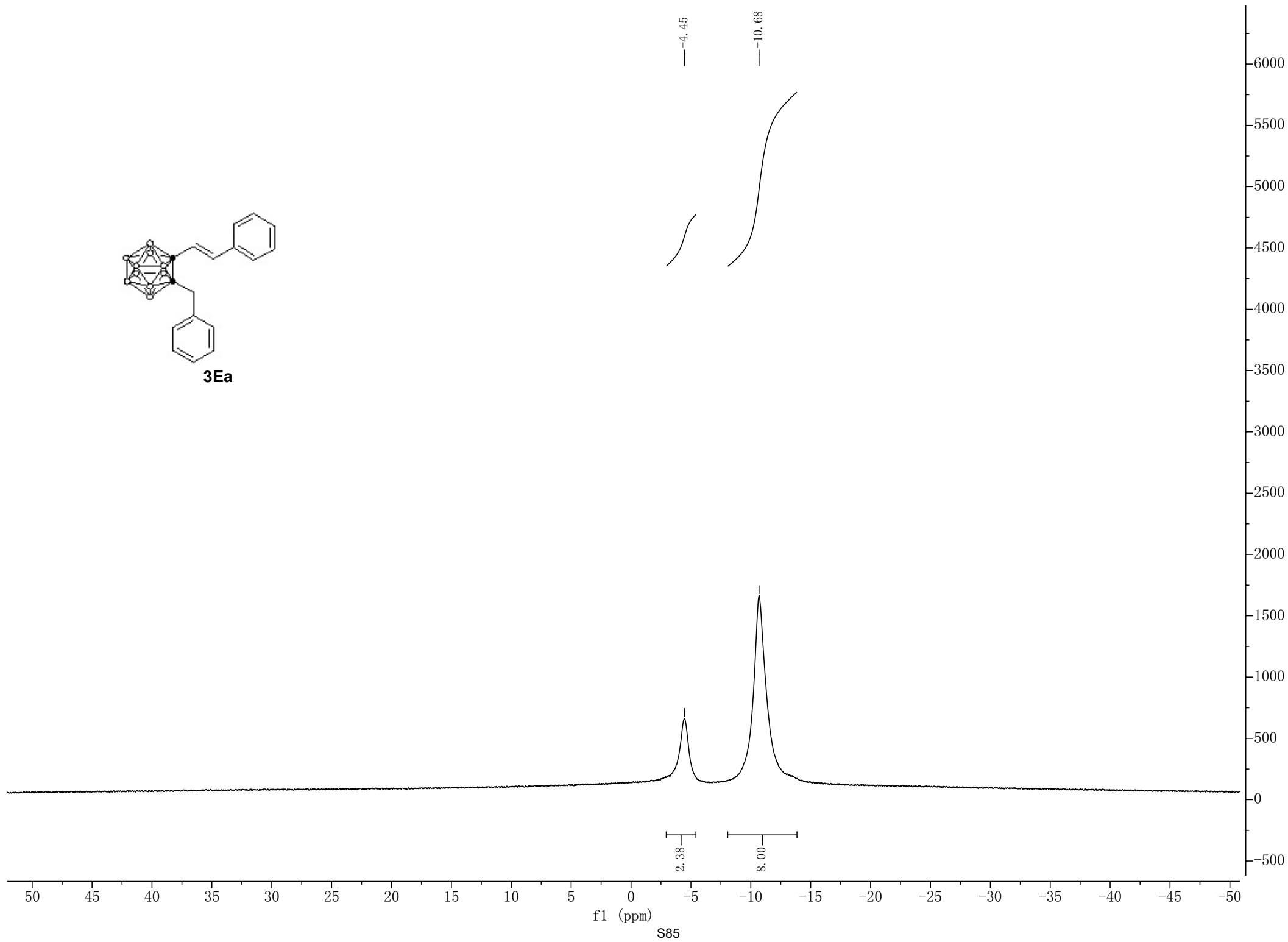
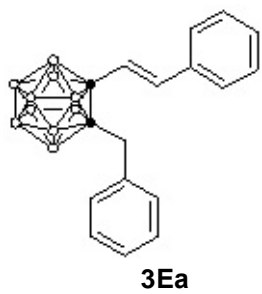


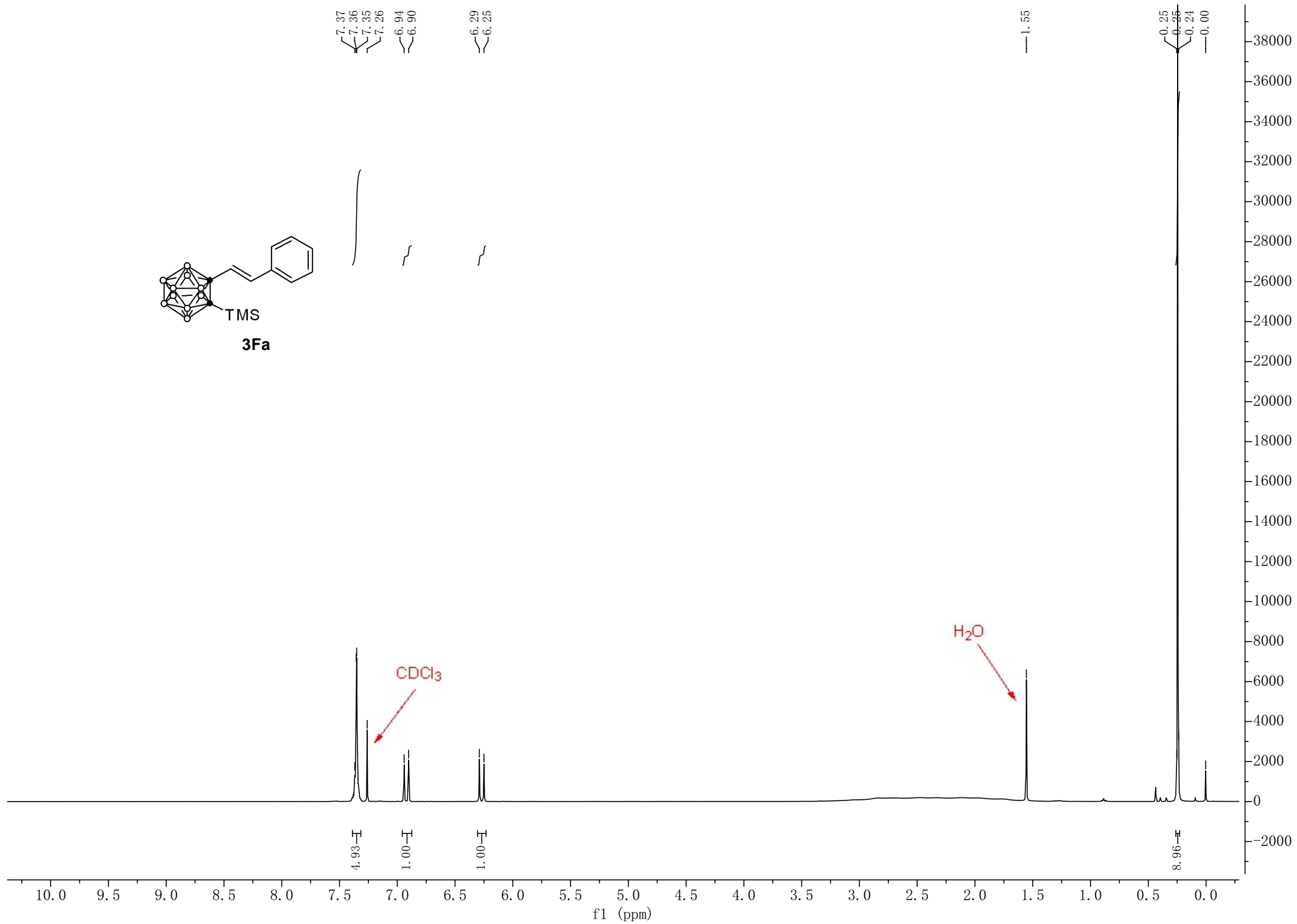
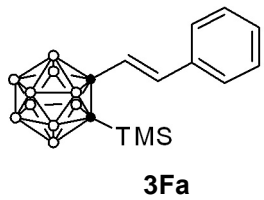
3Da

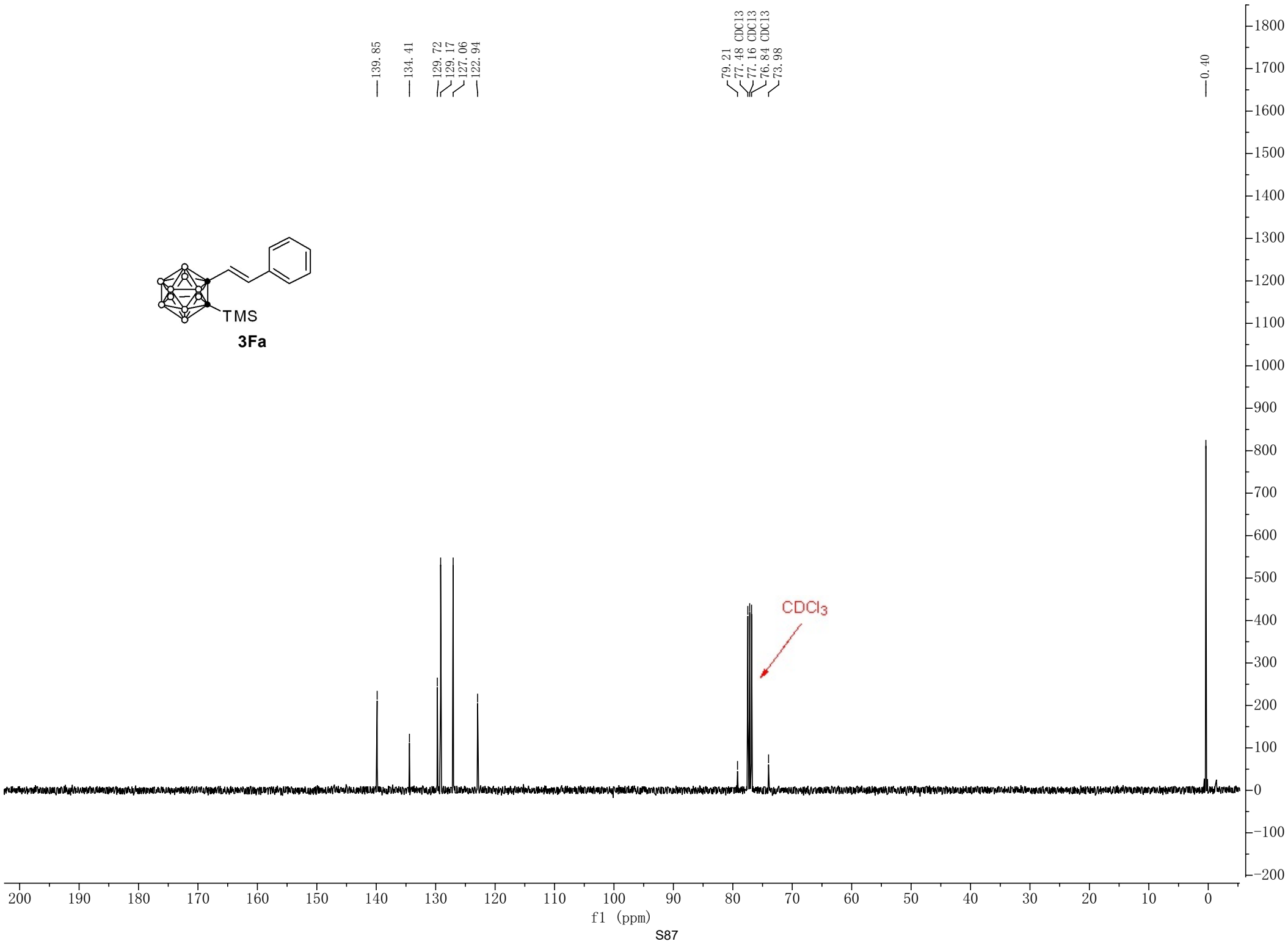
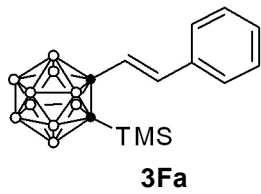


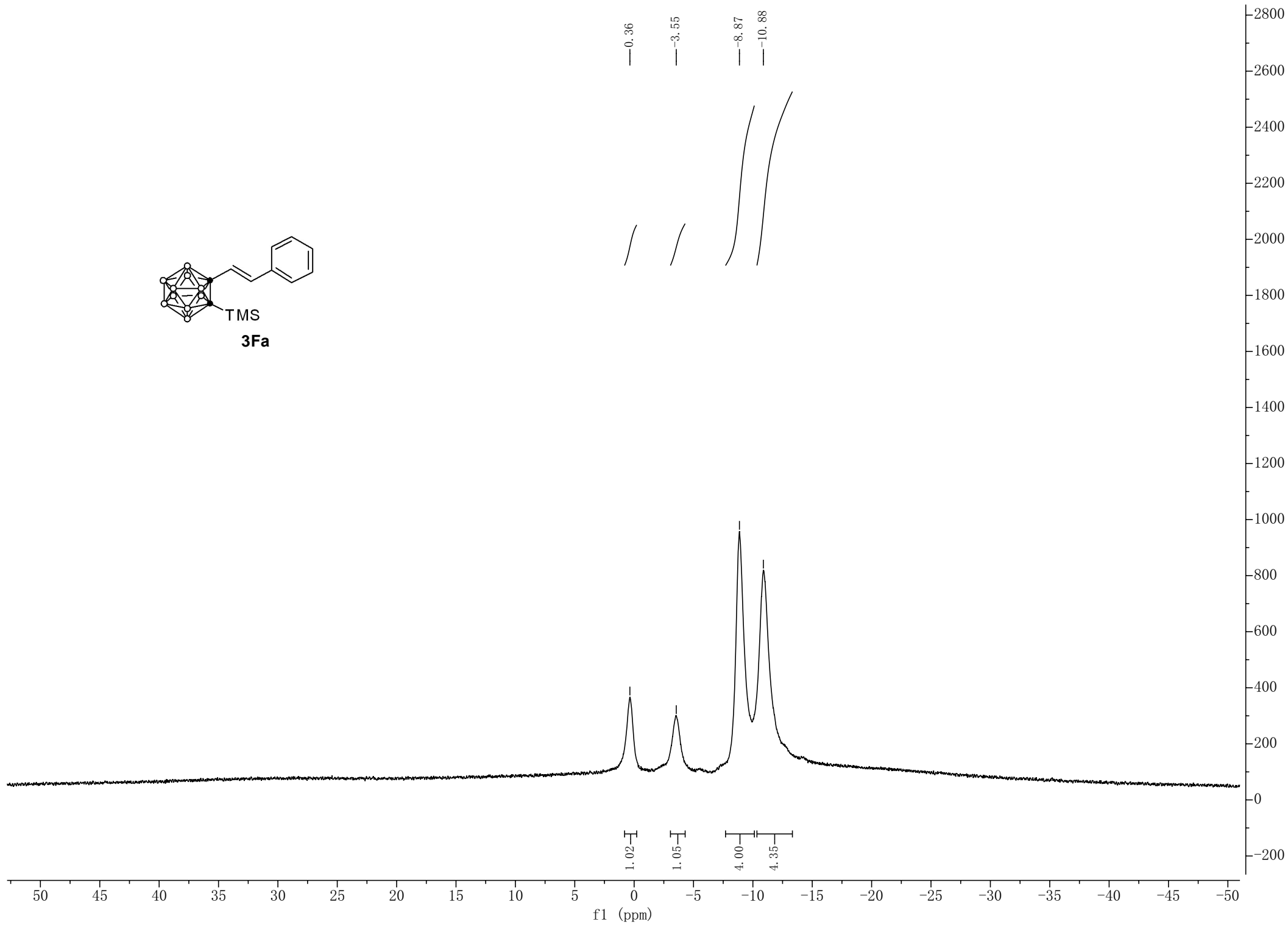
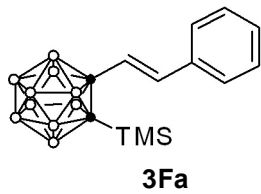


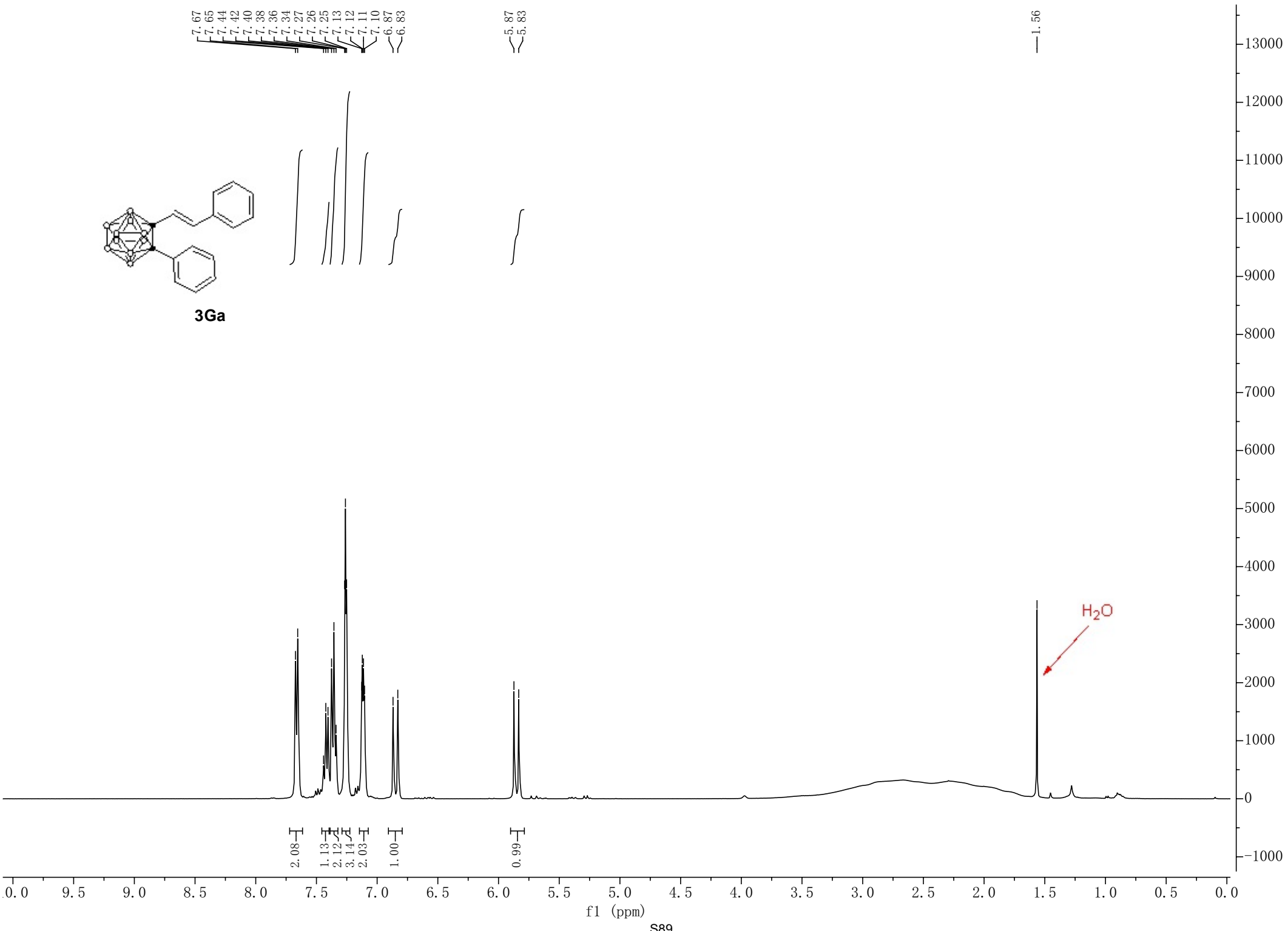


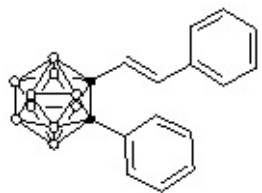




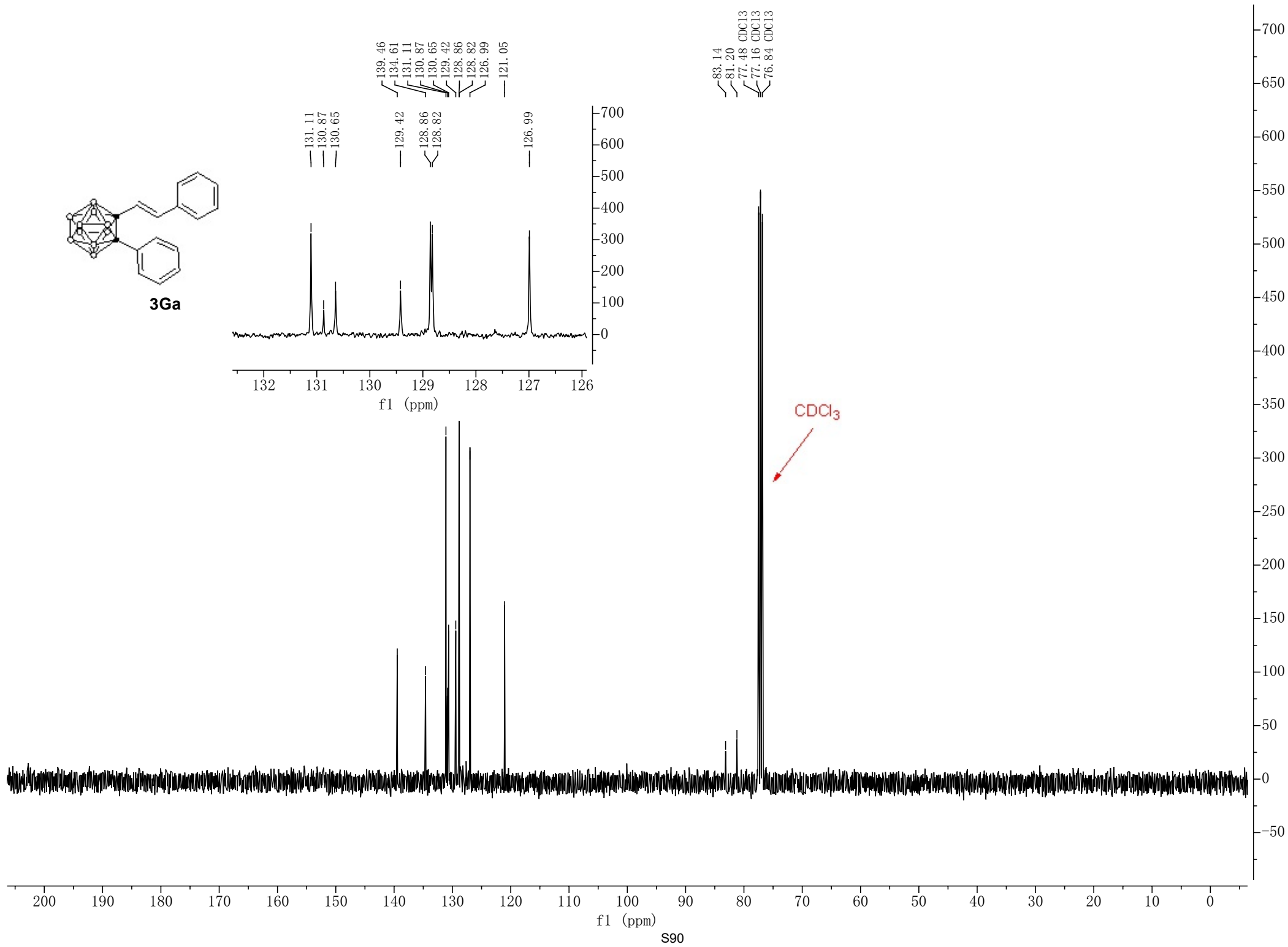
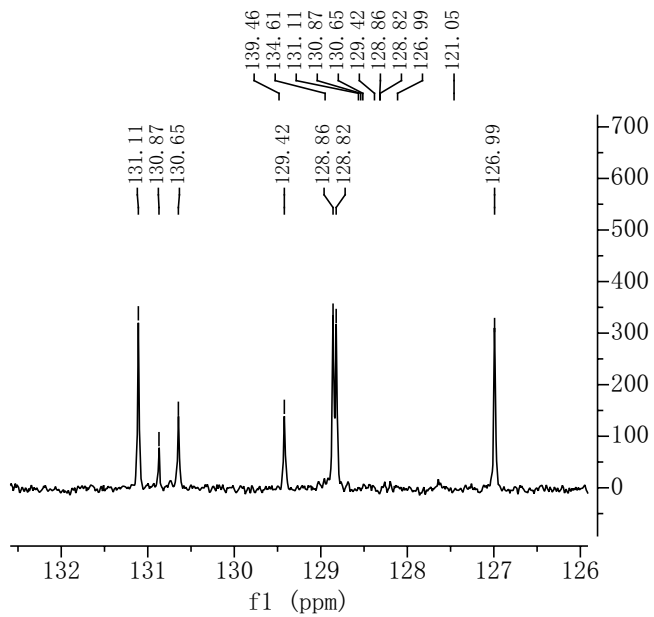


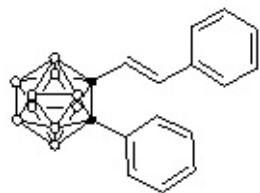




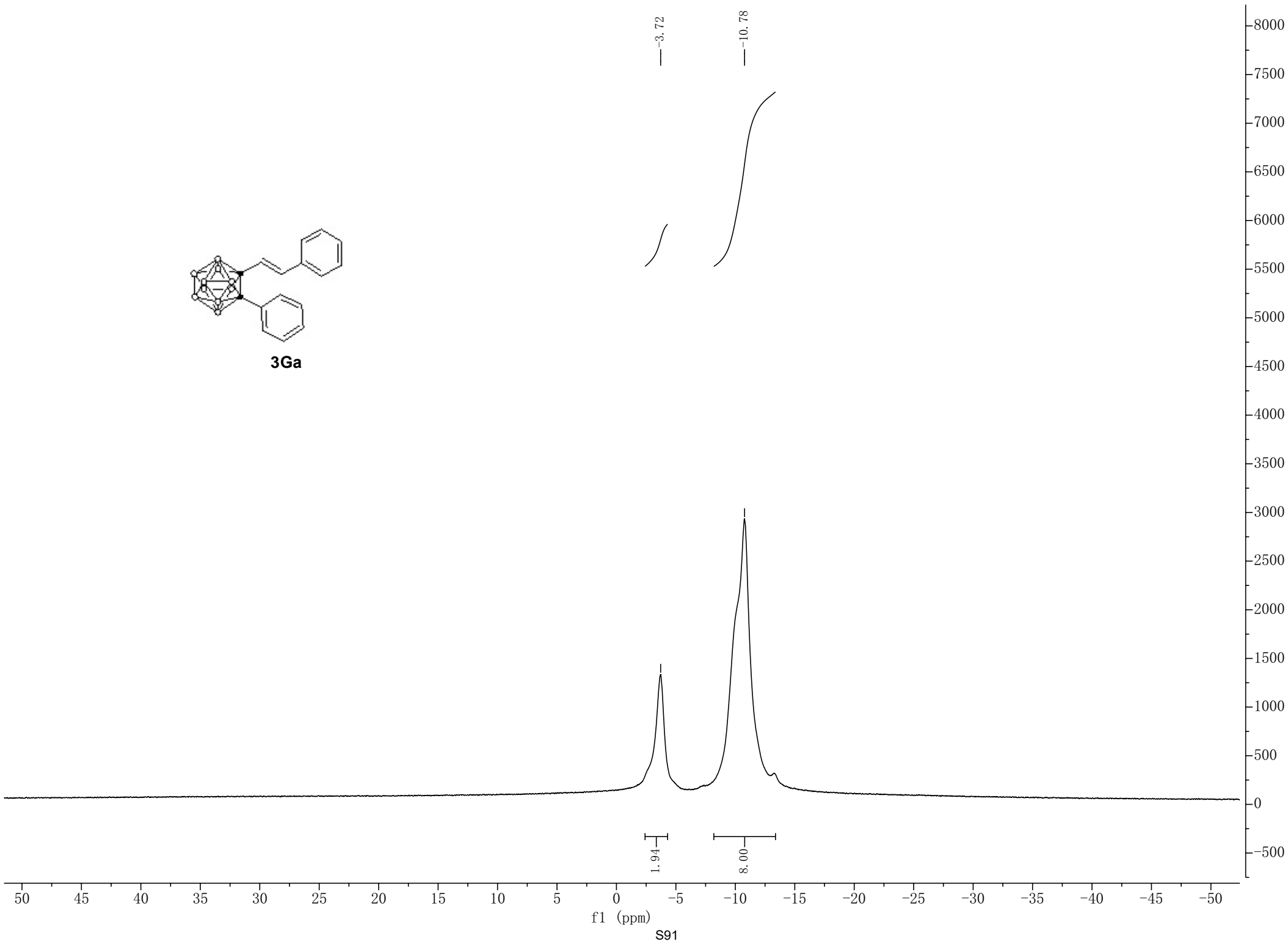


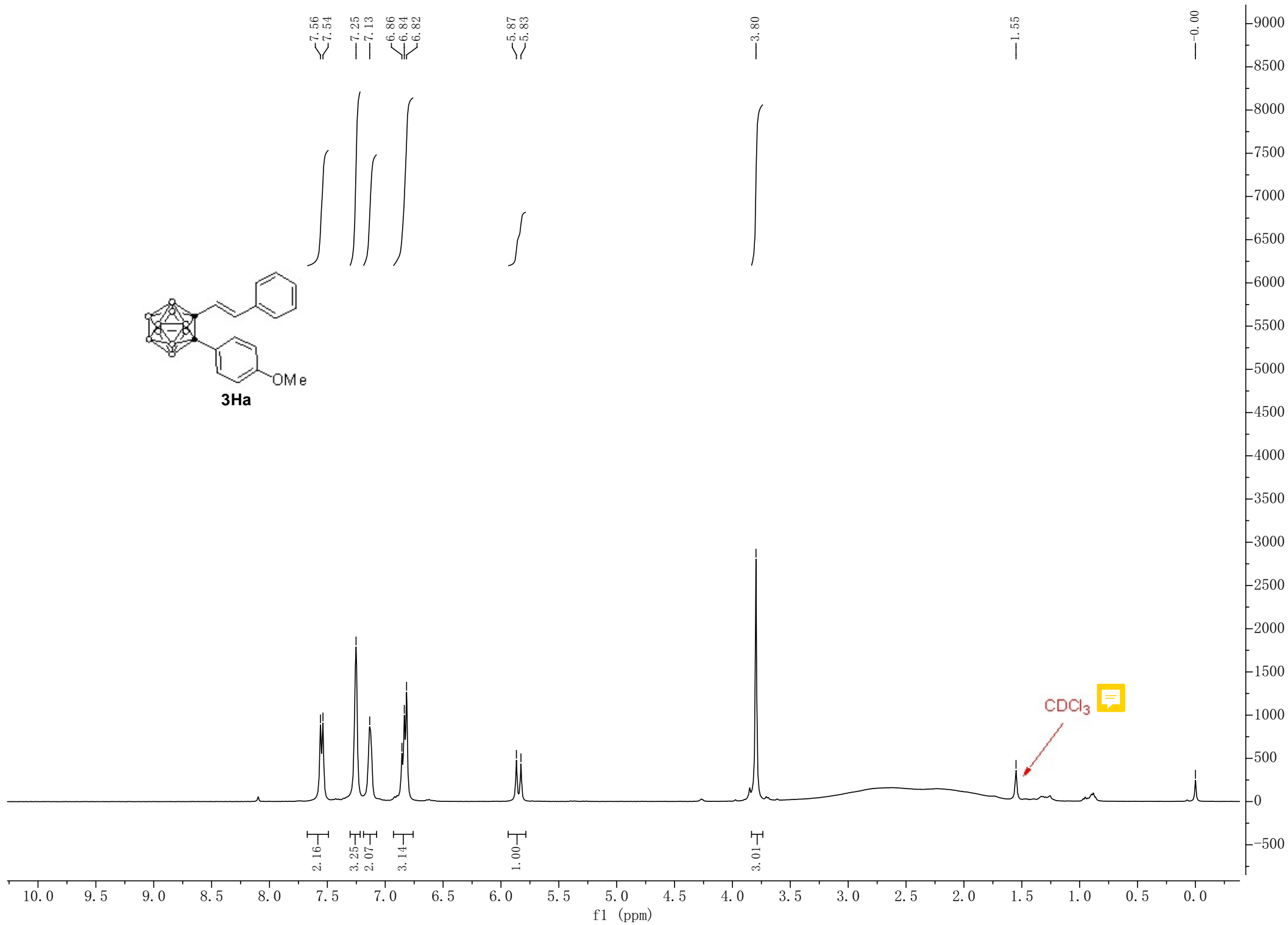
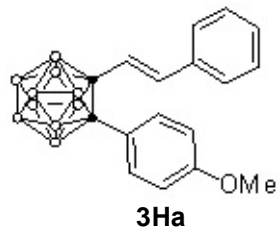
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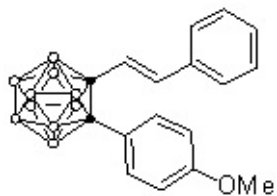




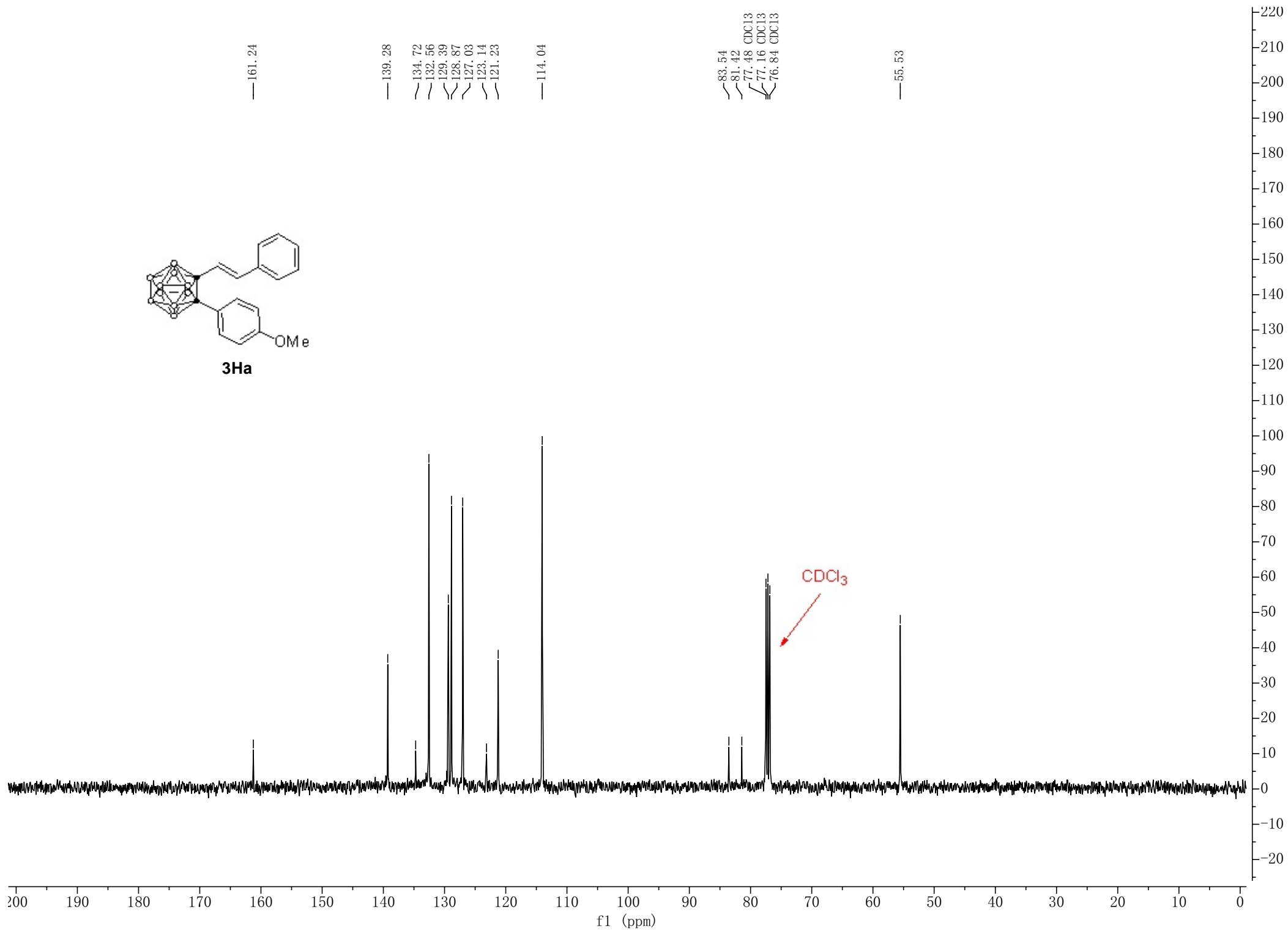
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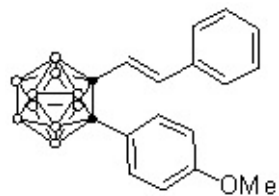




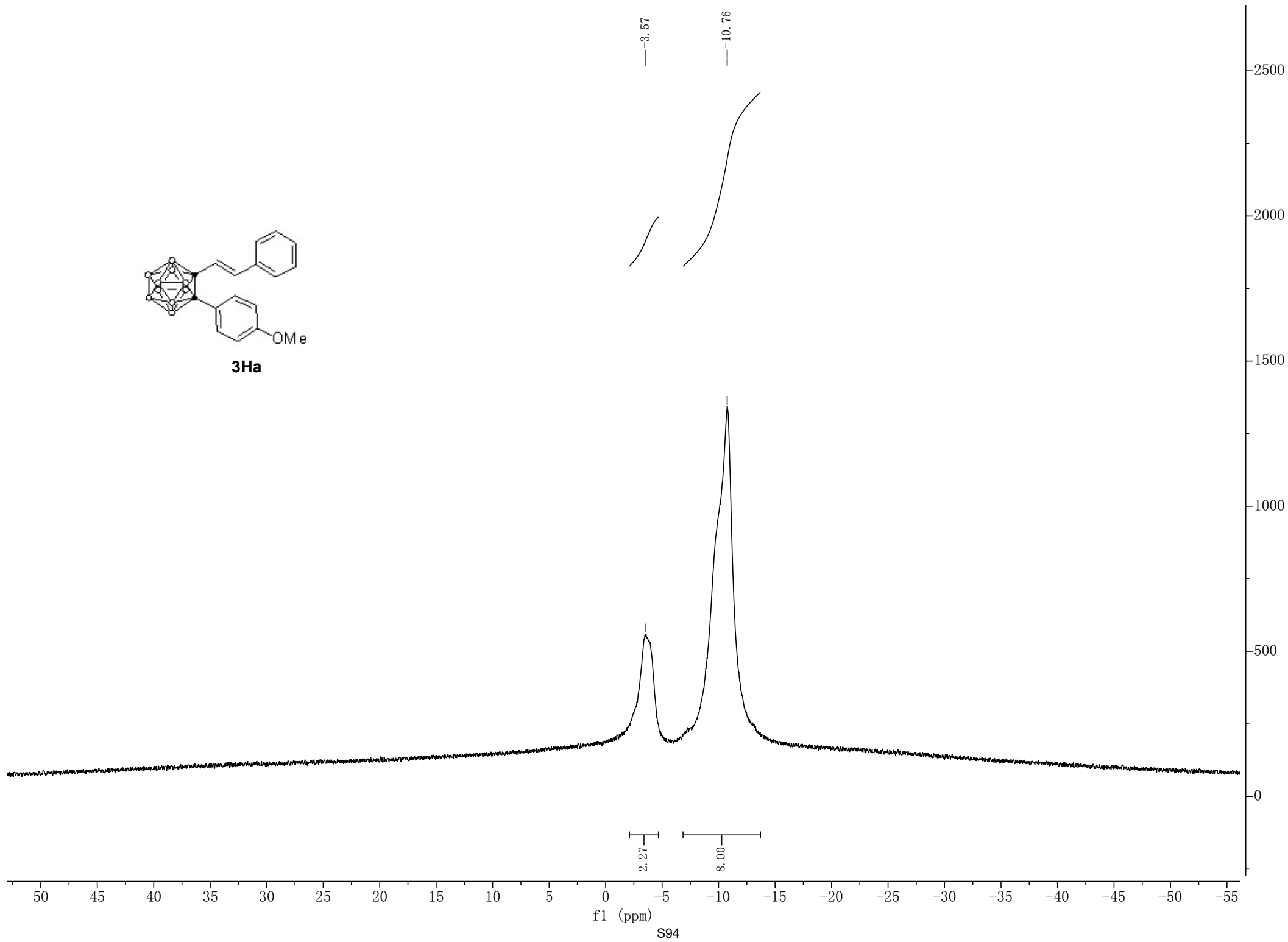


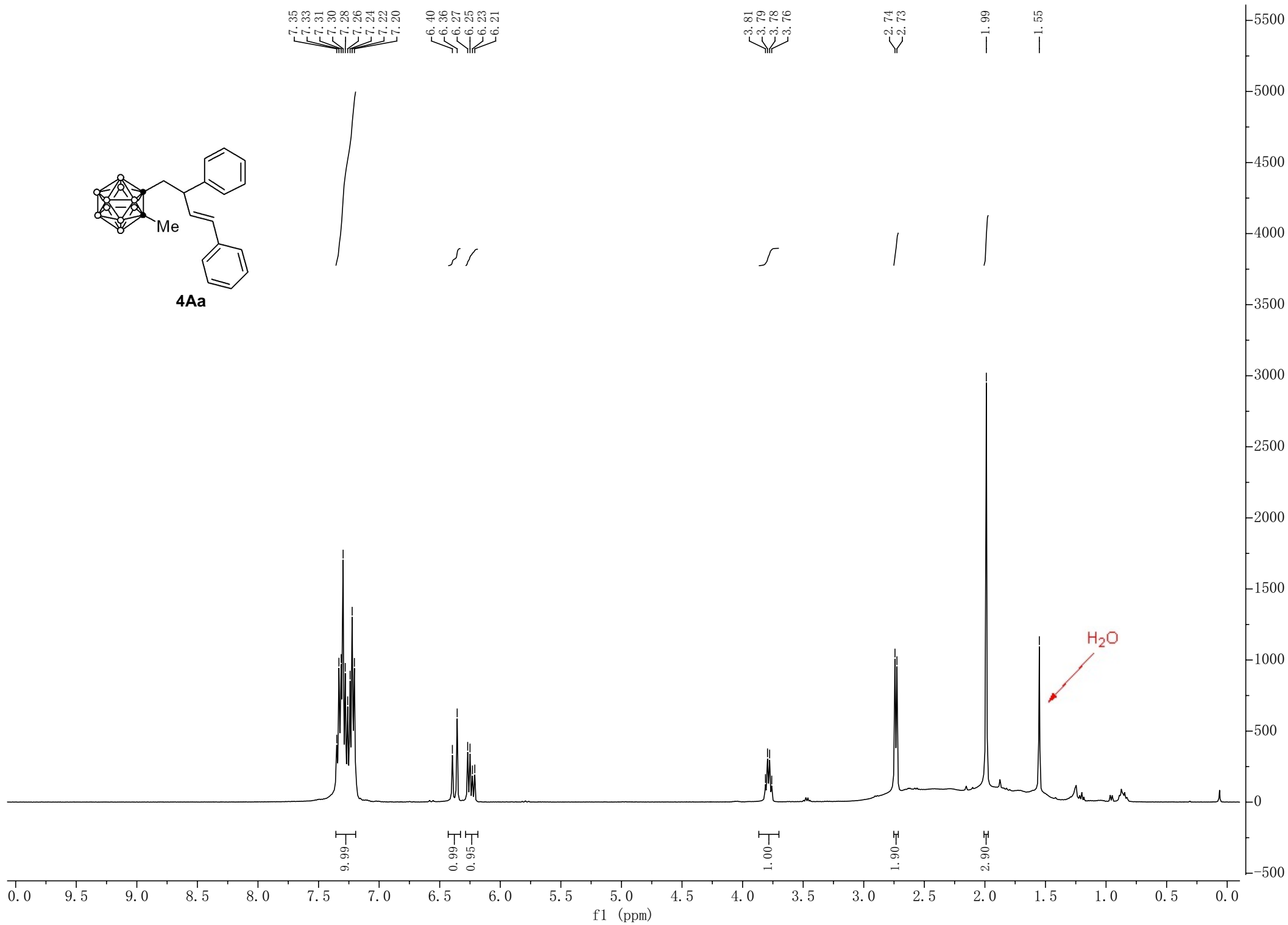
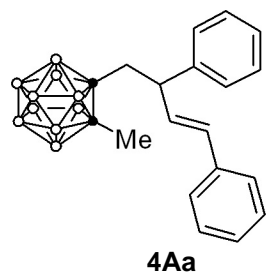
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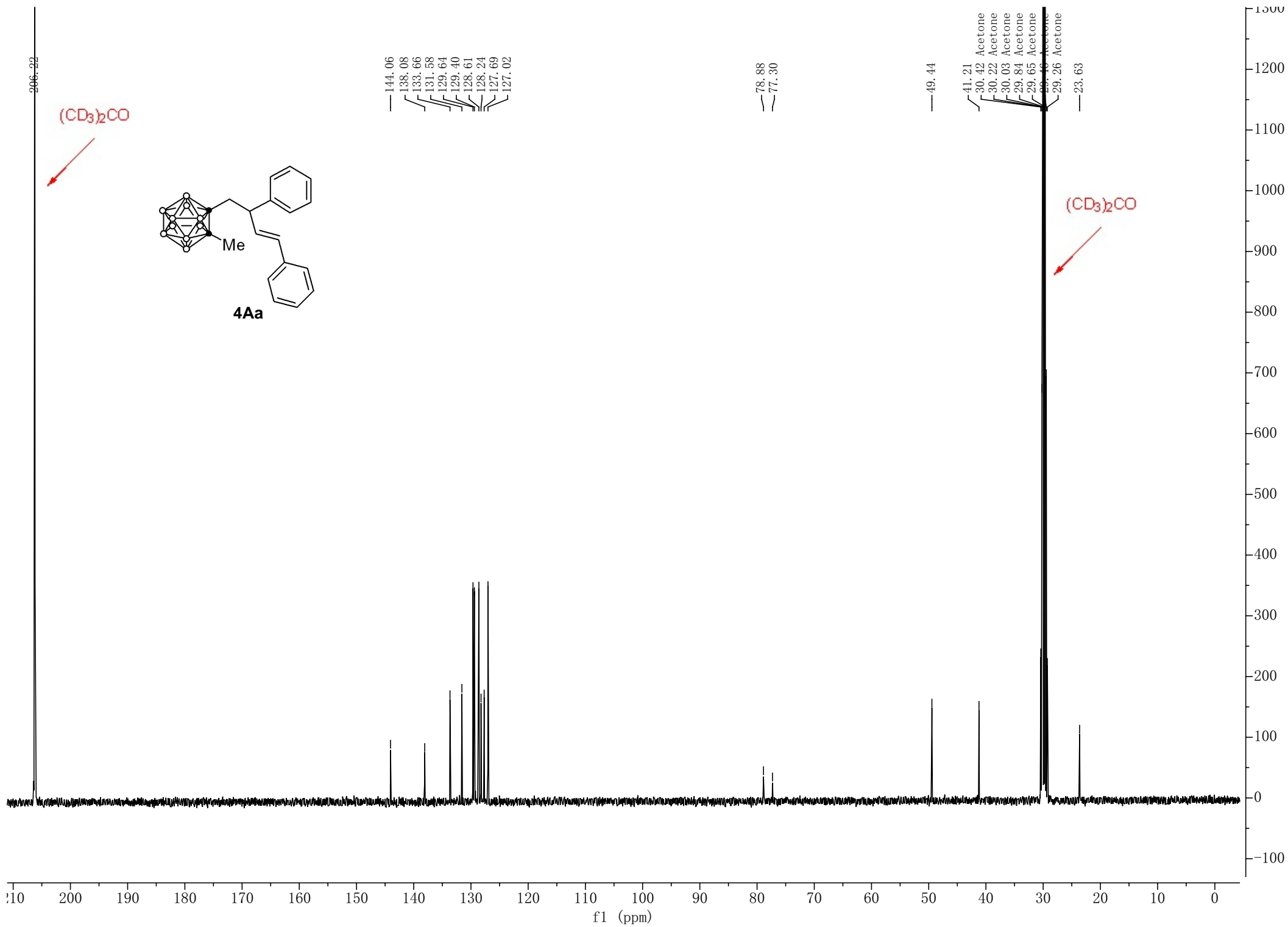


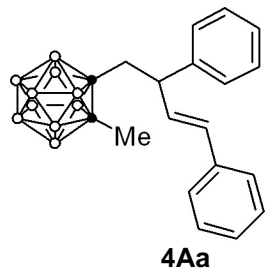


3Ha









—4.33
—6.08
—10.80

