Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Dendritic AIE-active luminogens with a POSS core: synthesis, characterization, and application as chemosensors

Kai Xiang,[ab] Lijuan He,[ab] Hongxia Yang,[c] Yanmin Li,[c] Caihong Xu*[a]

and Shuhong Li *[c]

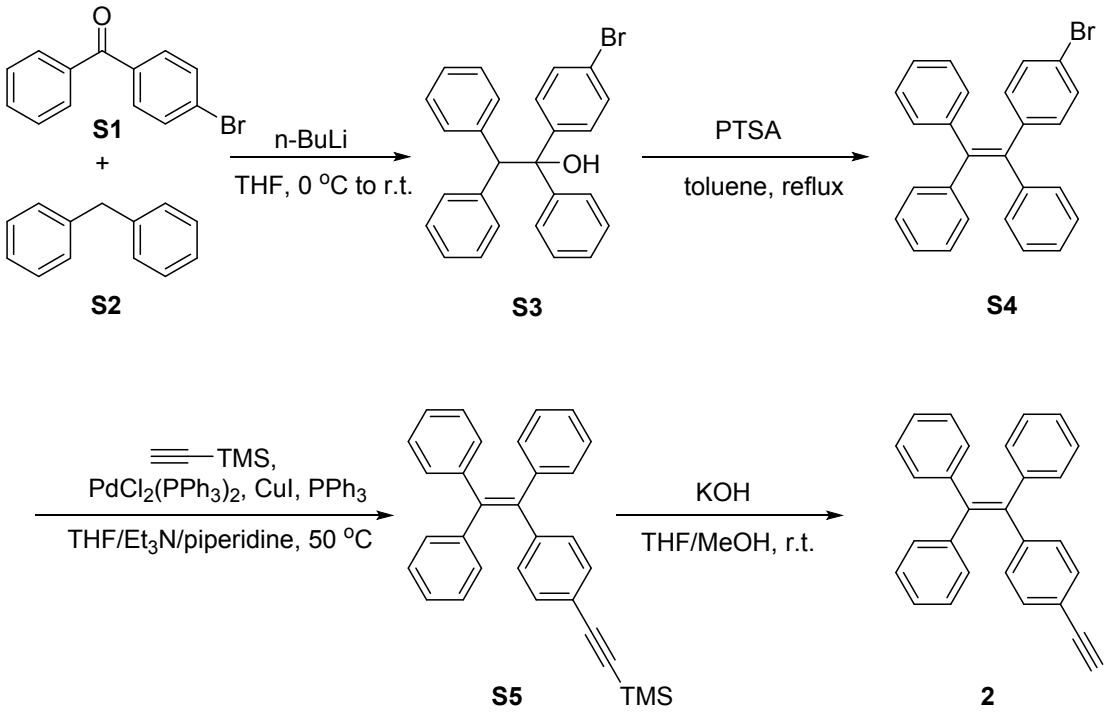
[a] Beijing National Laboratory for Molecular Sciences (BNLMS), Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China E-mail: caihong@iccas.ac.cn.

[b] University of Chinese Academy of Sciences, Beijing, 100049, P. R. China

[c] School of Science, Beijing Technology and Business University, Beijing 100037, P. R. China E-mail: lish@th.btbu.edu.cn.

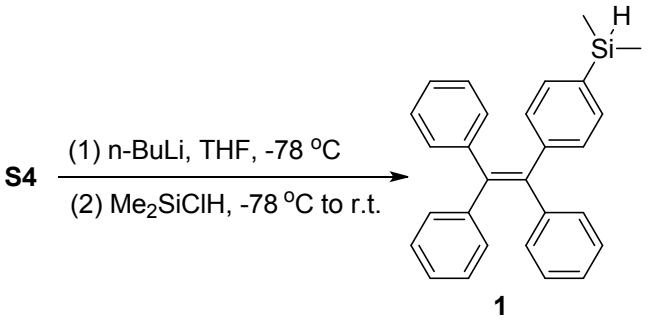
1. Preparation of Compound 1 and 2.

Preparation of compound 2



Scheme S1. Synthtic route to compound **2**. PTSA = *p*-toluenesulfonic acid.

Preparation of compound 1



To a THF (40 mL) solution **S4** (1.65 g, 4 mmol, 1.0 eq.) was added n-BuLi (1.6 M in hexane, 5 mL, 8 mmol, 2 eq.) at −78 °C. After being stirred for 8 h at −78 °C, chlorodimethylsilane (0.87 mL, 8 mmol, 2 eq) was then injected slowly to the solution at 78°C. The obtained solution was warmed gradually to room temperature and stirred overnight. The reaction mixture was quenched with saturated aqueous $NaHCO_3$ (15 mL). The organic layer was separated and aqueous layer was extracted with

petroleum ether (100 mL x 2). The combined organic layer was washed with brine (15 mL), dried over $MgSO_4$ and concentrated under vacuum to get residue. The residue was purified by silica gel column chromatography using hexane as eluent to give 1.40 g (89.7%) of compound **1** as a white solid. **m. p.** 115-116 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$), δ (ppm): 7.24 (d, 1H, Ar-H), 7.13-7.05 (m, 10H, Ar-H), 7.05-6.97 (m, 8H, Ar-H), 4.34 (quint, 1H), 0.28 (d, 6H, CH_3). **^{13}C NMR** (100 MHz, $CDCl_3$): δ (ppm) 144.5, 143.7, 143.7, 143.6, 141.1, 140.8, 135.1, 133.3, 131.3, 131.3, 130.7, 127.7, 127.6, 126.4, 126.4, -3.8. **IR** (KBr), υ (cm^{-1}): 3058, 2959, 2121, 1599, 1491, 1441, 1388, 1254 (Si-CH_3 bending), 1102 (Si-Ph stretching), 884 (Si-CH_3 stretching), 759, 700. **HRMS (MALDI-TOF)**: $[M]^+$ = 390.18013 (calcd for $C_{28}H_{26}Si$, 390.17983).

2. Differential Scanning Calorimetry (DSC) Curves of 1, 2, POSS2 and POSS4.

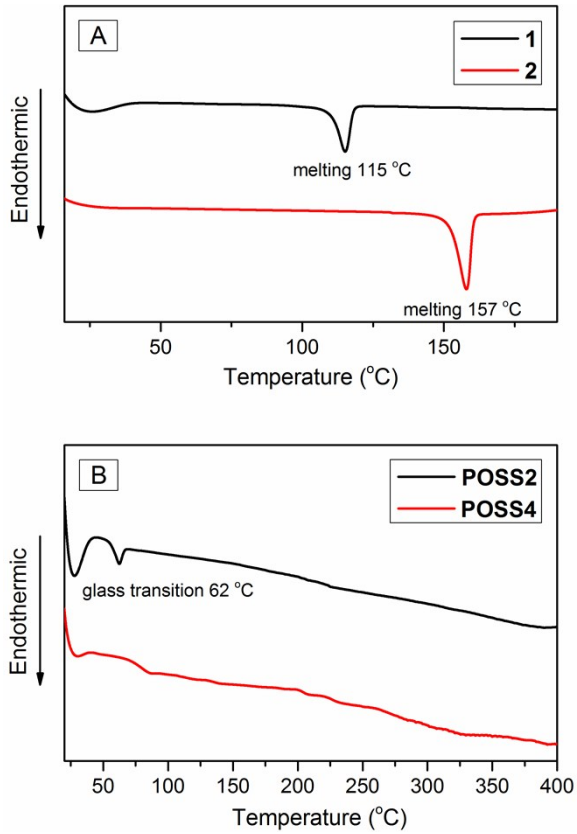
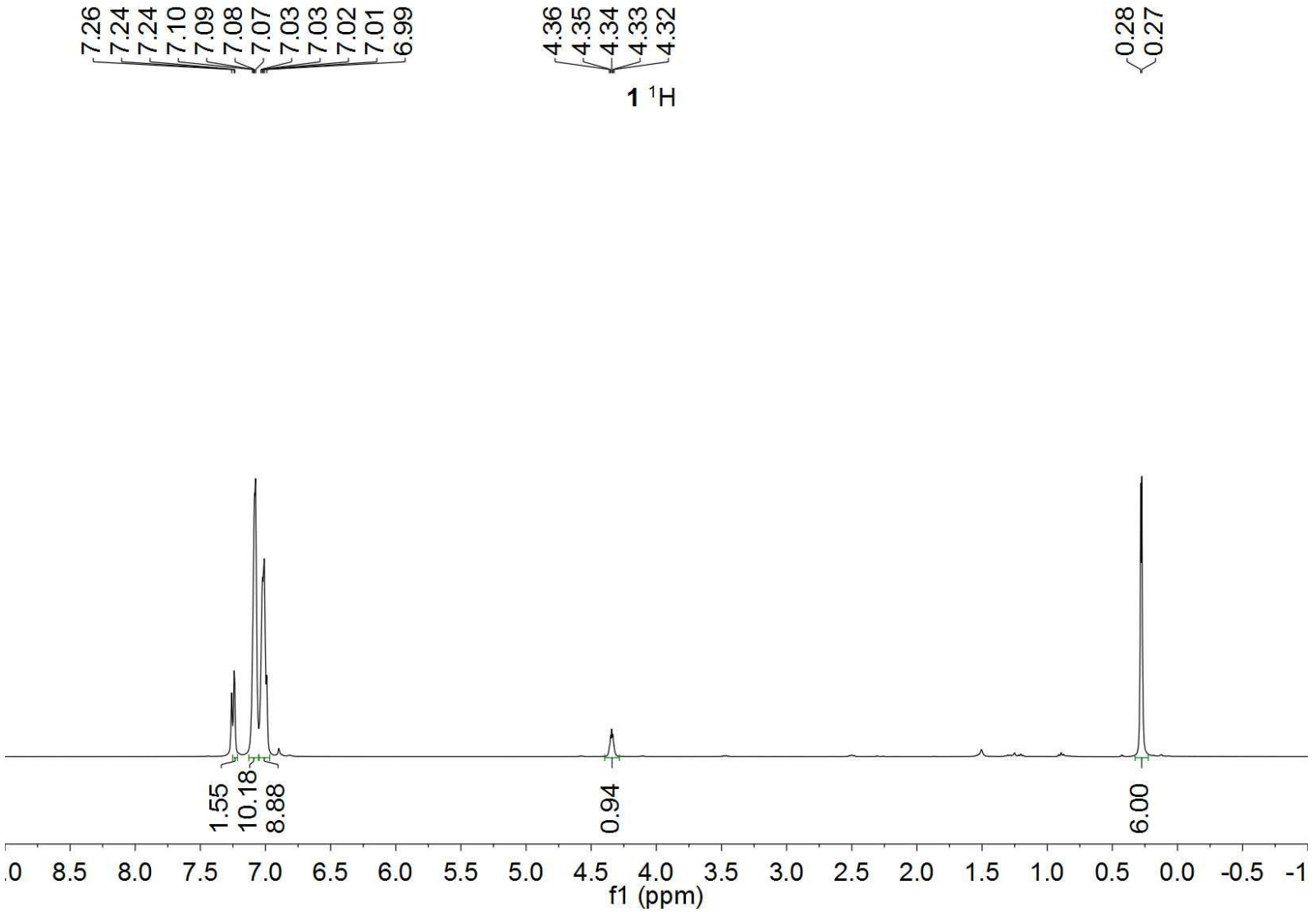
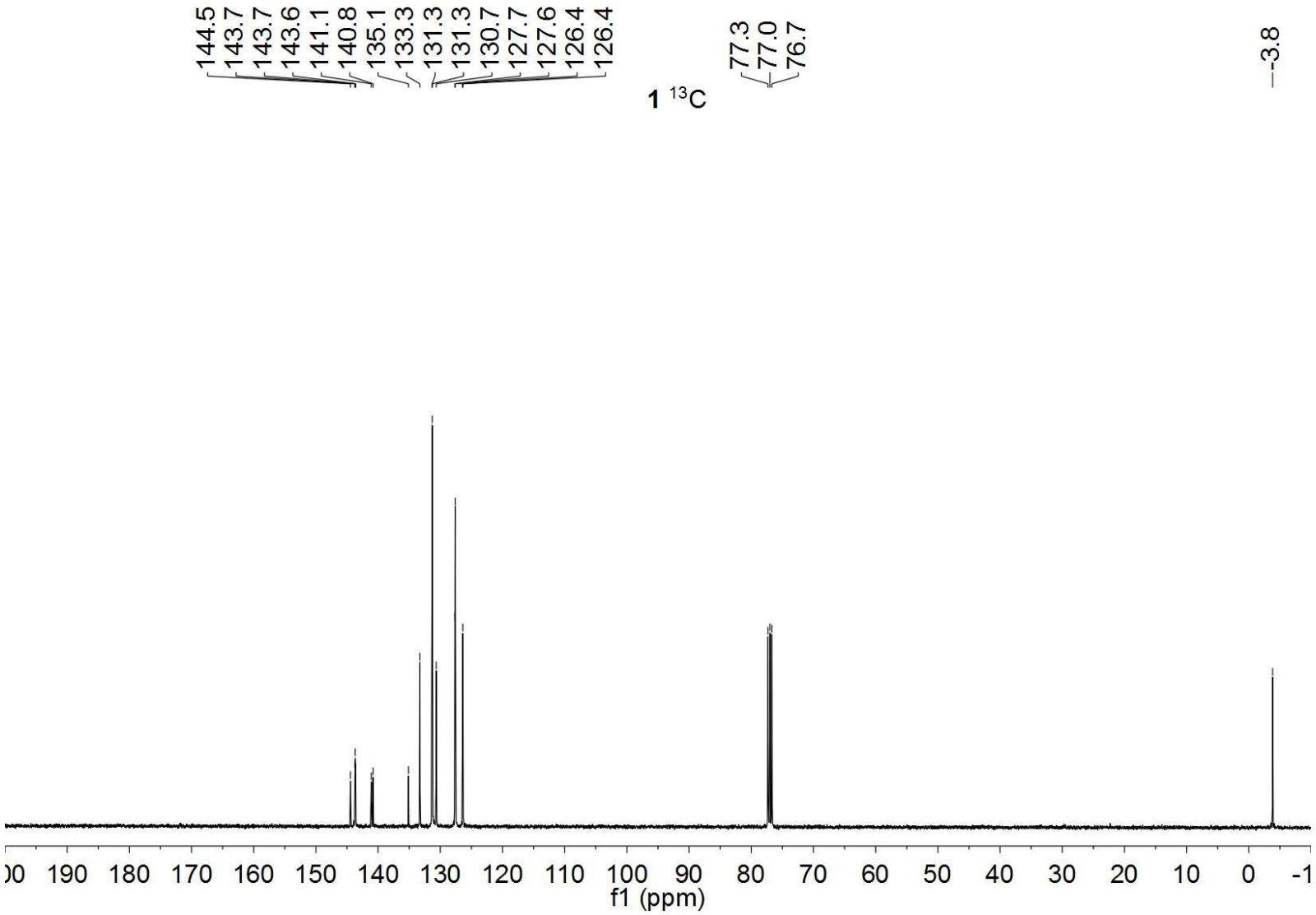
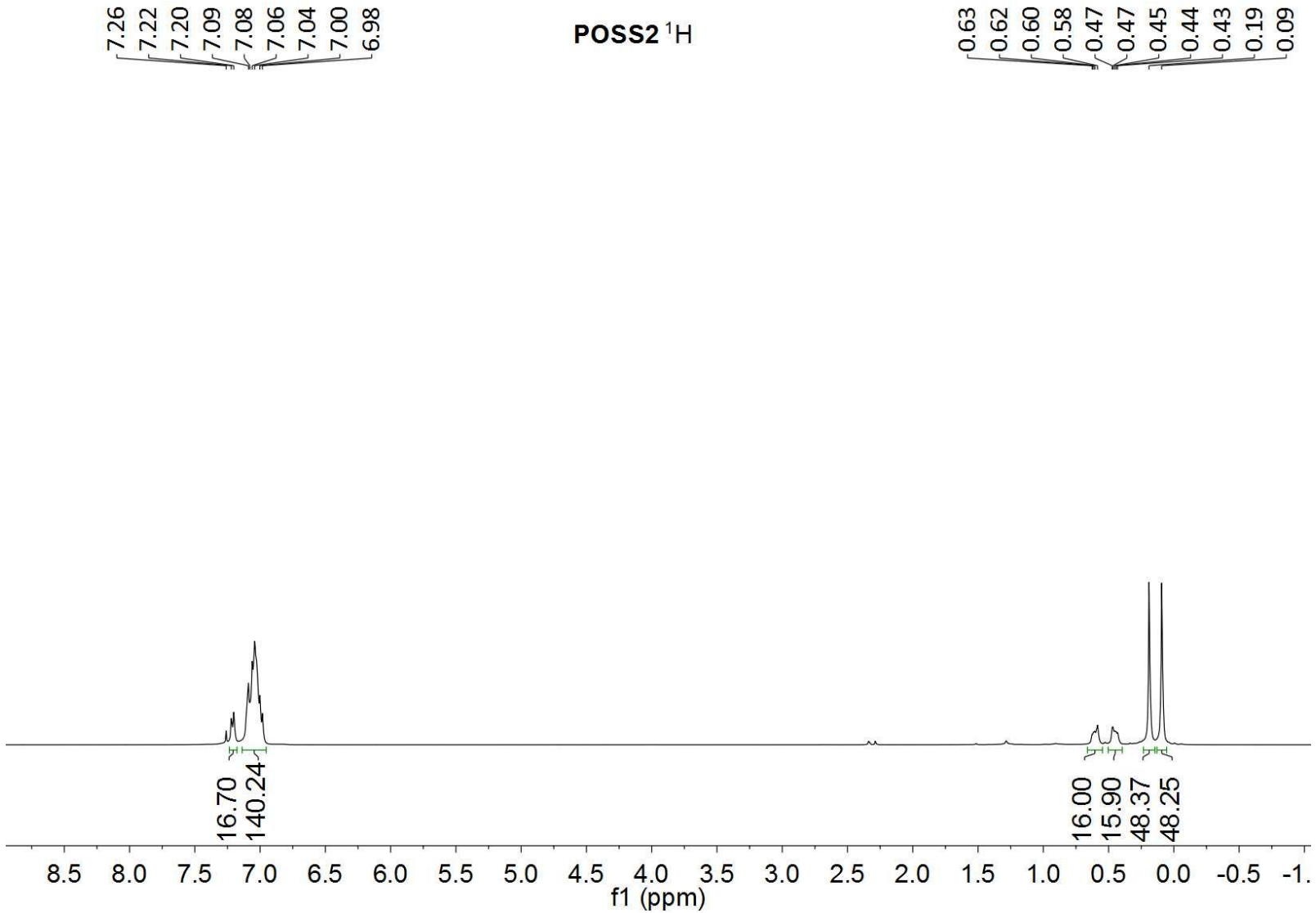


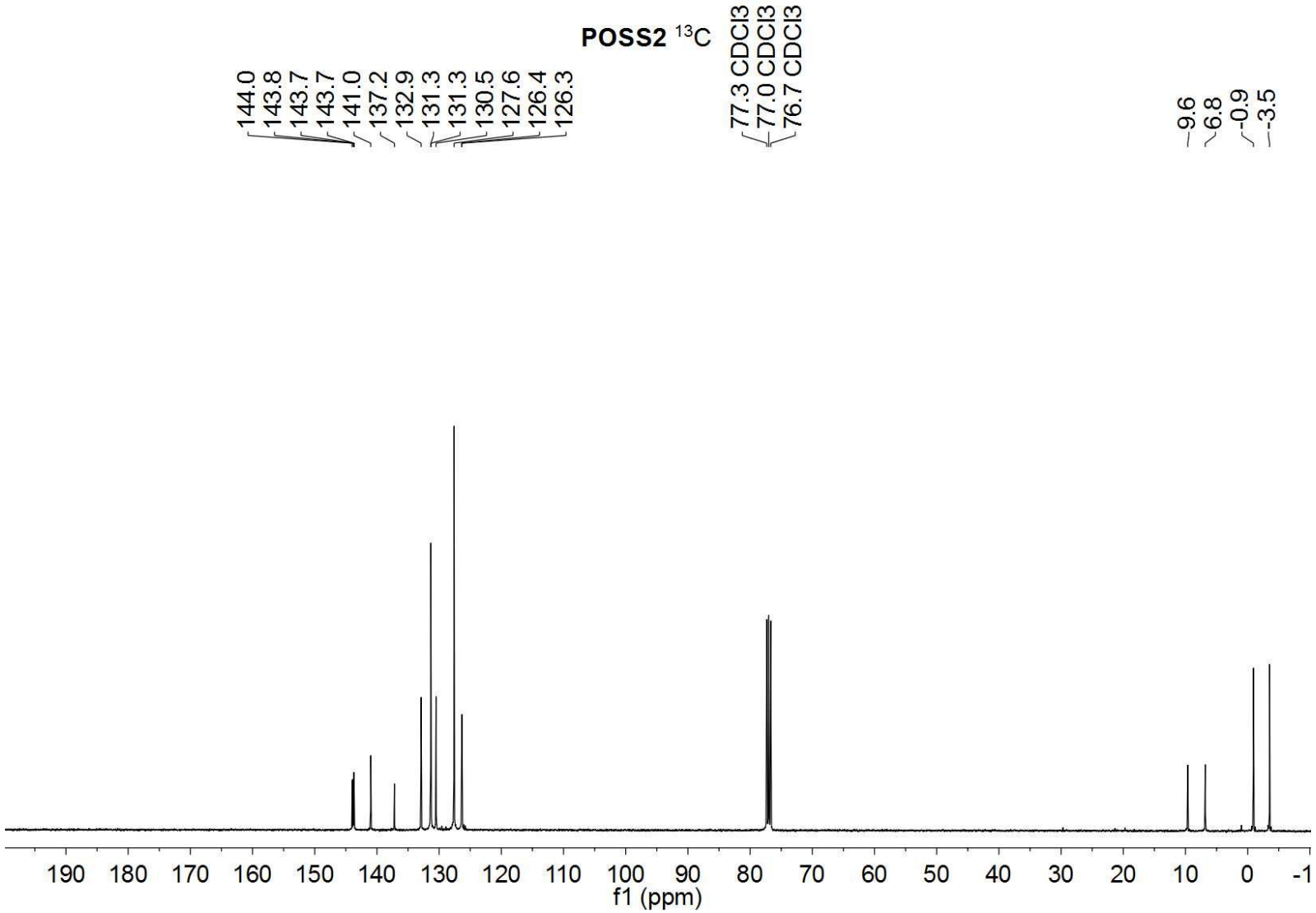
Figure S1. DSC curves of **1**, **2**, **POSS2**, **POSS4** under N_2 at a heating rate of 10 °C/min.

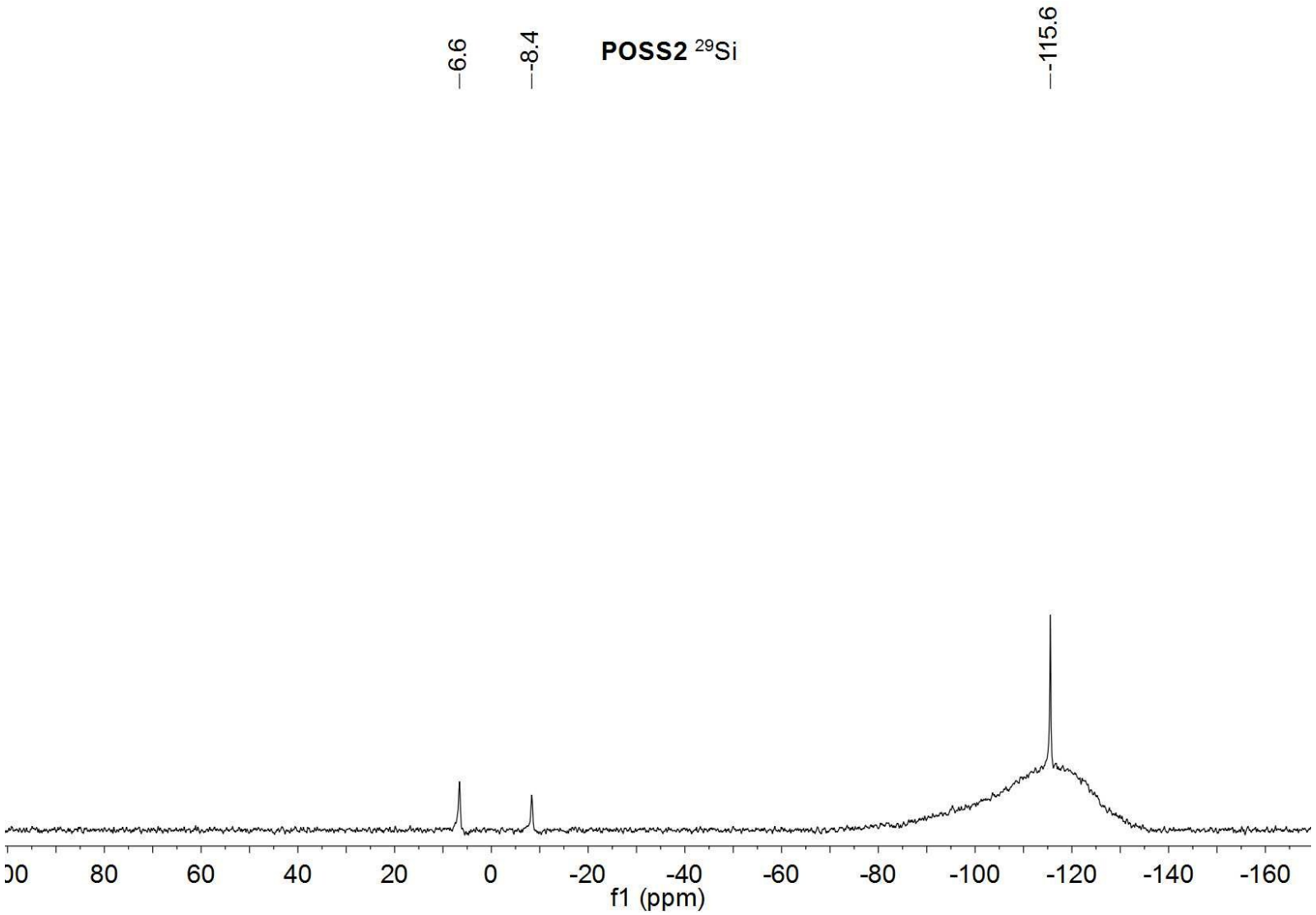
3. ^{1}H, ^{13}C, ^{29}SiNMR Spectra of Synthetic Compounds.

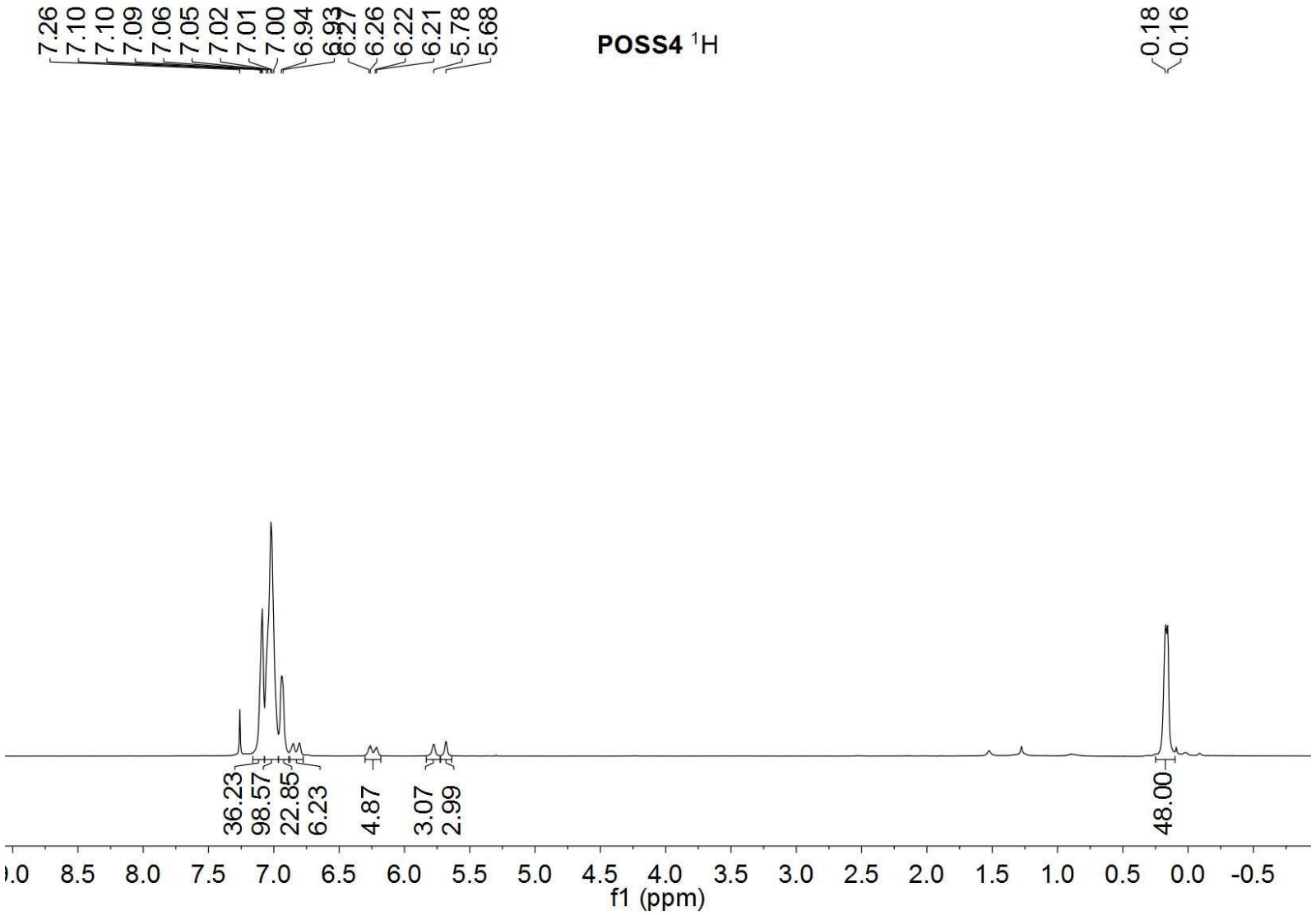

7.26
7.24
7.24
7.10
7.09
7.08
7.07
7.03
7.03
7.02
7.01
6.99
4.36
4.35
4.34
4.33
4.32
0.28
0.27
1 ^{1}H
1.55
10.18
8.88
0.94
6.00
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

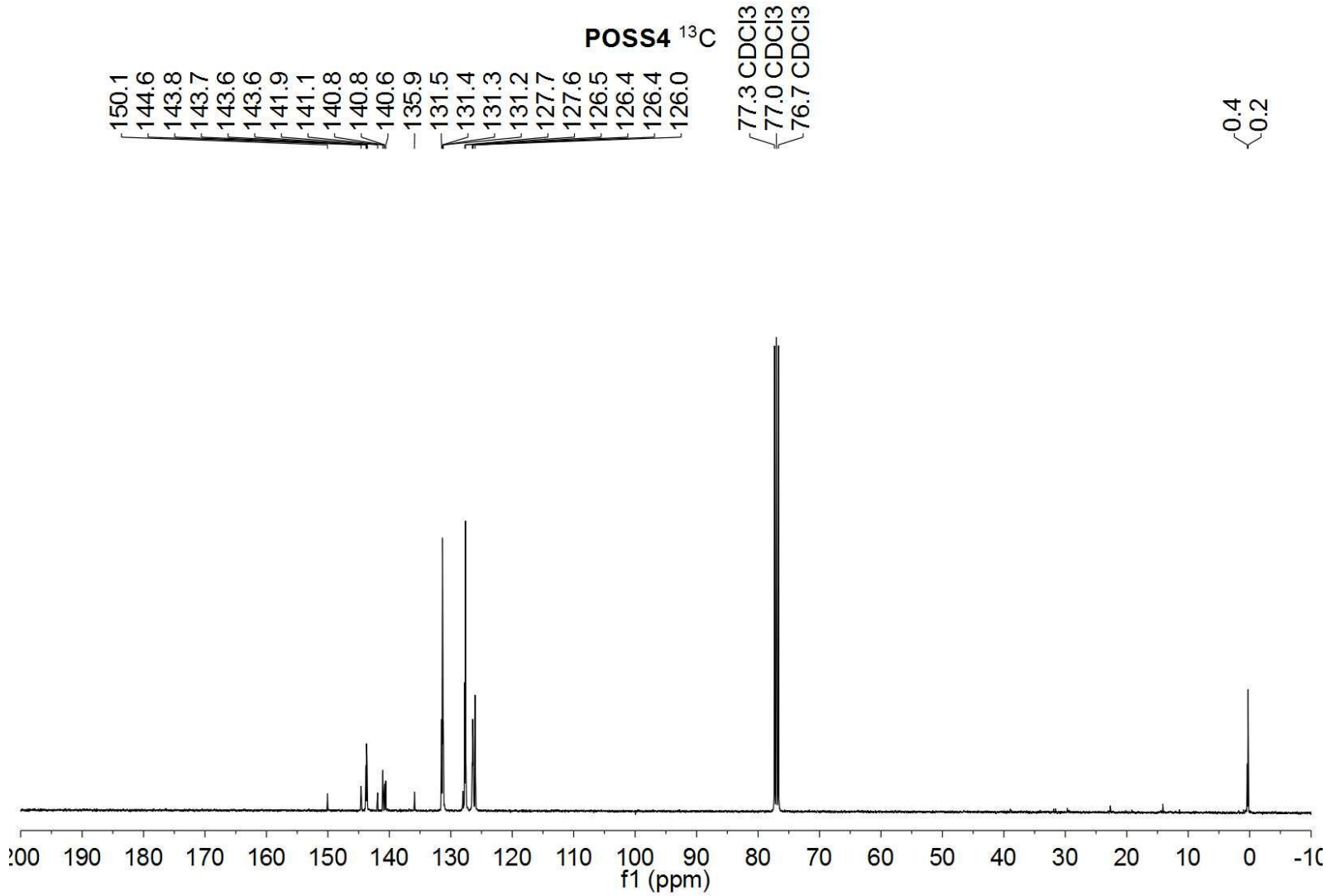

144.5
143.7
143.7
143.6
141.1
140.8
135.1
133.3
131.3
131.3
130.7
127.7
127.6
126.4
126.4
77.3
77.0
76.7
-3.8
1 13C
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

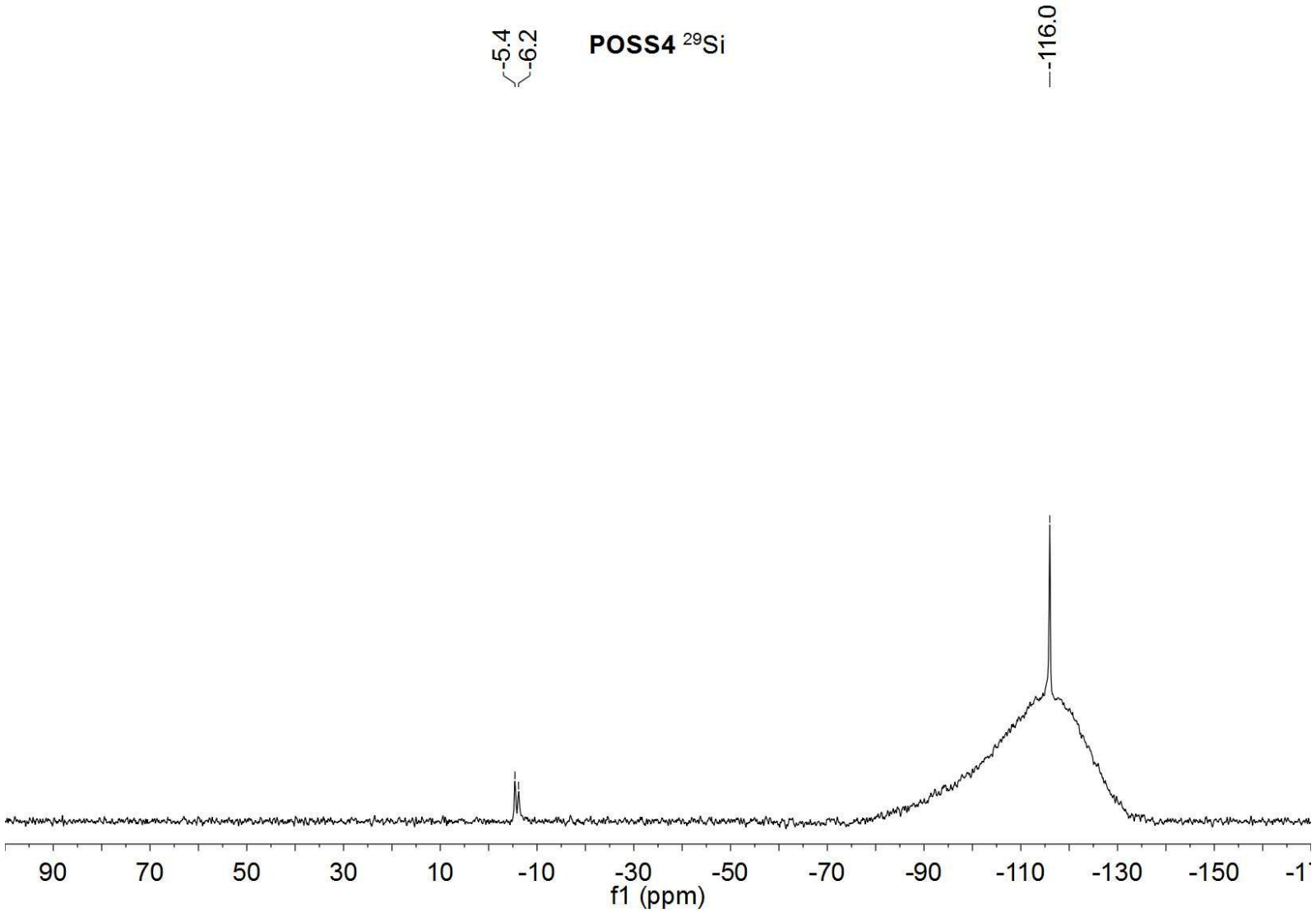

7.26
7.22
7.20
7.09
7.08
7.06
7.04
7.00
6.98
POSS2 1H
0.63
0.62
0.60
0.58
0.47
0.47
0.45
0.44
0.43
0.19
0.09
16.70
140.24
16.00
15.90
48.37
48.25
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


POSS2 13C
144.0
143.8
143.7
143.7
141.0
137.2
132.9
131.3
131.3
130.5
127.6
126.4
126.3
77.3 CDCl3
77.0 CDCl3
76.7 CDCl3
9.6
6.8
-0.9
-3.5
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


-6.6
-8.4
POSS2 29Si
-115.6
00
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
f1 (ppm)


7.26
7.10
7.10
7.09
7.06
7.05
7.02
7.01
7.00
6.94
6.93
6.27
6.26
6.22
6.21
5.78
5.68
POSS4 1H
0.18
0.16
36.23
98.57
22.85
6.23
4.87
3.07
2.99
48.00
f1 (ppm)


POSS4 13C
150.1
144.6
143.8
143.7
143.6
143.6
141.9
141.1
140.8
140.8
140.6
135.9
131.5
131.4
131.3
131.2
127.7
127.6
126.5
126.4
126.4
126.0
77.3 CDCl3
77.0 CDCl3
76.7 CDCl3
0.4
0.2
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-5.4
-6.2
POSS4 29Si
-116.0
90
70
50
30
10
-10
-30
-50
-70
-90
-110
-130
-150
f1 (ppm)