Supporting Information

Dithia[3.3]paracyclophane-Based Monometal Ruthenium Acetylide Complexes: Synthesis, Characterization and Substituent Effects

Xingxun Zhu, Yaping Ou, Jing Zhang, Jian-Long Xia, Jun Yin, Guang-Ao Yu*, Sheng Hua Liu*

Received (in XXX, XXX) Xth XXXXXXXXX 201X, Accepted Xth XXXXXXXXX 201X
First published on the web Xth XXXXXXXXX 201X

Crystallographic Information

Table S1 partial datas for Bond lengths (Å) and bond angles (°) of complex **2a**

Bond distances (Å)			
Ru(1)-C(37)	2.010(4)	Ru(1)-P(2)	2.267(9)
Ru(1)-C(29)	2.227(3)	C(37)-C(38)	1.205(5)
Ru(1)-C(28)	2.235(3)	C(38)-C(39)	1.449(5)
Bond angles (°)			
C(37)-Ru(1)-C(29)	93.87(14)	C(38)-C(37)-Ru(1)	170.4(3)
C(37)-Ru(1)-C(28)	89.98(14)	C(37)-C(38)-C(39)	166.6(4)
C(29)-Ru(1)-C(28)	37.19(13)	C(44)-C(39)-C(40)	118.1(3)

S2 partial datas for Bond lengths (Å) and bond angles (°) of complex **3e**

Bond distances (Å)			
Ru(1)-C(37)	2.021(2)	Ru(1)-P(2)	2.2636(8)
Ru(1)-C(30)	2.217(3)	Ru(1)-C(31)	2.266(3)
Ru(1)-P(1)	2.2528(7)	Ru(1)-C(27)	2.268(2)
Bond angles (°)			
C(37)-Ru(1)-C(30)	97.67(10)	C(38)-C(37)-Ru(1)	175.2(2)
C(37)-Ru(1)-C(29)	89.28(10)	C(37)-C(38)-C(39)	177.2(3)
C(30)-Ru(1)-C(29)	36.93(13)	C(44)-C(39)-C(40)	117.9(3)

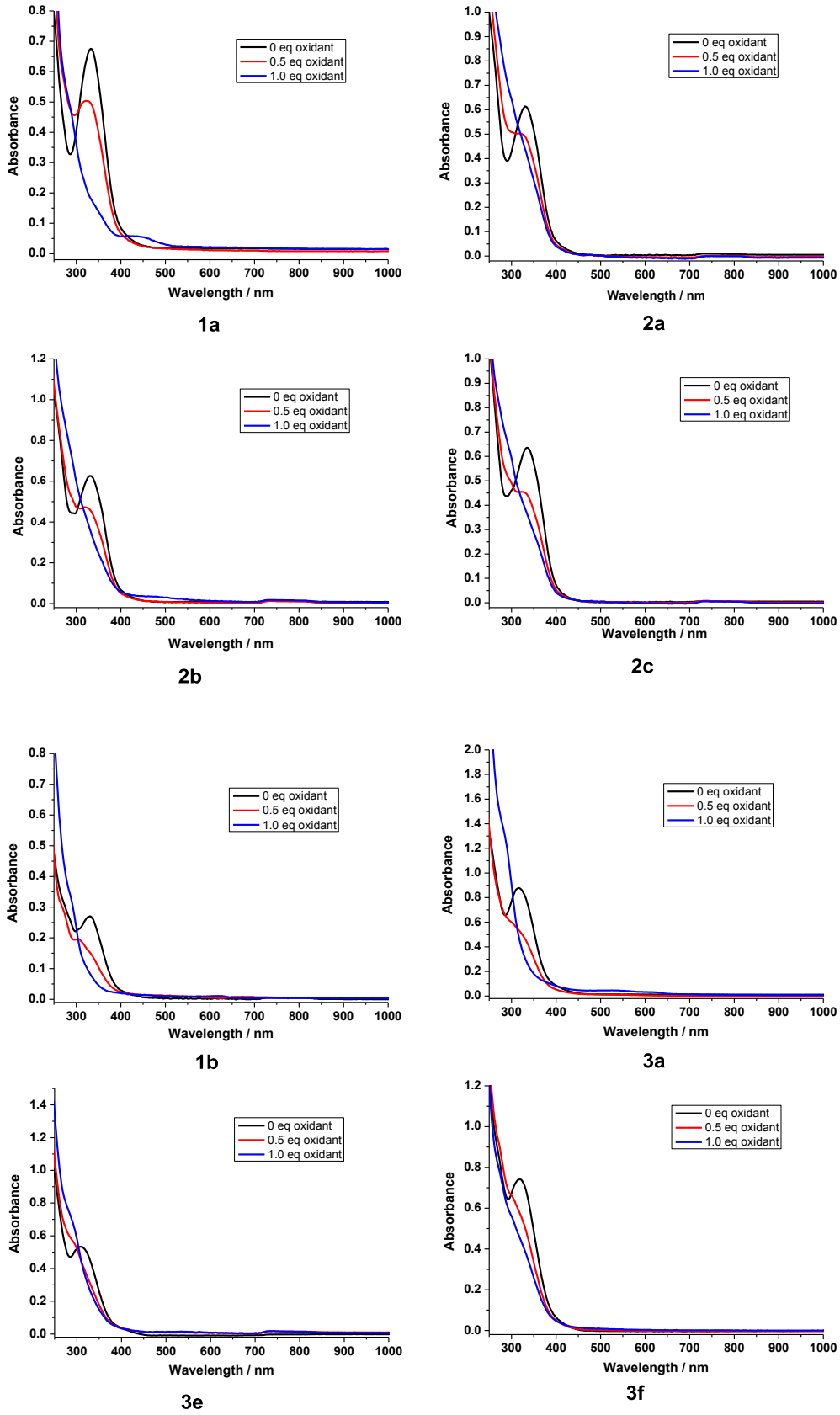
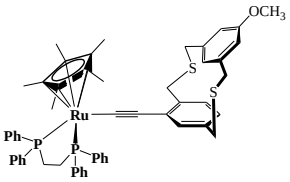
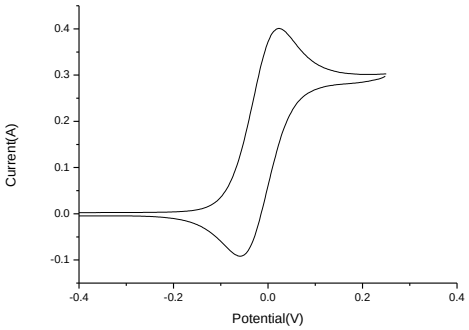
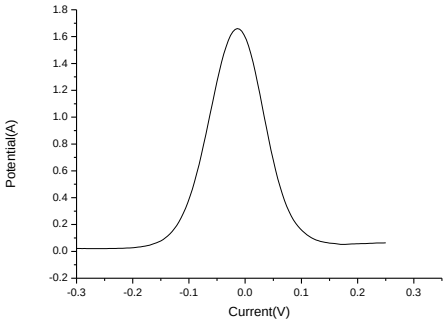


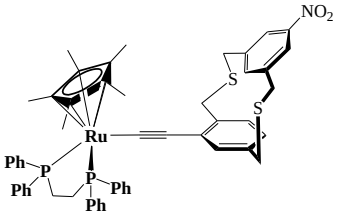
Figure S1. UV/Vis absorption spectrum changes of complexes **1a, 2a-2c** and **1b**, **3a**, **3e**, **3f** in the presence of increasing amounts of ferrocenium hexafluorophosphate as a chemical oxidant: Black lines, neat compounds before adding any oxidant; red lines, after addition of 0.5 equiv of oxidant; blue traces, after addition of 1 equiv of oxidant.

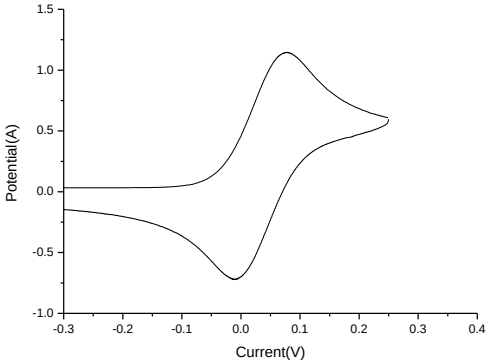
Electrochemistry Information

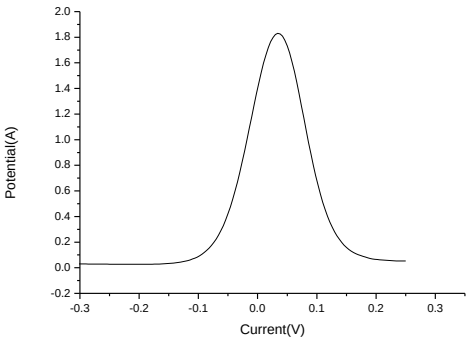


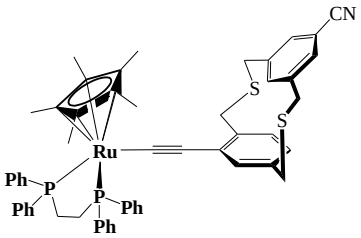


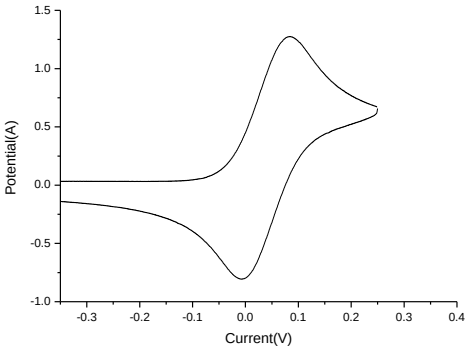


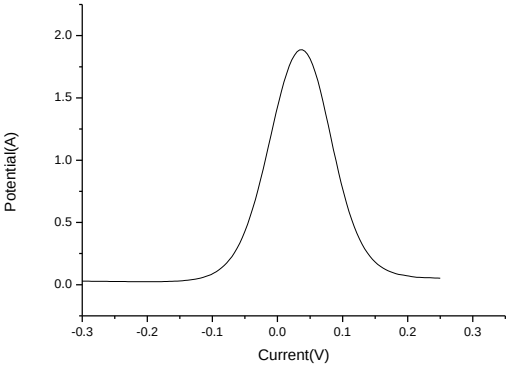


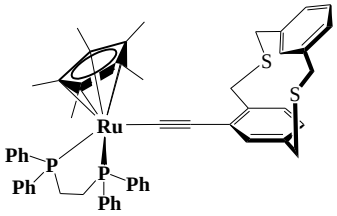


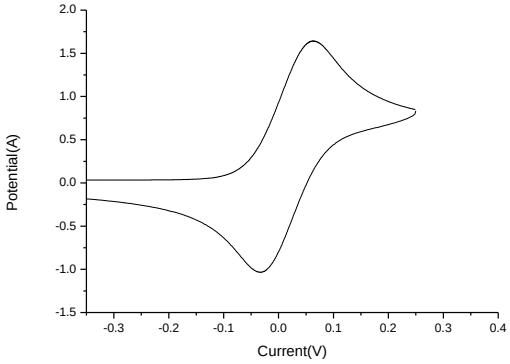


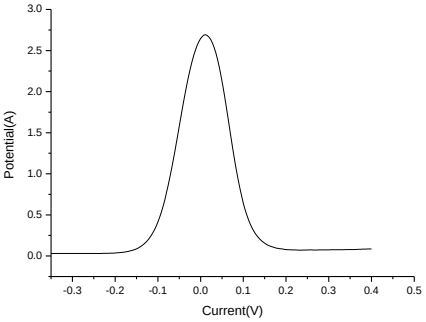


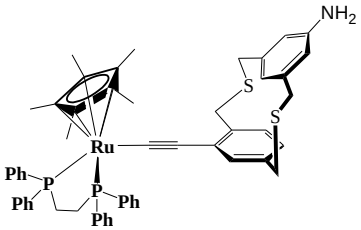


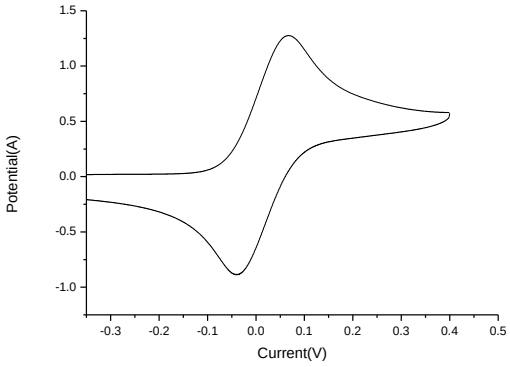


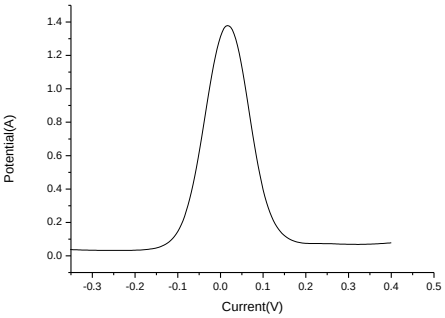


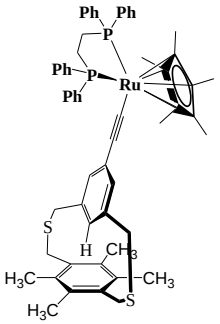


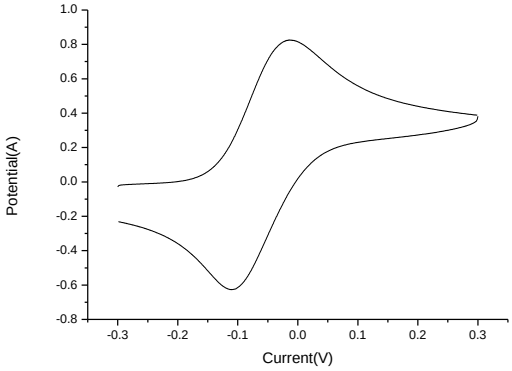


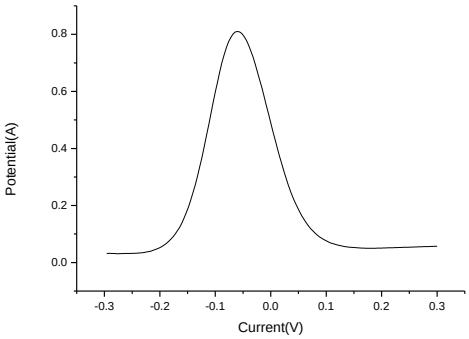


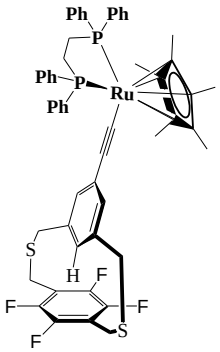


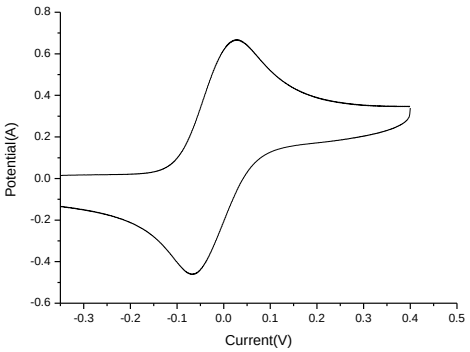


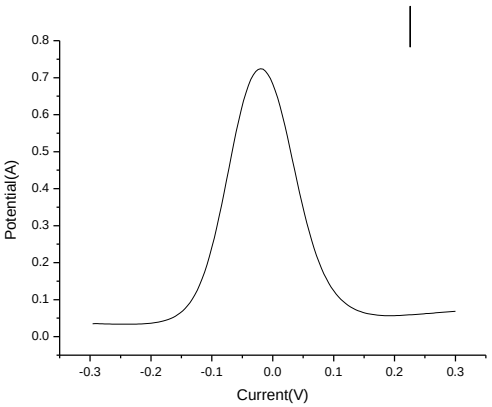


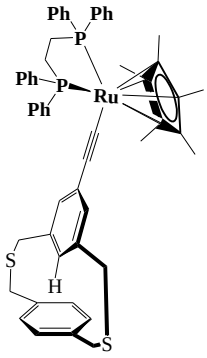


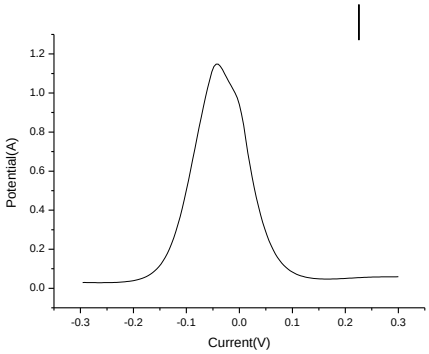


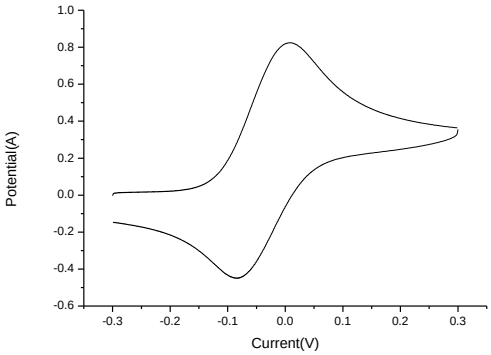


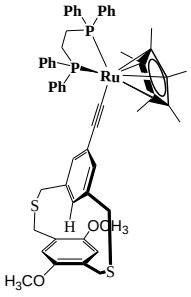


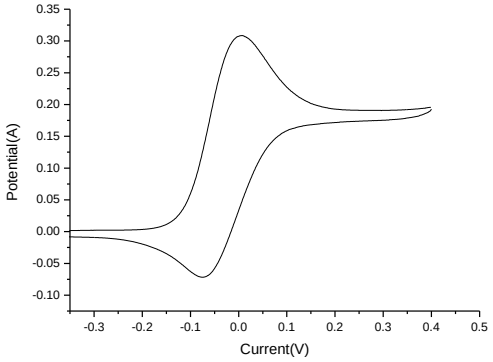


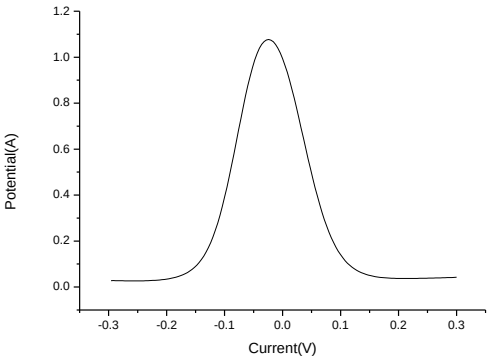


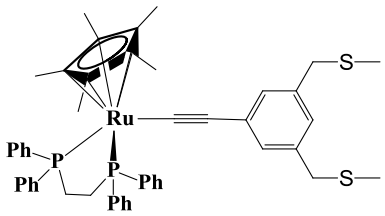












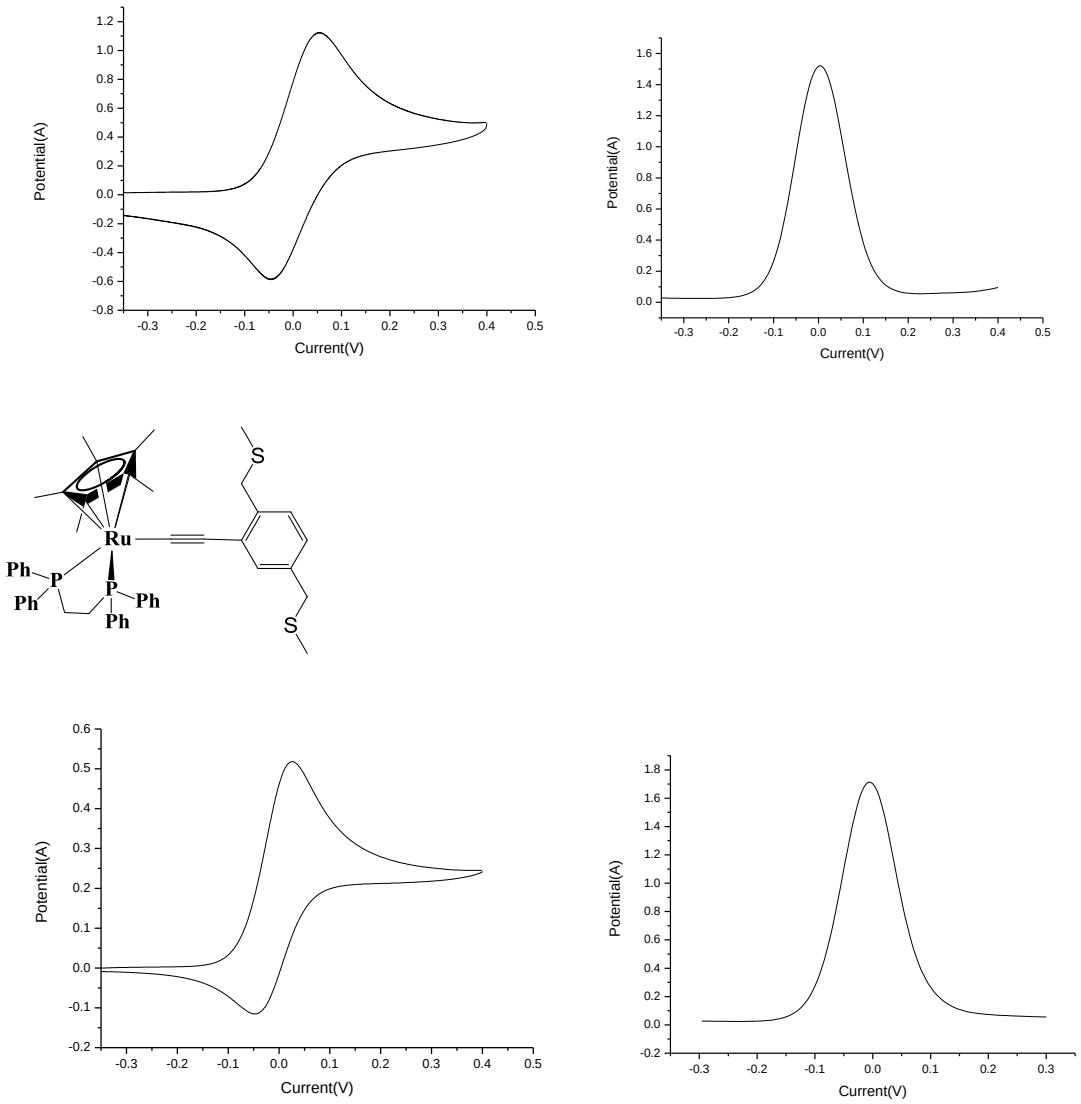


Figure S2. Cyclic voltammograms (CV) of complexes **1a**, **2a-e** and **1b, 3a-f** in CH_2Cl_2/Bu_4NPF_6 at v=0.1 V s^{-1}. Square-wave voltammograms (SWV) at f =10 Hz. Potentials are given relative to the Ag/Ag^+ standard.

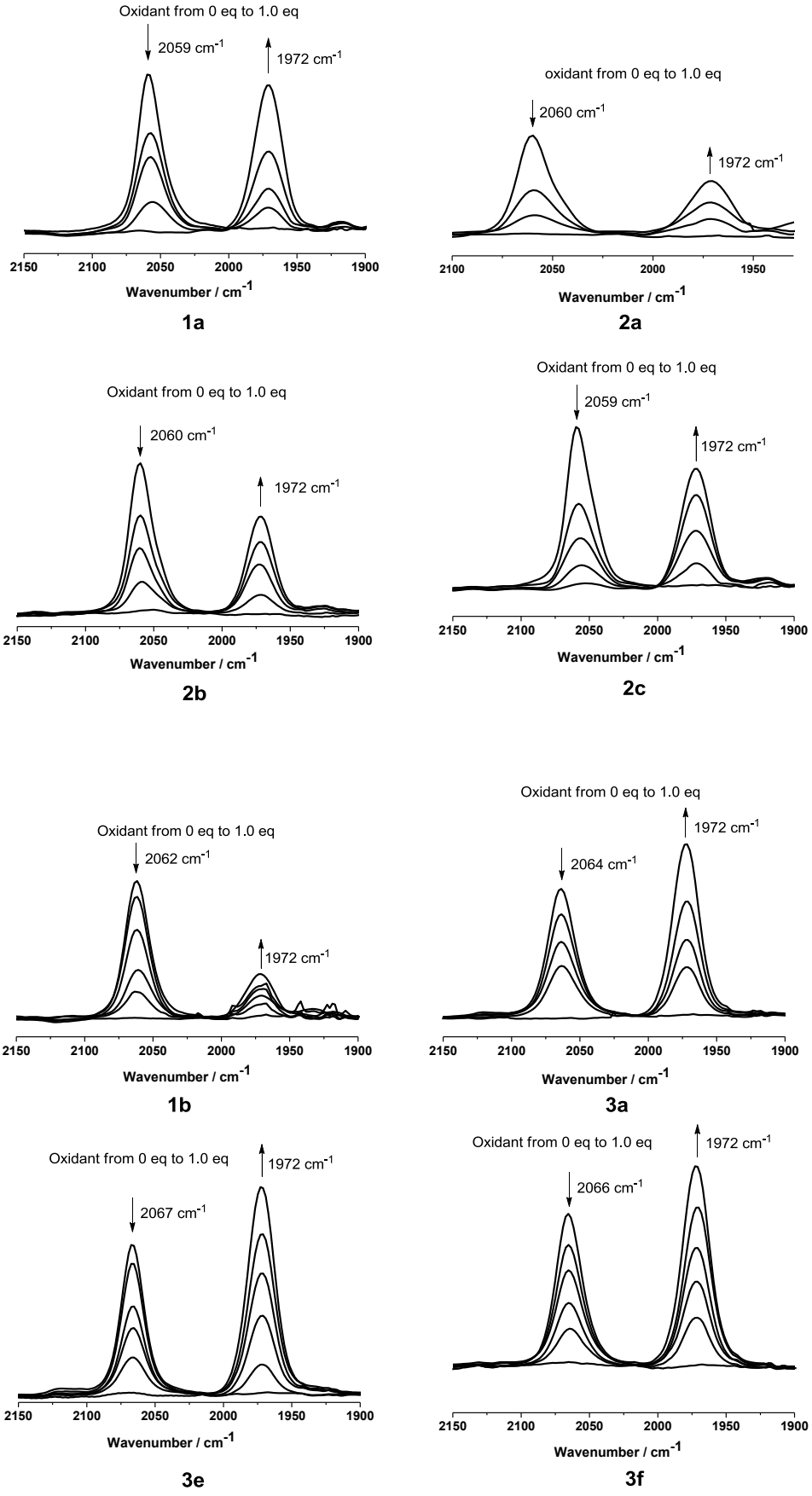
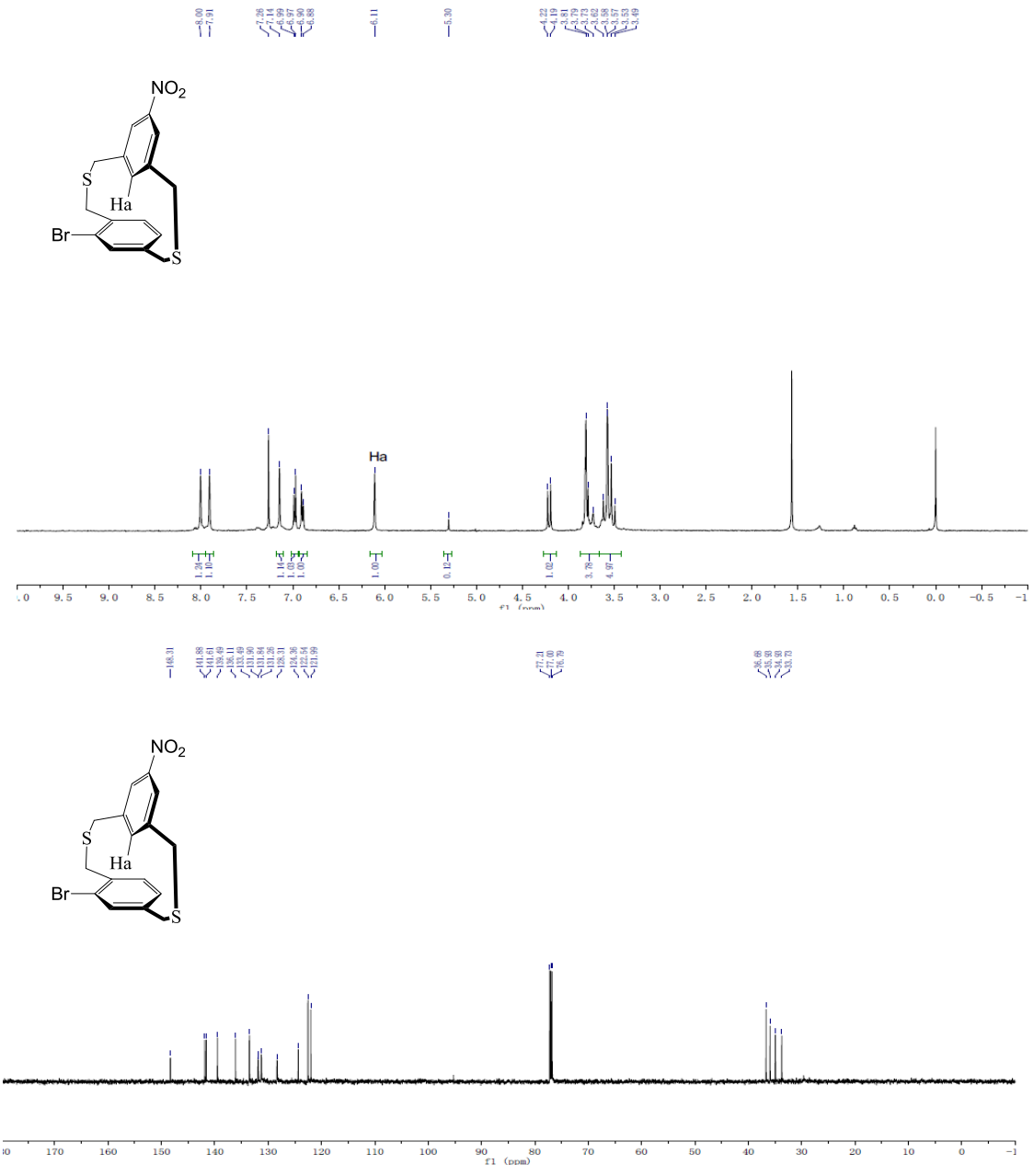
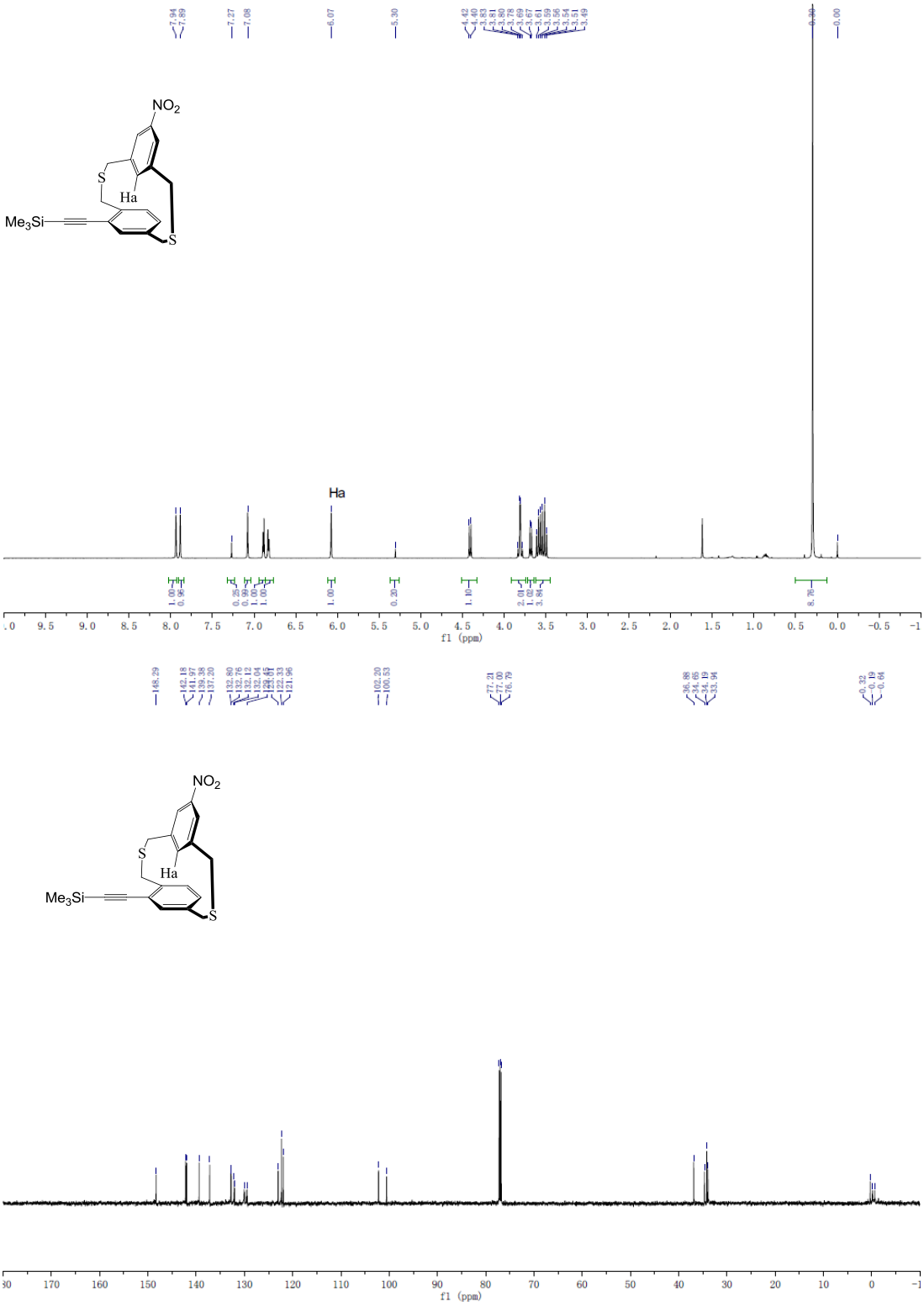


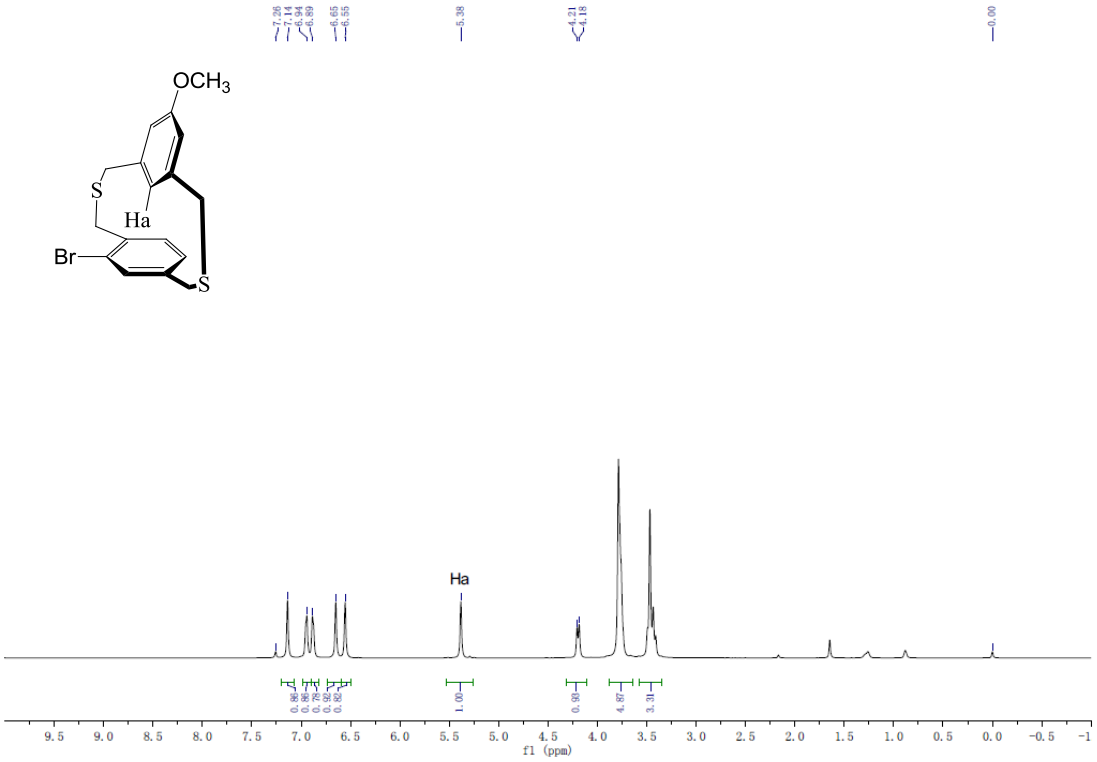
Figure S3 IR spectroscopy changes of complexes **1a, 2a-c** and **1b, 3a, 3e, 3f** in the presence of increasing amounts of ferrocenium

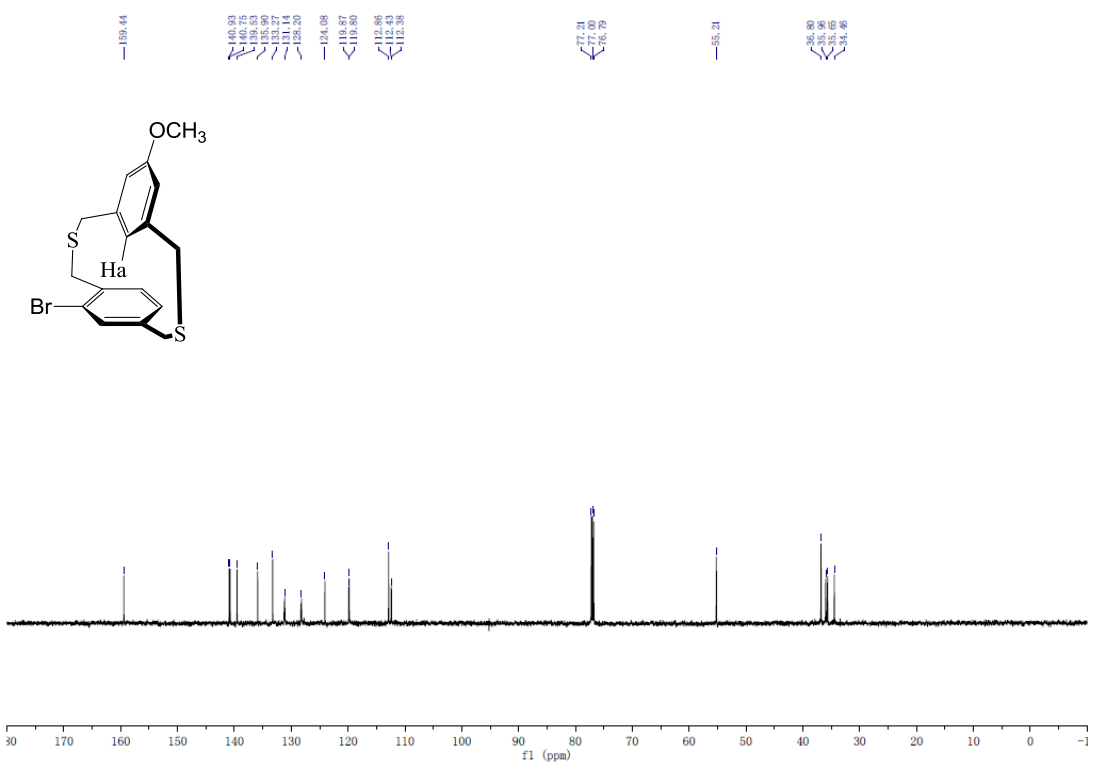
hexafluorophosphate as a chemical oxidant from 0 eq to 1.0 eq

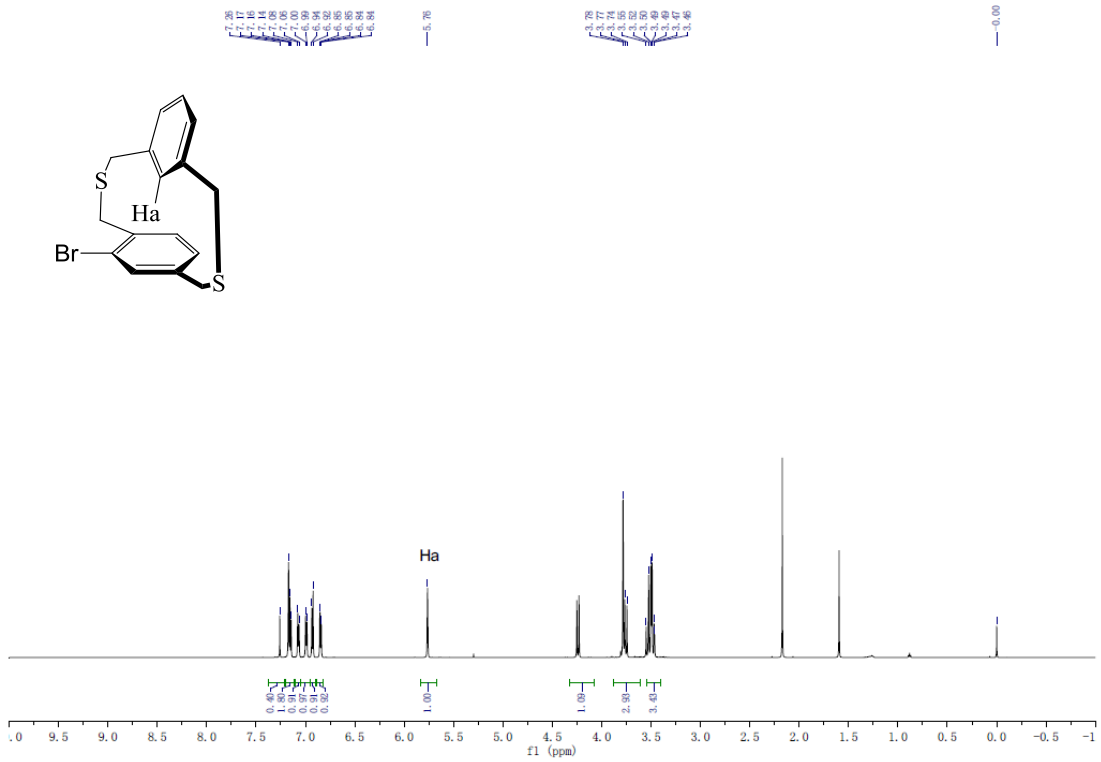
NMR Information

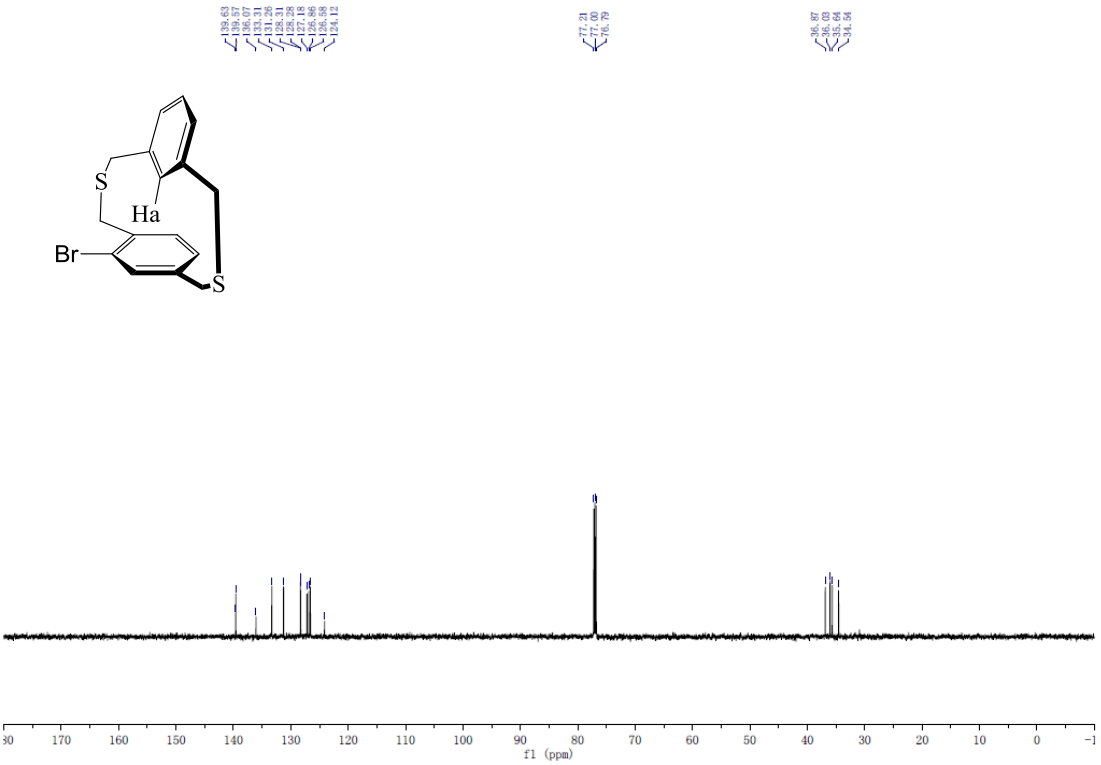


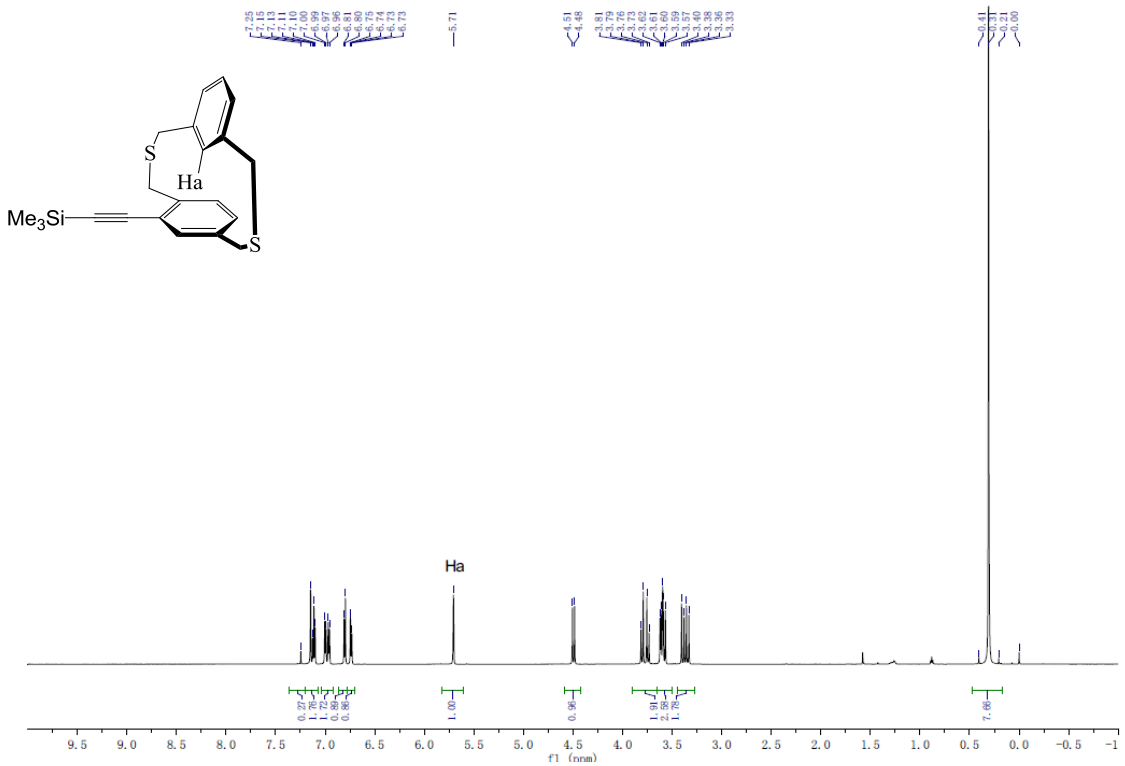

NO2
S
Ha
Me3Si
S
Ha
f1 (ppm)
NO2
S
Ha
Me3Si
S
f1 (ppm)

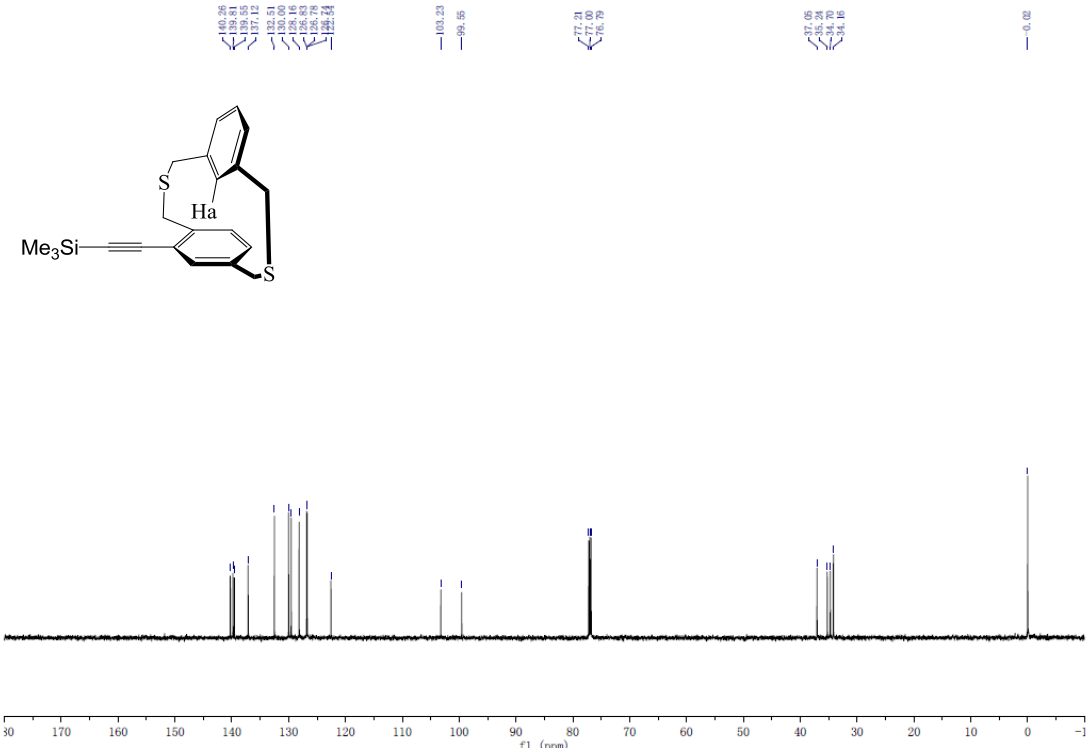


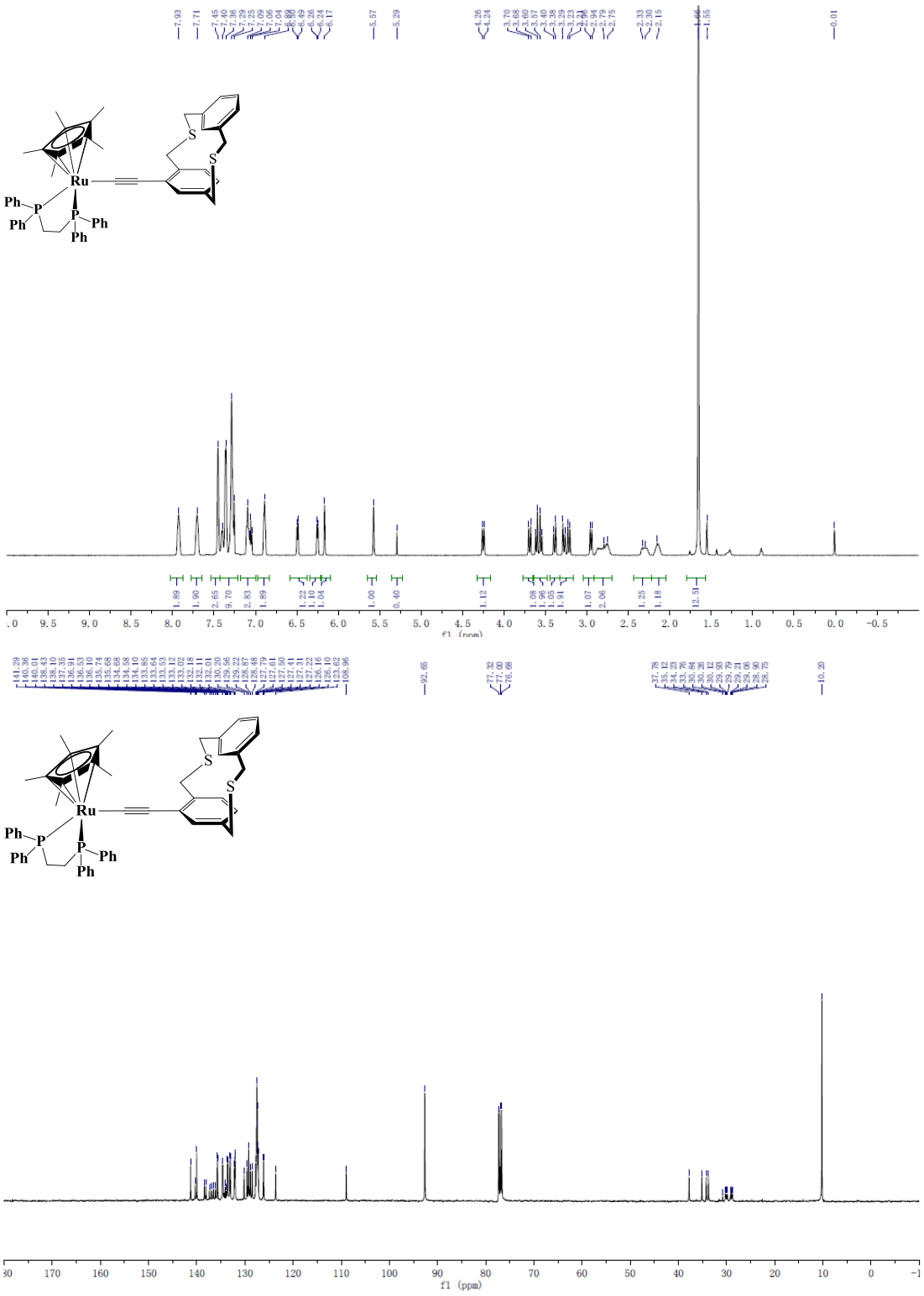


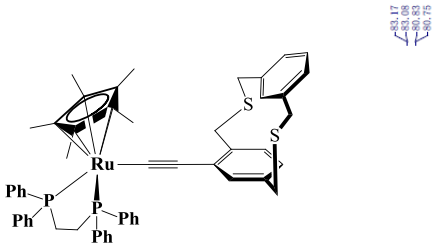


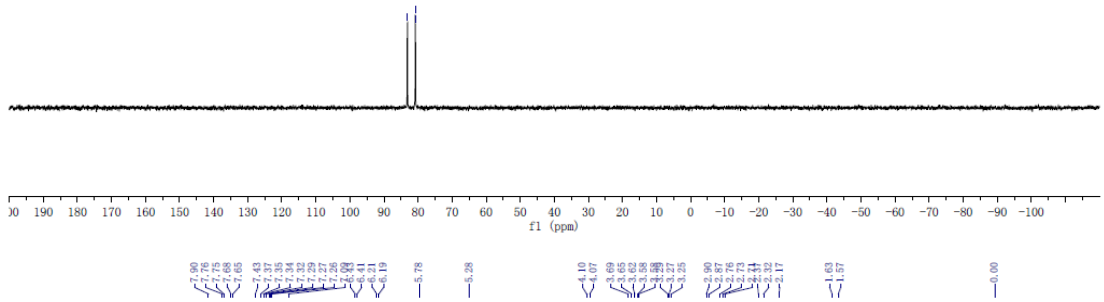


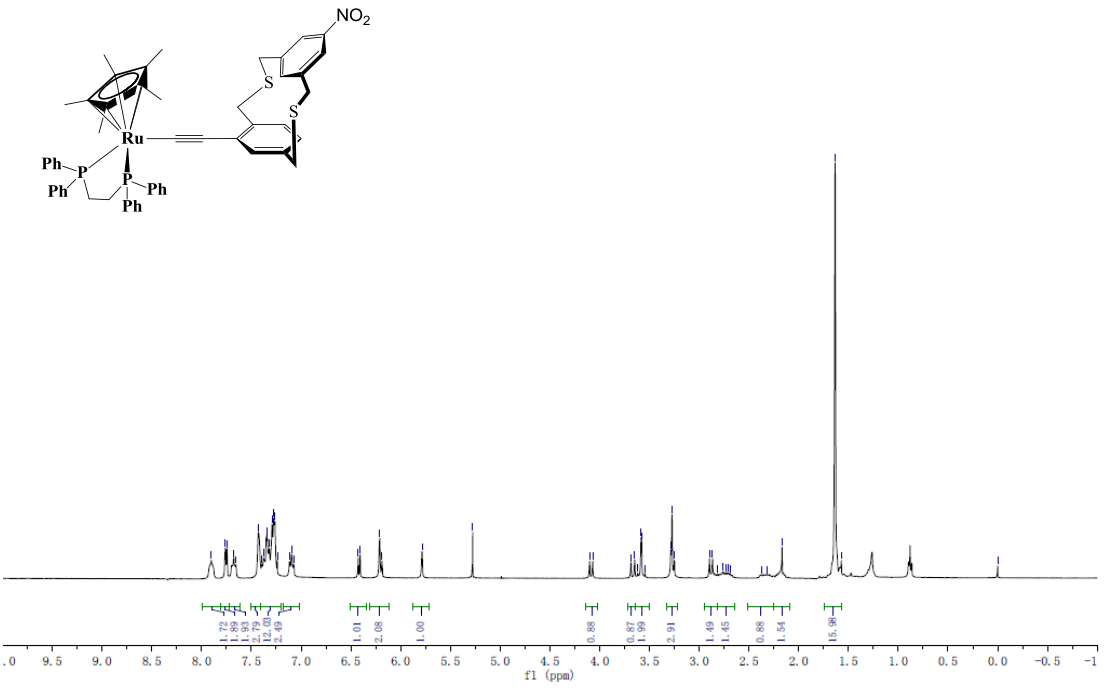

Ha
Me3Si
S
S
Ha
f1 (ppm)

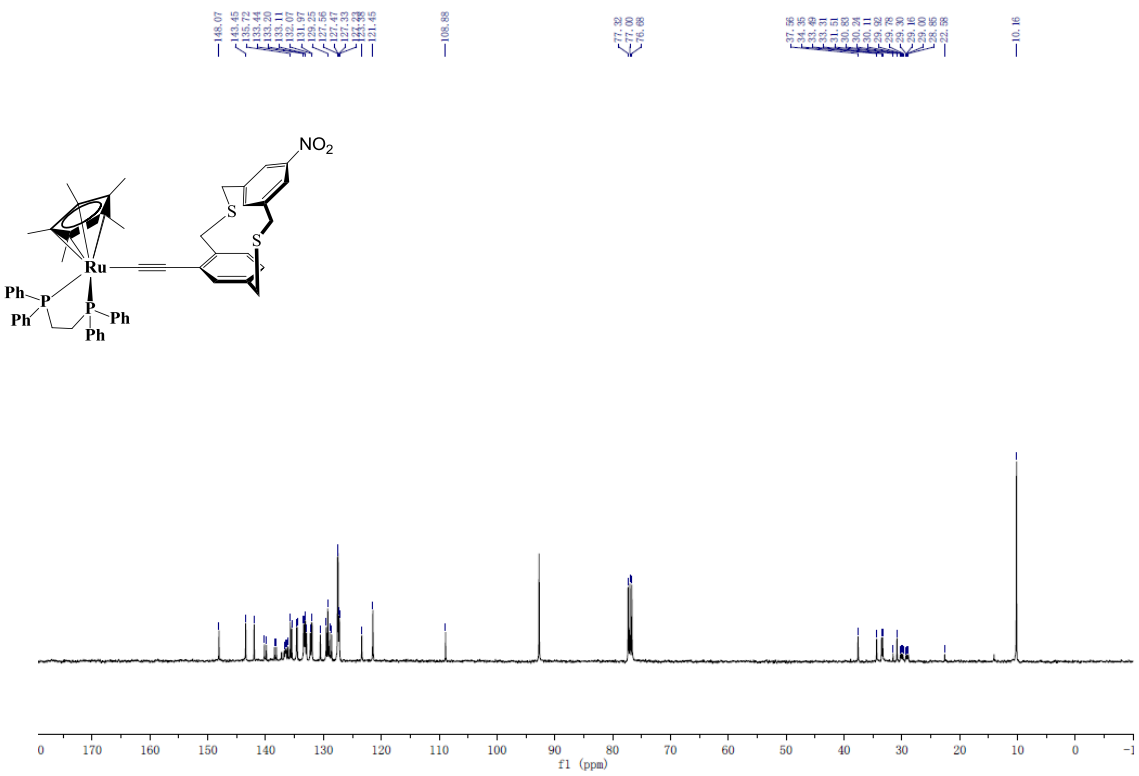

Me3Si
S
S
Ha
f1 (ppm)

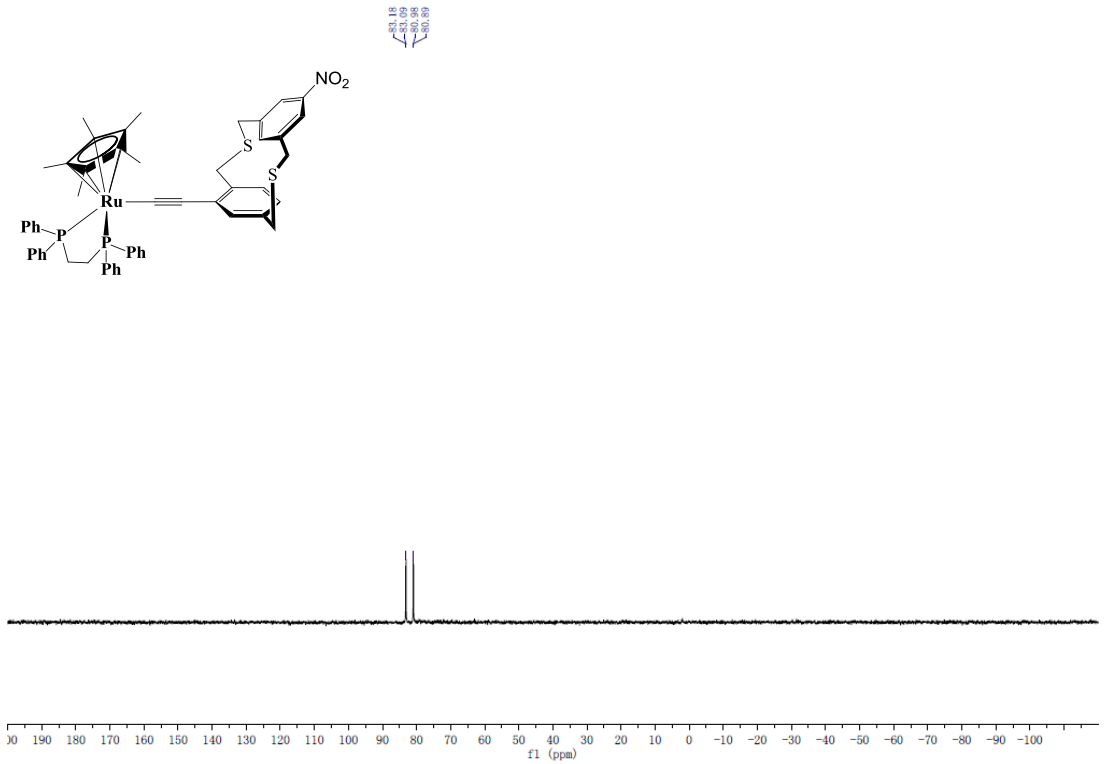


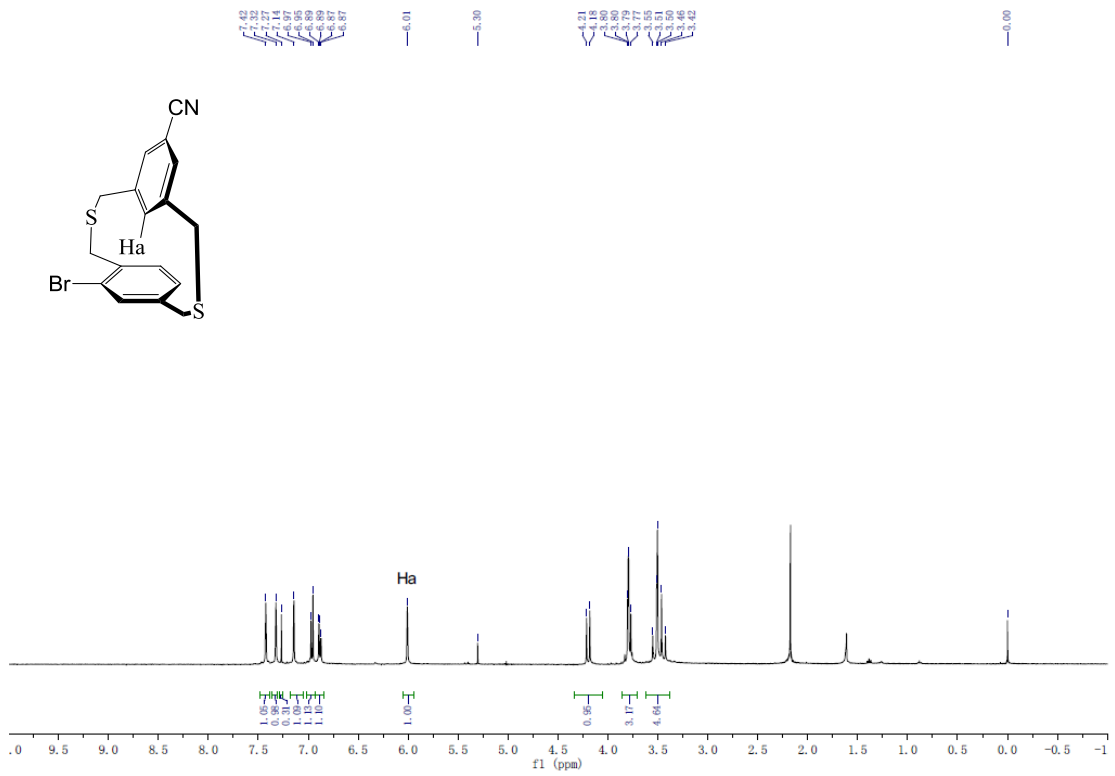


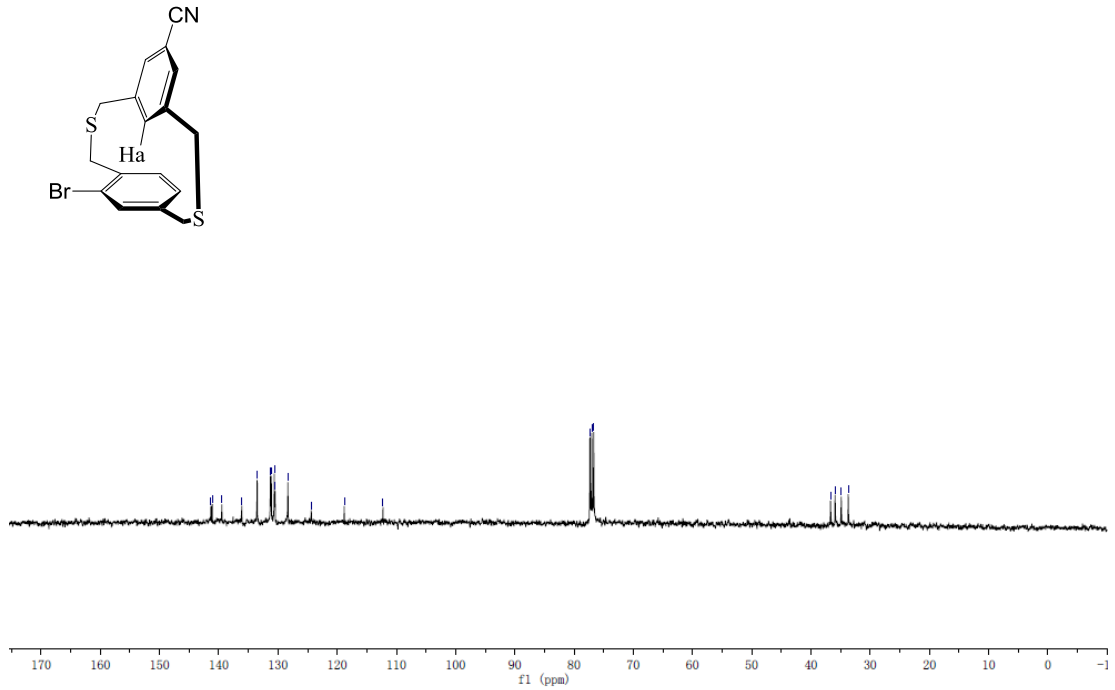


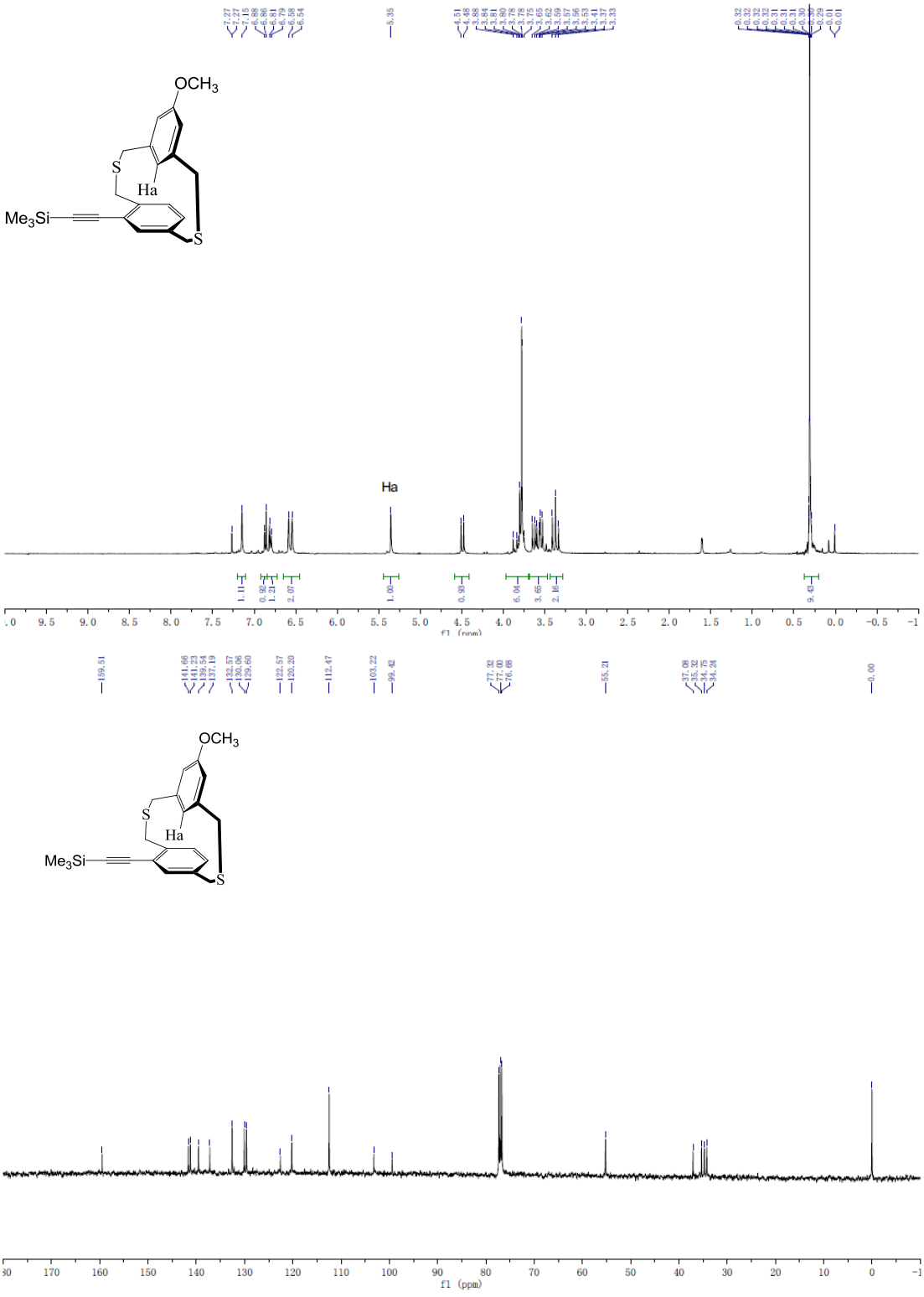


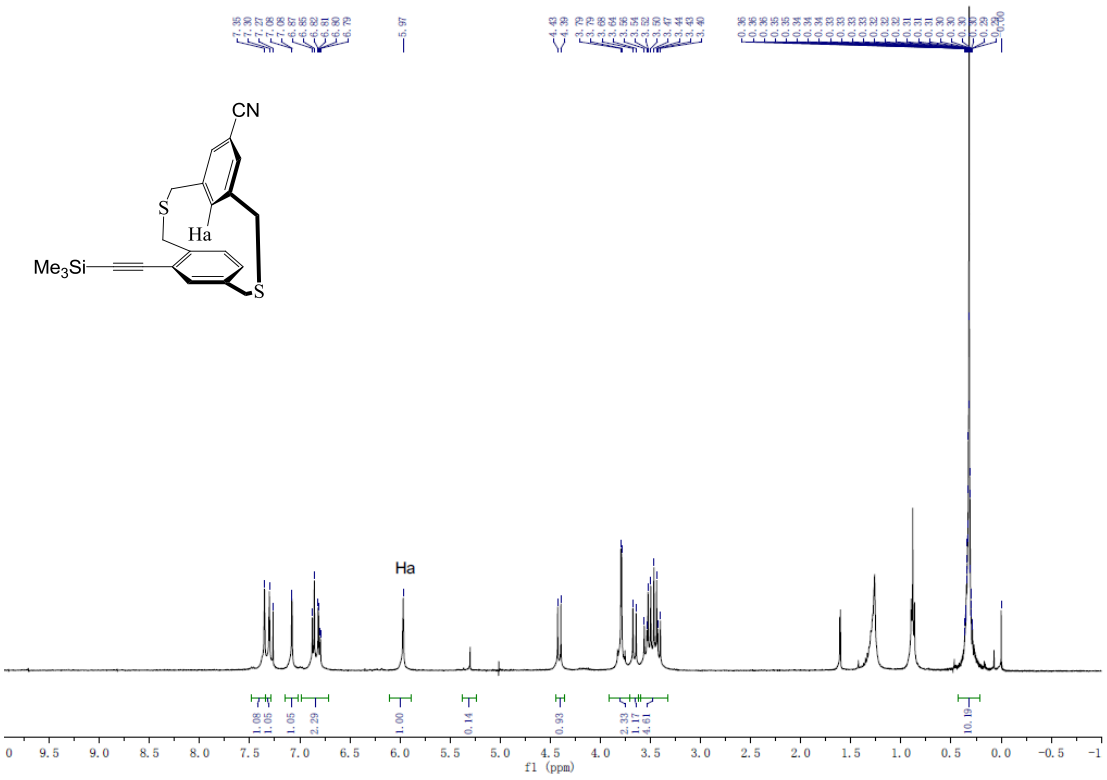


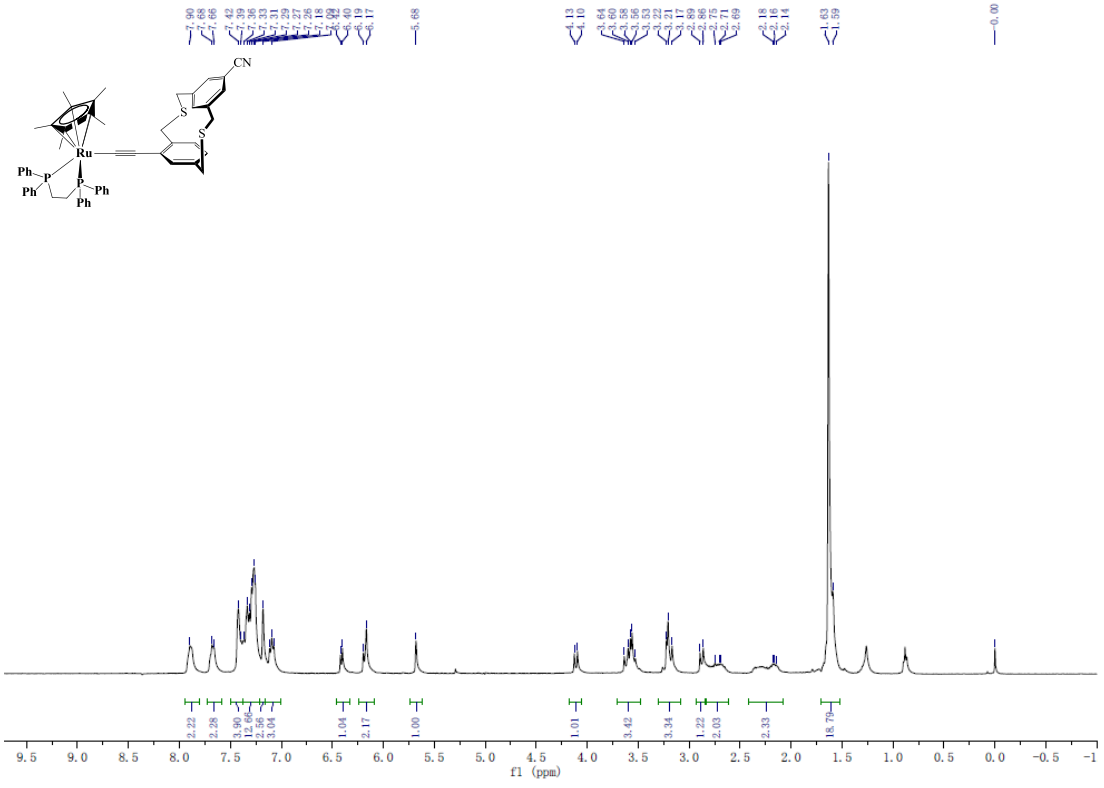


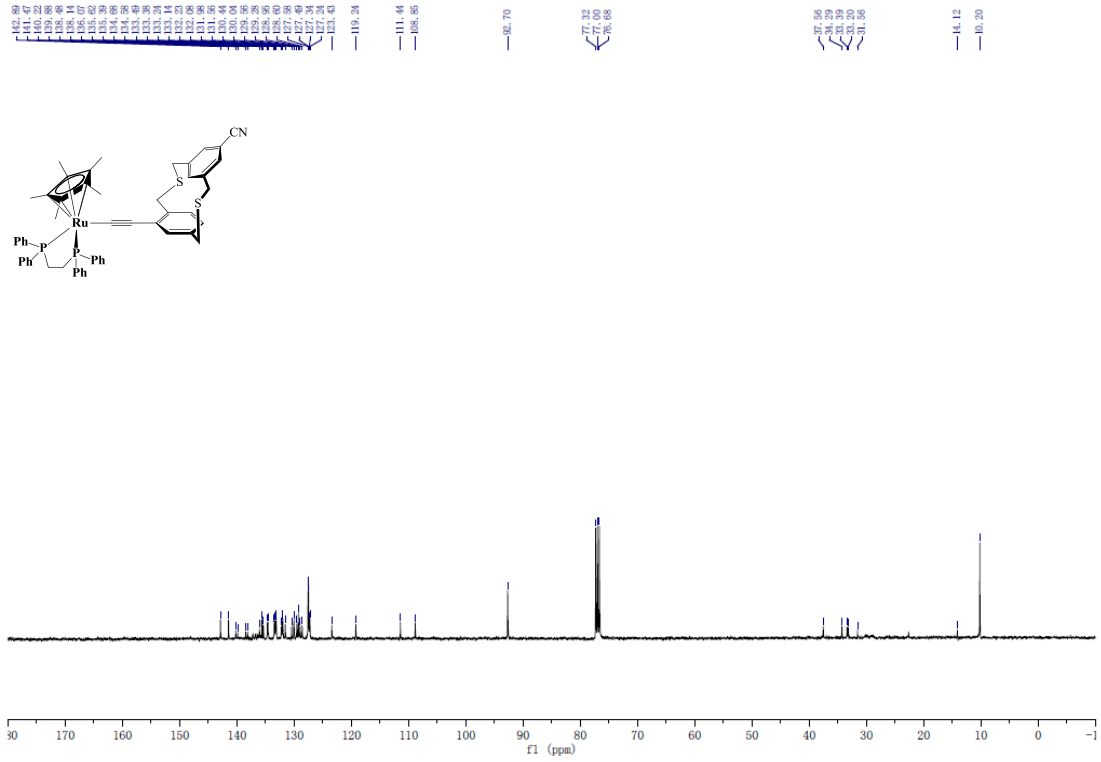


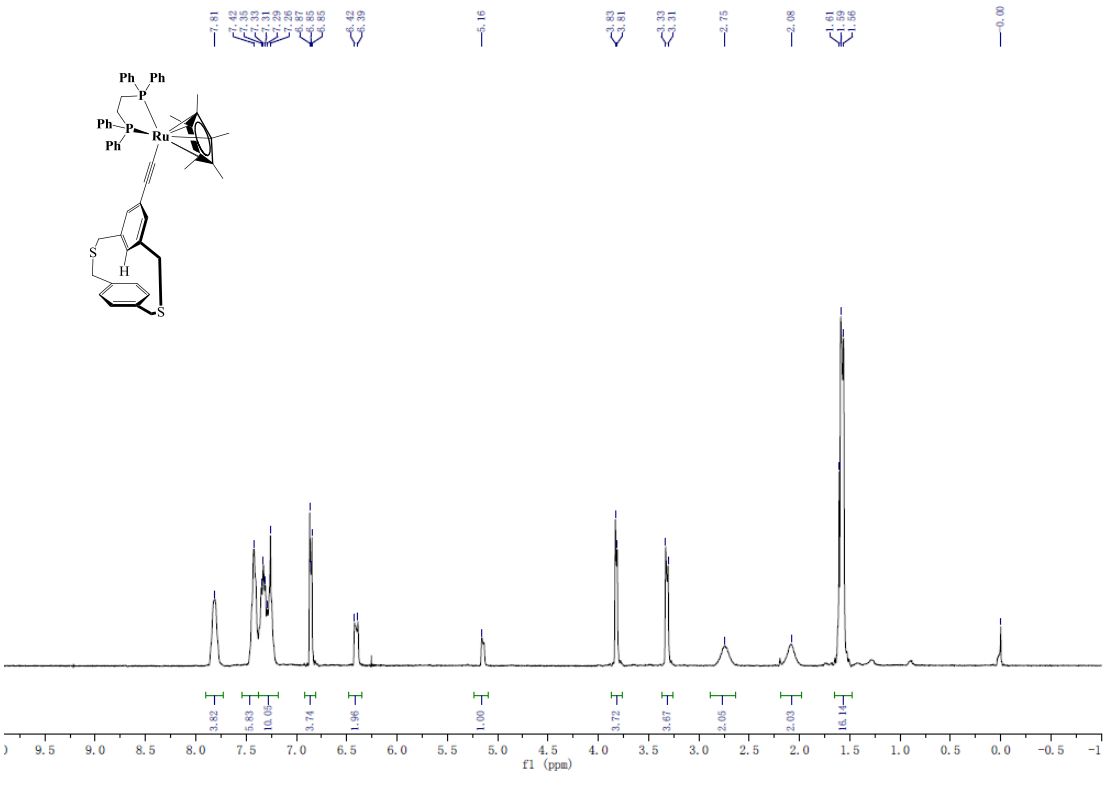


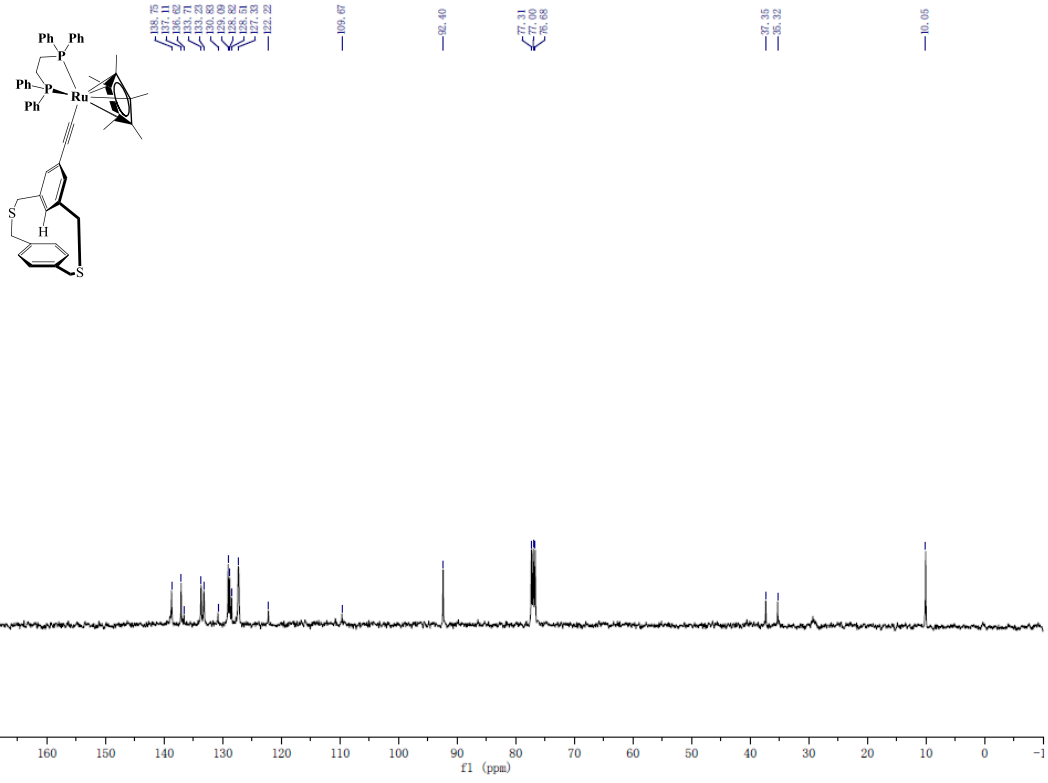

OCH3
S
Ha
Me3Si
S
Ha
f1 (ppm)
OCH3
S
Ha
Me3Si
S
f1 (ppm)

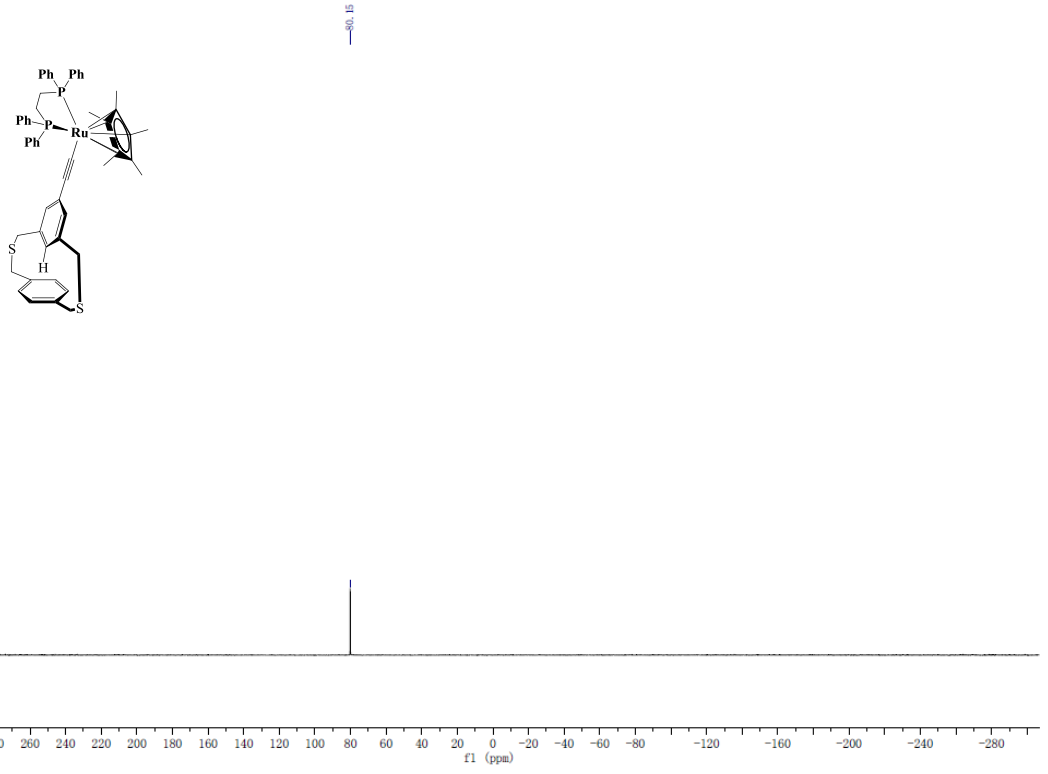


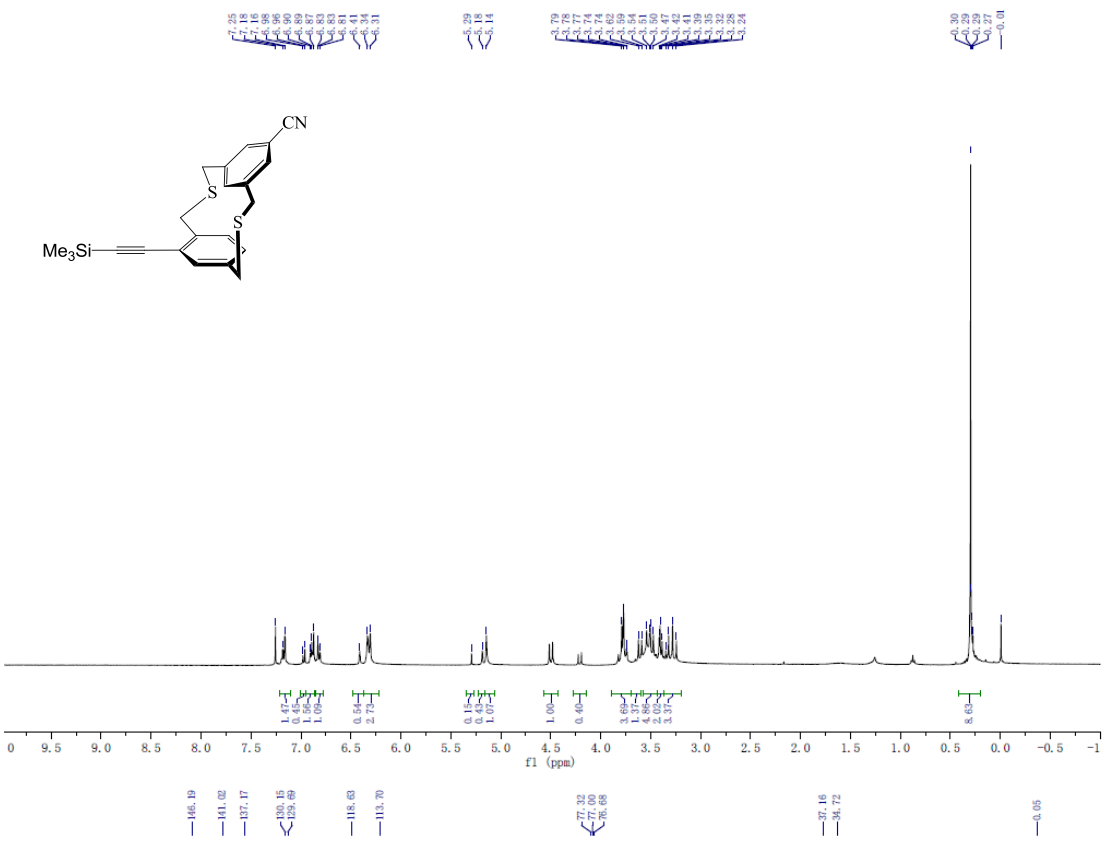


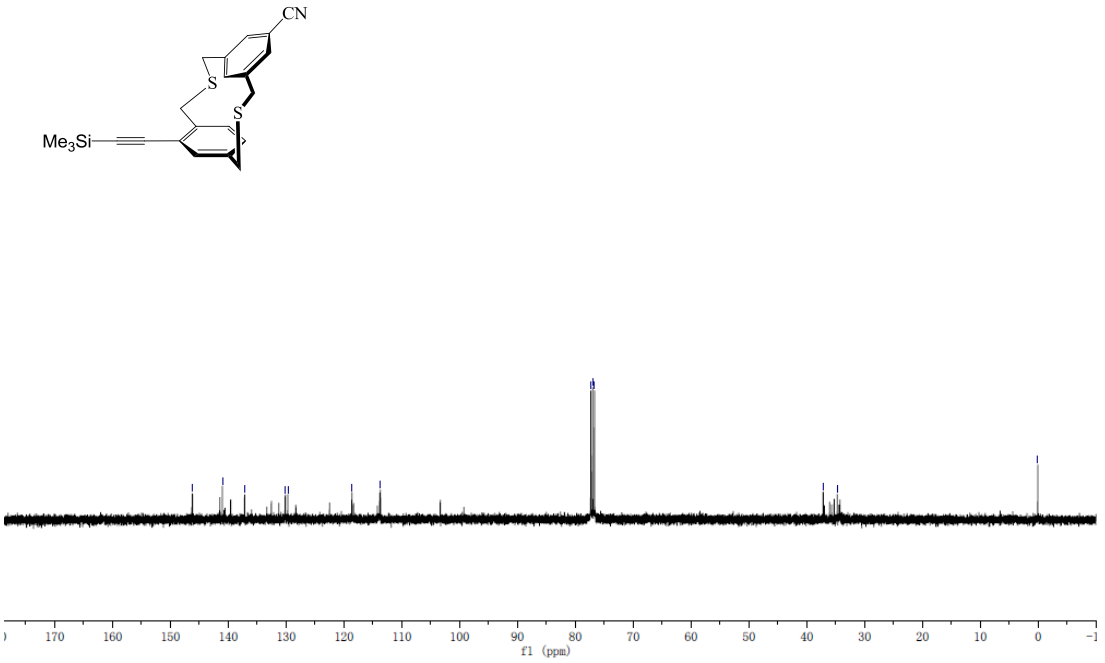


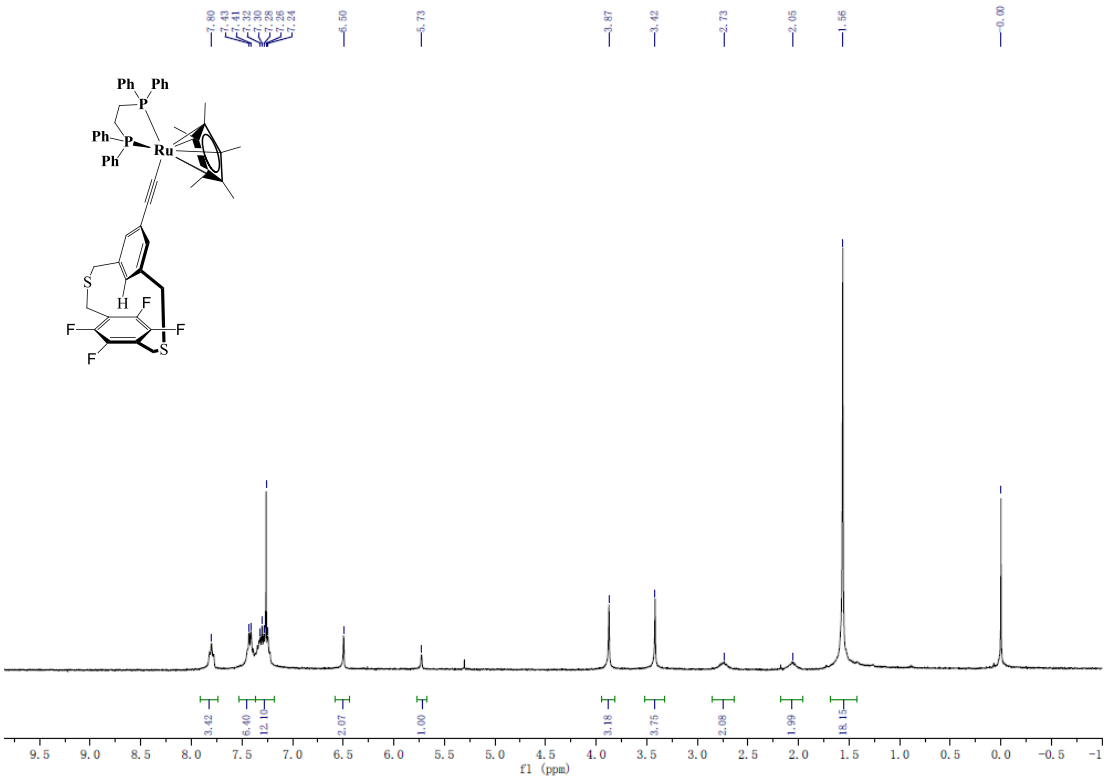


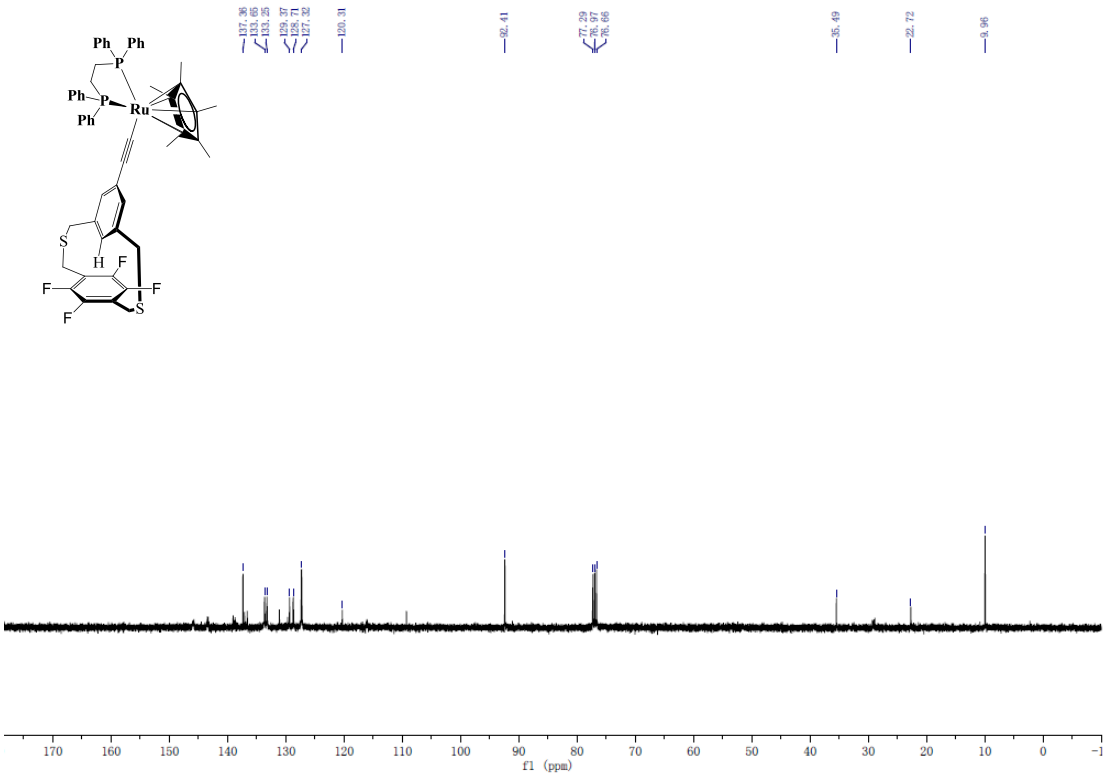


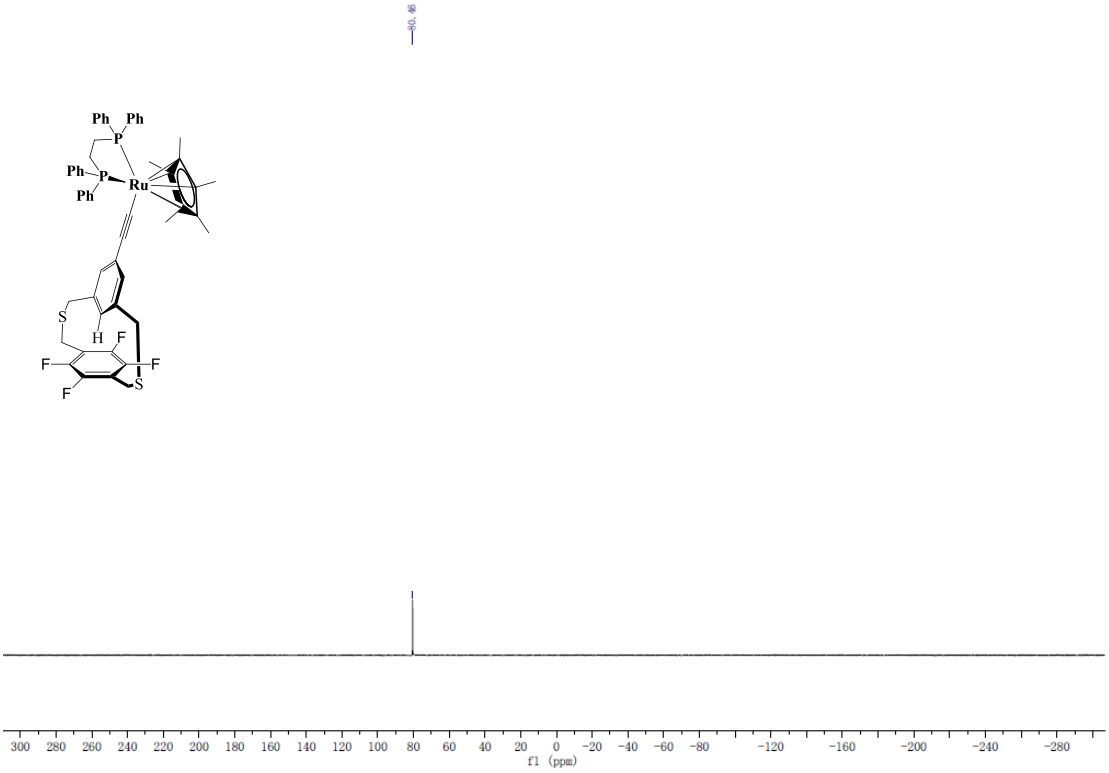


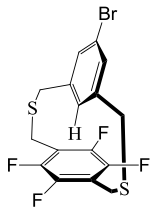


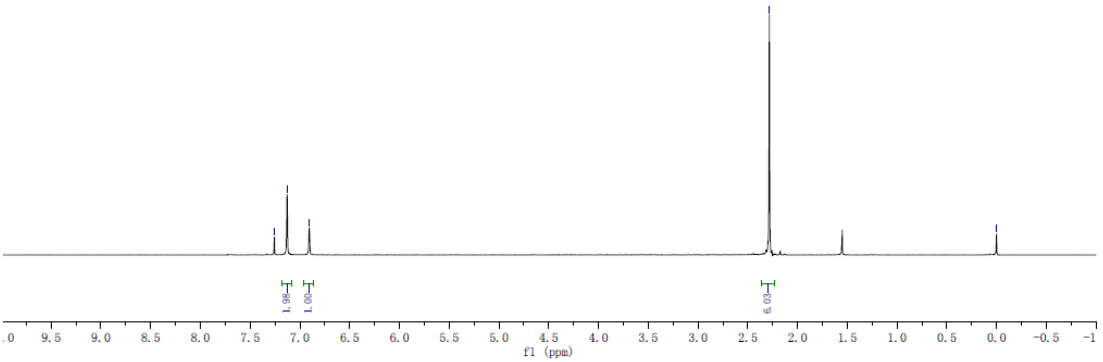


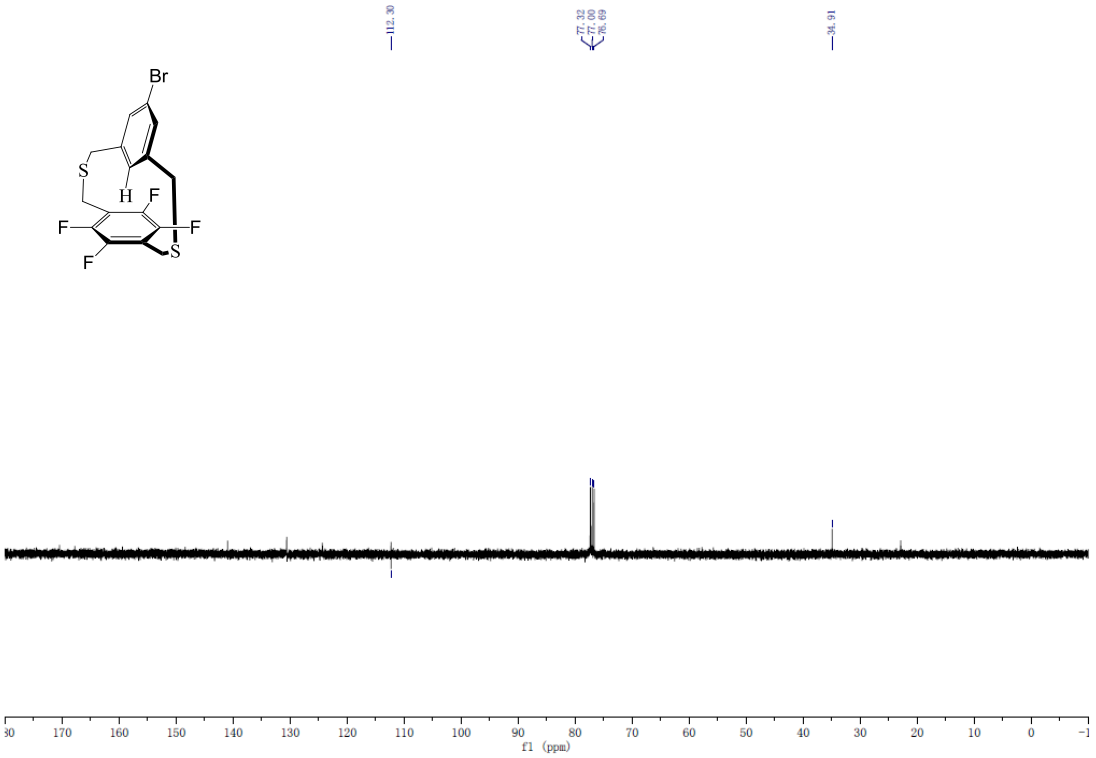


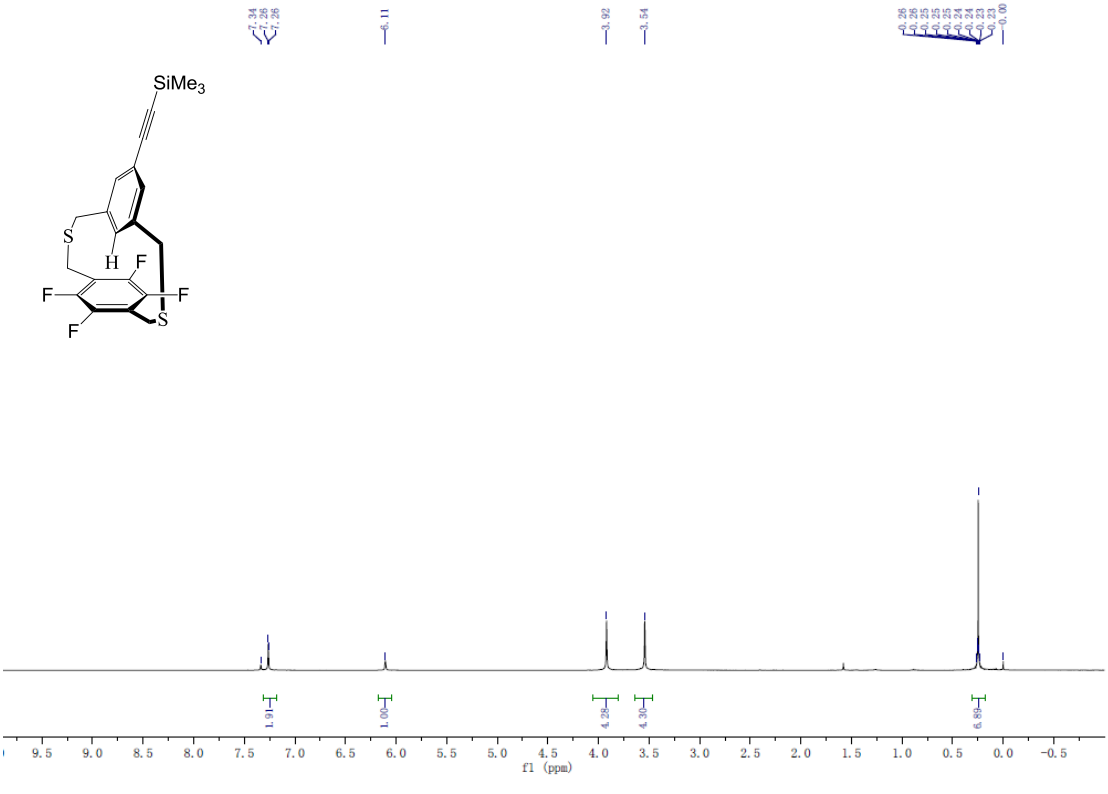


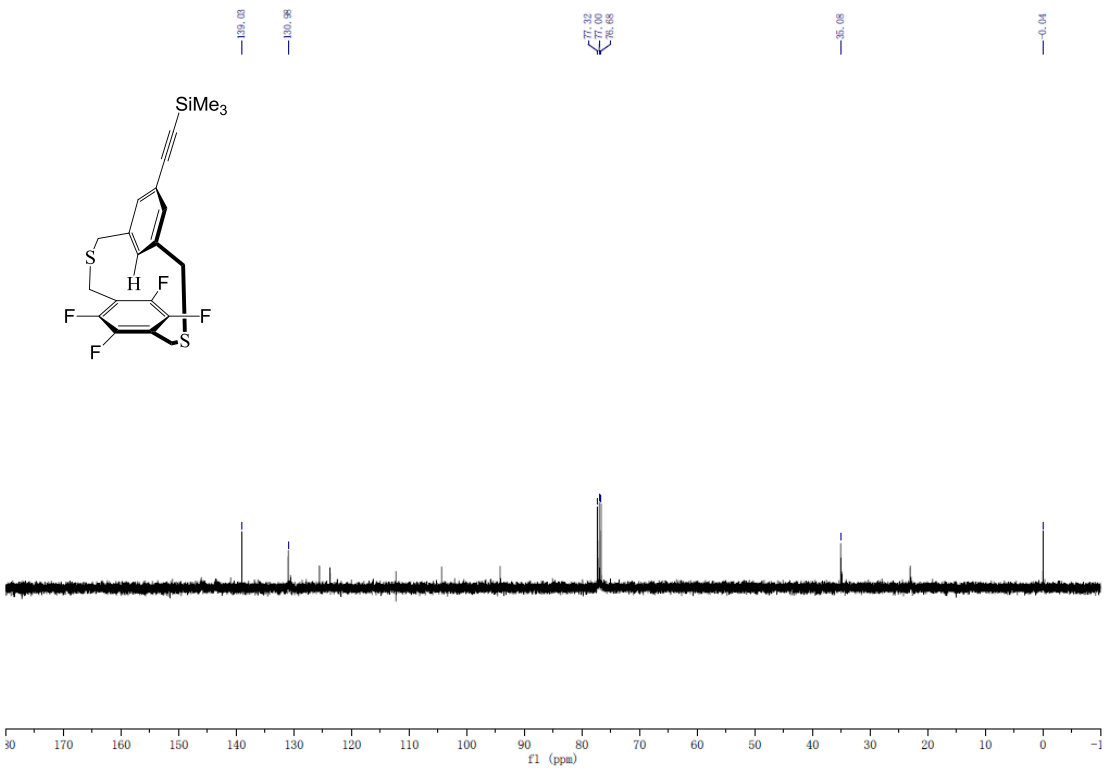


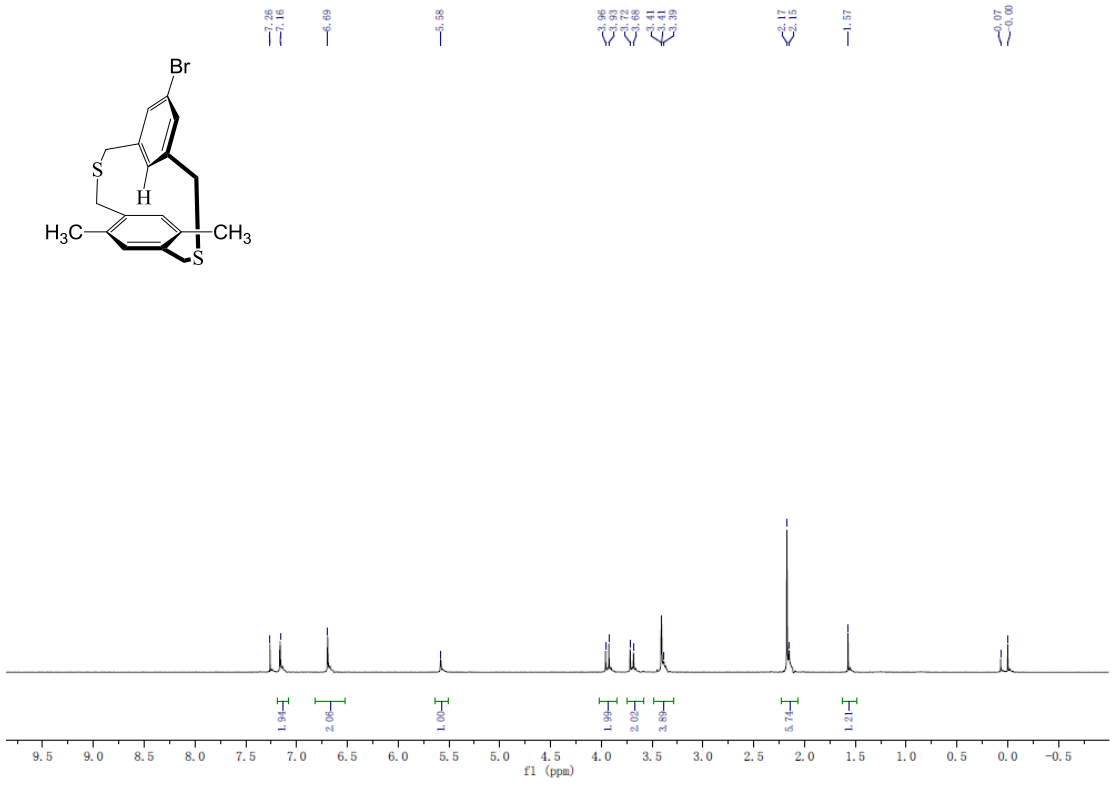


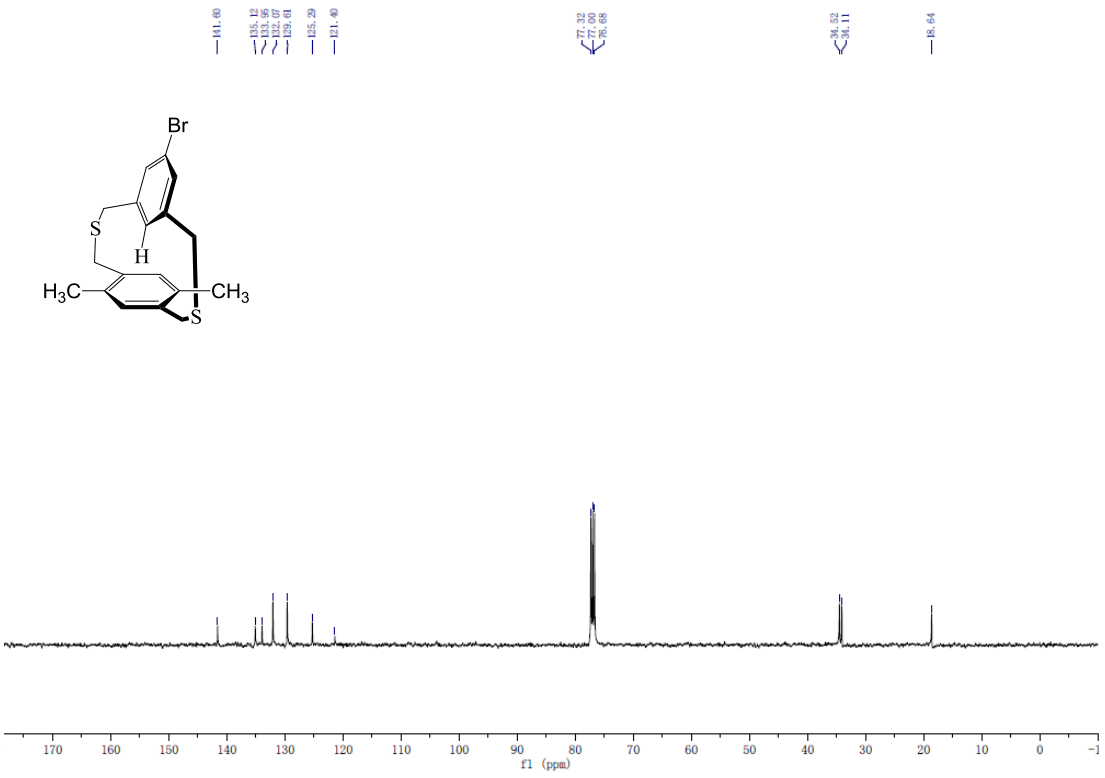


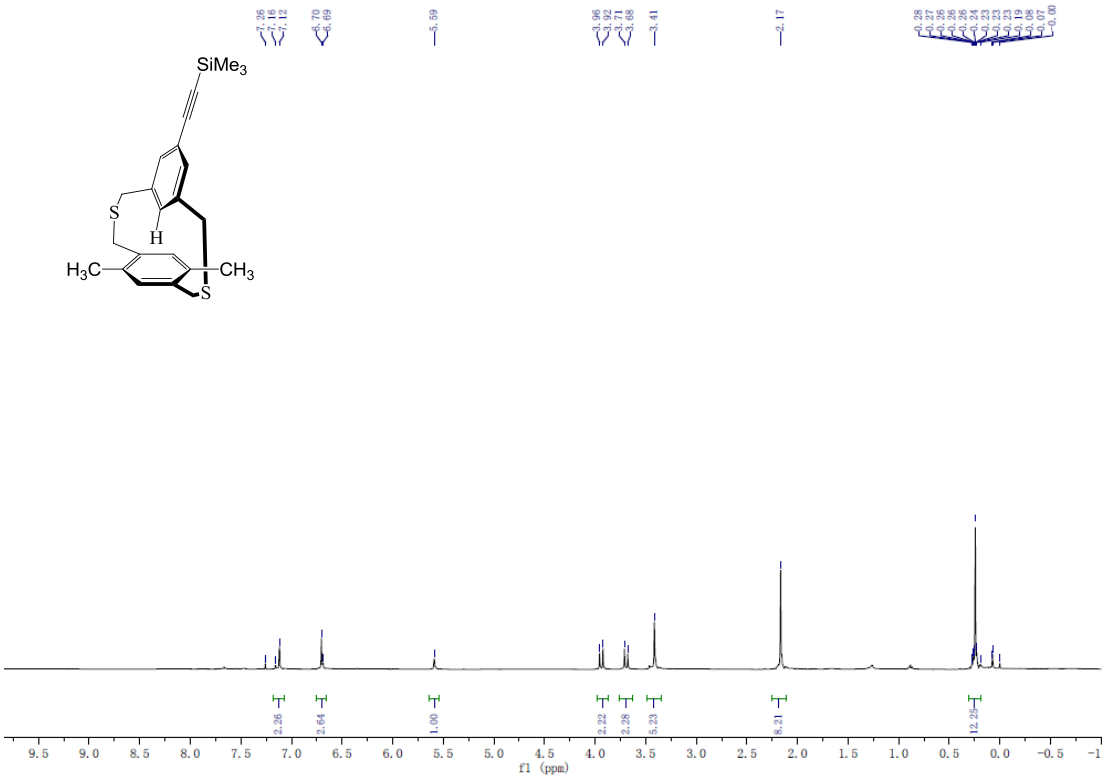





139.03
130.98
77.32
77.00
76.68
35.08
-0.04
SiMe3
S
H
F
F
F
S
f1 (ppm)


7.26
7.16
6.69
5.58
3.96
3.93
3.72
3.68
3.41
3.44
3.39
2.17
2.15
1.57
0.07
0.00
Br
S
H
H3C
CH3
S
1.94
2.06
1.00
1.99
2.02
3.89
5.74
1.21
f1 (ppm)


Br
S
H
H3C
CH3
S
f1 (ppm)


SiMe3
S
H
H3C
CH3
S
f1 (ppm)