Supporting Information

Copper *β*-Octakis(trifluoromethyl)corroles: New Paradigms for Ligand Substituent Effects in Transition Metal Complexes

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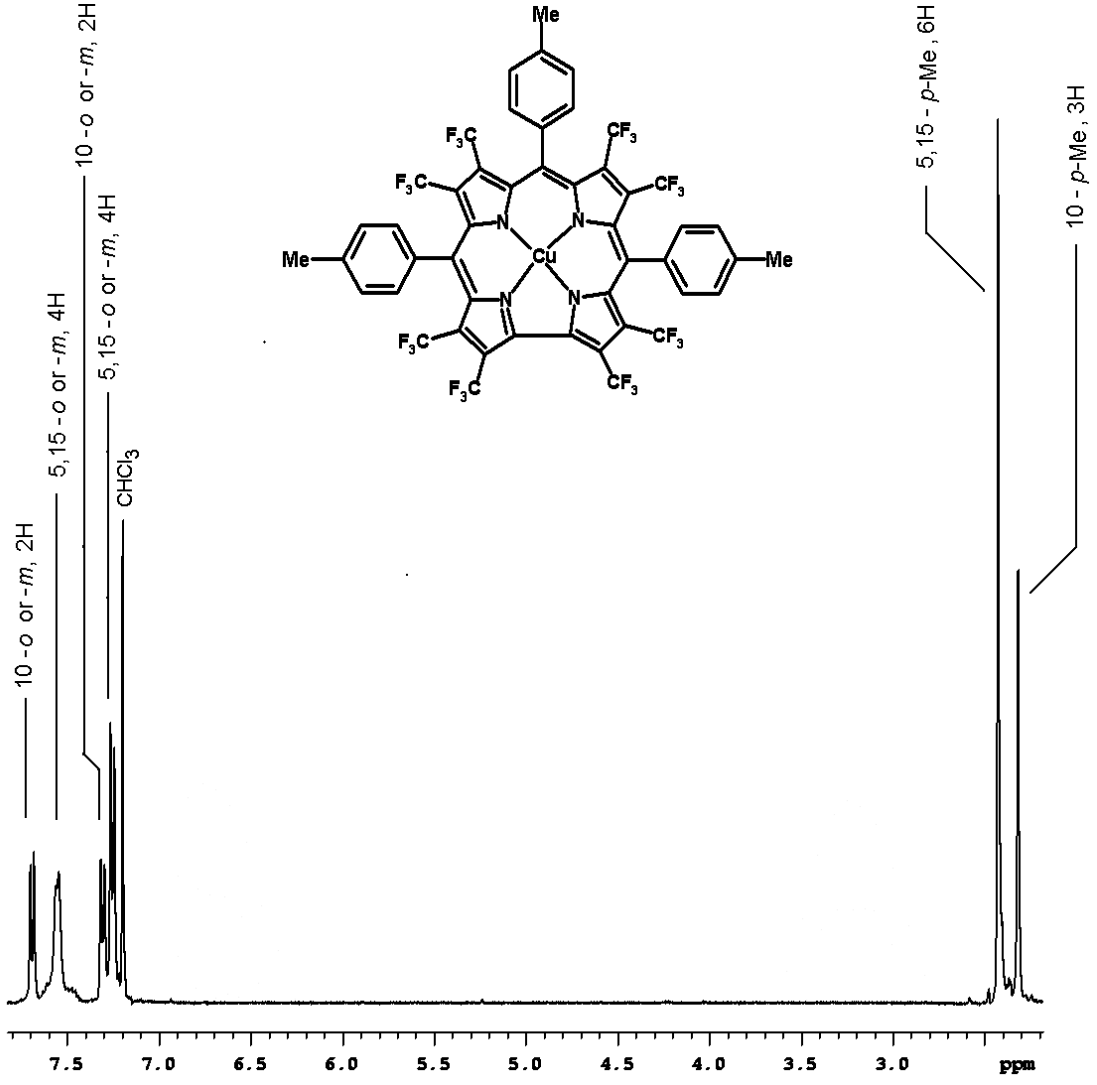
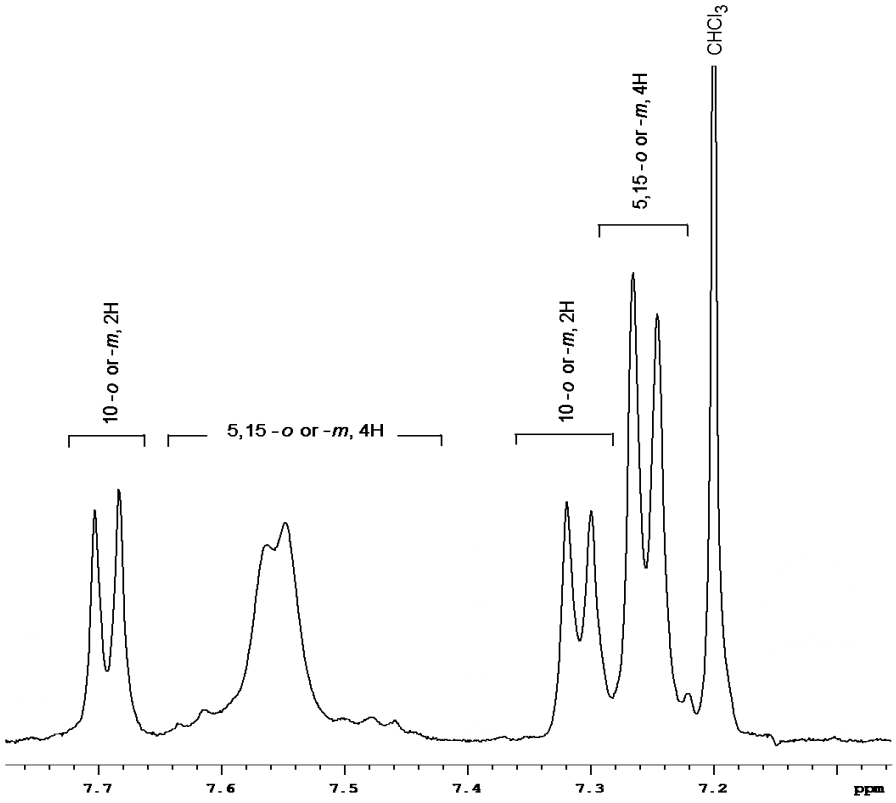
Proton NMR Spectra

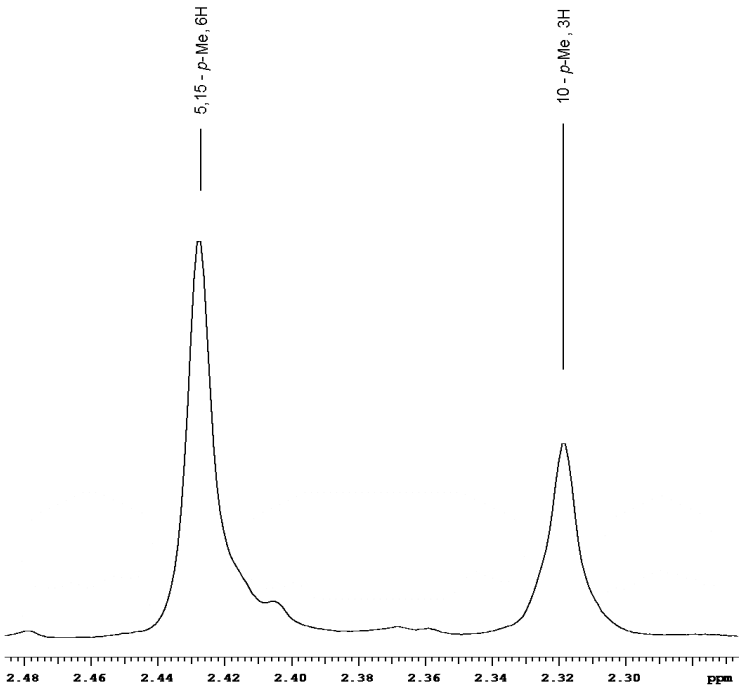
Figure S1. ^{1}H NMR spectra of Cu[$(CF_3)_8$T(*p*-MeP)C]: (a) the full range, (b) expanded views of the peaks, and (c) the ^{1}H - ^{1}H COSY.

(a)



(b)


10 -o or -m, 2H
5,15 -o or -m, 4H
10 -o or -m, 2H
5,15 -o or -m, 4H
CHCl3
7.7
7.6
7.5
7.4
7.3
7.2
ppm


5,15 - p-Me, 6H
10 - p-Me, 3H
2.48
2.46
2.44
2.42
2.40
2.38
2.36
2.34
2.32
2.30
ppm

(c)

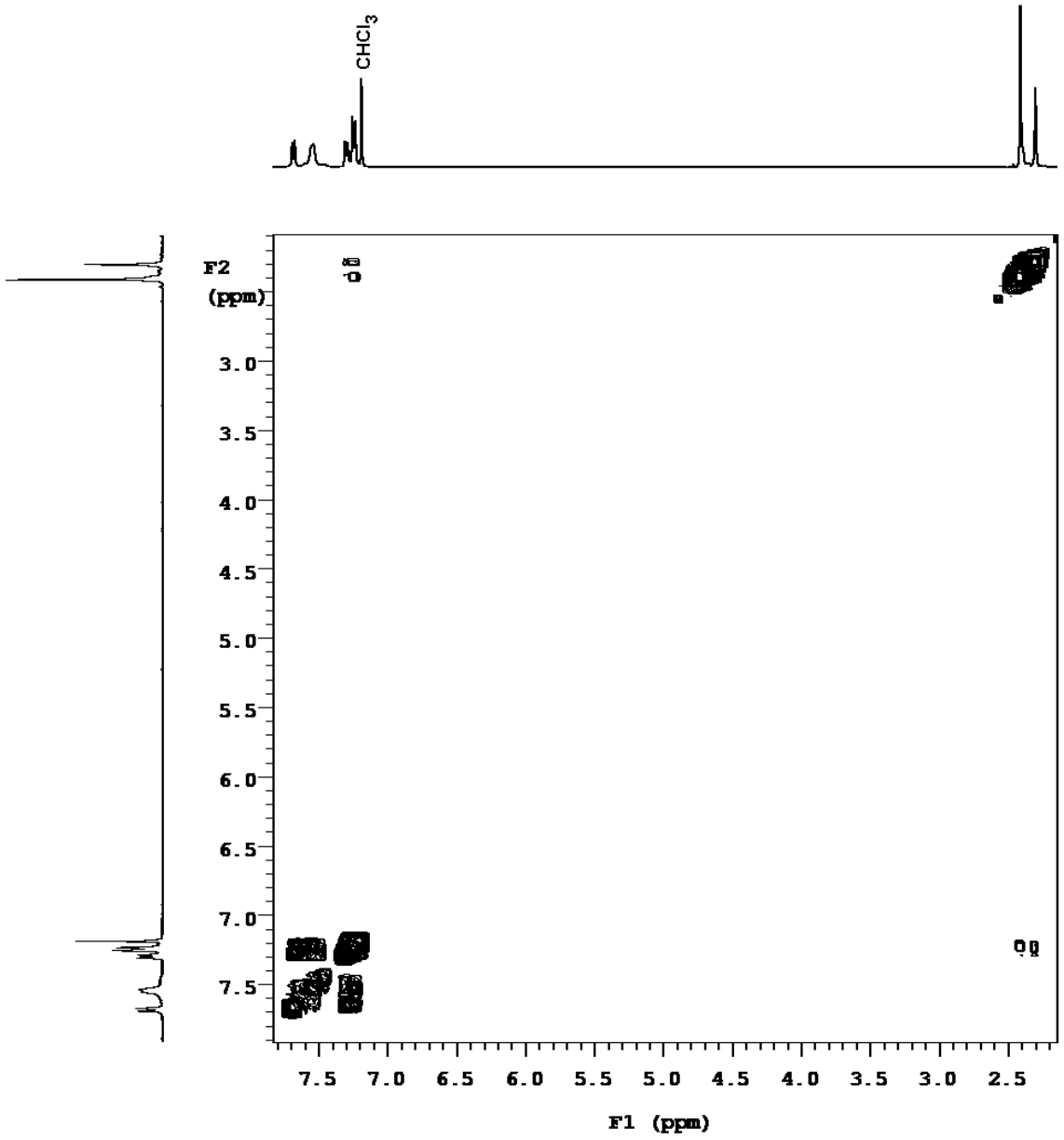
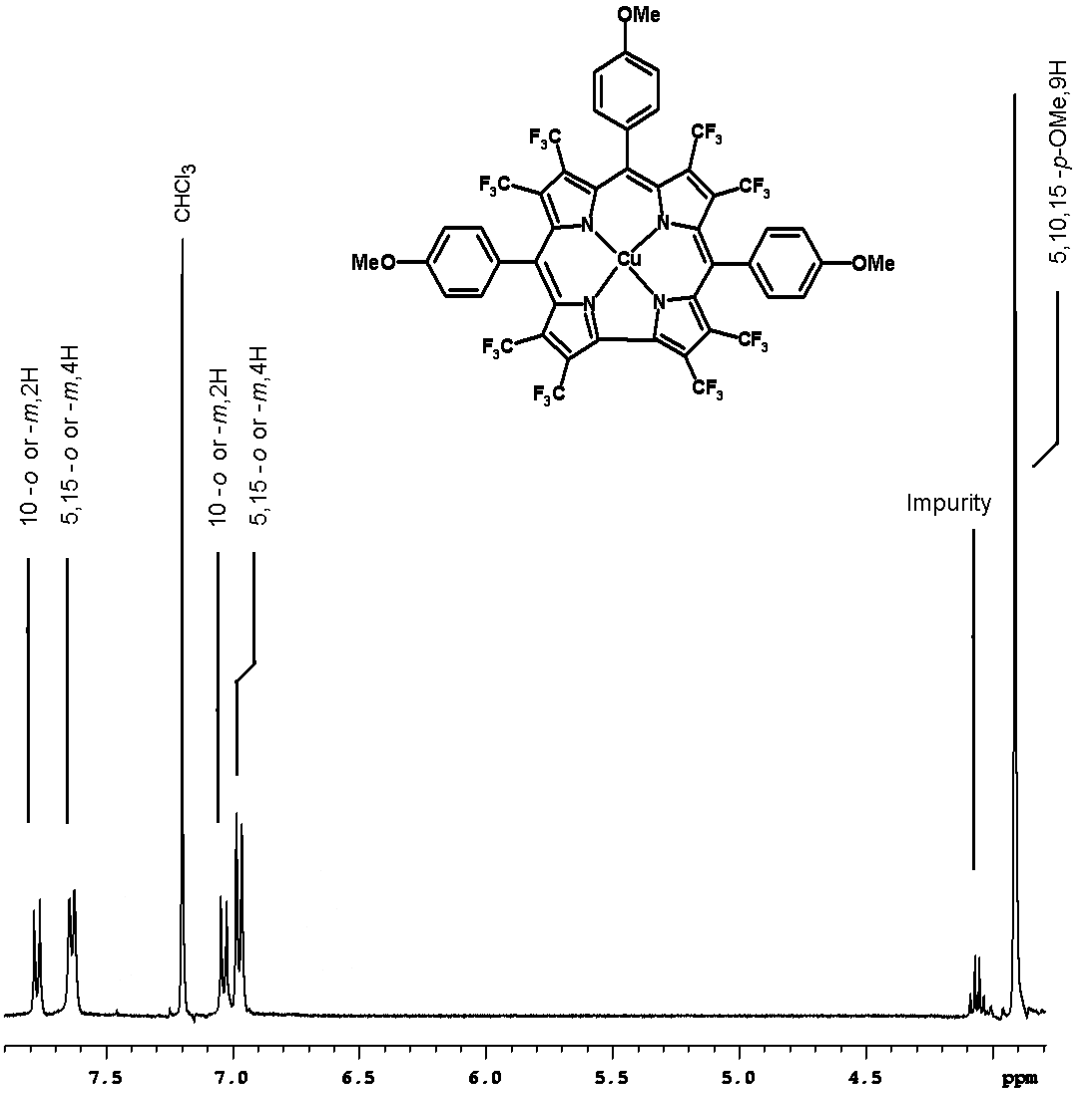
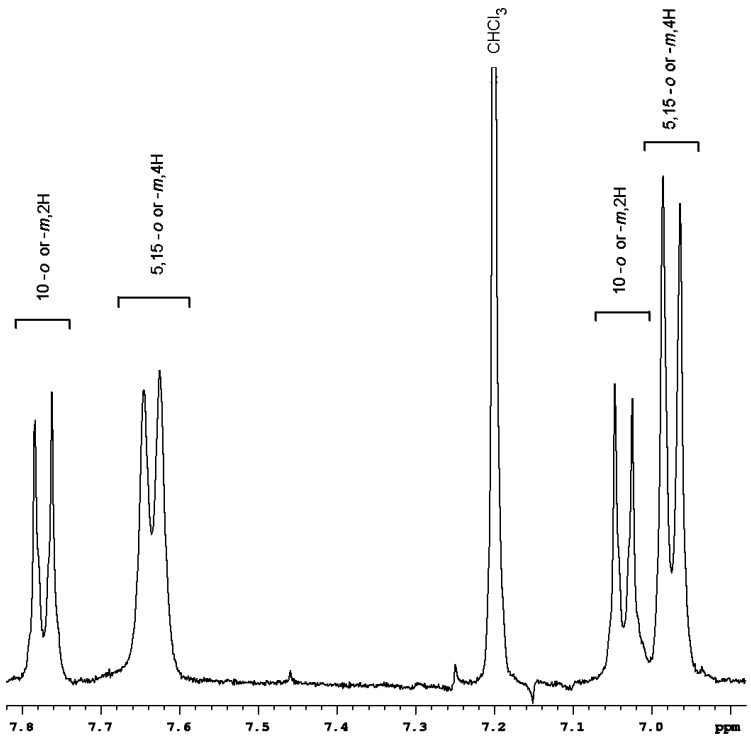

CHCl3
F2
(ppm)
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5
F1 (ppm)

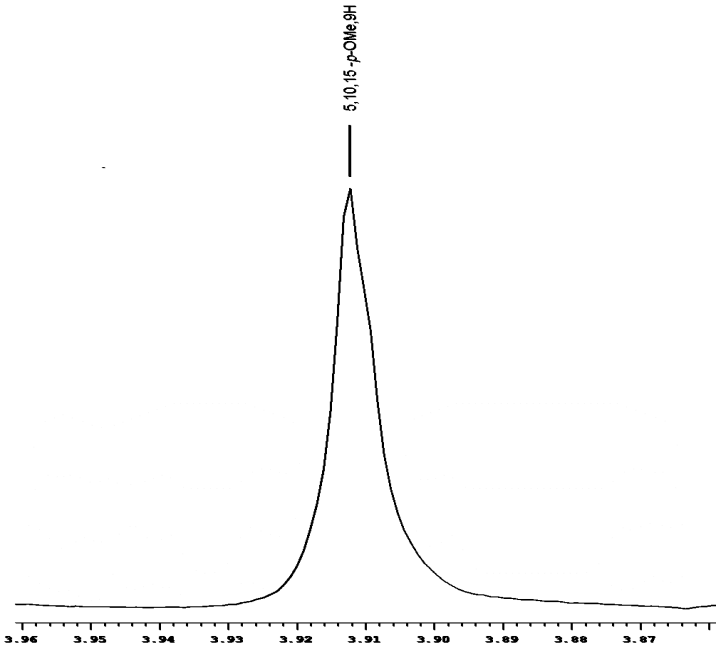
Figure S2. ^{1}H NMR spectra of Cu[$(CF_3)_8$T(*p*-OMeP)C]: (a) the full range, (b) expanded views of the peaks, and (c) the ^{1}H -^{1}H COSY.

(a)



(b)


10 -o or -m,2H
5,15 -o or -m,4H
CHCl3
10 -o or -m,2H
5,15 -o or -m,4H
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm


5,10,15 -p-OMe,9H
3.96
3.95
3.94
3.93
3.92
3.91
3.90
3.89
3.88
3.87

(c)

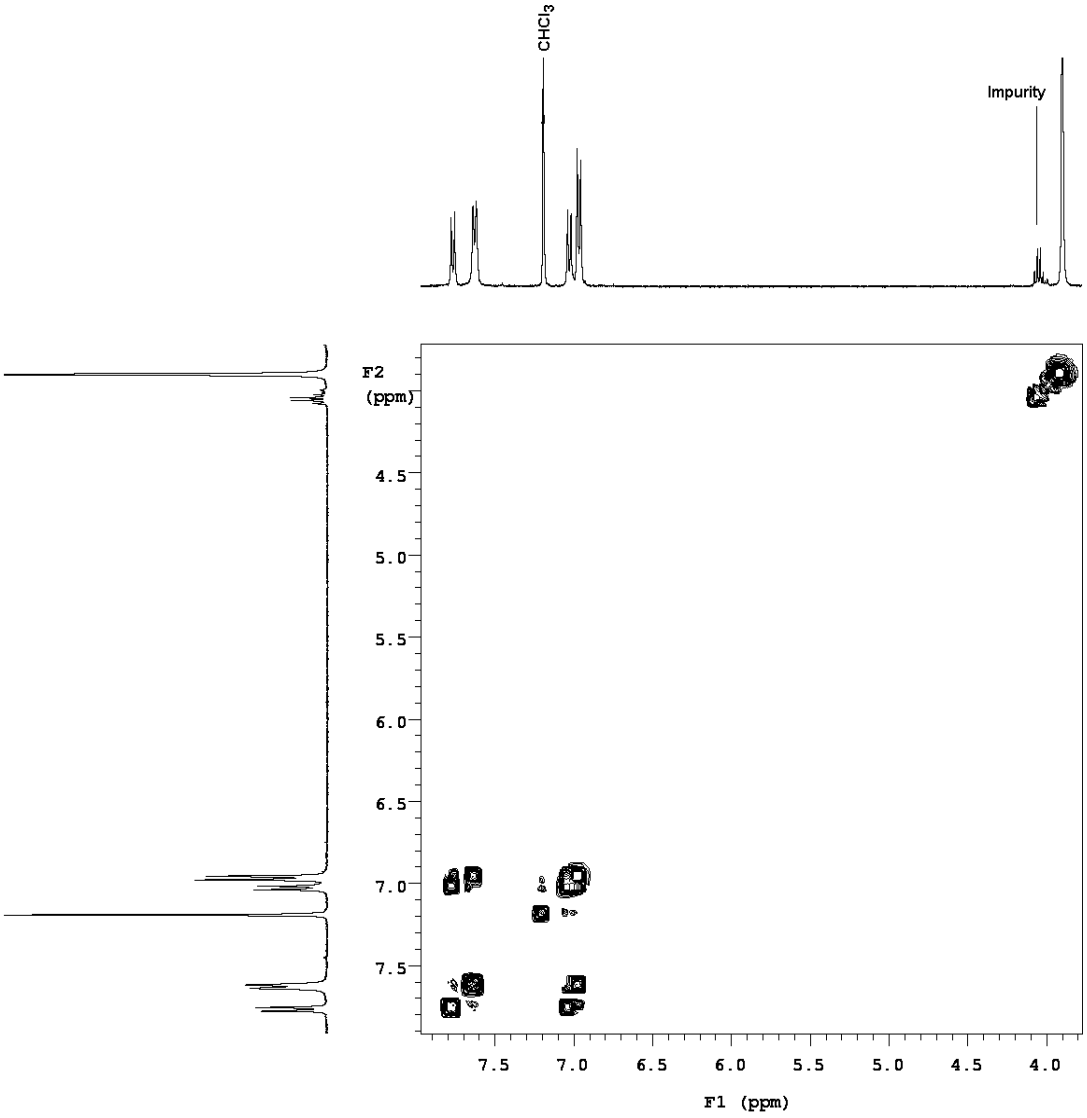
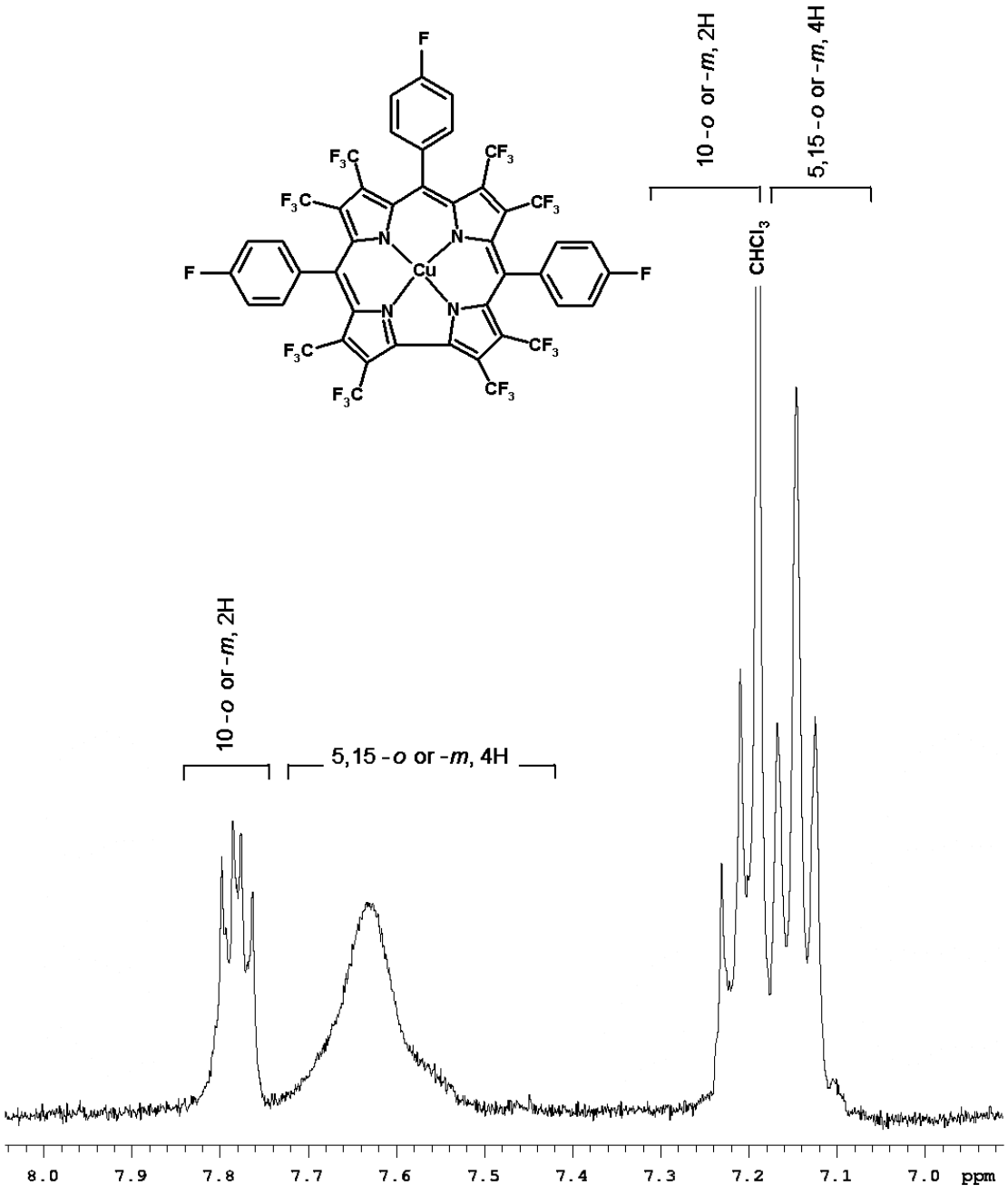
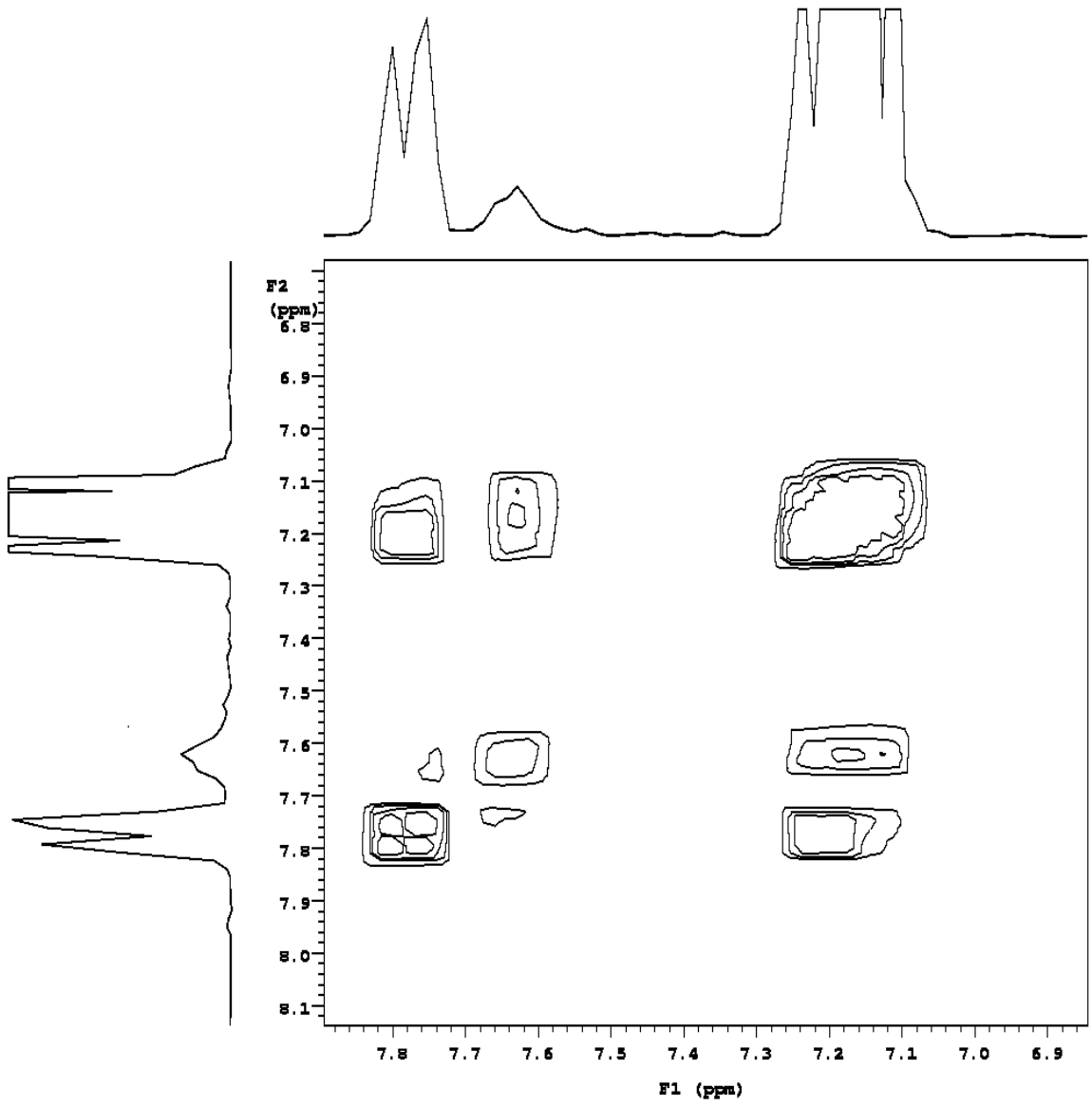

CHCl3
Impurity
F2
(ppm)
4.5
5.0
5.5
6.0
6.5
7.0
7.5
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
F1 (ppm)

Figure S3. ^{1}H NMR spectra of Cu[$(CF_3)_8$T(*p*-FP)C]: (a) the full range, and (b) the ^{1}H -^{1}H COSY.

(a)



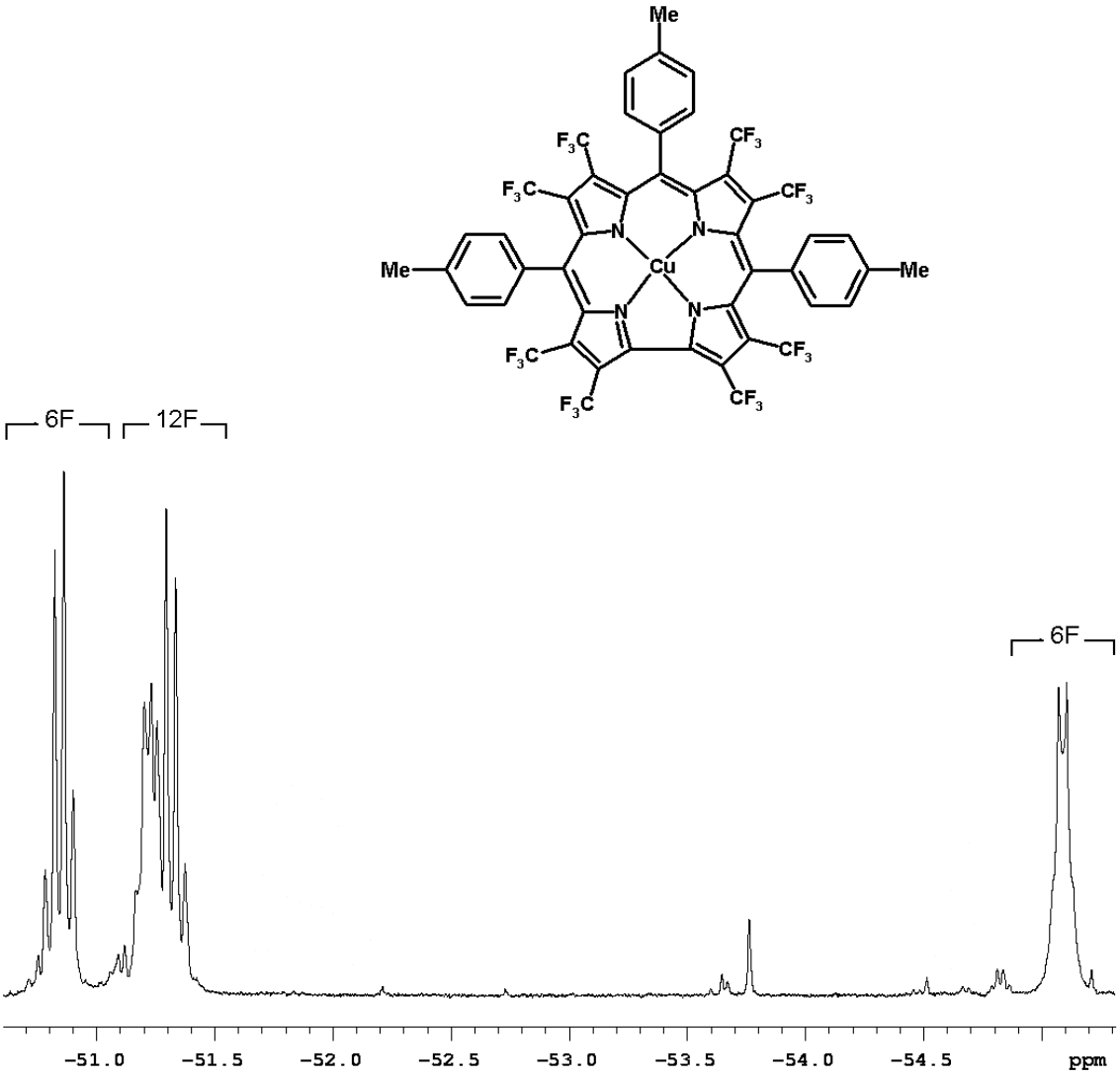
(b)


F2
(ppm)
6.8
6.9
7.0
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
F1 (ppm)

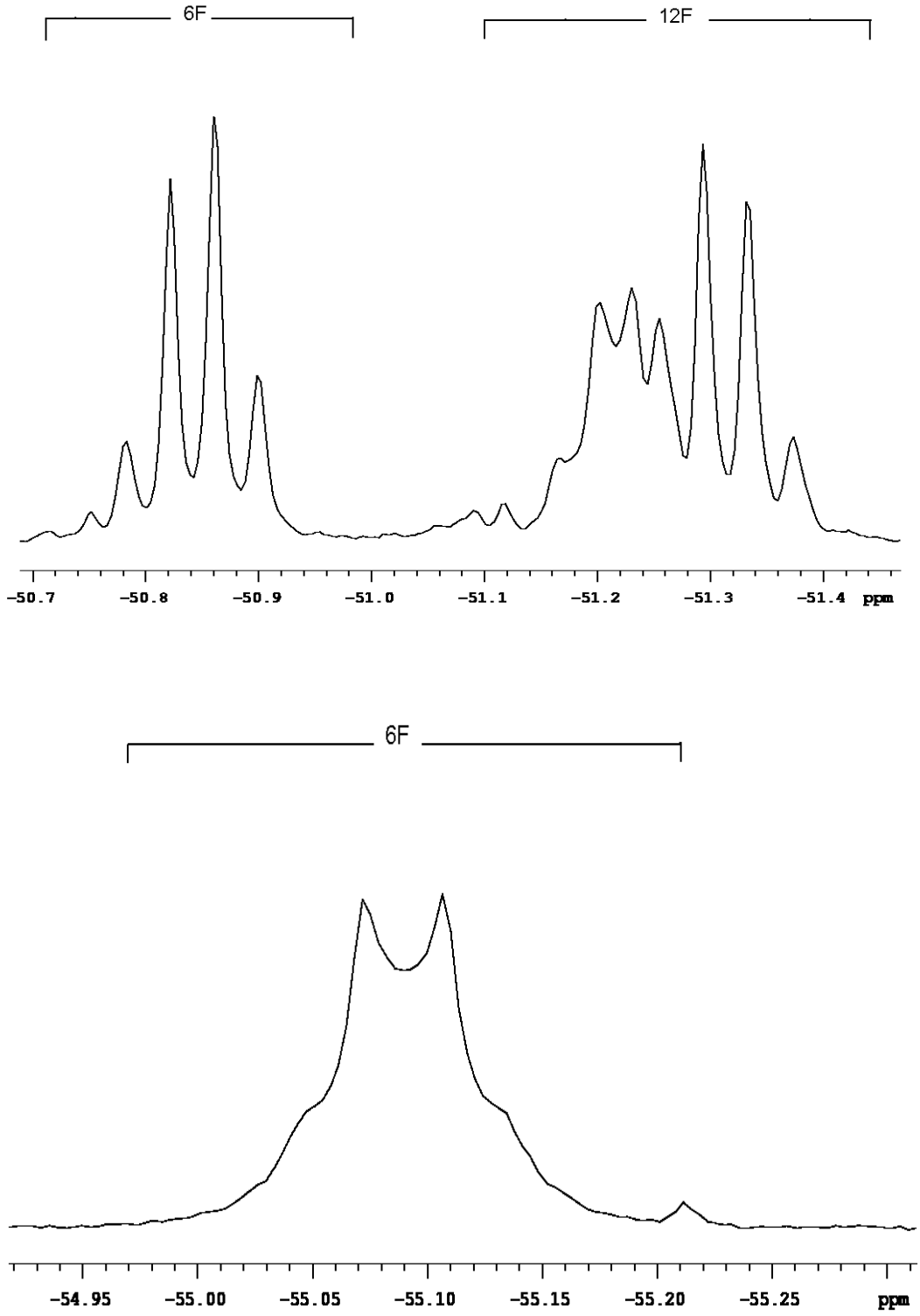
Fluorine-19 NMR Spectra

Figure S4. ^{19}F NMR spectra of Cu[$(CF_3)_8$T(*p*-MeP)C]: (a) the full range, (b) expanded views of the peaks, and (c) the ^{19}F-^{19}F COSY.

(a)



(b)


6F
12F
-50.7
-50.8
-50.9
-51.0
-51.1
-51.2
-51.3
-51.4
ppm
6F
-54.95
-55.00
-55.05
-55.10
-55.15
-55.20
-55.25
ppm

(c)

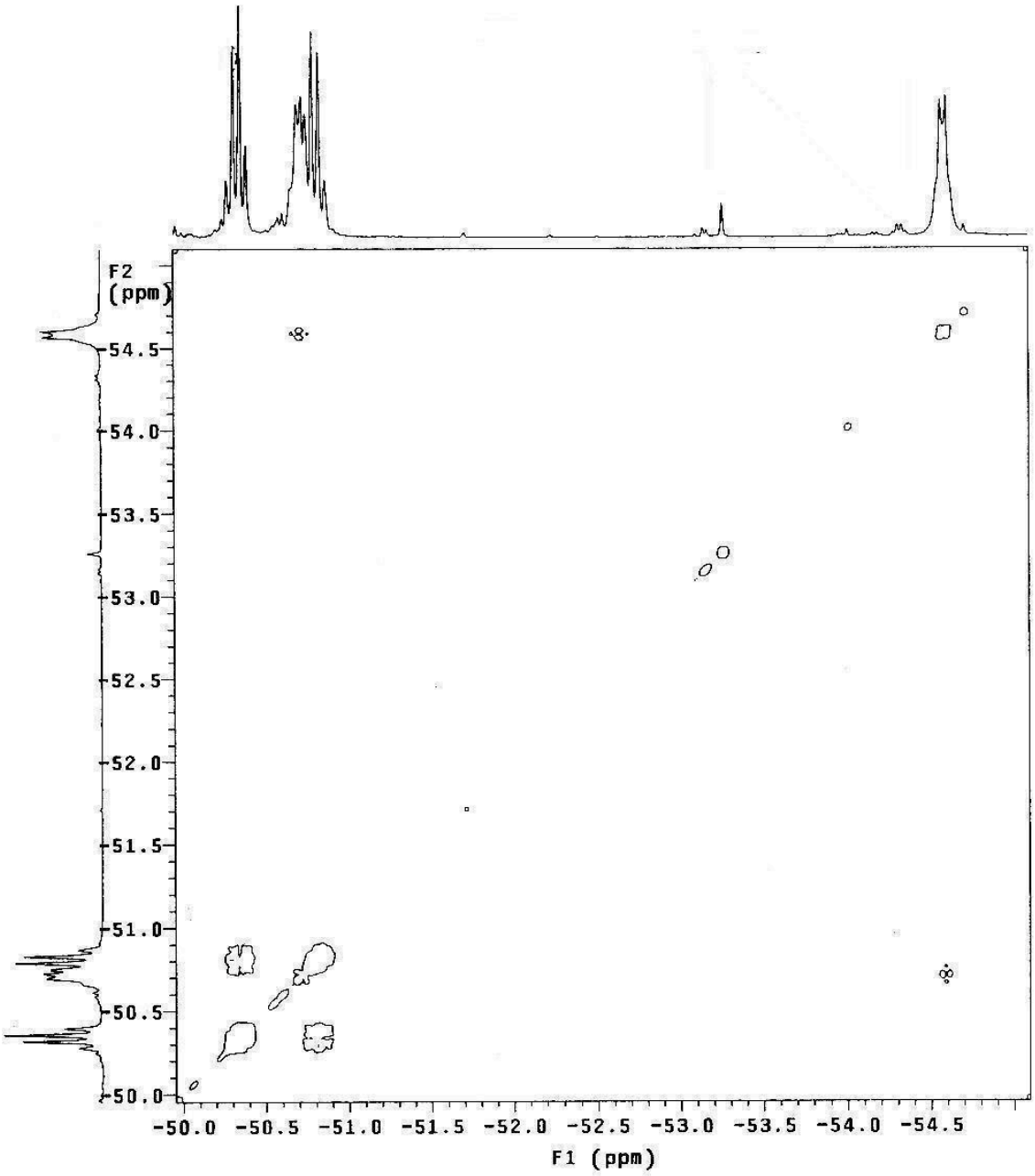
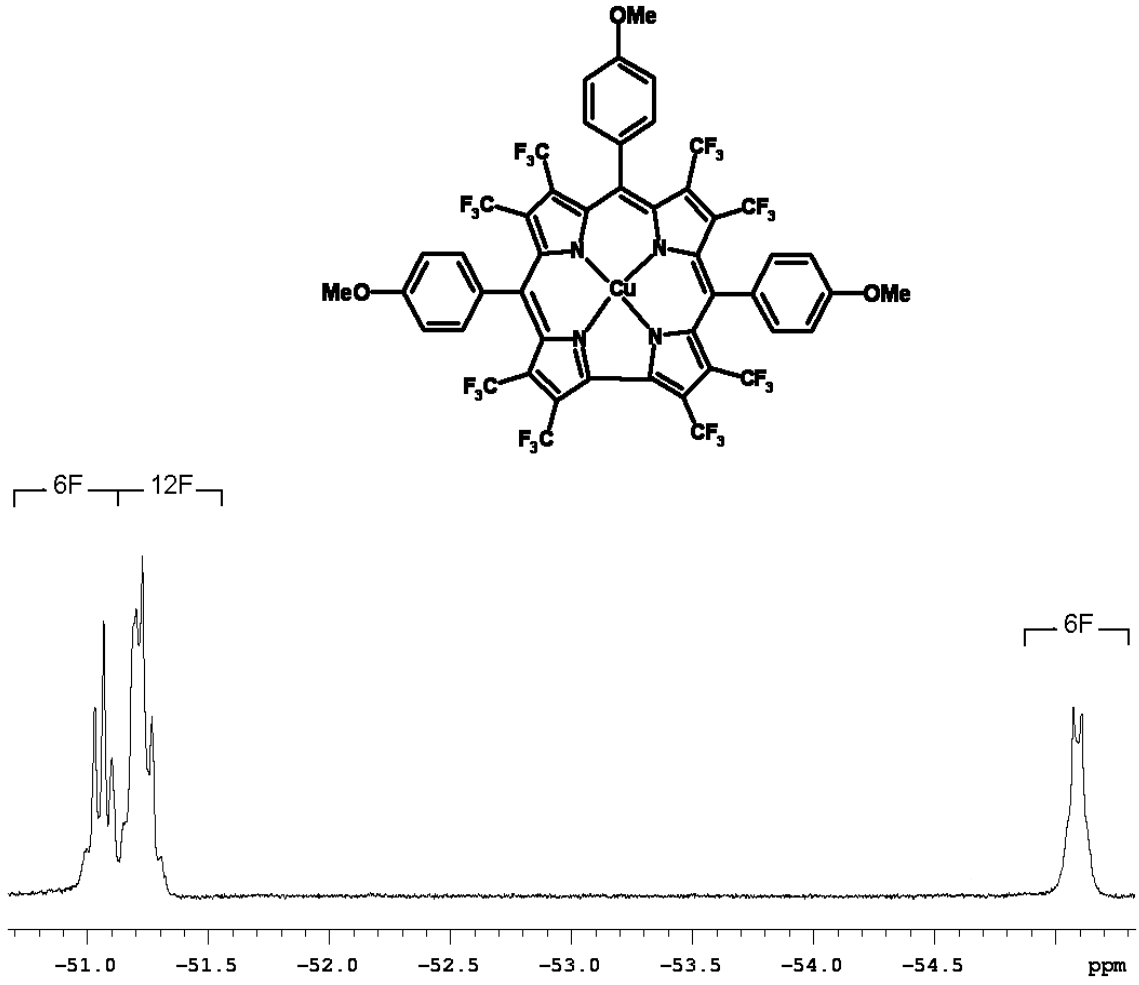
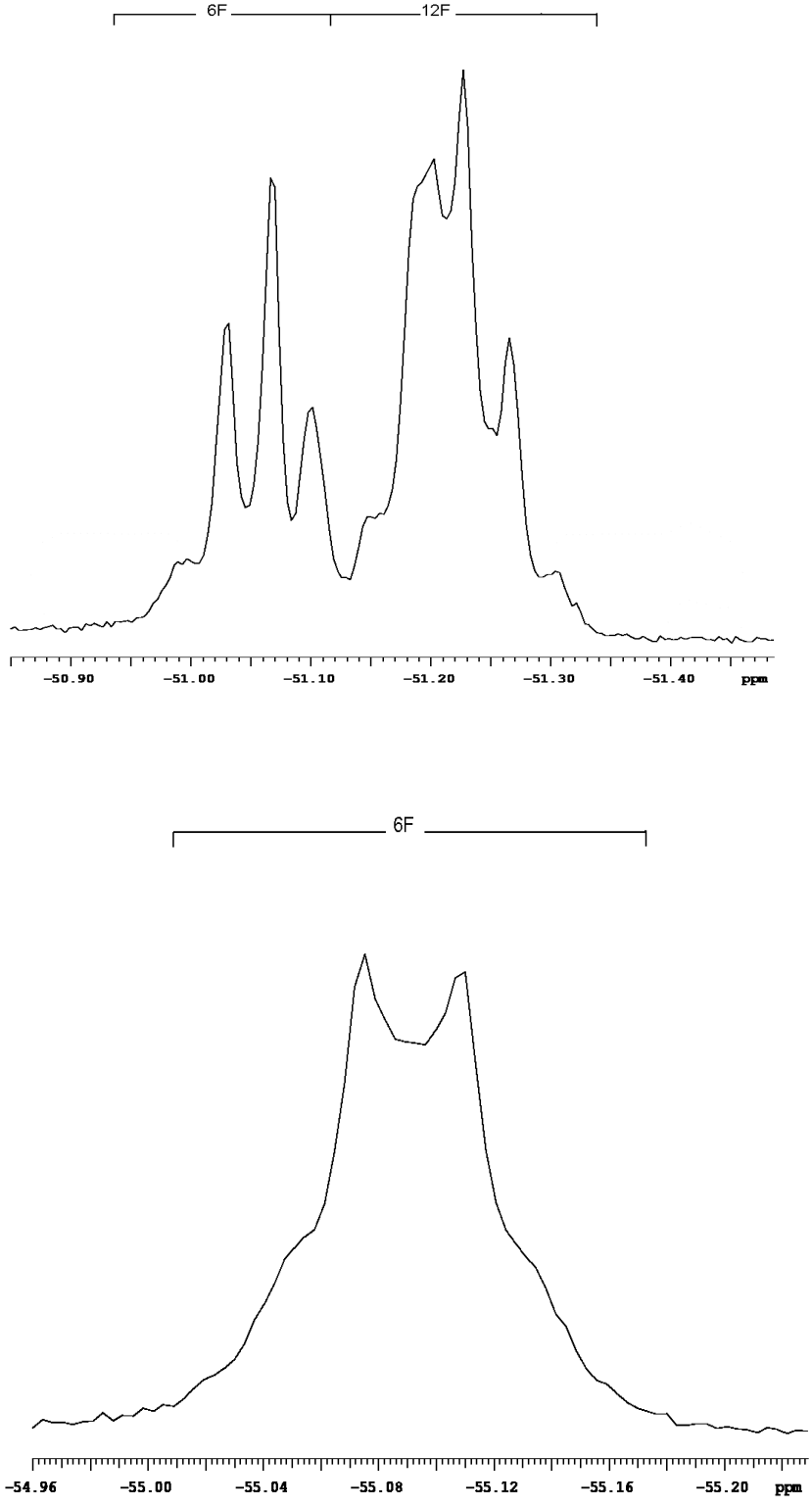

F2
(ppm)
-54.5
-54.0
-53.5
-53.0
-52.5
-52.0
-51.5
-51.0
-50.5
-50.0
-50.0 -50.5 -51.0 -51.5 -52.0 -52.5 -53.0 -53.5 -54.0 -54.5
F1 (ppm)

Figure S5. ^{19}F NMR spectra of Cu[$(CF_3)_8$T(*p*-OMeP)C]: (a) the full range, (b) expanded views of the peaks, and (c) the ^{19}F-^{19}F COSY.

(a)



(b)


6F
12F
-50.90
-51.00
-51.10
-51.20
-51.30
-51.40
ppm
6F
-54.96
-55.00
-55.04
-55.08
-55.12
-55.16
-55.20
ppm

(c)

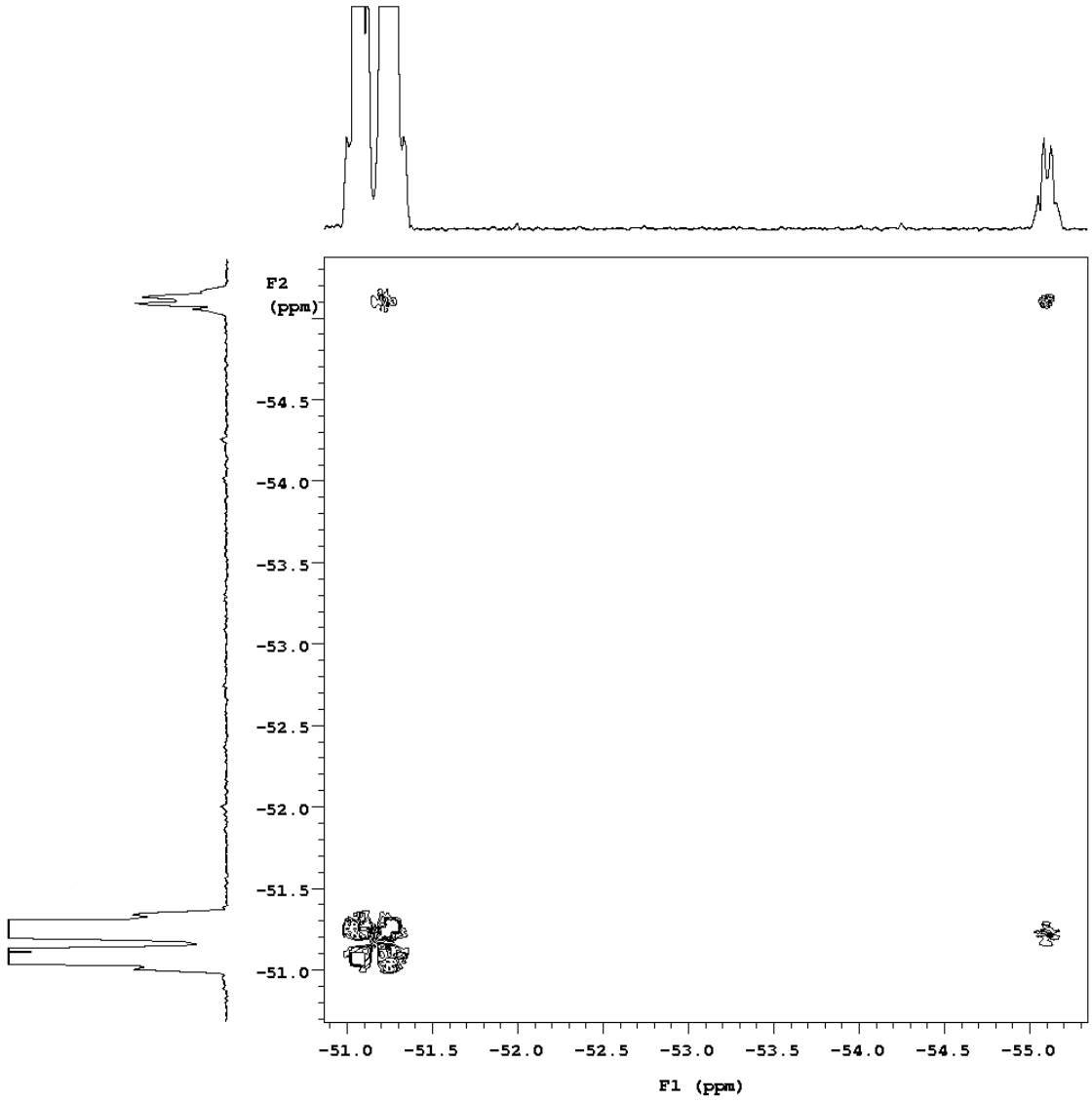
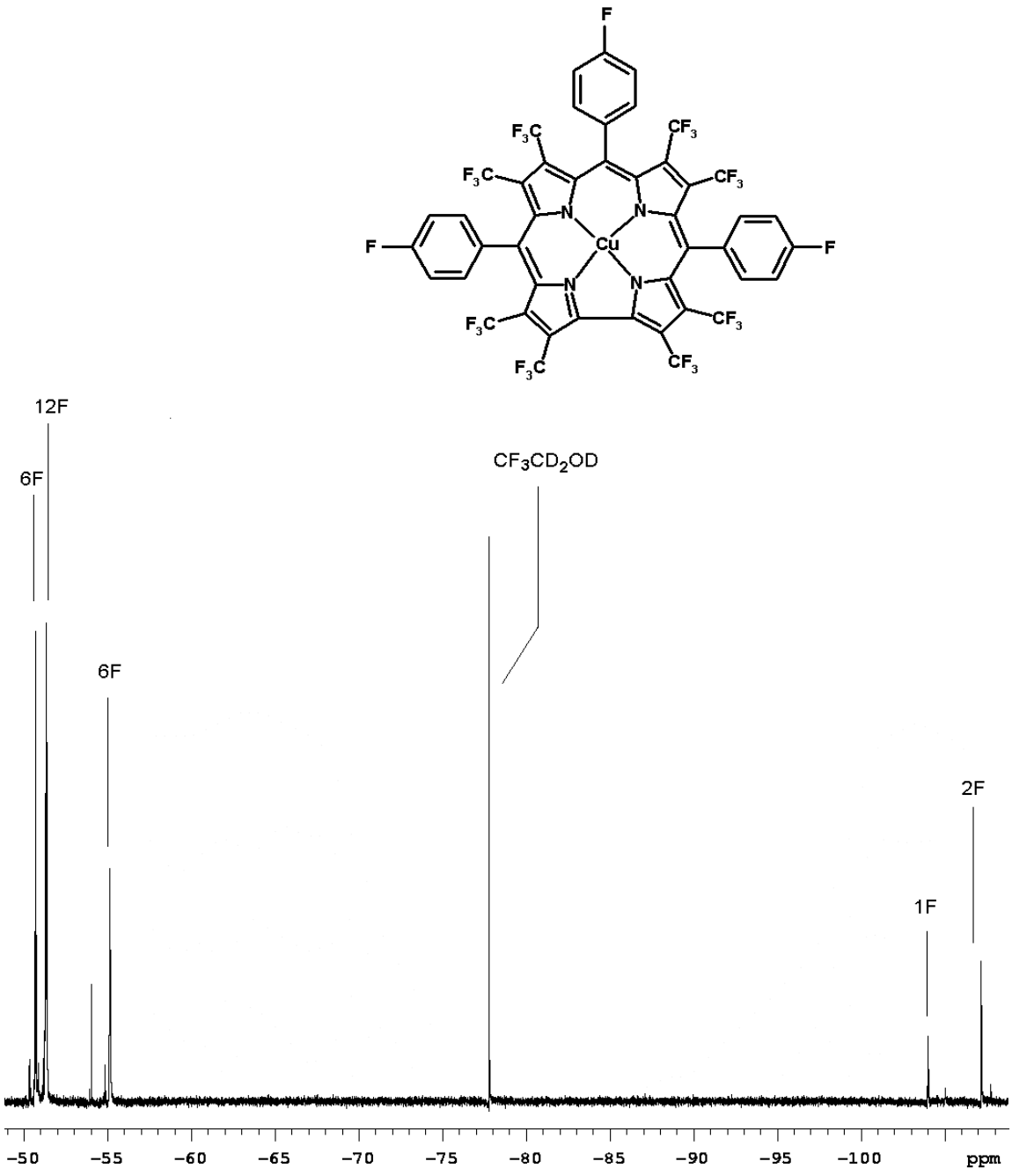
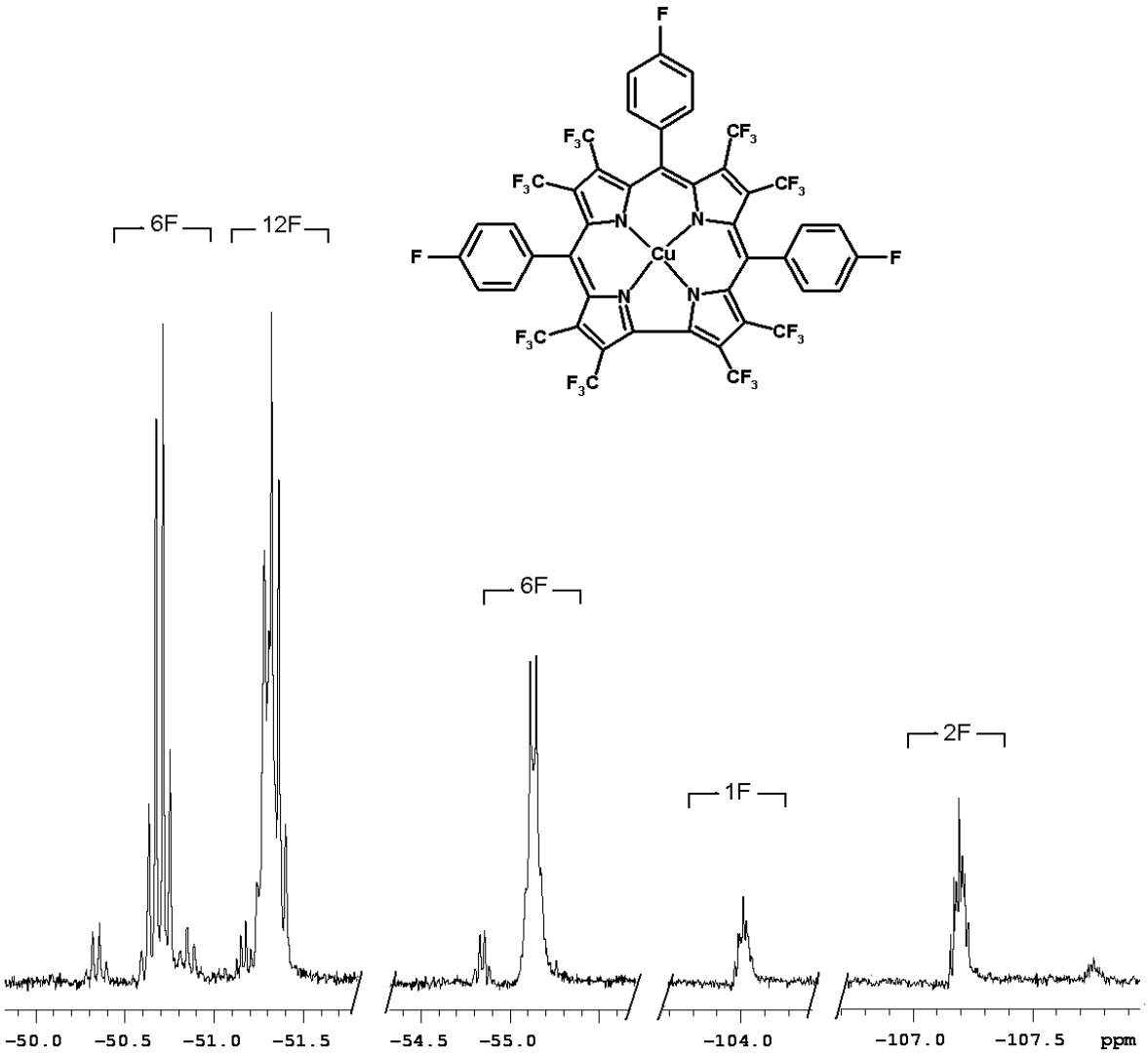

F2
(ppm)
-54.5
-54.0
-53.5
-53.0
-52.5
-52.0
-51.5
-51.0
-51.0
-51.5
-52.0
-52.5
-53.0
-53.5
-54.0
-54.5
-55.0
F1 (ppm)

Figure S6. ^{19}F NMR spectra of Cu[$(CF_3)_8$T(*p*-F-P)C]: (a) the full range, (b) (i) and (ii) are expanded views of the peaks, and (c) the ^{19}F-^{19}F COSY of the region between -55.2 and -50.5 ppm.

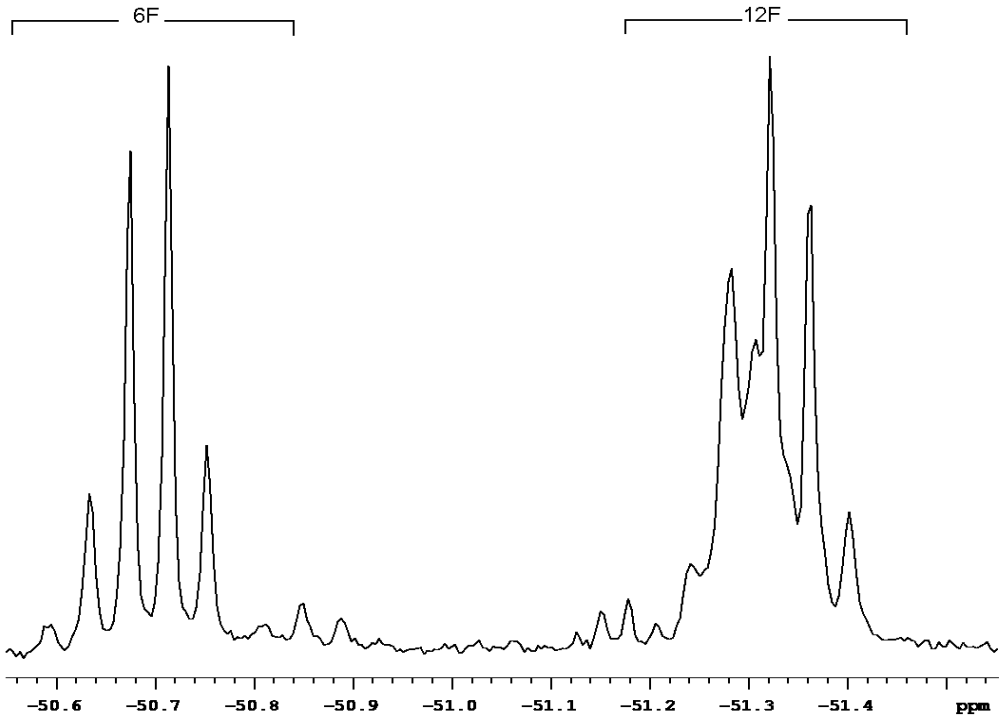
(a)

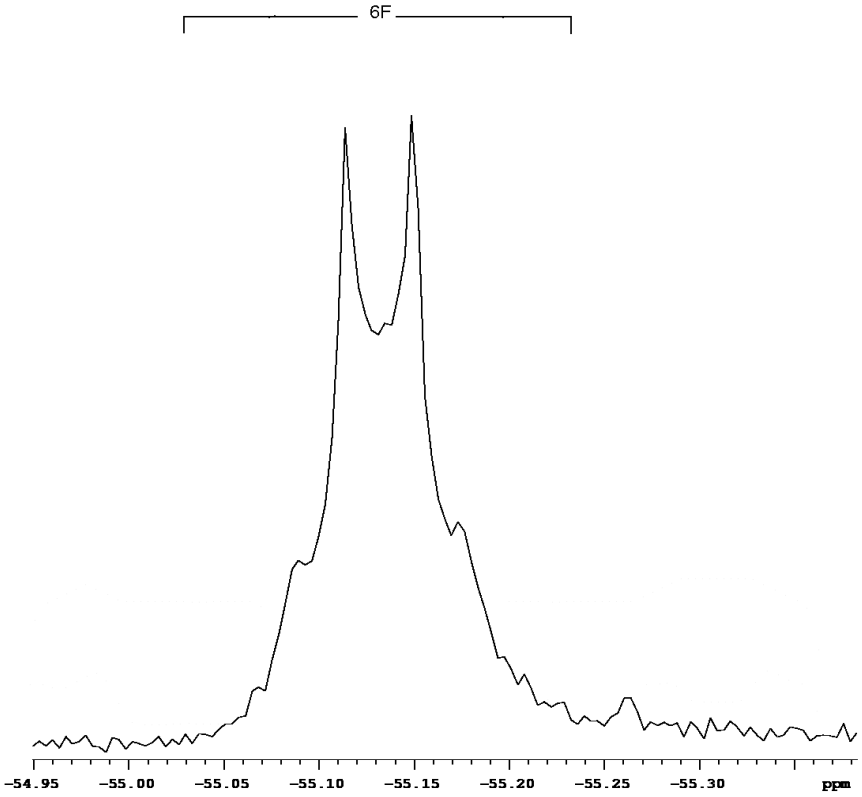


(b) (i)

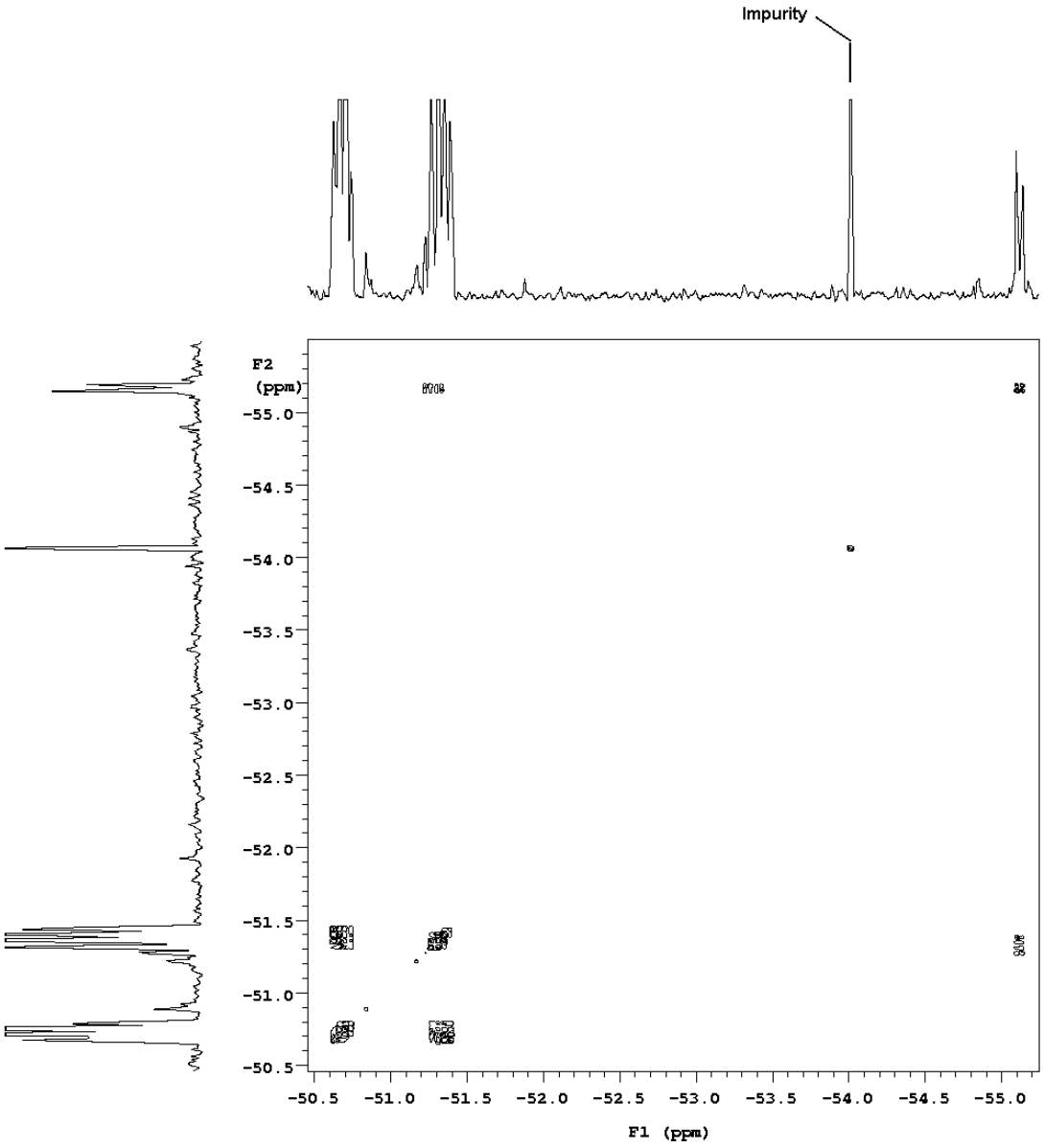

F
F3C
CF3
F3C
CF3
N
N
Cu
F
F
N
N
F3C
CF3
F3C
CF3
6F
12F
6F
1F
2F
−50.0
−50.5
−51.0
−51.5
−54.5
−55.0
−104.0
−107.0
−107.5
ppm

(b) (ii)


6F
12F
-50.6
-50.7
-50.8
-50.9
-51.0
-51.1
-51.2
-51.3
-51.4
ppm


6F
-54.95
-55.00
-55.05
-55.10
-55.15
-55.20
-55.25
-55.30
ppm

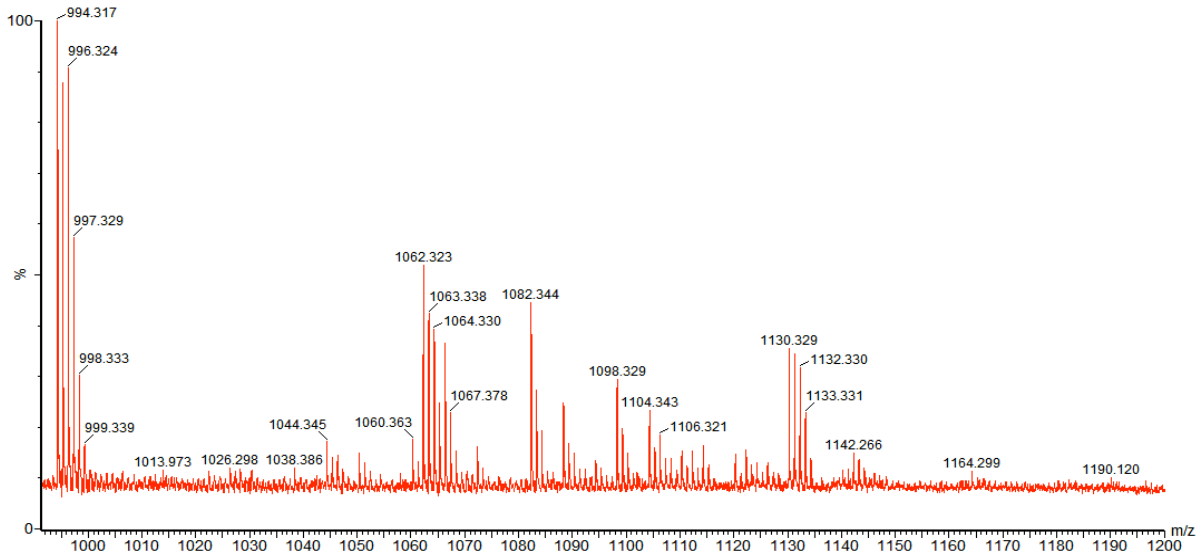
(c)


Impurity
F2
(ppm)
-55.0
-54.5
-54.0
-53.5
-53.0
-52.5
-52.0
-51.5
-51.0
-50.5
-50.5
-51.0
-51.5
-52.0
-52.5
-53.0
-53.5
-54.0
-54.5
-55.0
F1 (ppm)

Mass Spectra

Figure S7. Mass spectra of Cu[$(CF_3)_8$TPC]: (a) the full range, (b) an expanded view of isotopomers with inserted theoretical mass spectrum.

(a)



(b)

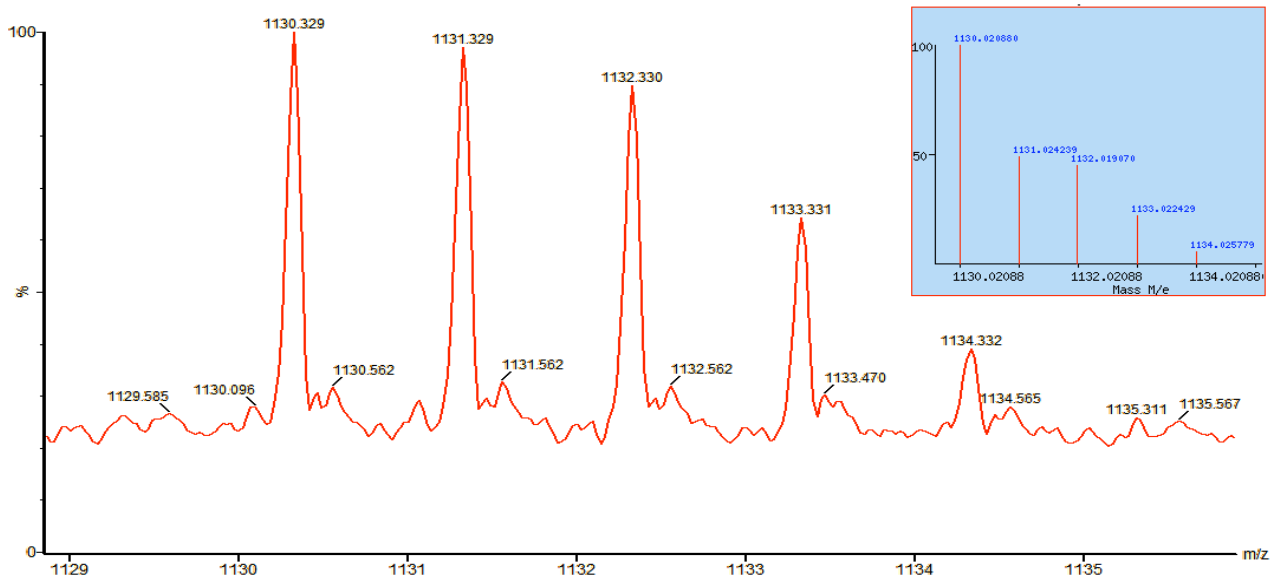
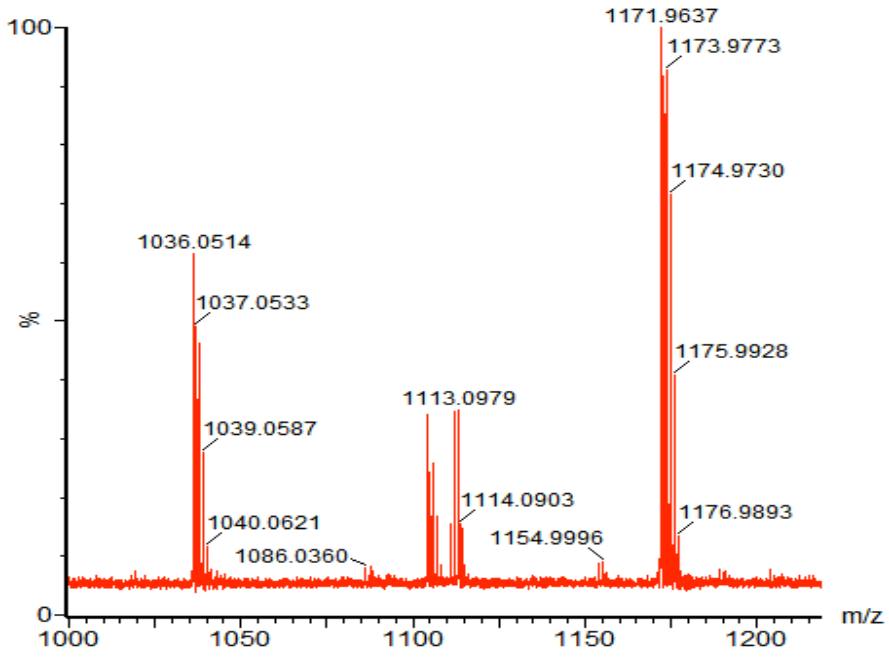


Figure S8. Mass spectra of Cu[$(CF_3)_8$T(*p*-MeP)C]: (a) the full range, (b) an expanded view of isotopomers with inserted theoretical mass spectrum.

(a)



(b)

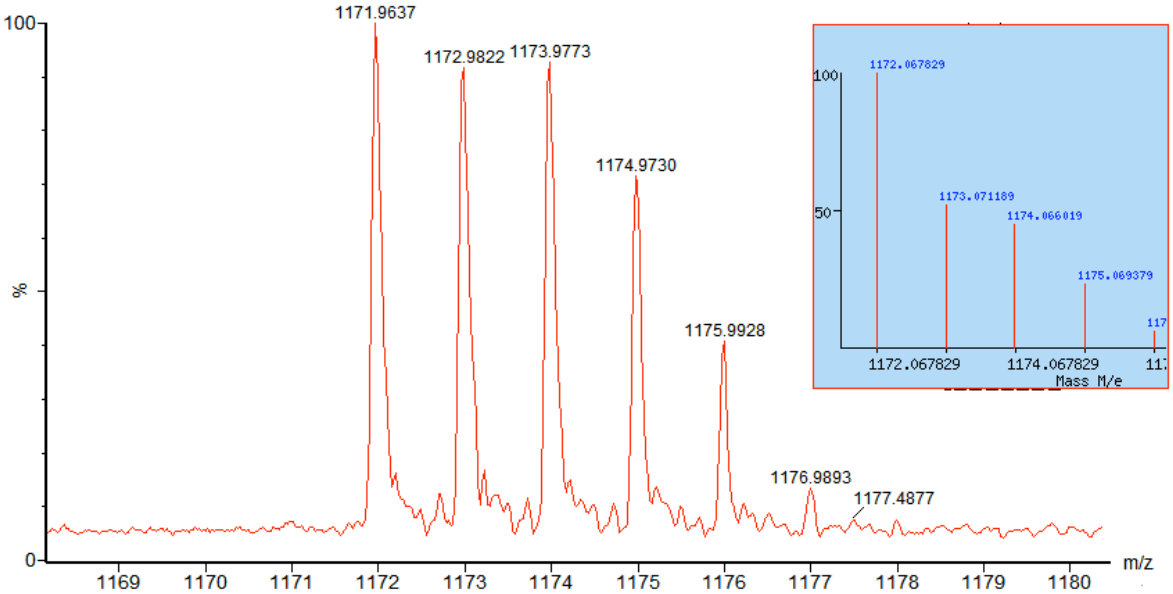
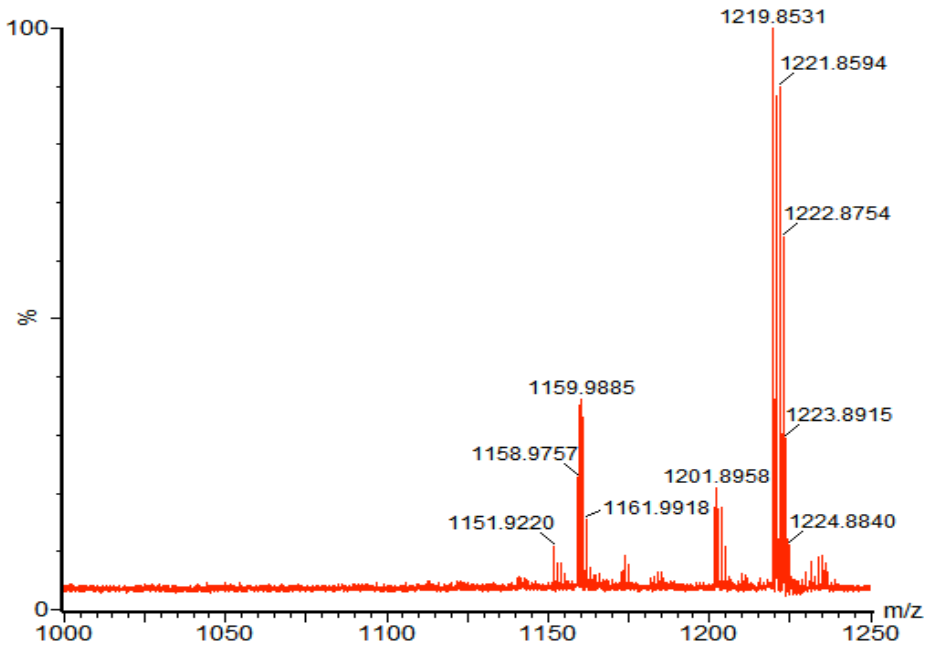


Figure S9. Mass spectra of Cu[$(CF_3)_8$T(*p*-OMeP)C]: (a) the full range, (b) an expanded view of isotopomers with inserted theoretical mass spectrum.

(a)



(b)

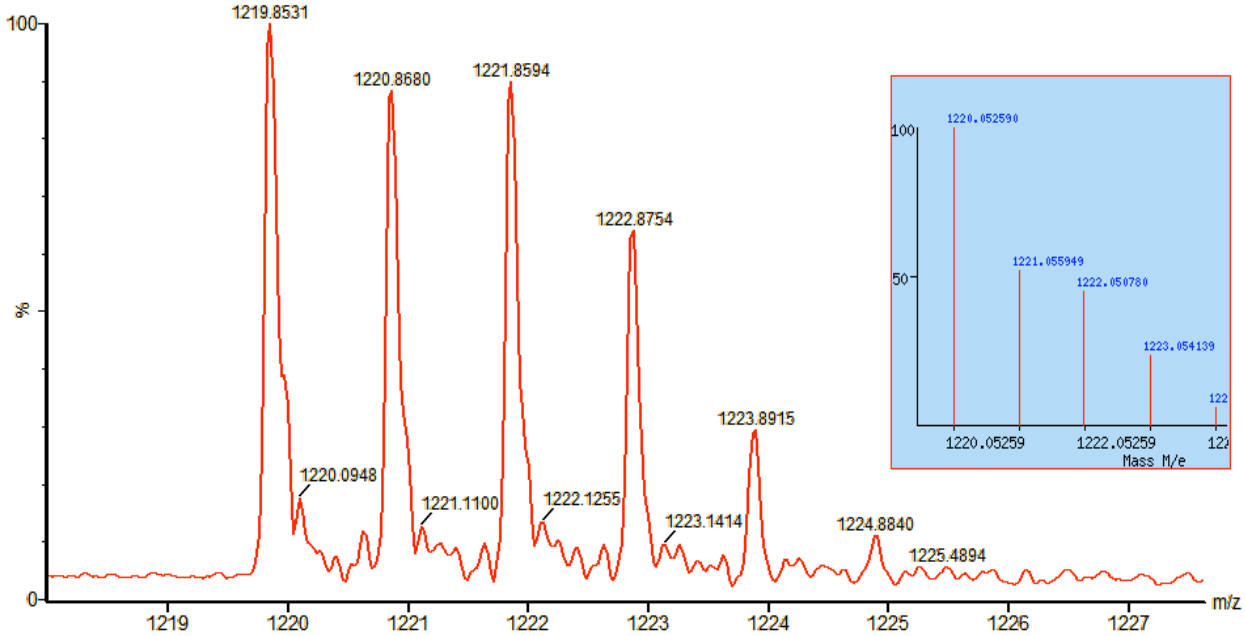
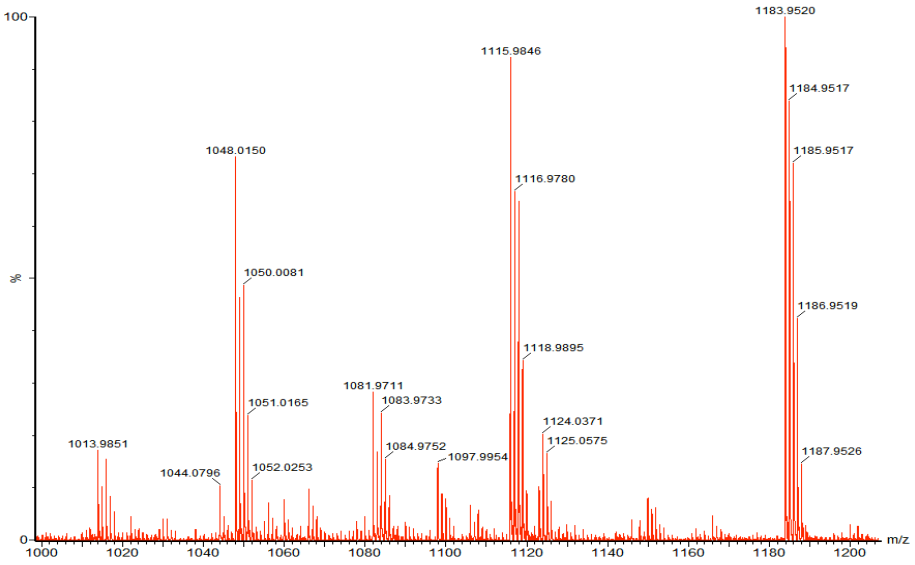
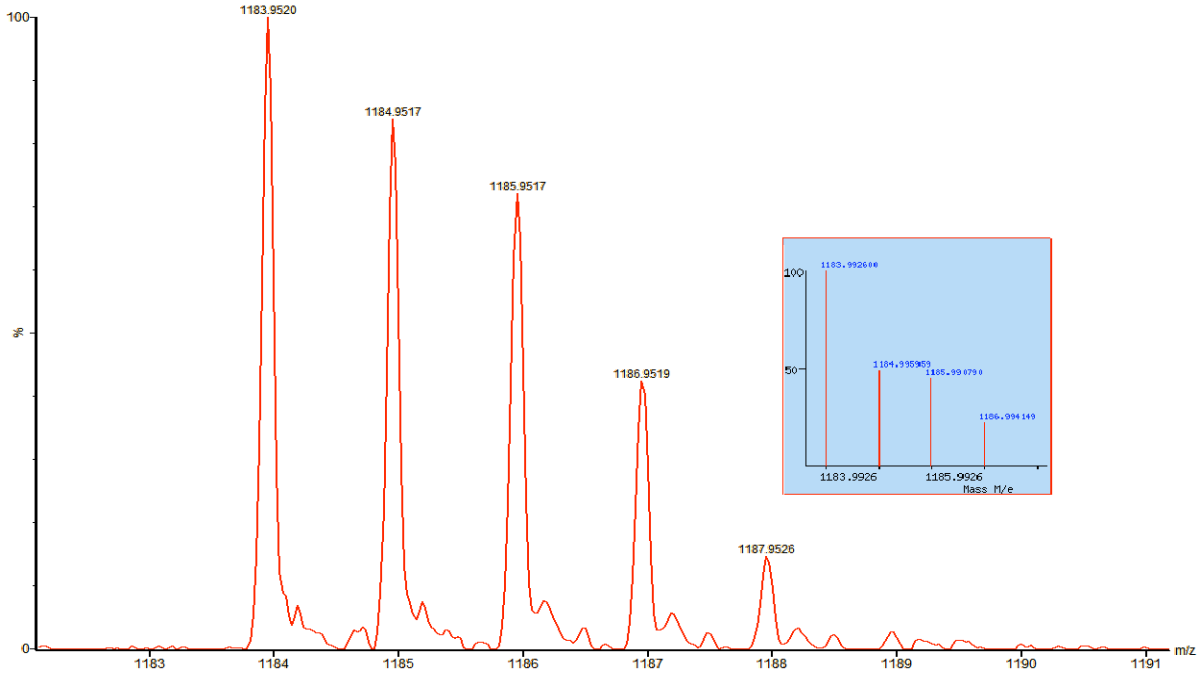


Figure S10. Mass spectra of Cu[$(CF_3)_8$T(*p*-FP)C]: (a) the full range, (b) an expanded view of isotopomers with inserted theoretical mass spectrum.

(a)

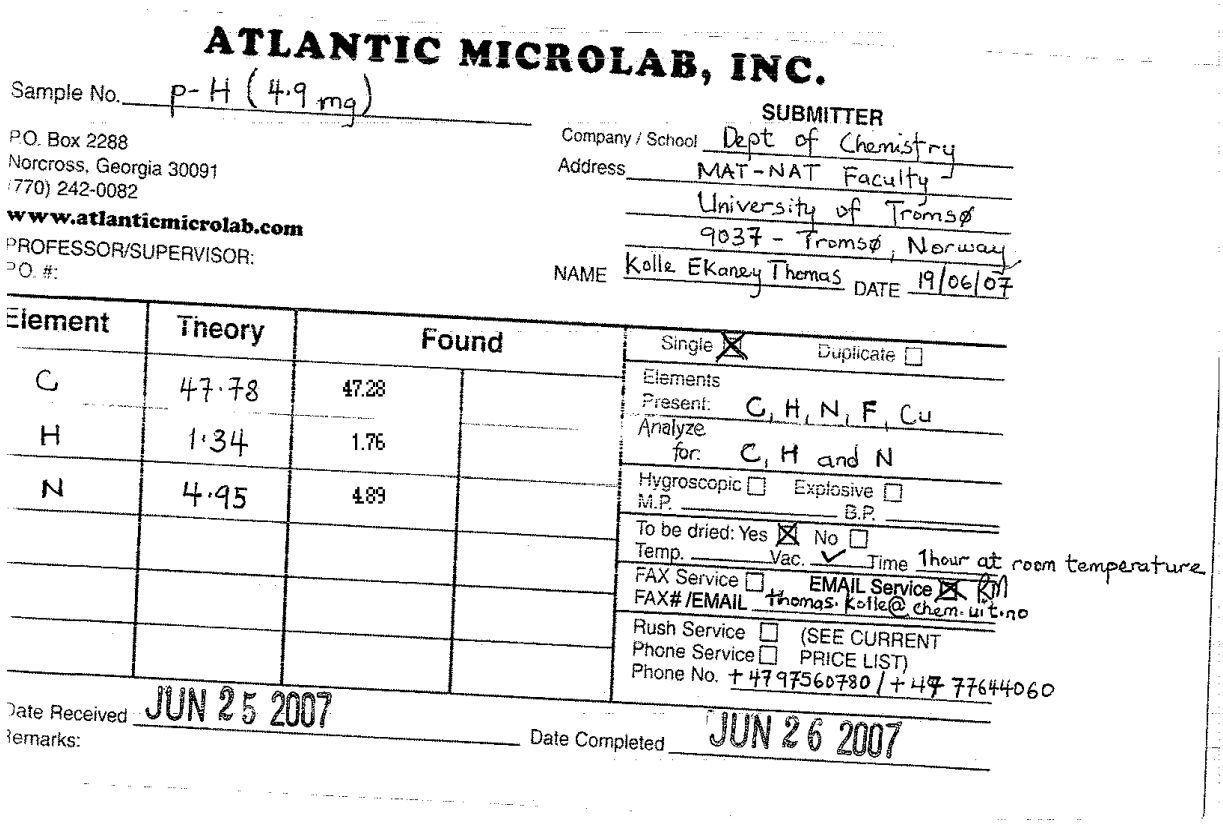


(b)



Elemental Analyses

Figure S11. Elemental Composition of $Cu[(CF_3)_8TPC]$



ATLANTIC MICROLAB, INC.

Sample No. p-H (4.9 mg)

P.O. Box 2288
Norcross, Georgia 30091
(770) 242-0082
www.atlanticmicrolab.com
PROFESSOR/SUPERVISOR:
P.O. #:

SUBMITTER
Company / School Dept of Chemistry
Address MAT-NAT Faculty
University of Tromsø
9037 - Tromsø, Norway
NAME Kolle Ekaney Thomas DATE 19/06/07

Element	Theory	Found	
C	47.78	47.28	
H	1.34	1.76	
N	4.95	4.89	

Single ☒ Duplicate ☐
Elements Present: C, H, N, F, Cu
Analyze for: C, H and N
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☒ No ☐
Temp. _____ Vac. ✓ Time 1hour at room temperature
FAX Service ☐ EMAIL Service ☒ KM
FAX# /EMAIL thomas.kolle@chem.uit.no
Rush Service ☐ (SEE CURRENT
Phone Service ☐ PRICE LIST)
Phone No. +4797560780 / +47 77644060

Date Received JUN 25 2007
Remarks:
Date Completed JUN 26 2007

Figure S12. Elemental Composition of Cu[$(CF_3)_8$T(*p*-MeP)C]

ATLANTIC MICROLAB, INC.

Sample No. P-Me (5.1mg)

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PROFESSOR/SUPERVISOR:
P.O. #:

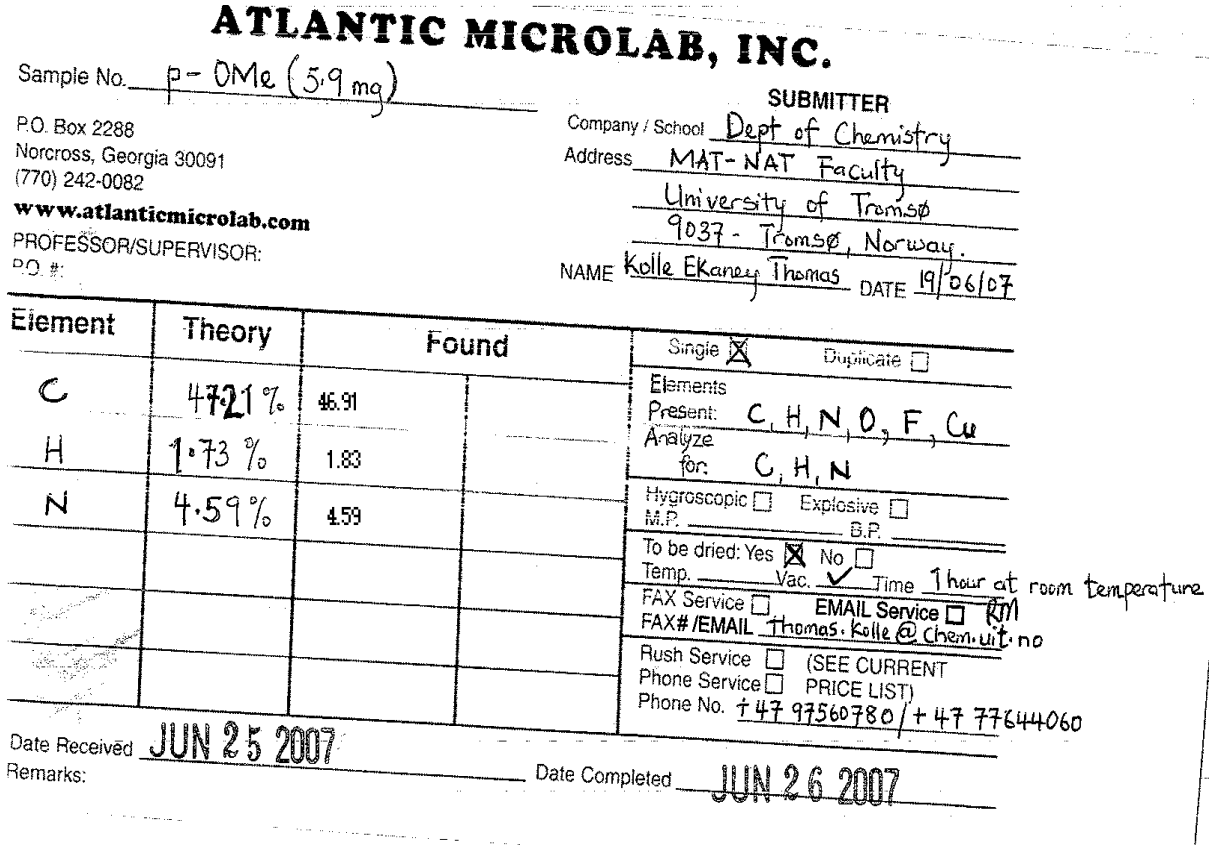
SUBMITTER
Company / School Dept of Chemistry
Address Maths & Natural Science Faculty
University of Tromsø
9037- Tromsø, NORWAY
NAME Kolle Ekaney Thomas DATE 27/04/2007
email: thomas.kolle@chem.uit.no

Element	Theory	Found	
C	49.14%	50.34	50.52
H	1.80%	2.25	2.22
N	4.78%	4.58	4.69
F	38.86%	38.50	
		NO CHARGE FOR DUPLICATES	

Single ☒ Duplicate ☐
Elements Present: C, H, N, F, Cu
Analyze for: C, H, N and F (if possible)
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
FAX Service ☐
FAX Phone # _____
Rush Service ☐ (SEE CURRENT
Phone Service ☒ PRICE LIST)
Phone No. +47 77644060 / +47 97560780

Date Received MAY 03 2007 Date Completed MAY 07 2007
Remarks:

Figure S13. Elemental Composition of Cu[$(CF_3)_8$T(*p*-OMeP)C]



ATLANTIC MICROLAB, INC.

Sample No. p-OMe (5.9 mg)

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Norcross, Georgia 30091
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PROFESSOR/SUPERVISOR:
P.O. #:

SUBMITTER
Company / School Dept of Chemistry
Address MAT-NAT Faculty
University of Tromsø
9037 - Tromsø, Norway.
NAME Kolle Ekaney Thomas DATE 19/06/07

Element	Theory	Found	
C	47.21 %	46.91	
H	1.73 %	1.83	
N	4.59 %	4.59	

Single ☒ Duplicate ☐
Elements Present: C, H, N, O, F, Cu
Analyze for: C, H, N
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☒ No ☐
Temp. _____ Vac. ✓ Time 1 hour at room temperature
FAX Service ☐ EMAIL Service ☐ RM
FAX# /EMAIL Thomas.Kolle@chem.uit.no
Rush Service ☐ (SEE CURRENT
Phone Service ☐ PRICE LIST)
Phone No. †47 97560780 / +47 77644060

Date Received JUN 25 2007
Remarks:
Date Completed JUN 26 2007

Figure S14. Elemental Composition of Cu[$(CF_3)_8$T(*p*-F-P)C]

ATLANTIC MICROLAB, INC.

Sample No. p-F₂(5.6mg)

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PROFESSOR/SUPERVISOR:
P.O. #:

SUBMITTER

Company / School Dept of Chemistry,MAT-NAT
Address University of Tromsø,
9037 Tromsø, Norway

NAME Kolle Ekaney Thomas DATE 03-06-08
thomas.kolle@chem.uit.no

Element	Theory	Found	
C	45.61 %	46.31	46.33
H	1.02 %	1.70	1.68
N	4.73 %	4.40	4.36
		NO CHARGE FOR DUPLICATES	

Single ☒ Duplicate ☐
Elements Present: C, H, N, F, Cu
Analyze for: C,H,N
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☑ No ☐
Temp. R.T Vac. ✓ Time 1 hour
FAX Service ☐ EMAIL Service ☒
FAX# /EMAIL thomas.kolle@chem.uit.no
Rush Service ☐ (SEE CURRENT PRICE LIST)
Phone Service ☒
Phone No. +47 77644060 / +47 77620910
+47 97560780

Date Received JUN 06 2008 Date Completed JUN 09 2008
Remarks: