

Supporting Information

KO^tBu-Promoted, Three-Component Domino Reaction of Arenes(indoles/phenols), C₆₀, and (Per/poly)fluoroarenes: Achieve Direct C-C Cross-Coupling of Fullerene with (Per/poly)fluoroarenes

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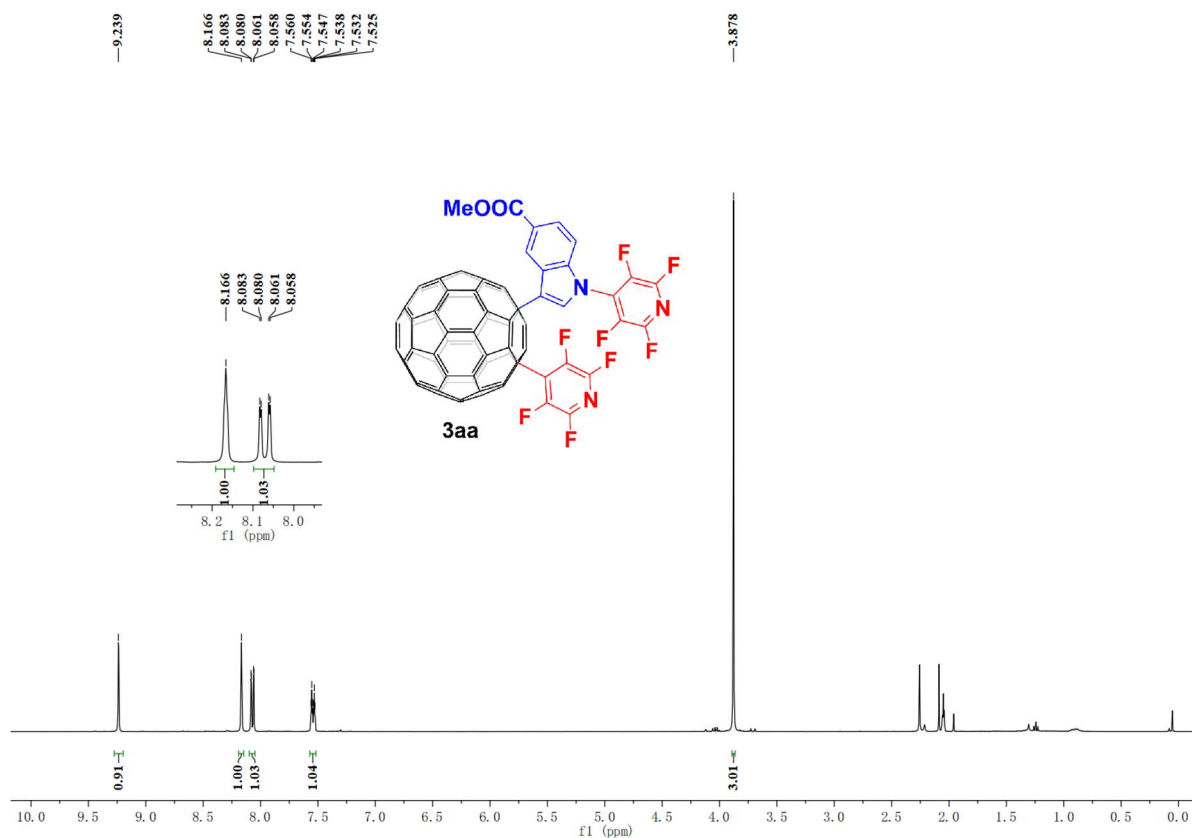
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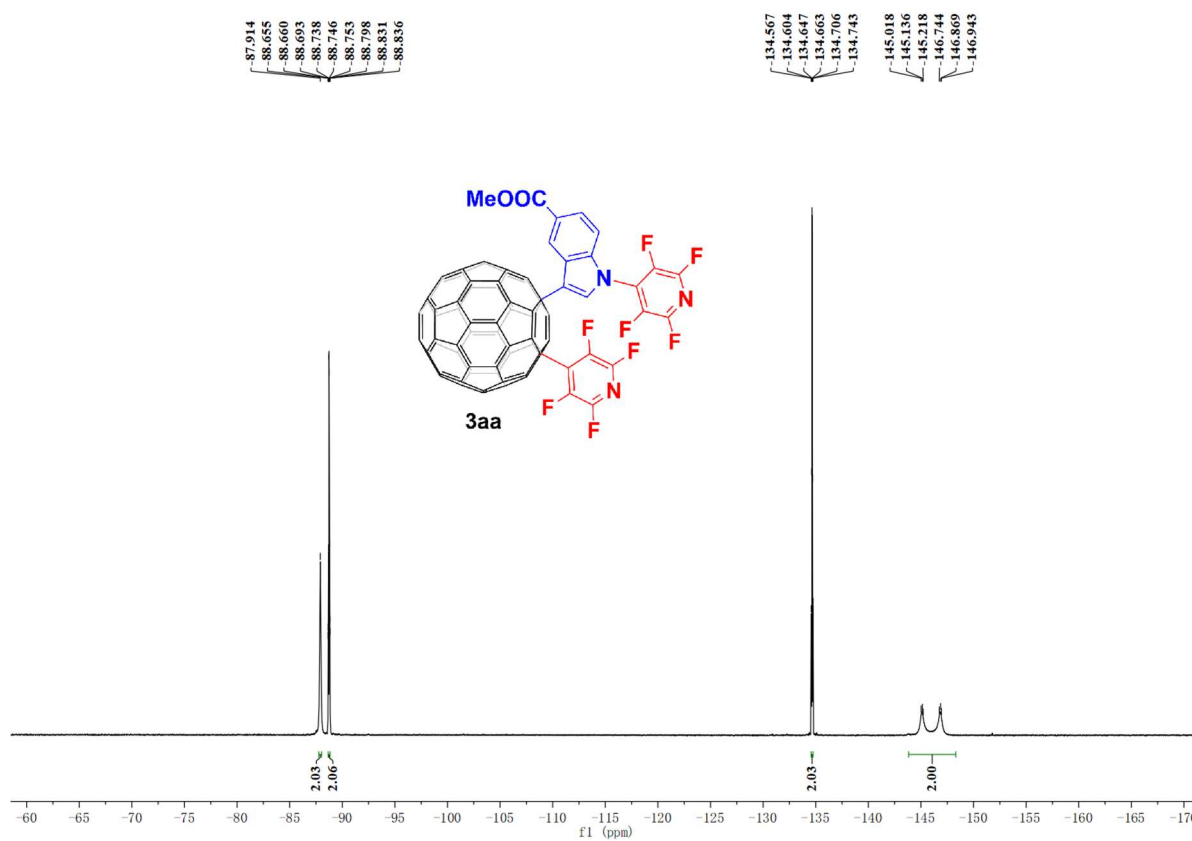
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1. NMR Spectra of 3aa-6ic

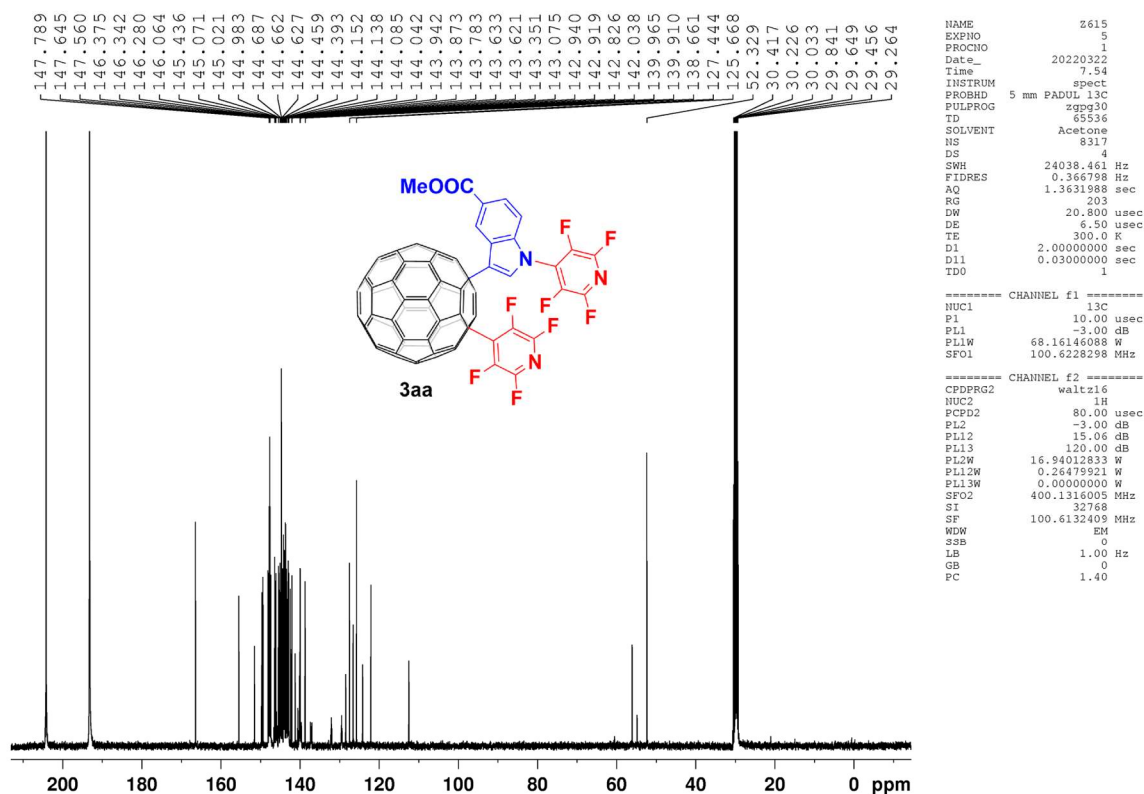
¹H NMR (400 MHz, CS₂/d₆-acetone) of compound 3aa



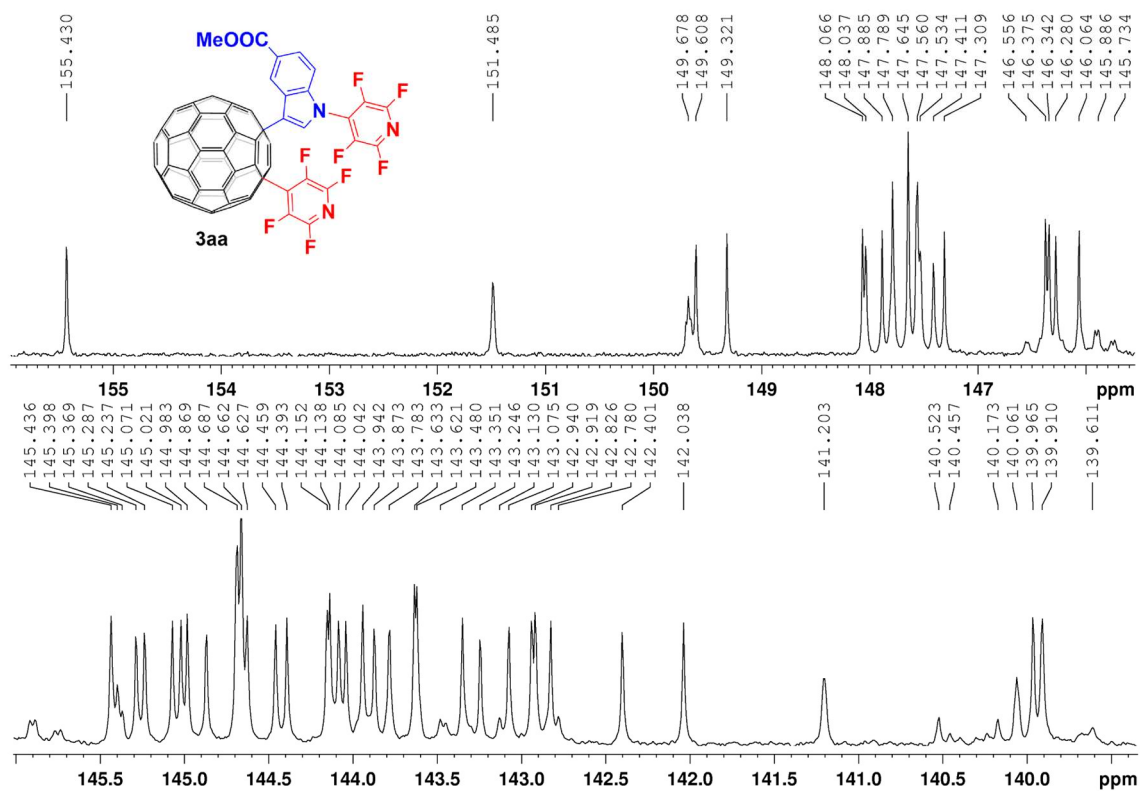
¹⁹F NMR (376 MHz, CS₂/d₆-acetone) of compound 3aa



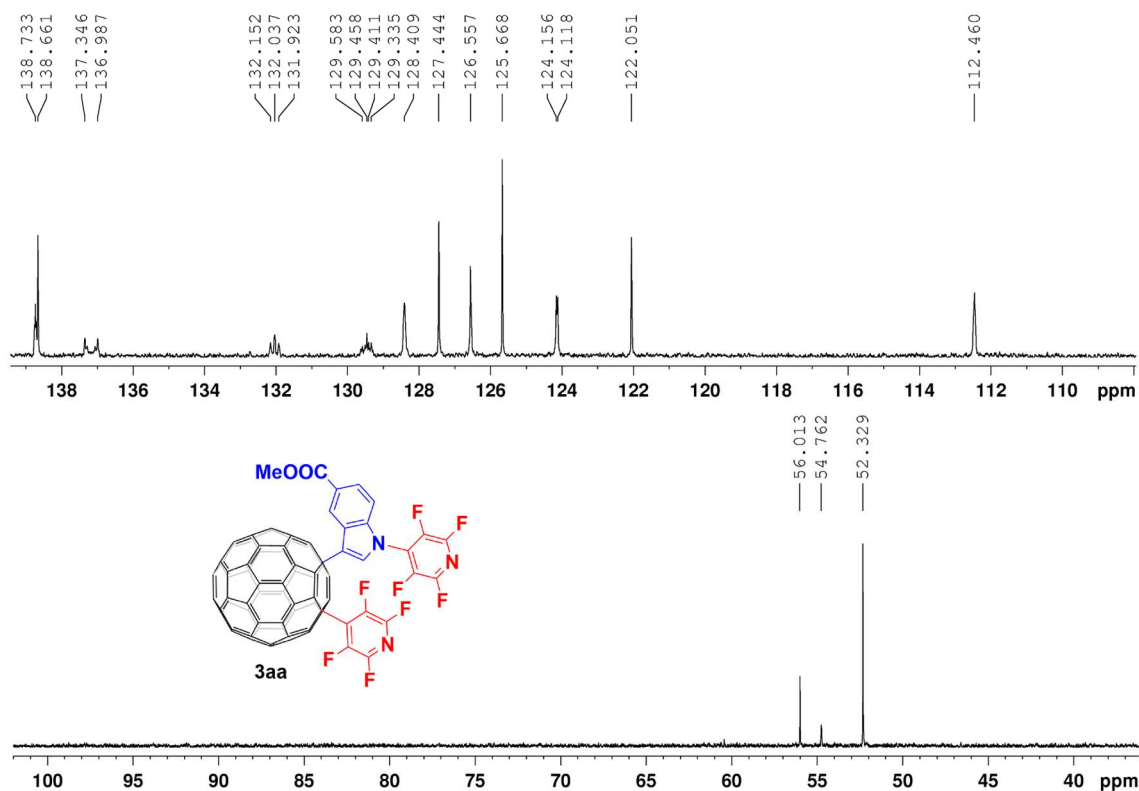
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3aa



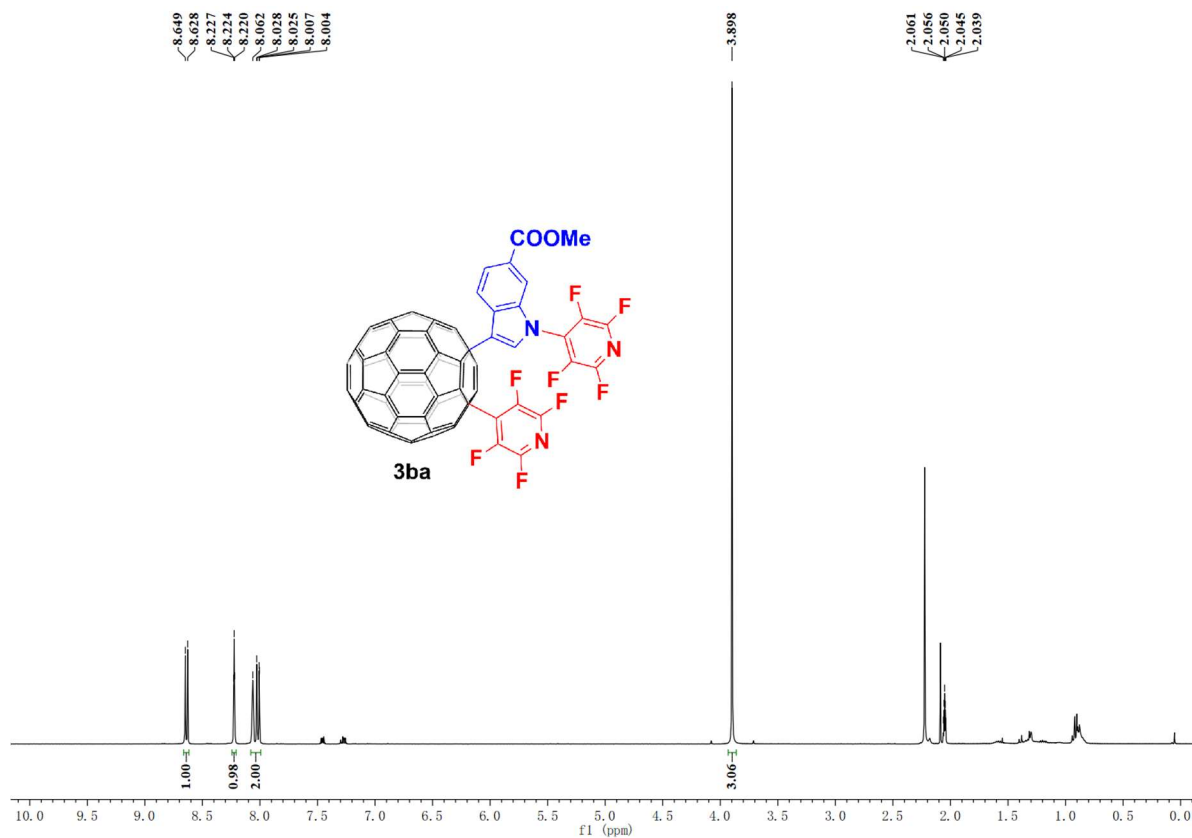
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3aa



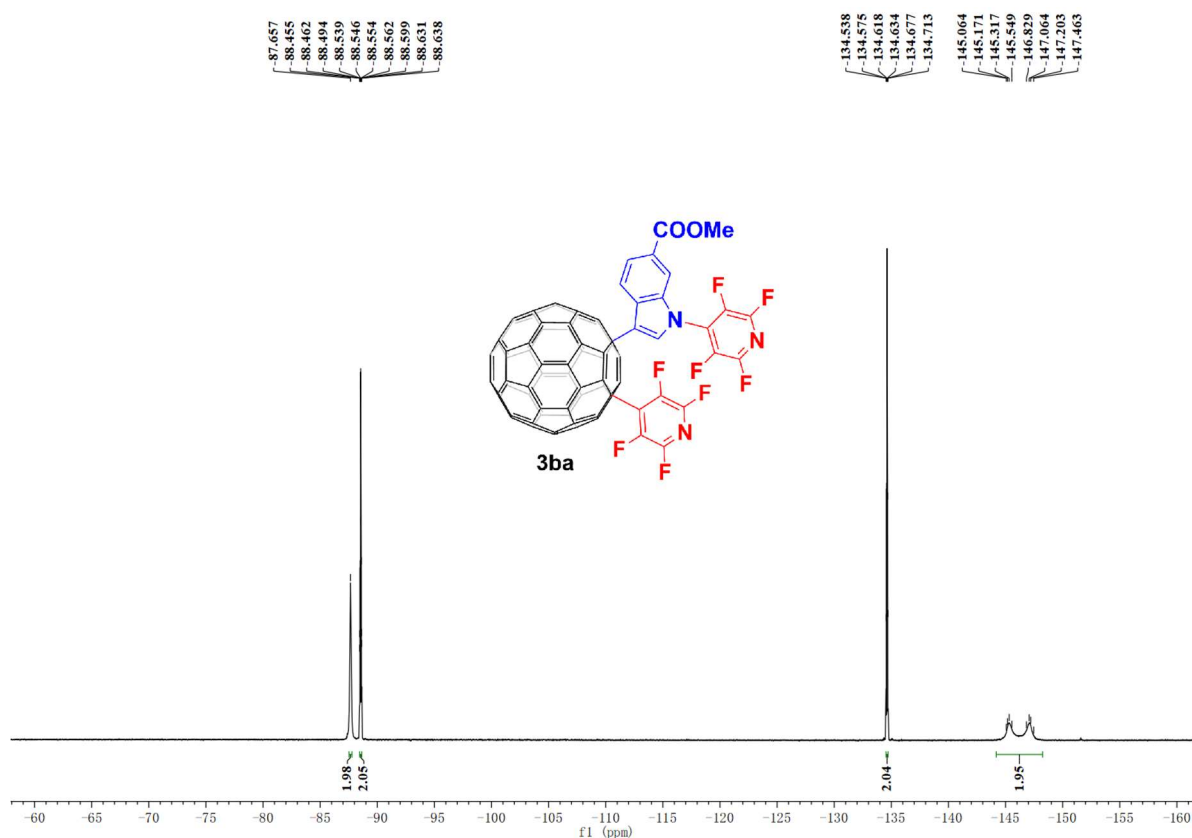
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3aa



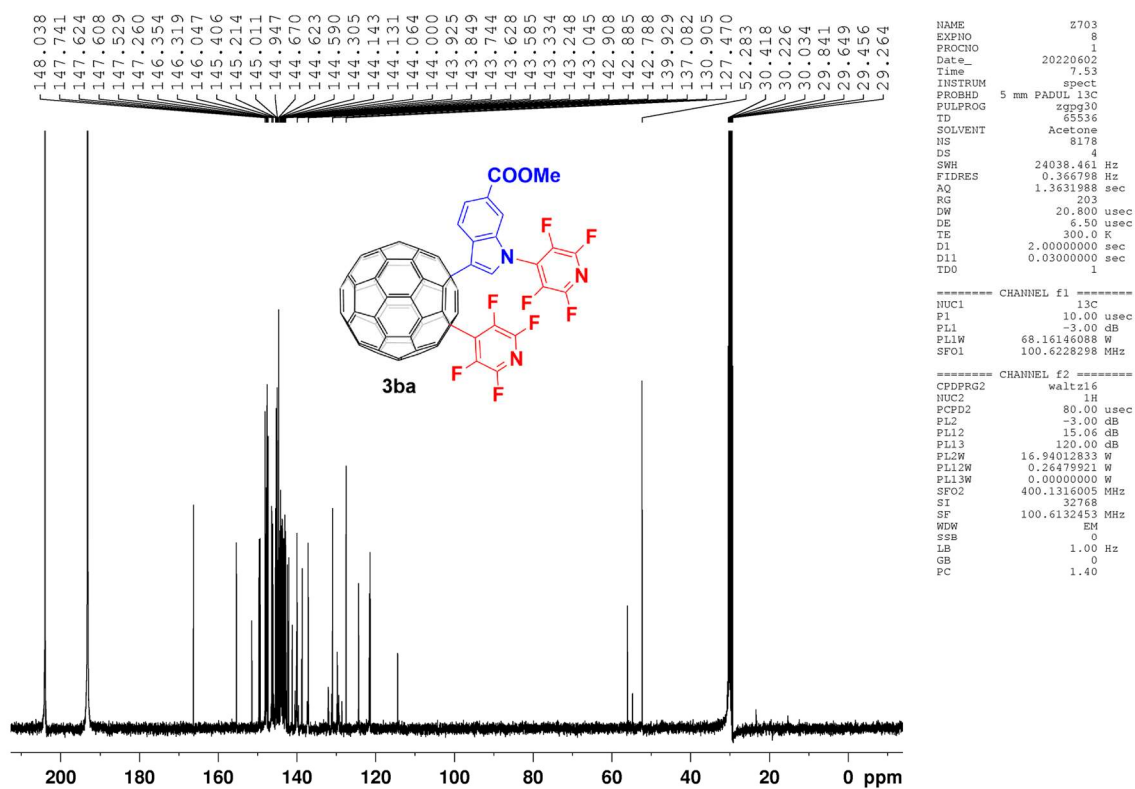
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 3ba



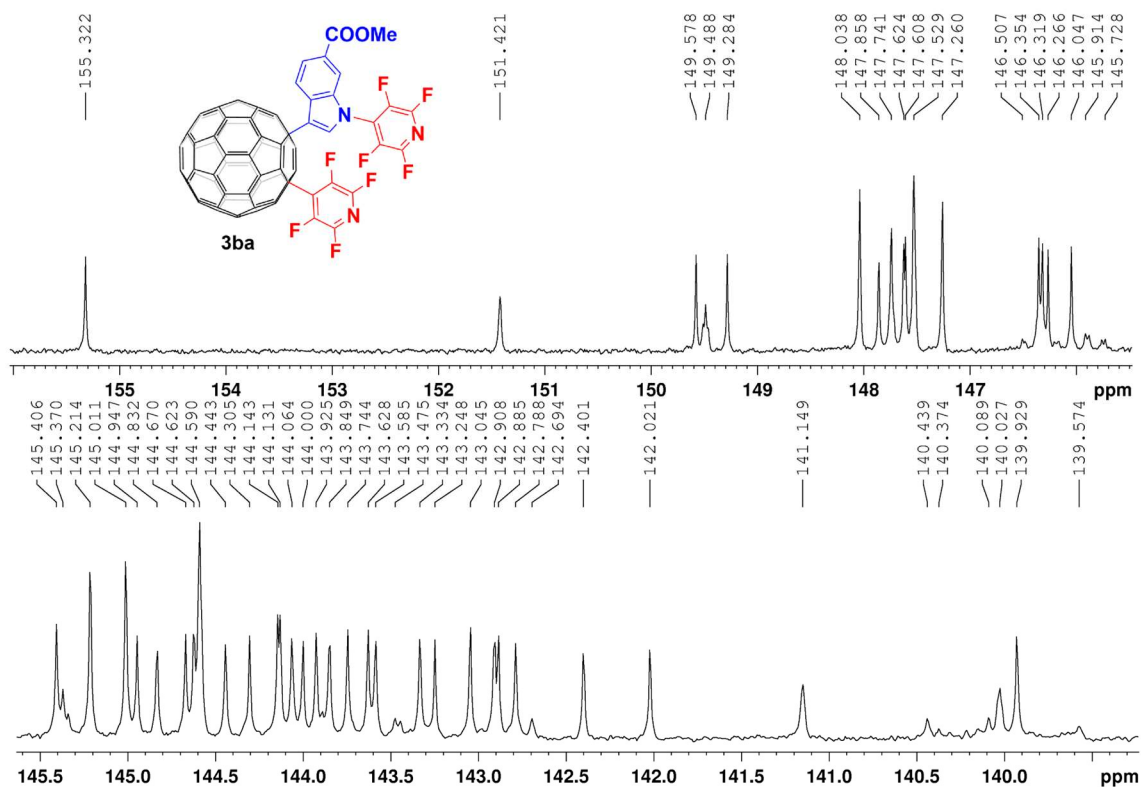
¹⁹F NMR (376 MHz, CS₂/d₆-acetone) of compound 3ba



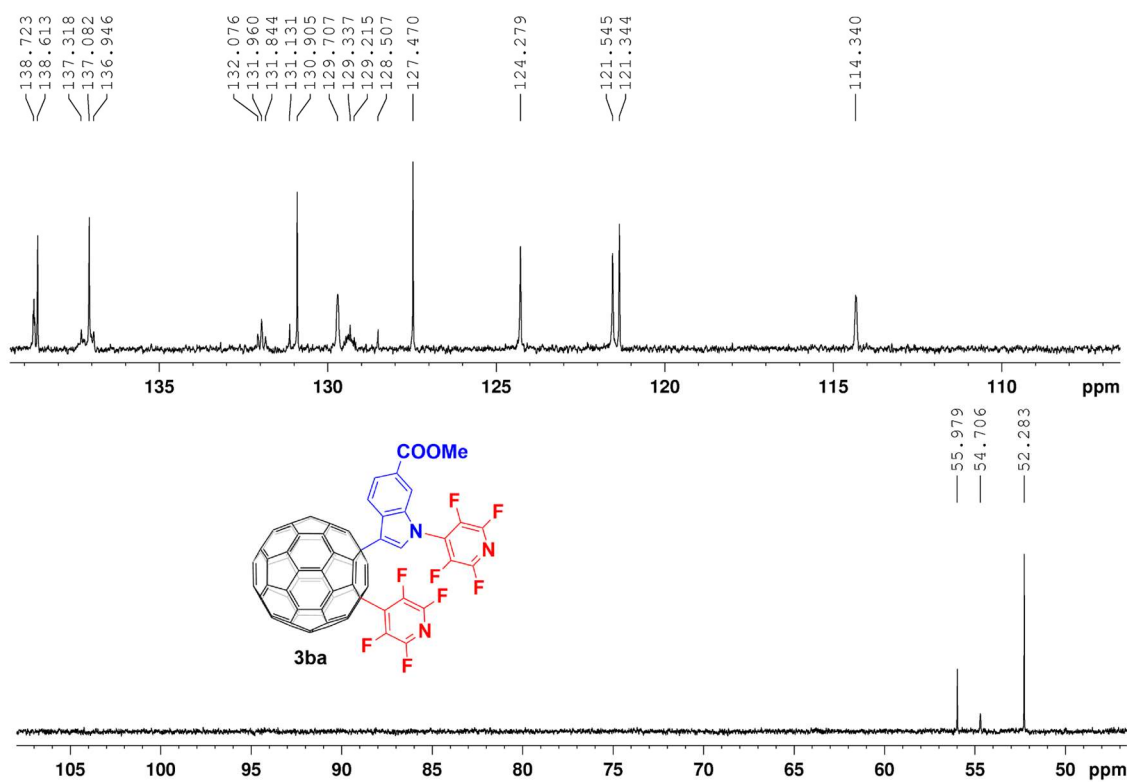
¹³C{¹H} NMR (100 MHz, CS₂/d₆-acetone) of compound 3ba



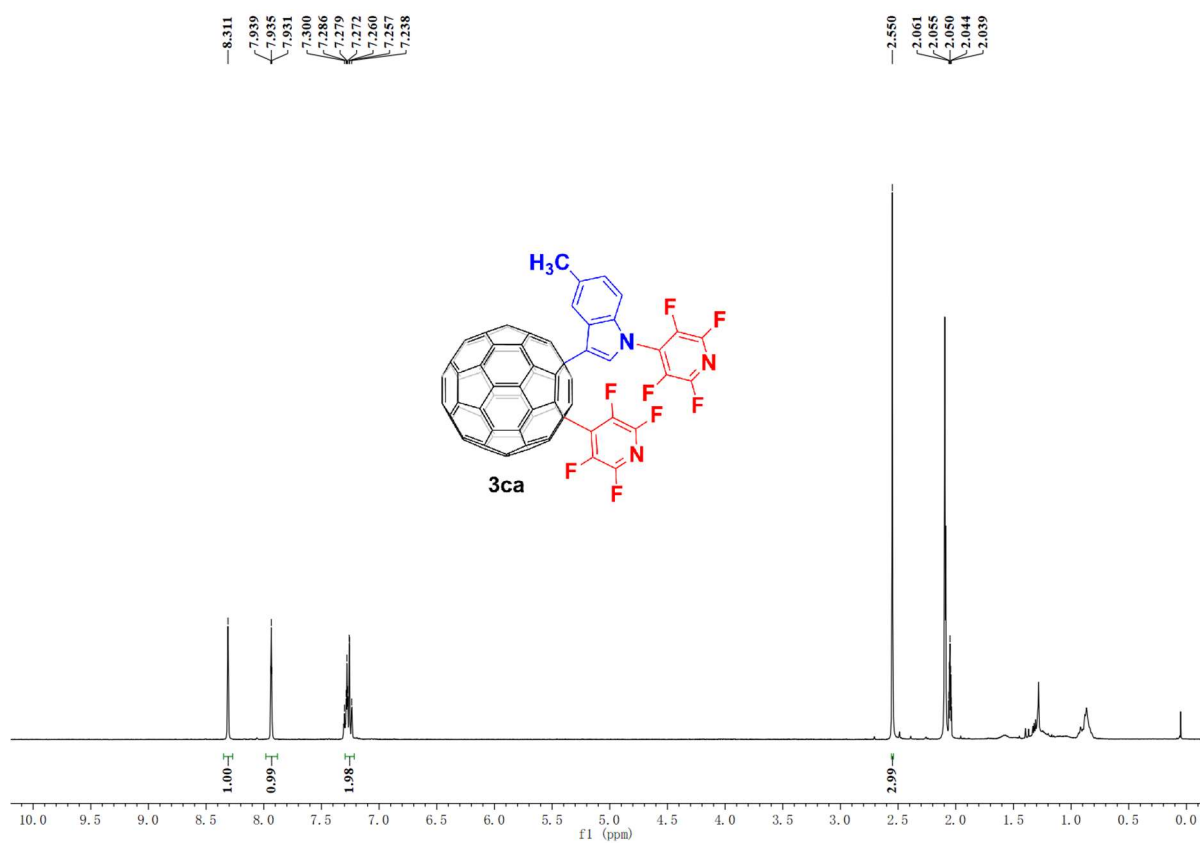
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3ba



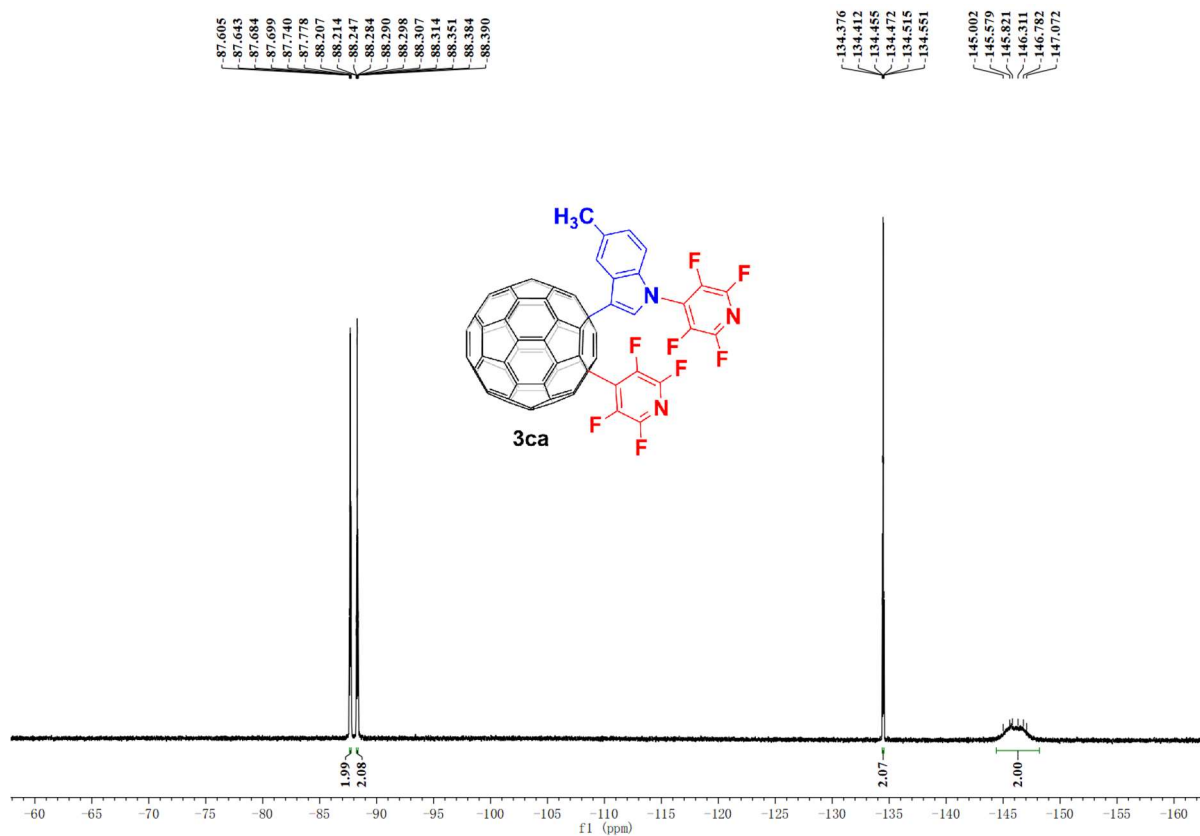
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3ba



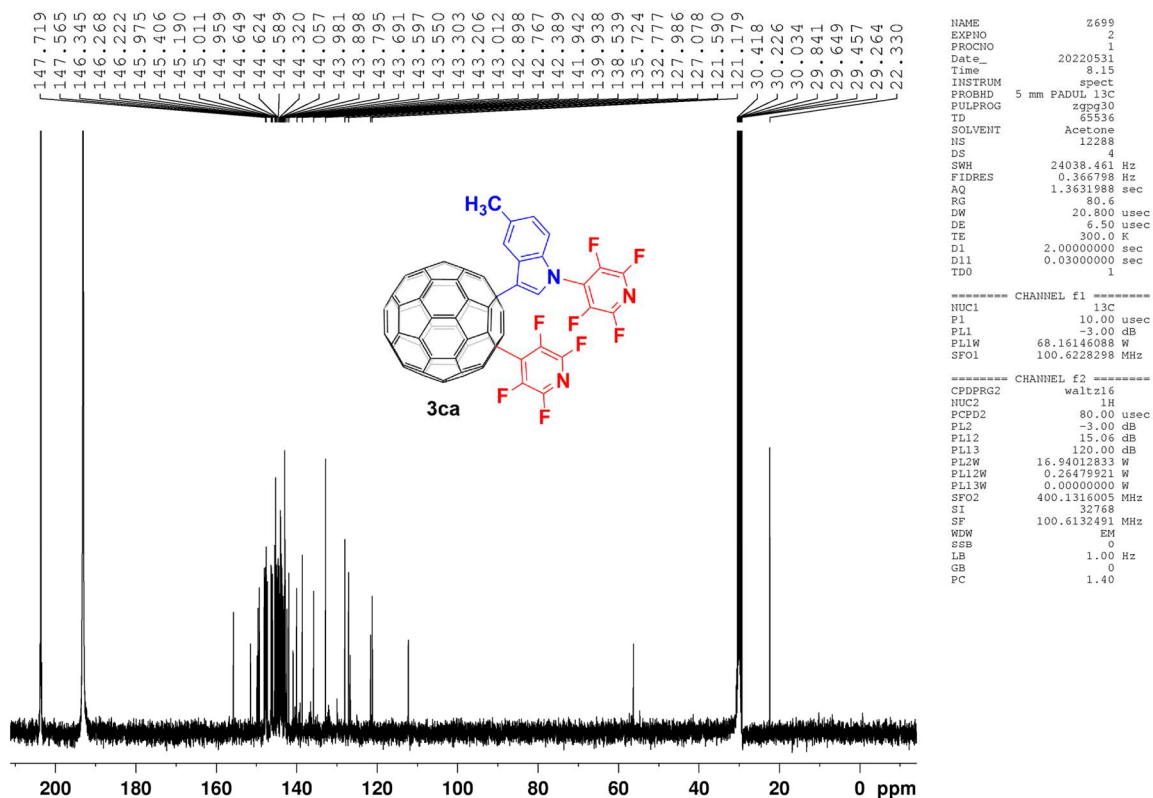
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 3ca



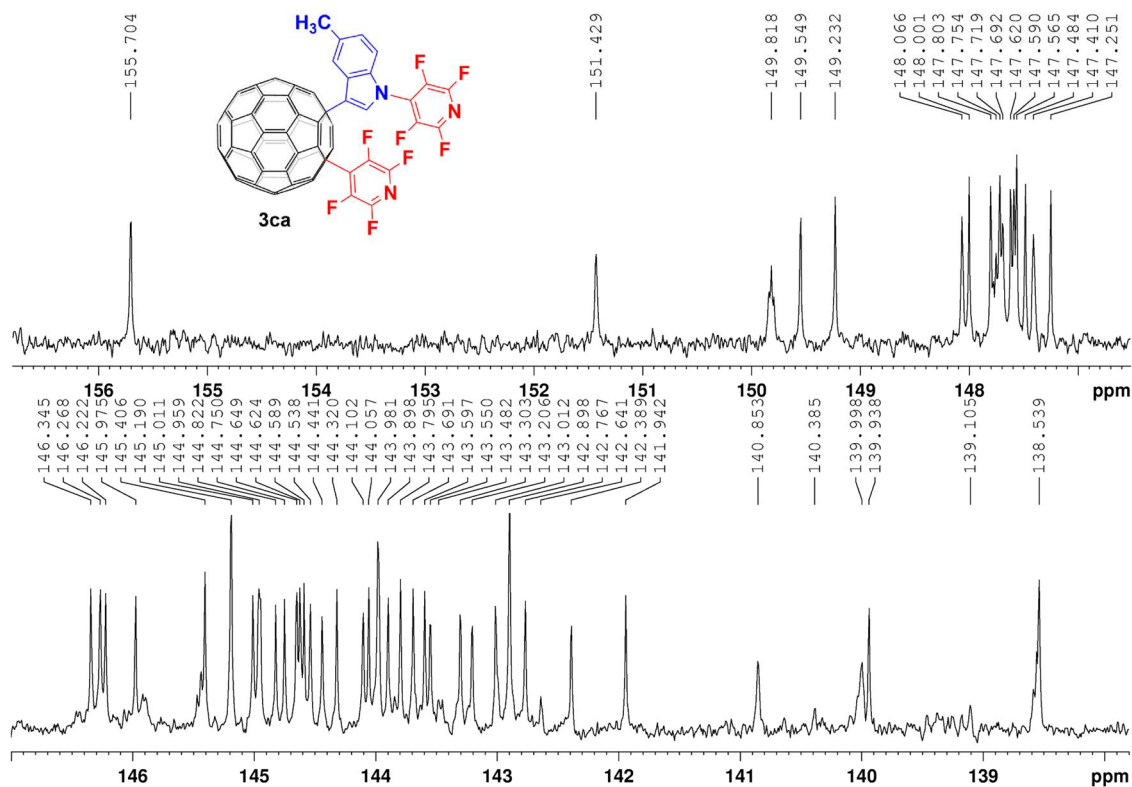
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 3ca



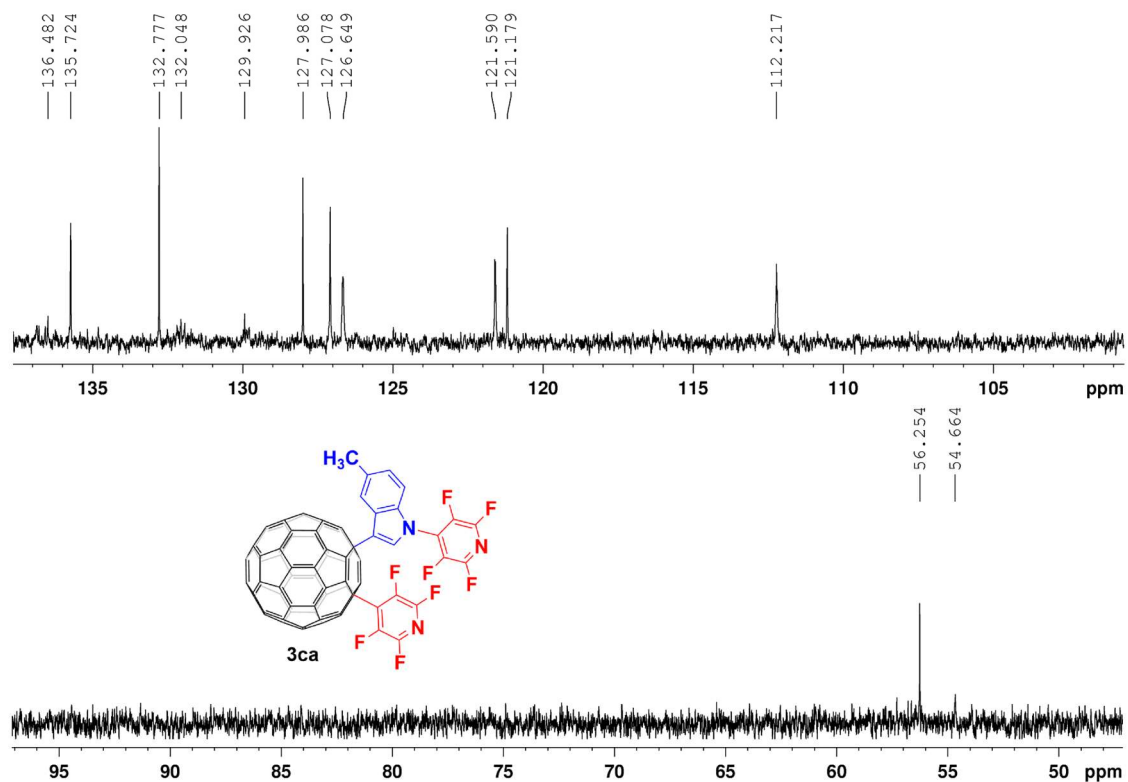
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 3ca



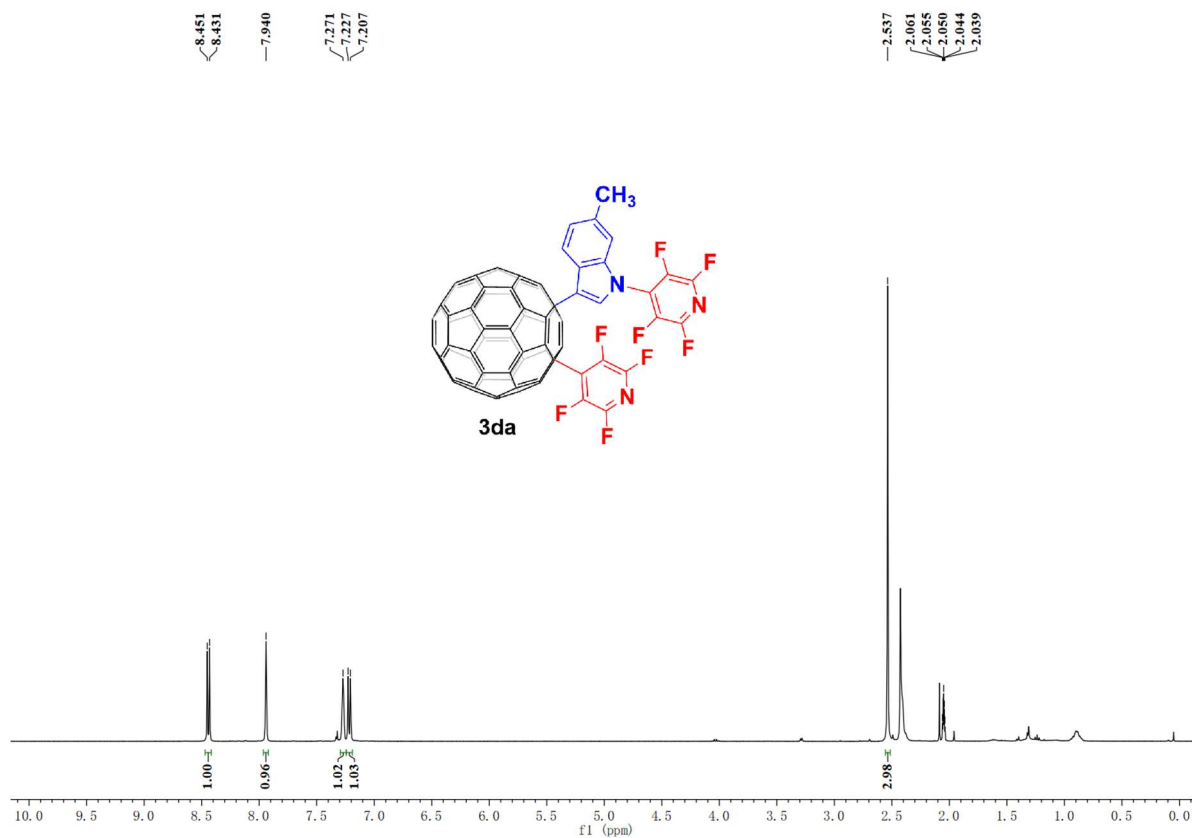
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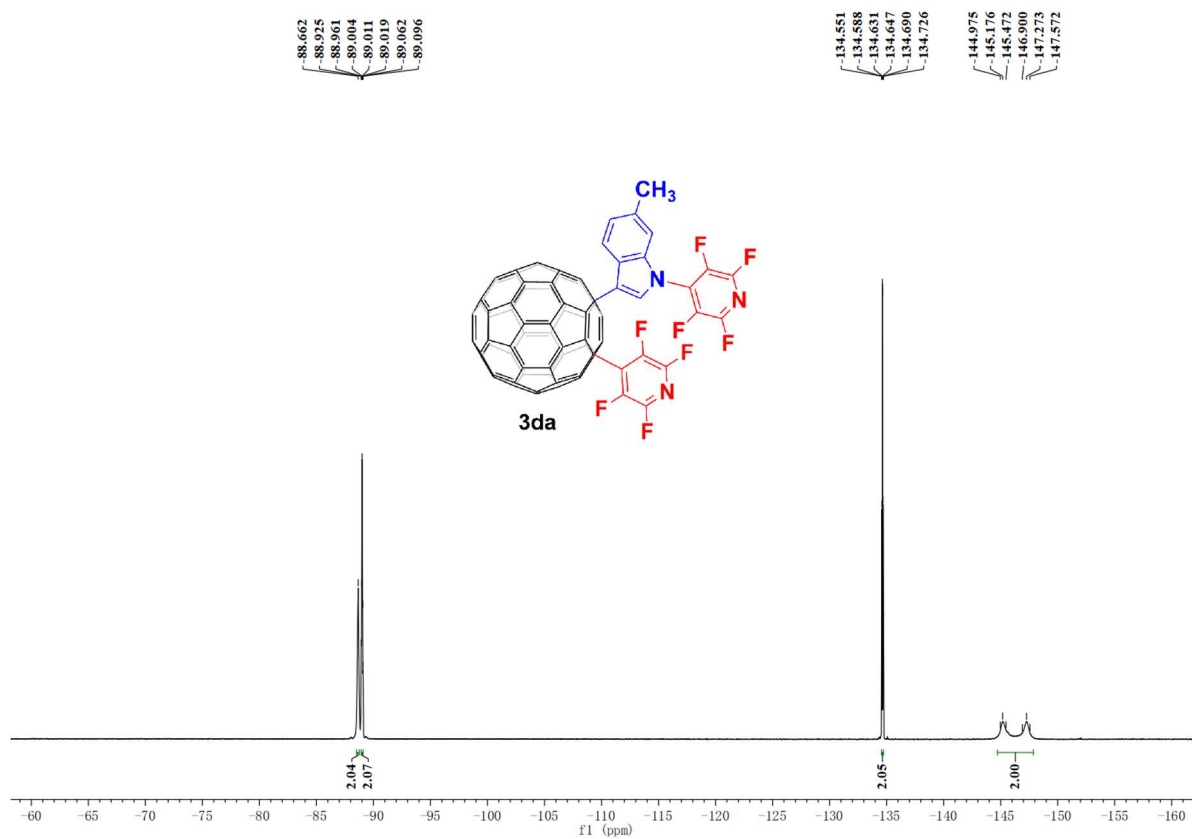
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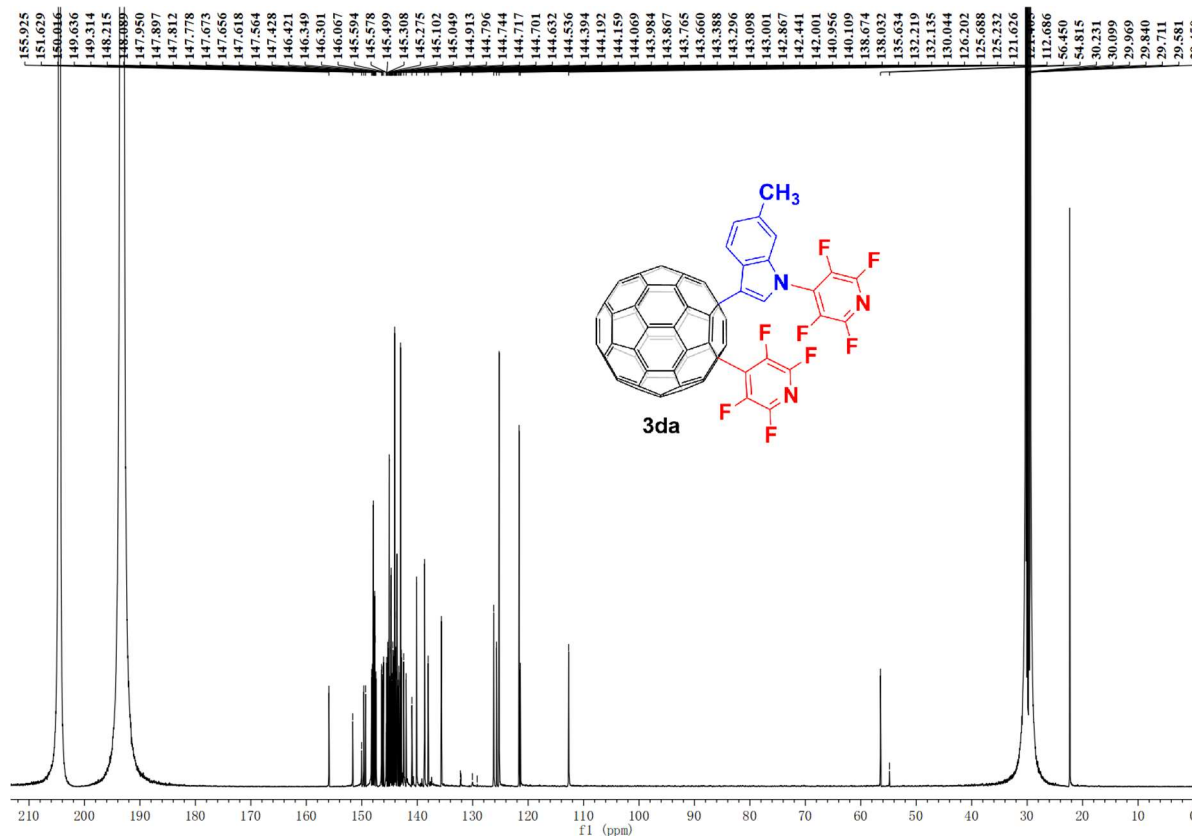
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 3da



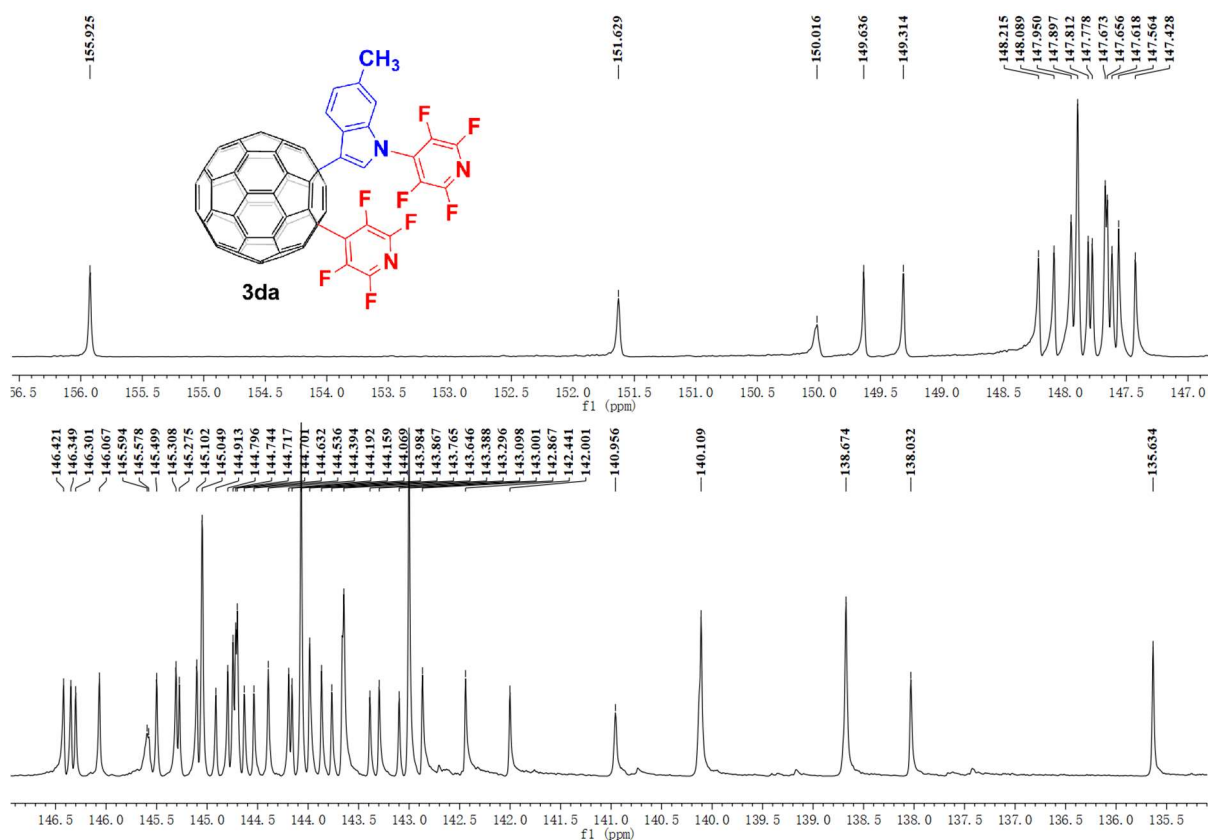
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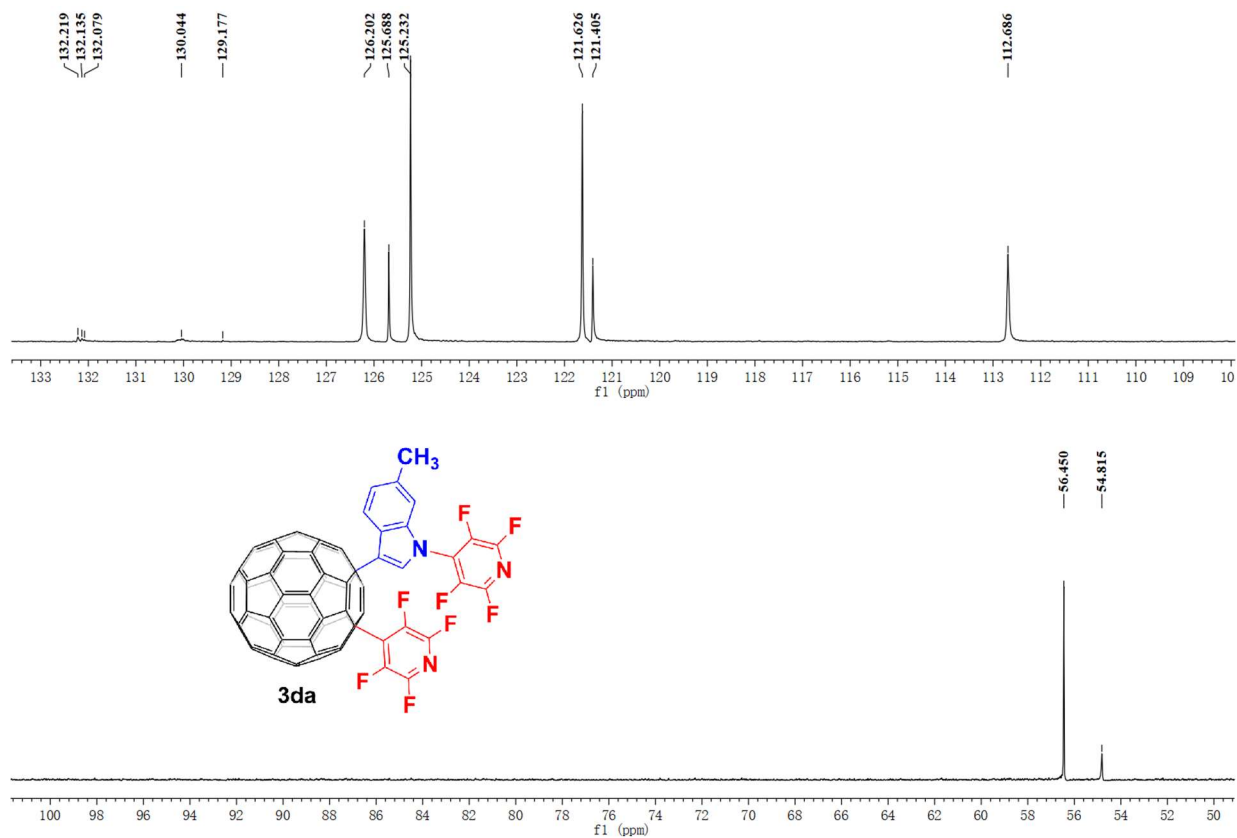
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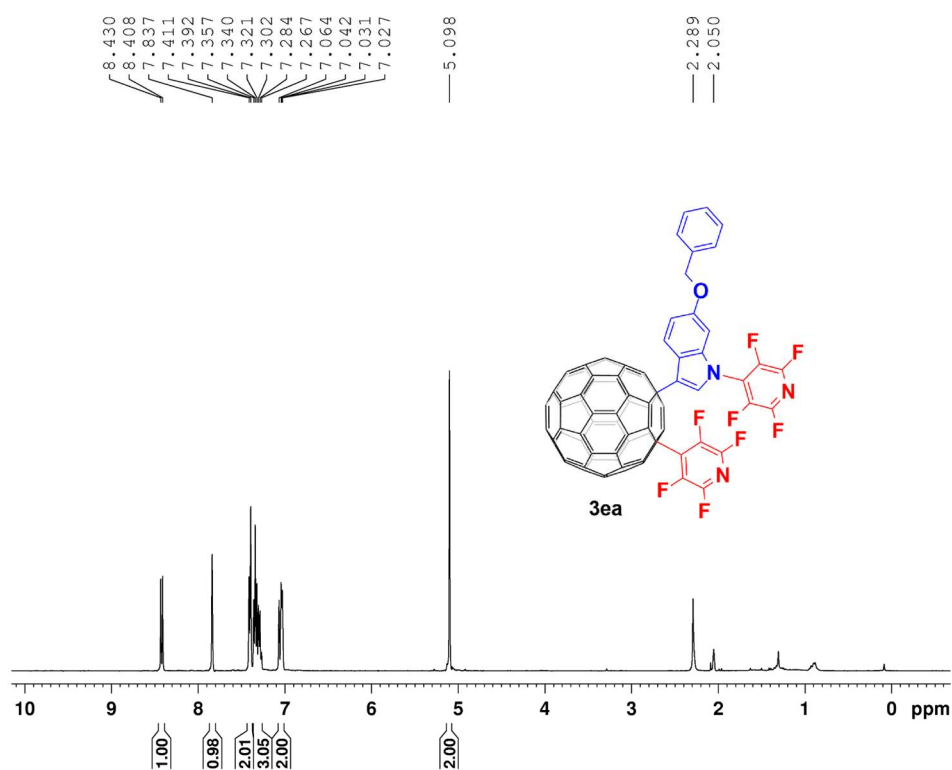
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3da



Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3da



¹H NMR (400 MHz, CS₂/d₆-acetone) of compound 3ea



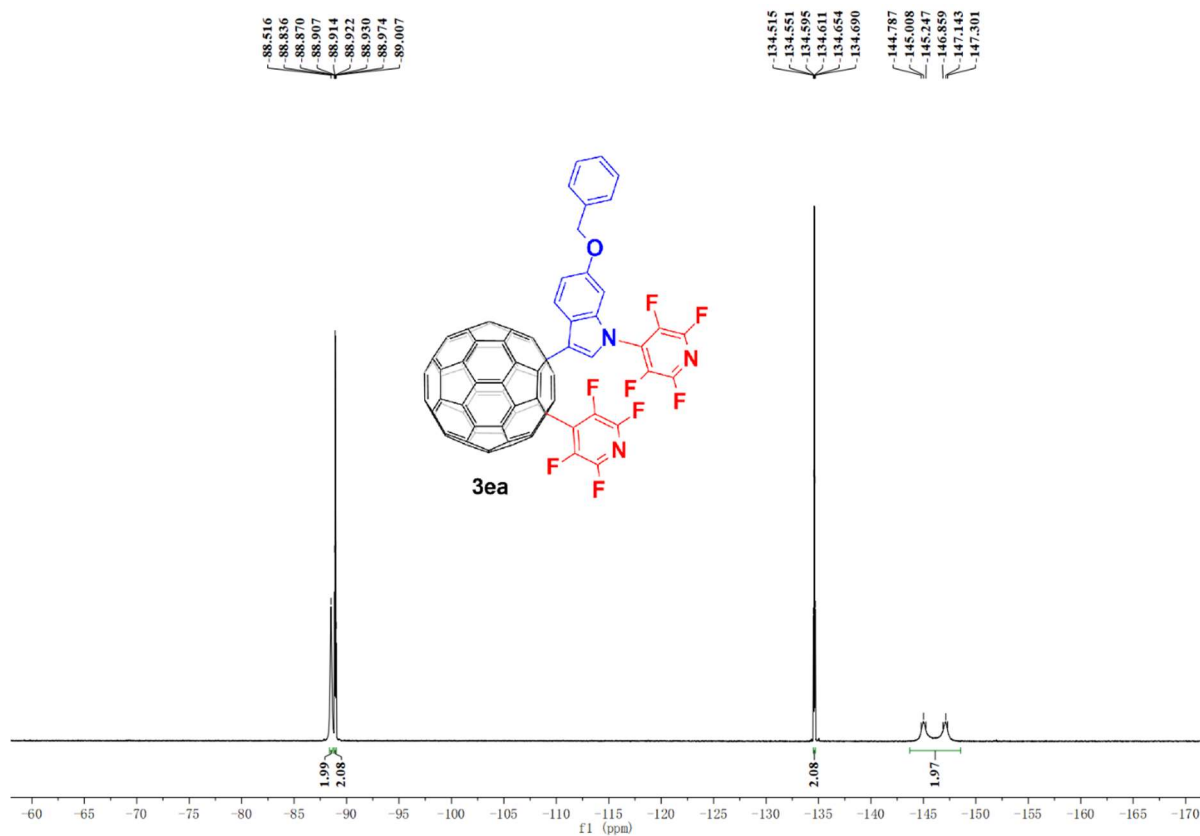
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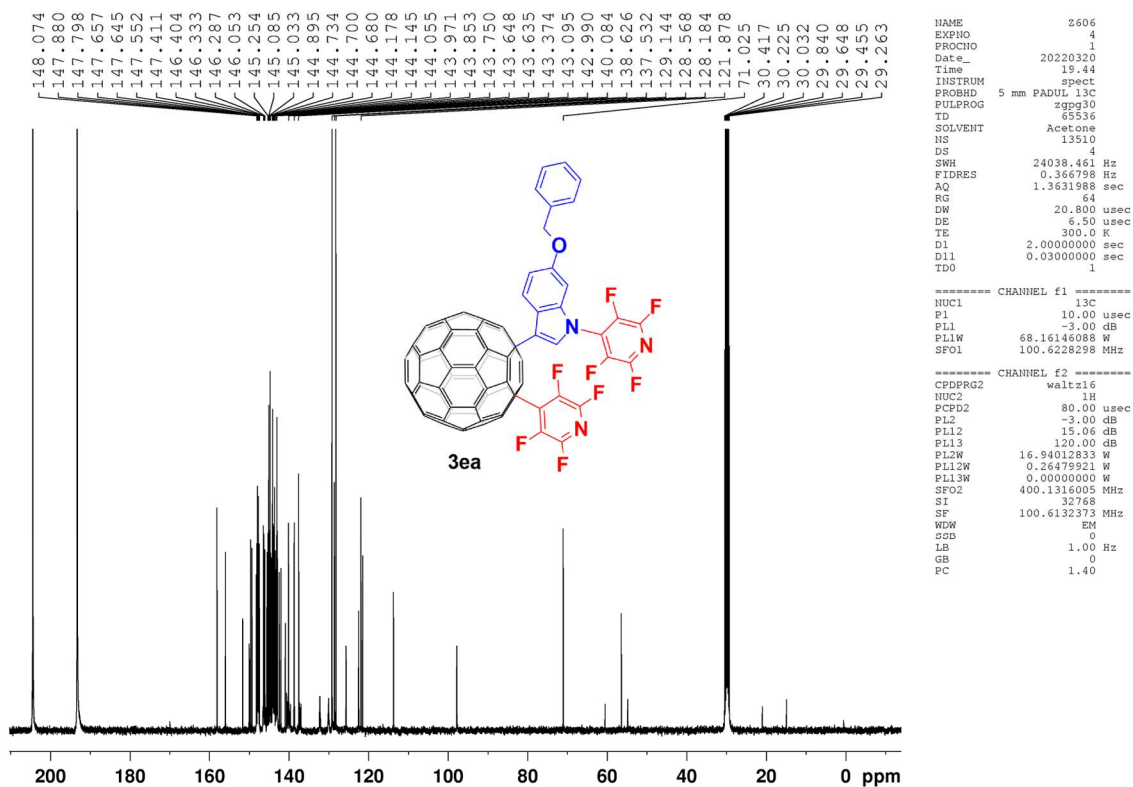
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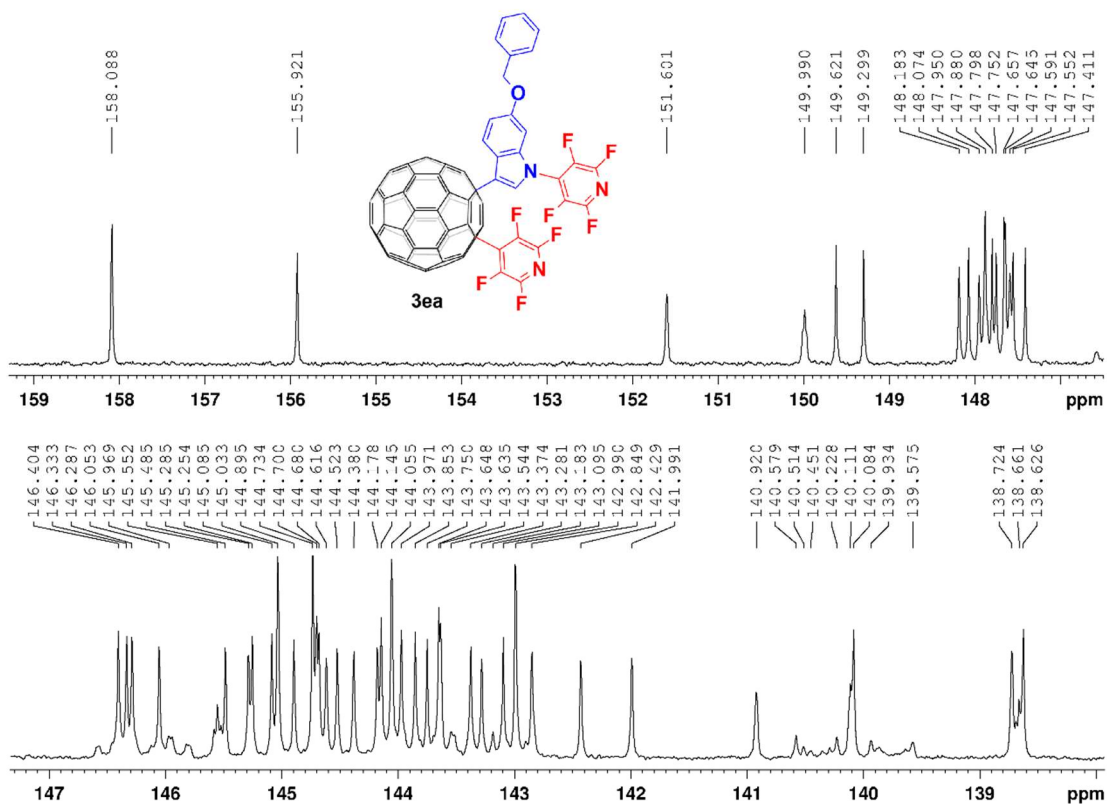
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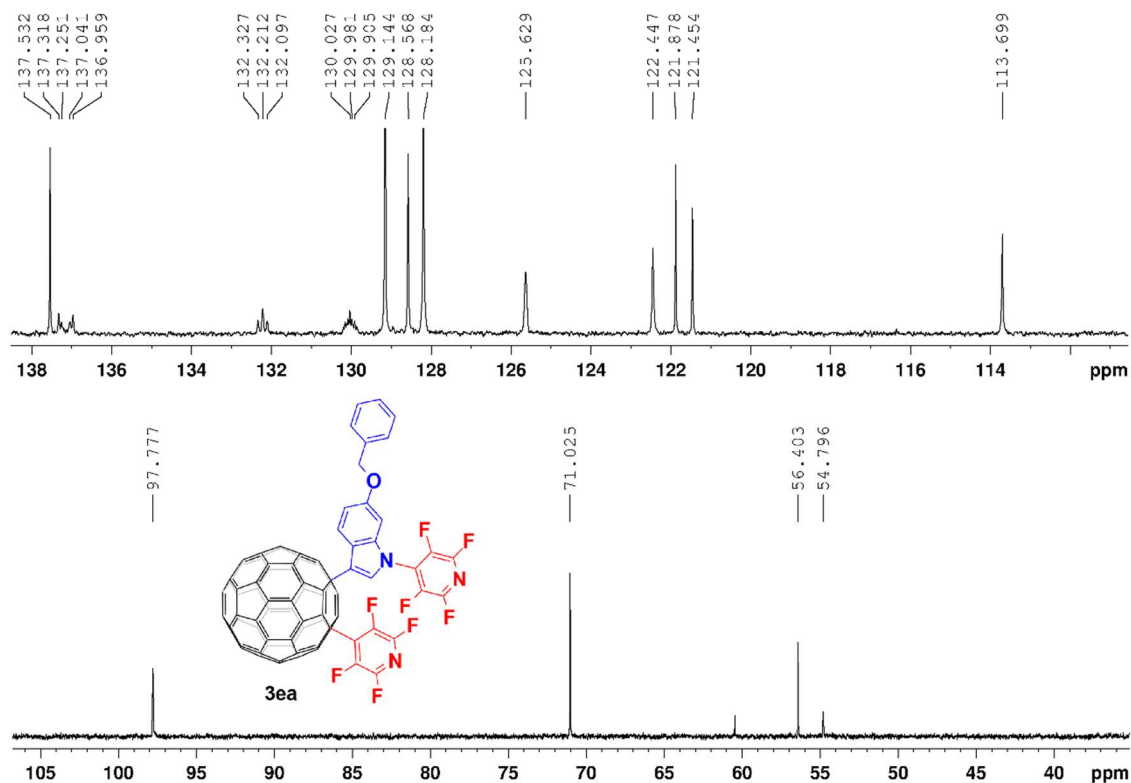
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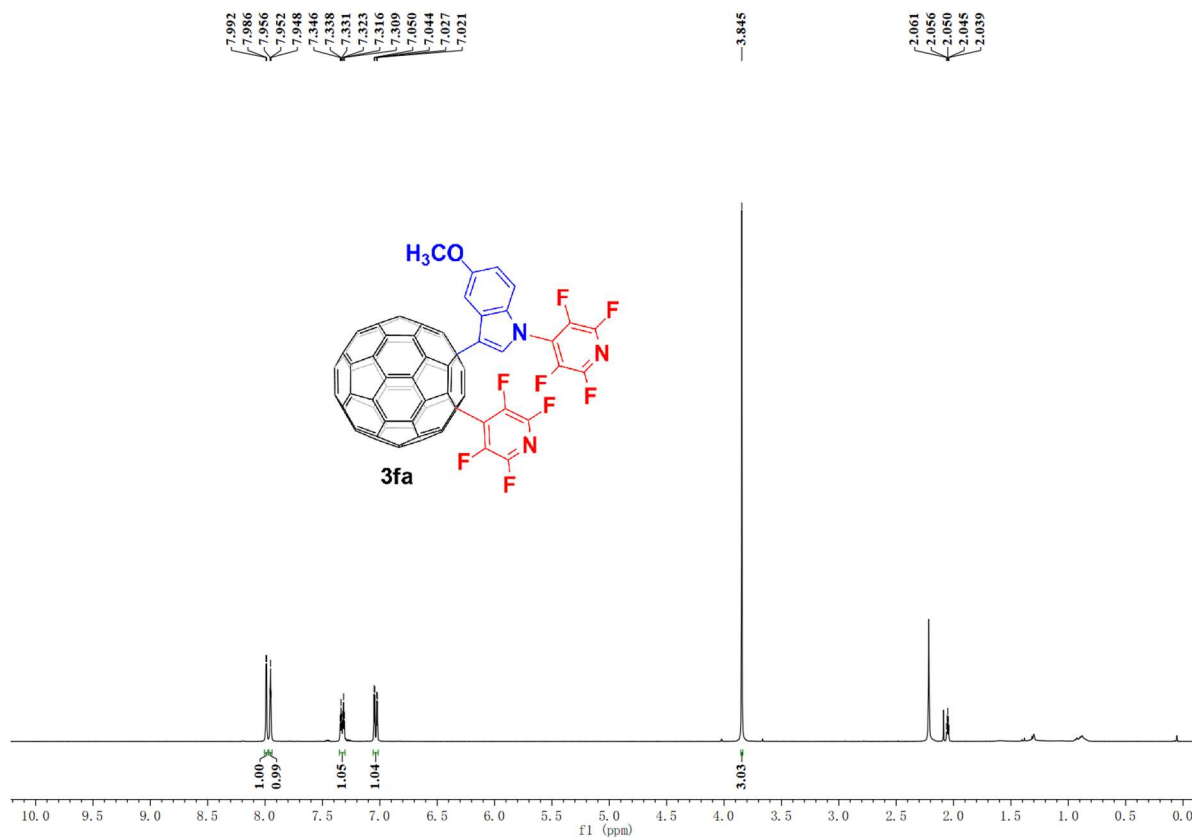
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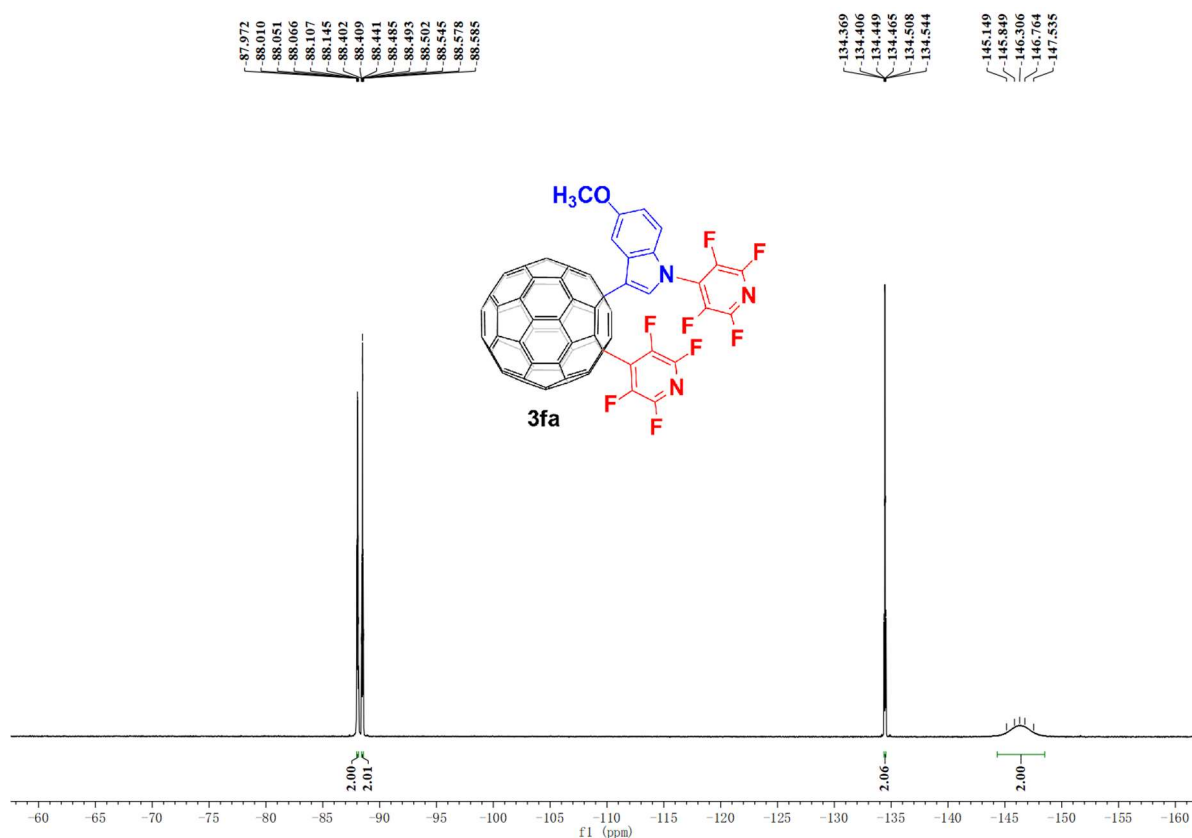
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3ea



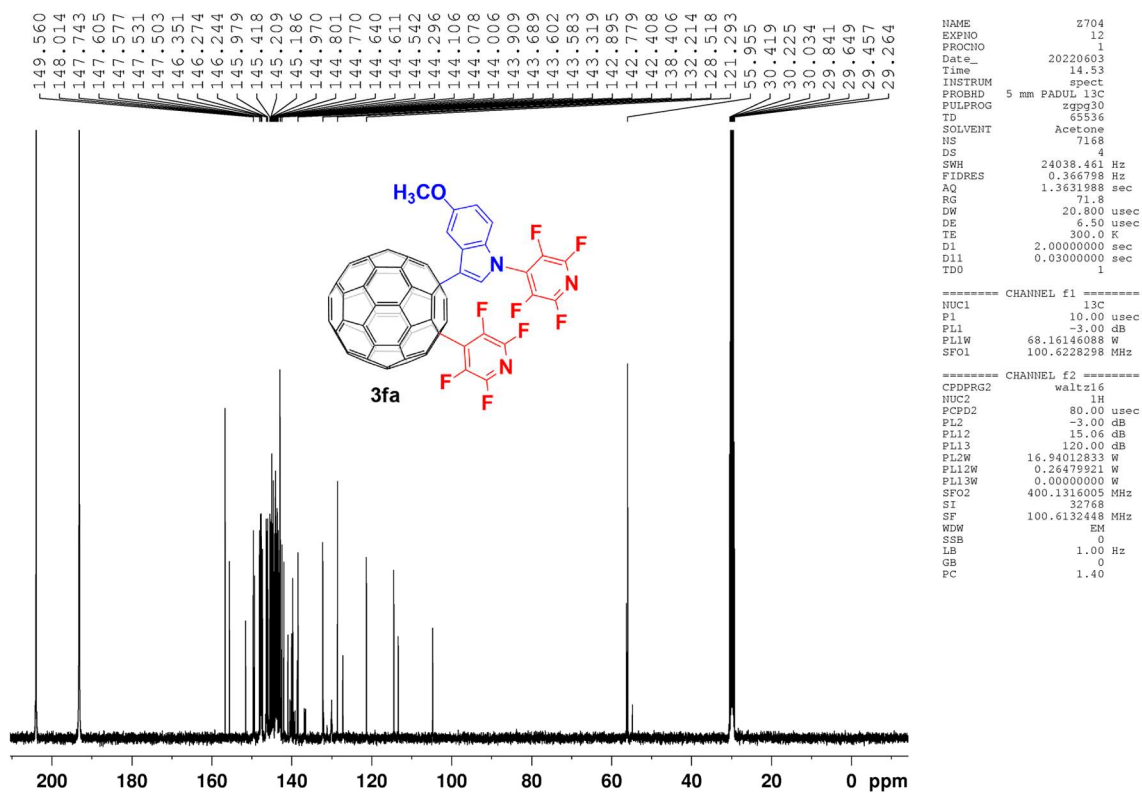
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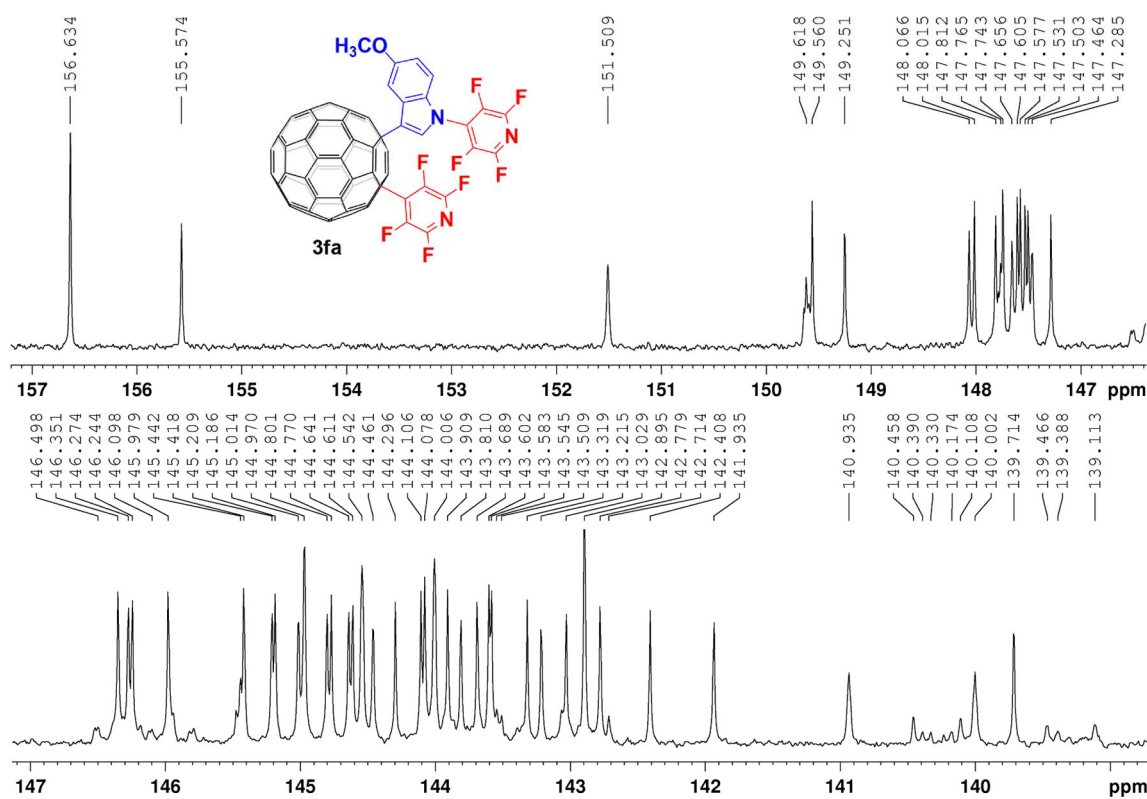
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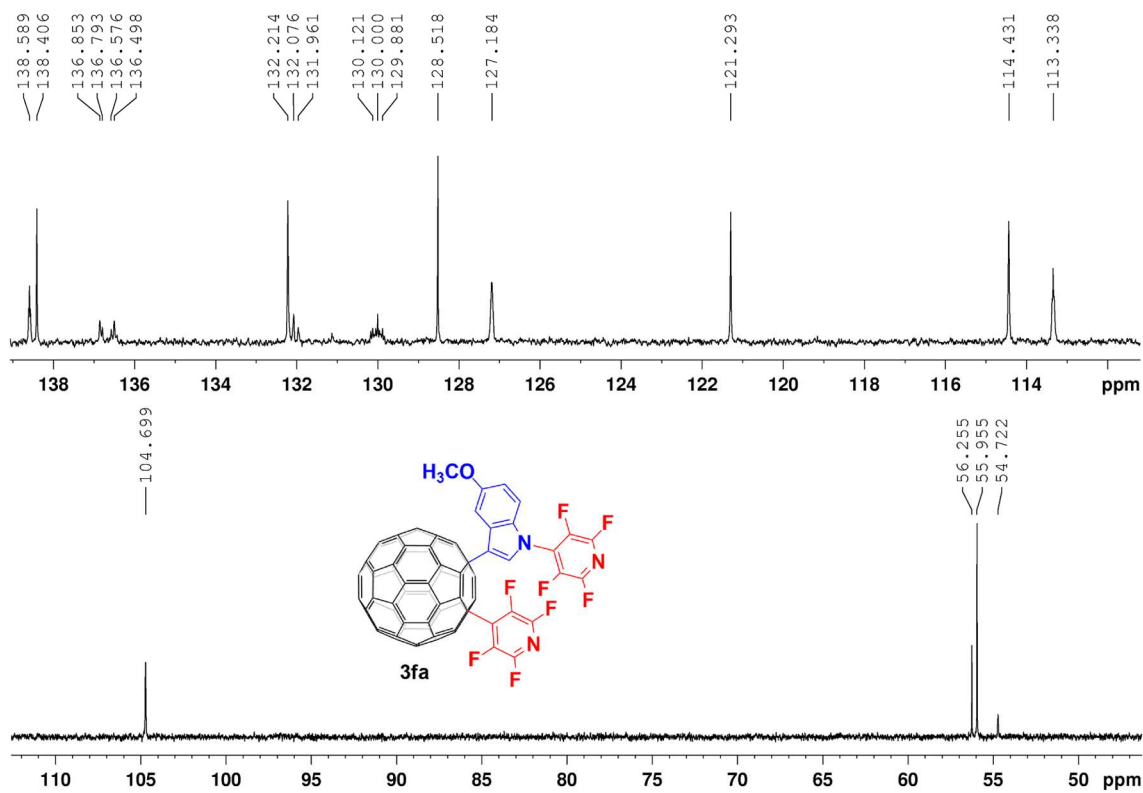
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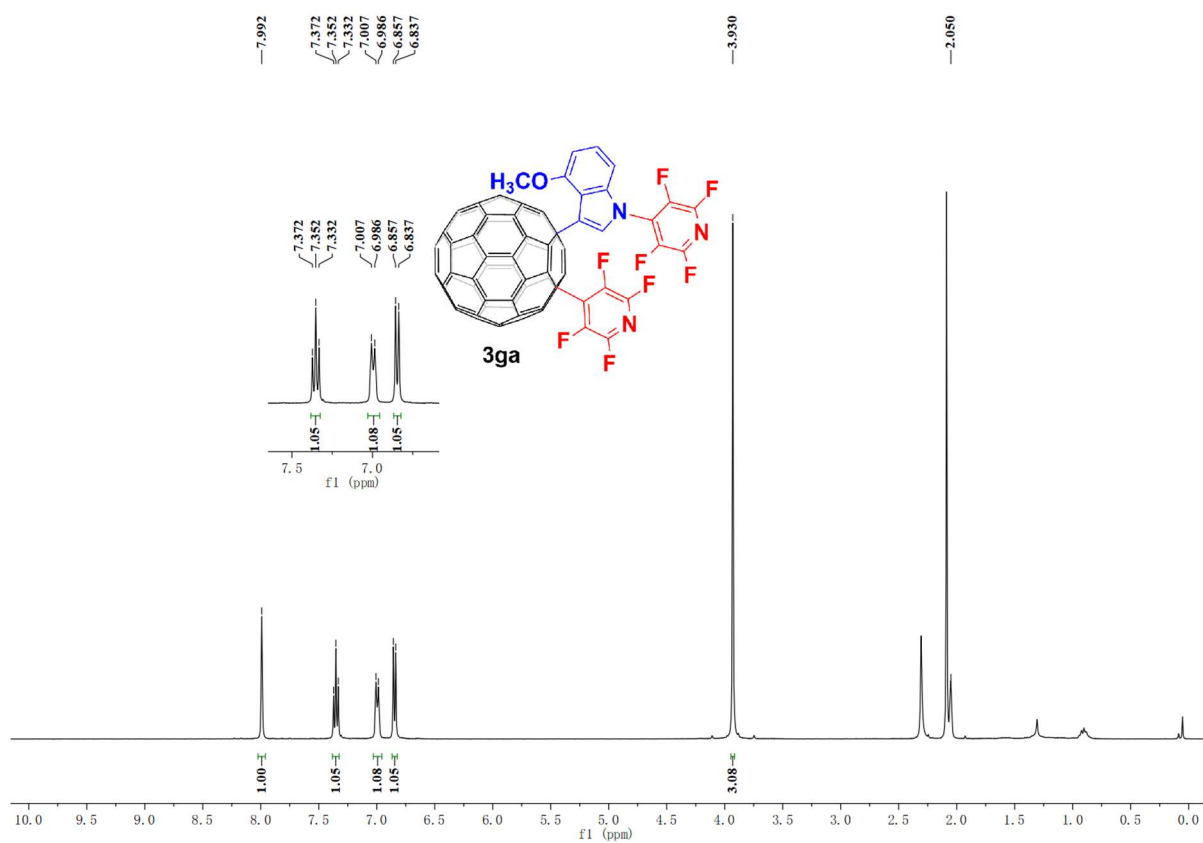
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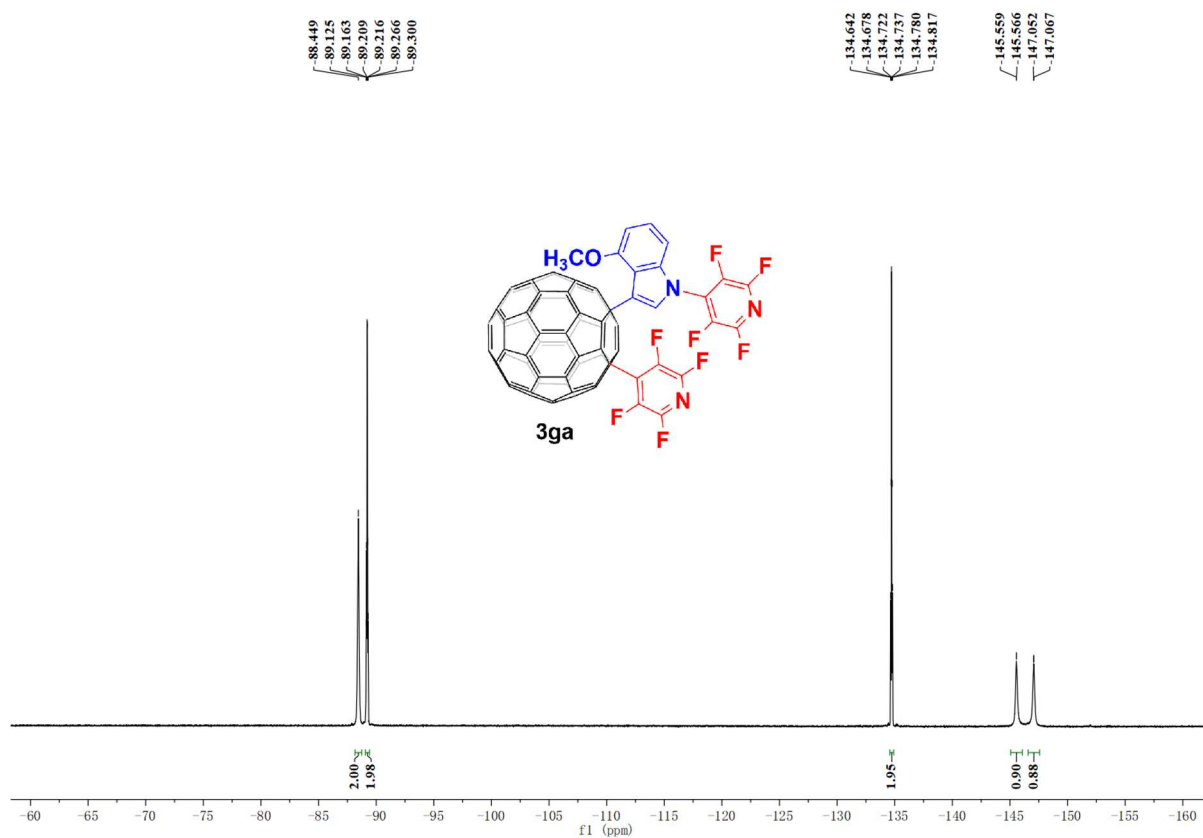
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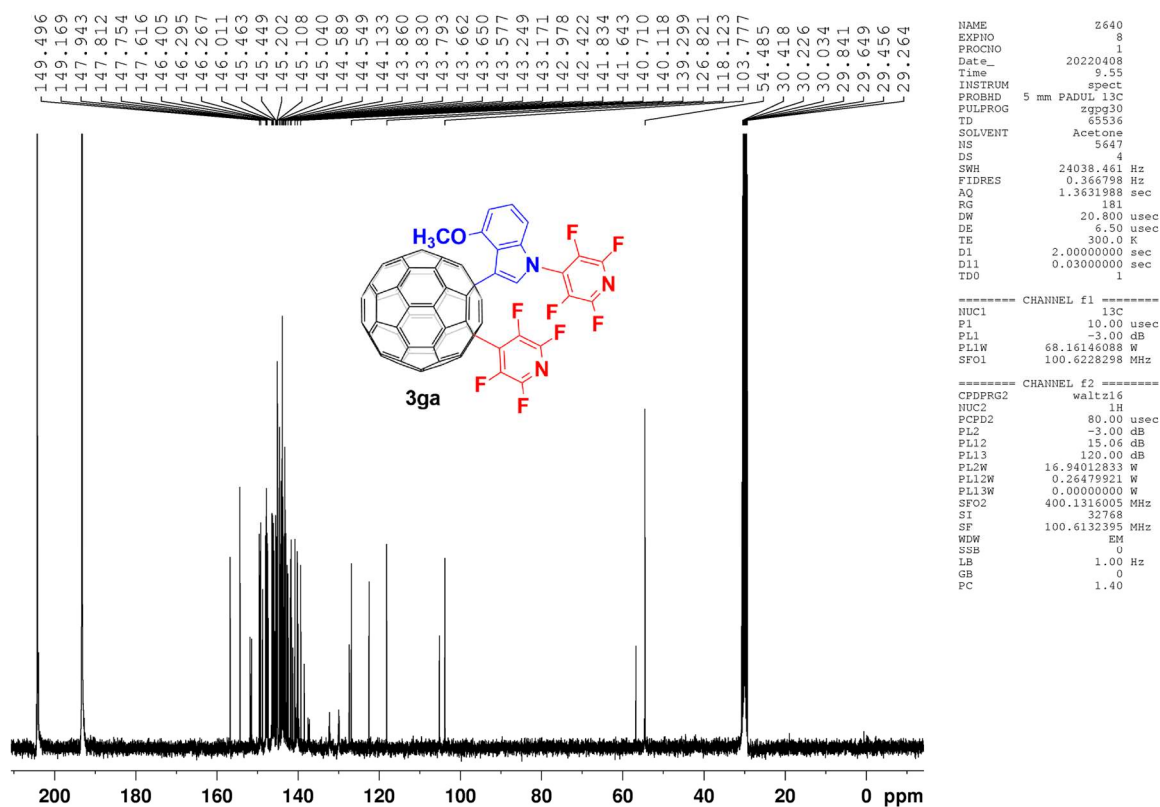
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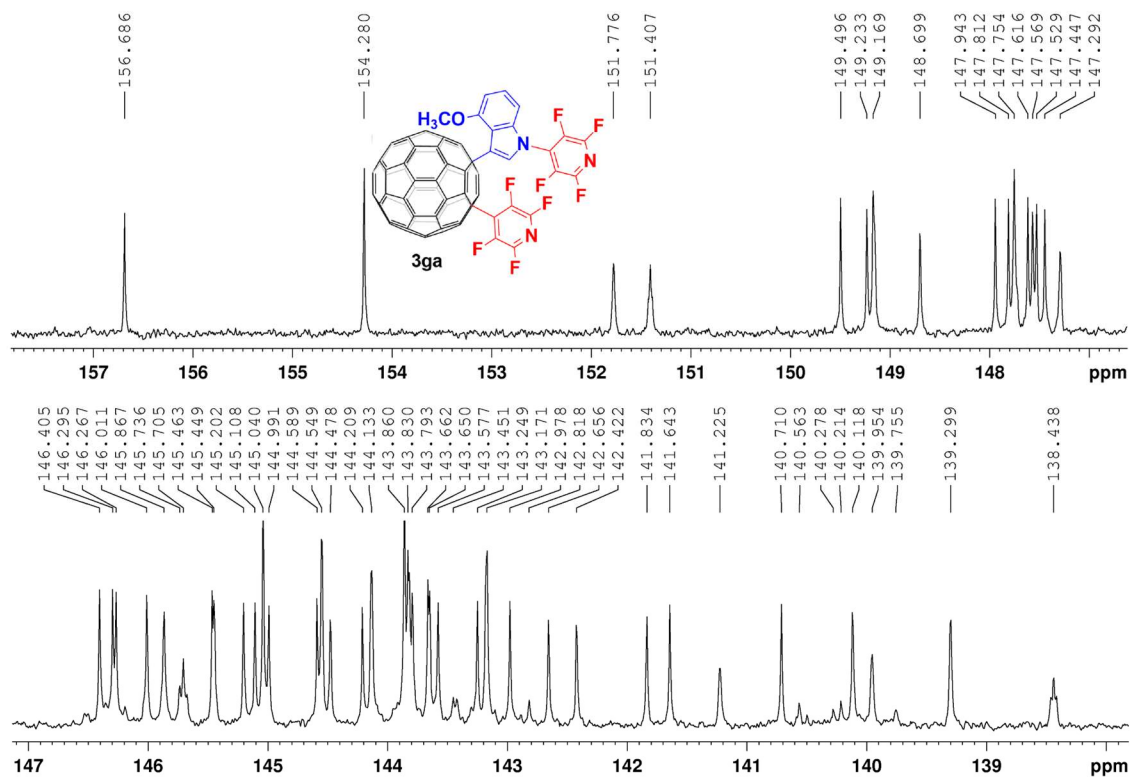
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 3ga



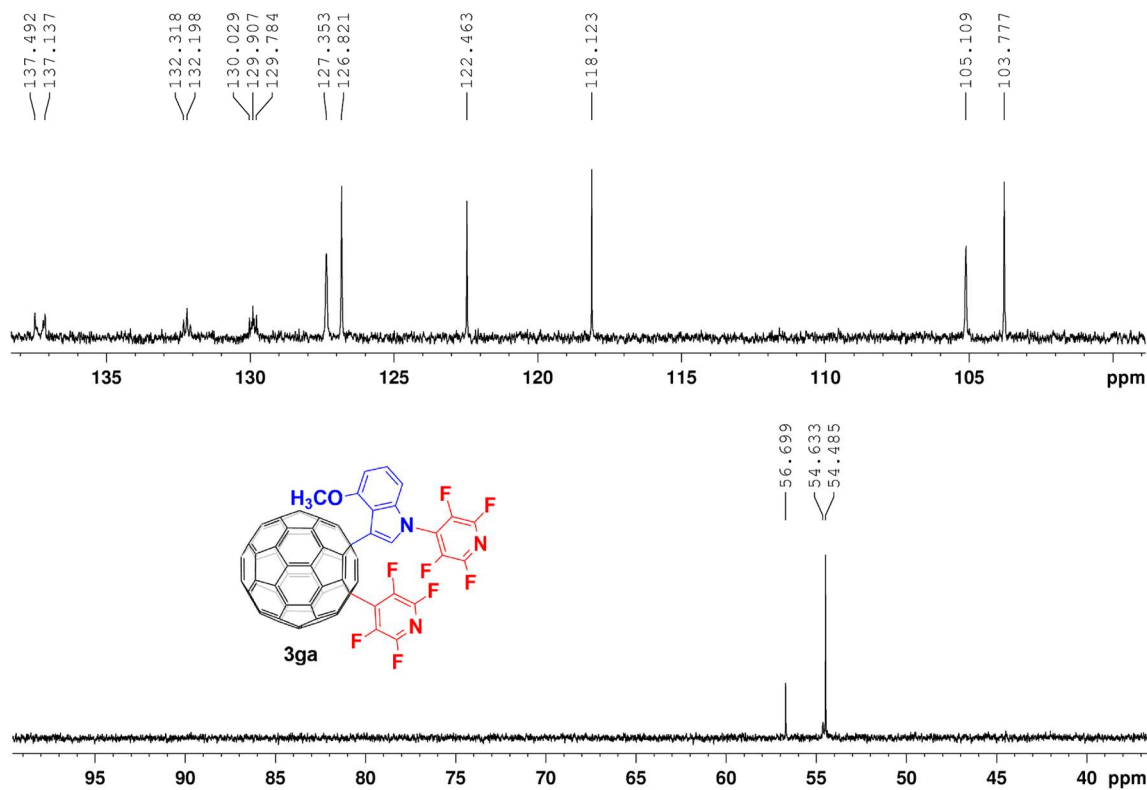
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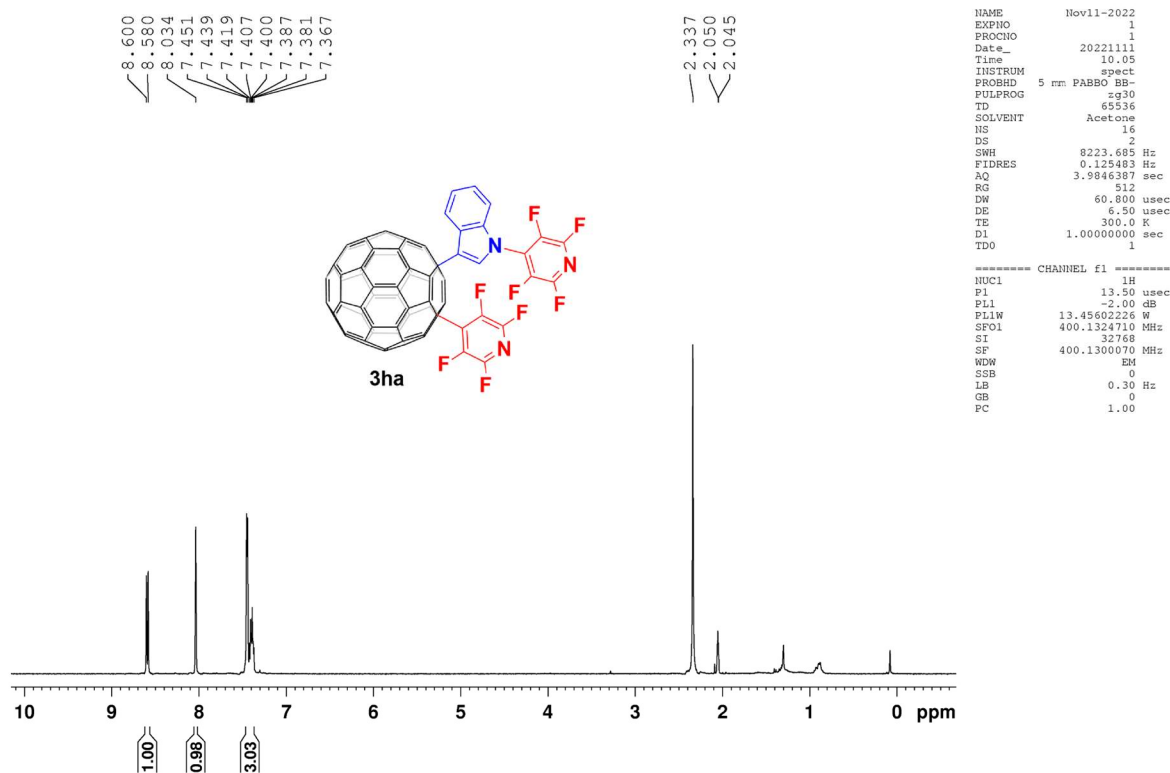
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3ga



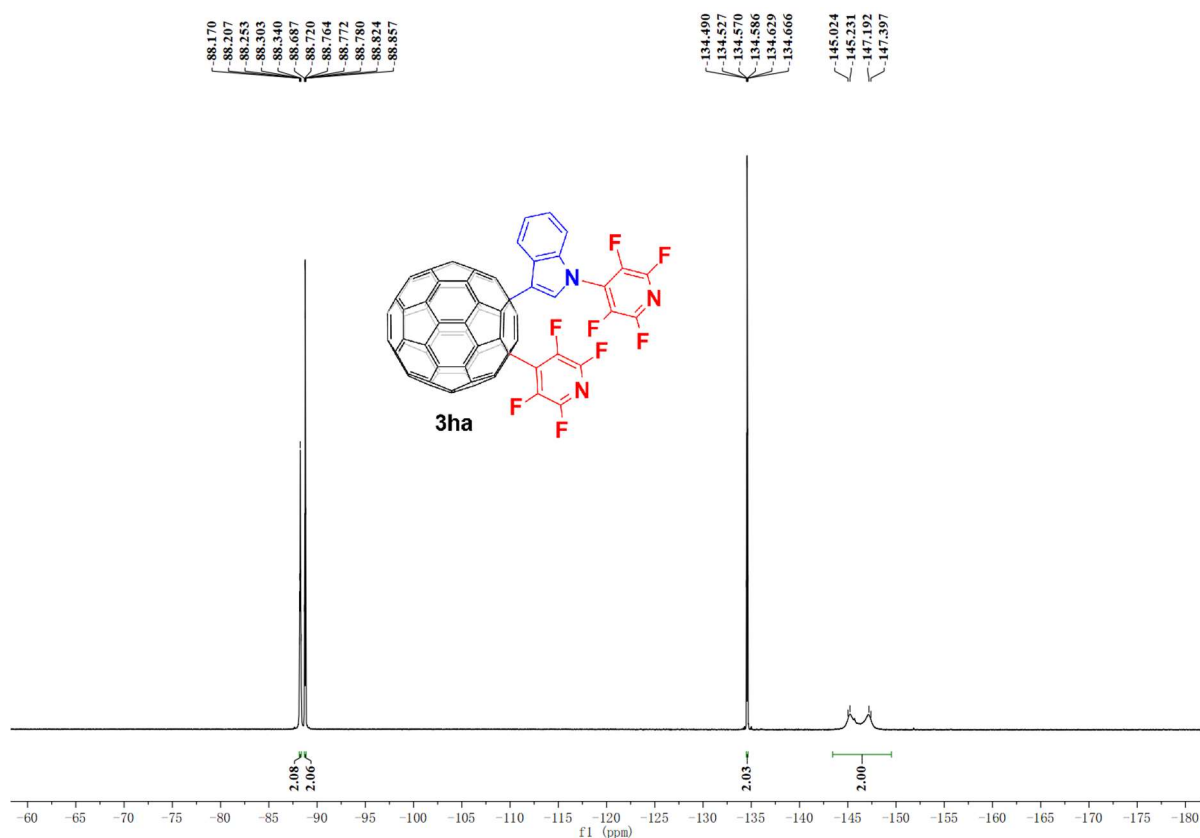
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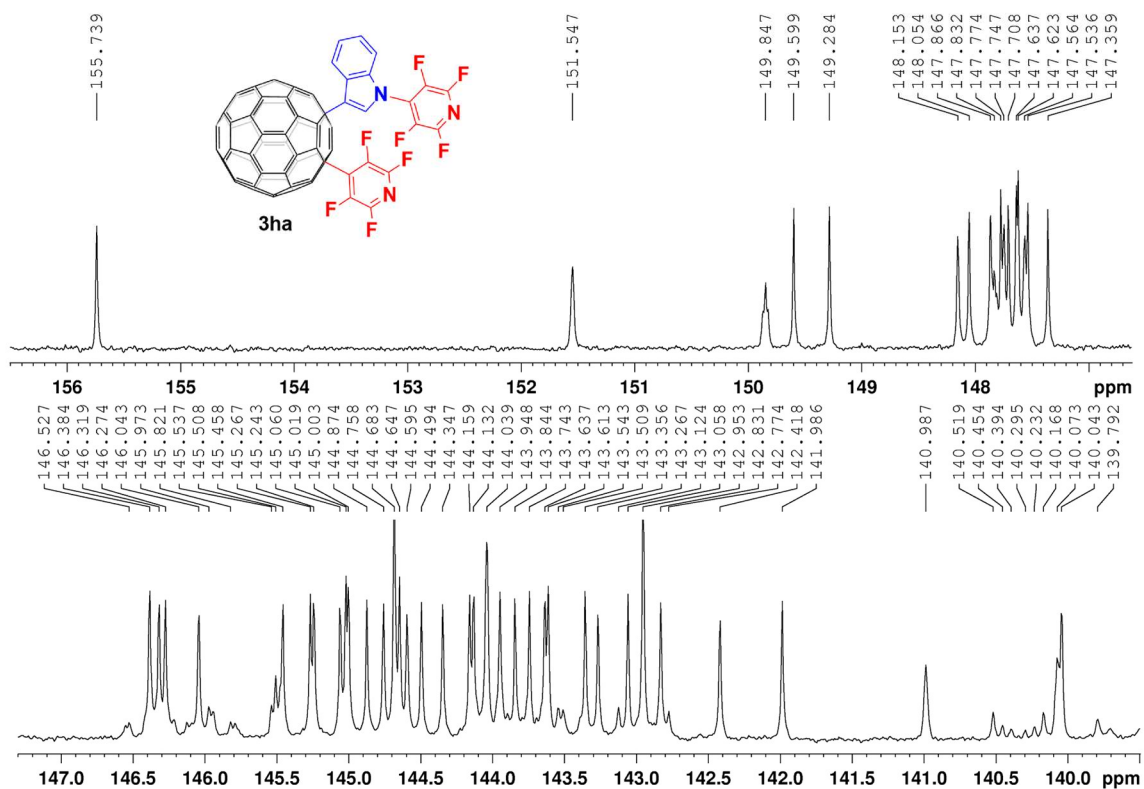
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 3ha



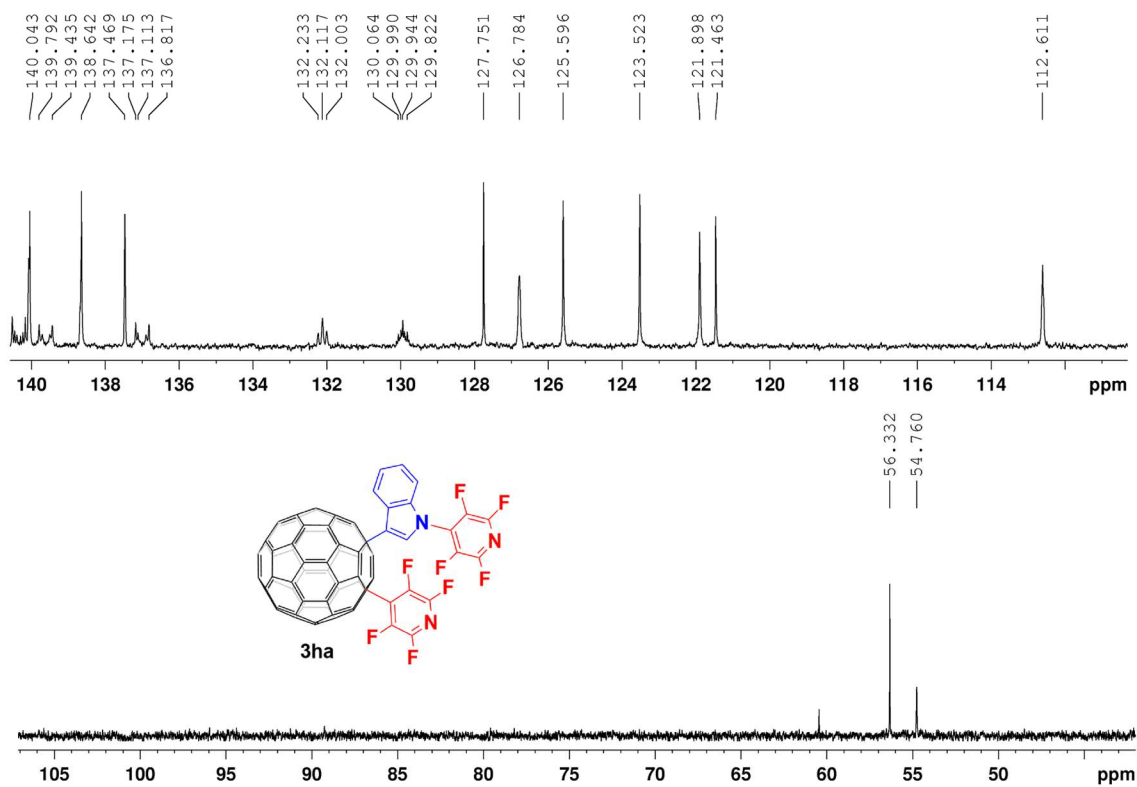
¹⁹F NMR (376 MHz, CS₂/d₆-acetone) of compound 3ha



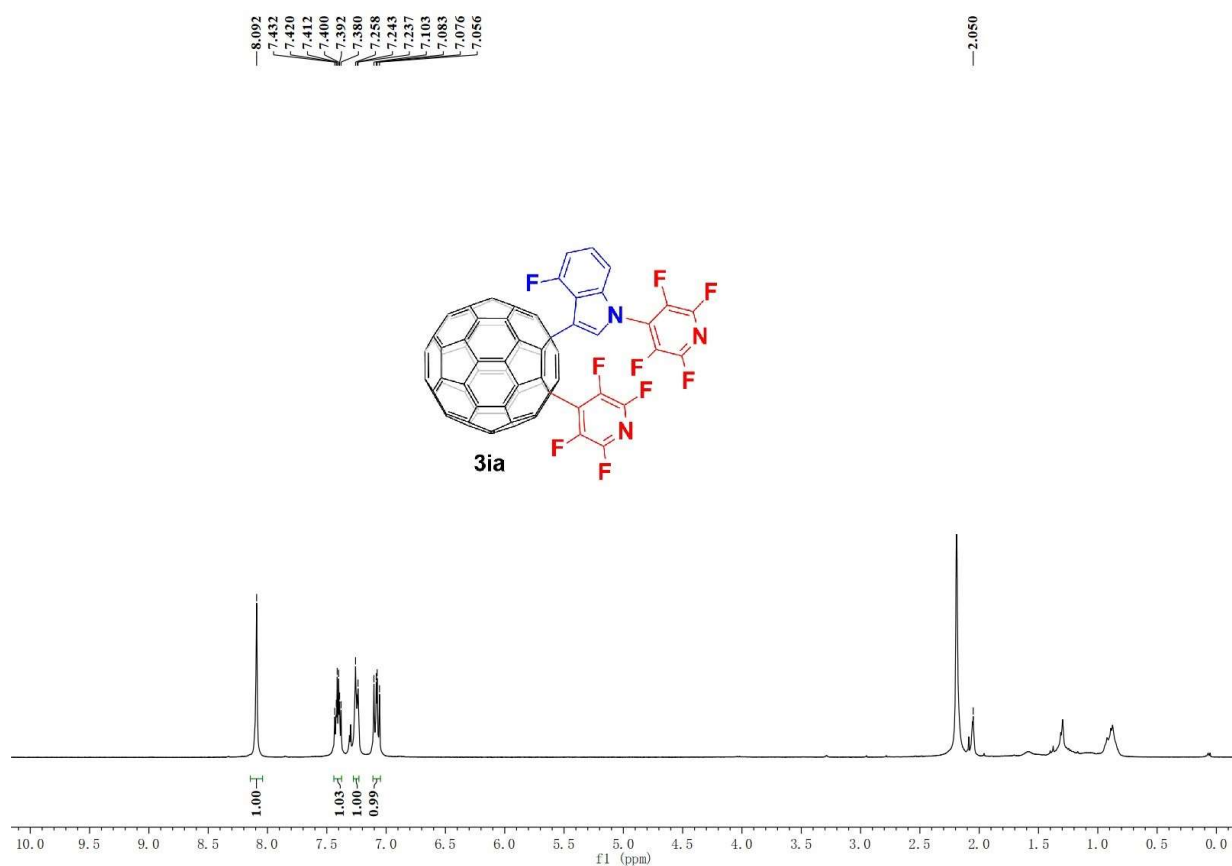
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3ha



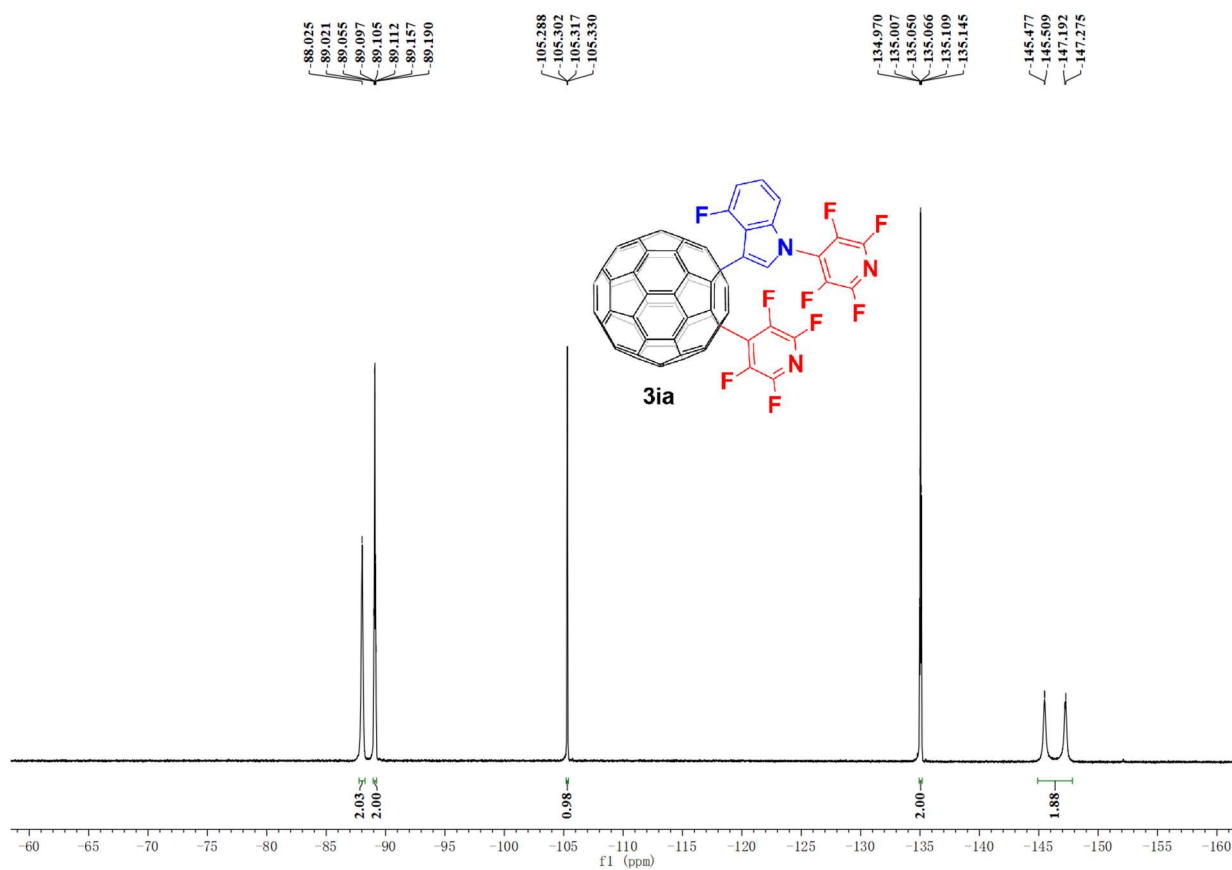
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3ha



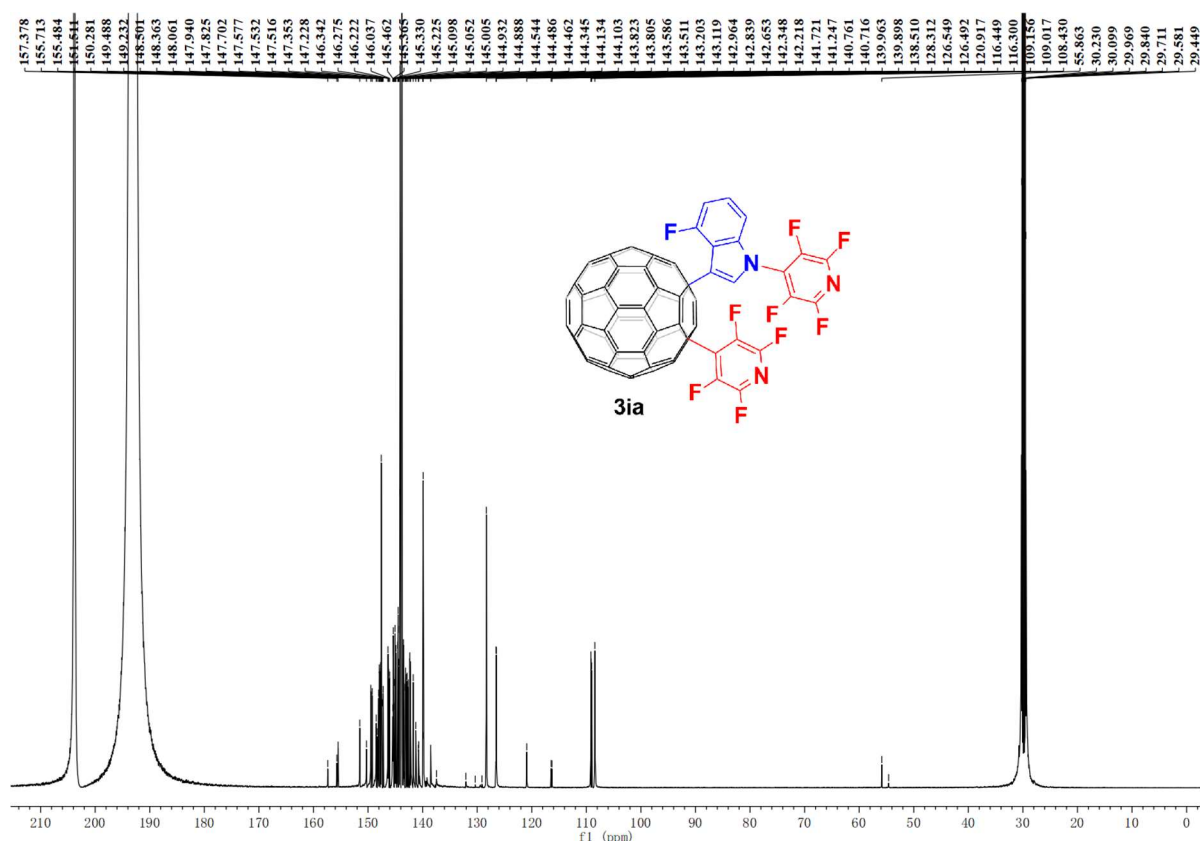
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **3ia**



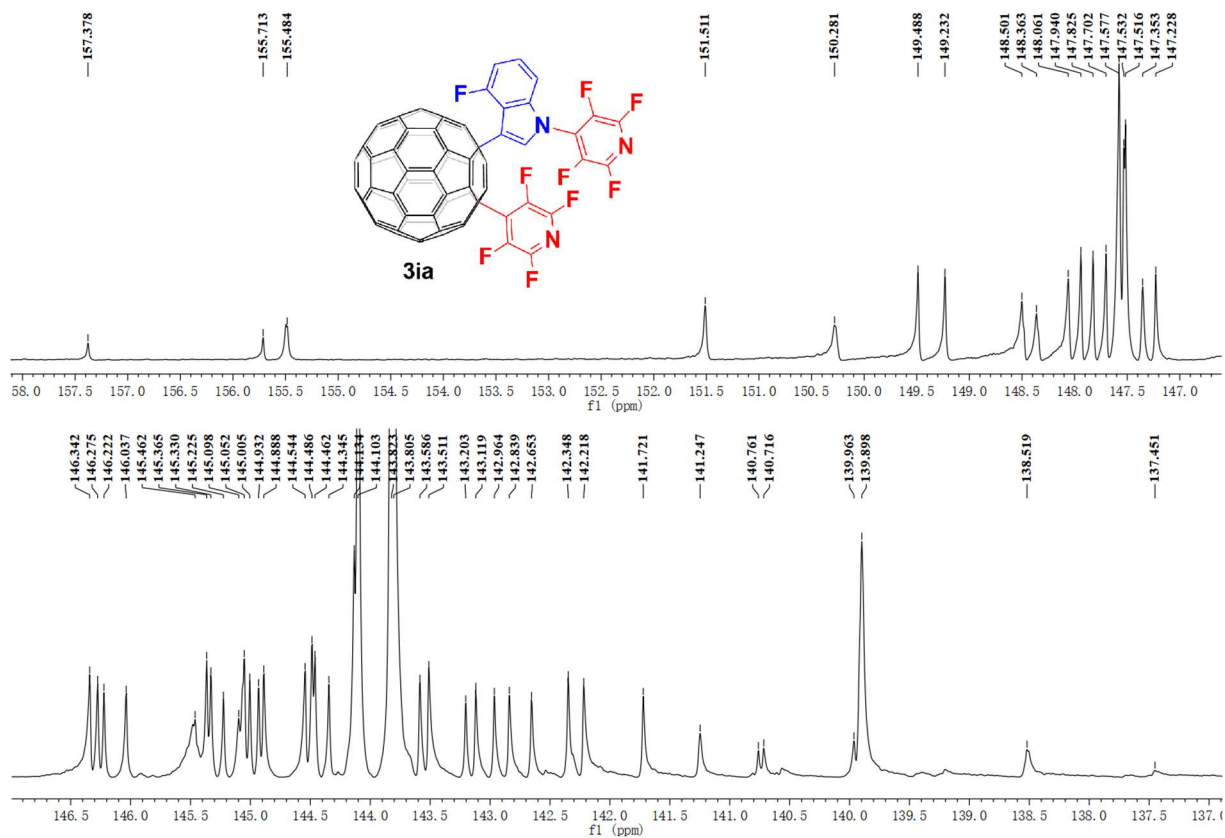
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound **3ia**



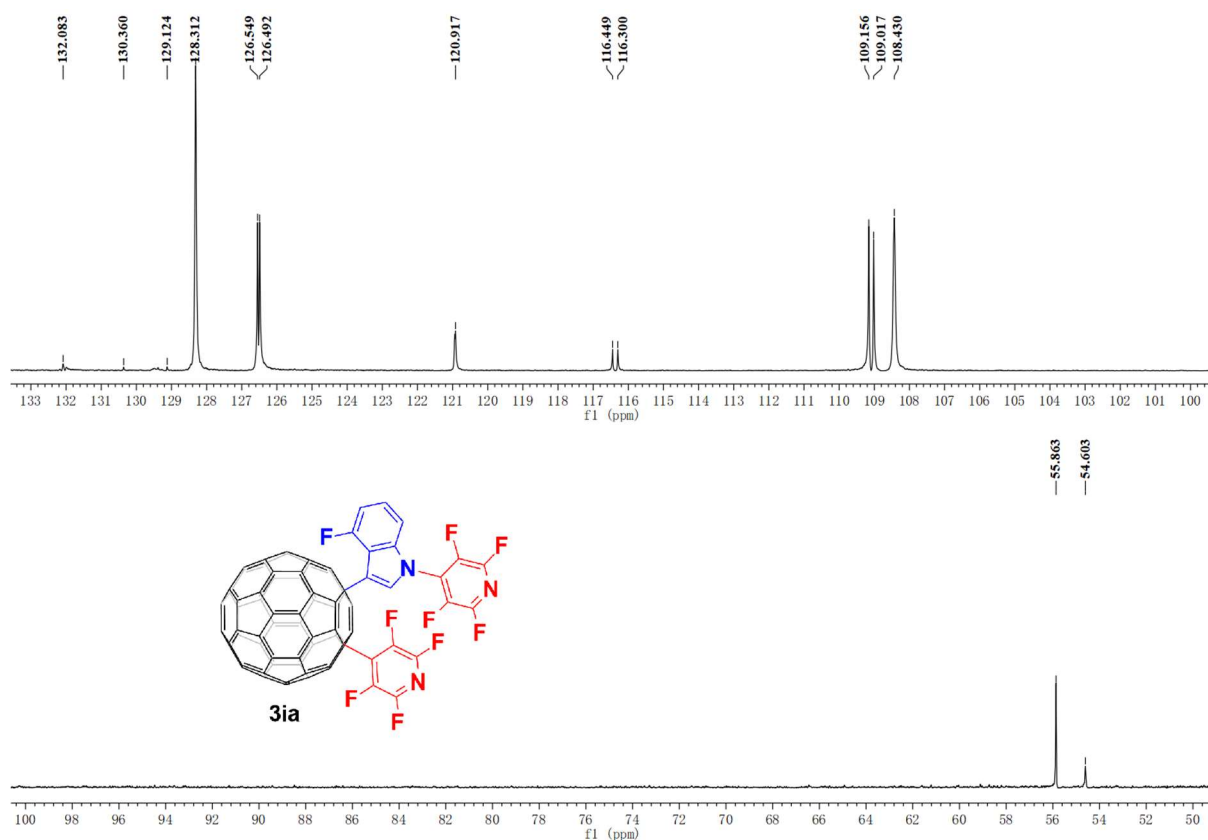
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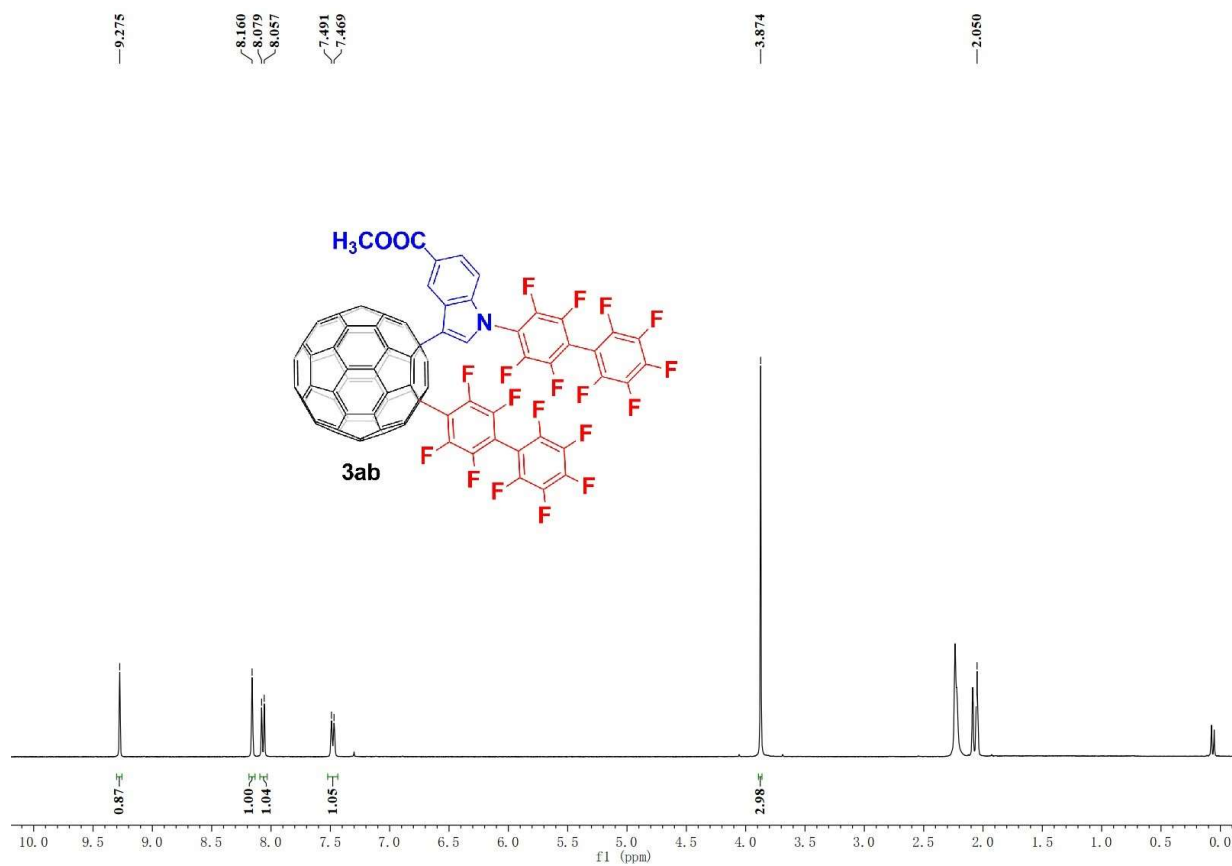
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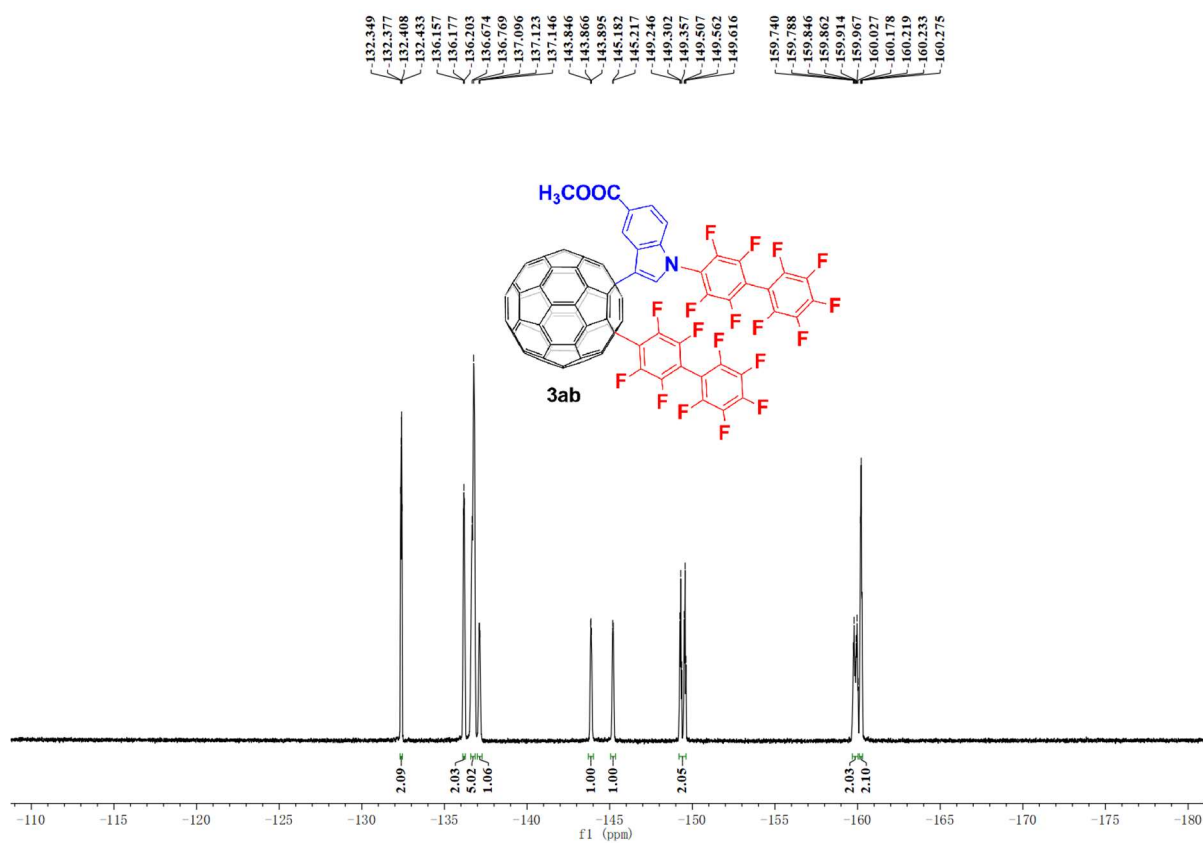
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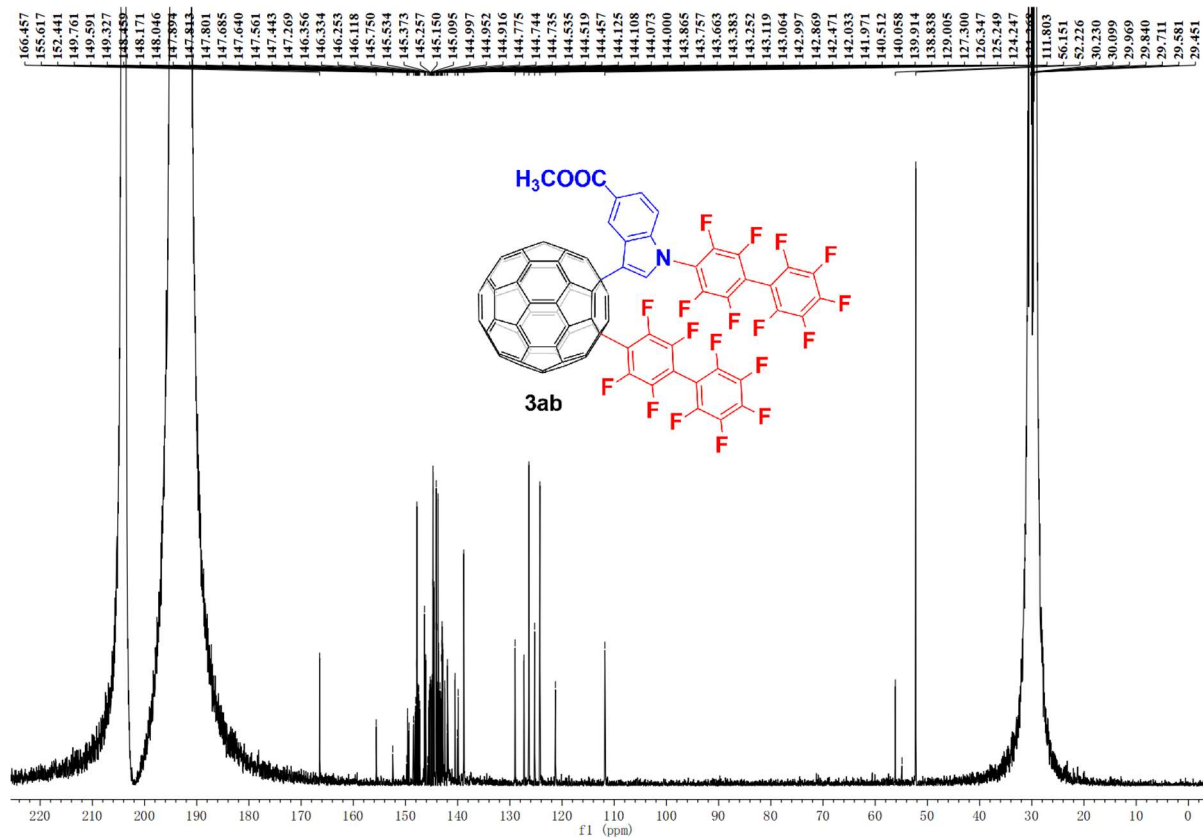
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **3ab**



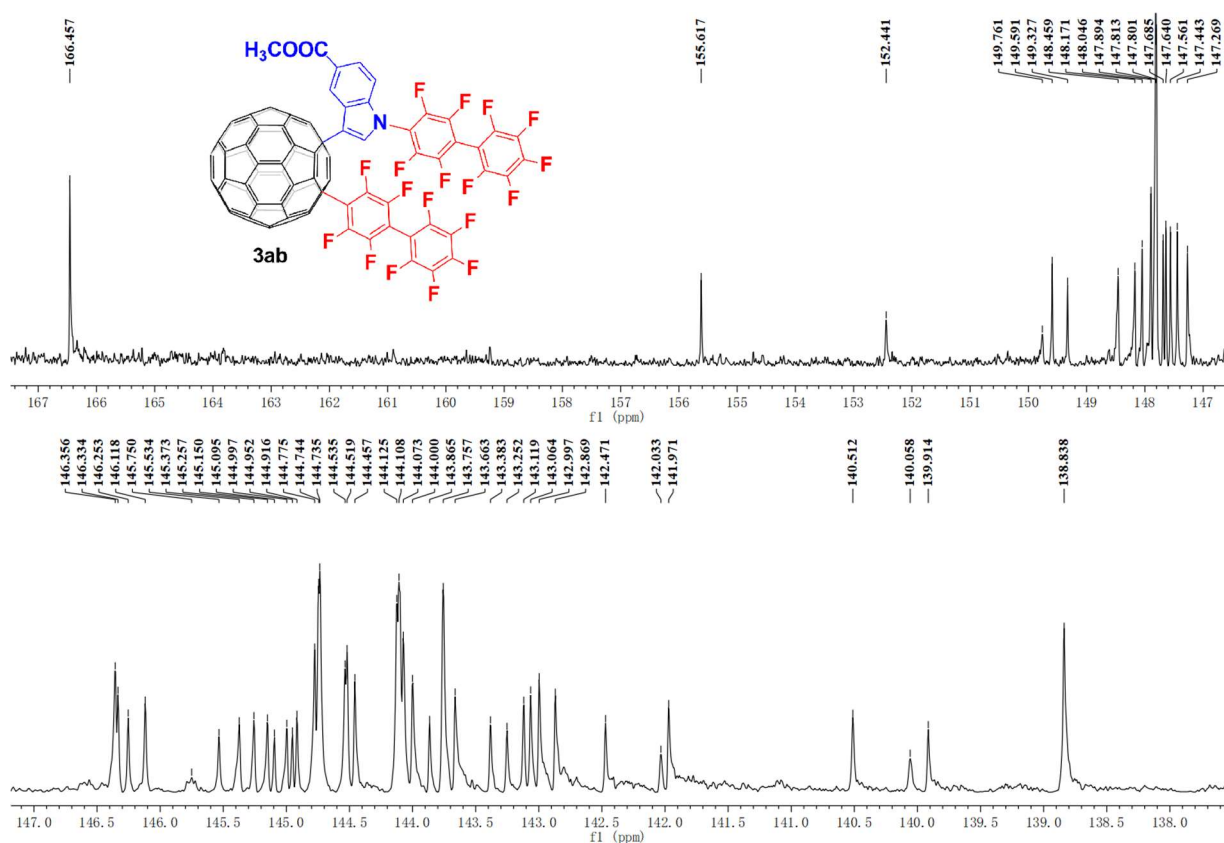
^{19}F NMR (376 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 3ab



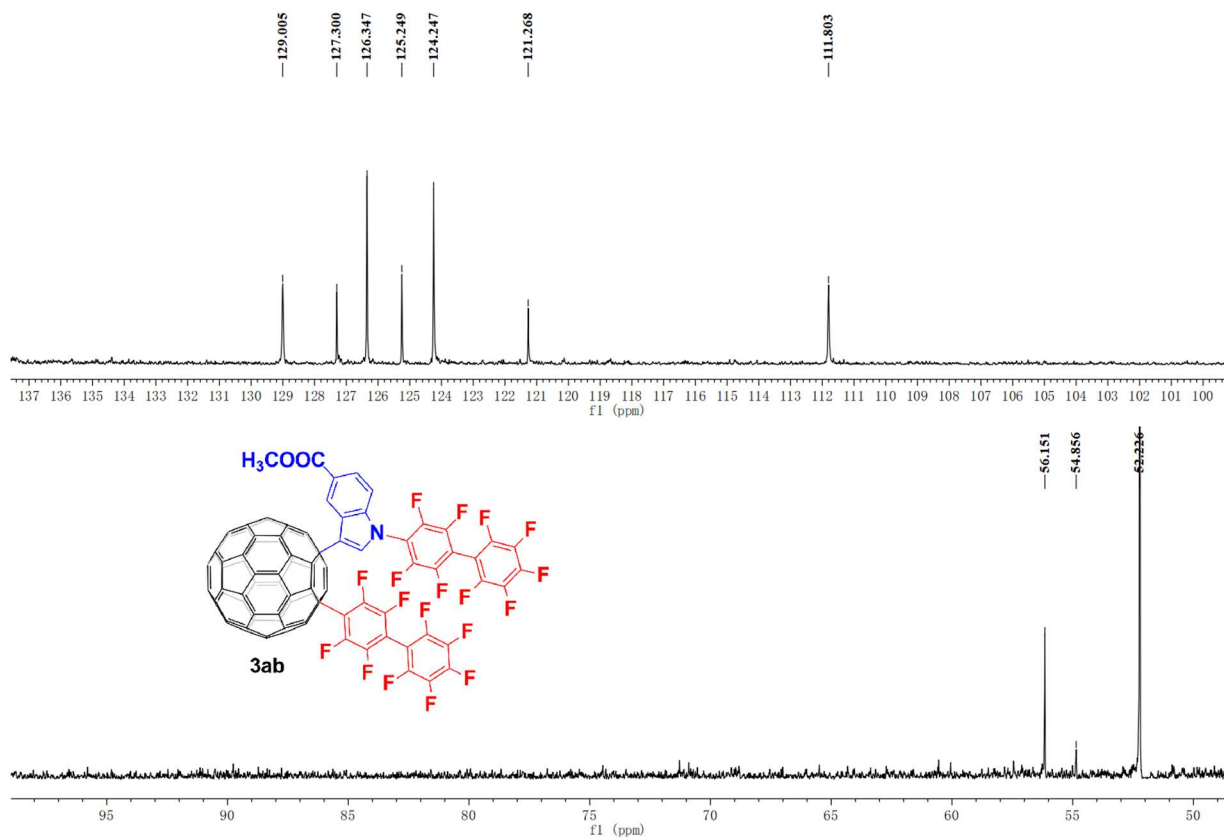
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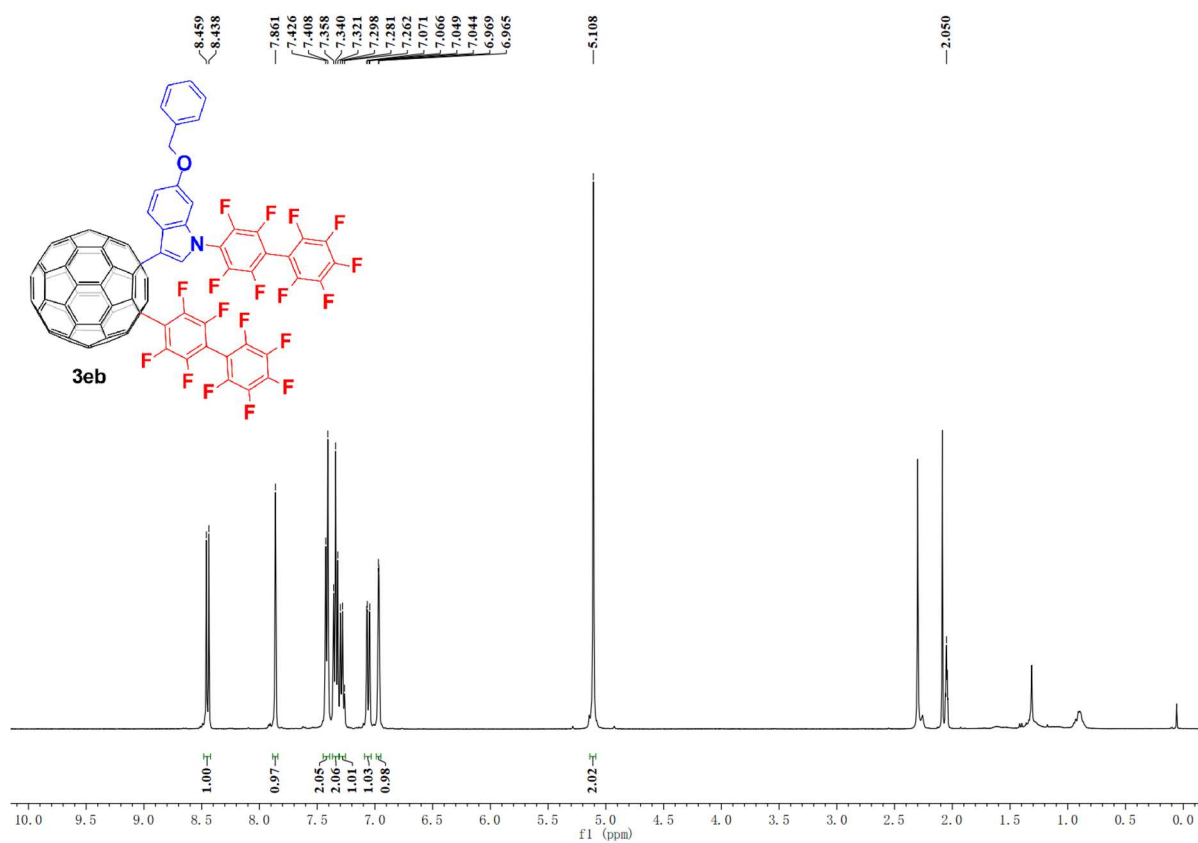
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound 3ab



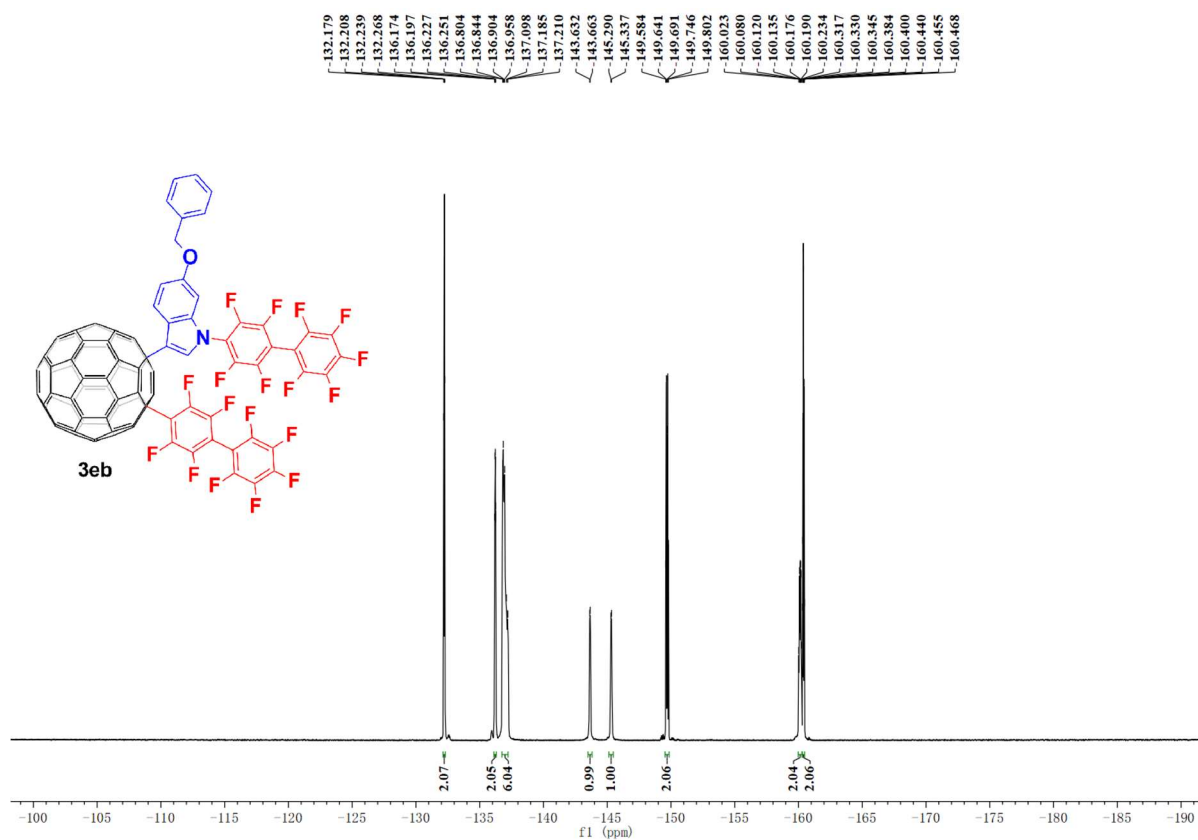
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound 3ab



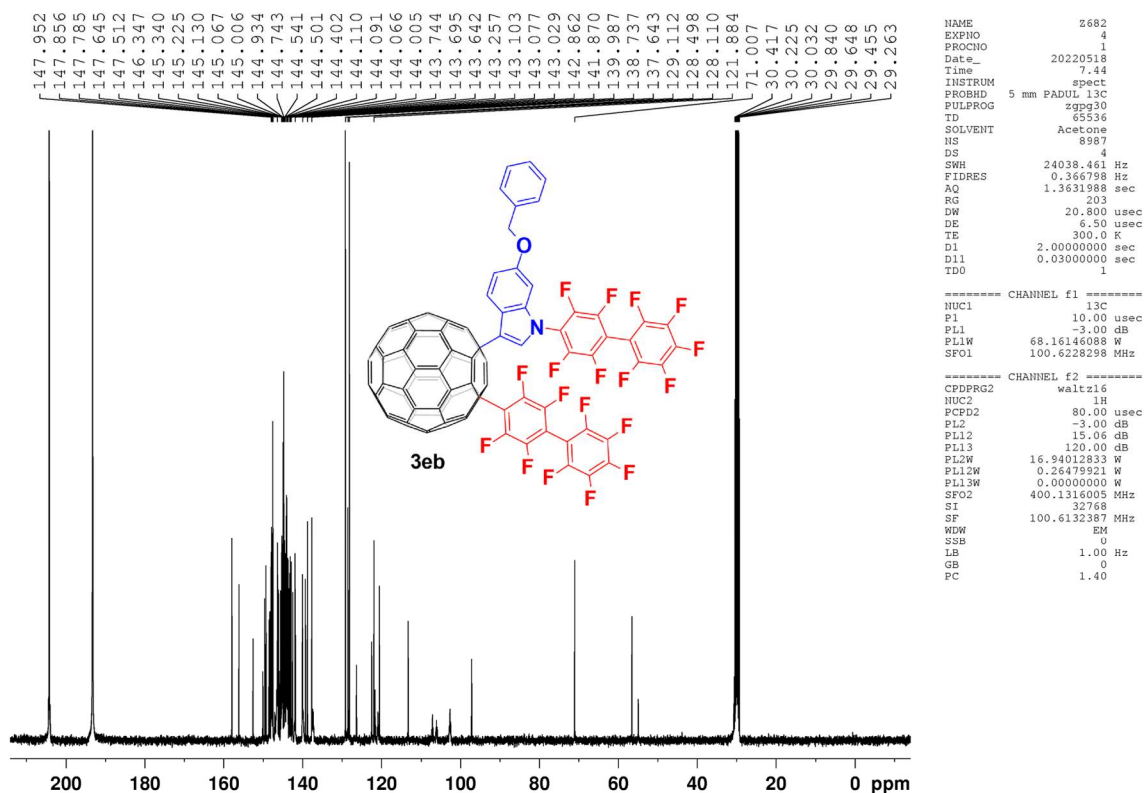
¹H NMR (400 MHz, CS₂/d₆-acetone) of compound 3eb



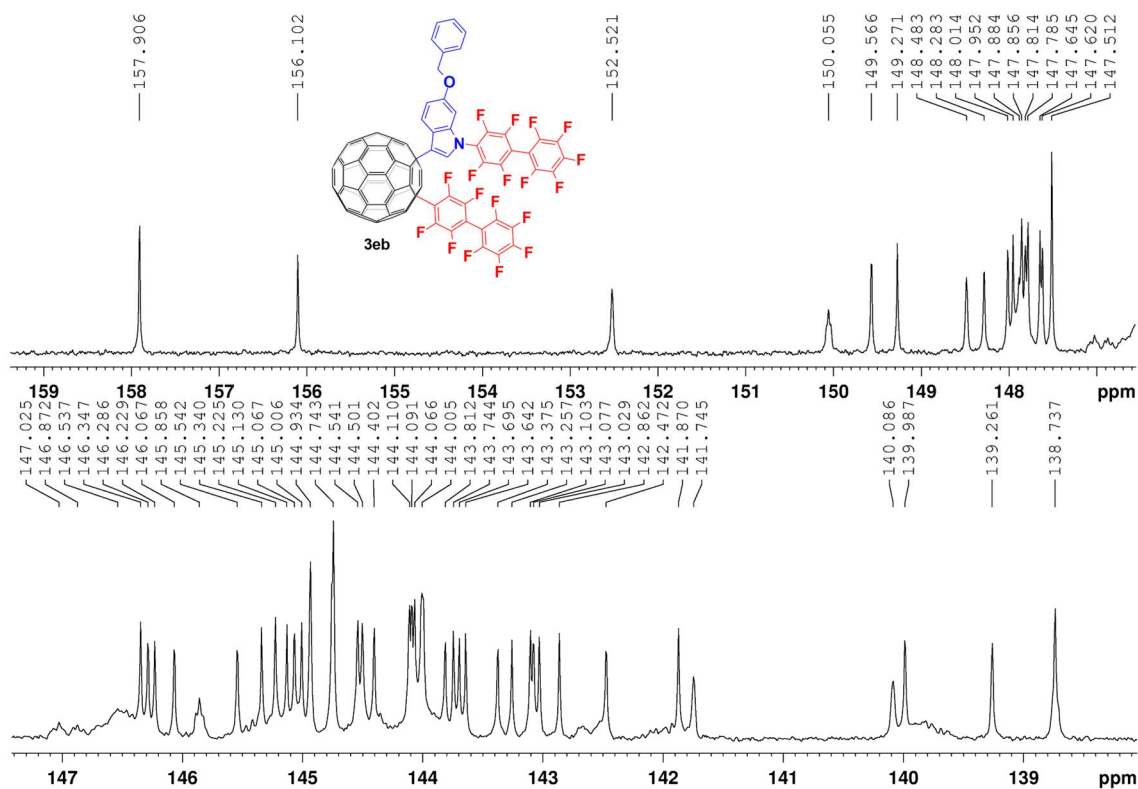
¹⁹F NMR (376 MHz, CS₂/d₆-acetone) of compound 3eb



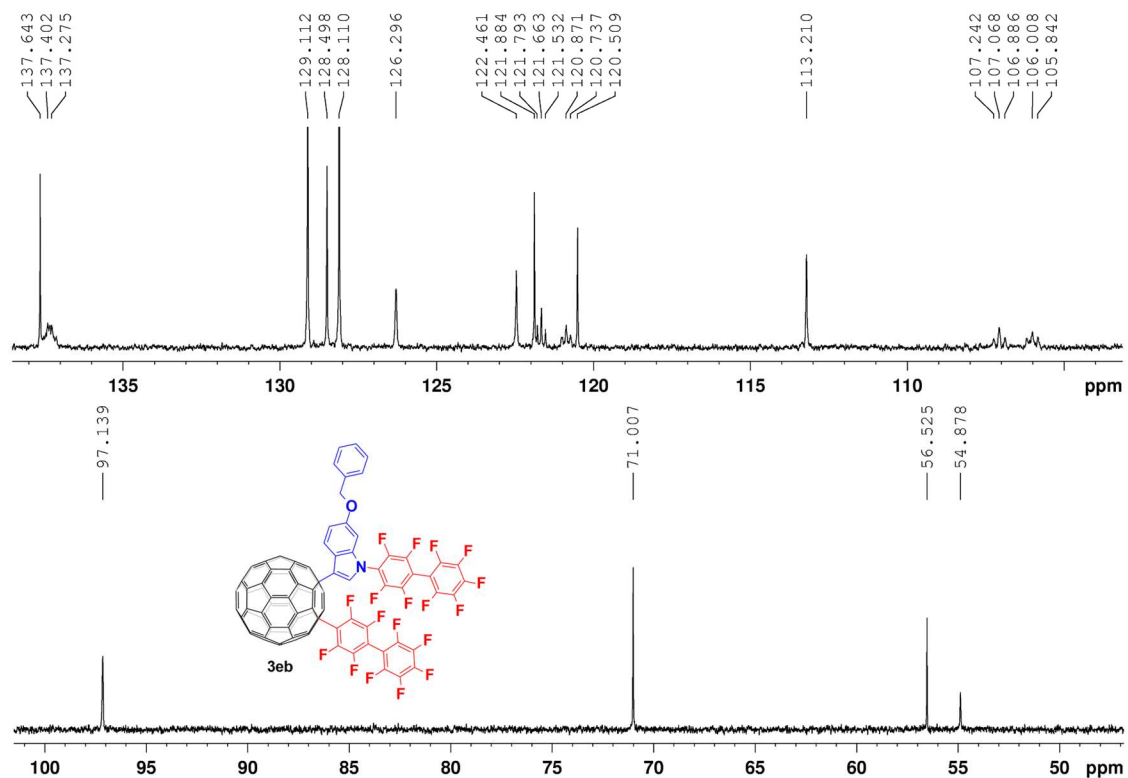
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 3eb



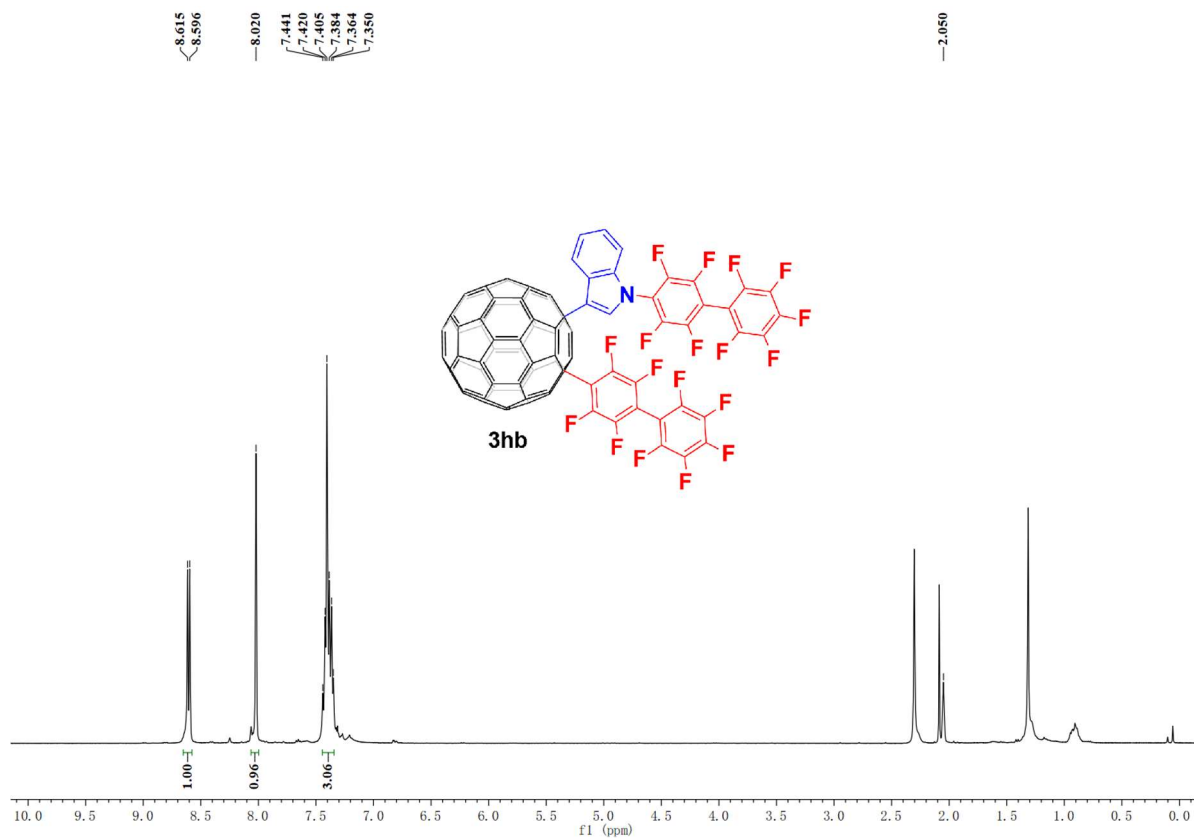
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 3eb



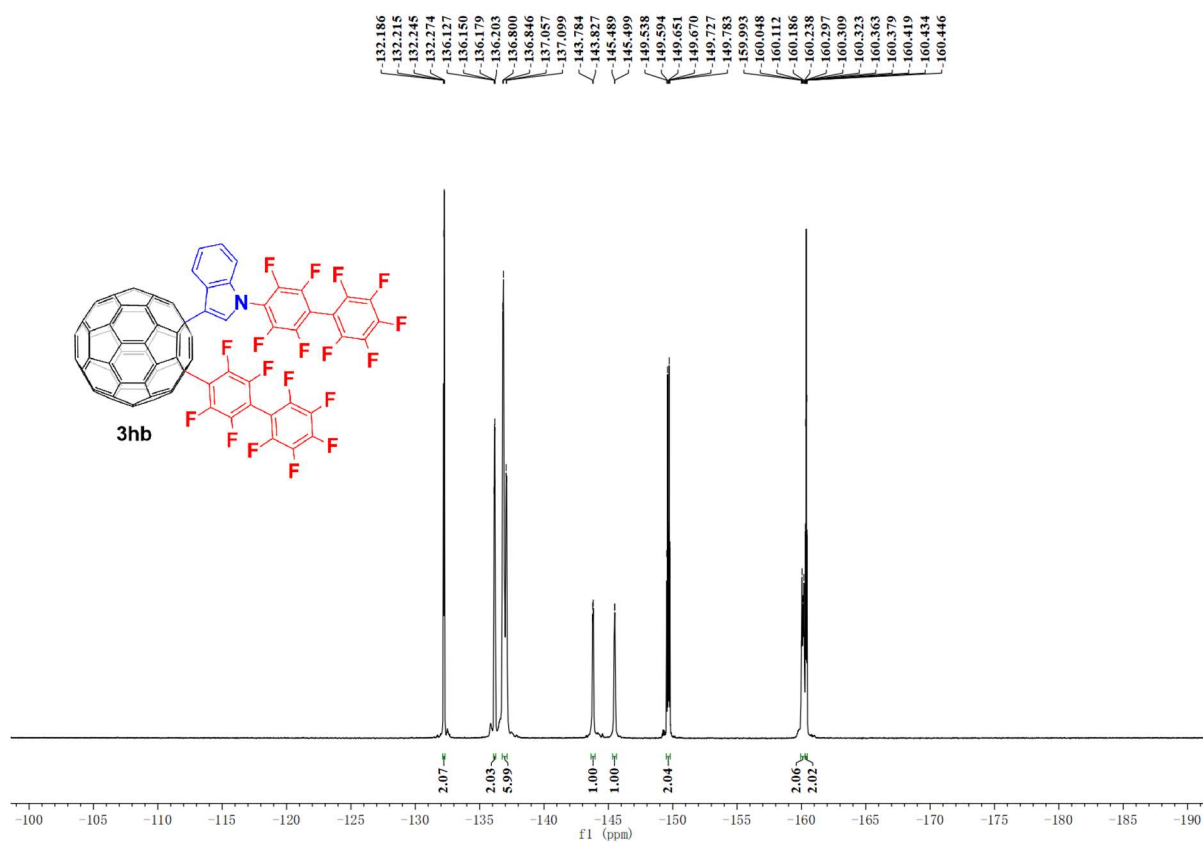
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 3eb



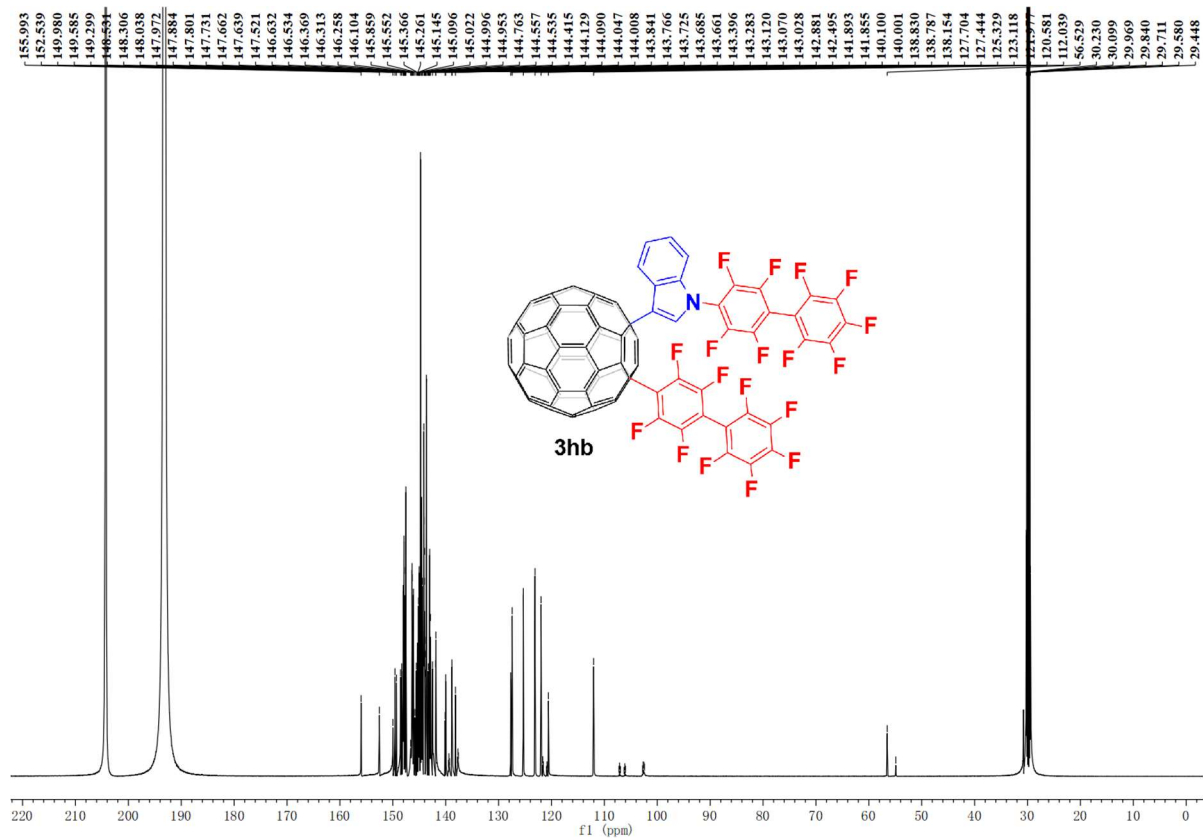
^1H NMR (400 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 3hb



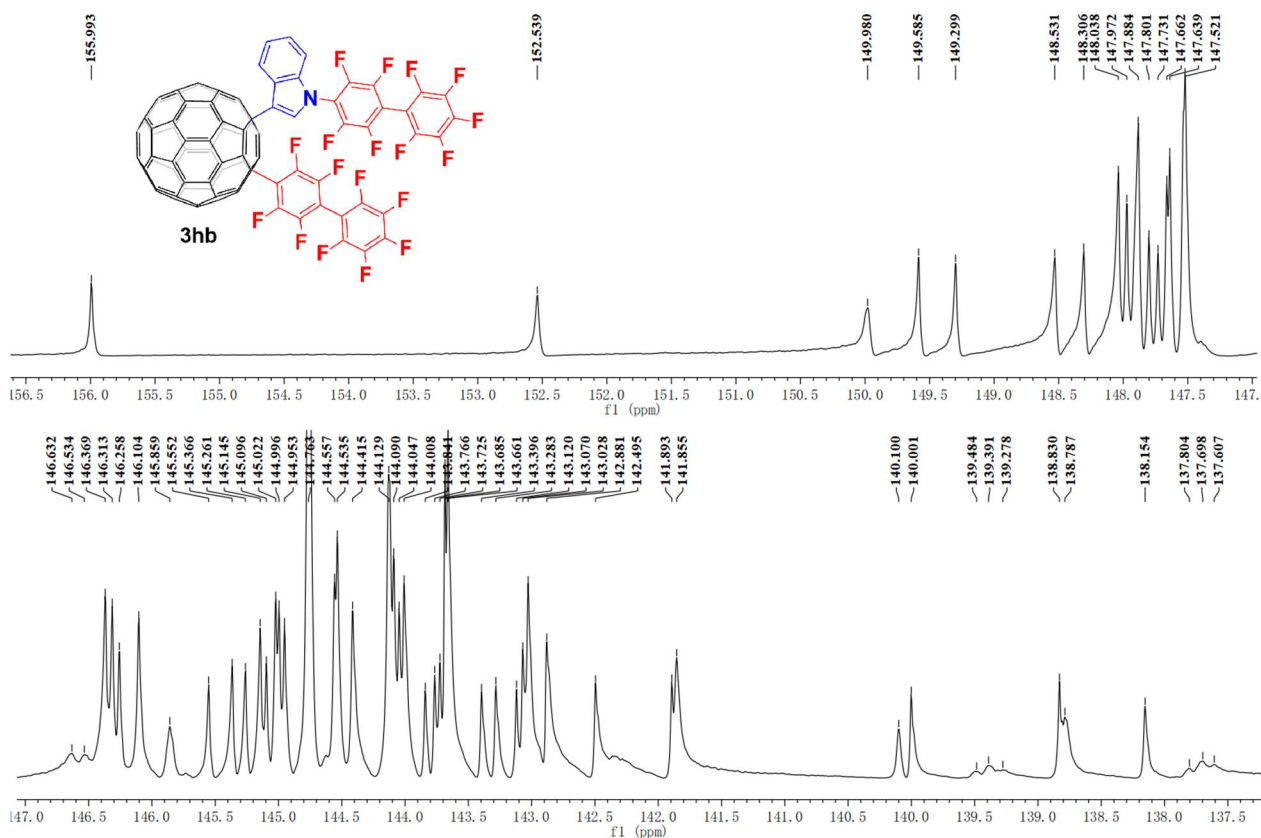
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 3hb



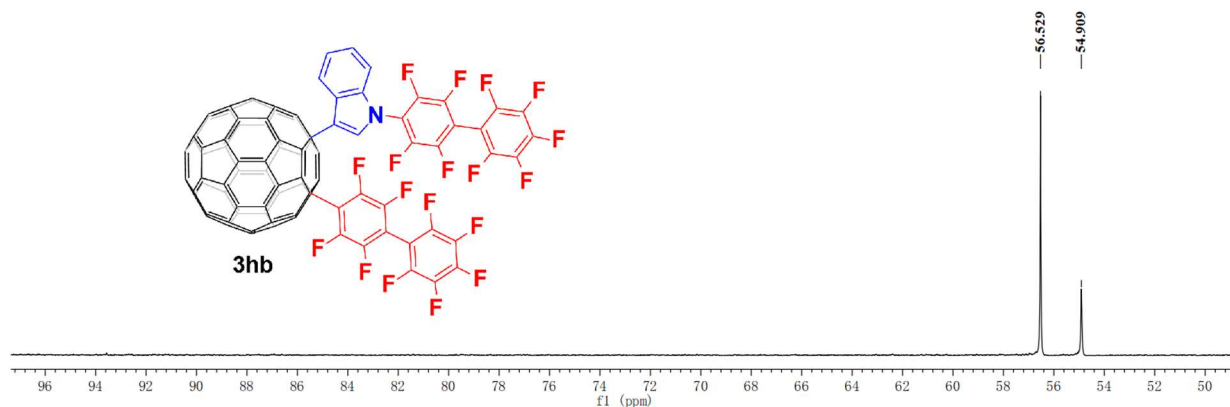
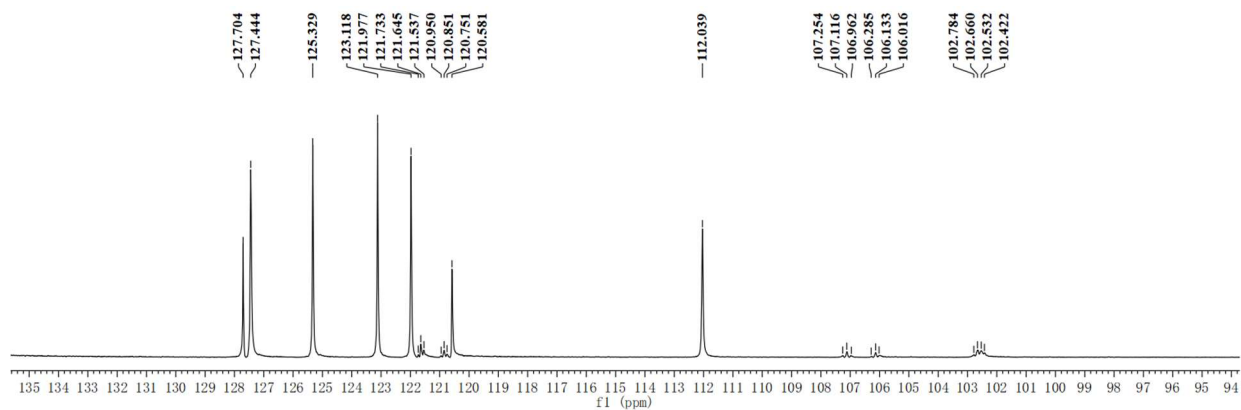
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3hb



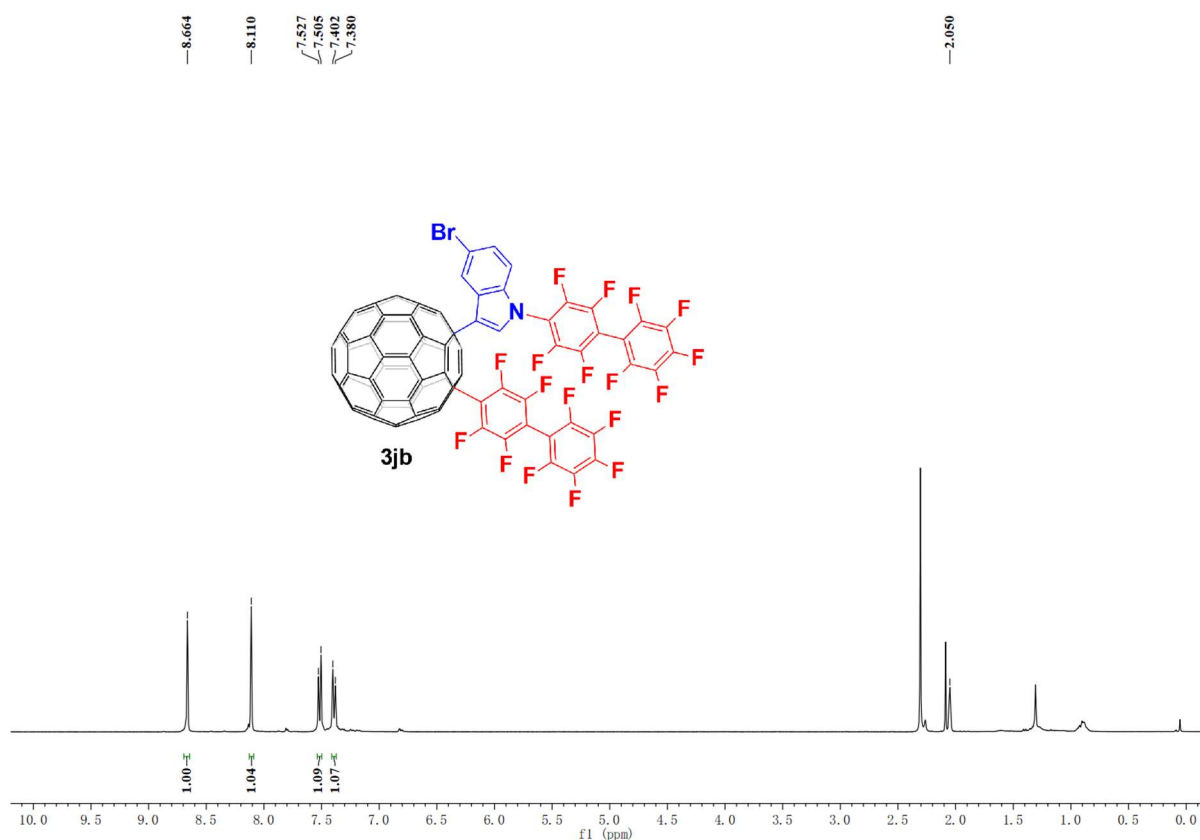
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3hb



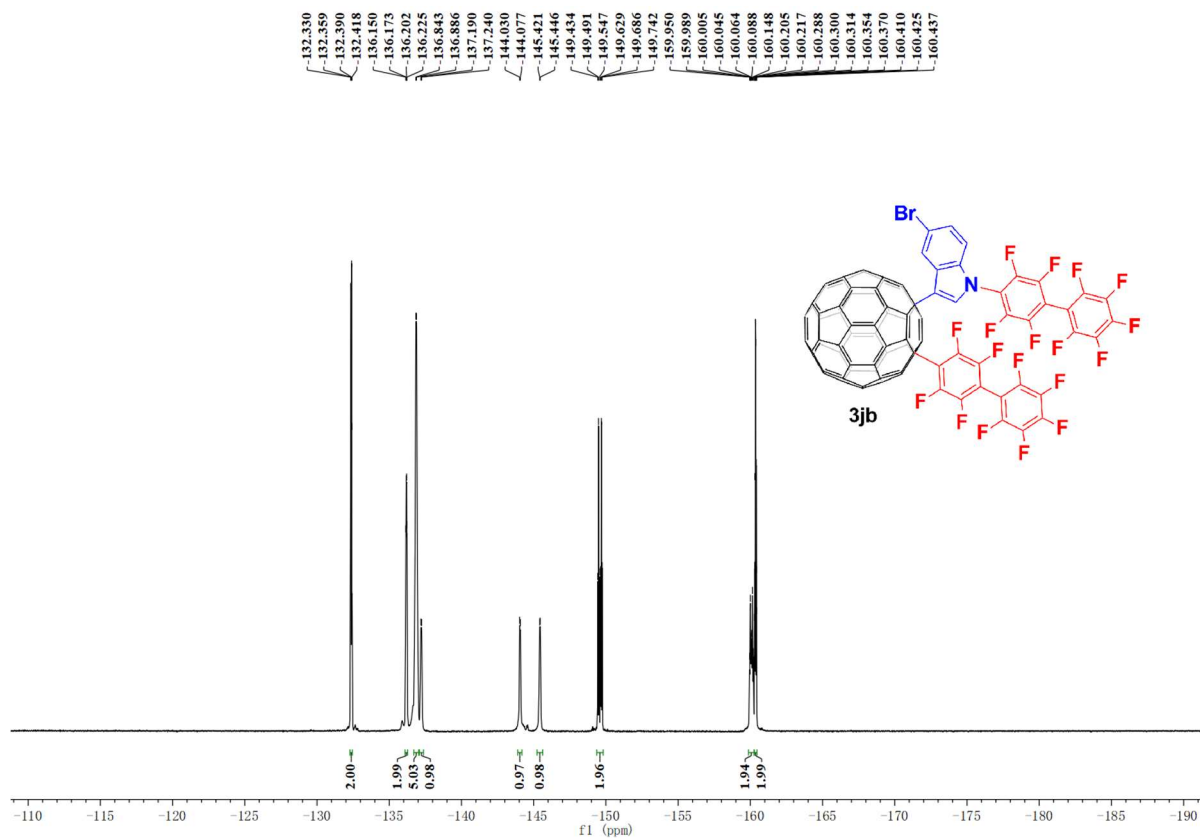
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3hb



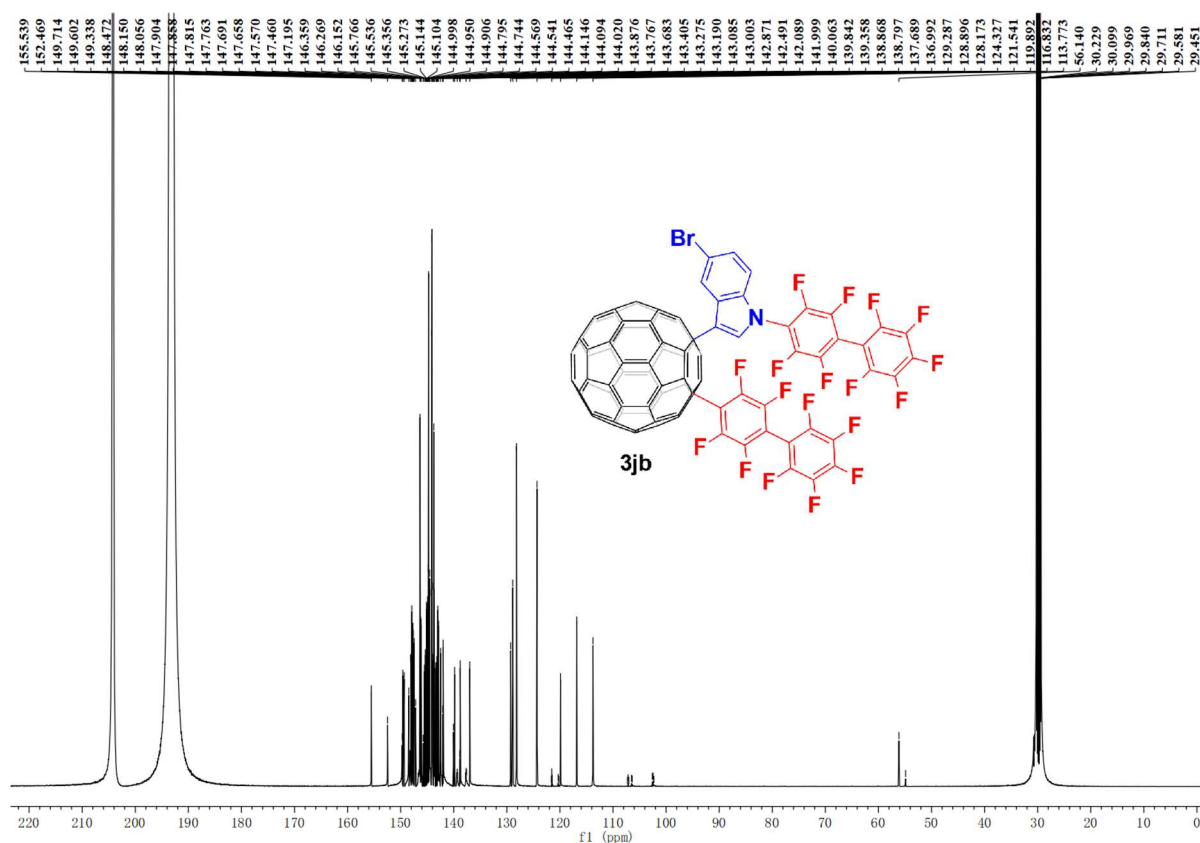
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 3jb



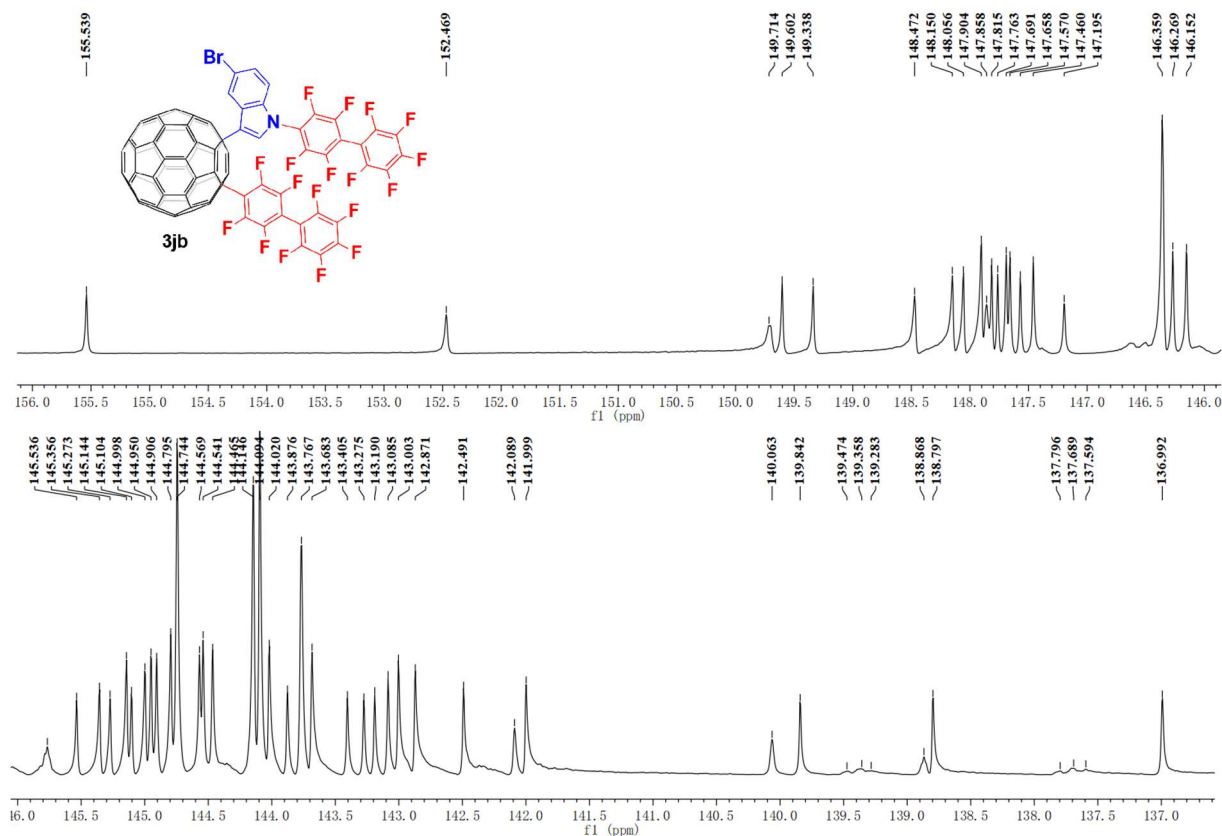
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 3jb



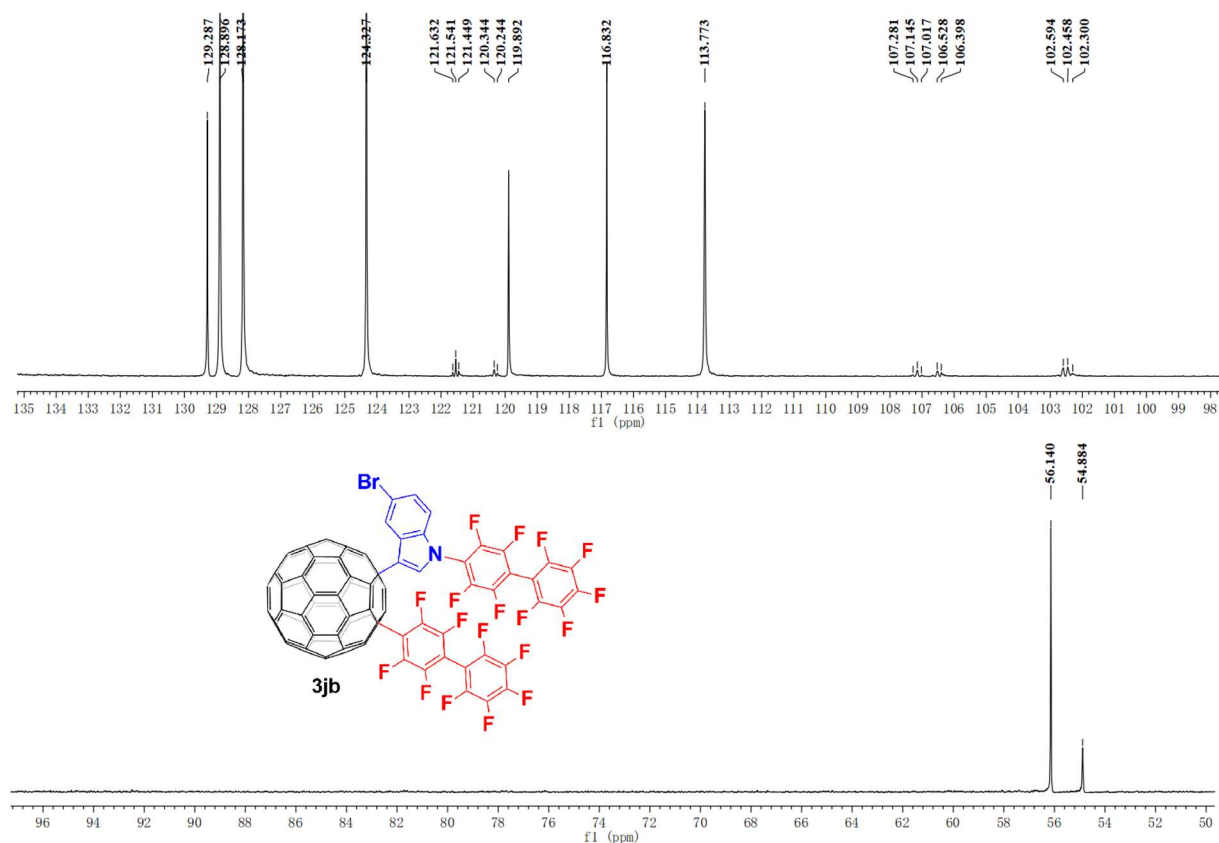
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 3jb



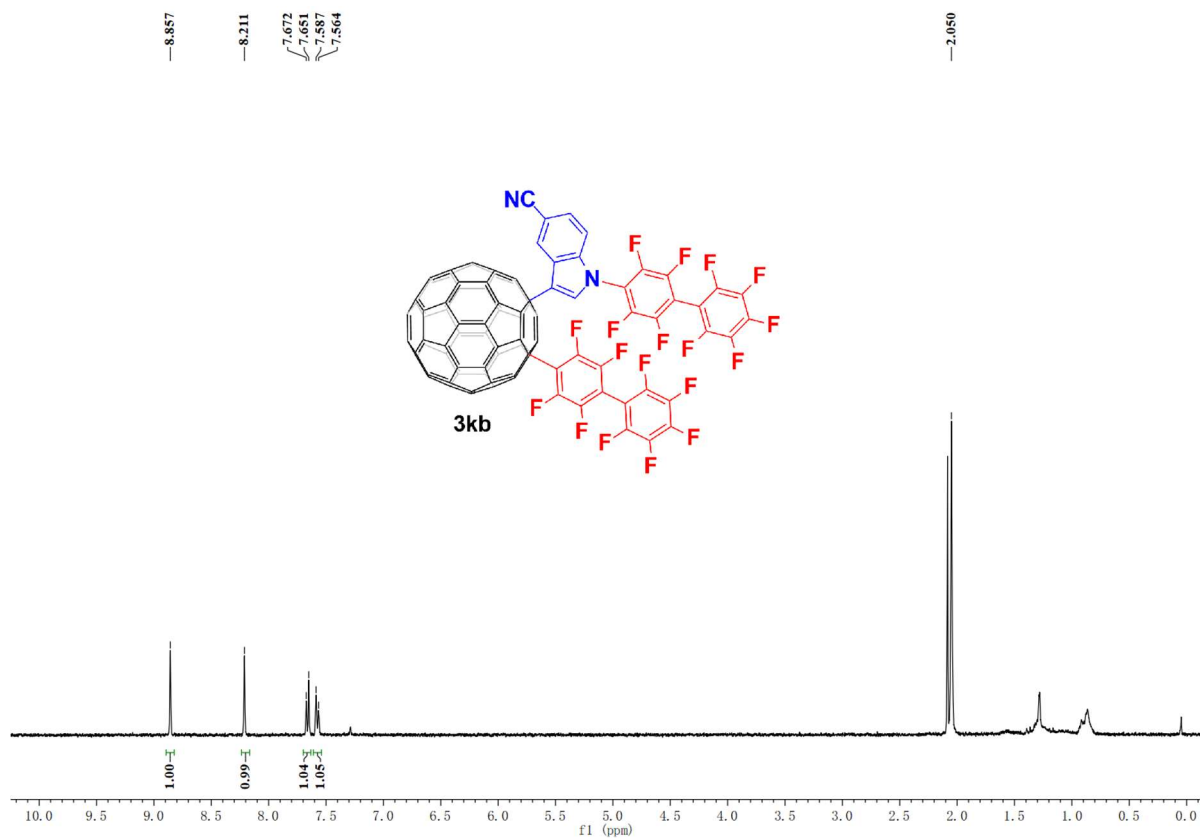
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 3jb



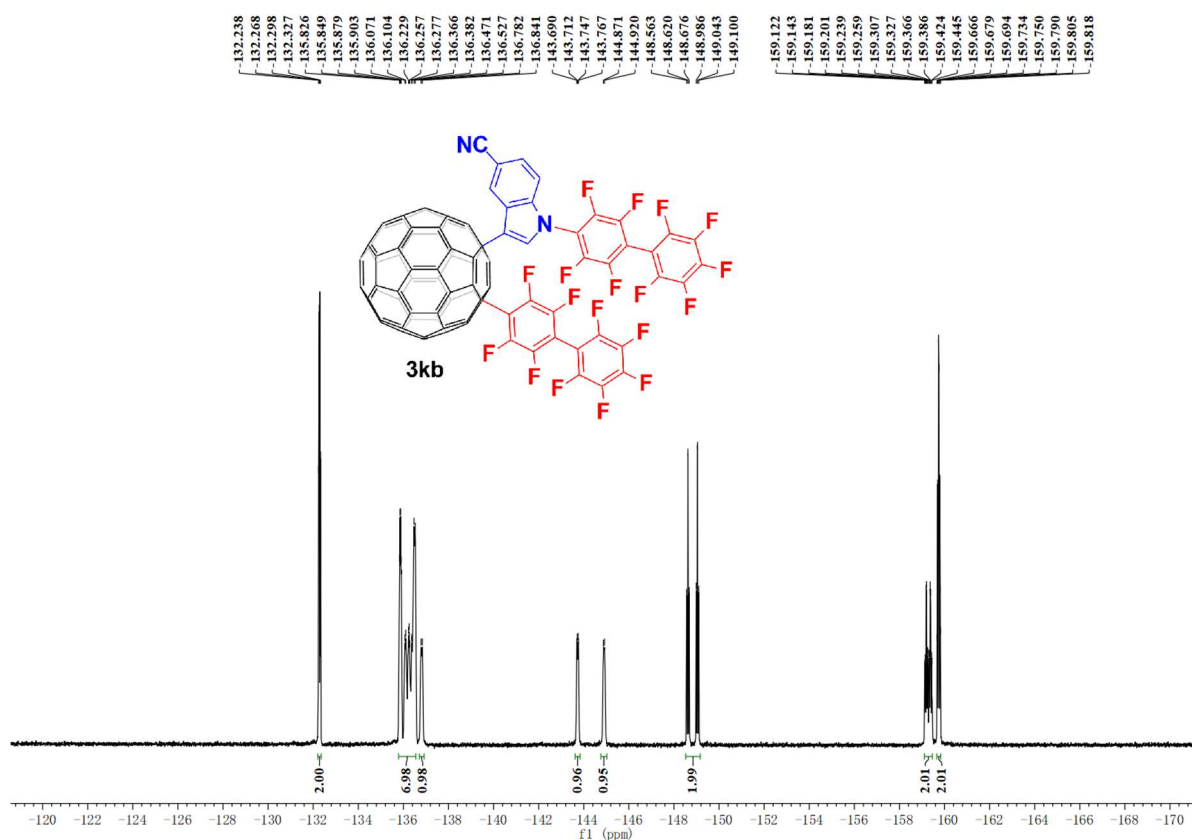
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3jb



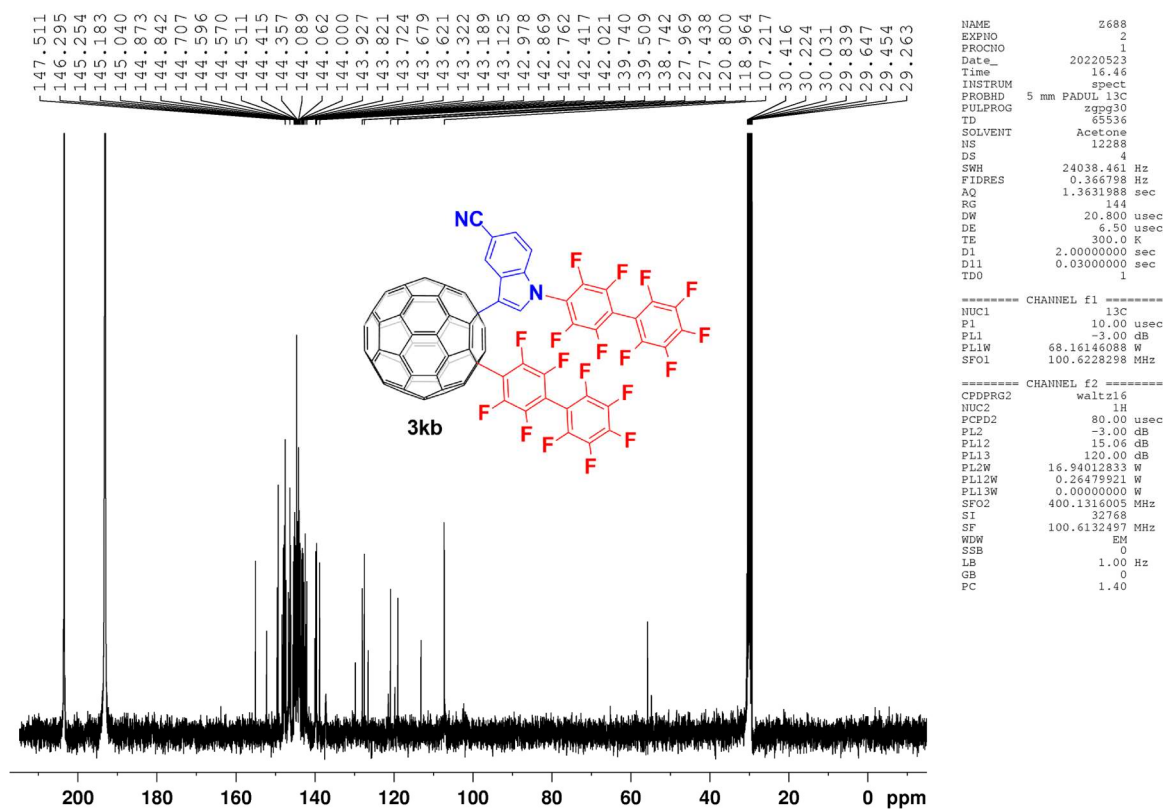
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 3kb



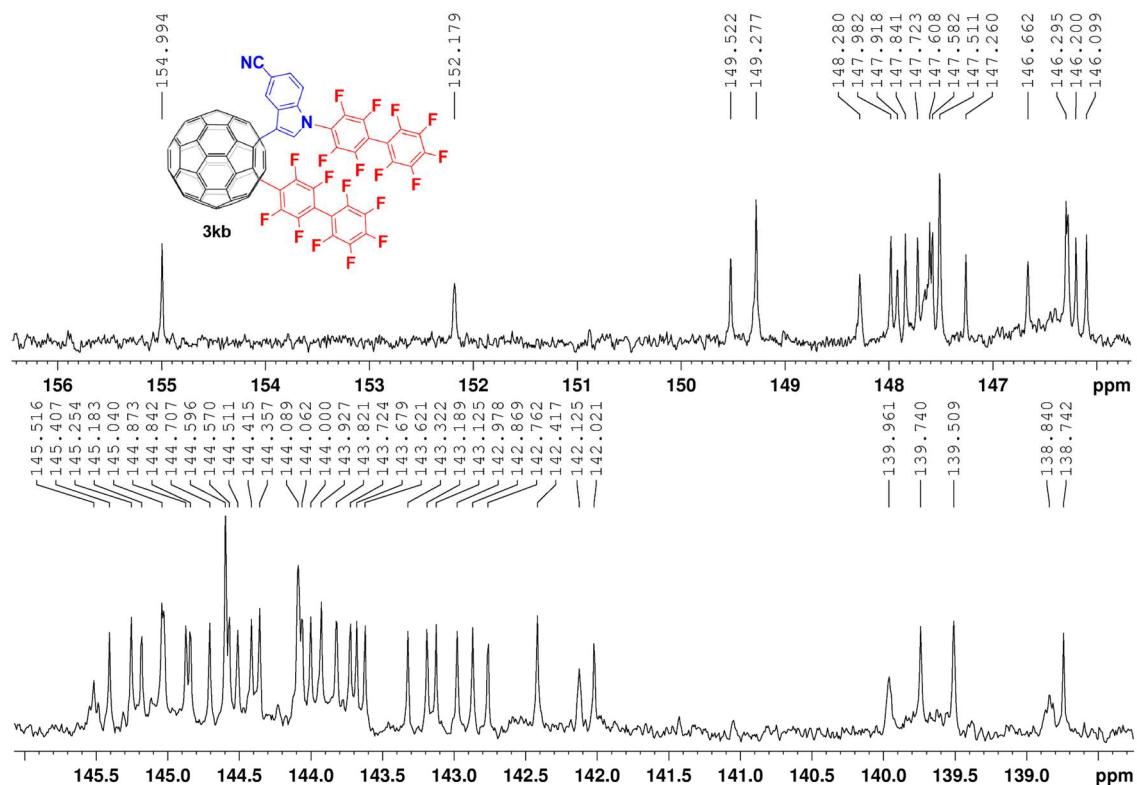
¹⁹F NMR (376 MHz, CS₂/d₆-acetone) of compound 3kb



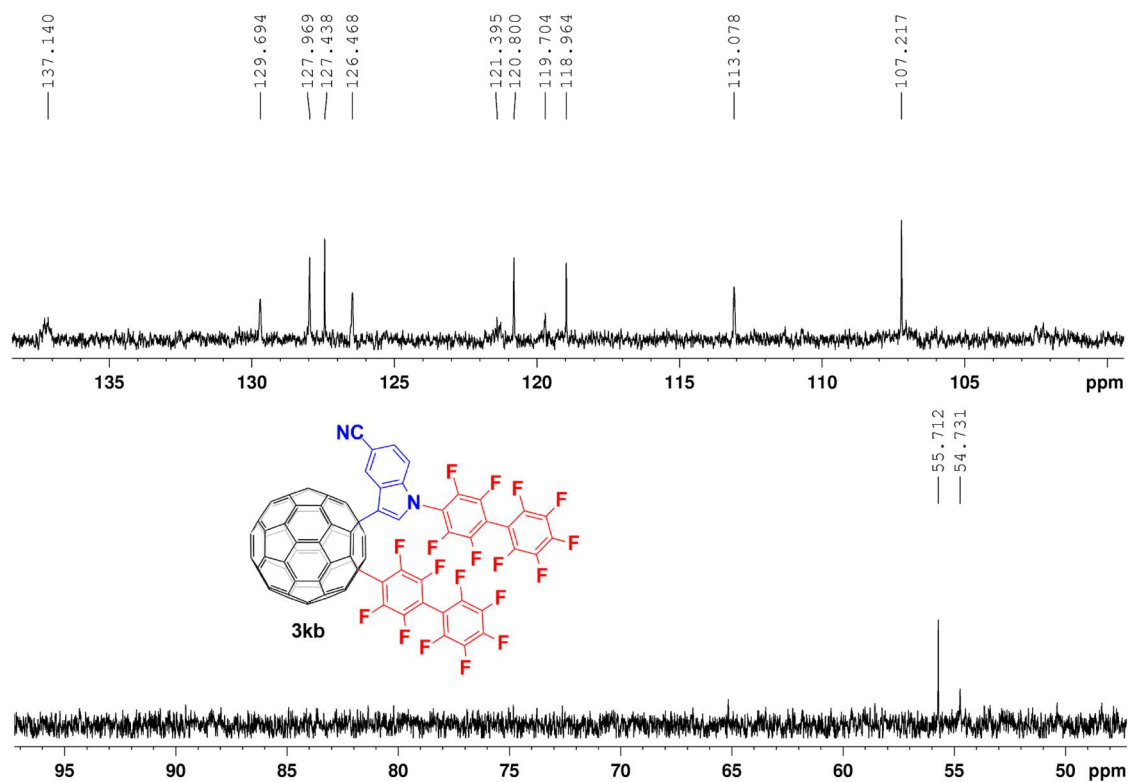
¹³C{¹H} NMR (100 MHz, CS₂/d₆-acetone) of compound 3kb



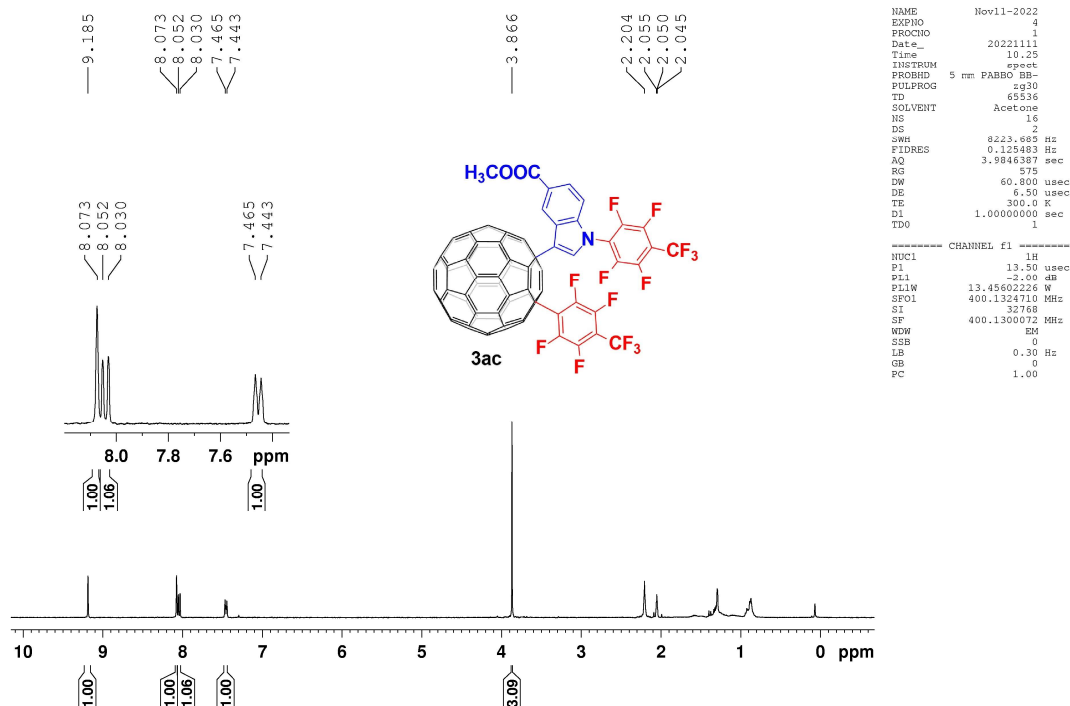
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3kb



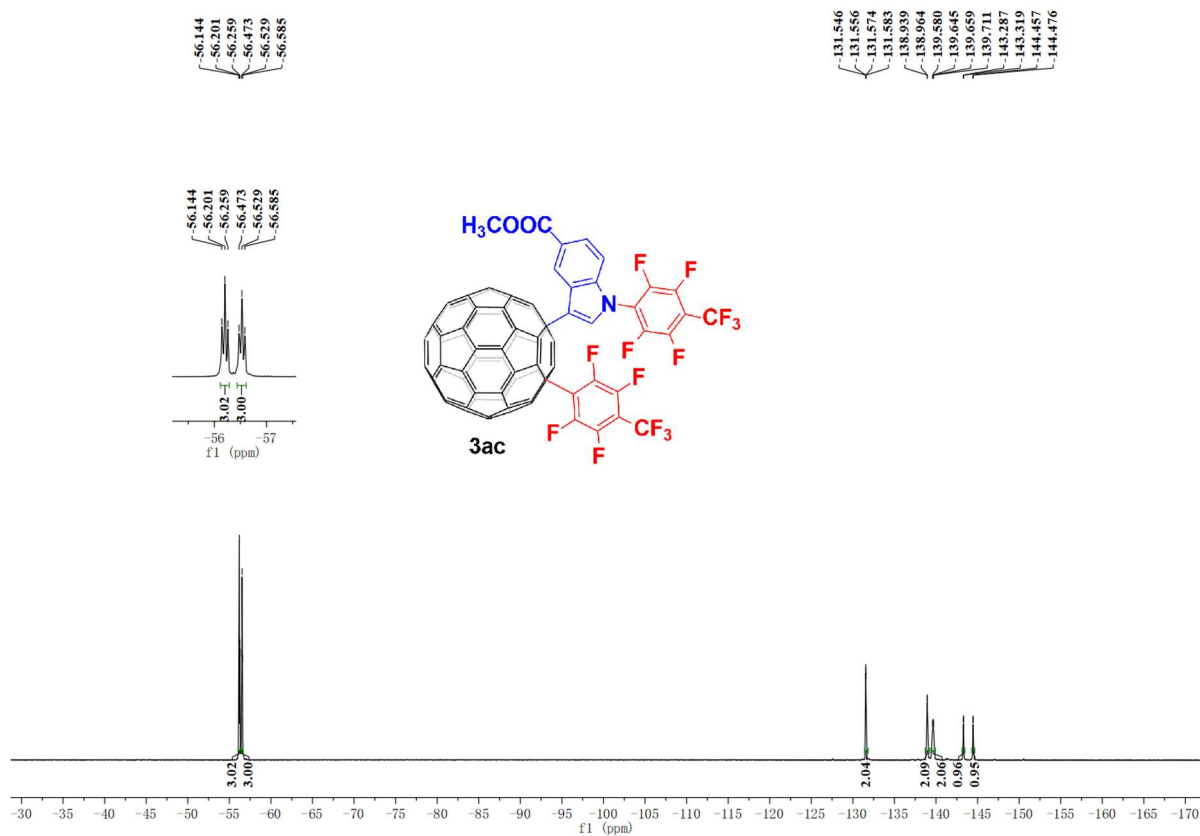
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3kb



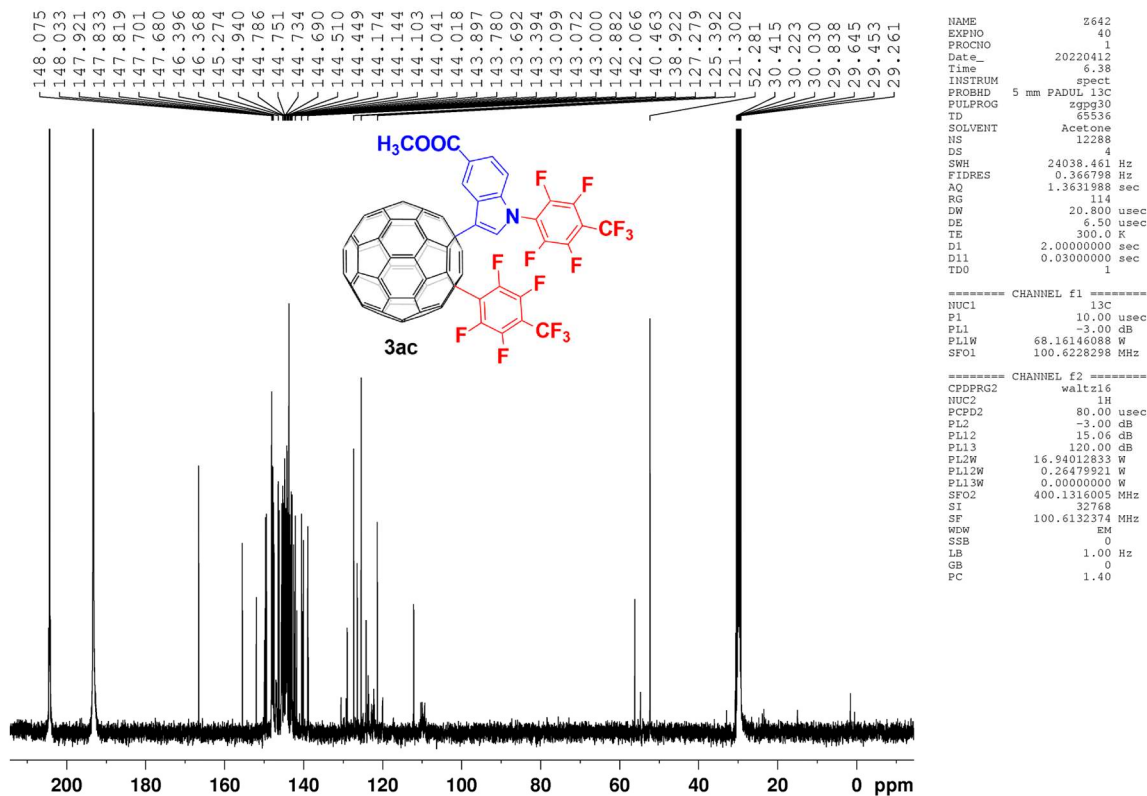
¹H NMR (400 MHz, CS₂/d₆-acetone) of compound 3ac



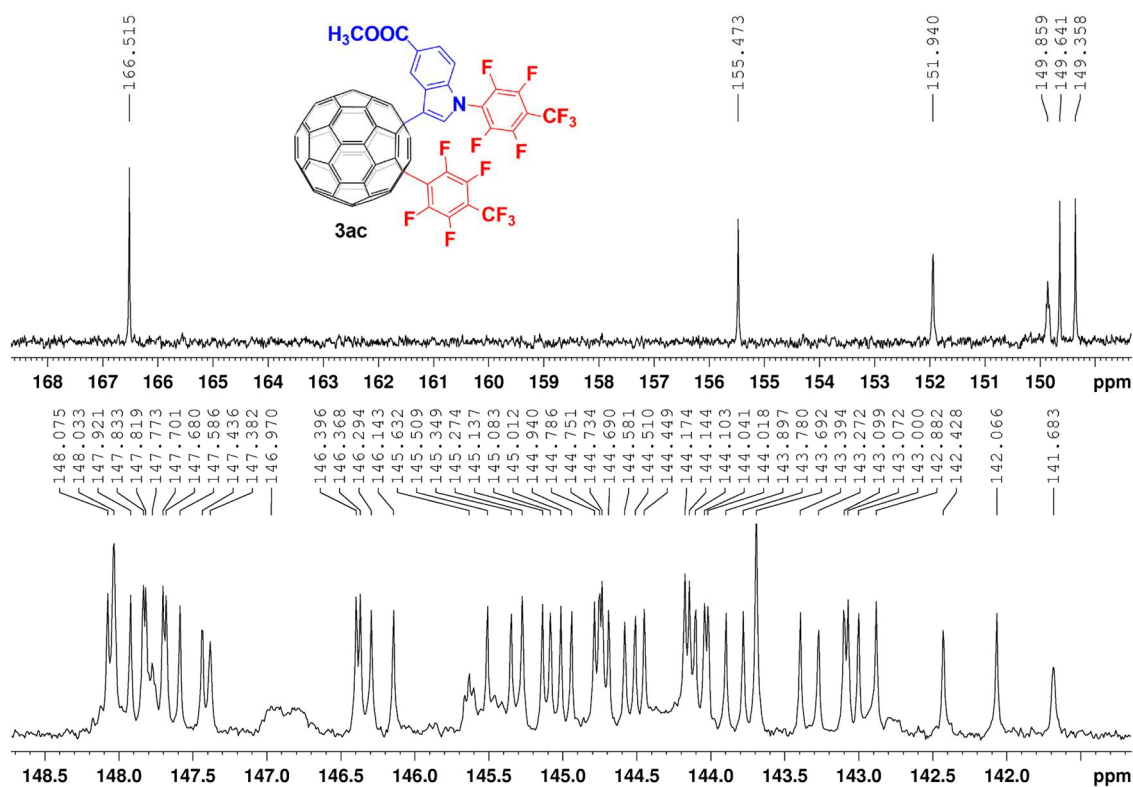
¹⁹F NMR (376 MHz, CS₂/d₆-acetone) of compound 3ac



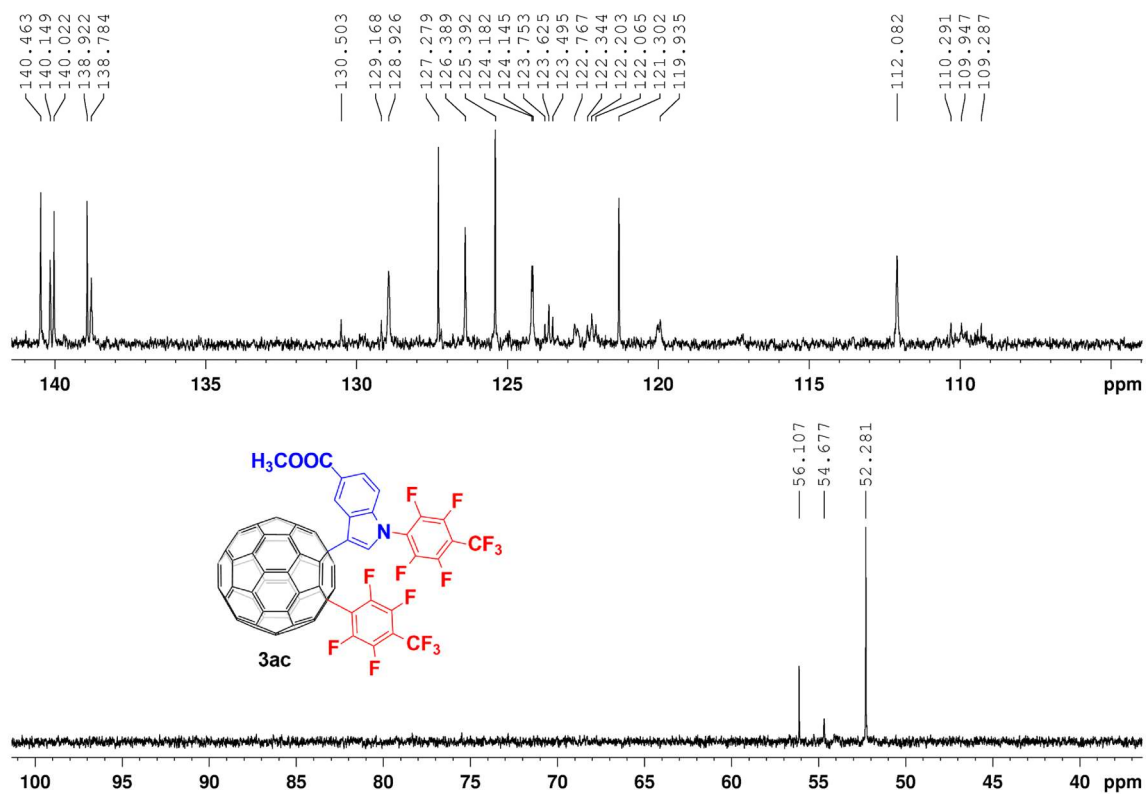
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **3ac**



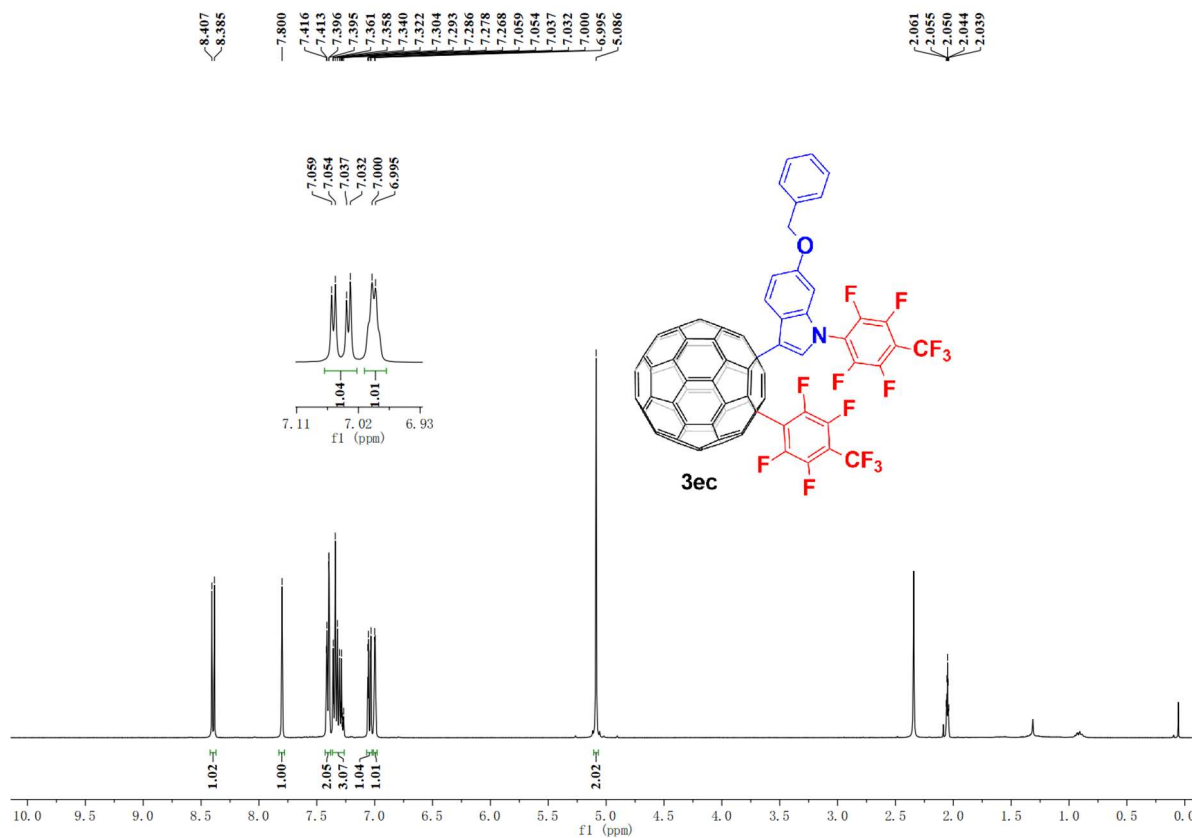
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **3ac**



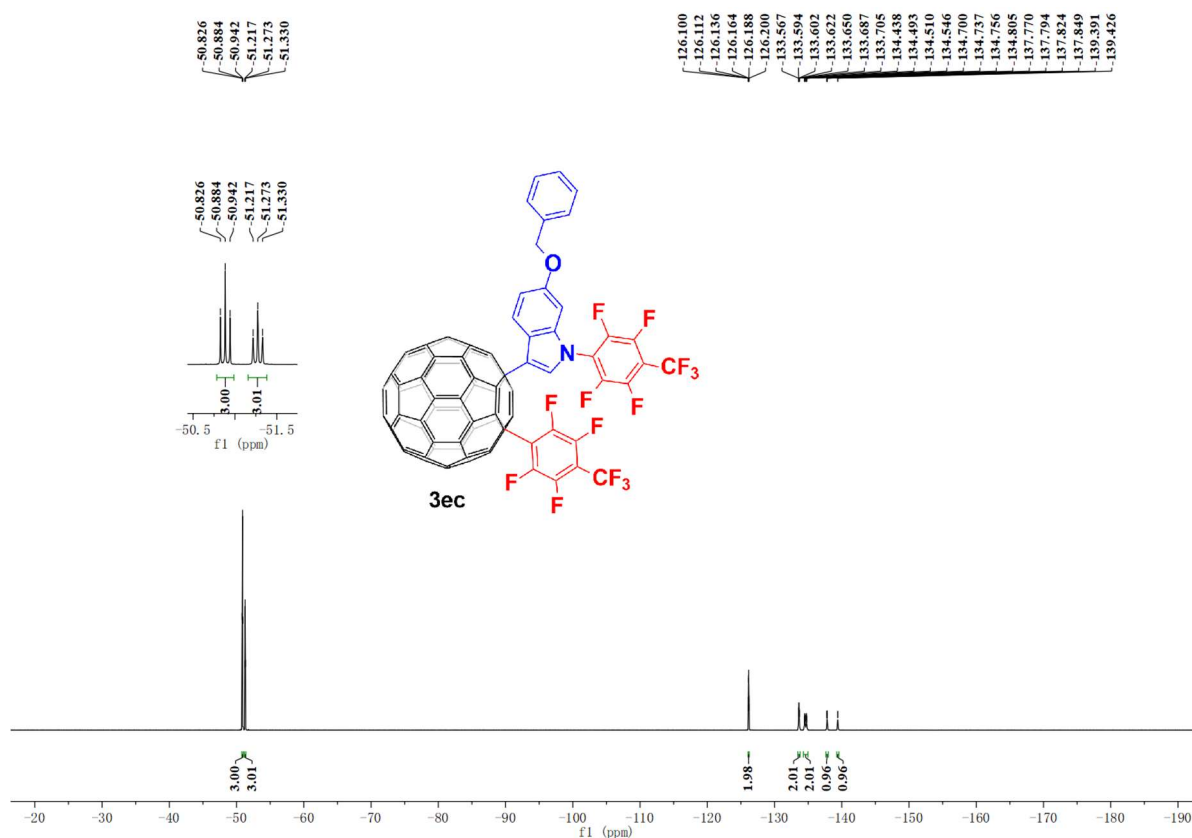
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **3ac**



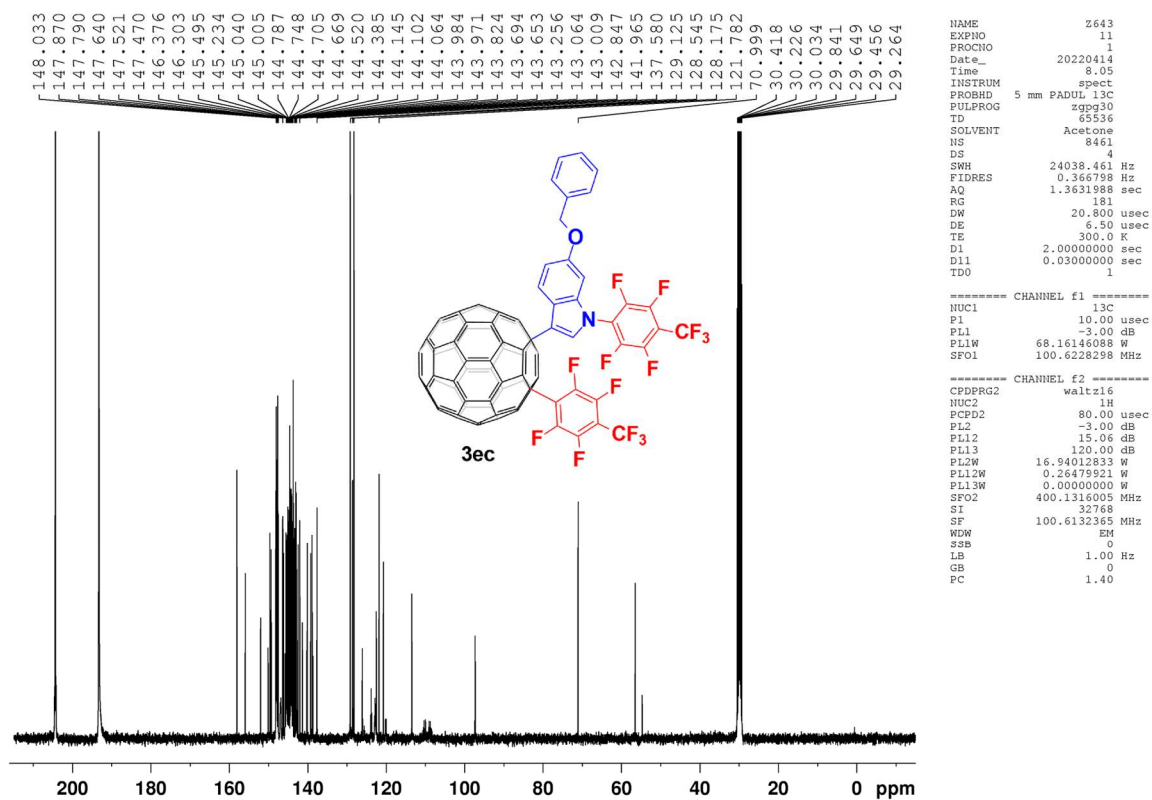
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **3ec**



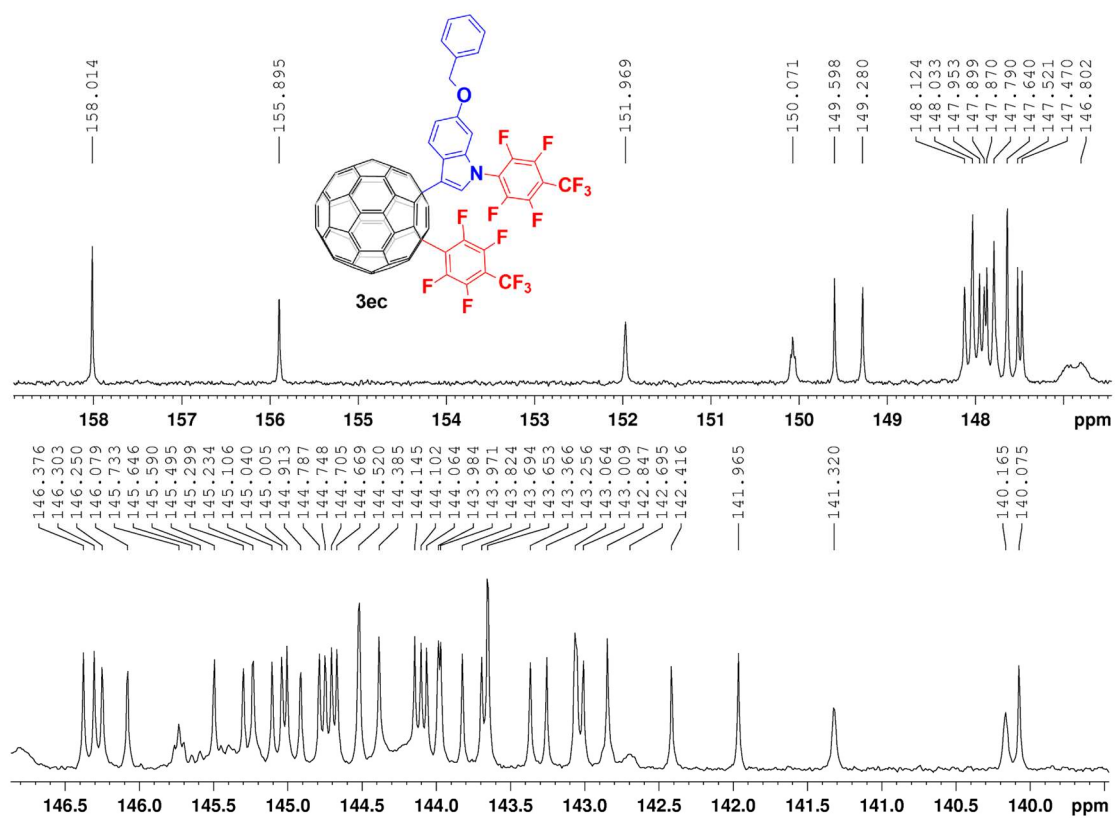
¹⁹F NMR (376 MHz, CS₂/d₆-acetone) of compound 3ec



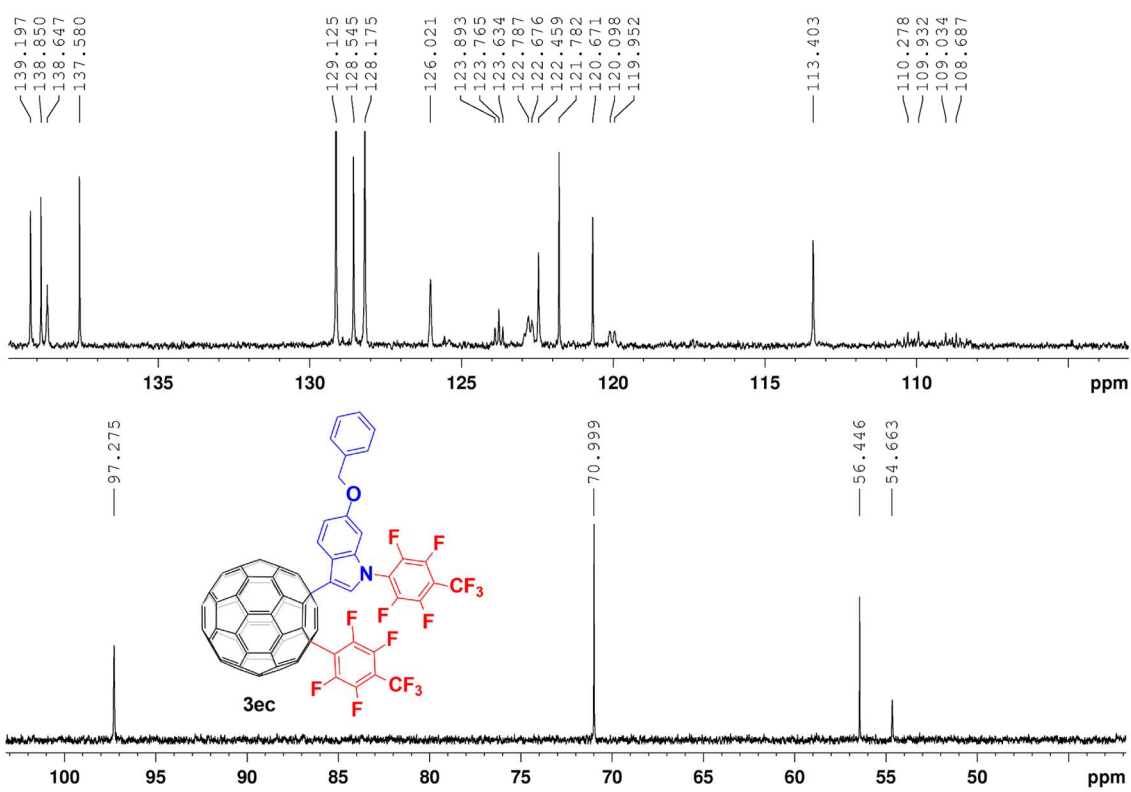
¹³C{¹H} NMR (100 MHz, CS₂/d₆-acetone) of compound 3ec



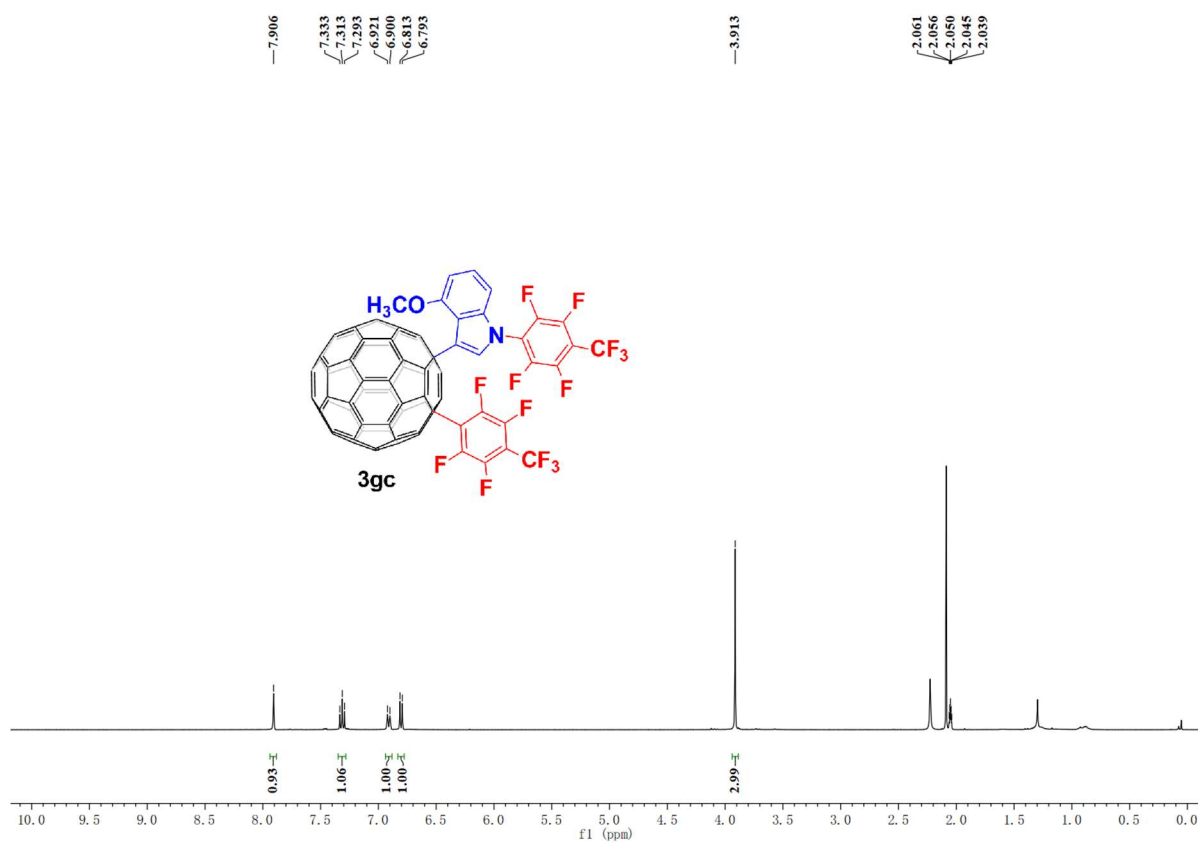
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **3ec**



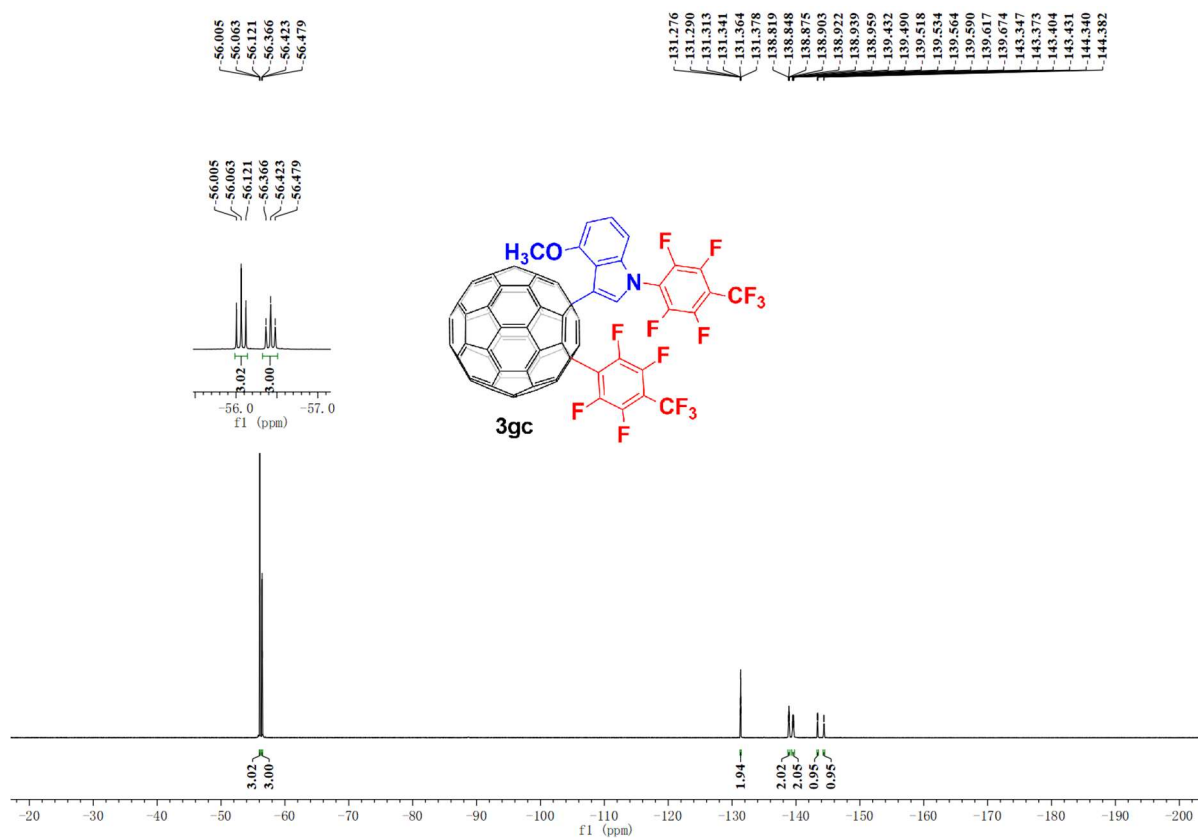
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **3ec**



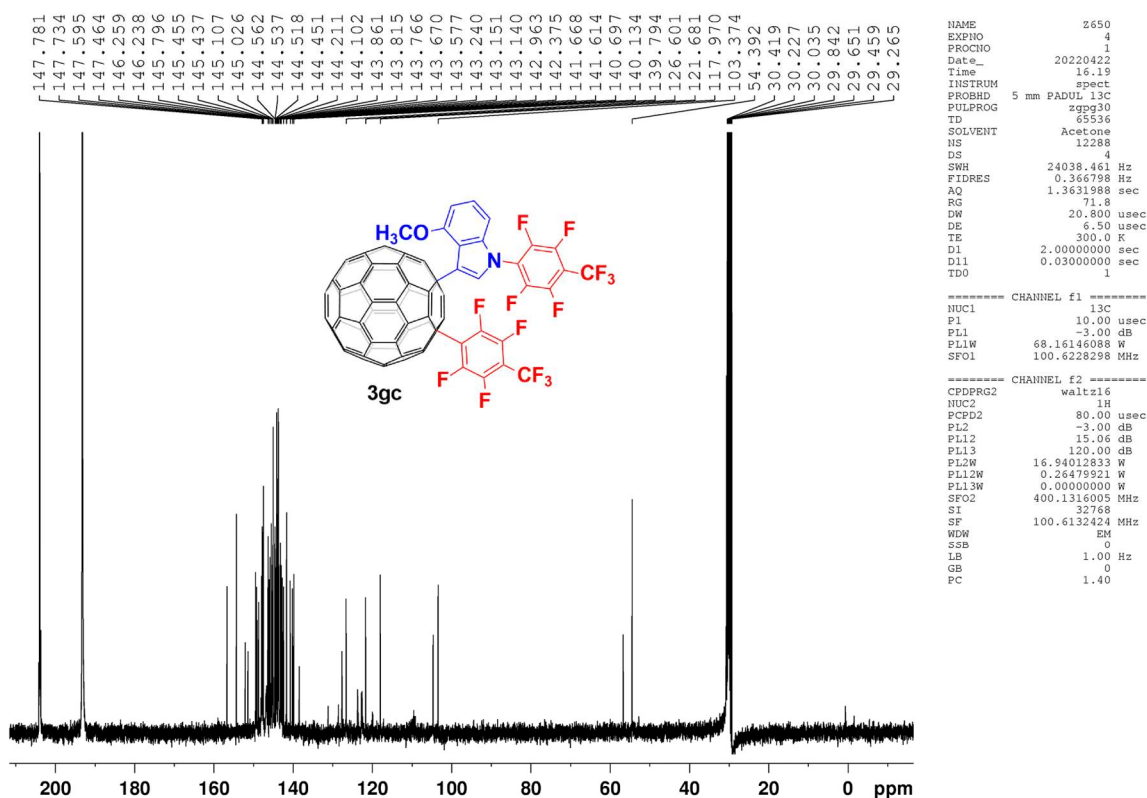
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **3gc**



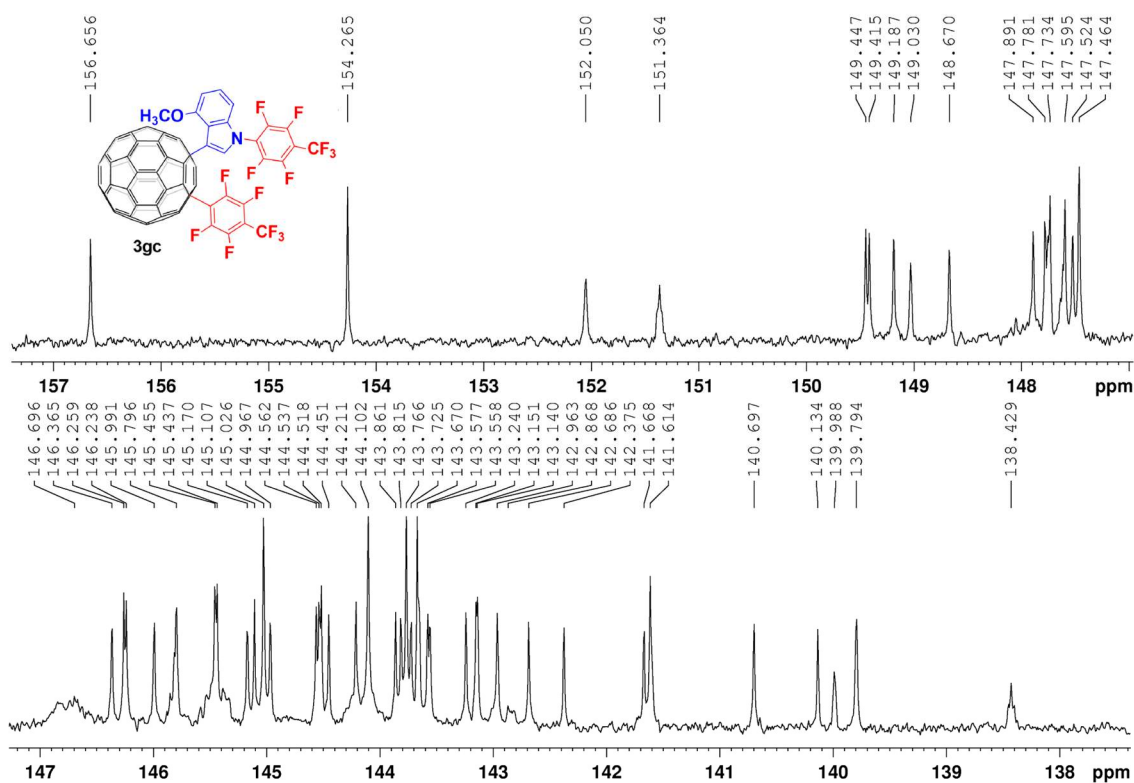
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound **3gc**



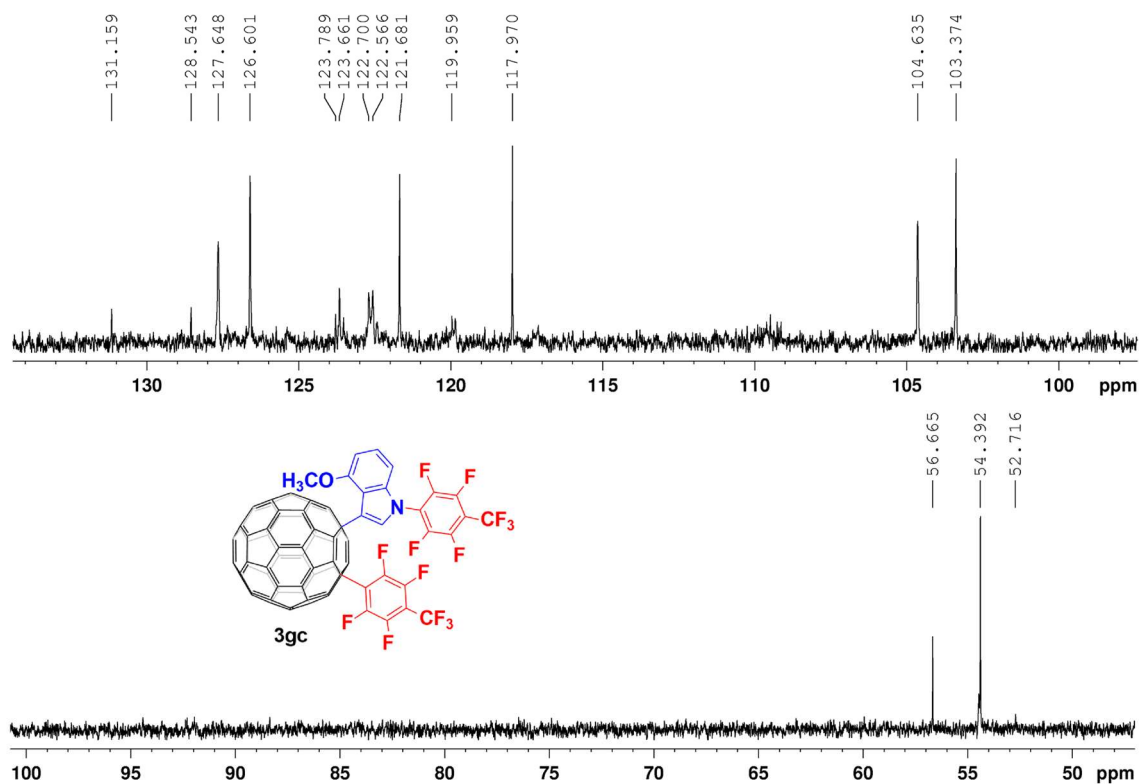
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **3gc**



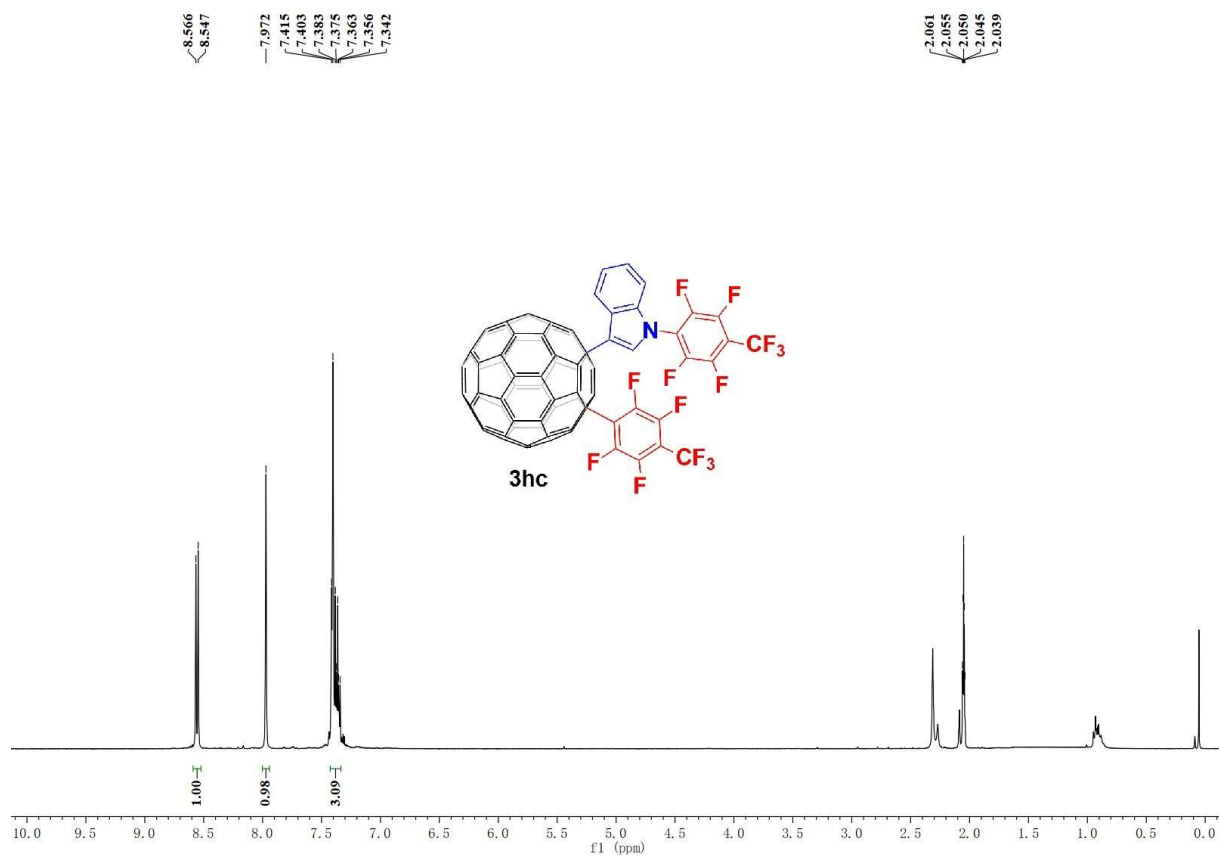
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **3gc**



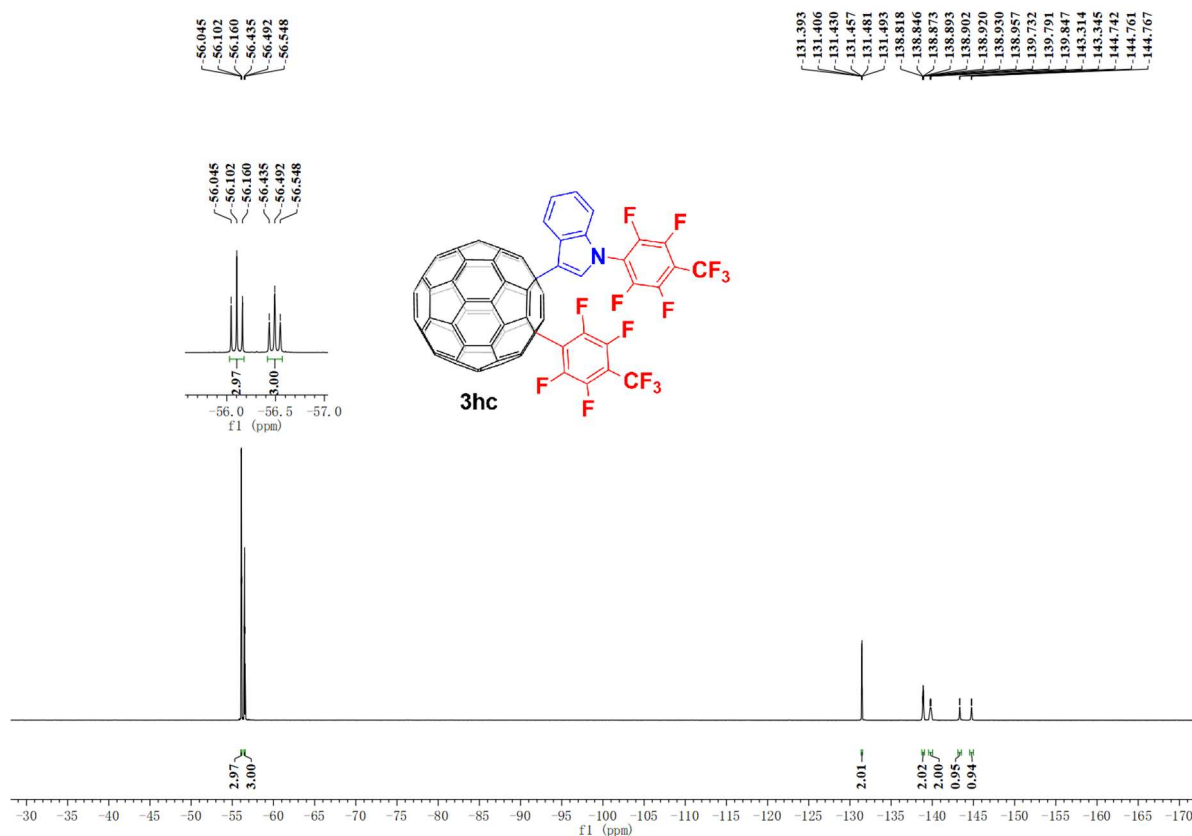
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **3gc**



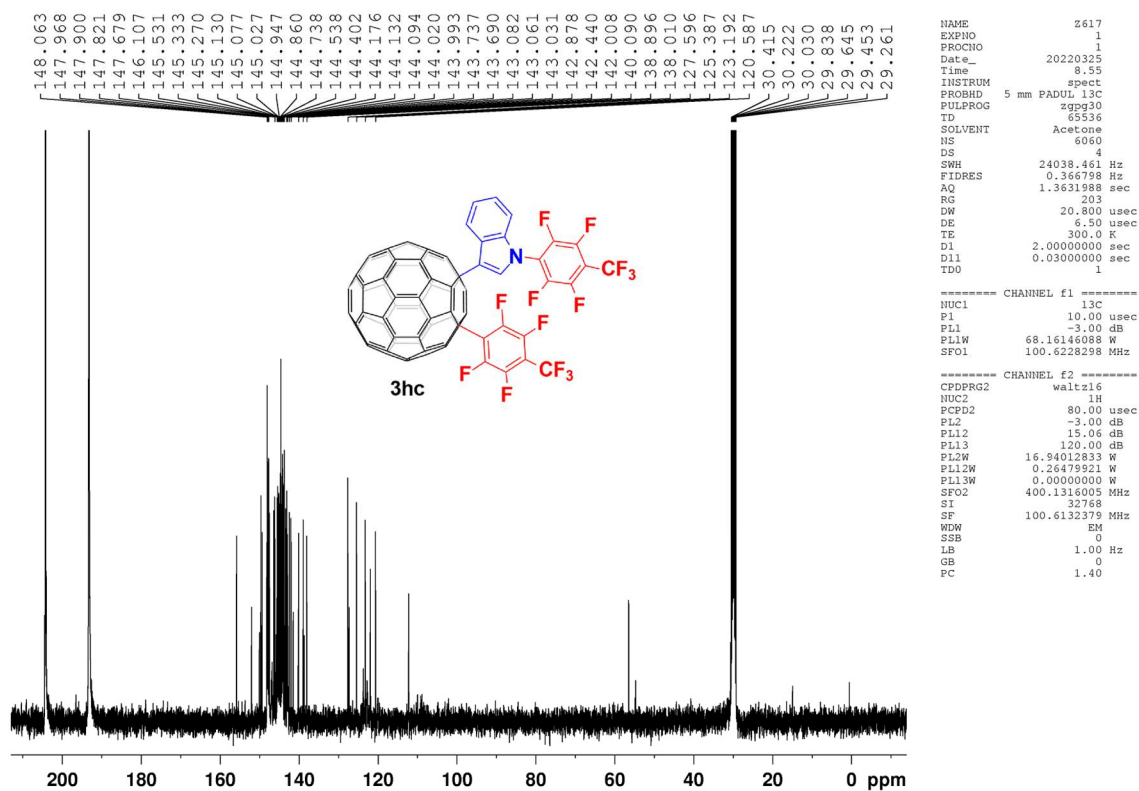
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **3hc**



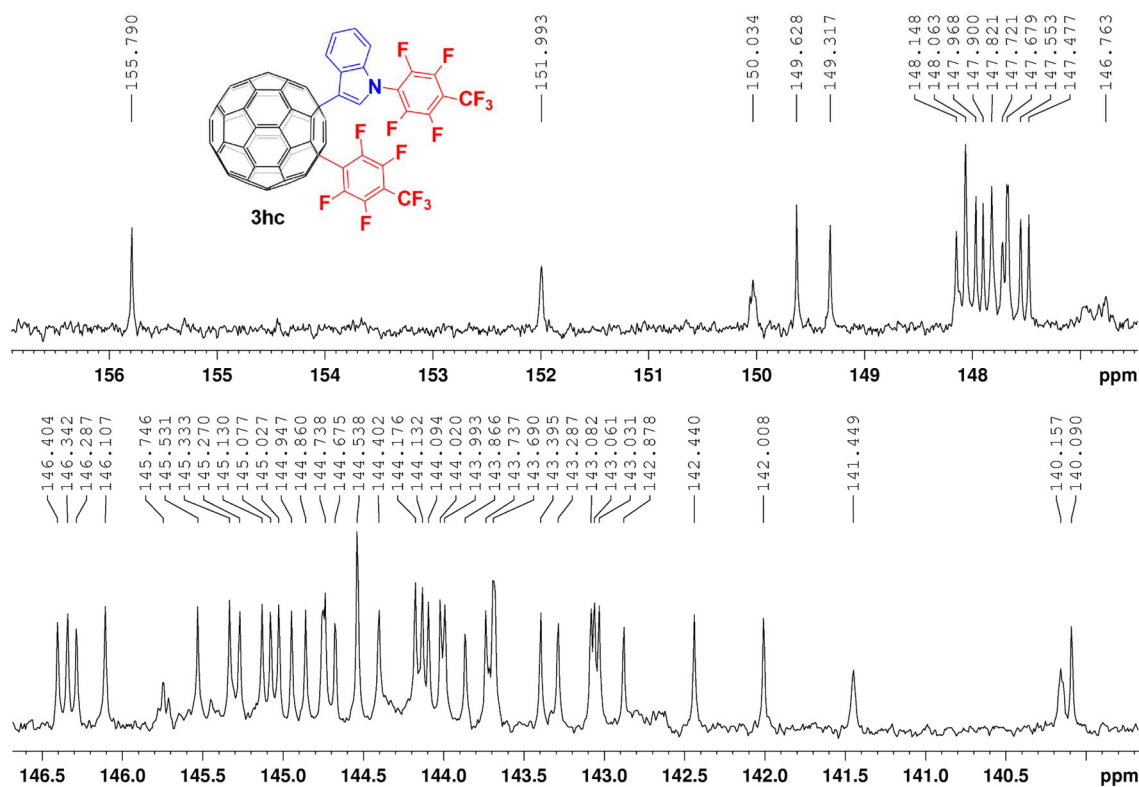
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 3hc



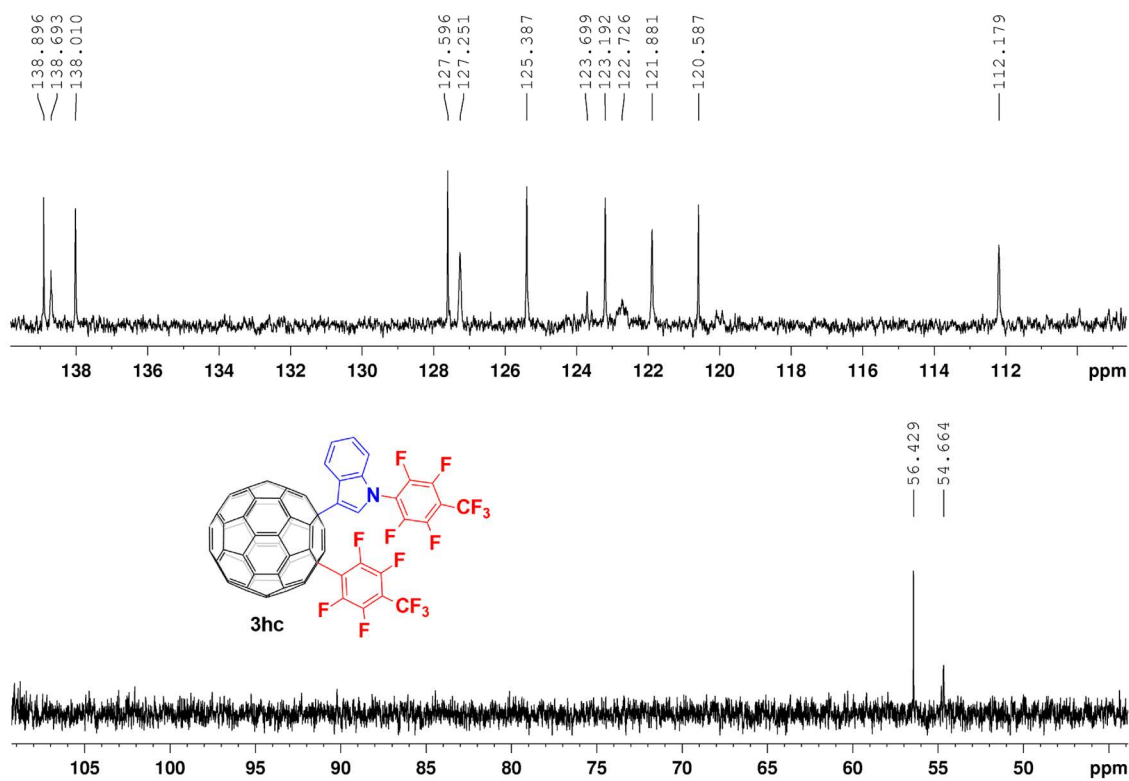
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3hc



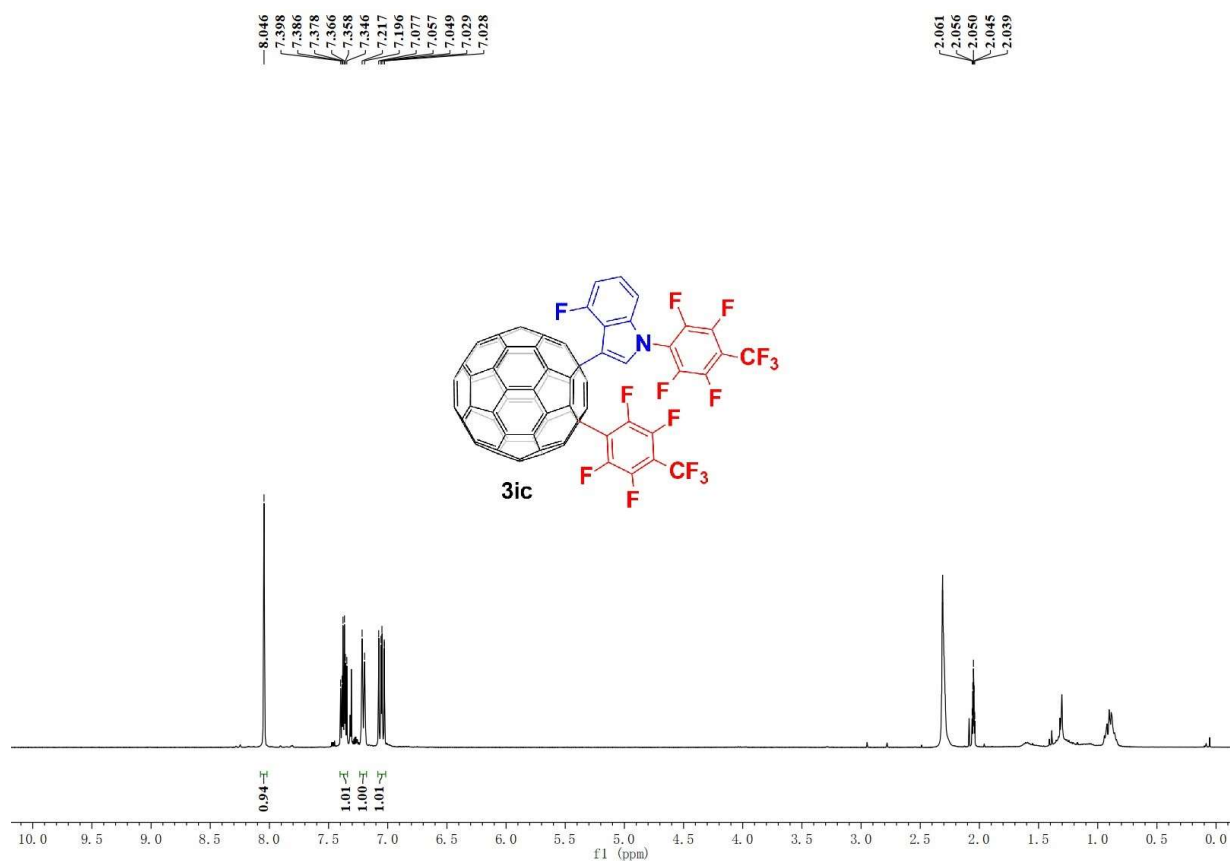
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3hc



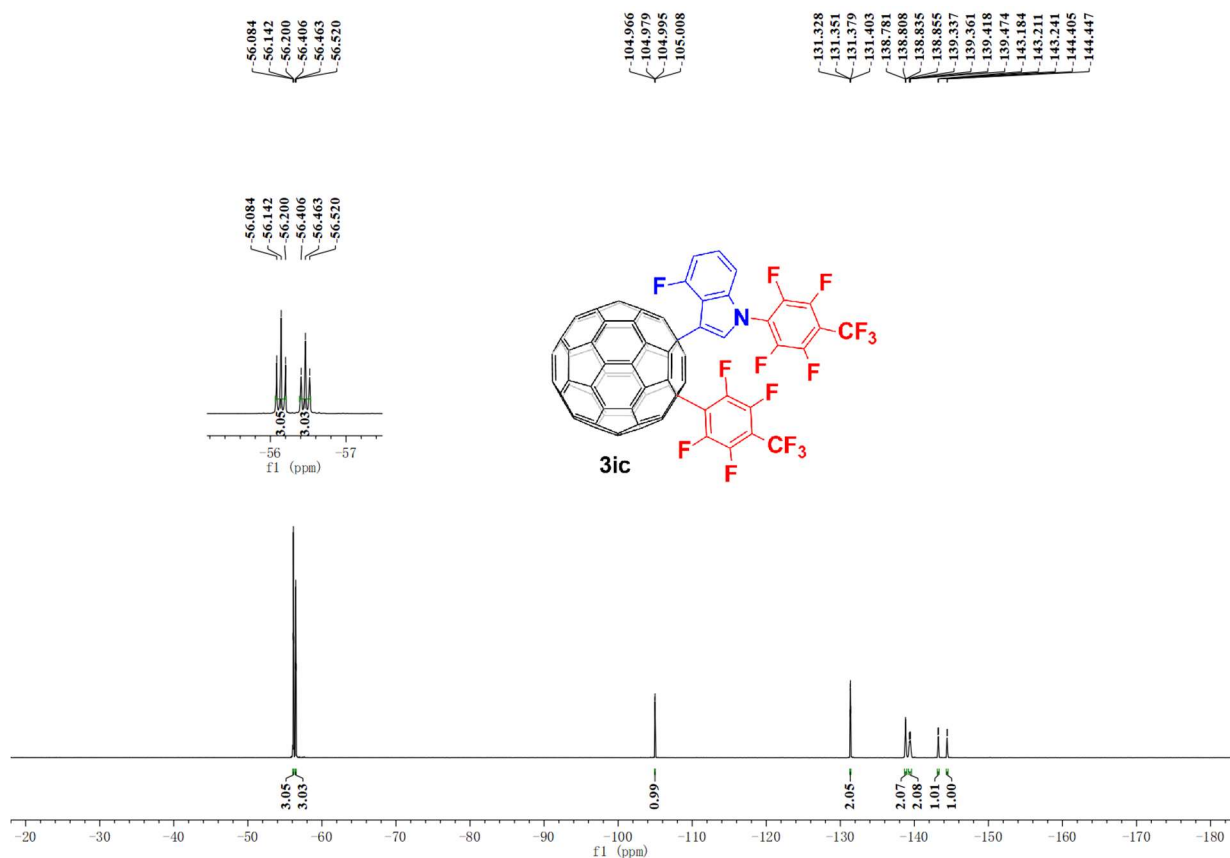
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3hc



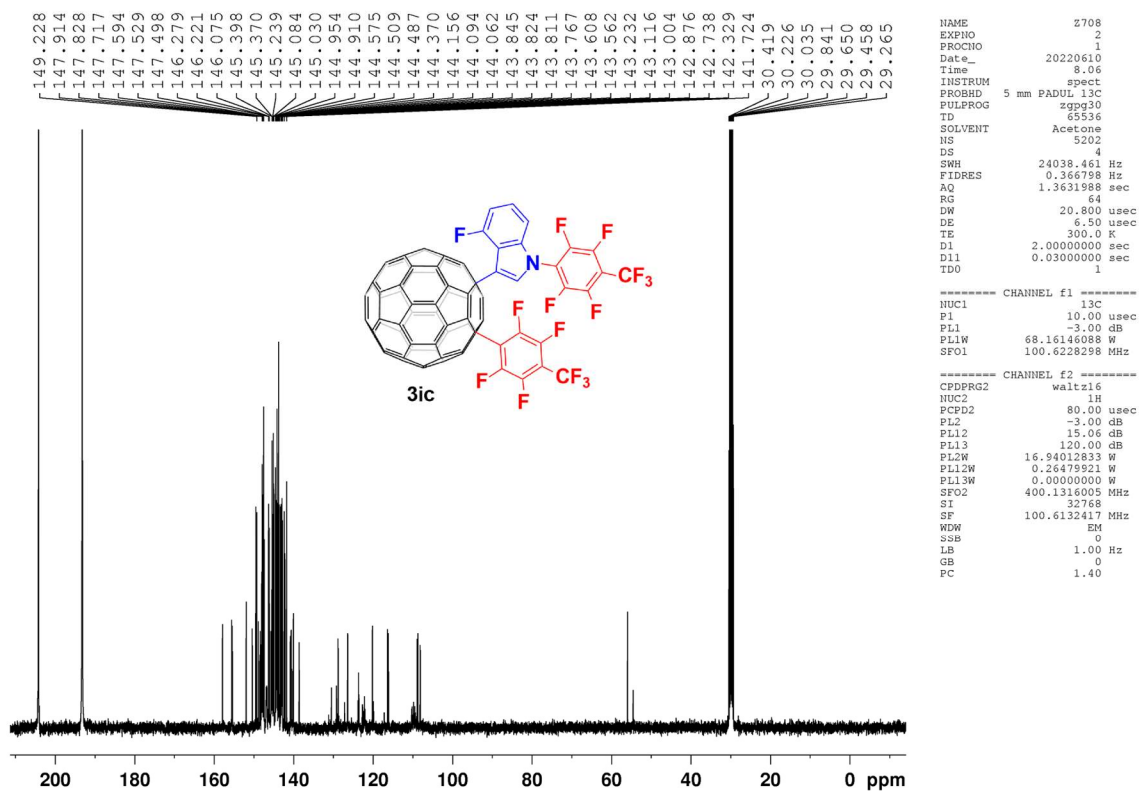
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **3ic**



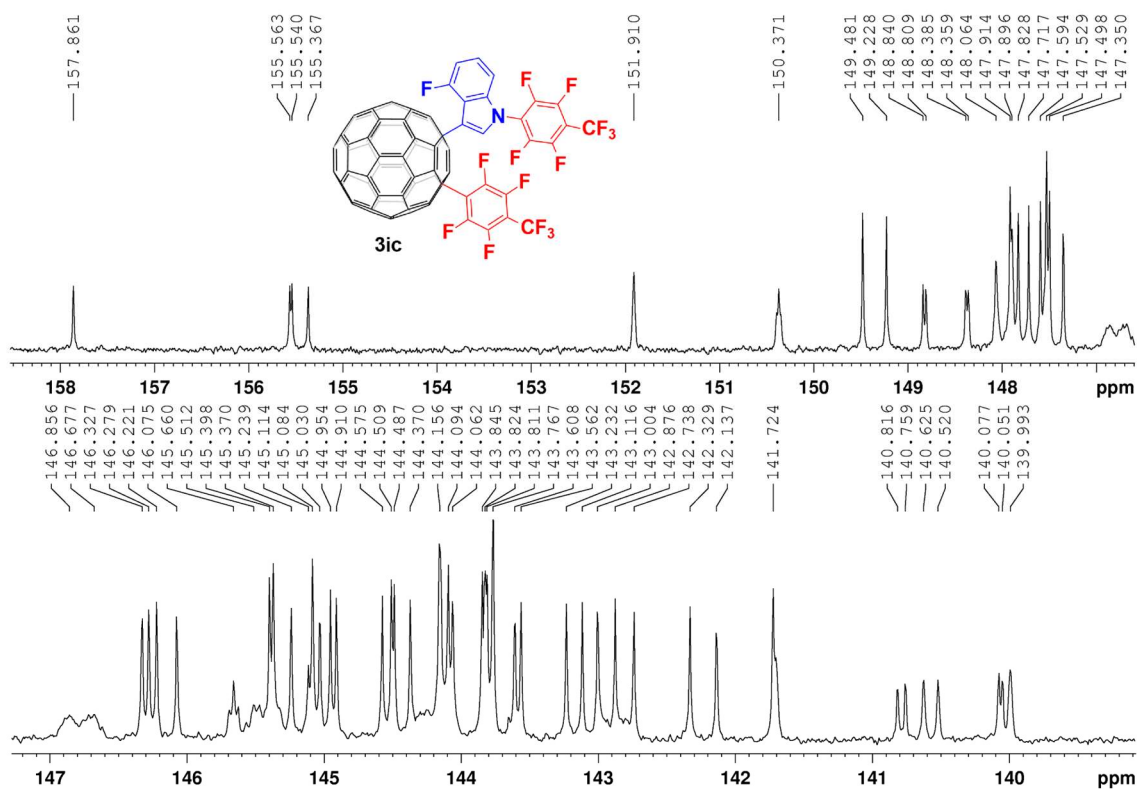
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound **3ic**



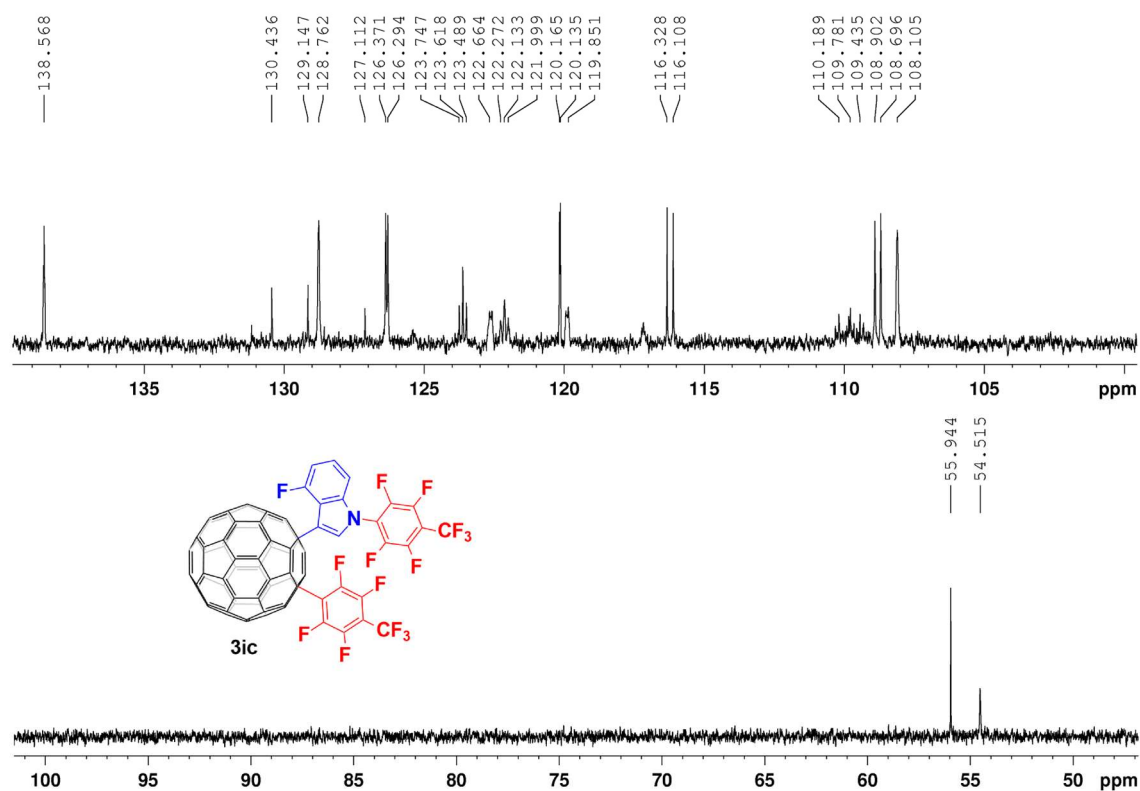
$^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound 3ic



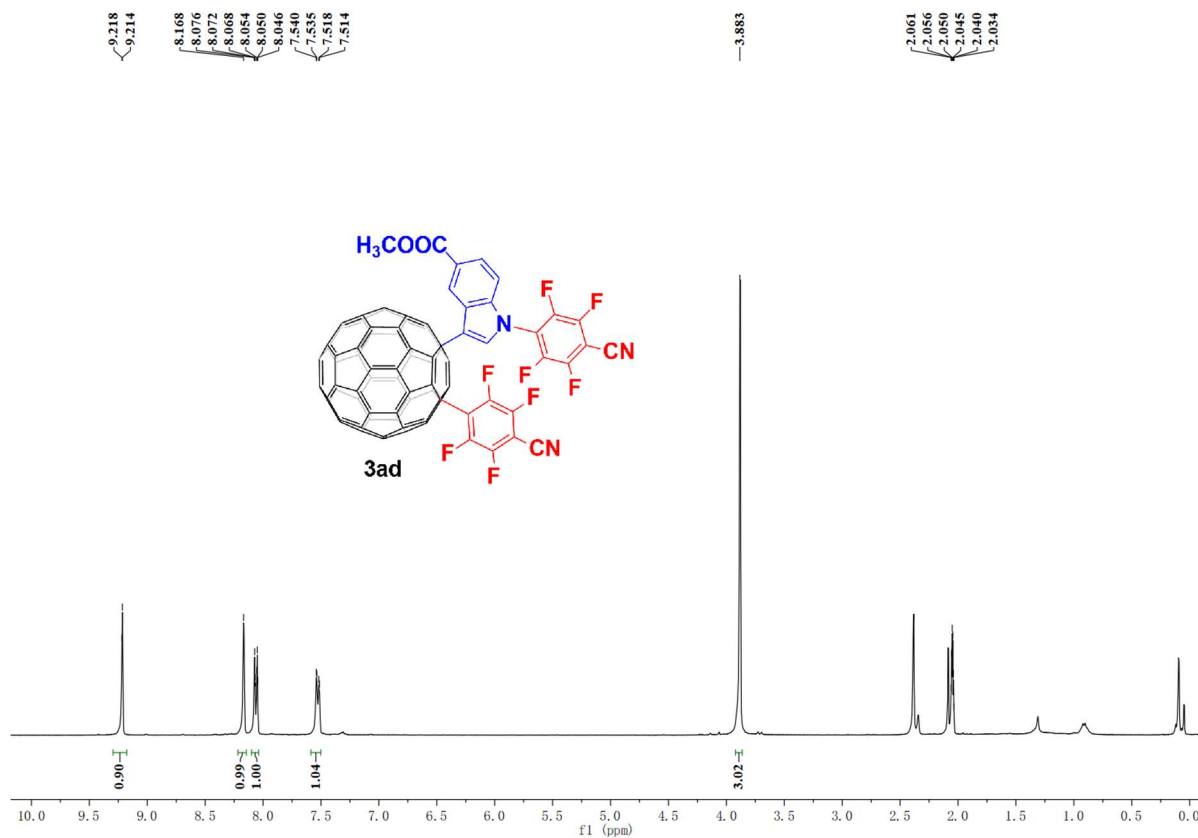
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound 3ic



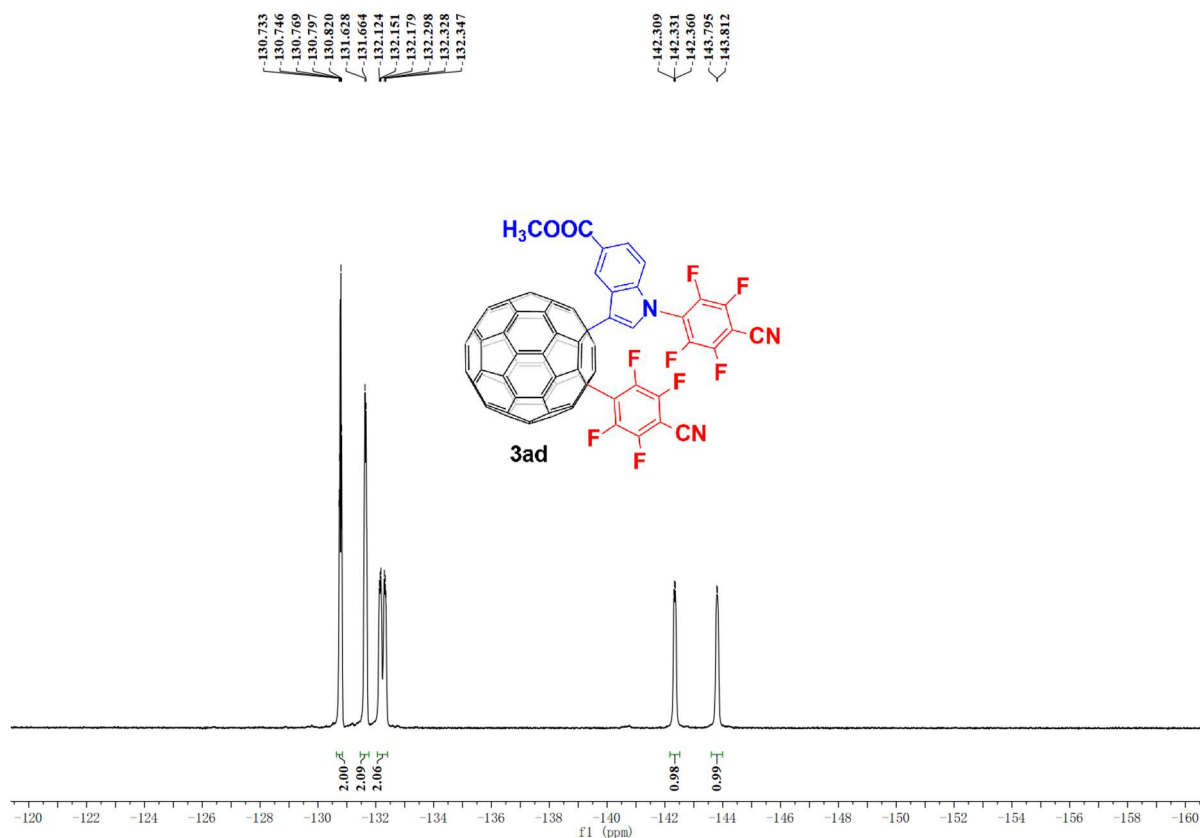
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound **3ic**



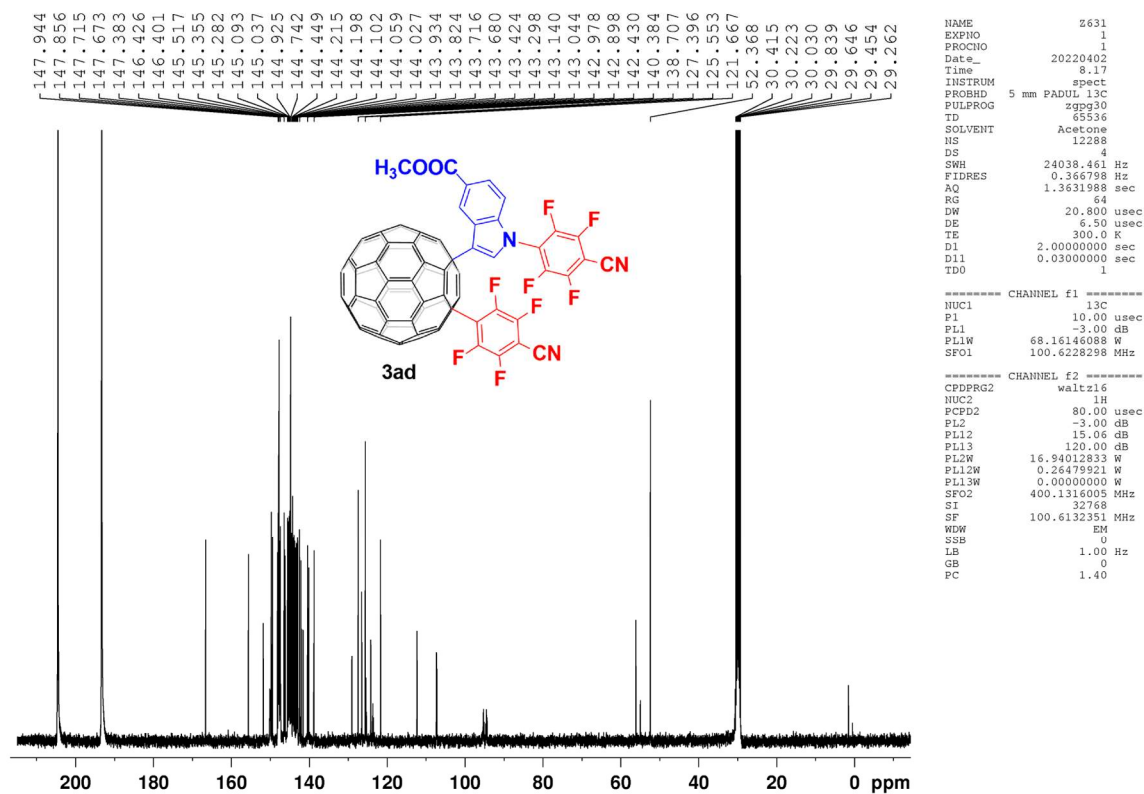
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **3ad**



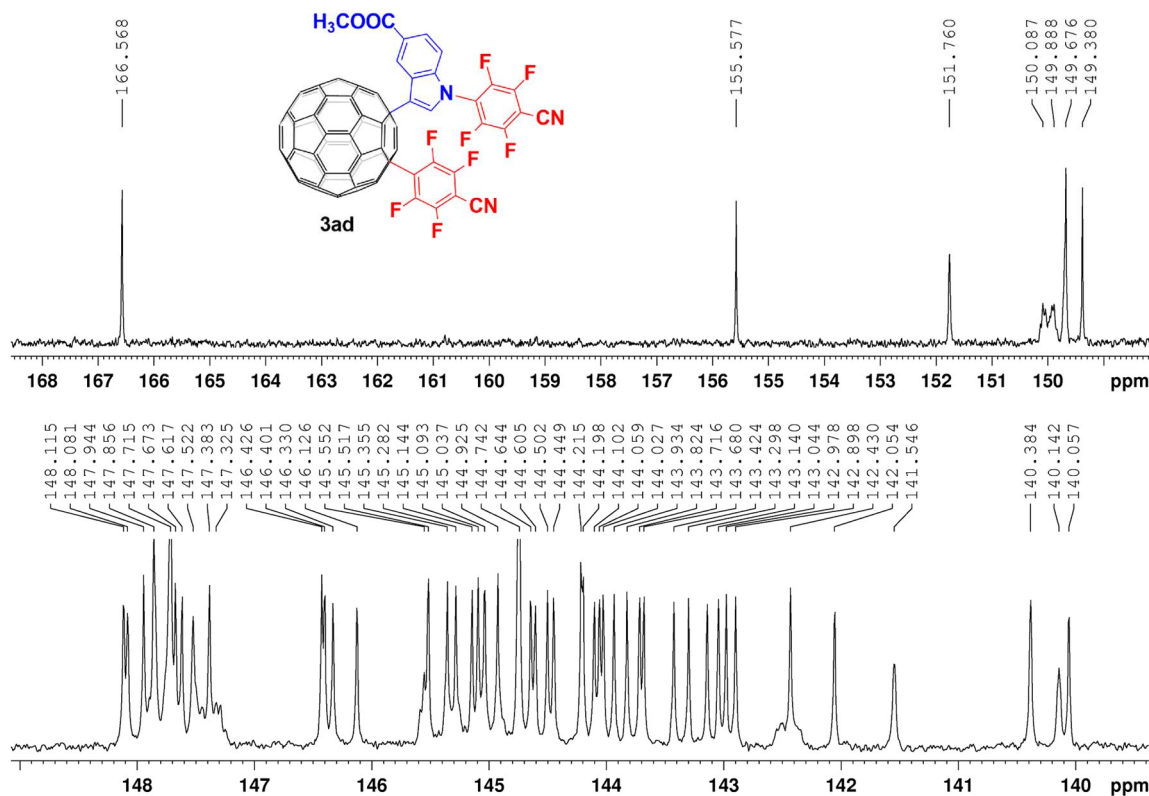
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 3ad



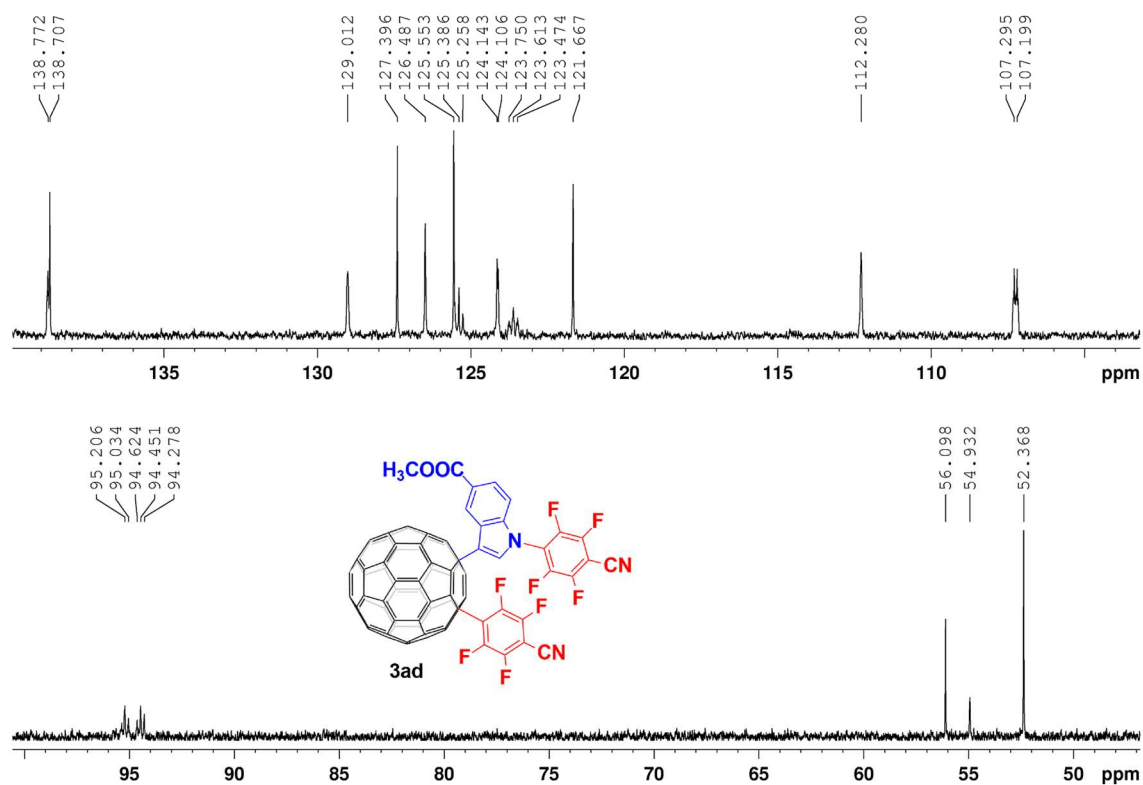
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3ad



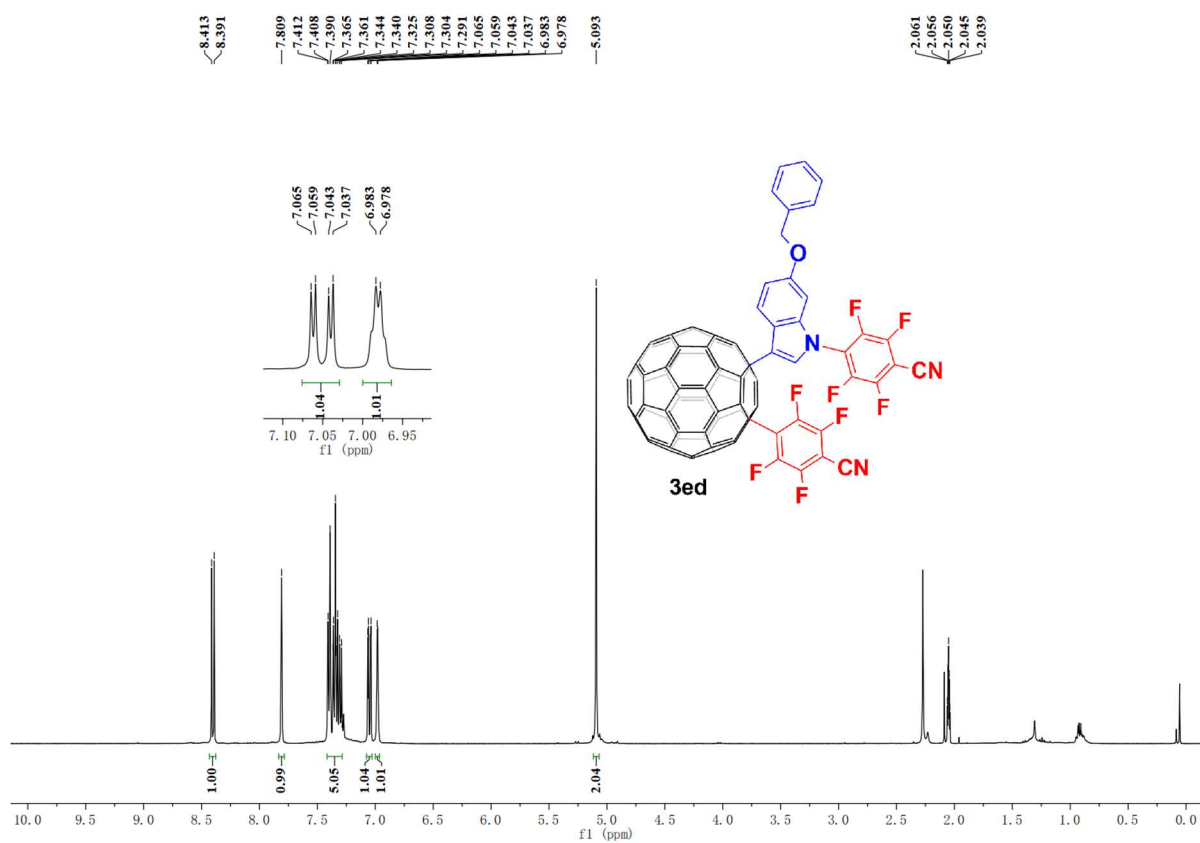
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3ad



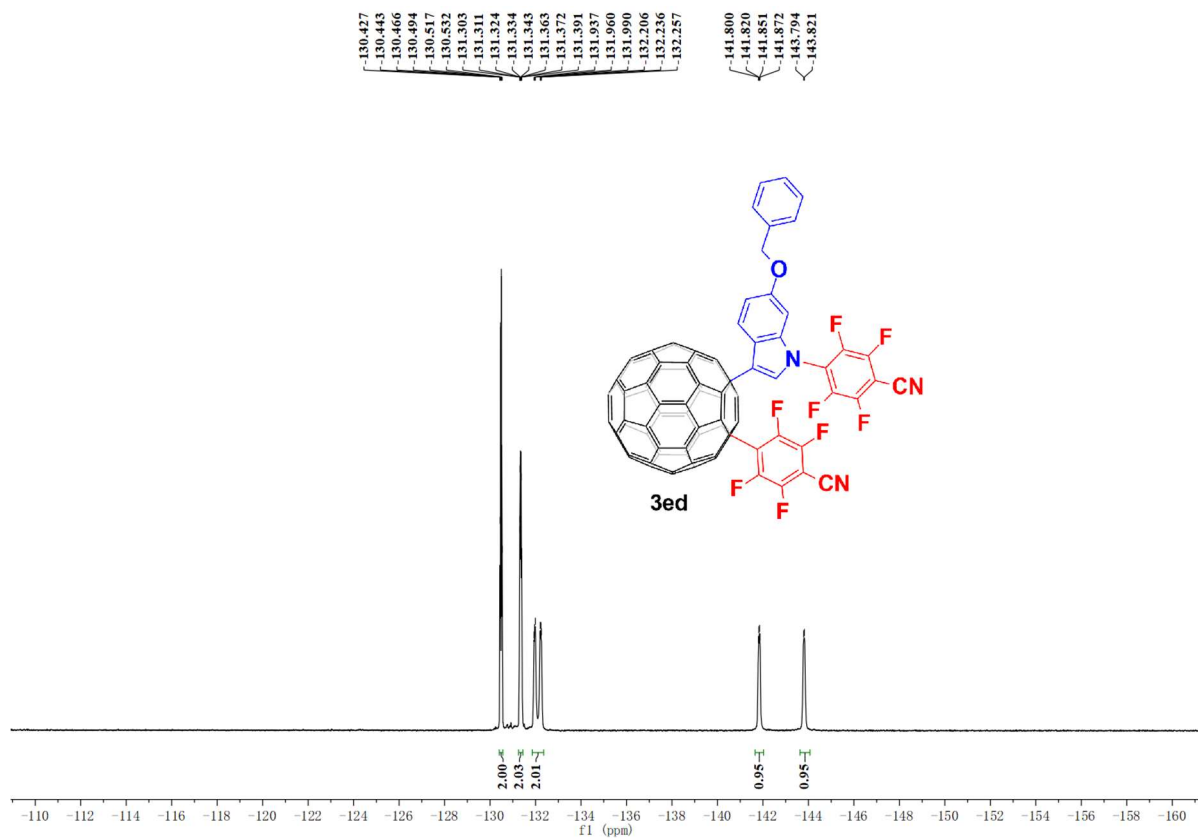
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3ad



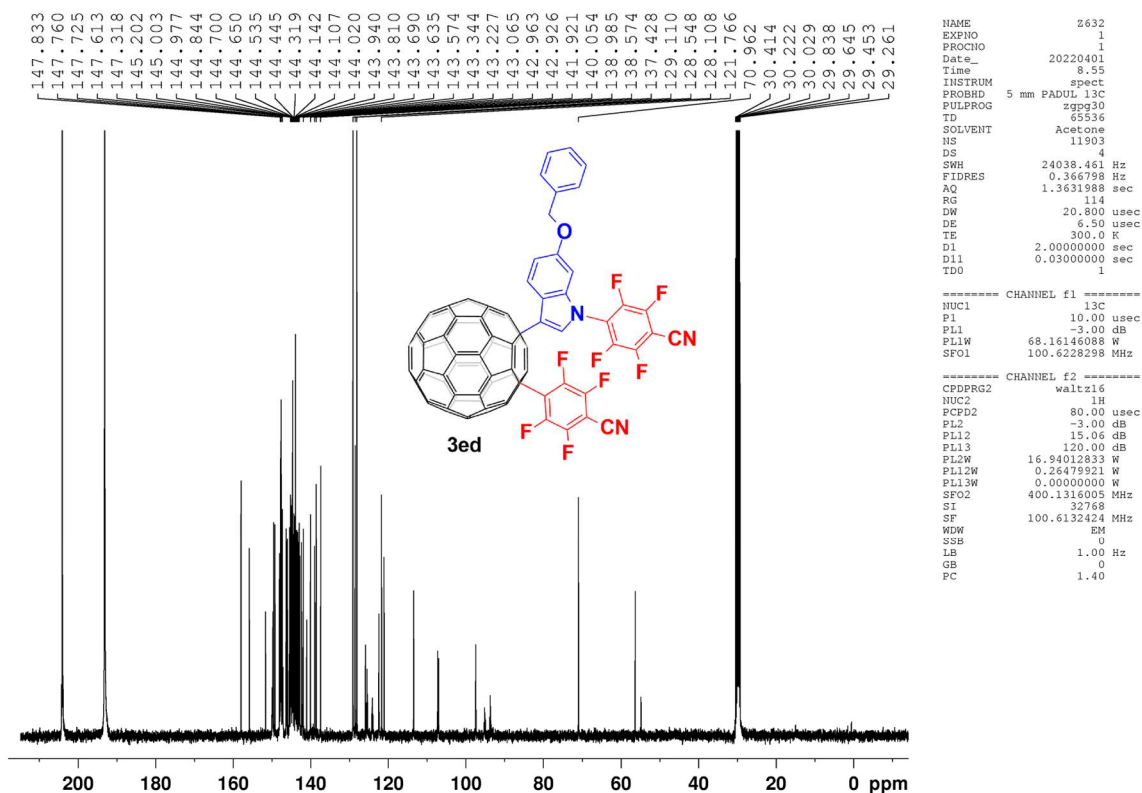
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 3ed



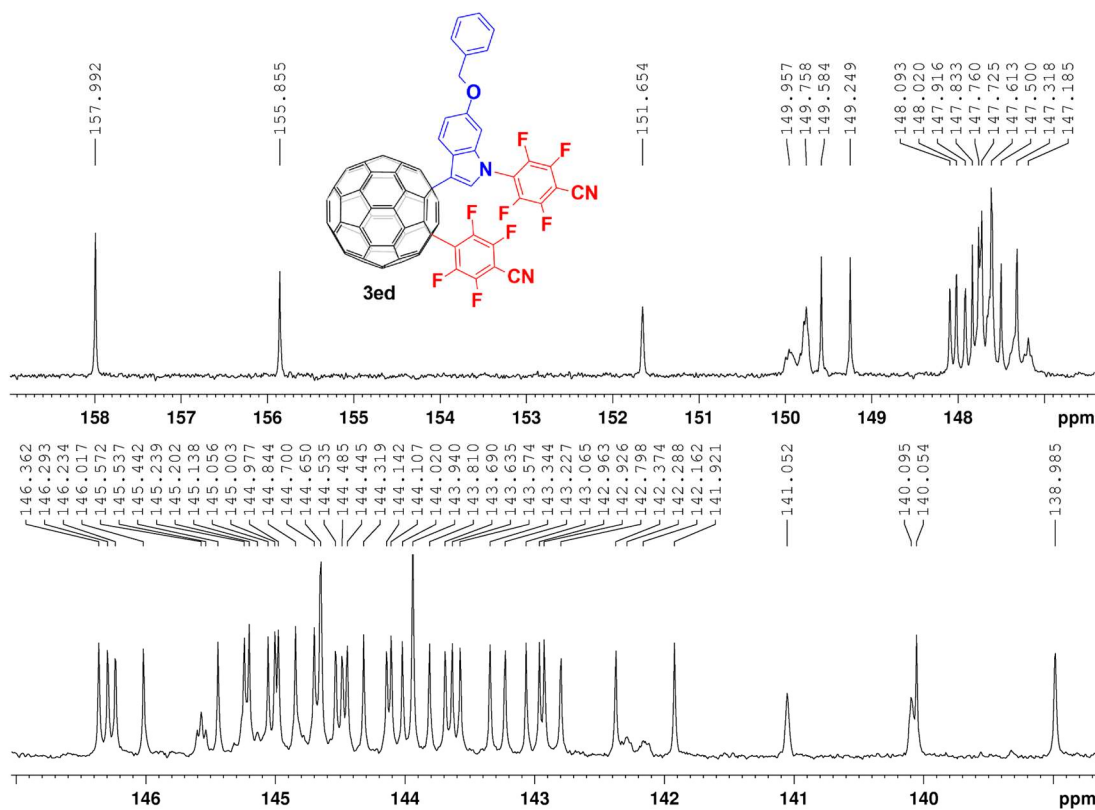
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 3ed



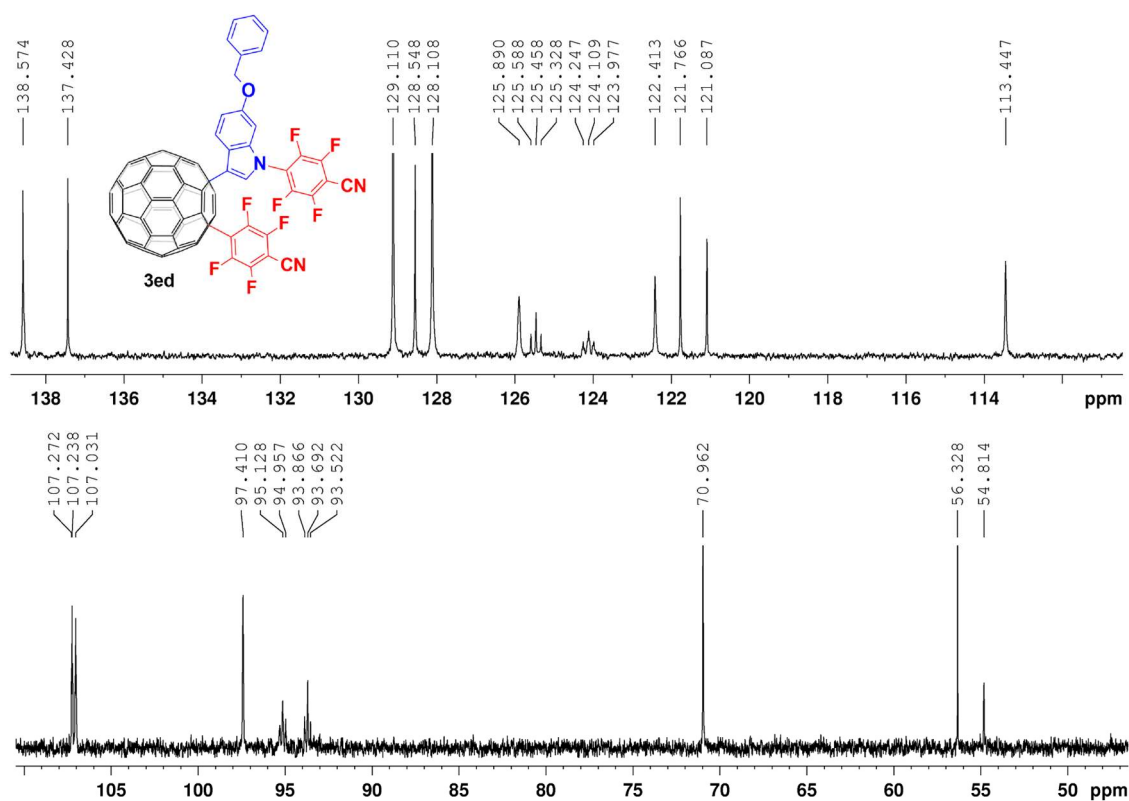
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 3ed



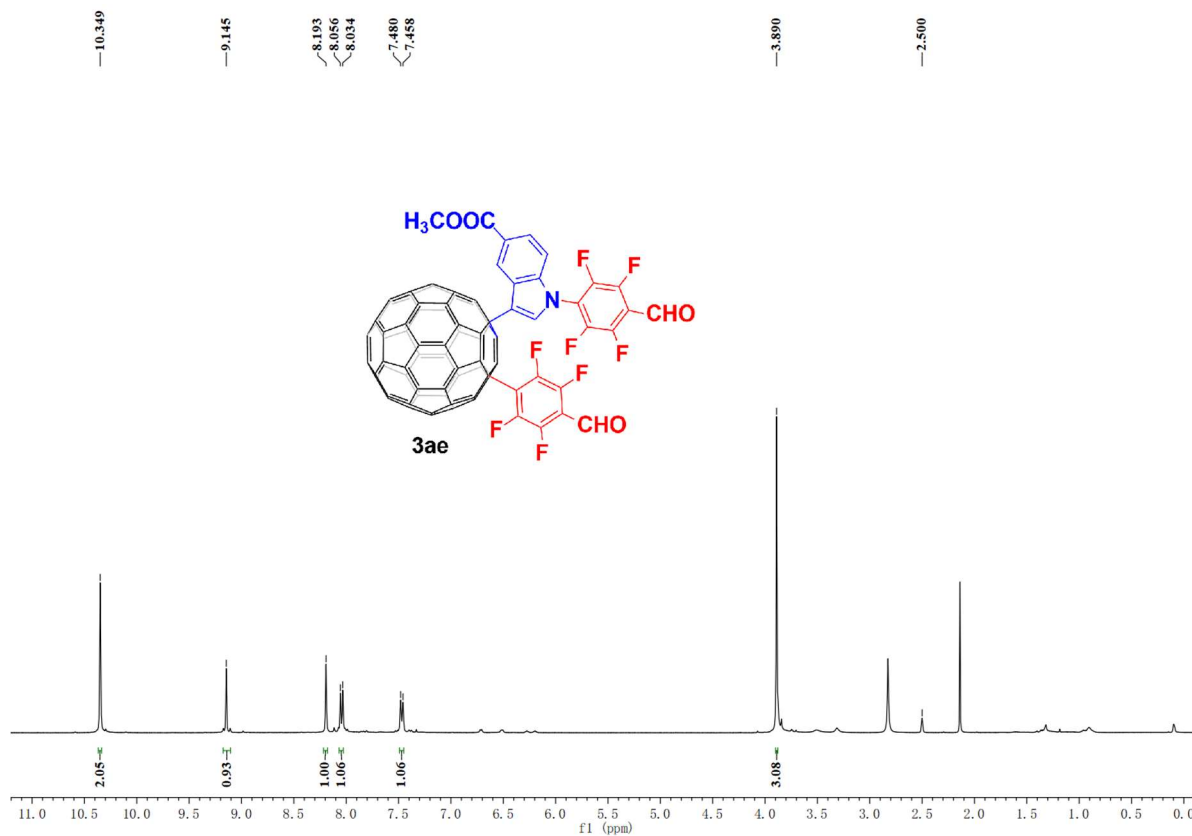
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 3ed



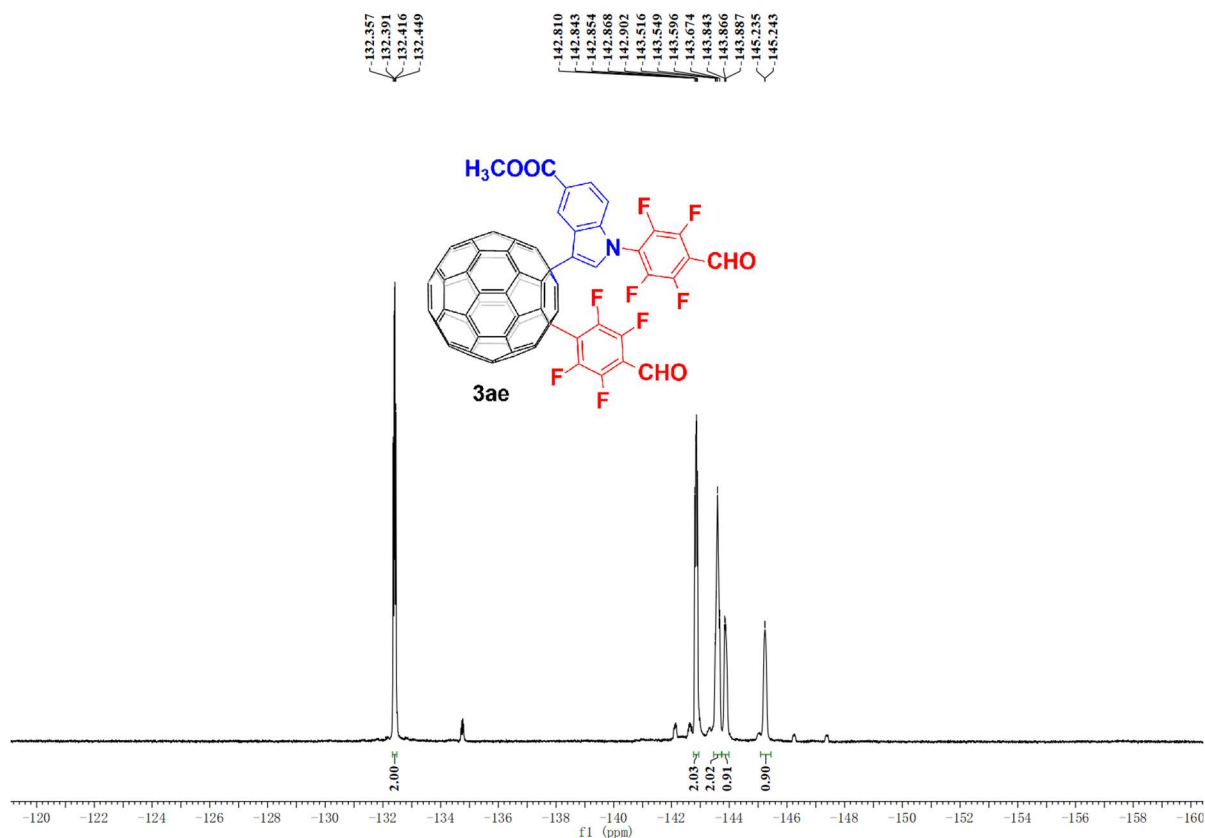
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **3ed**



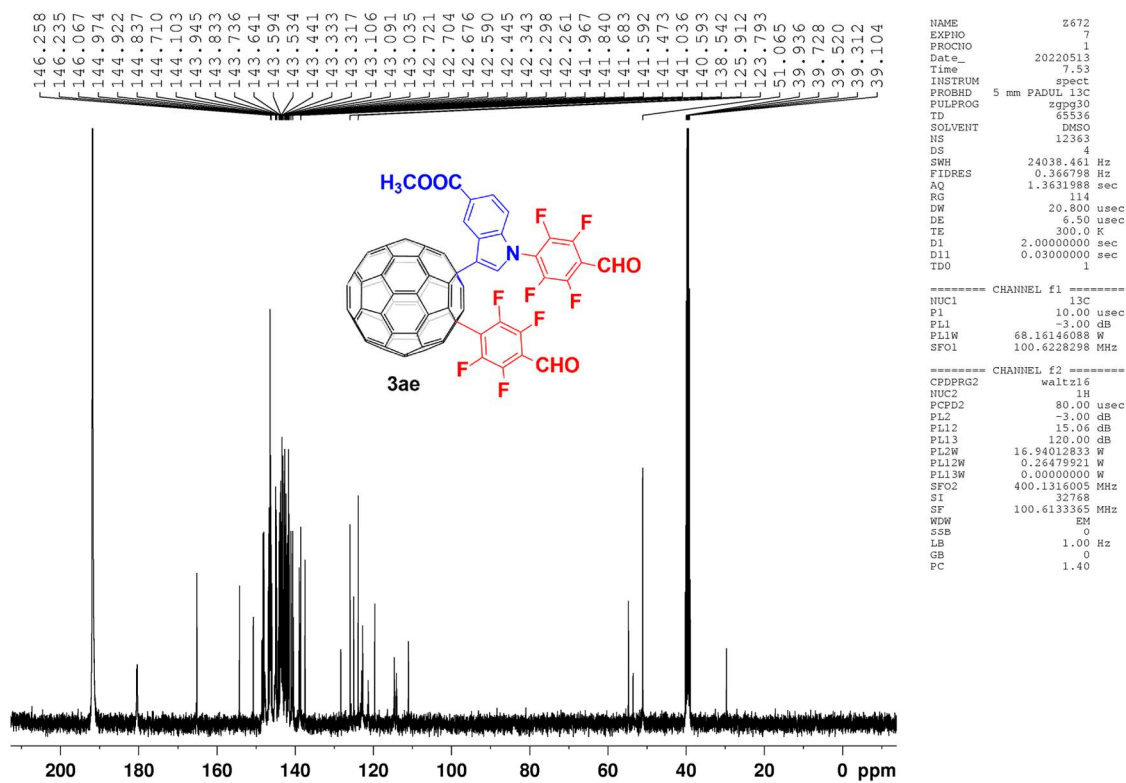
^1H NMR (400 MHz, CS_2/d_6 -DMSO) of compound **3ae**



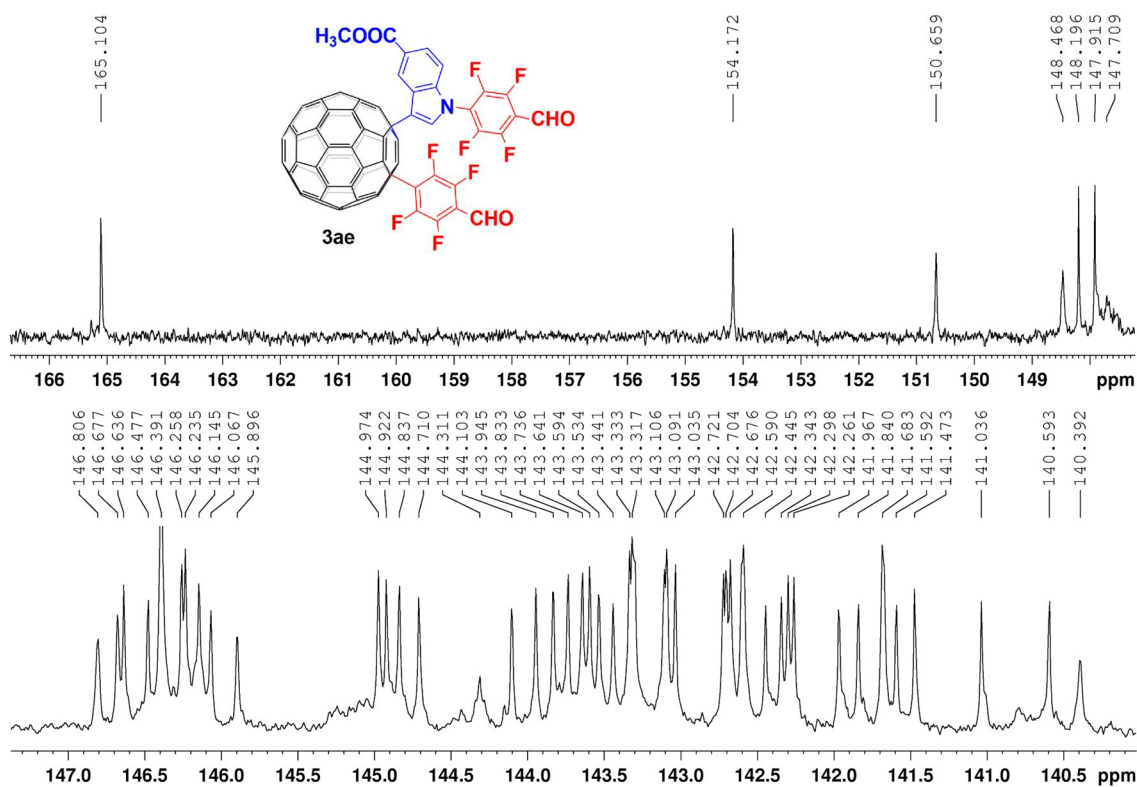
¹⁹F NMR (376 MHz, CS₂/d₆-DMSO) of compound 3ae



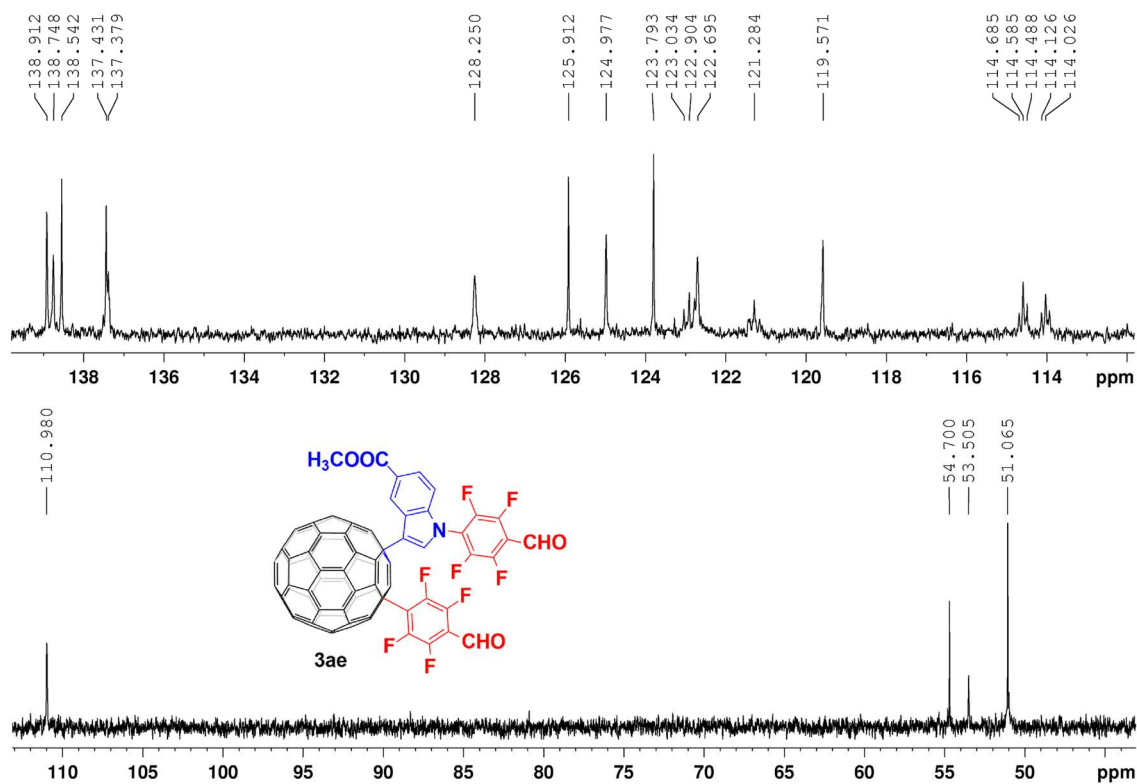
¹³C{¹H} NMR (100 MHz, CS₂/d₆-DMSO) of compound 3ae



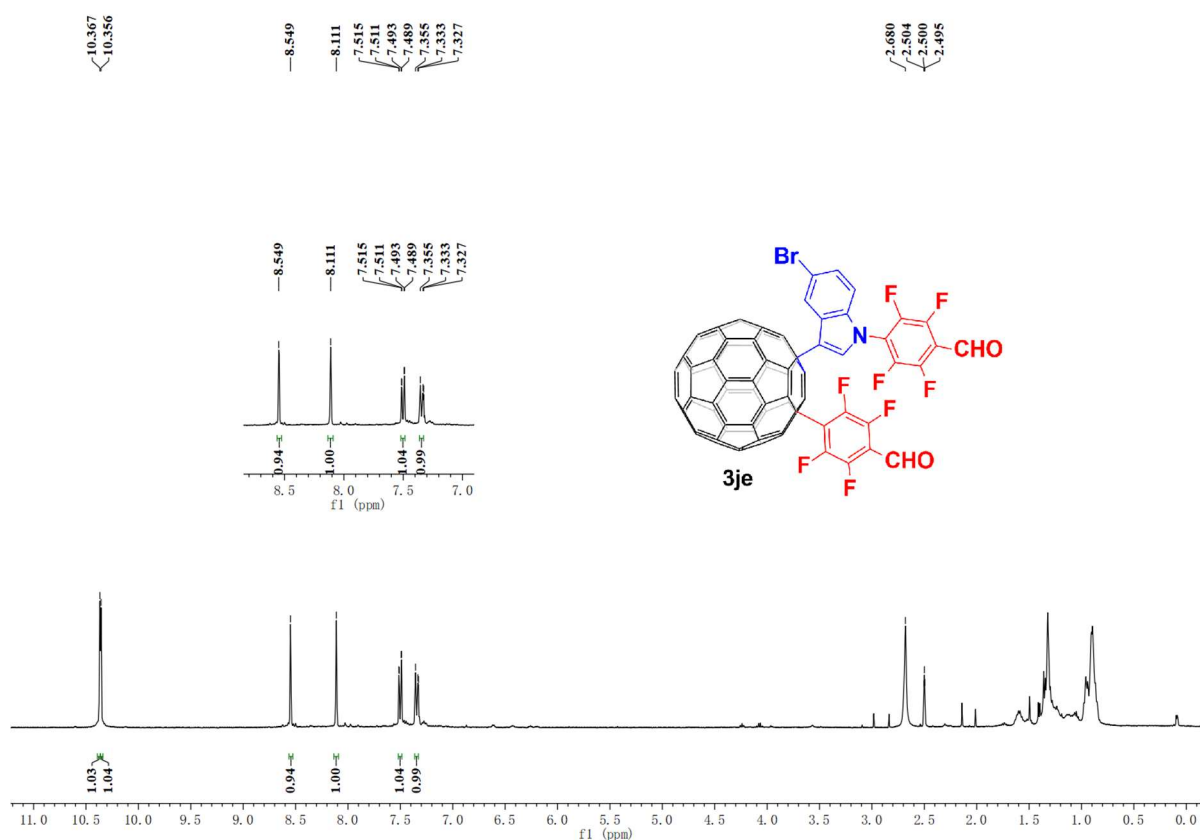
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound **3ae**



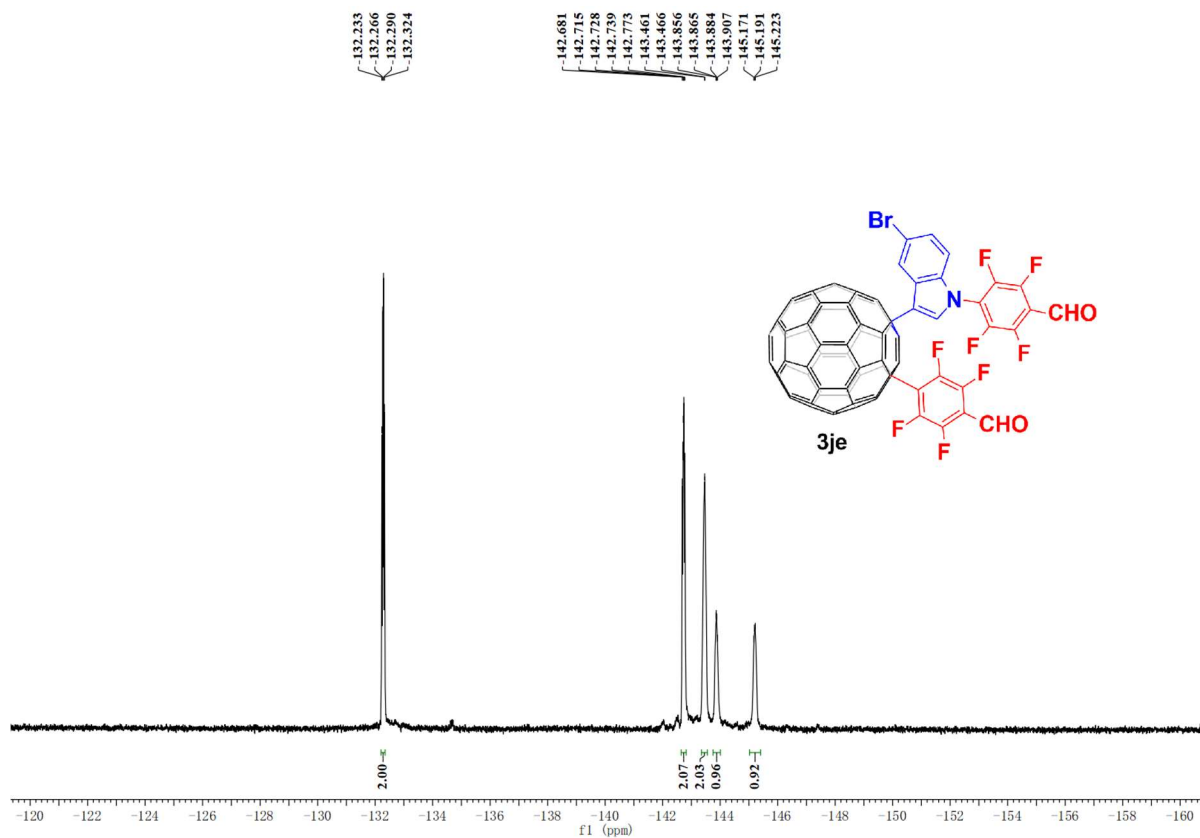
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound **3ae**



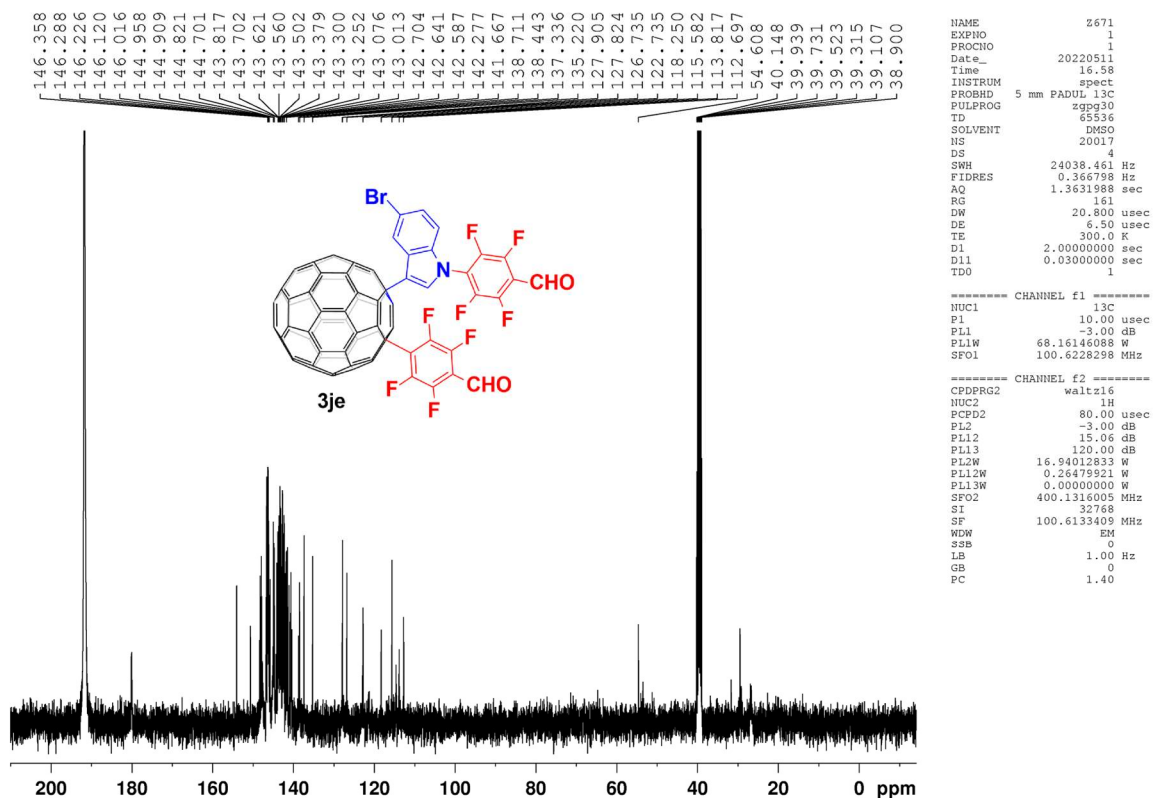
^1H NMR (400 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound 3je



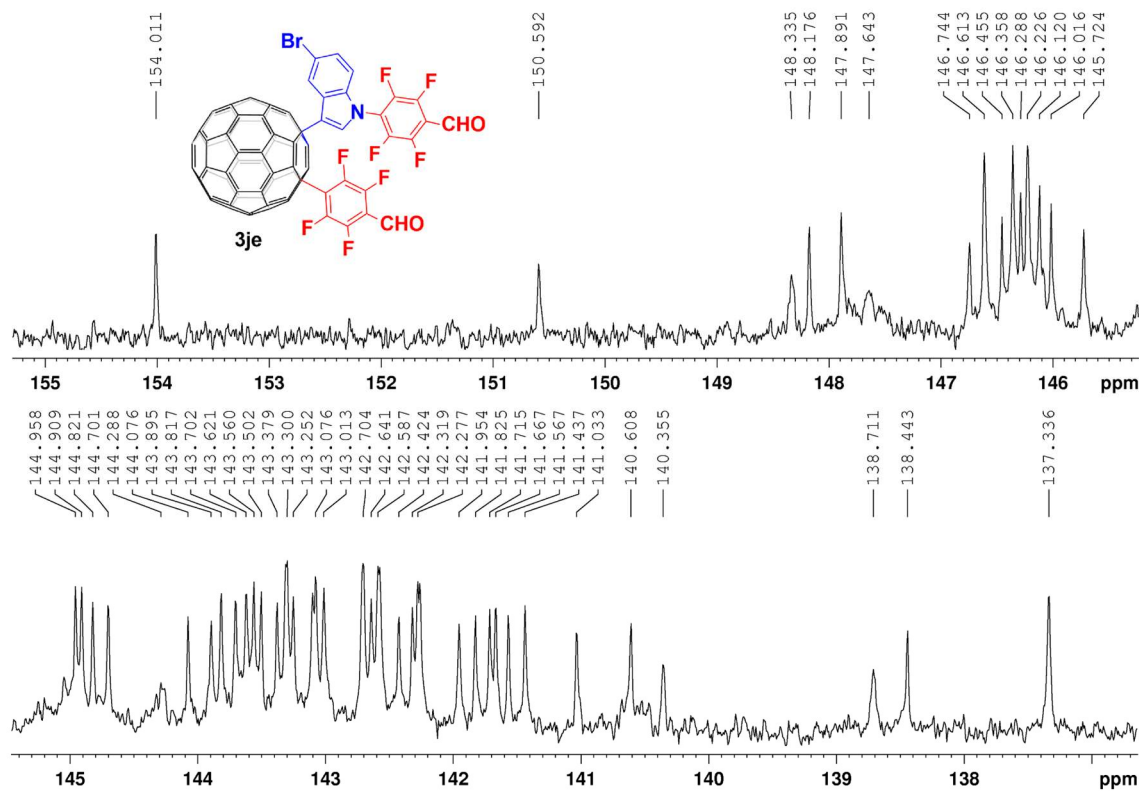
^{19}F NMR (376 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound 3je



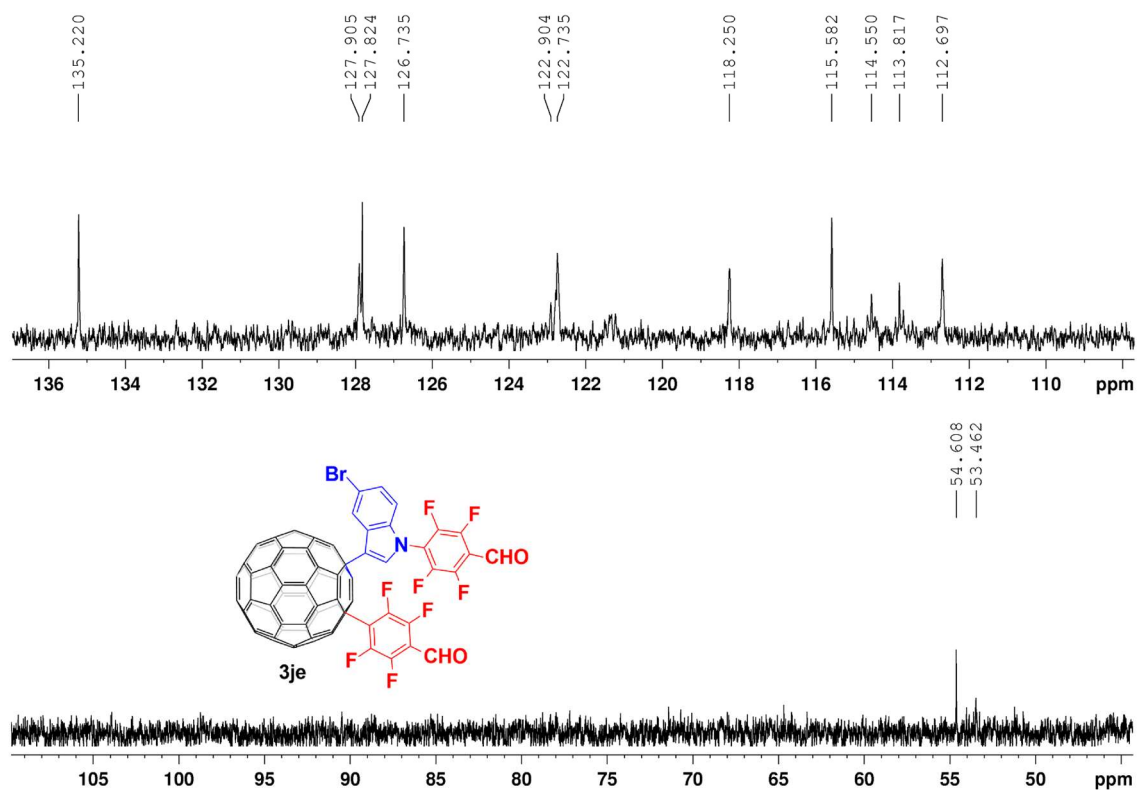
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound 3je



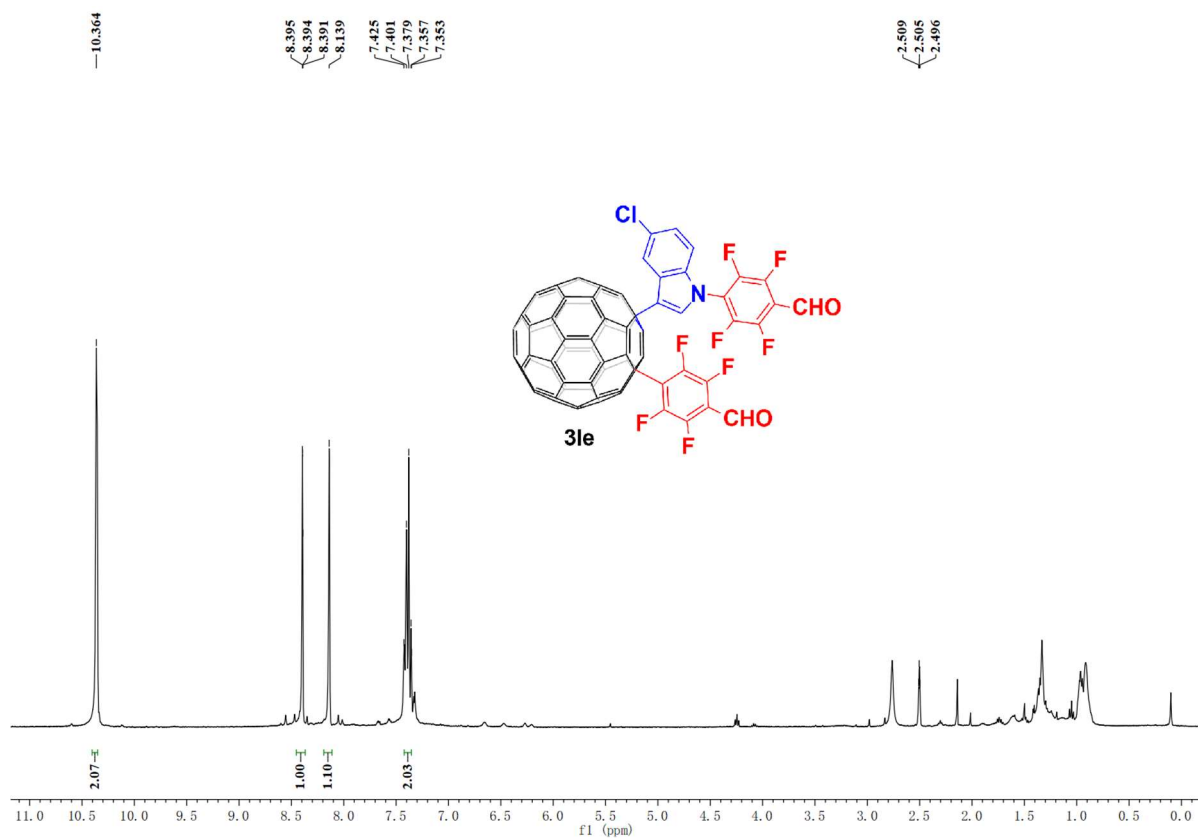
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound 3je



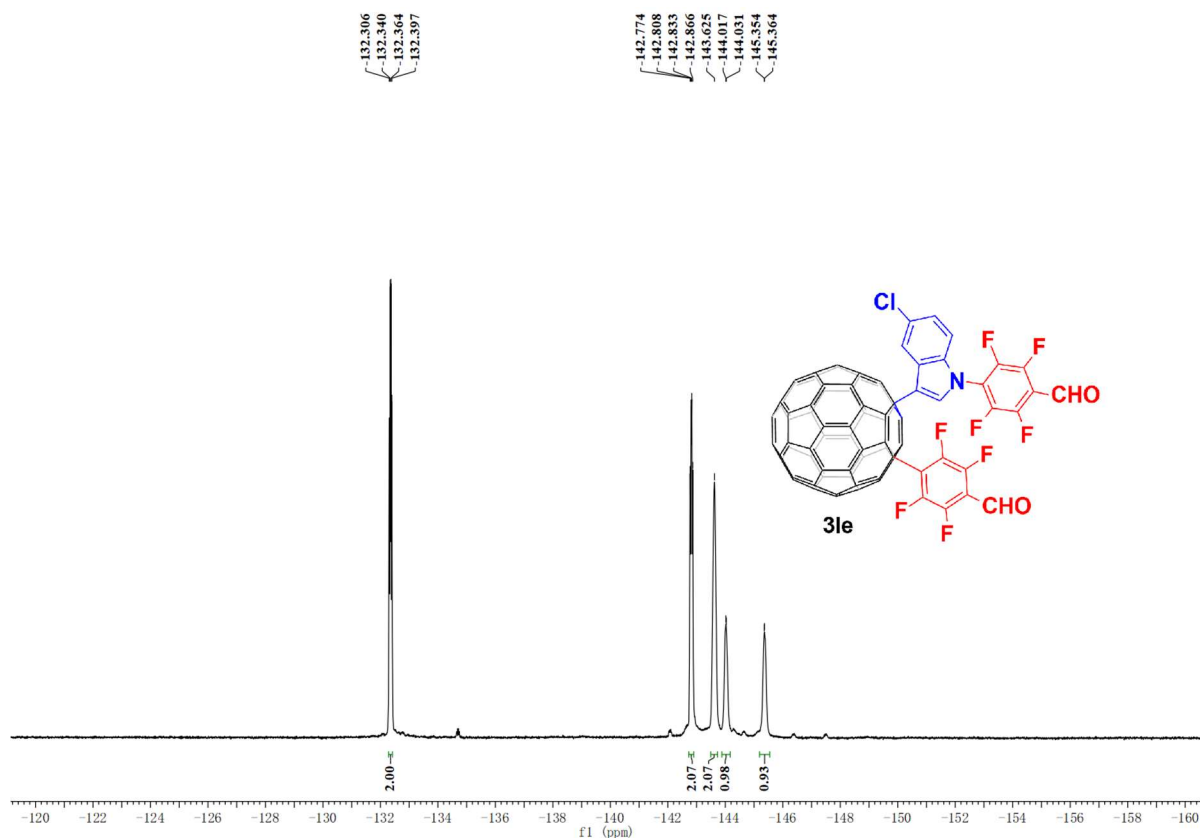
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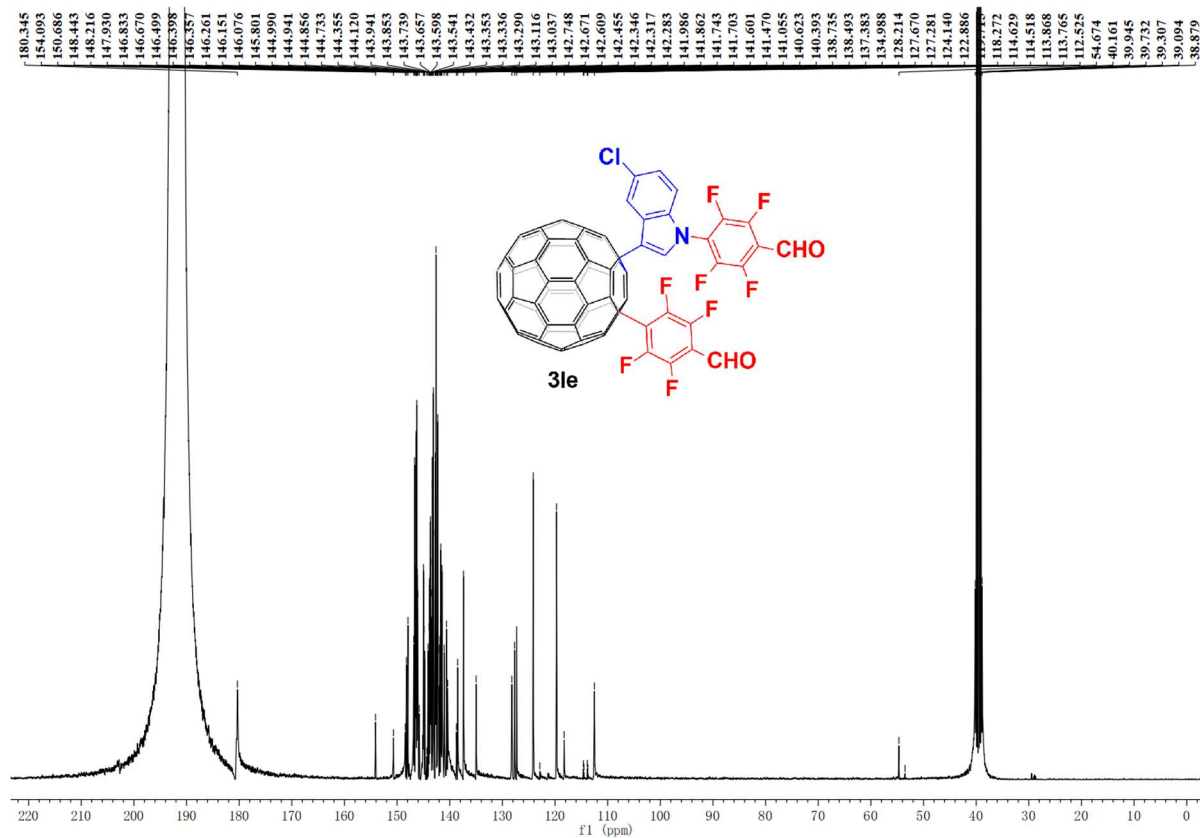
^1H NMR (400 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound **3le**



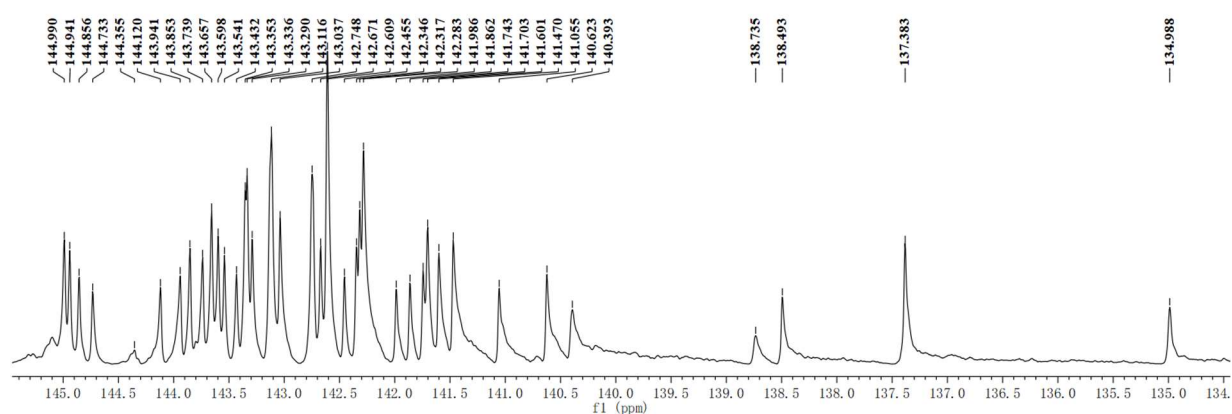
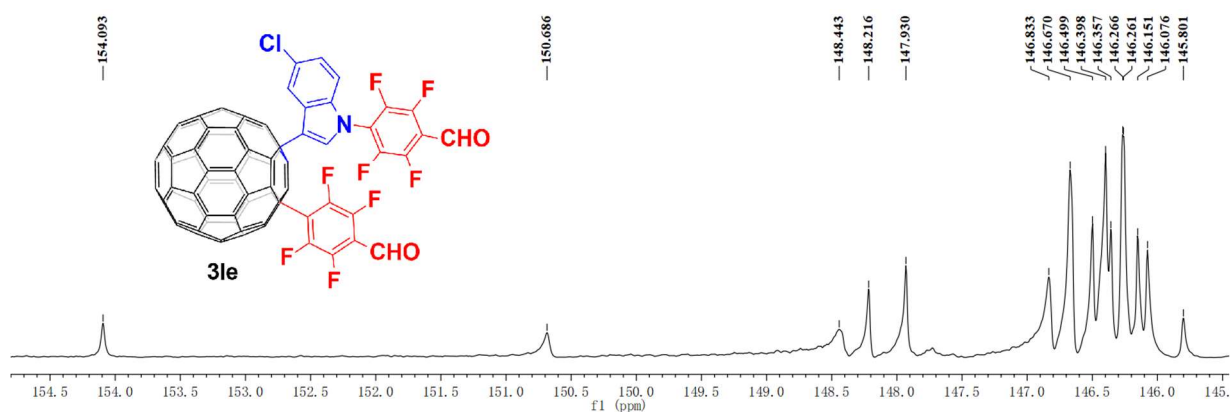
^{19}F NMR (376 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound 3le



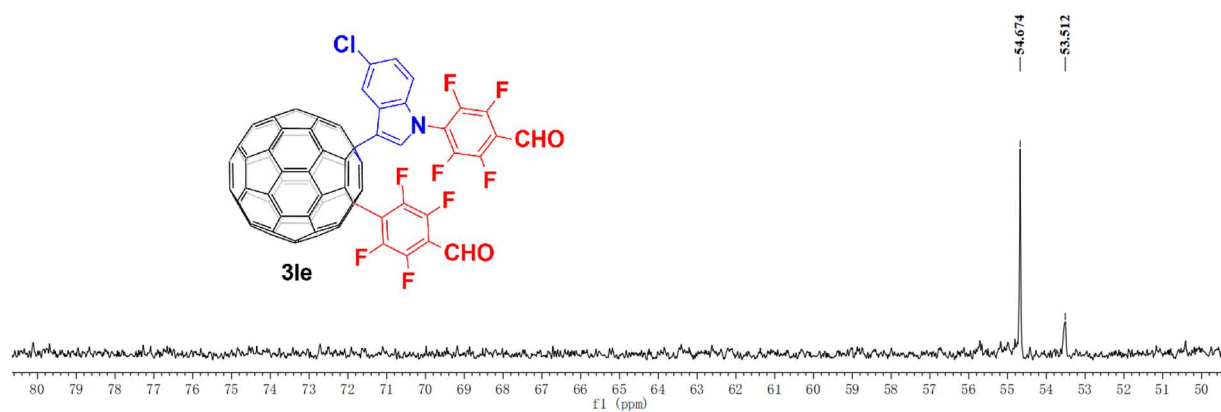
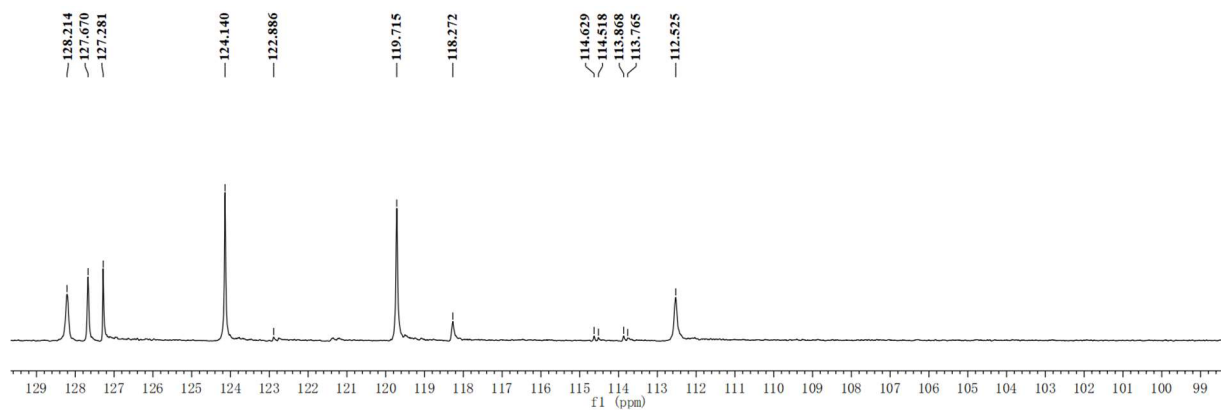
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound 3le



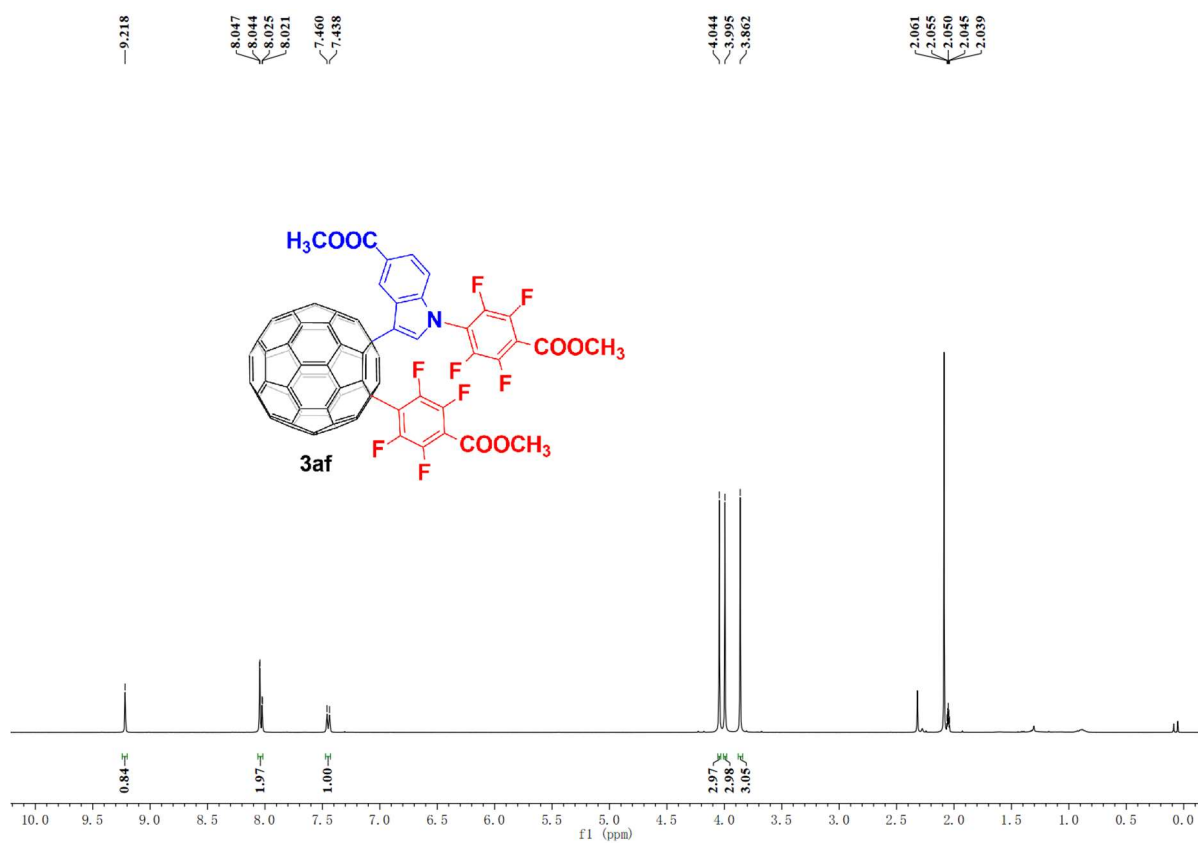
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound 3le



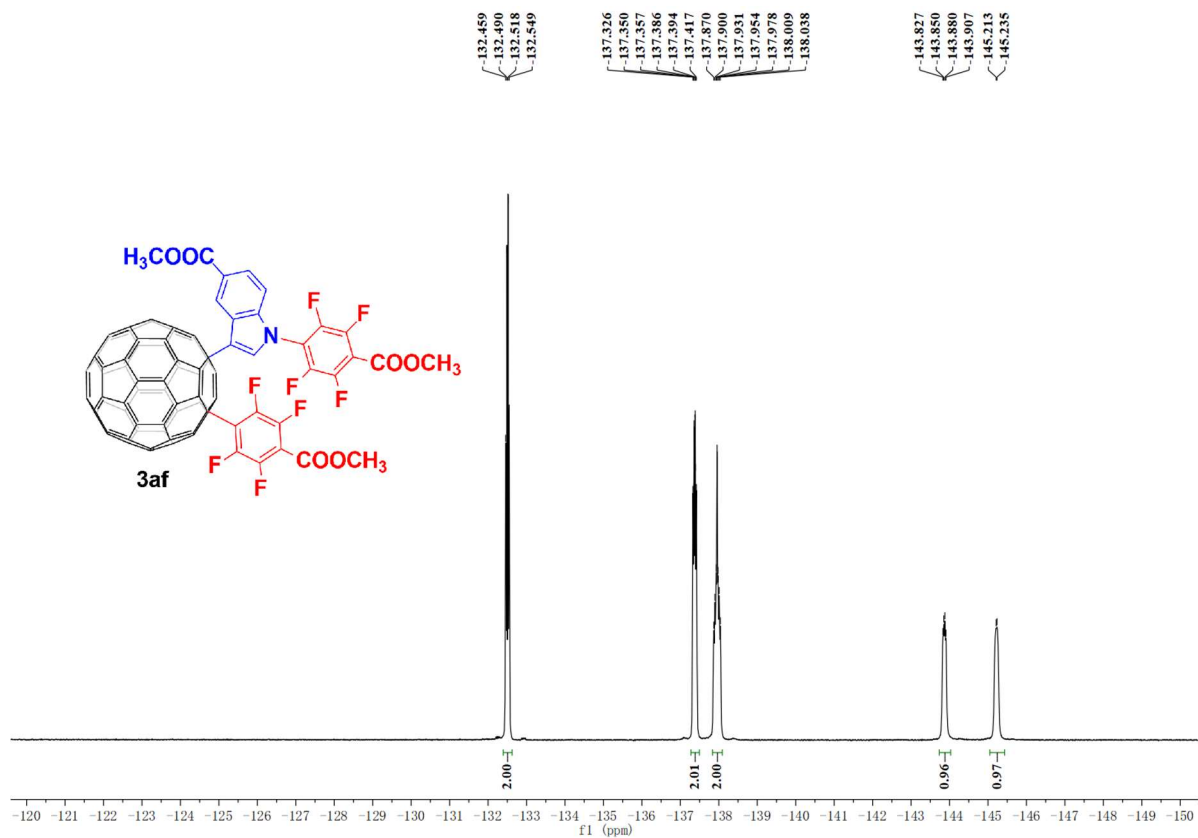
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-DMSO}$) of compound 3le



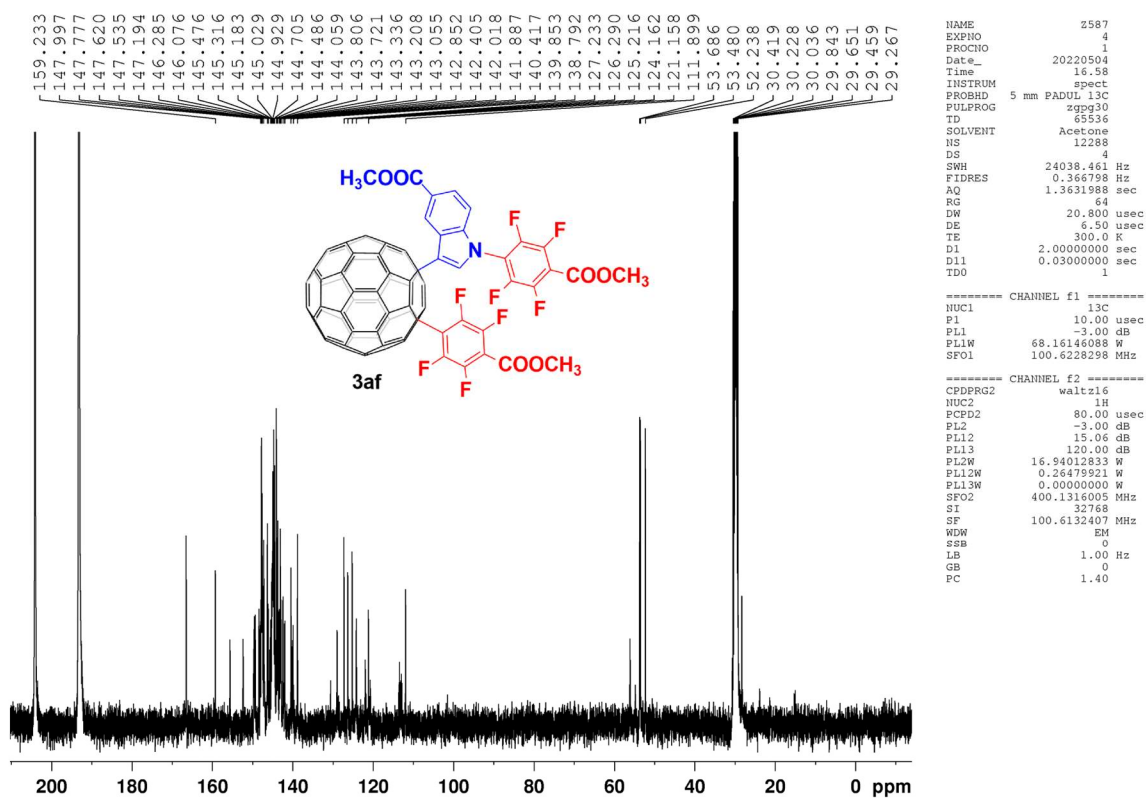
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 3af



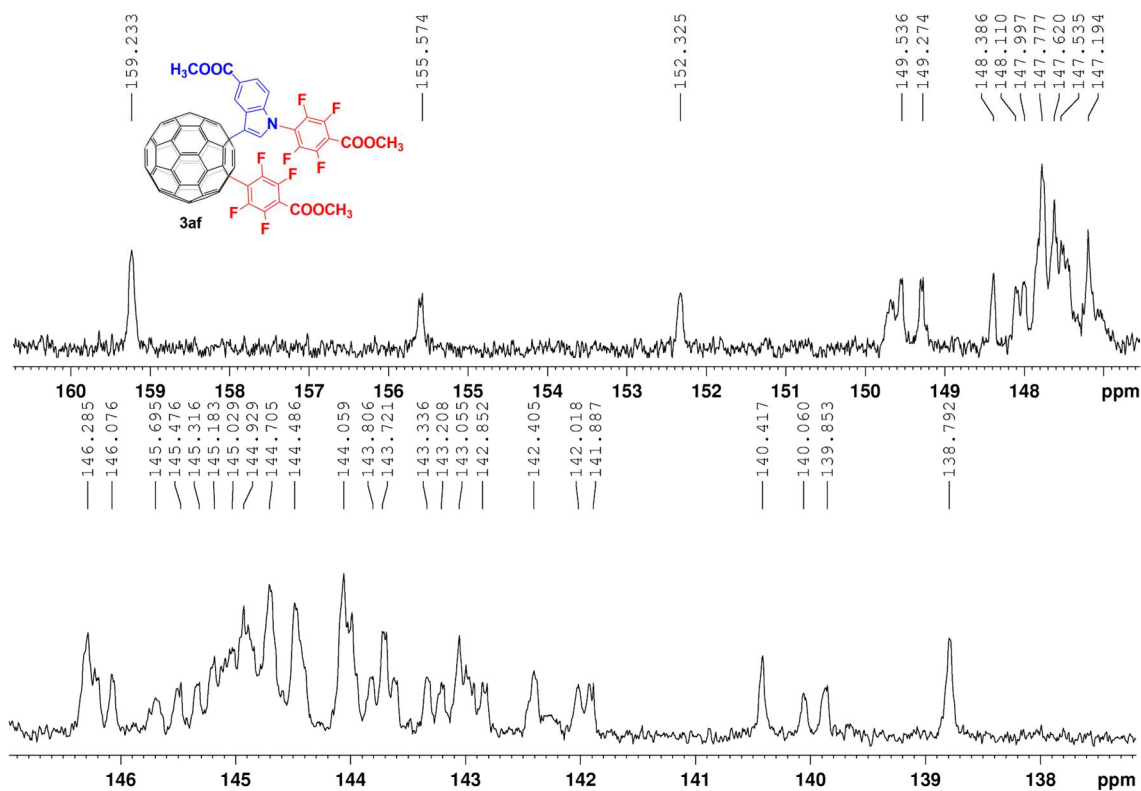
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 3af



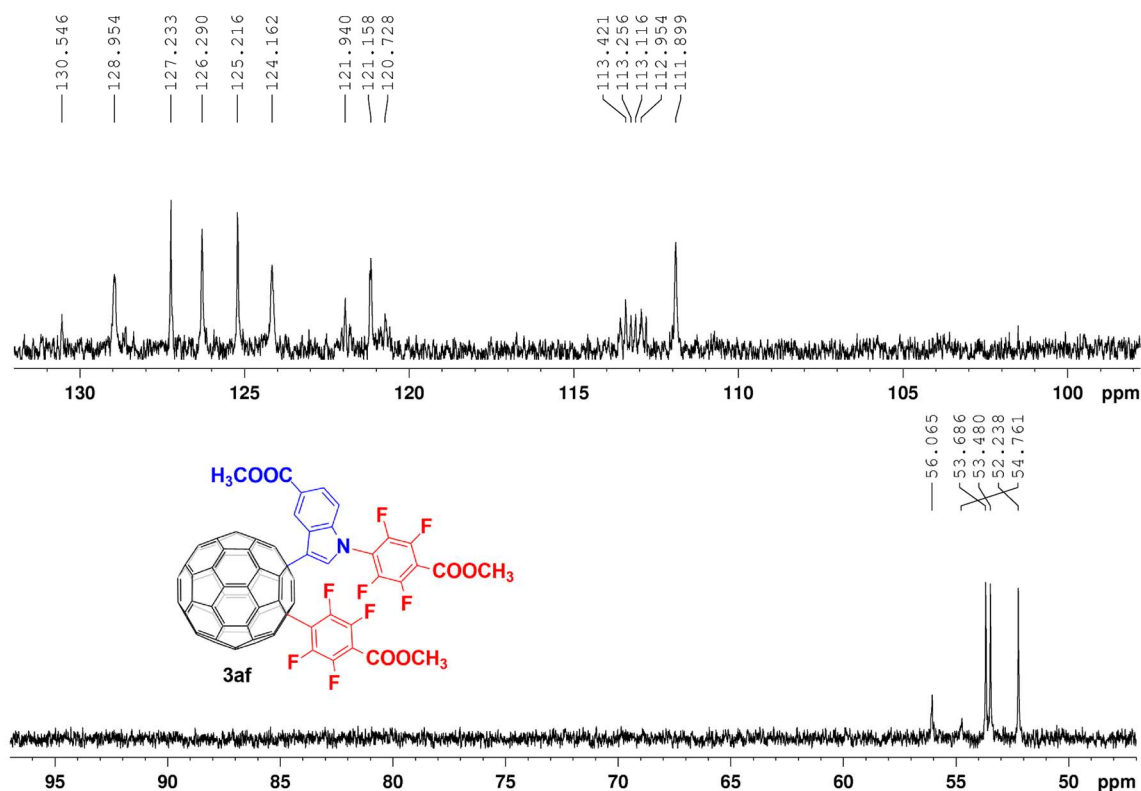
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3af



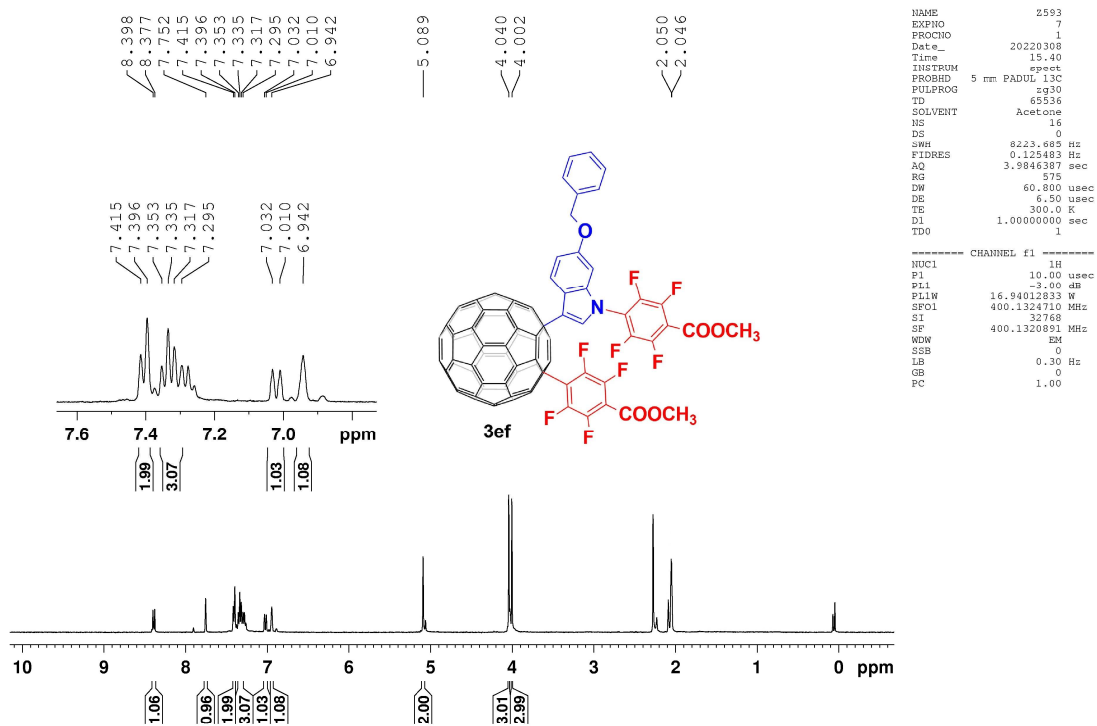
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3af



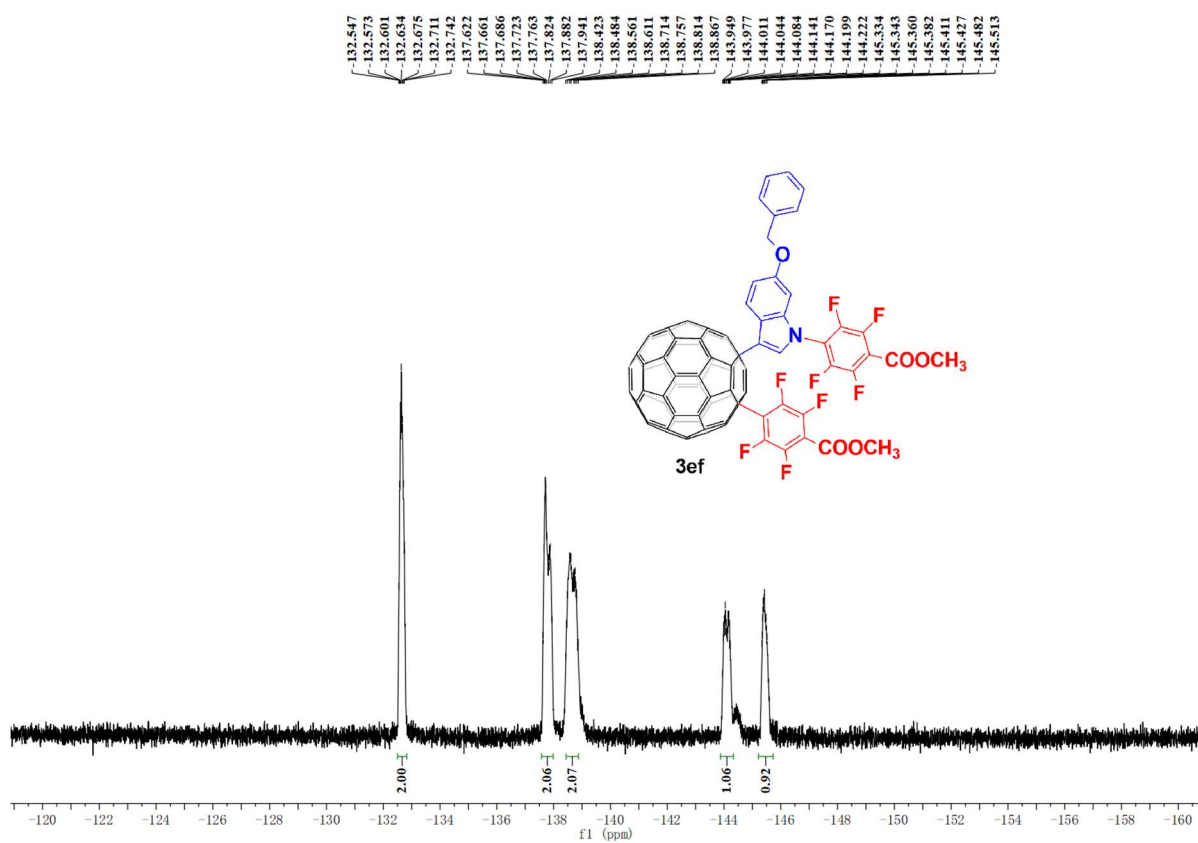
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 3af



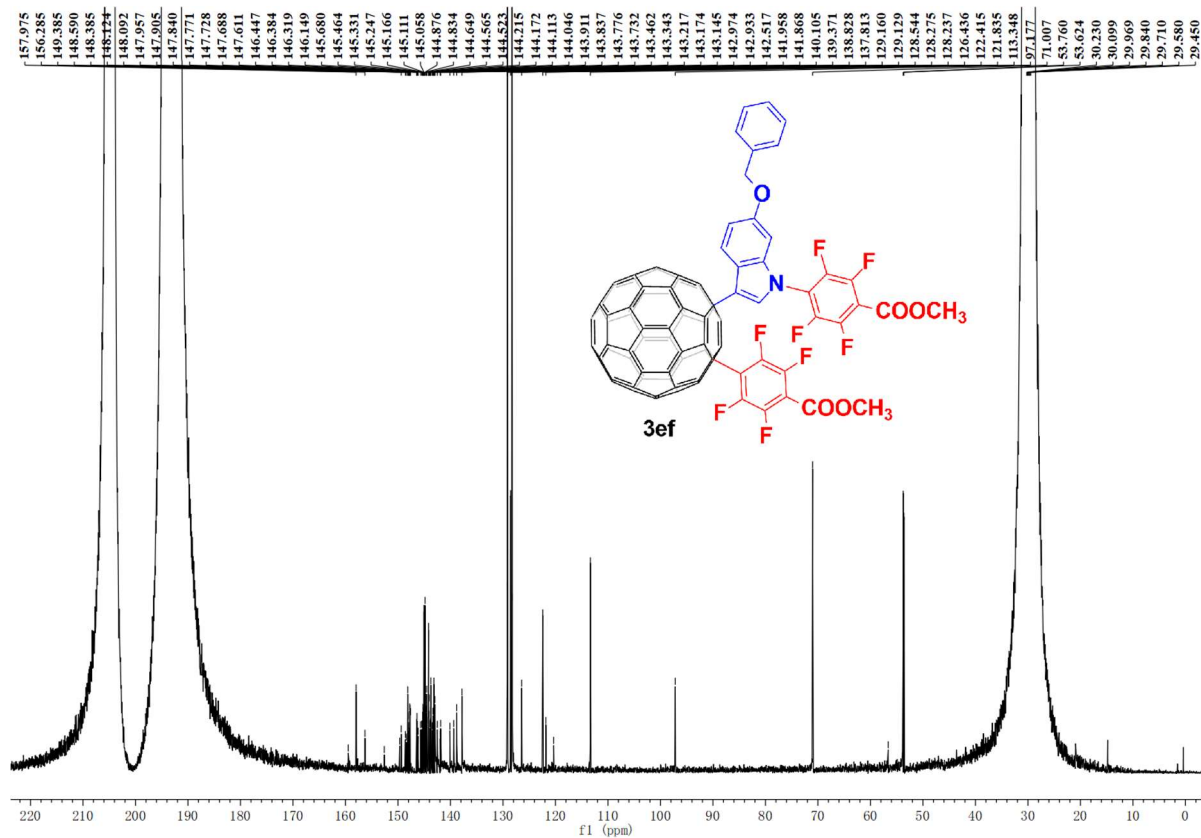
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 3ef



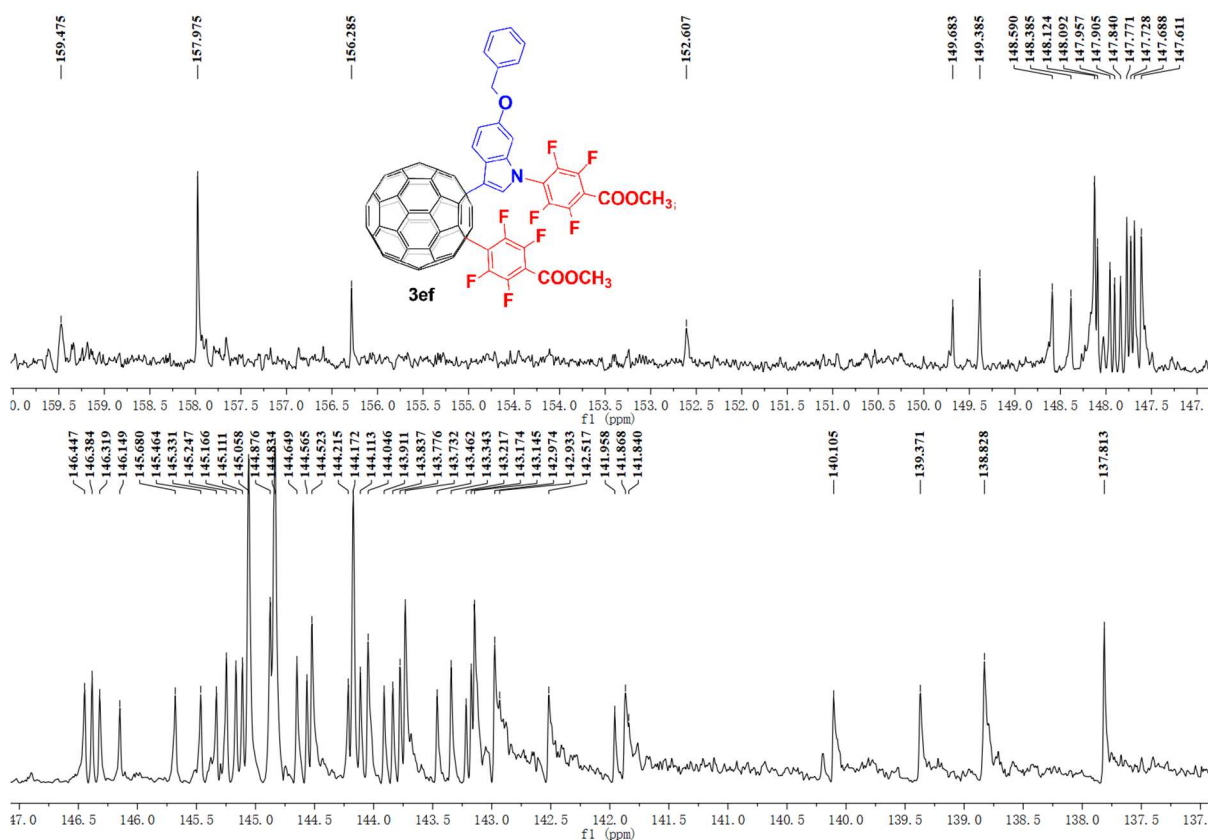
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 3ef



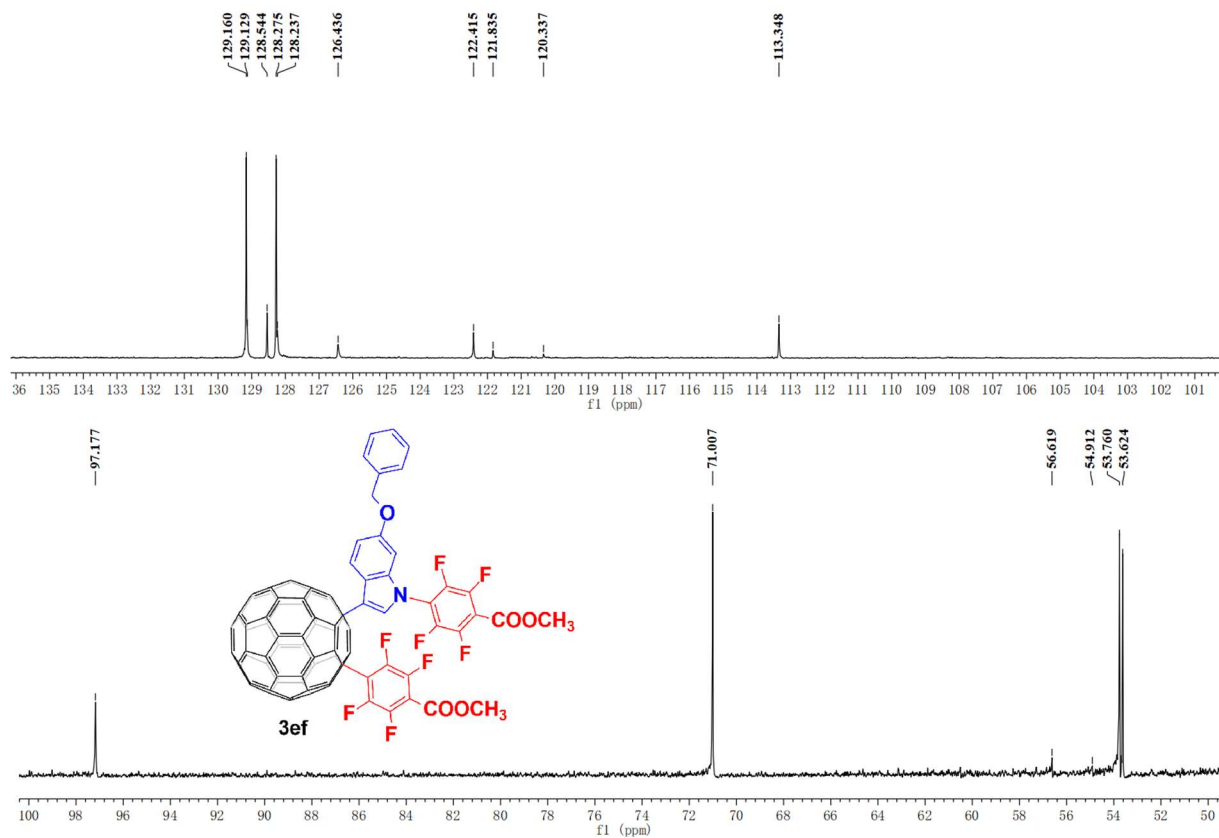
$^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound 3ef



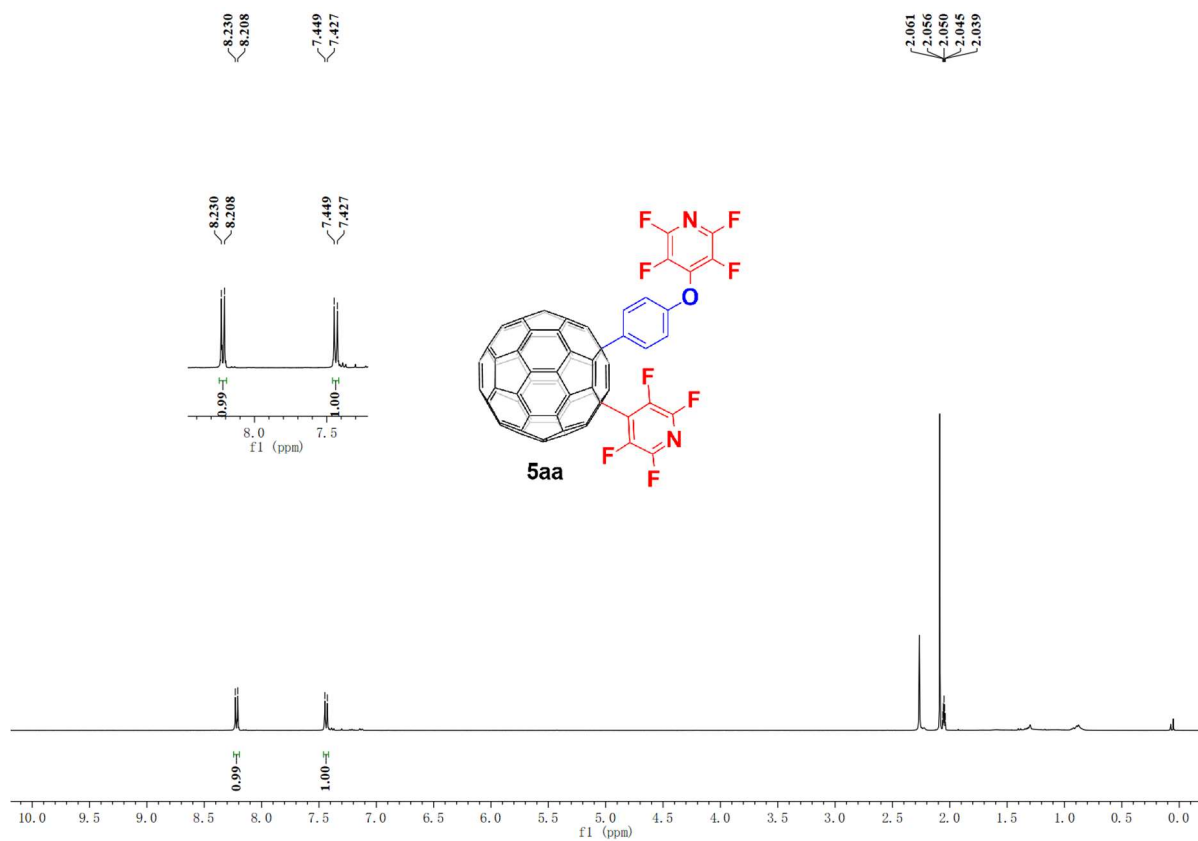
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound **3ef**



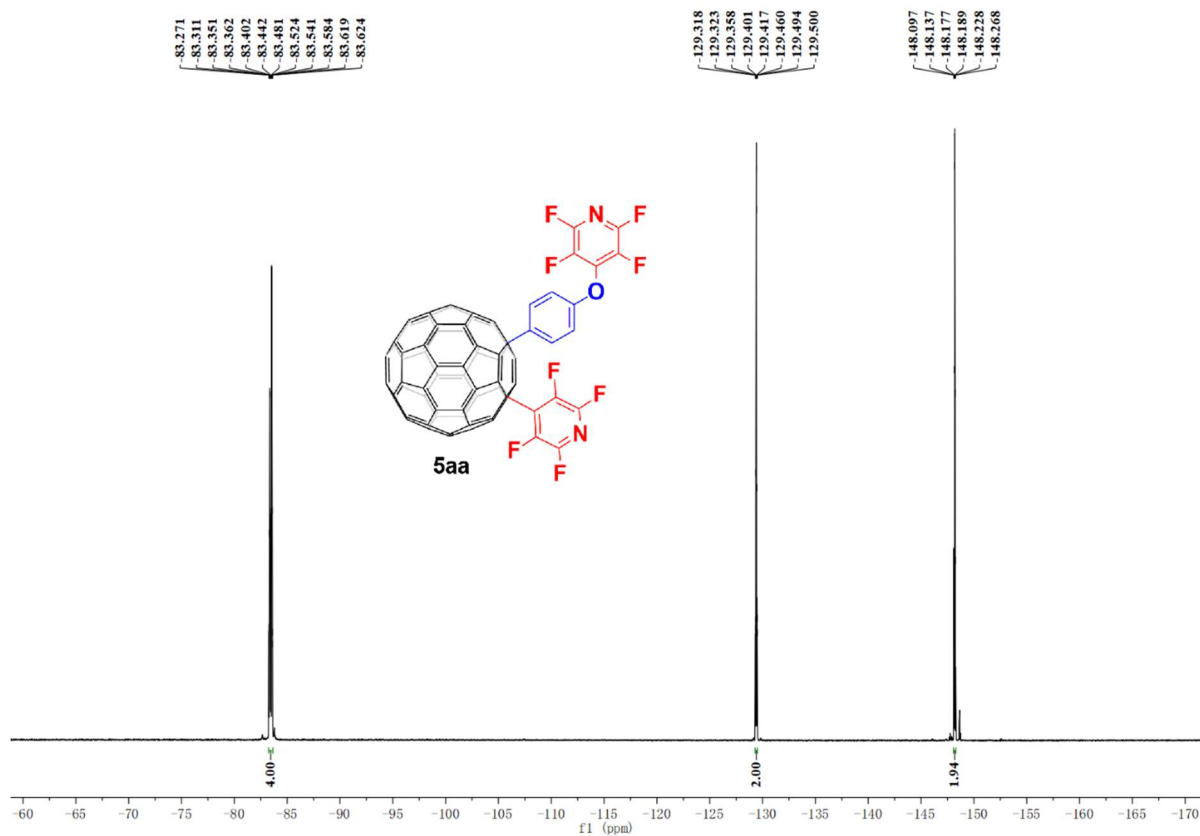
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound **3ef**



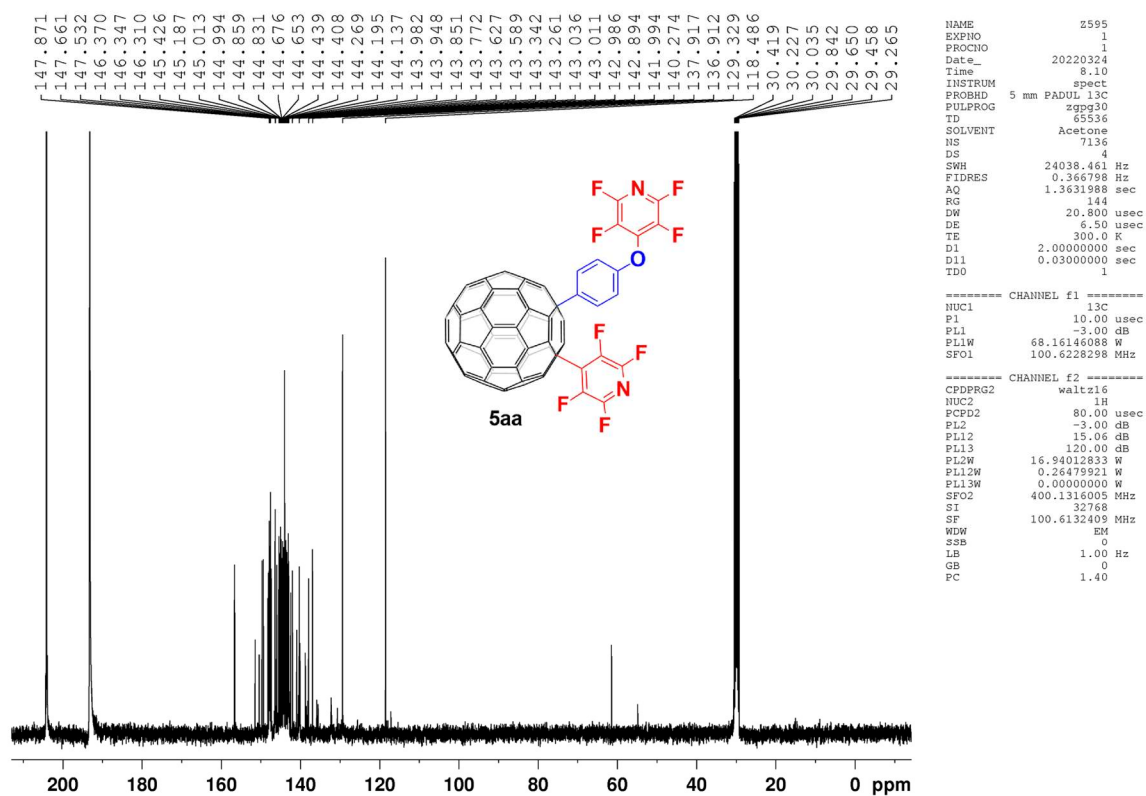
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 5aa



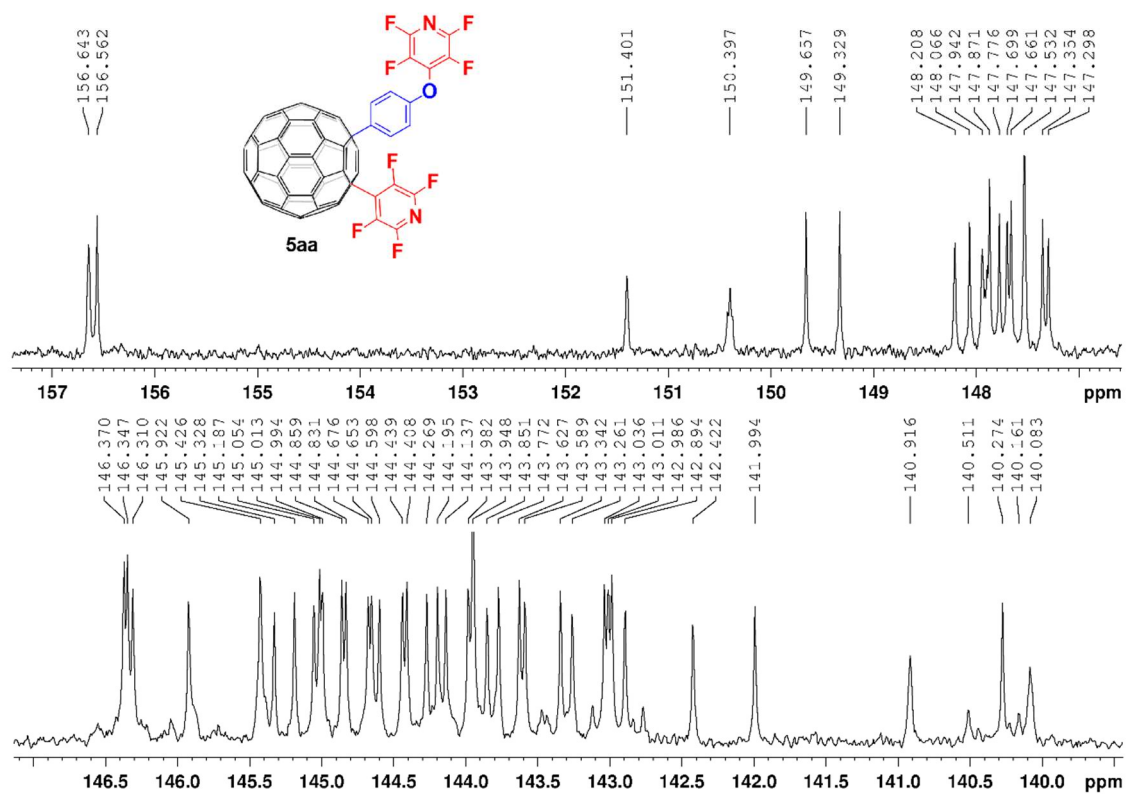
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 5aa



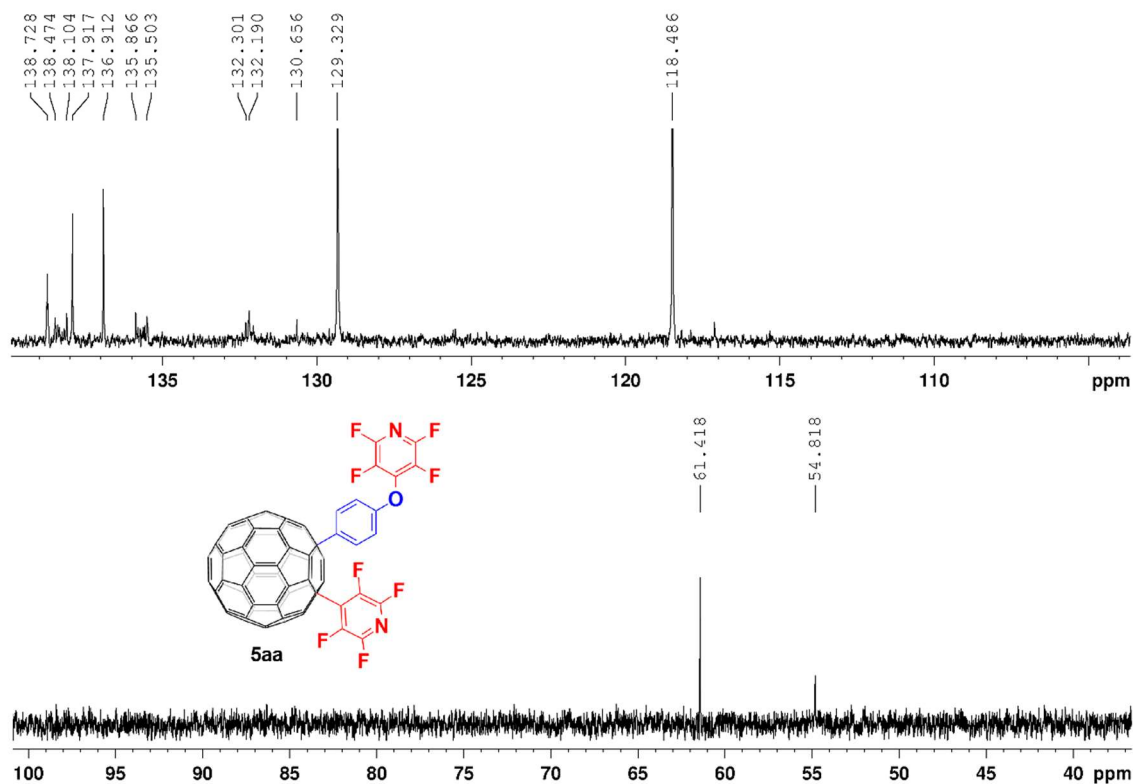
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 5aa



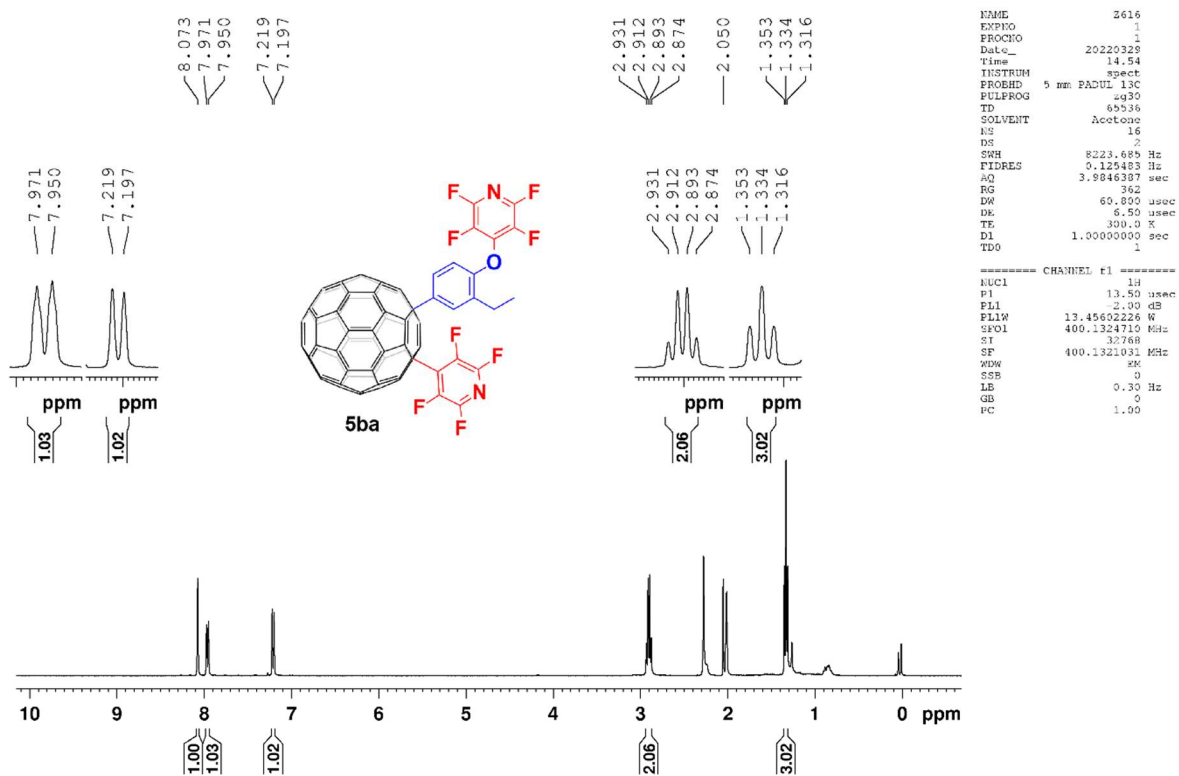
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 5aa



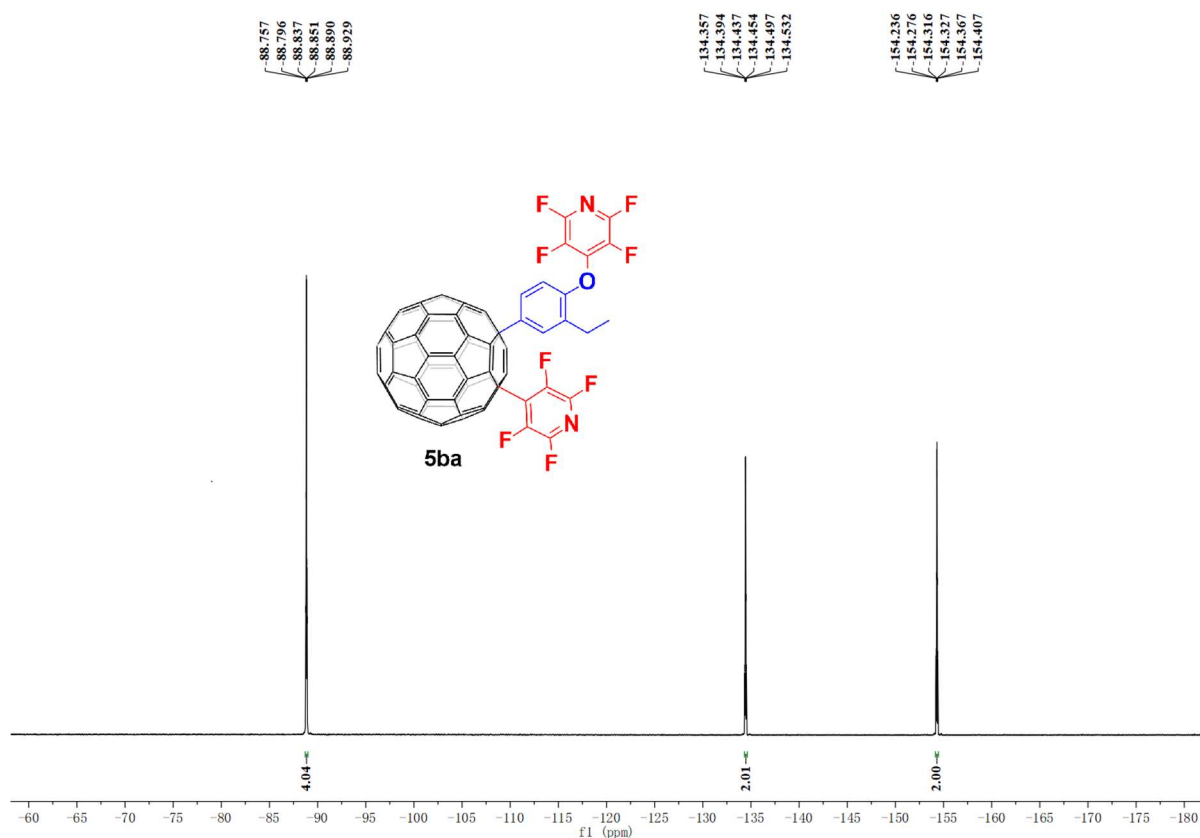
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5aa



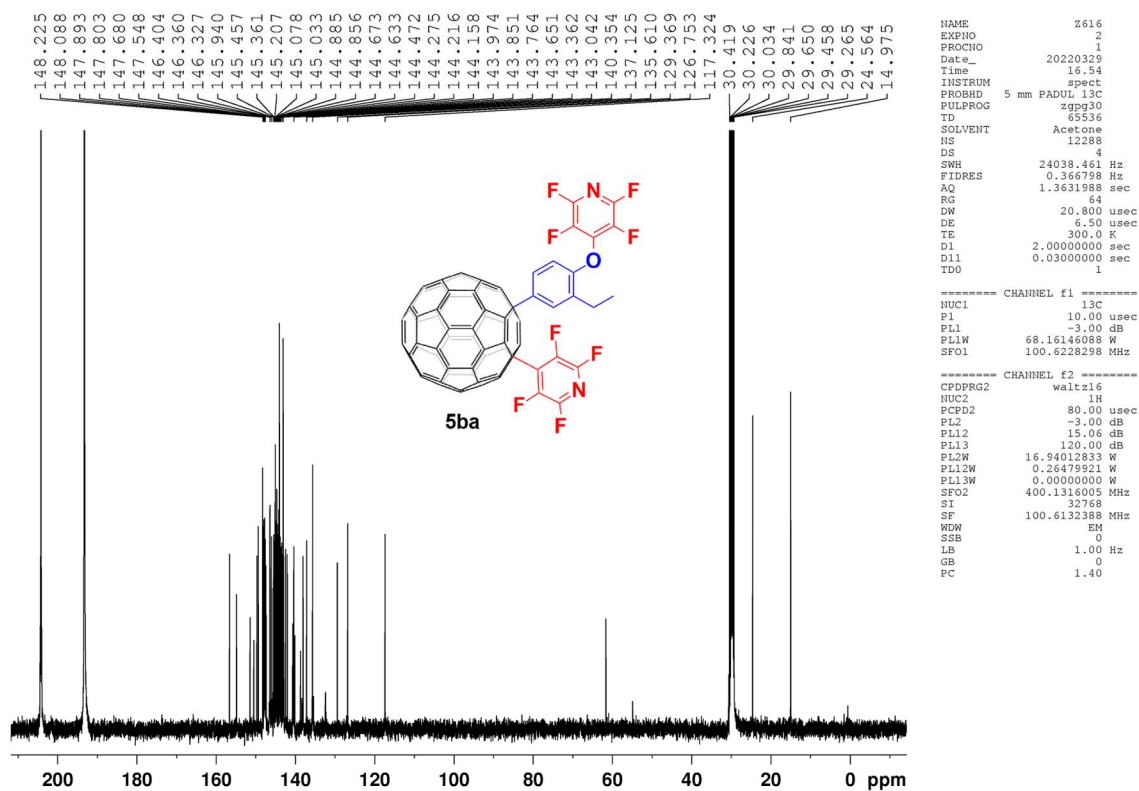
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 5ba



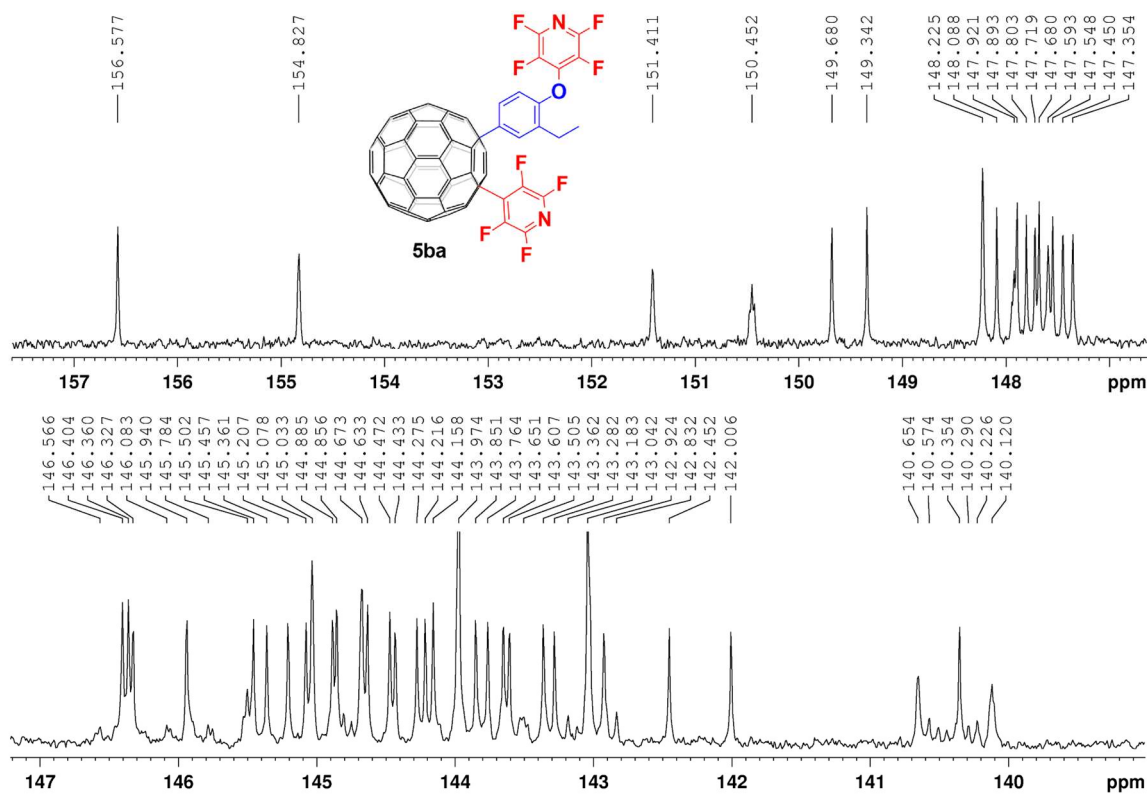
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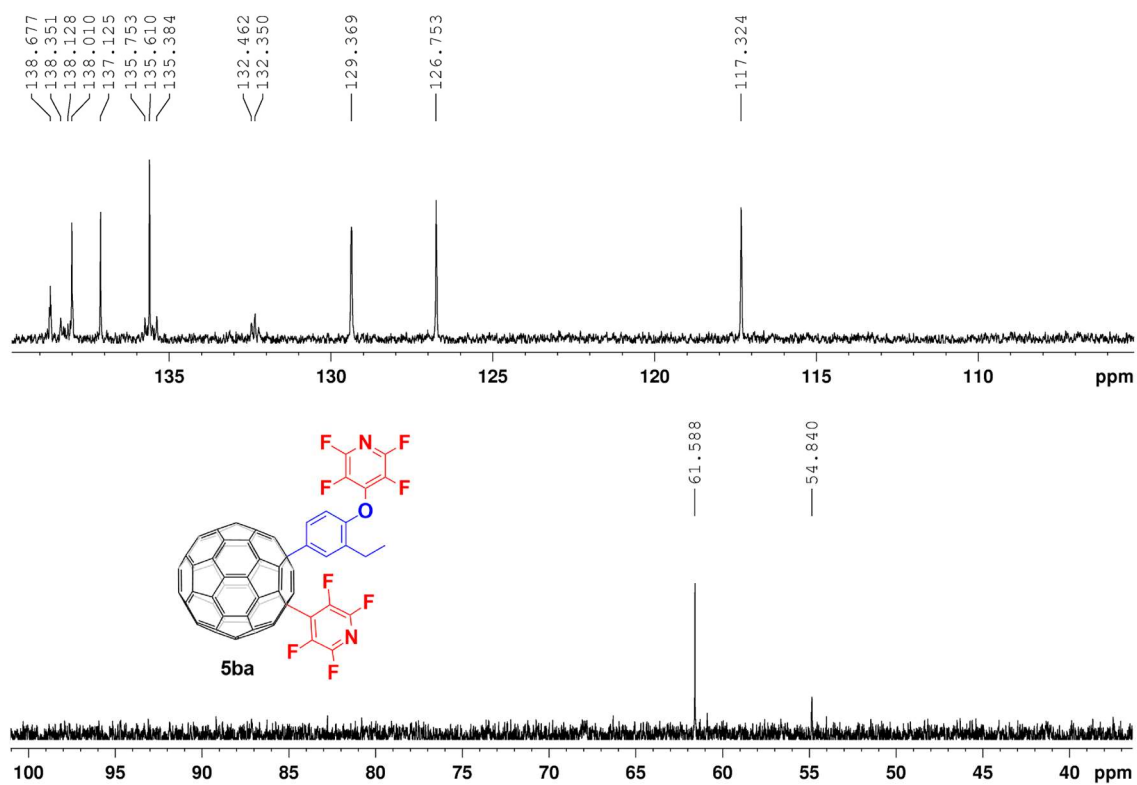
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5ba



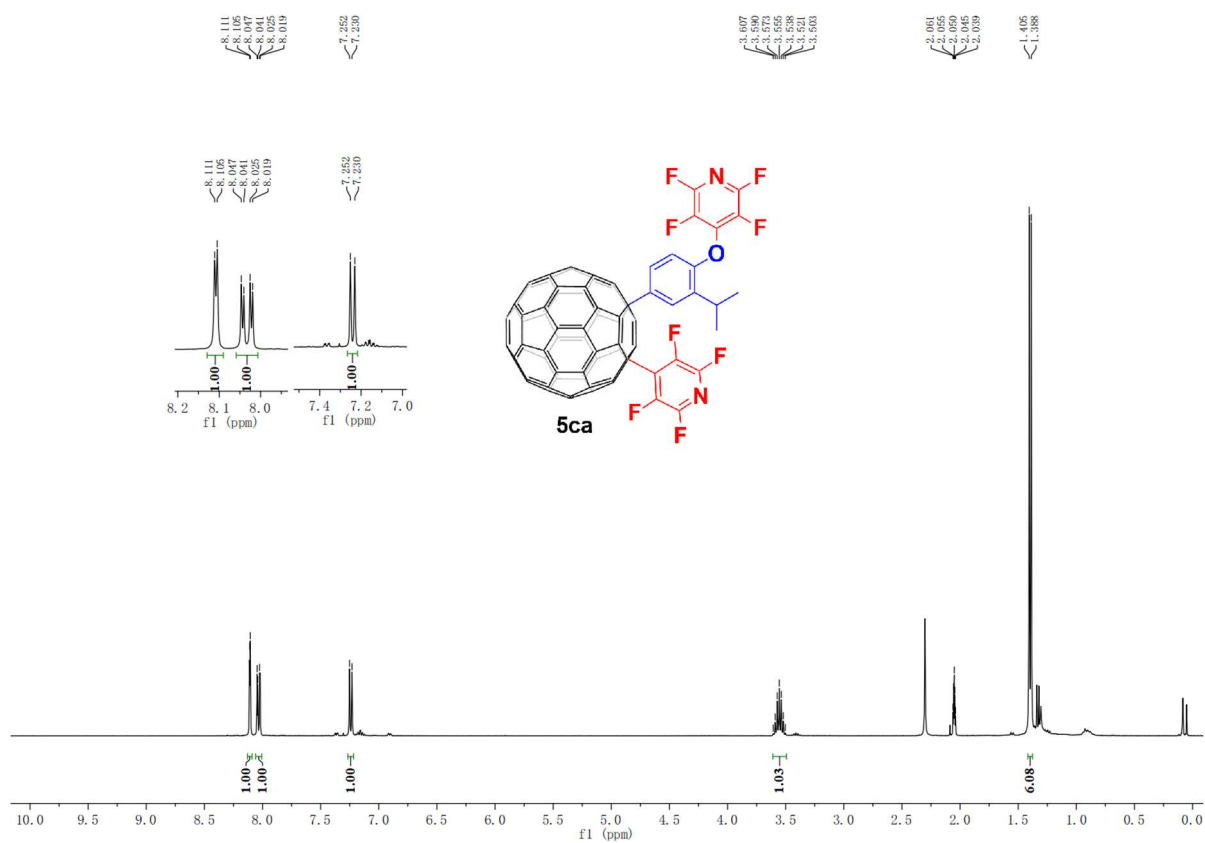
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5ba



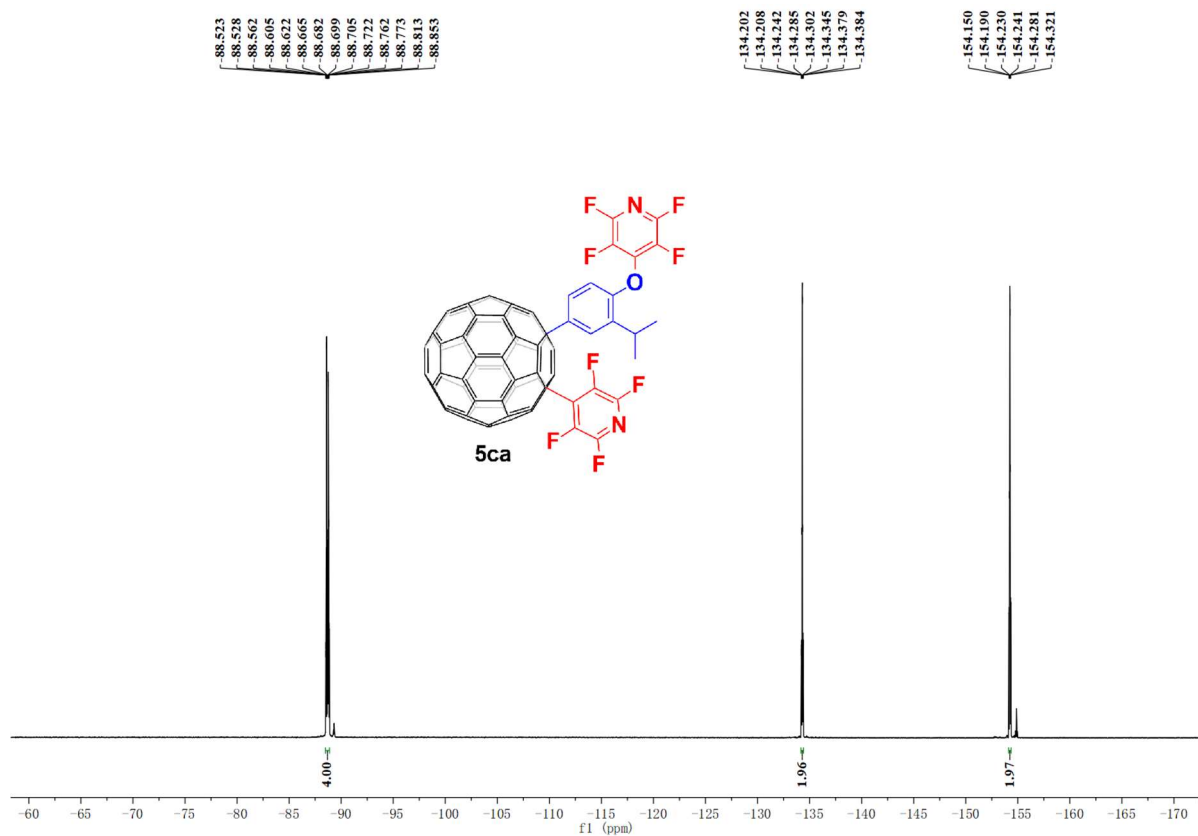
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5ba



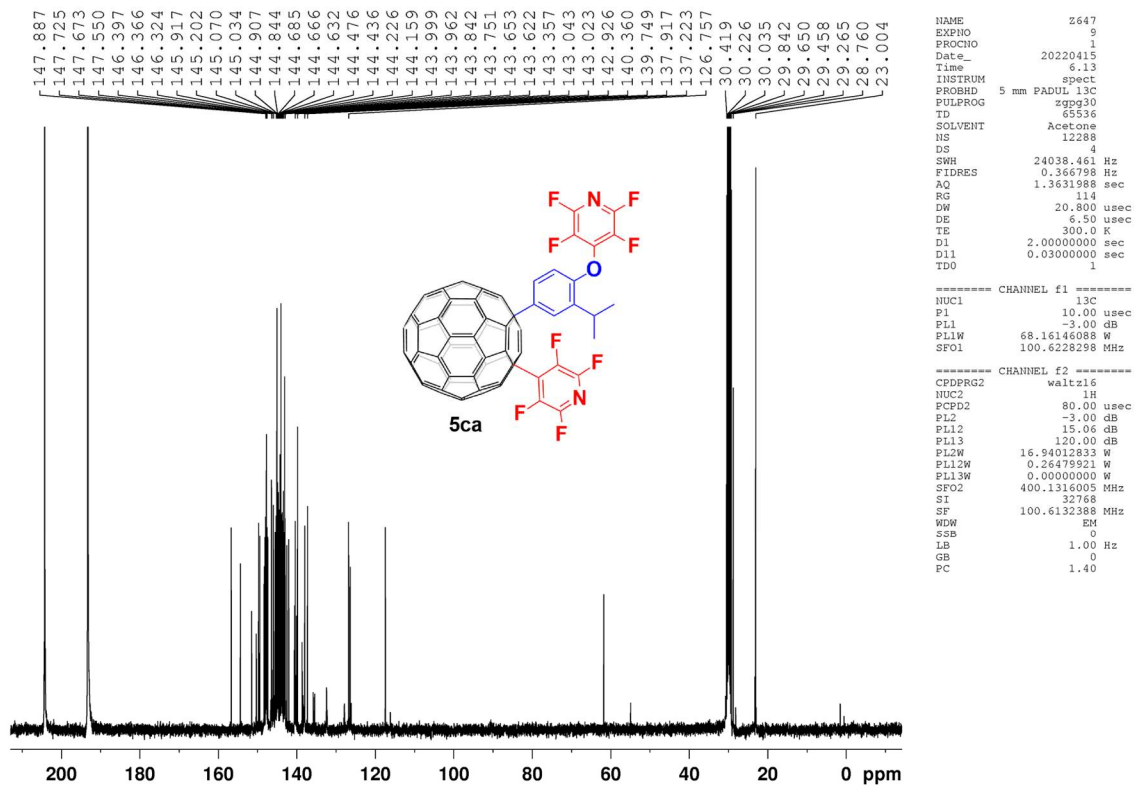
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 5ca



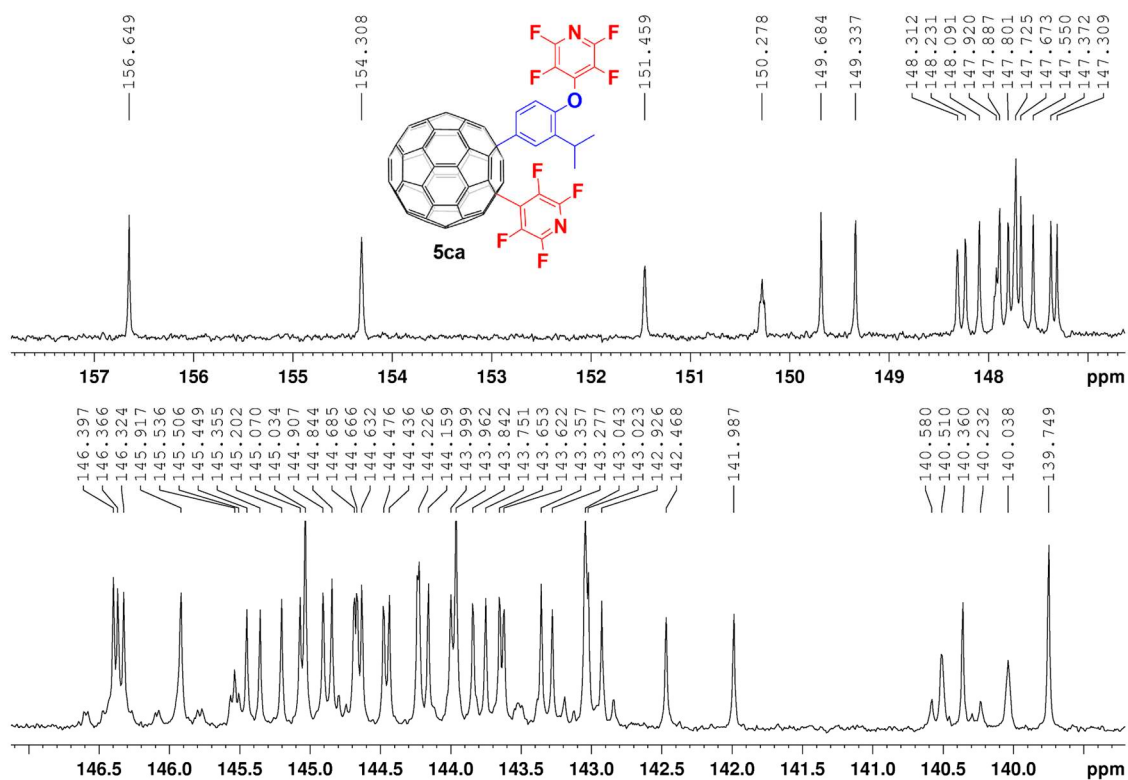
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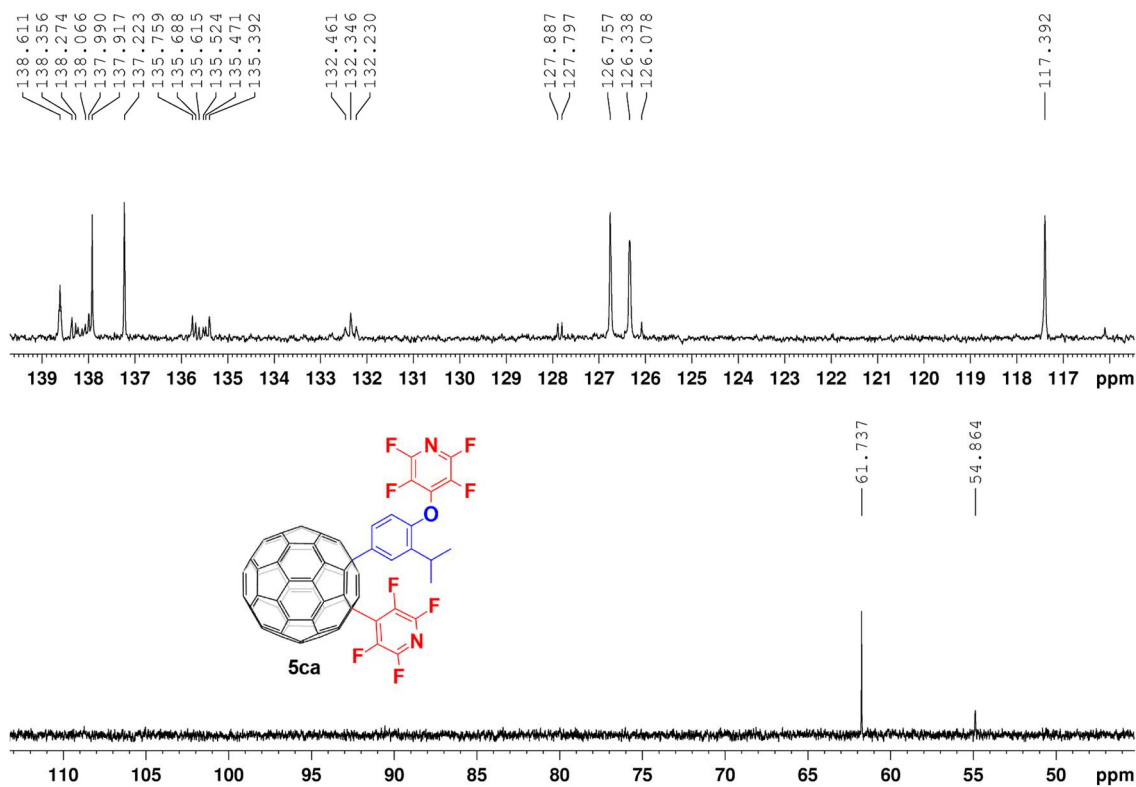
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 5ca



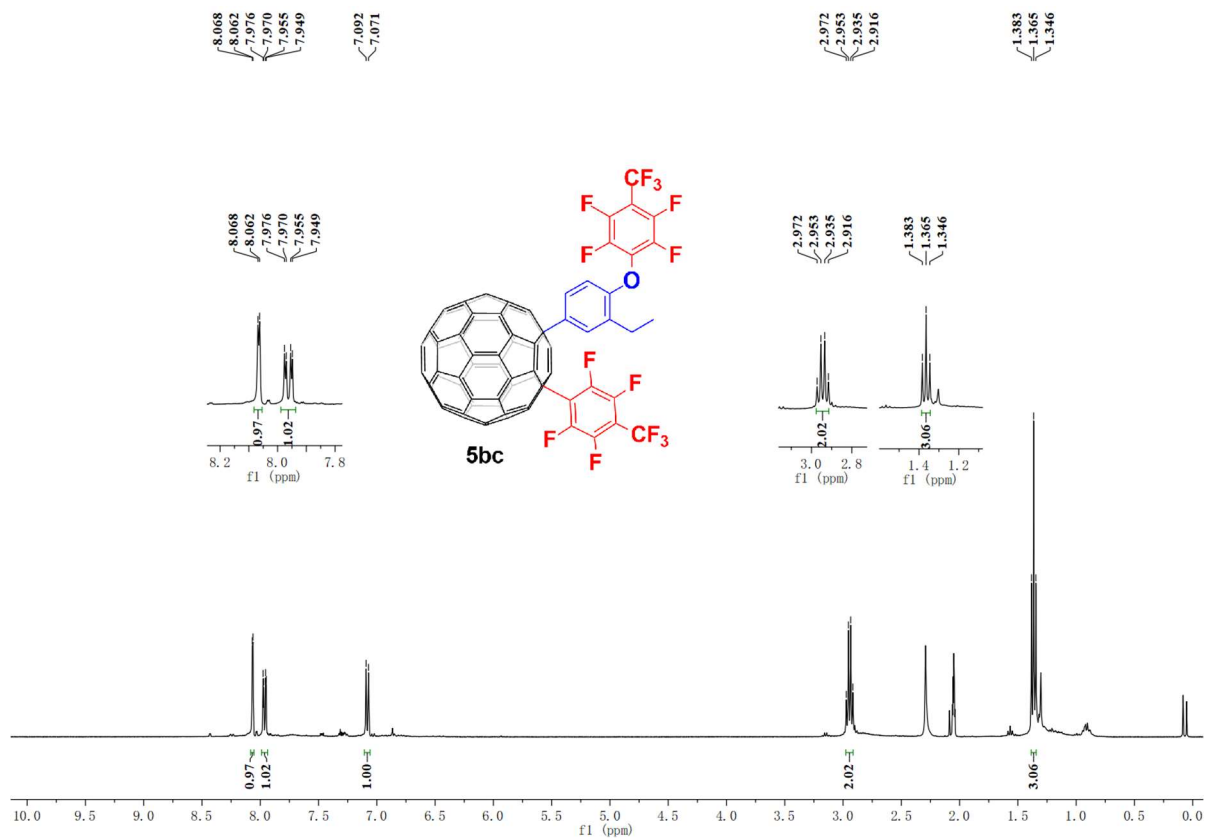
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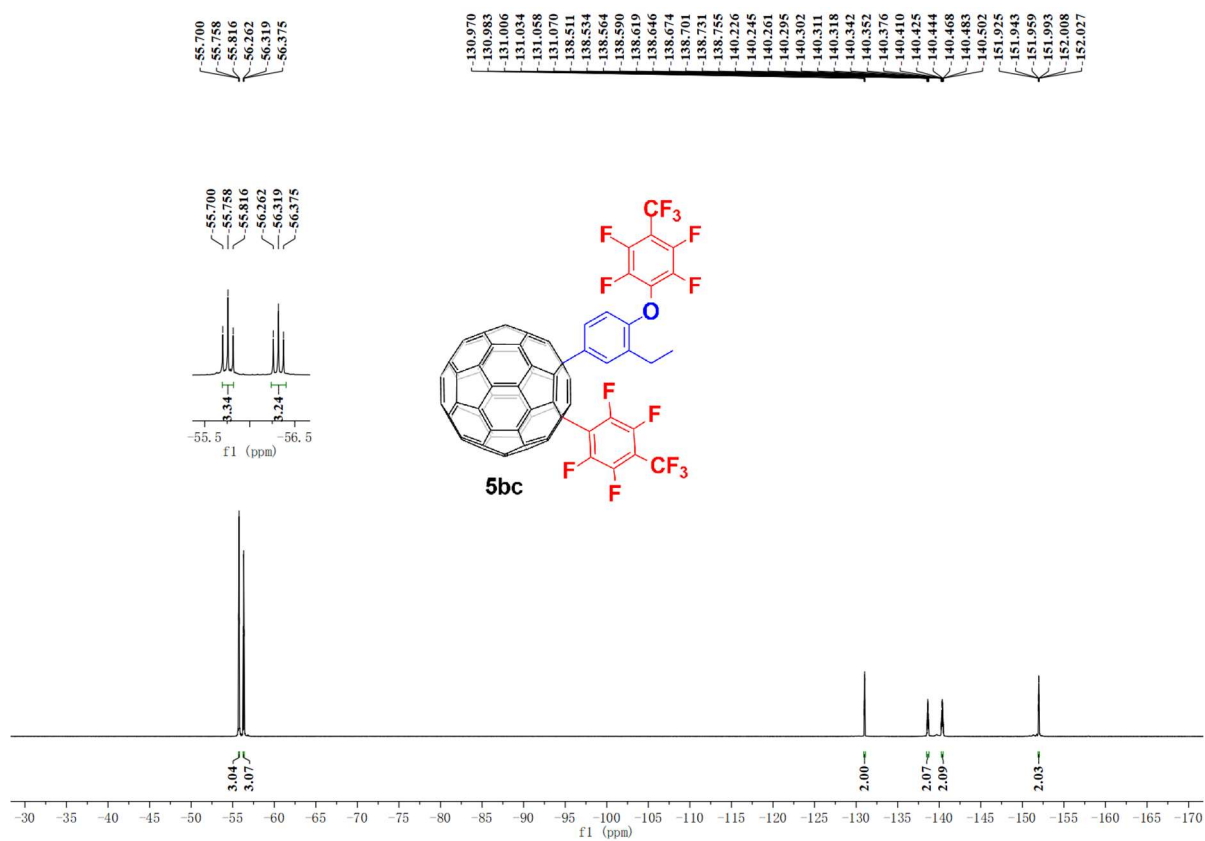
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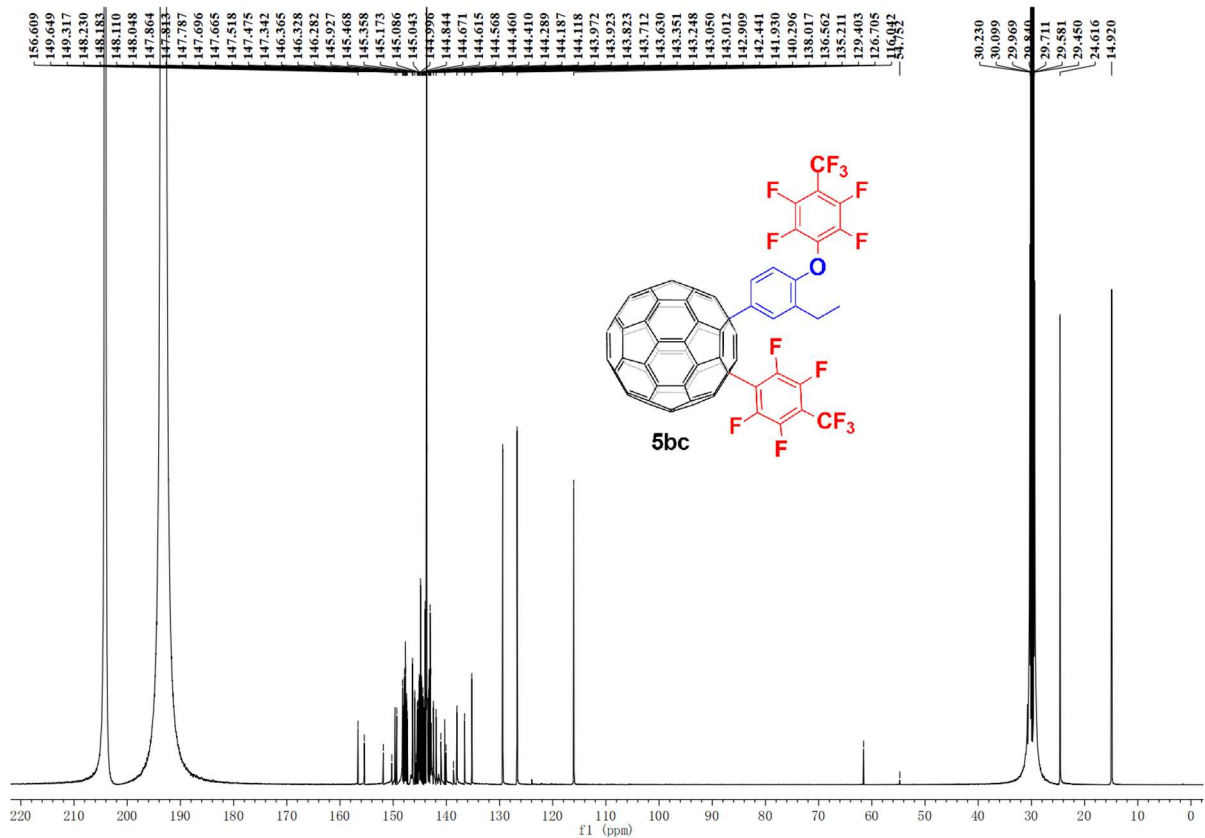
^1H NMR (400 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 5bc



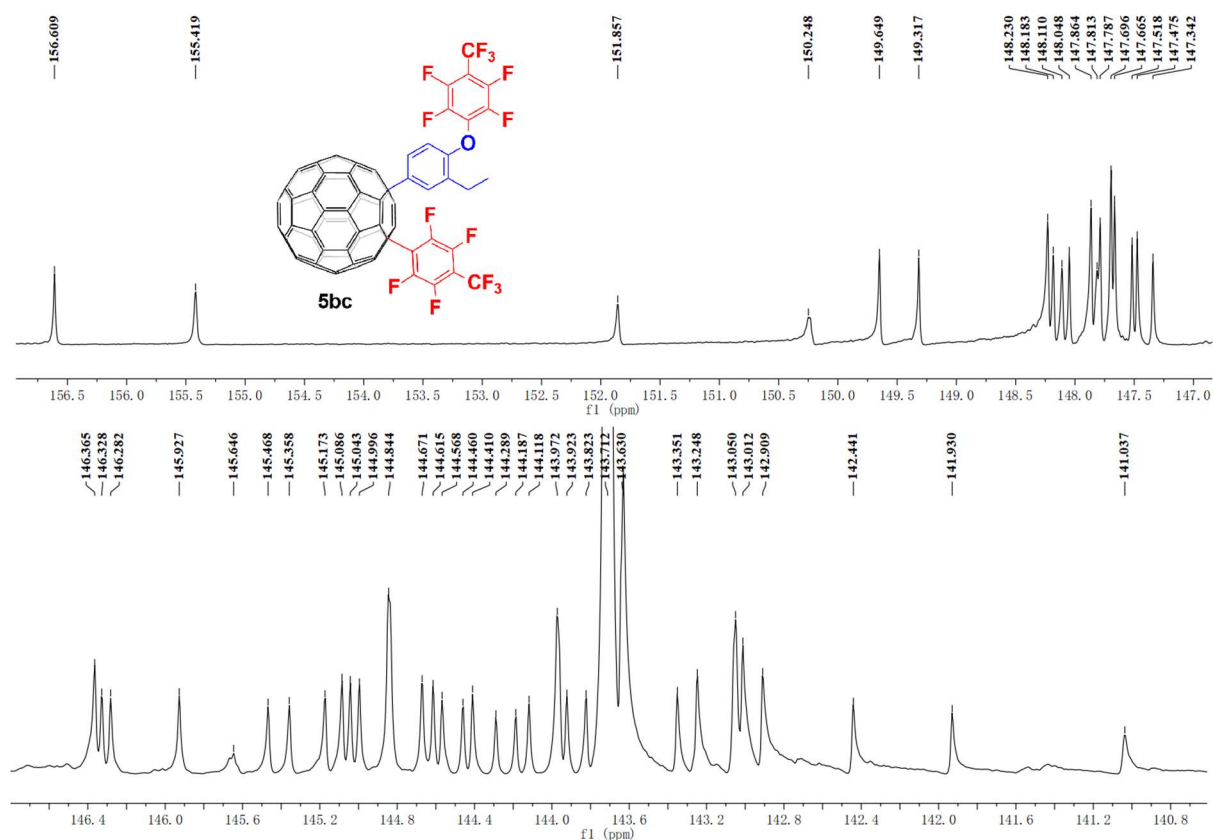
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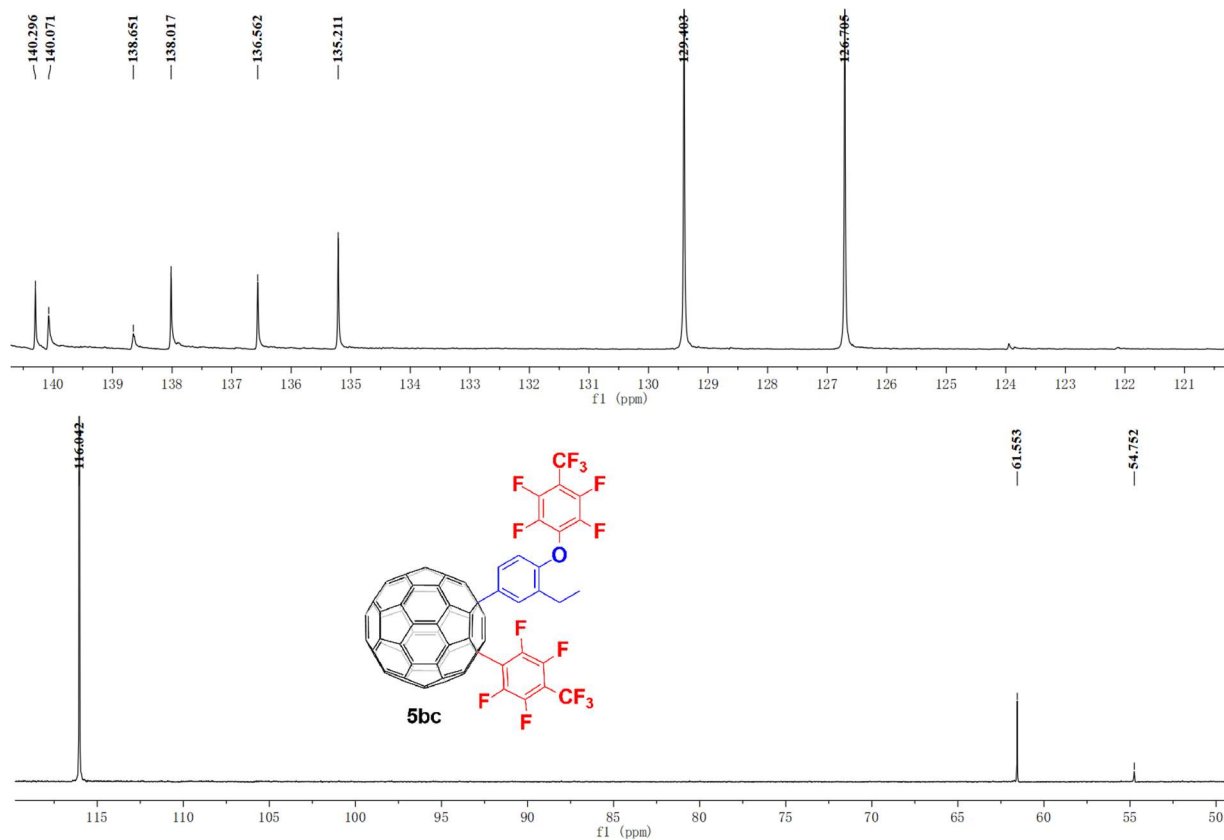
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5bc



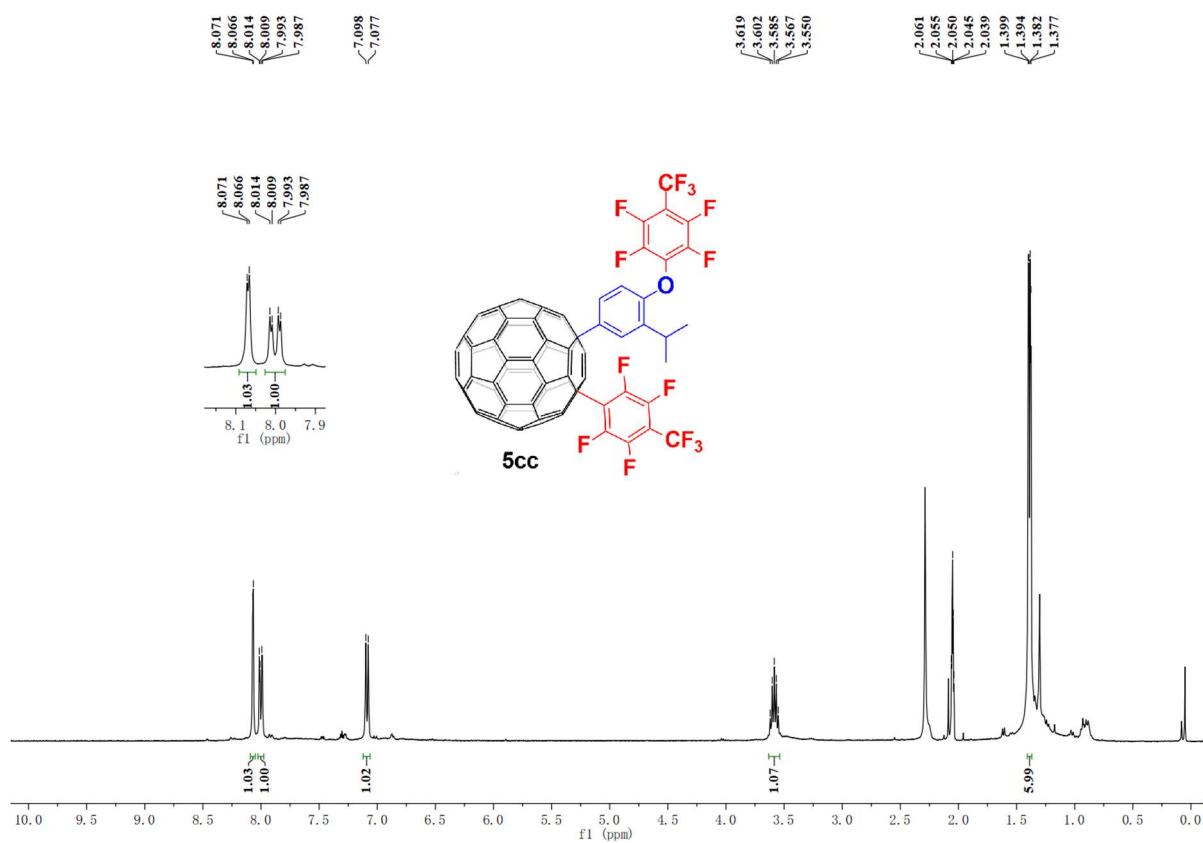
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **5bc**



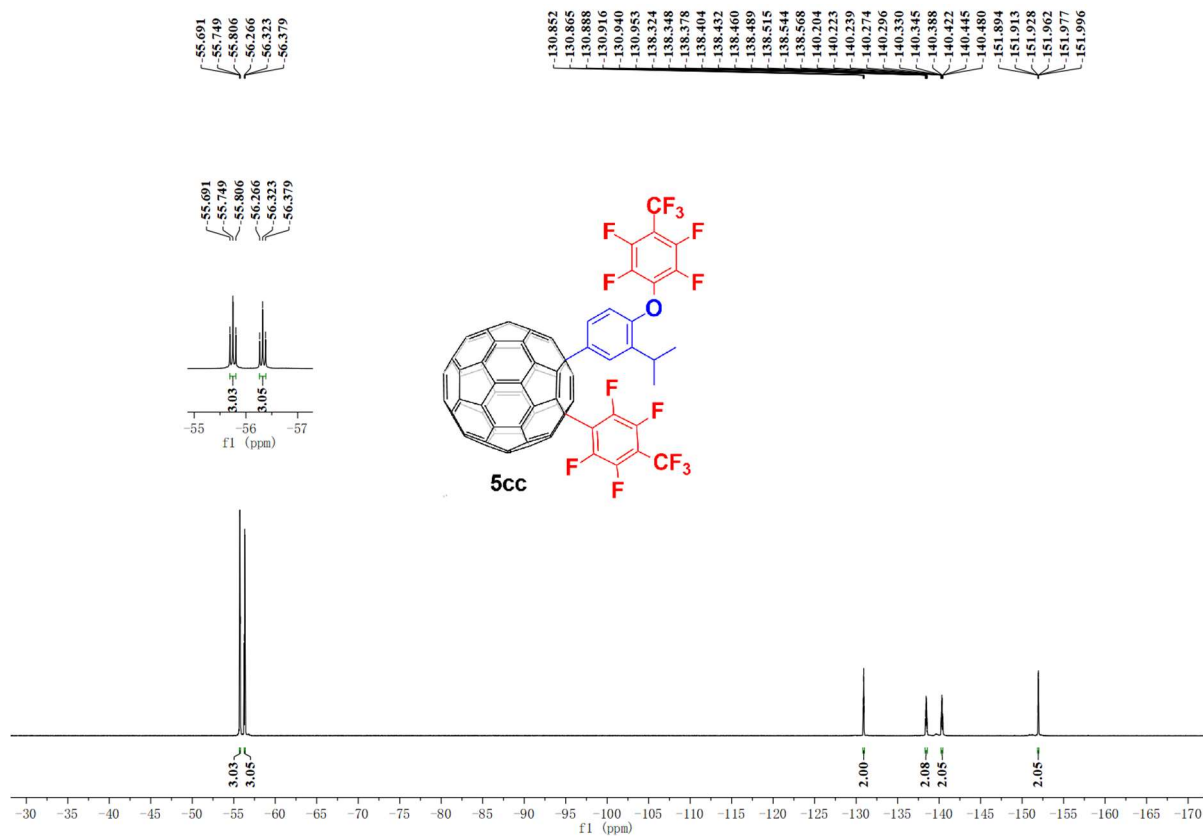
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **5bc**



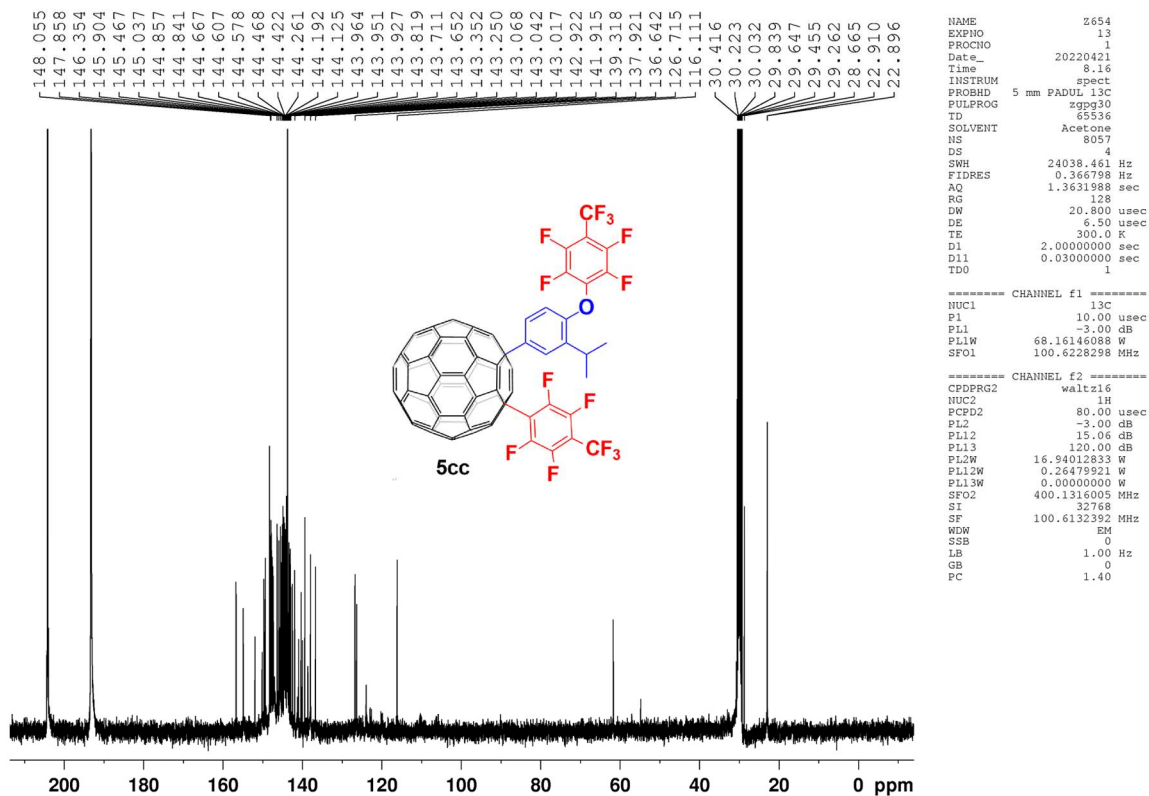
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **5cc**



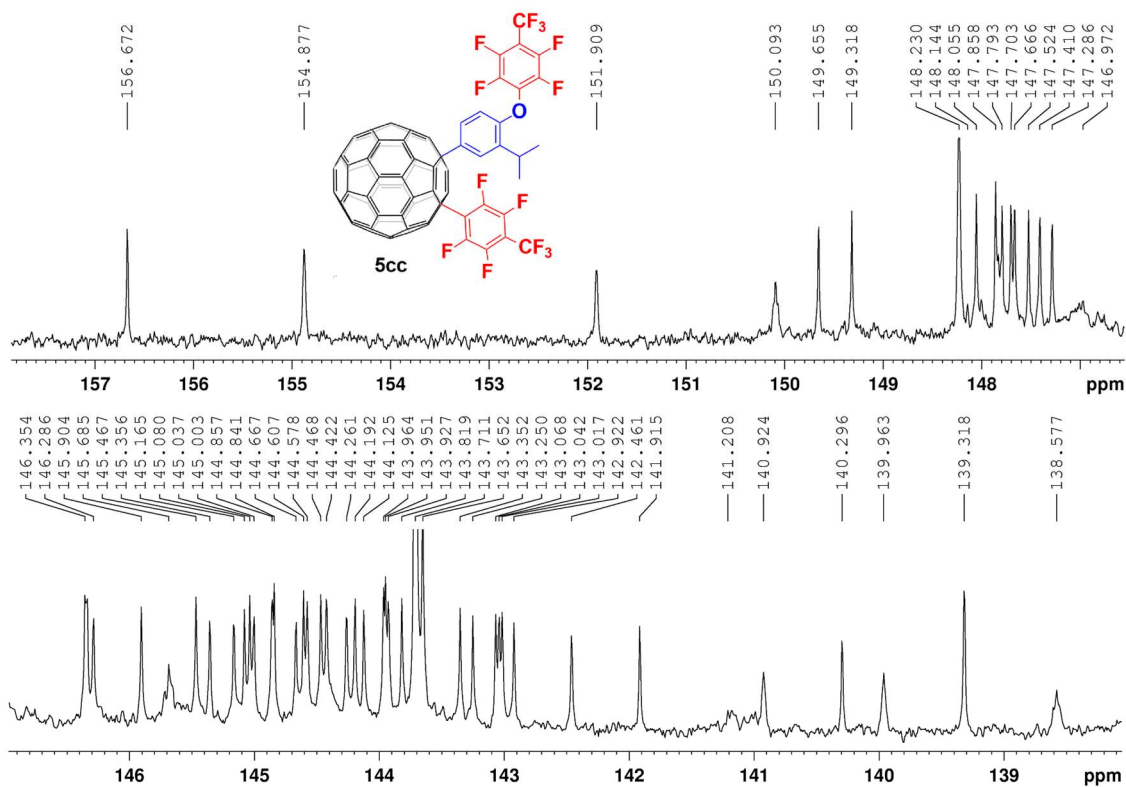
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound **5cc**



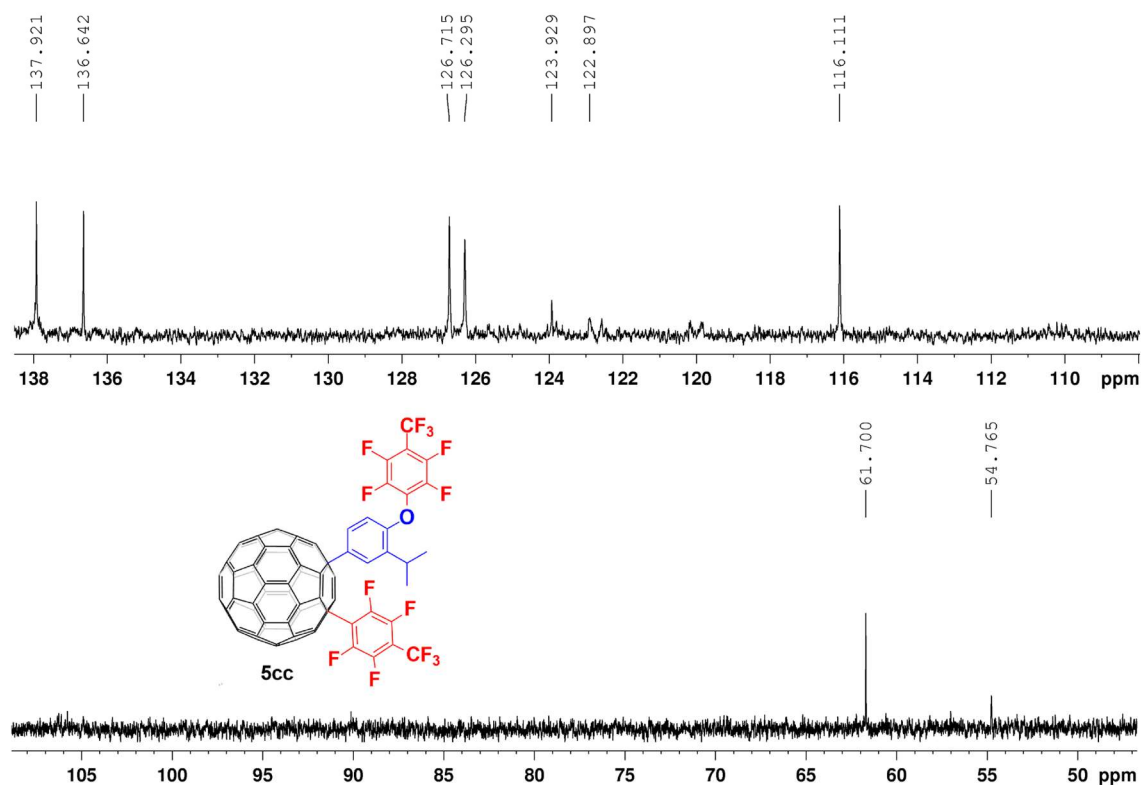
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 5cc



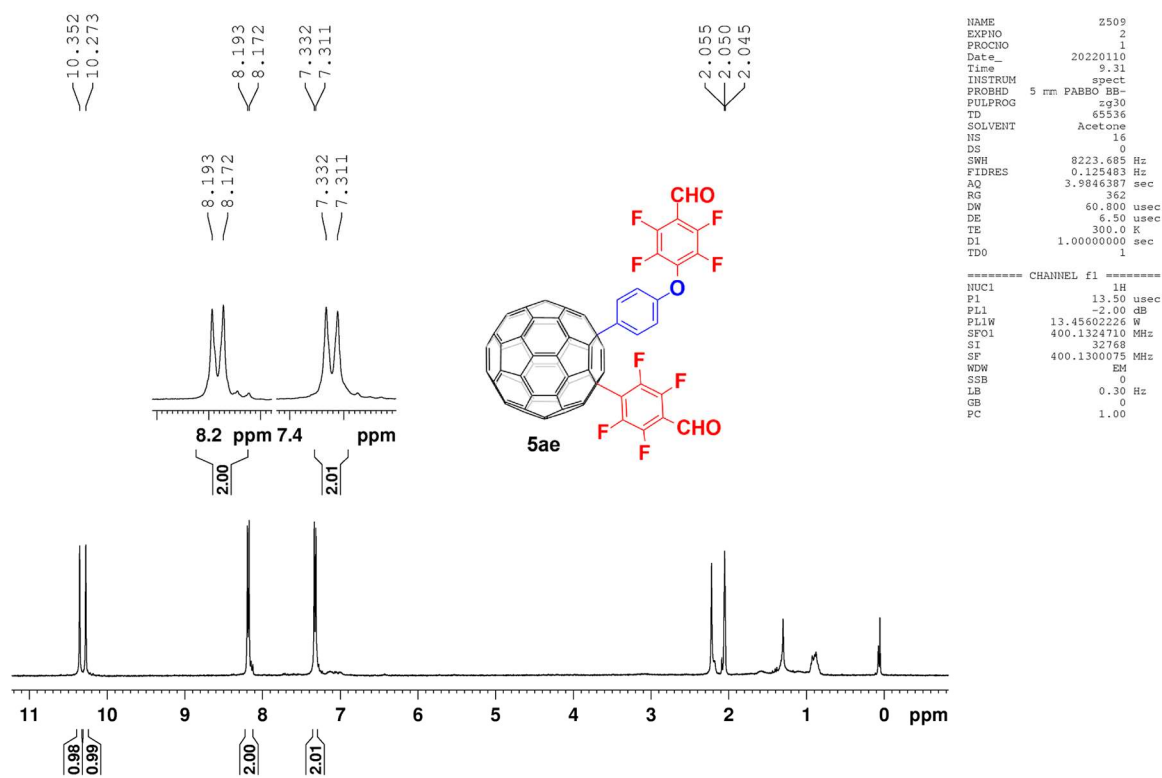
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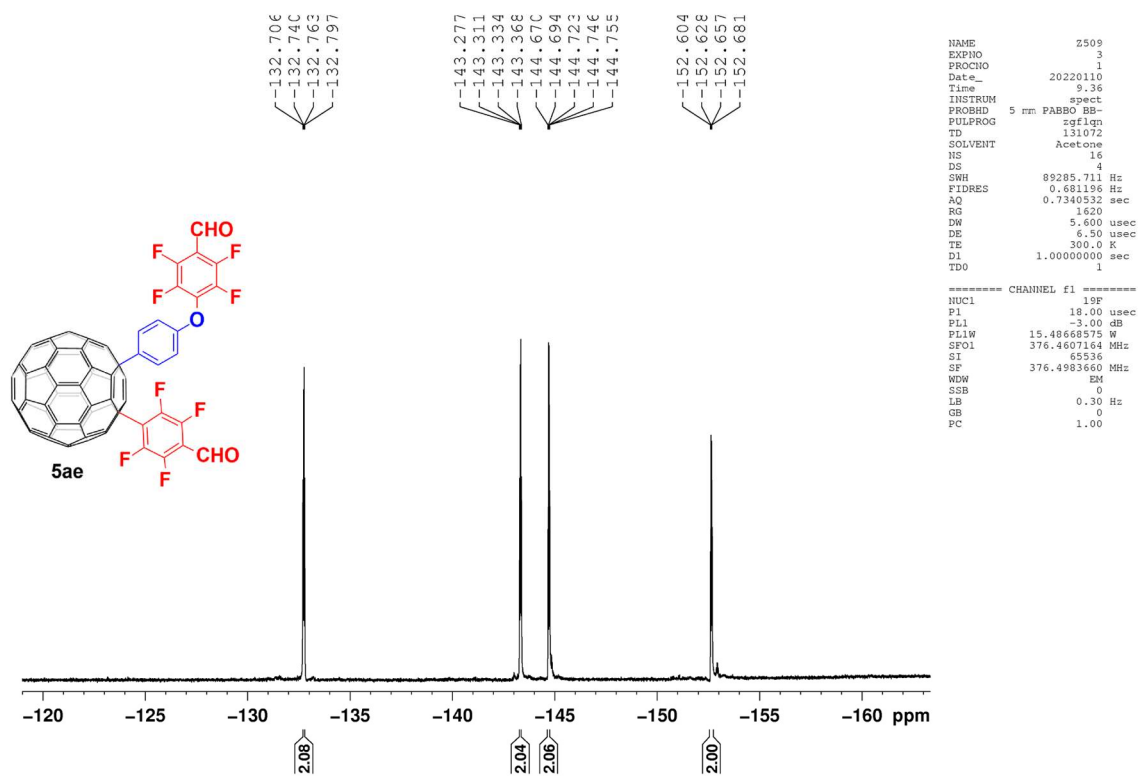
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5cc



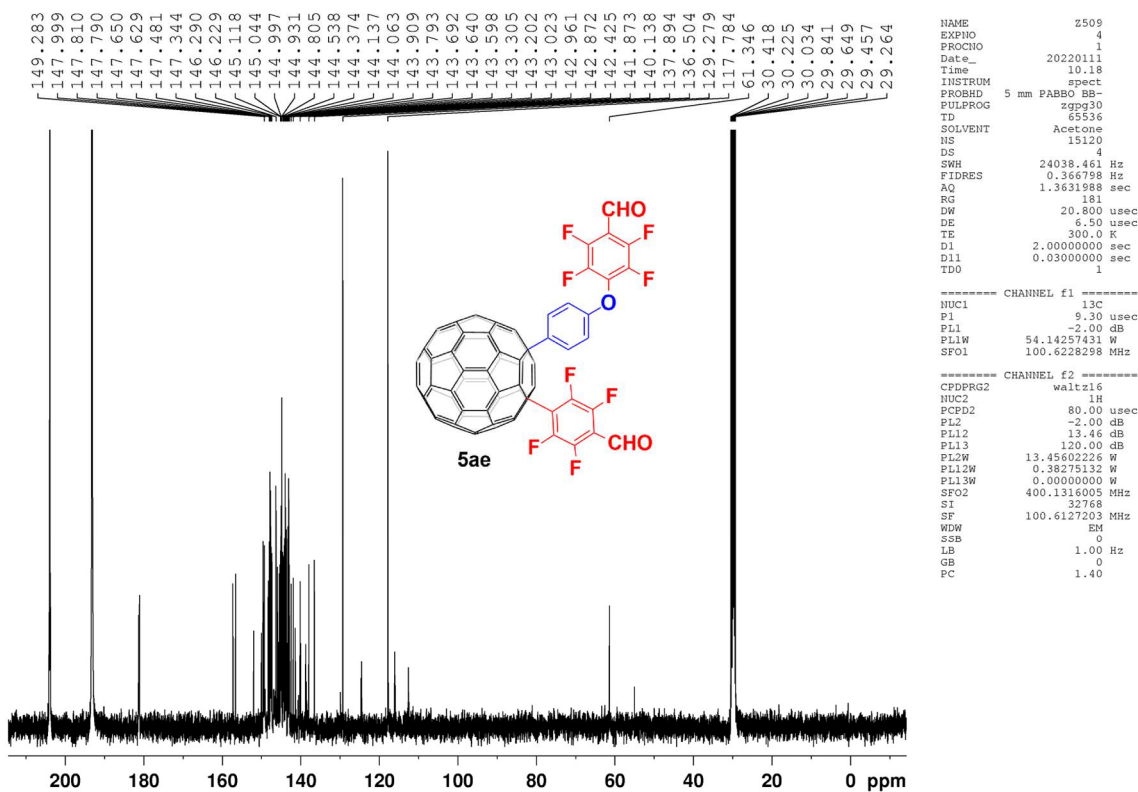
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 5ae



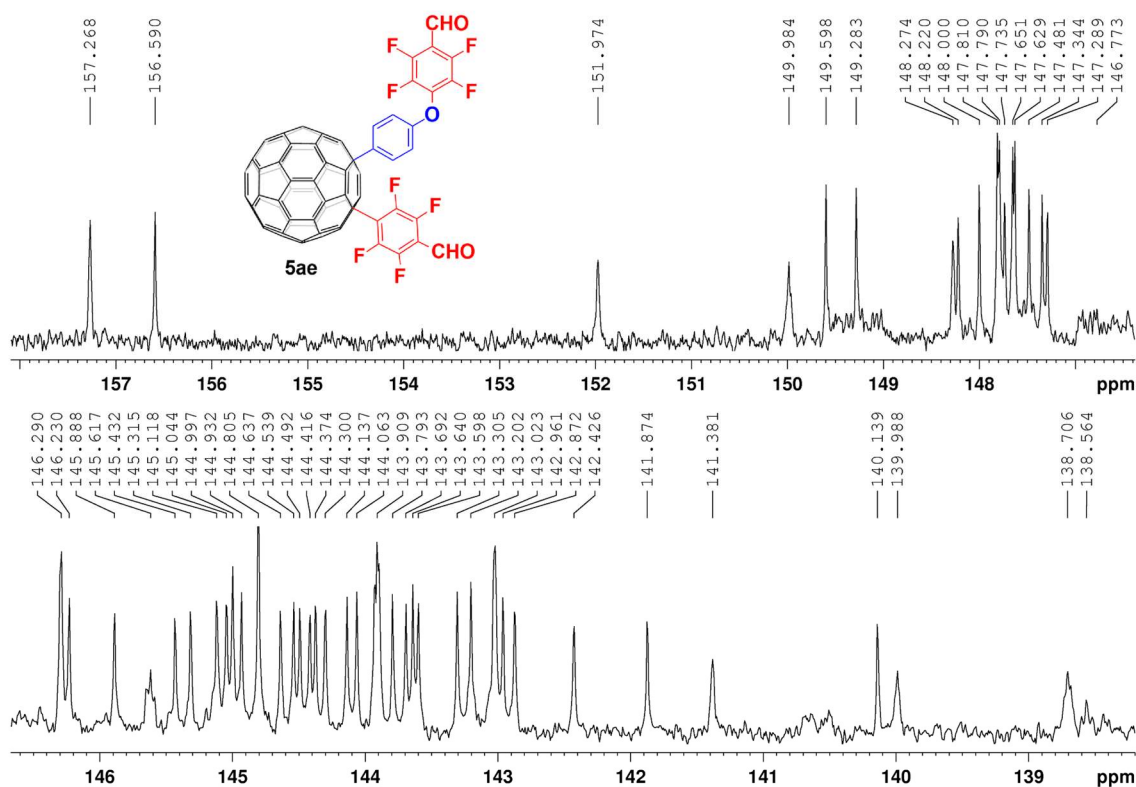
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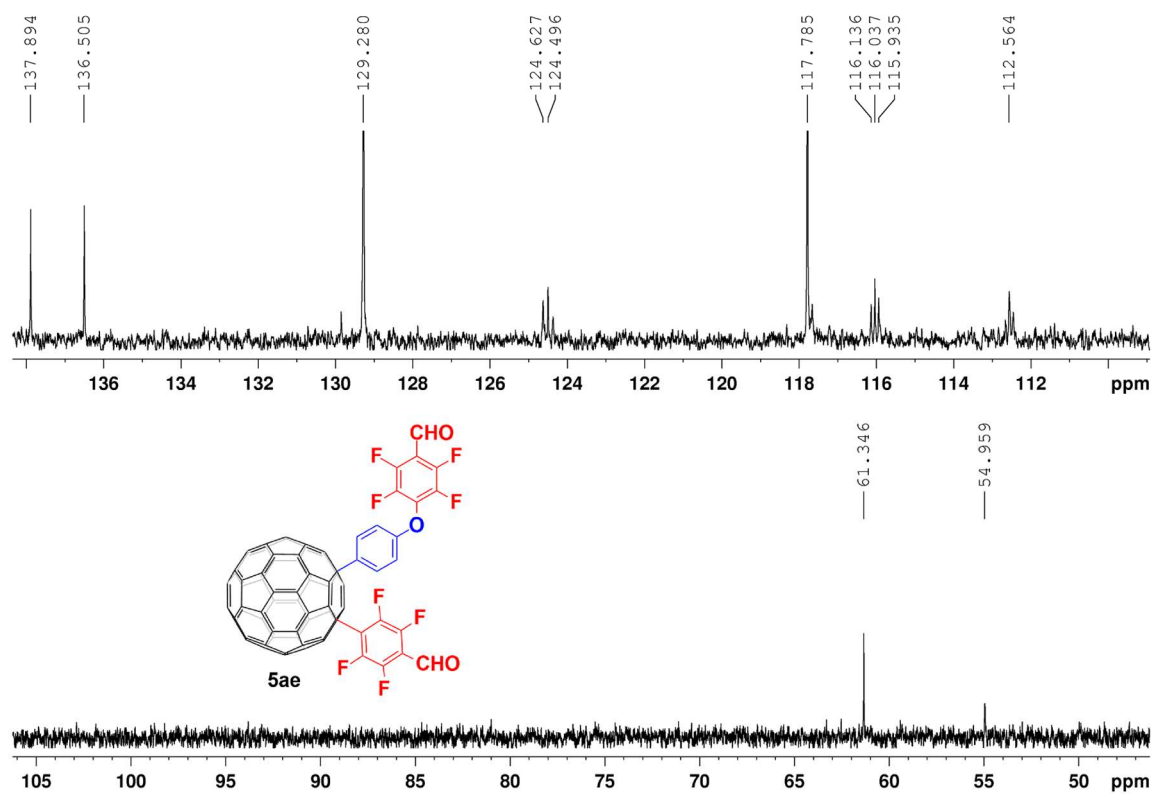
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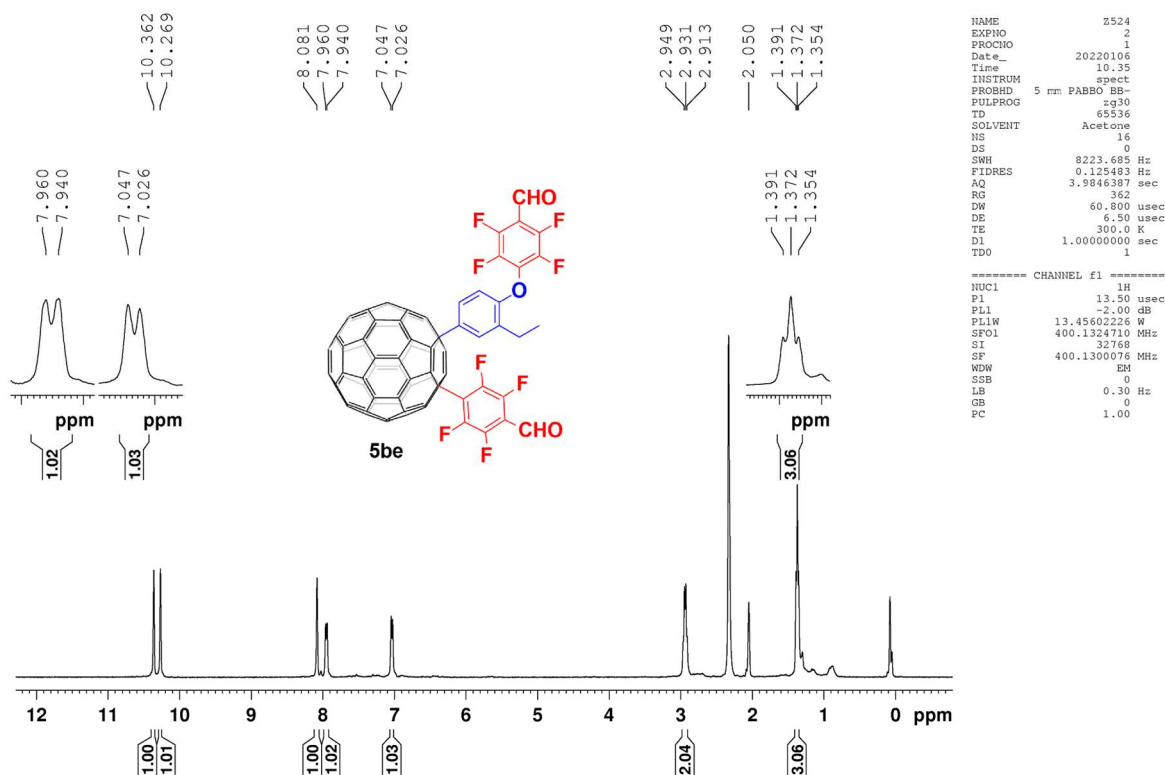
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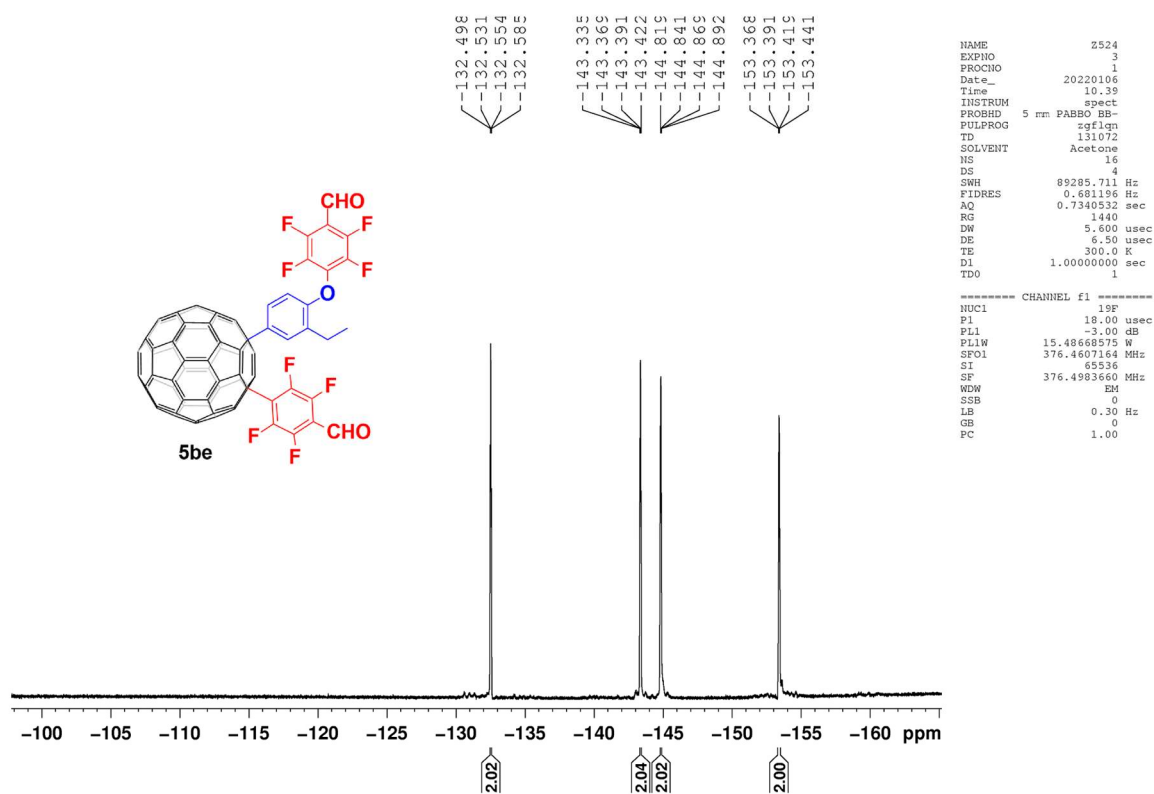
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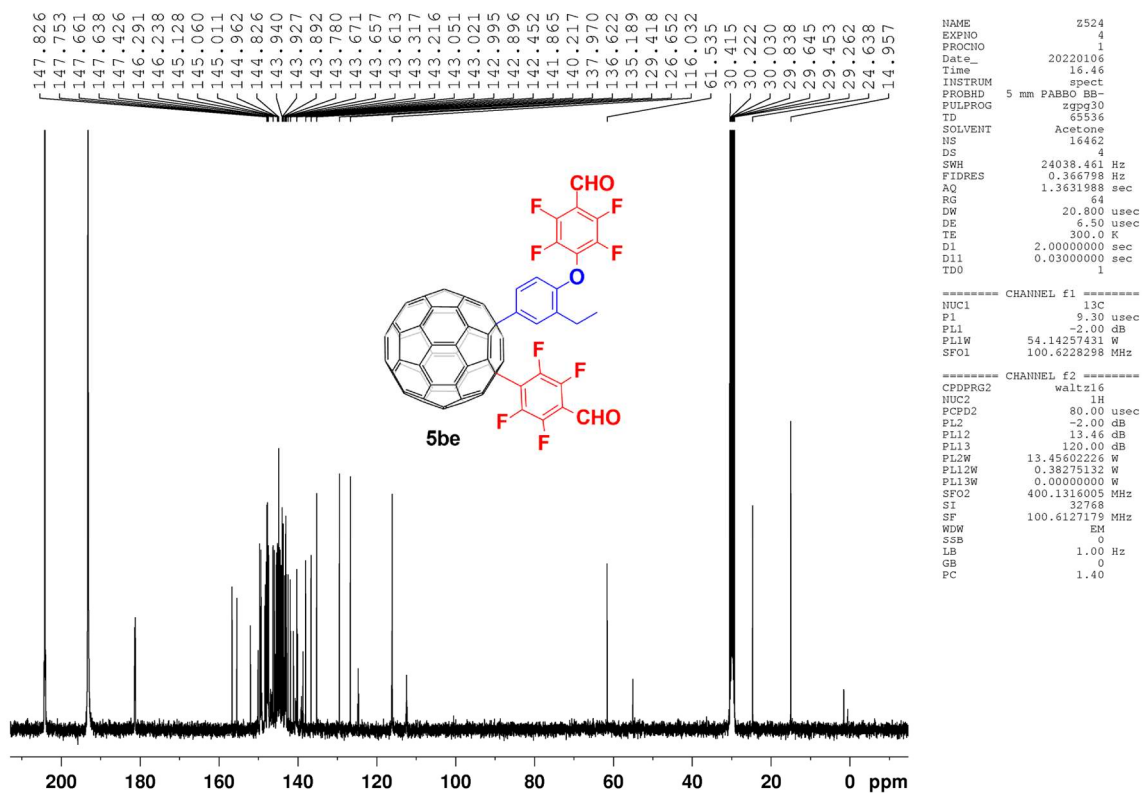
¹H NMR (400 MHz, CS₂/d₆-acetone) of compound 5be



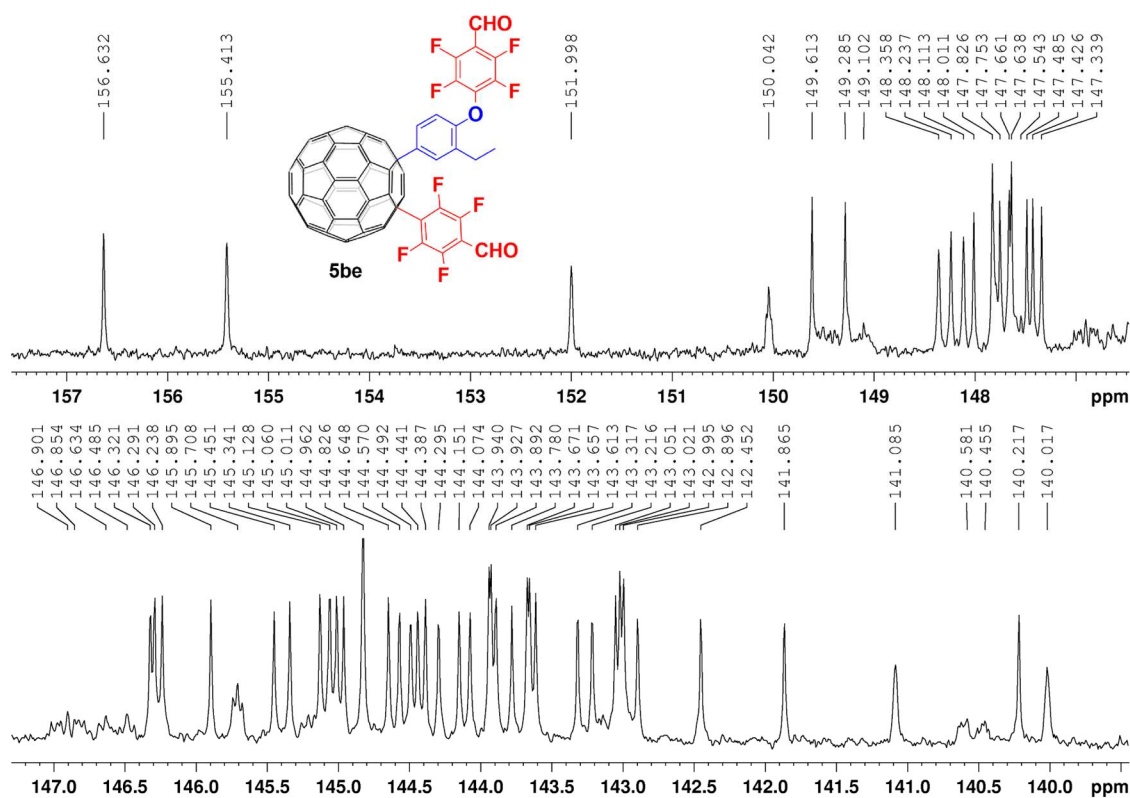
¹⁹F NMR (376 MHz, CS₂/d₆-acetone) of compound 5be



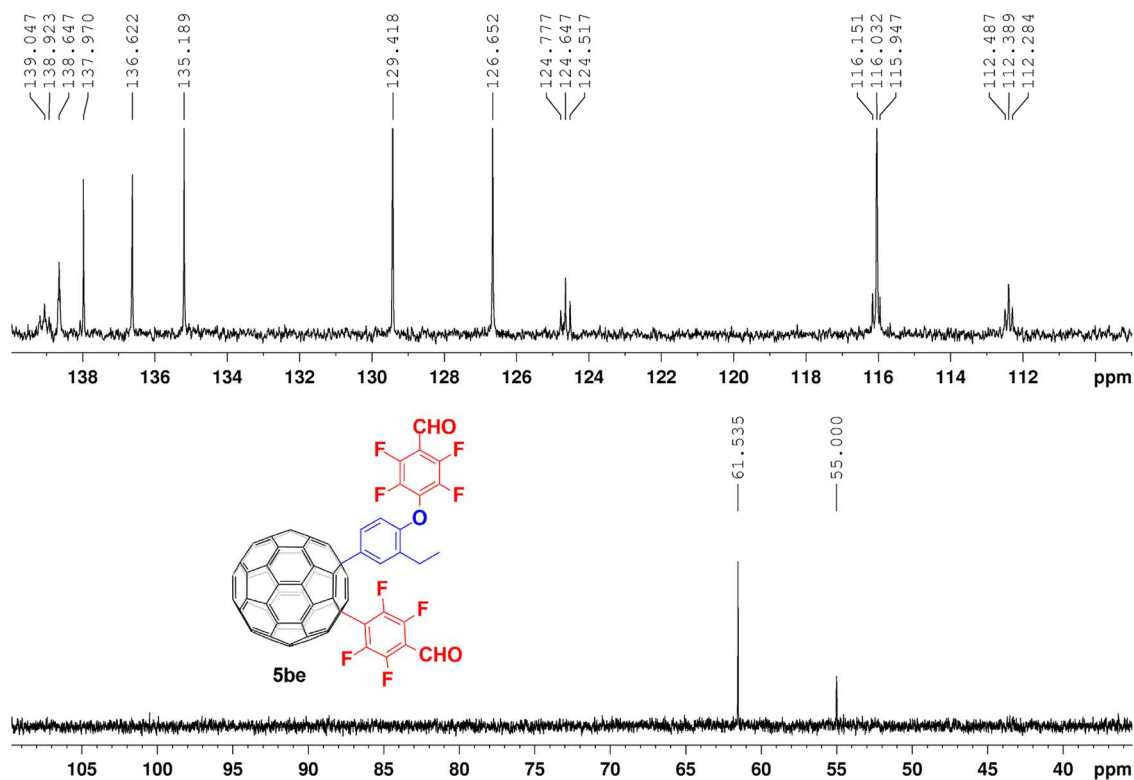
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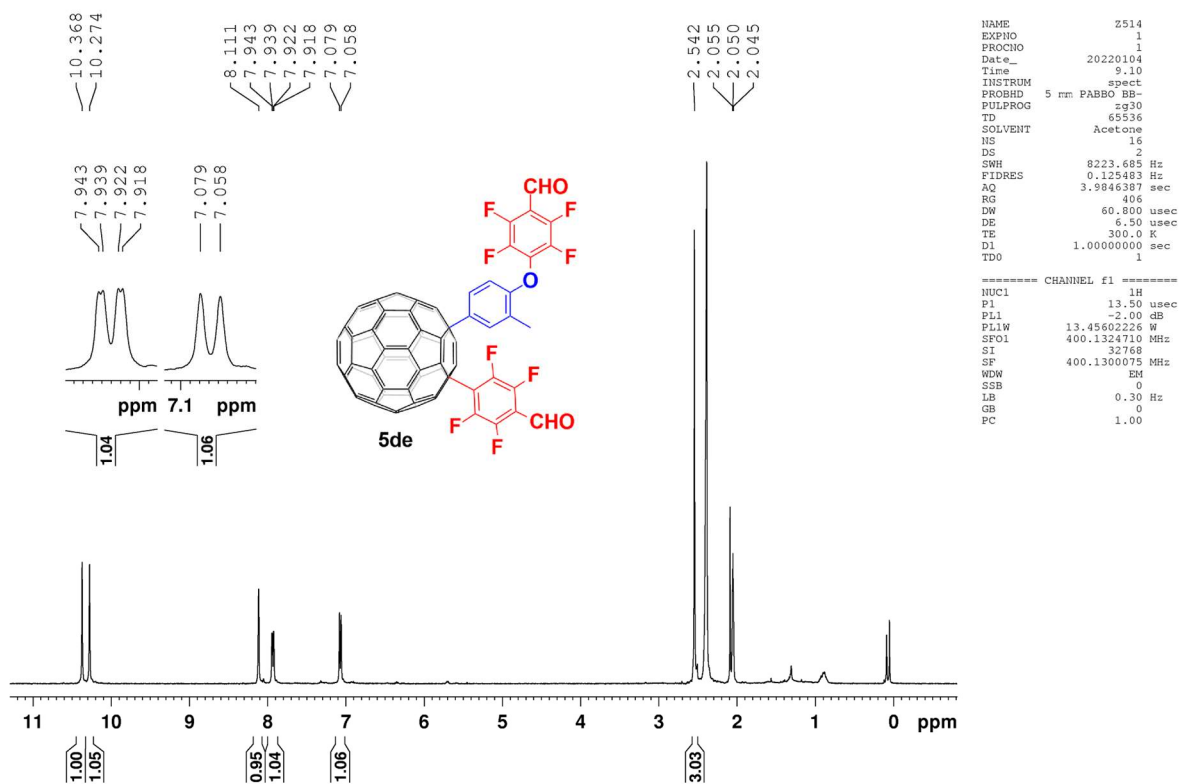
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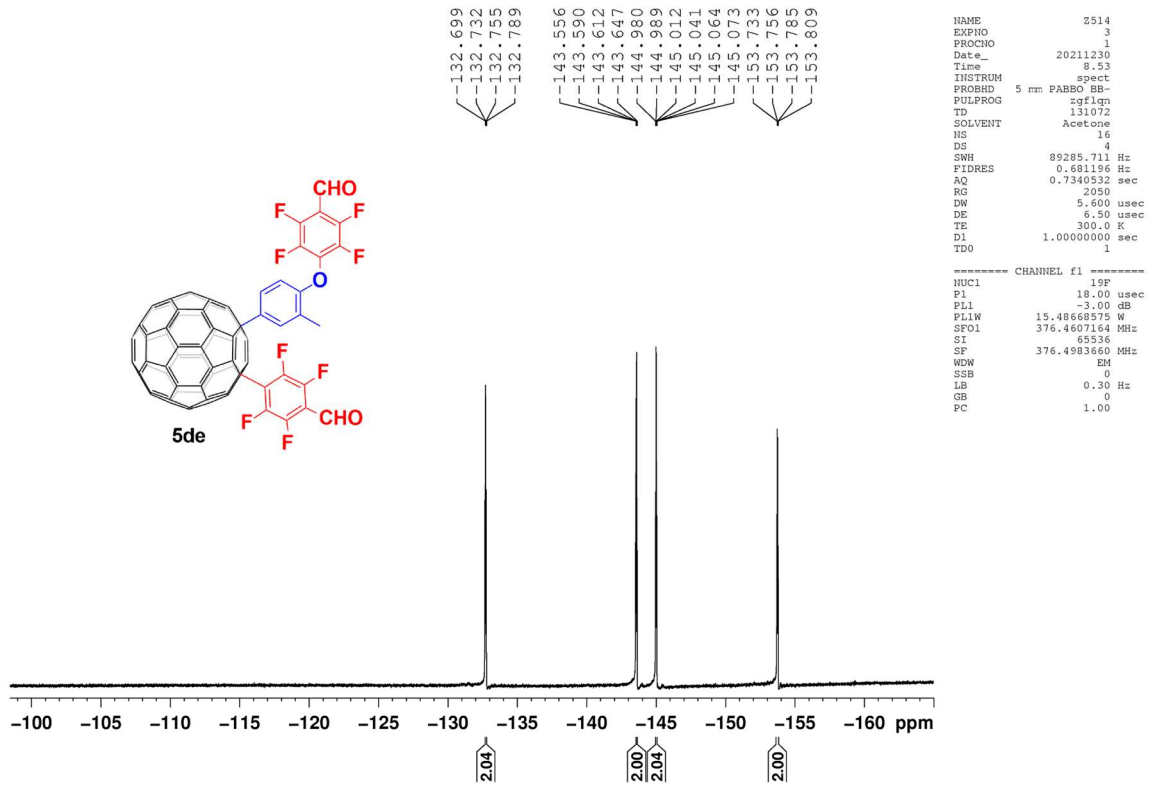
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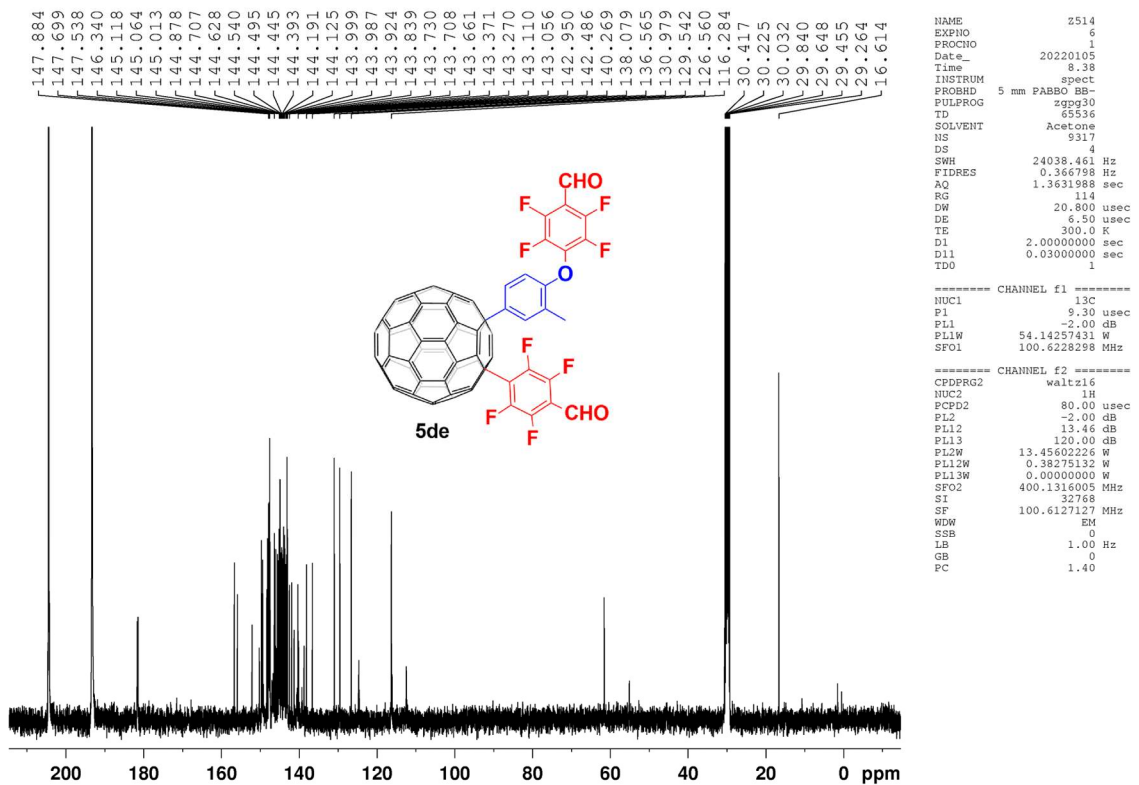
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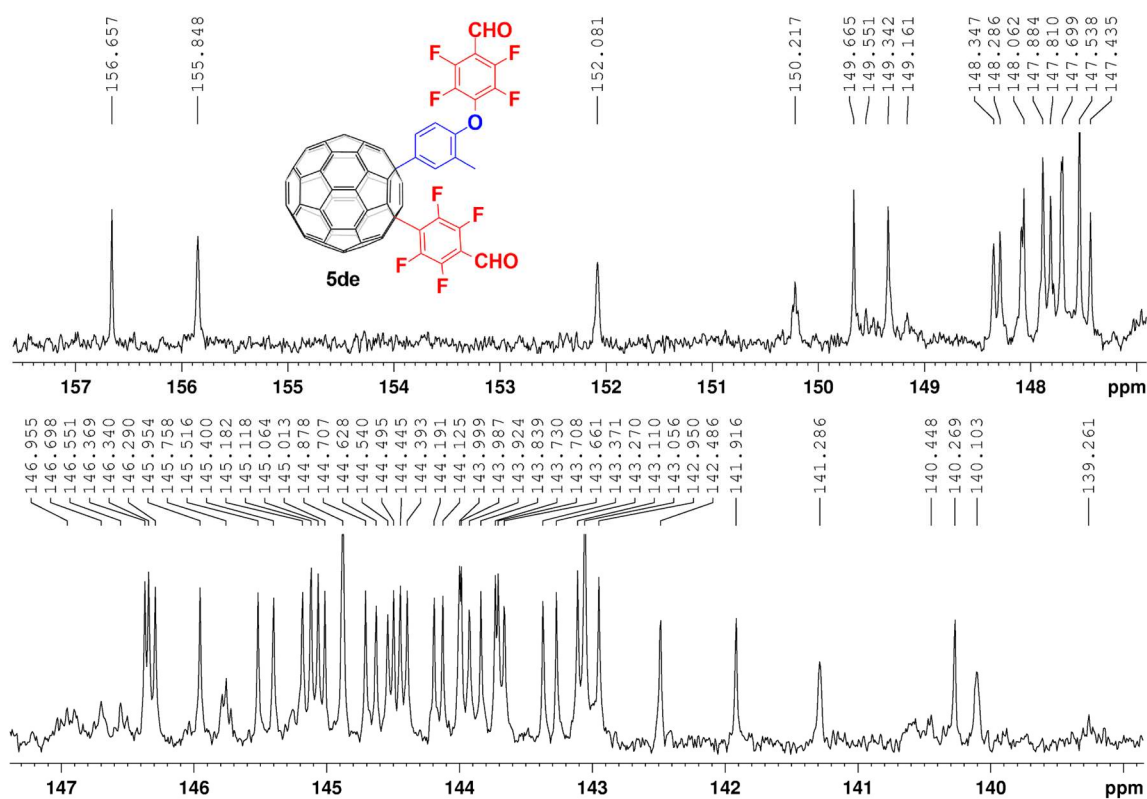
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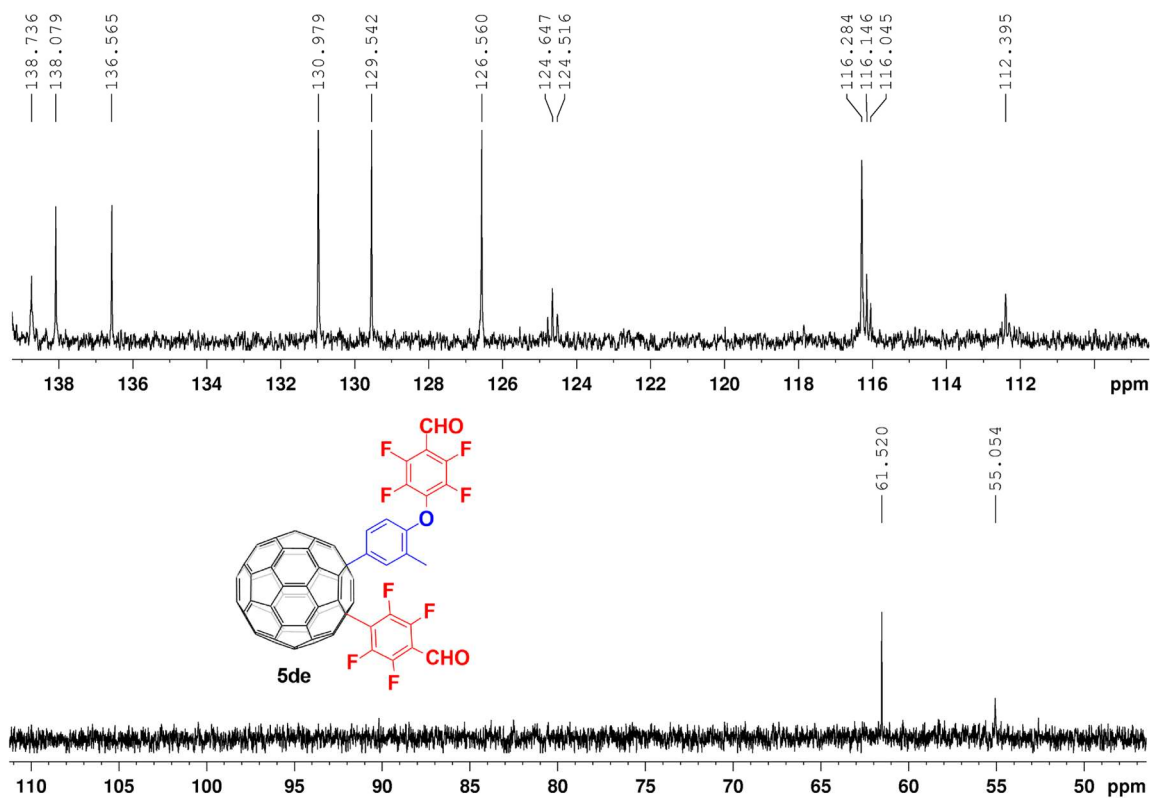
¹³C{¹H} NMR (100 MHz, CS₂/d₆-acetone) of compound 5de



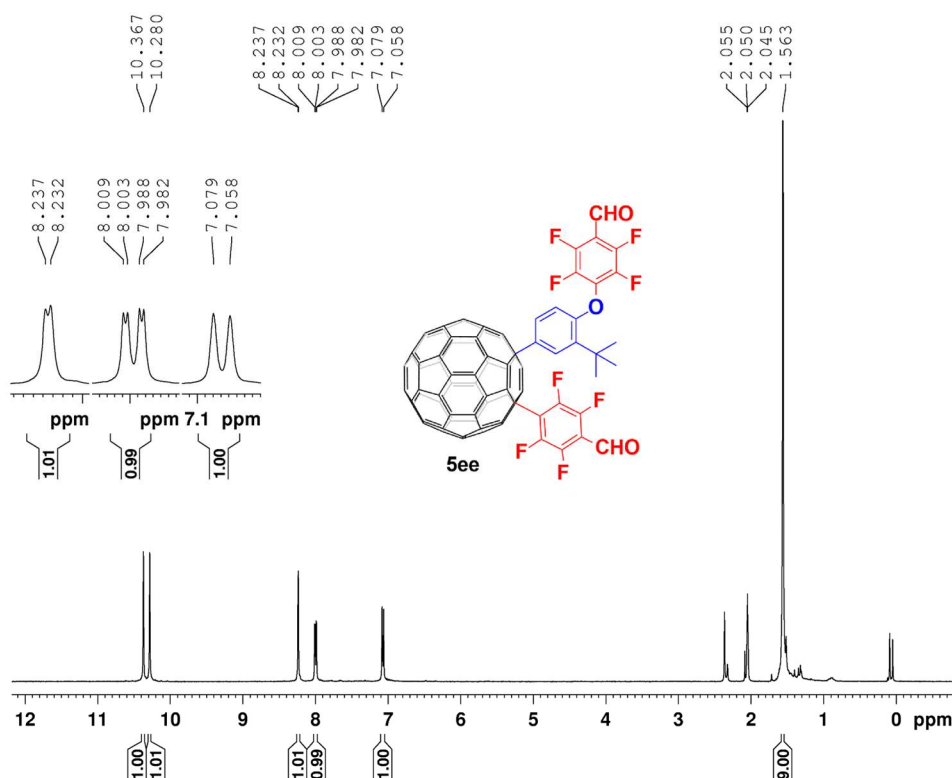
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5de



Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5de



¹H NMR (400 MHz, CS₂/d₆-acetone) of compound 5ee



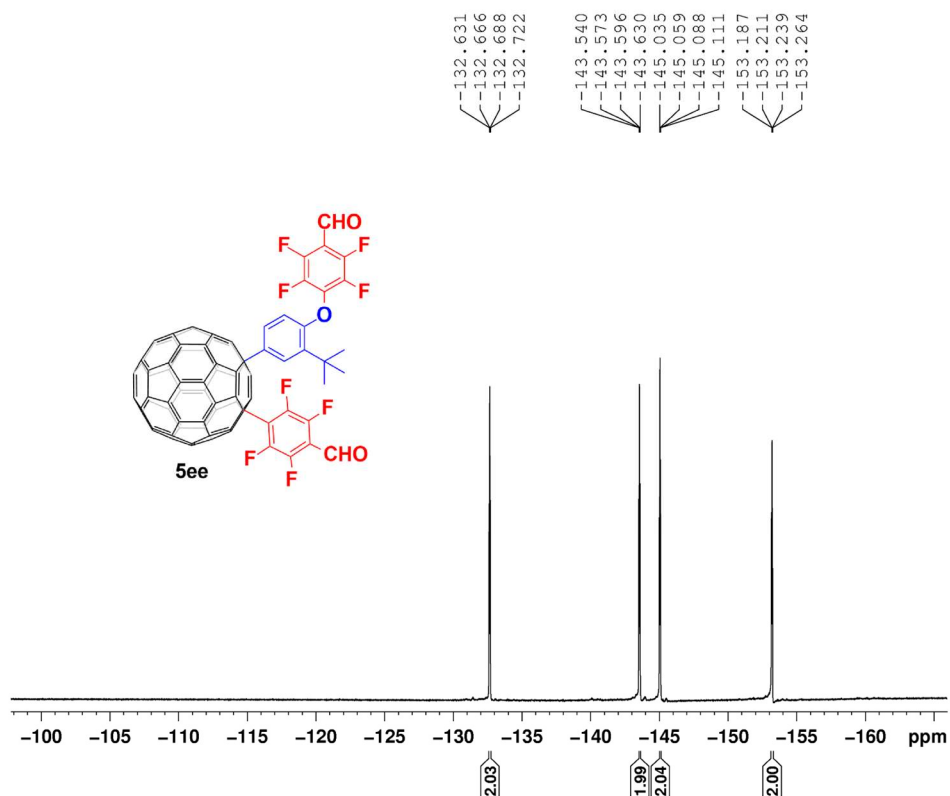
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NAME          Z515
EXPNO         1
PROCNO        1
Date_         20211229
Time          16.20
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       Acetone
NS            16
DS            0
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            322
DW            60.800 usec
DE            6.50 usec
TE            300.0 K
D1            1.00000000 sec
TDO           1
    
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```

===== CHANNEL f1 =====
NUC1          1H
P1            13.50 usec
PL1           -2.00 dB
PL1W          13.45602226 W
SFO1          400.1324710 MHz
SI            32768
SF            400.1300073 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
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¹⁹F NMR (376 MHz, CS₂/d₆-acetone) of compound 5ee



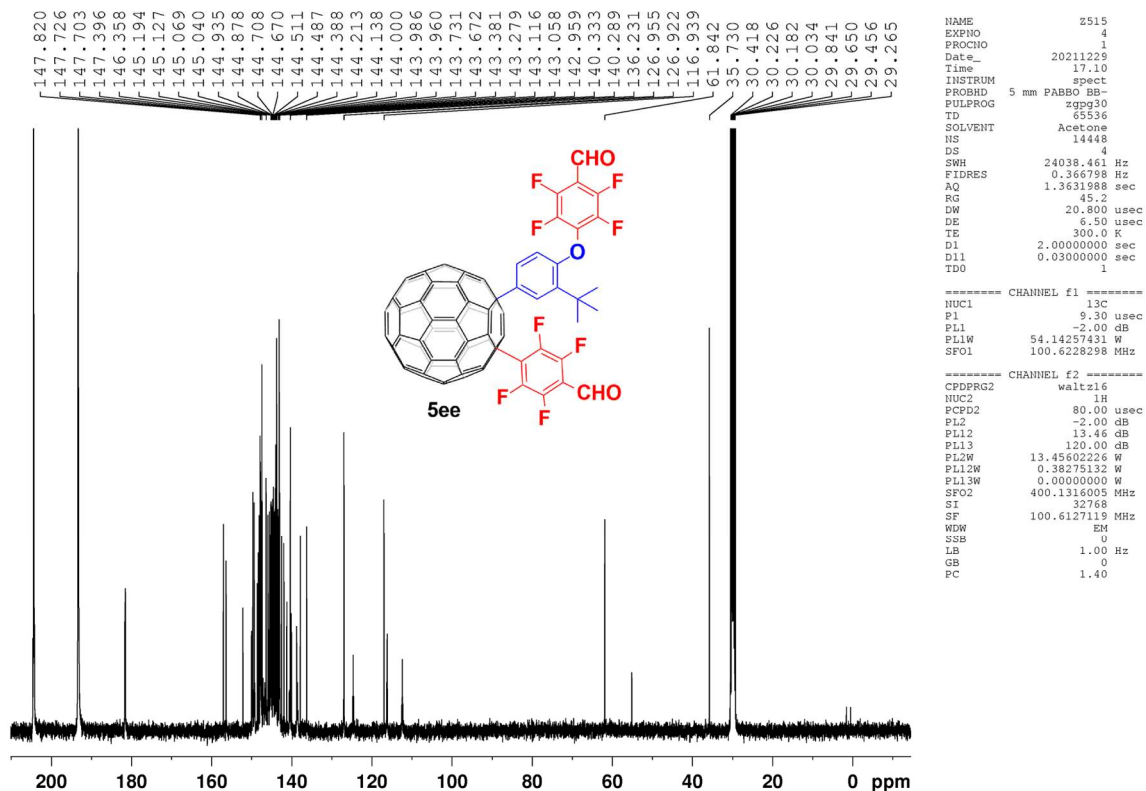
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NAME          Z515
EXPNO         2
PROCNO        1
Date_         20211229
Time          16.25
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            131072
SOLVENT       Acetone
NS            16
DS            4
SWH           89285.711 Hz
FIDRES        0.681196 Hz
AQ            0.7340532 sec
RG            1150
DW            5.600 usec
DE            6.50 usec
TE            300.0 K
D1            1.00000000 sec
TDO           1
    
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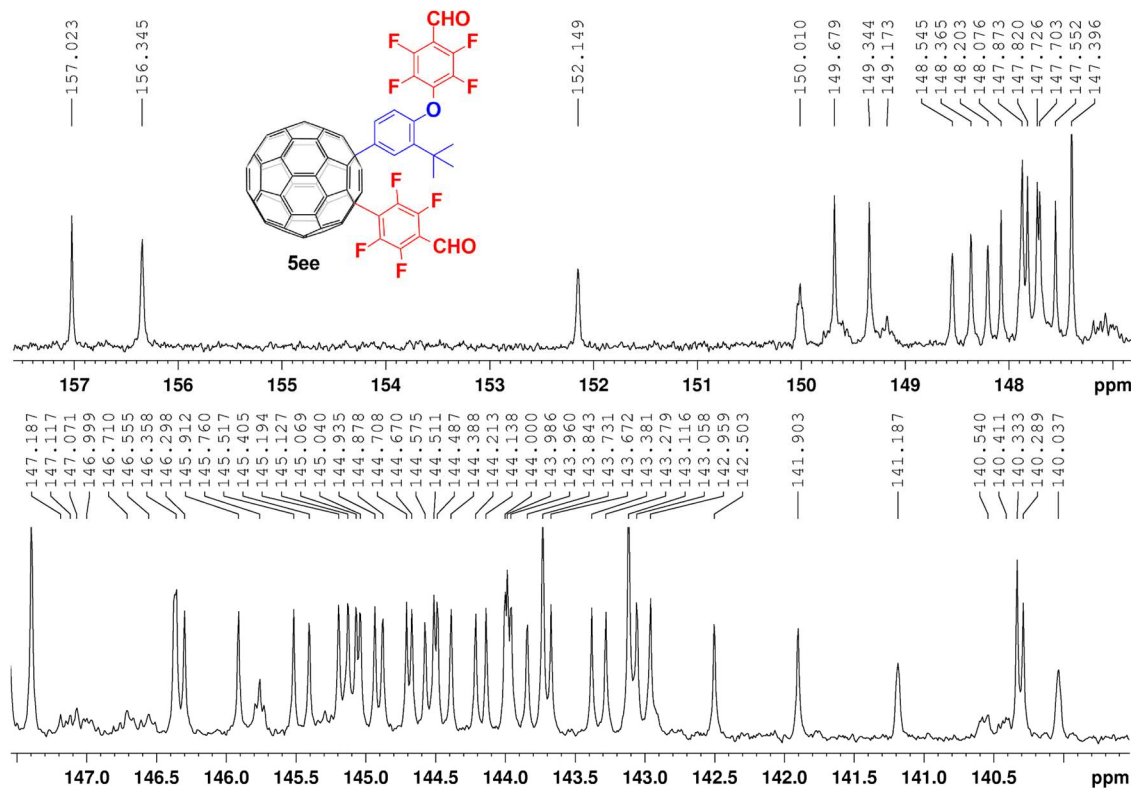
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===== CHANNEL f1 =====
NUC1          19F
P1            19.50 usec
PL1           -4.00 dB
PL1W          19.49658203 W
SFO1          376.4607164 MHz
SI            65536
SF            376.4983660 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
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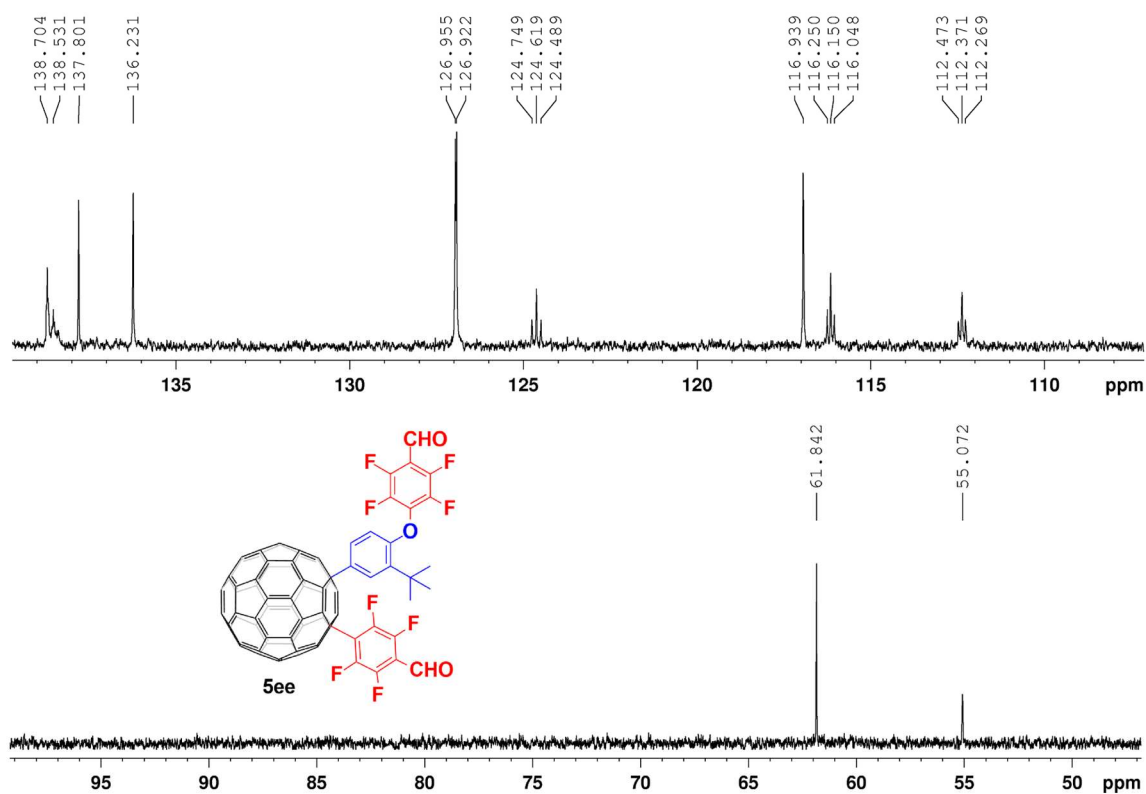

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound **5ee**



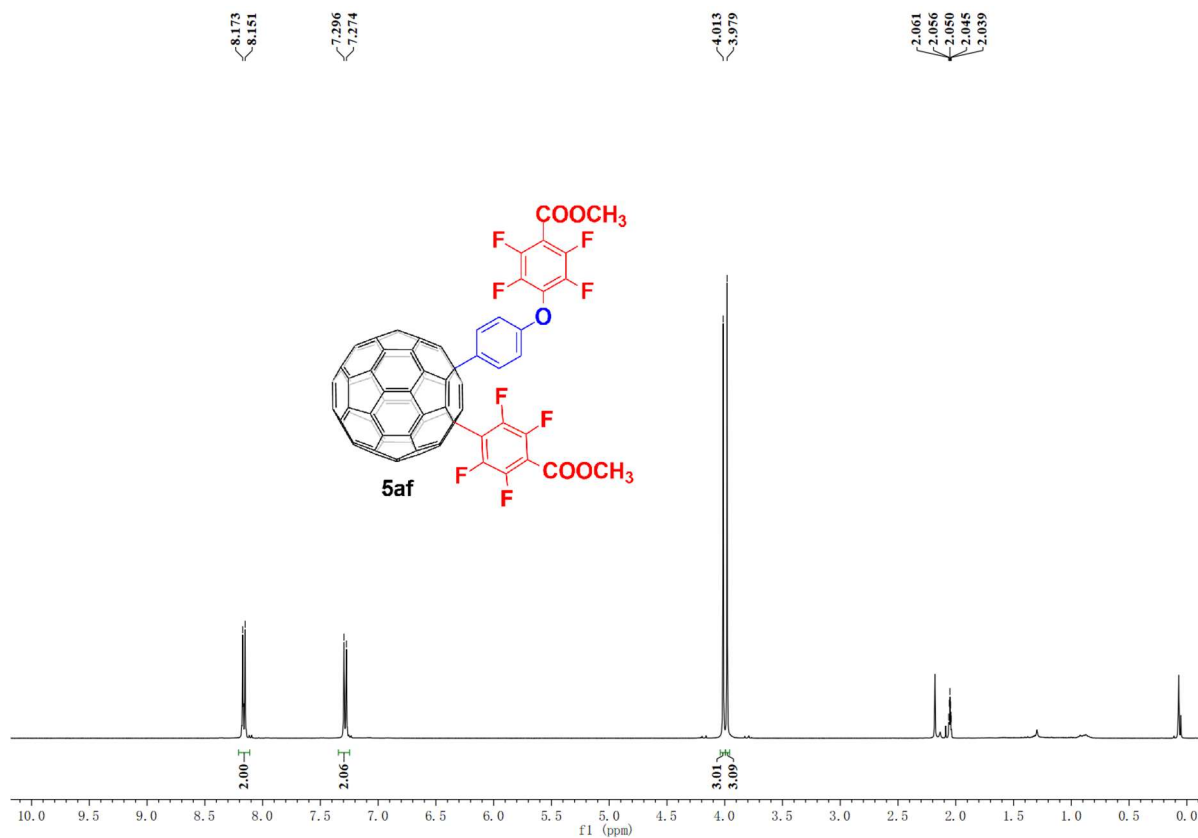
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound **5ee**



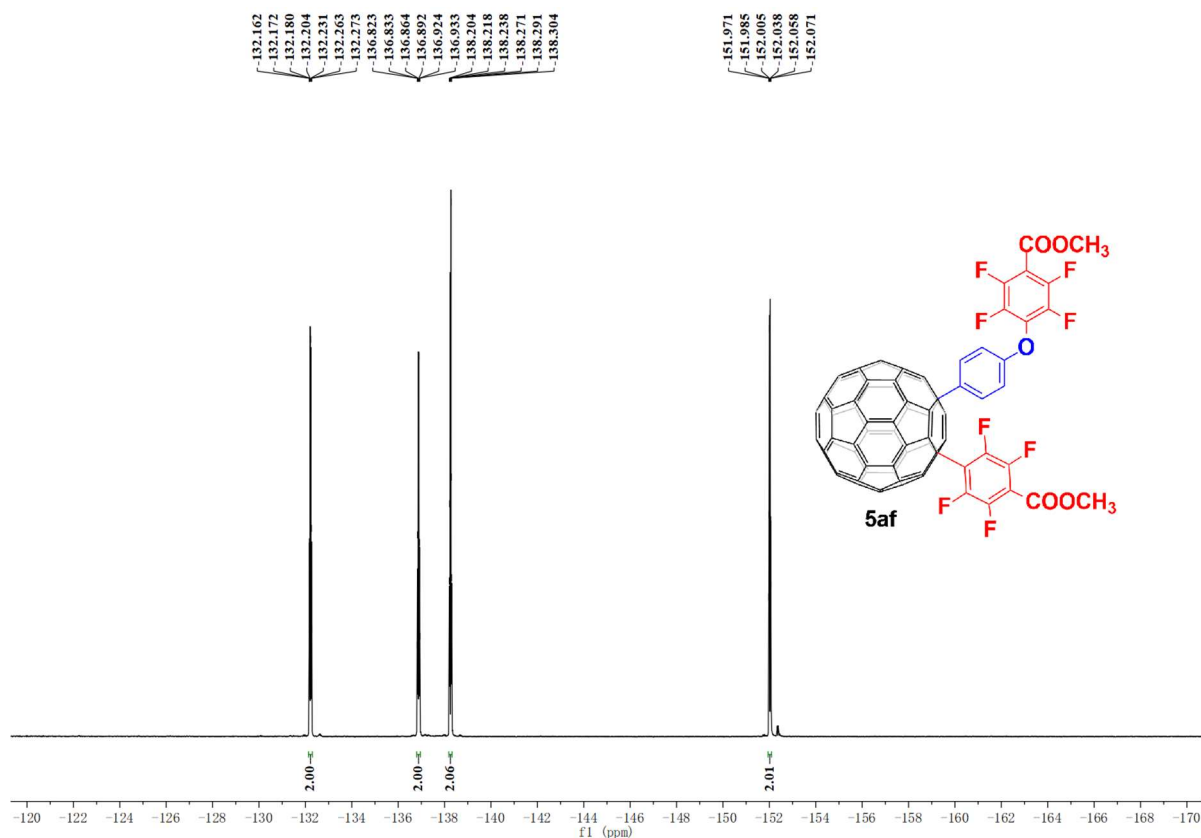
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **5ee**



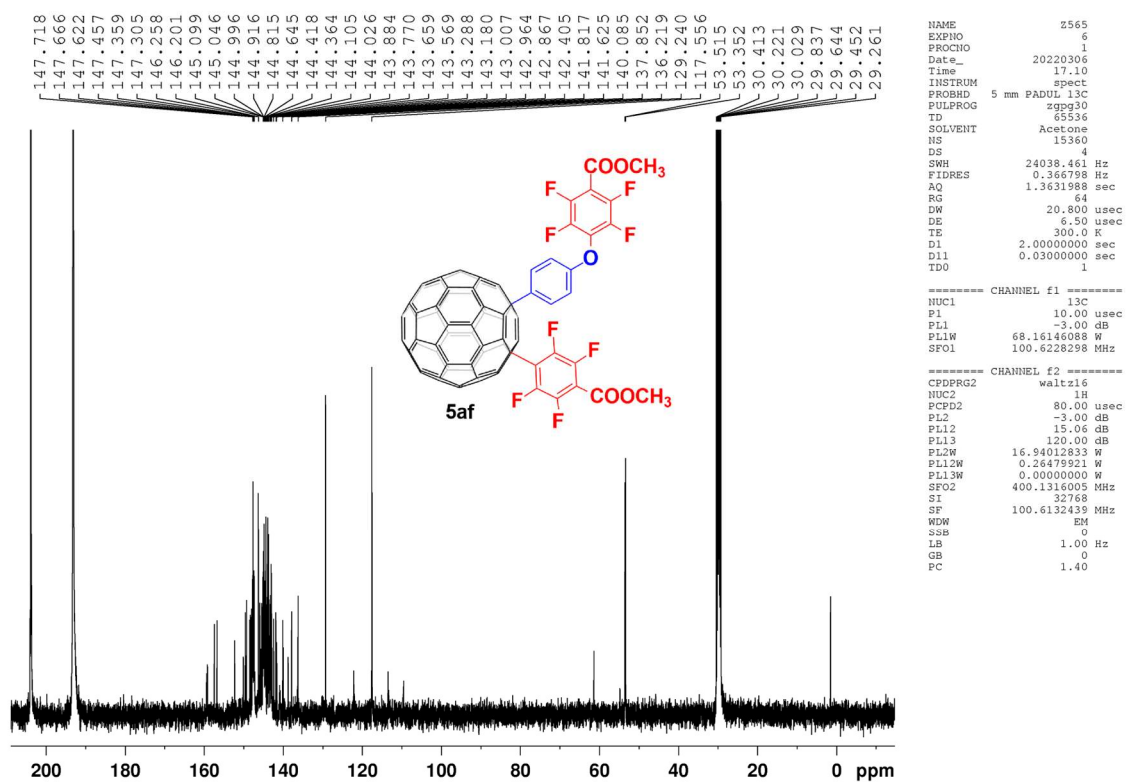
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **5af**



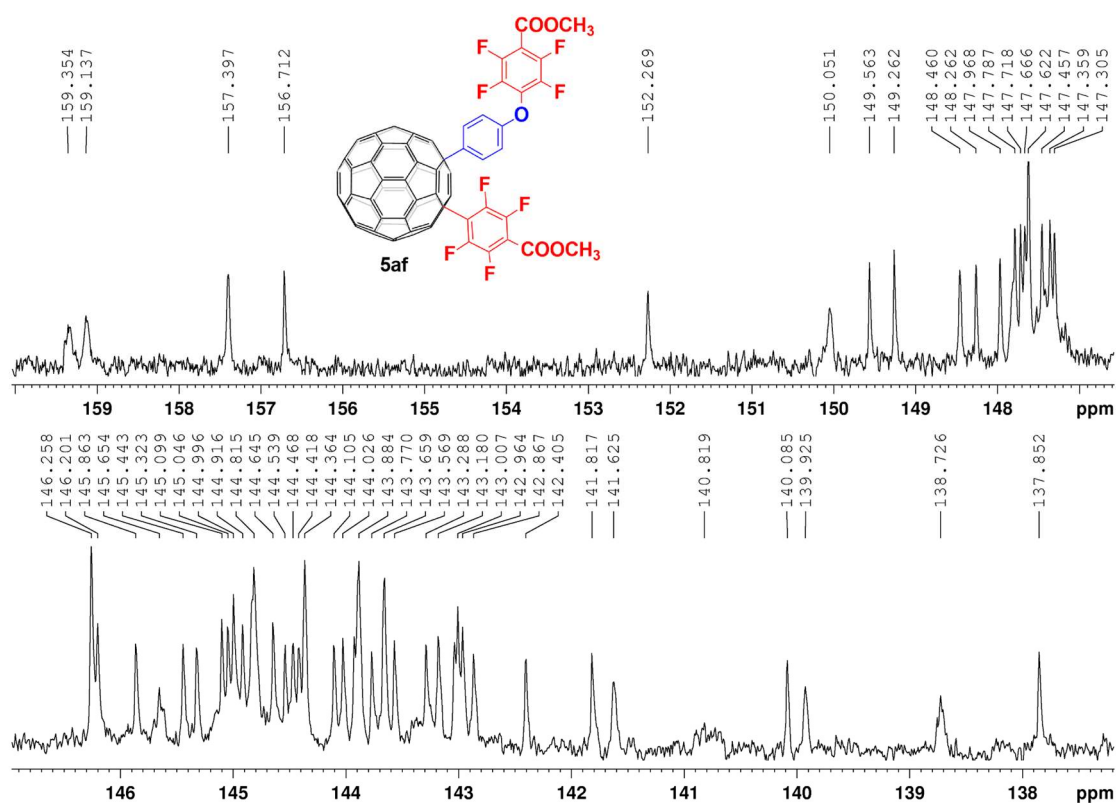
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 5af



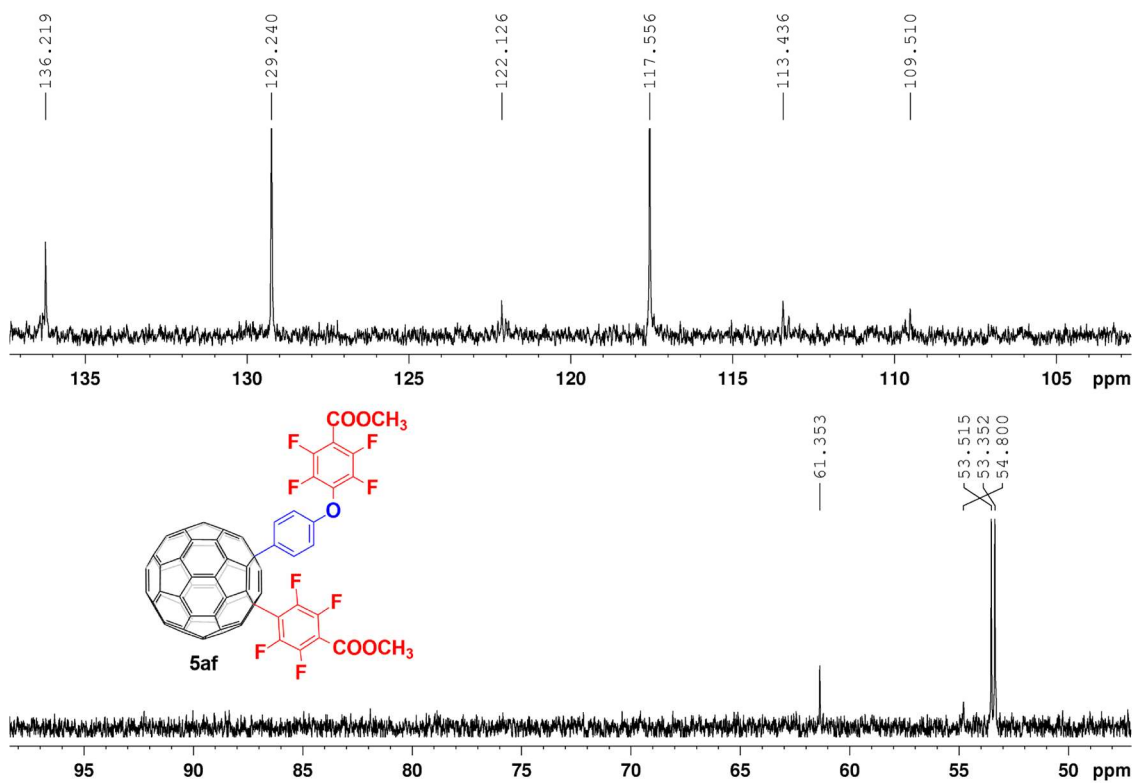
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5af



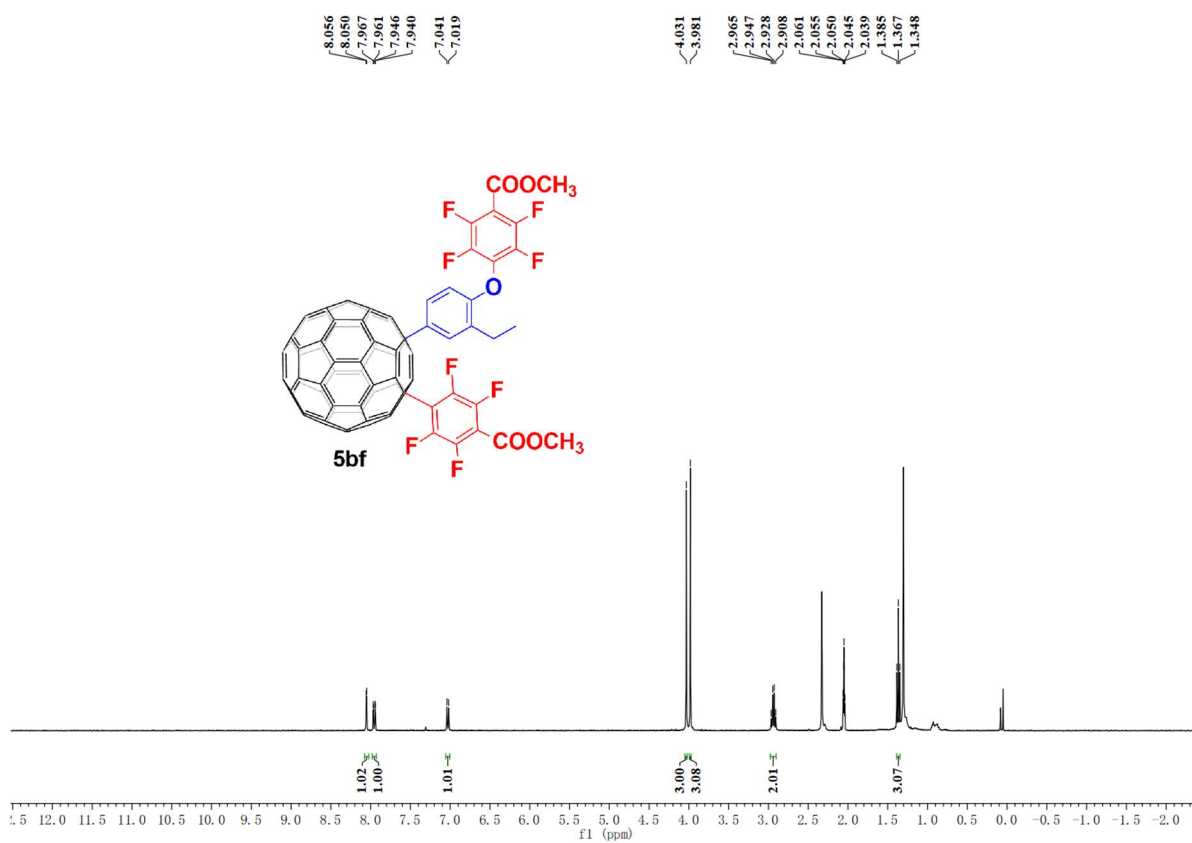
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **5af**



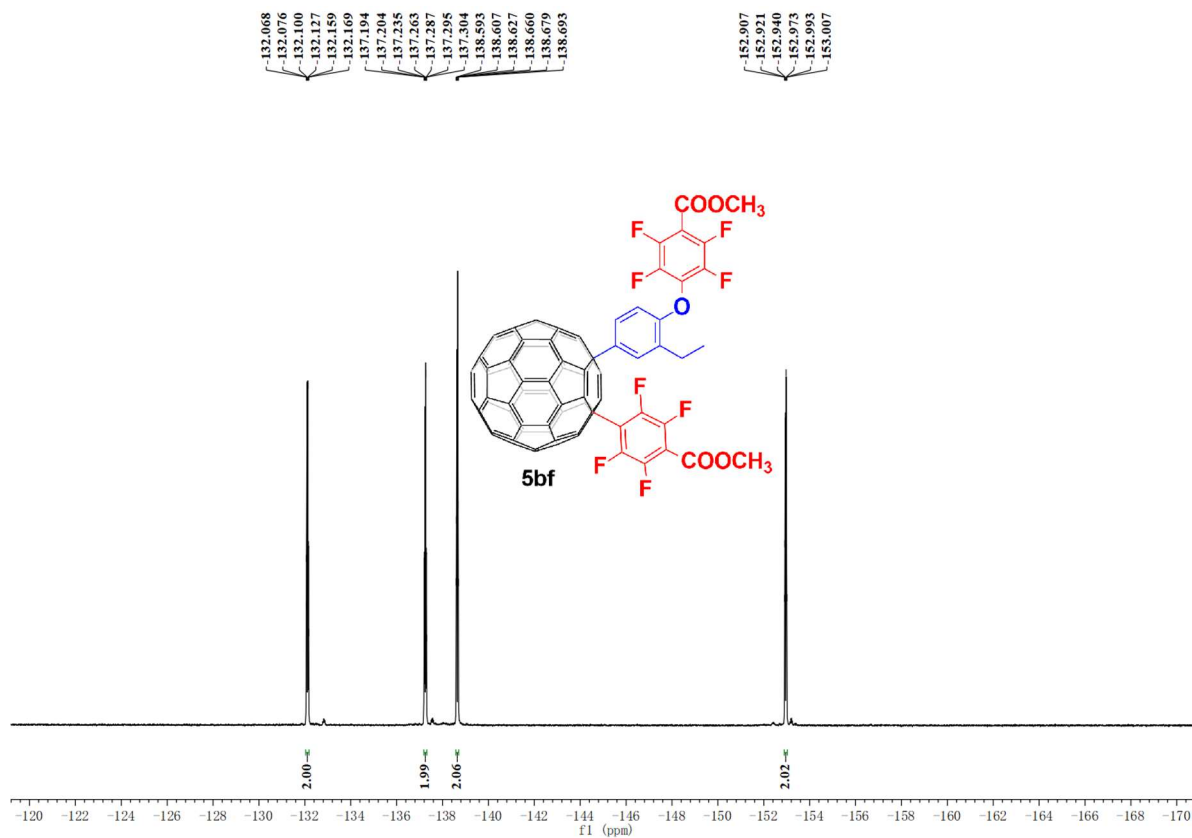
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **5af**



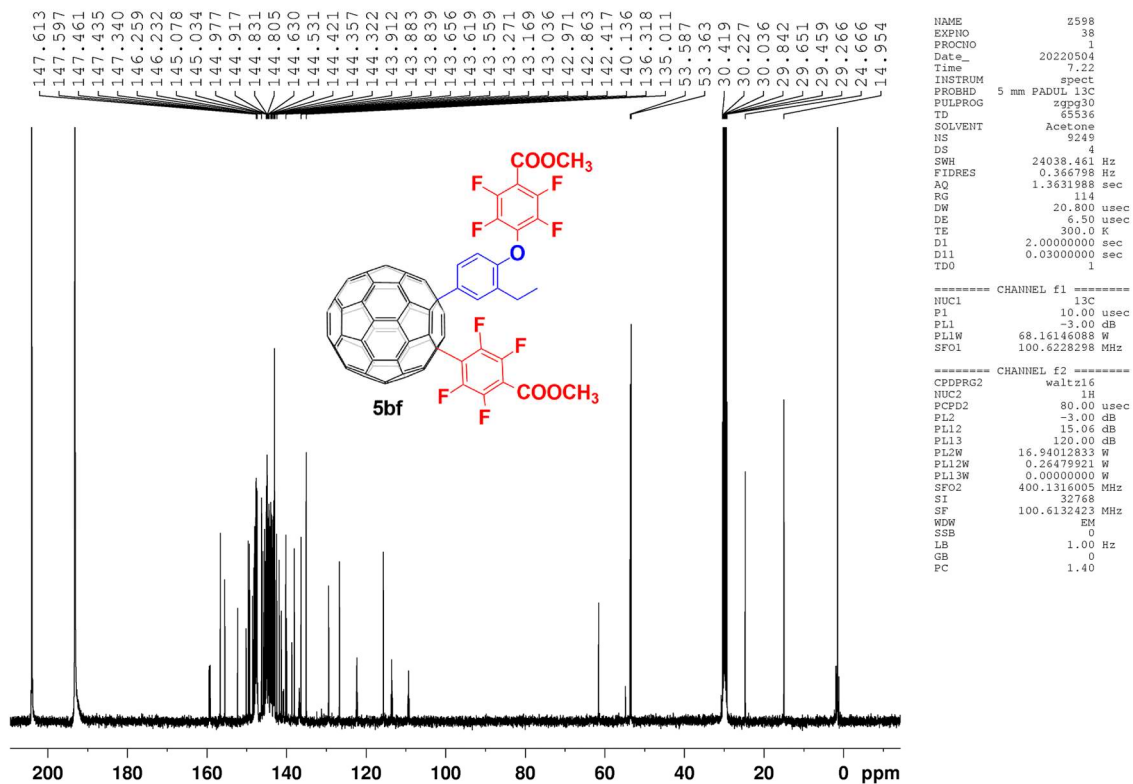
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 5bf



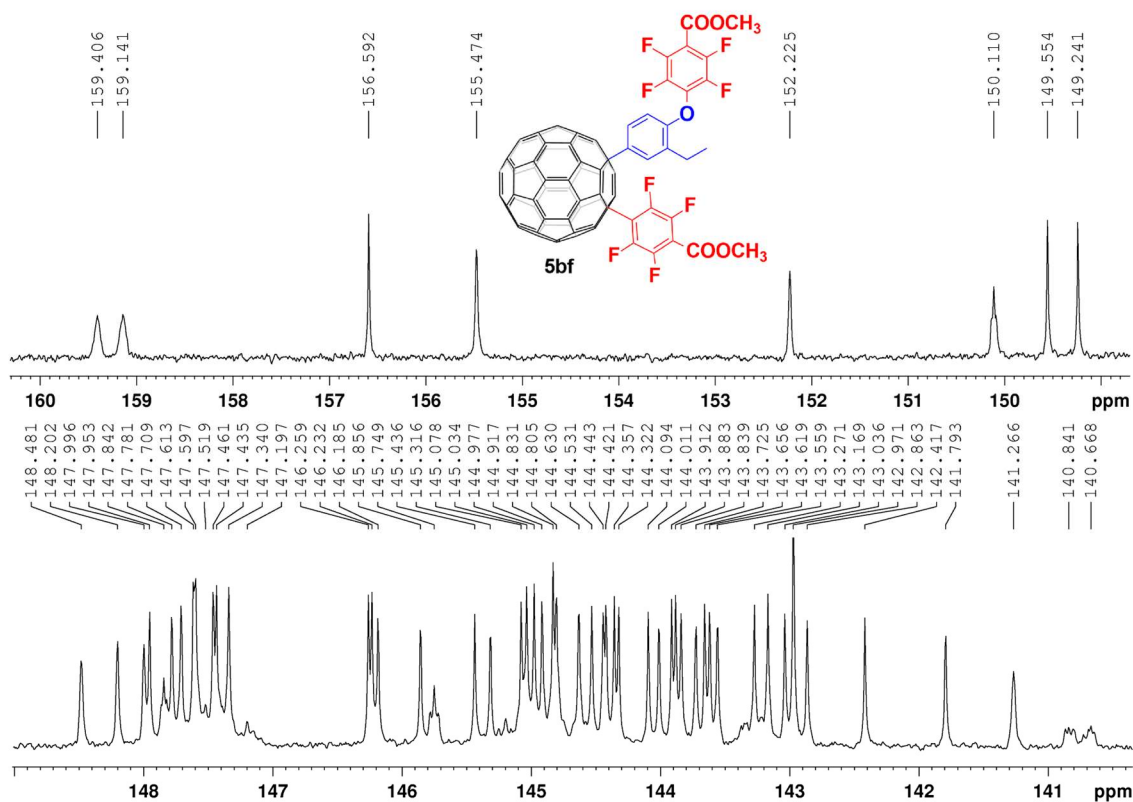
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 5bf



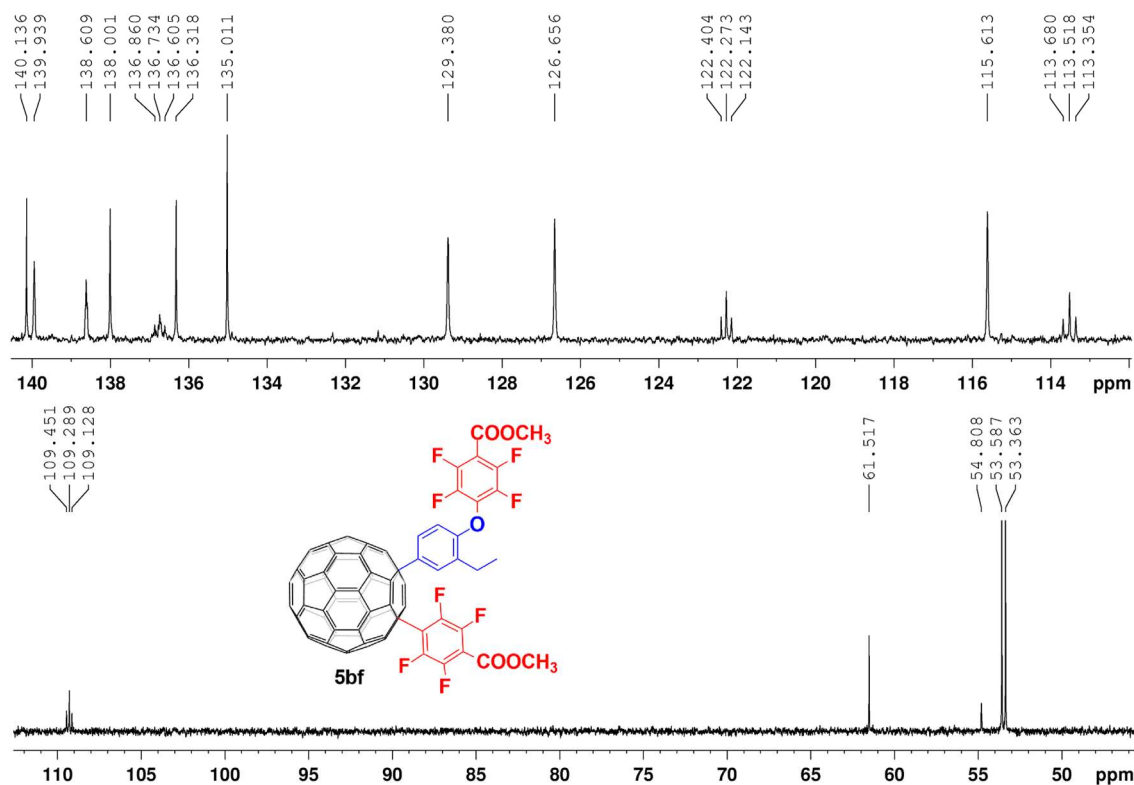
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 5bf



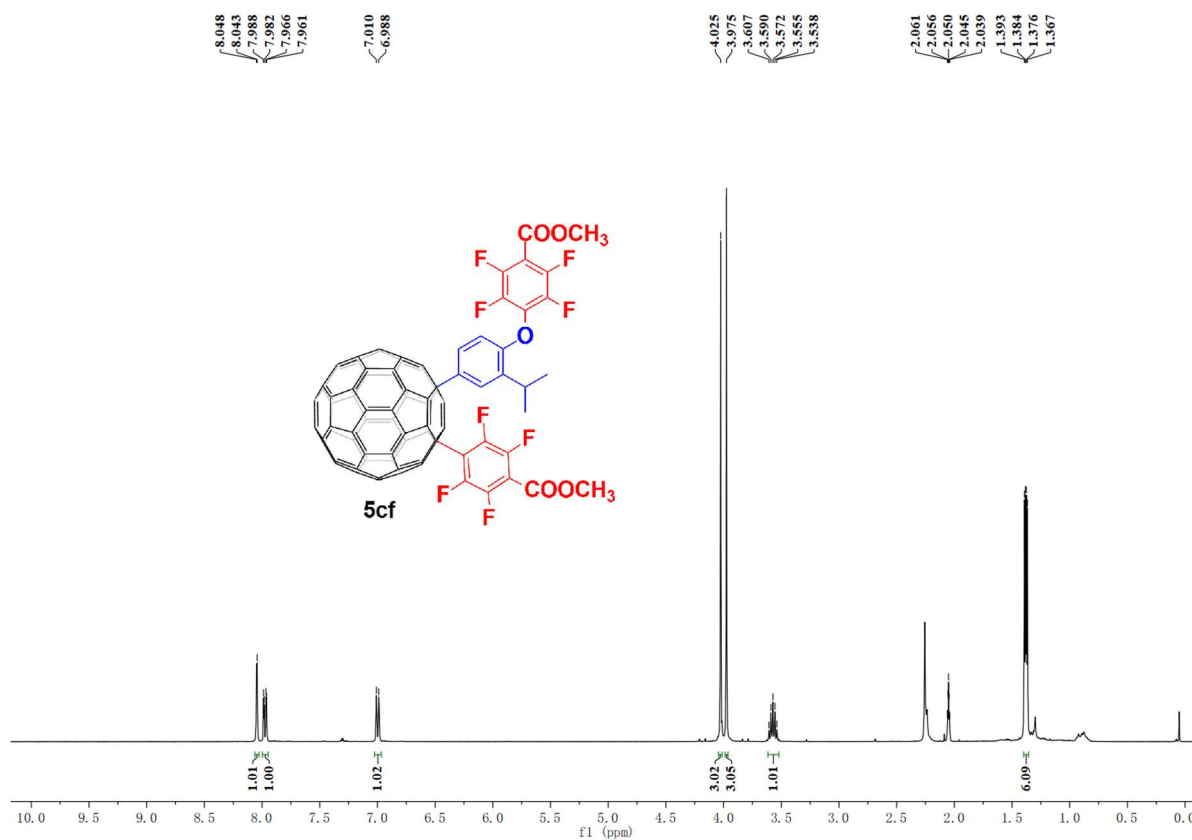
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{CS}_2/d_6\text{-acetone}$) of compound 5bf



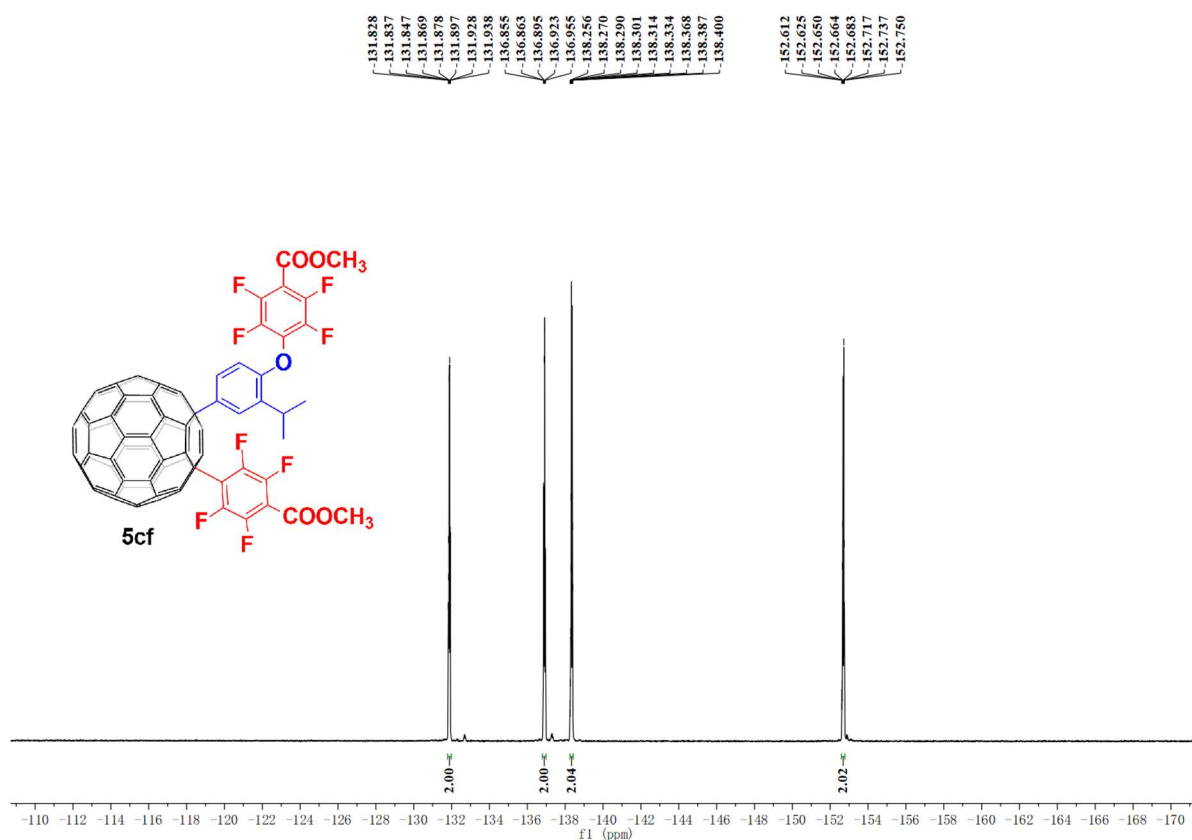
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **5bf**



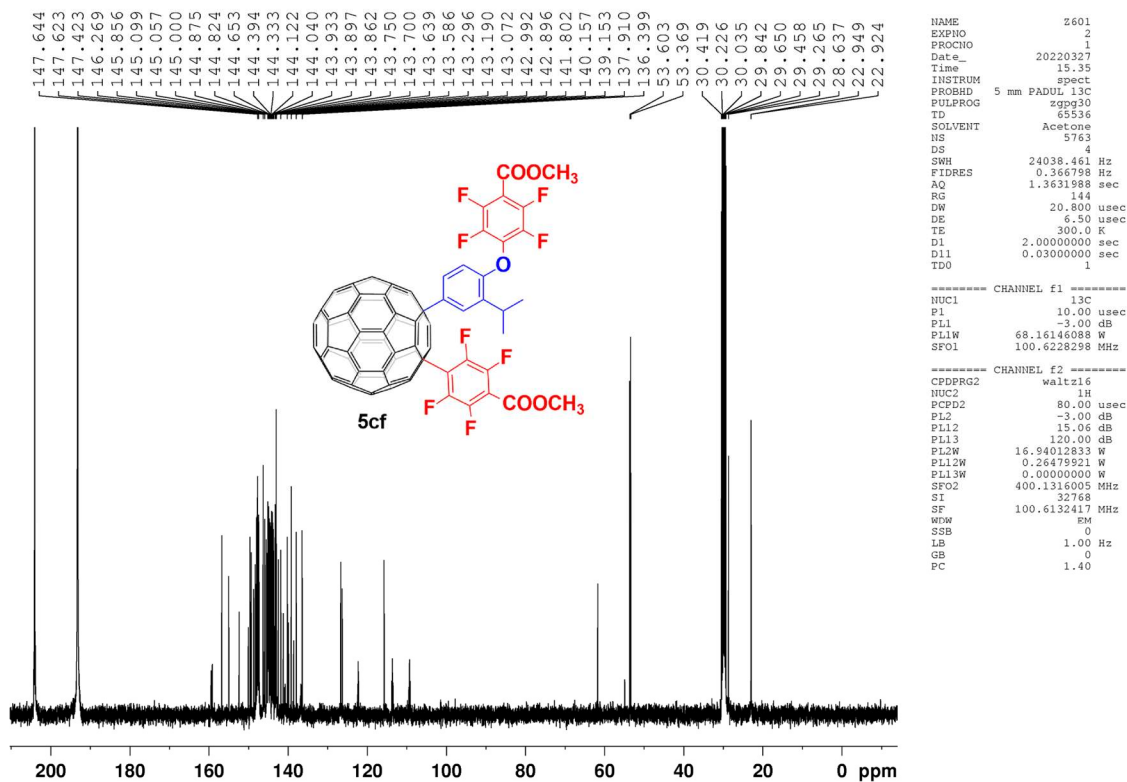
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **5cf**



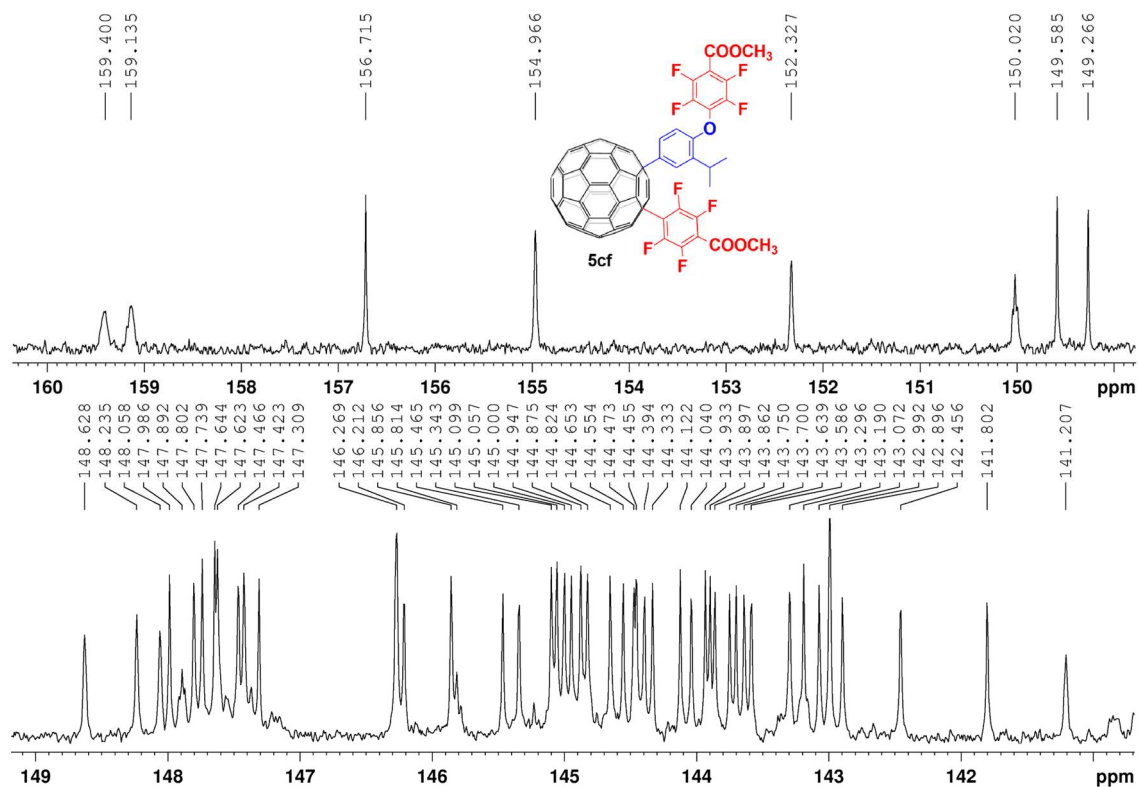
¹⁹F NMR (376 MHz, CS₂/d₆-acetone) of compound 5cf



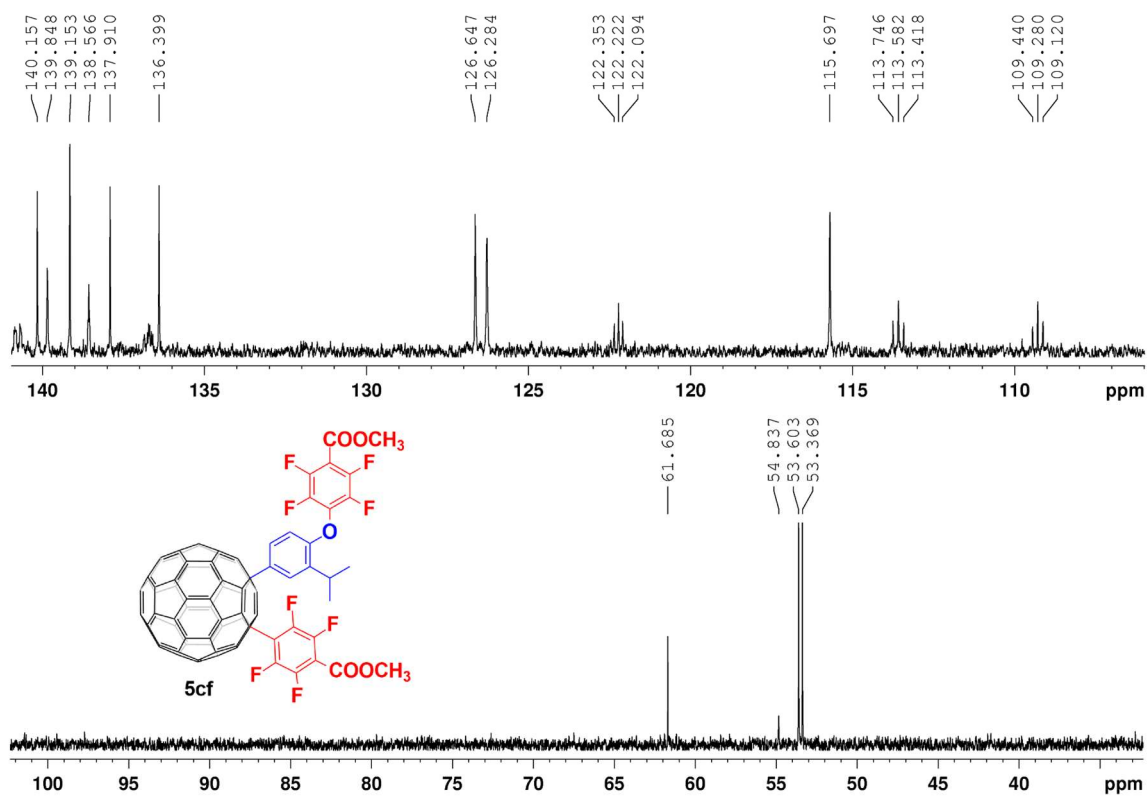
¹³C{¹H} NMR (100 MHz, CS₂/d₆-acetone) of compound 5cf



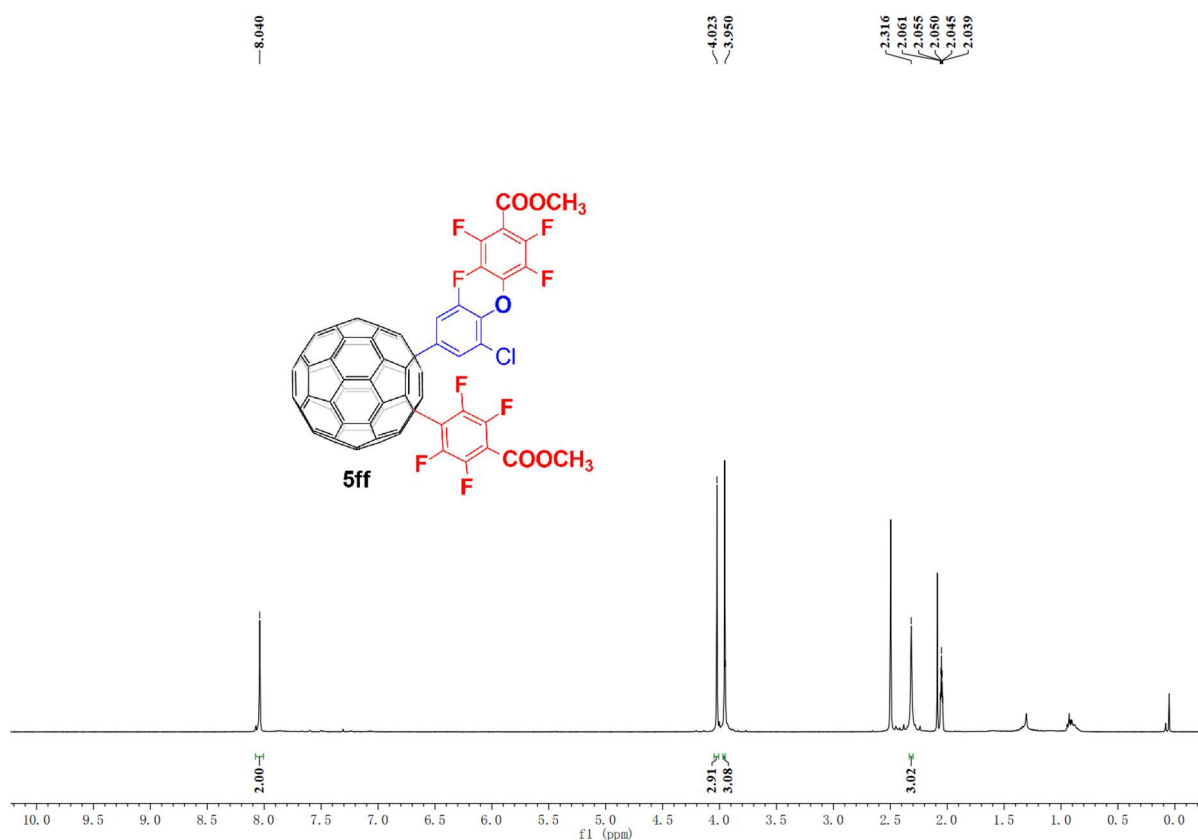
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **5cf**



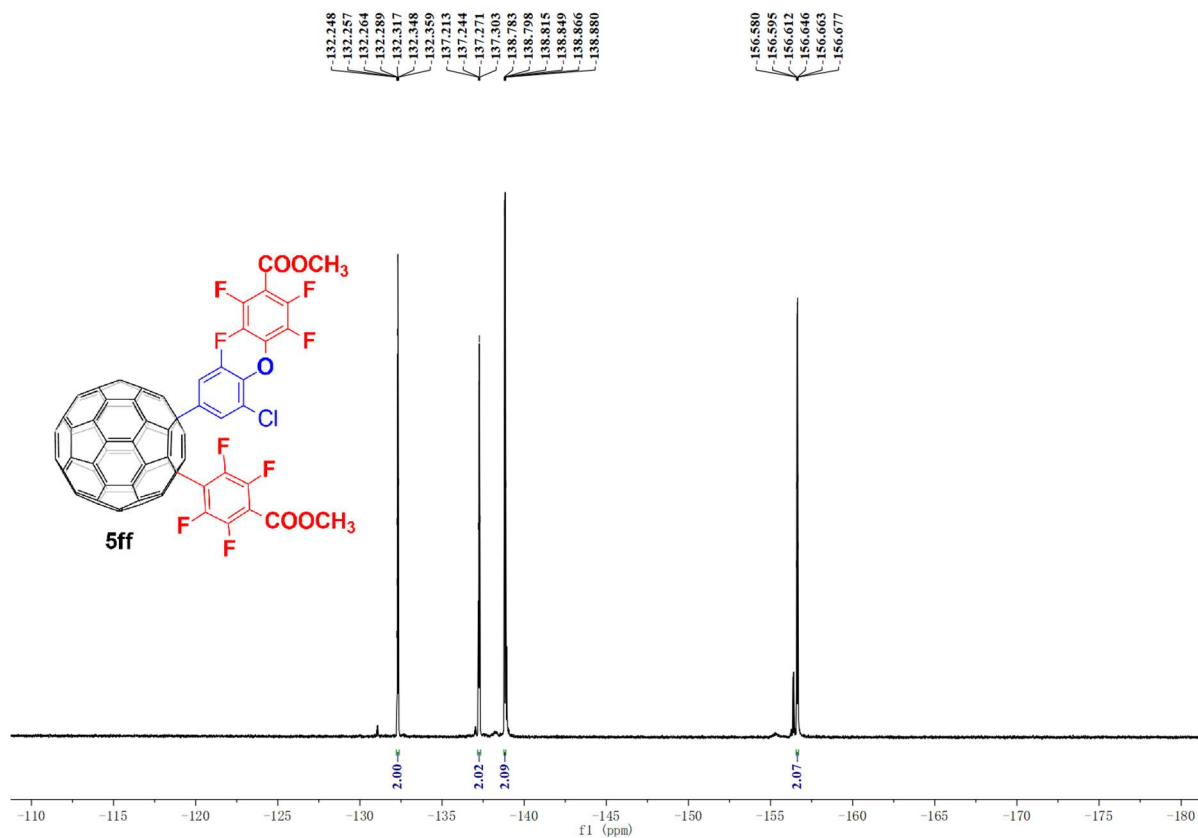
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **5cf**



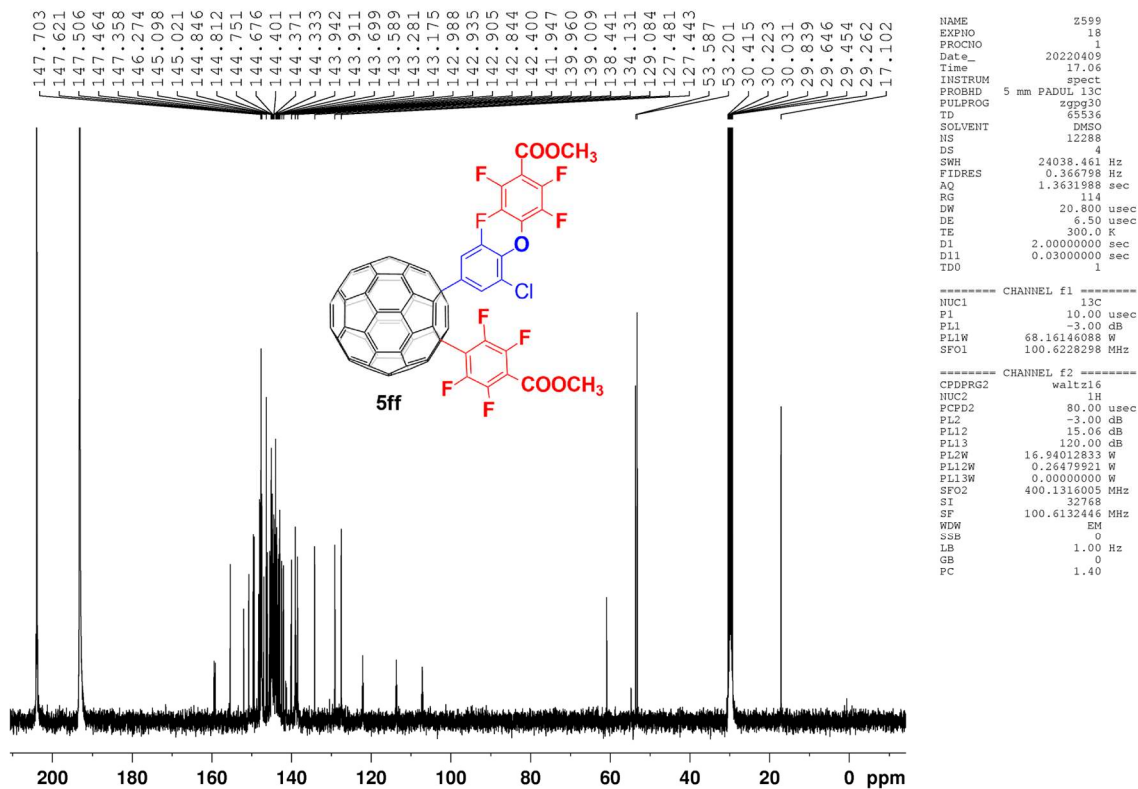
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 5ff



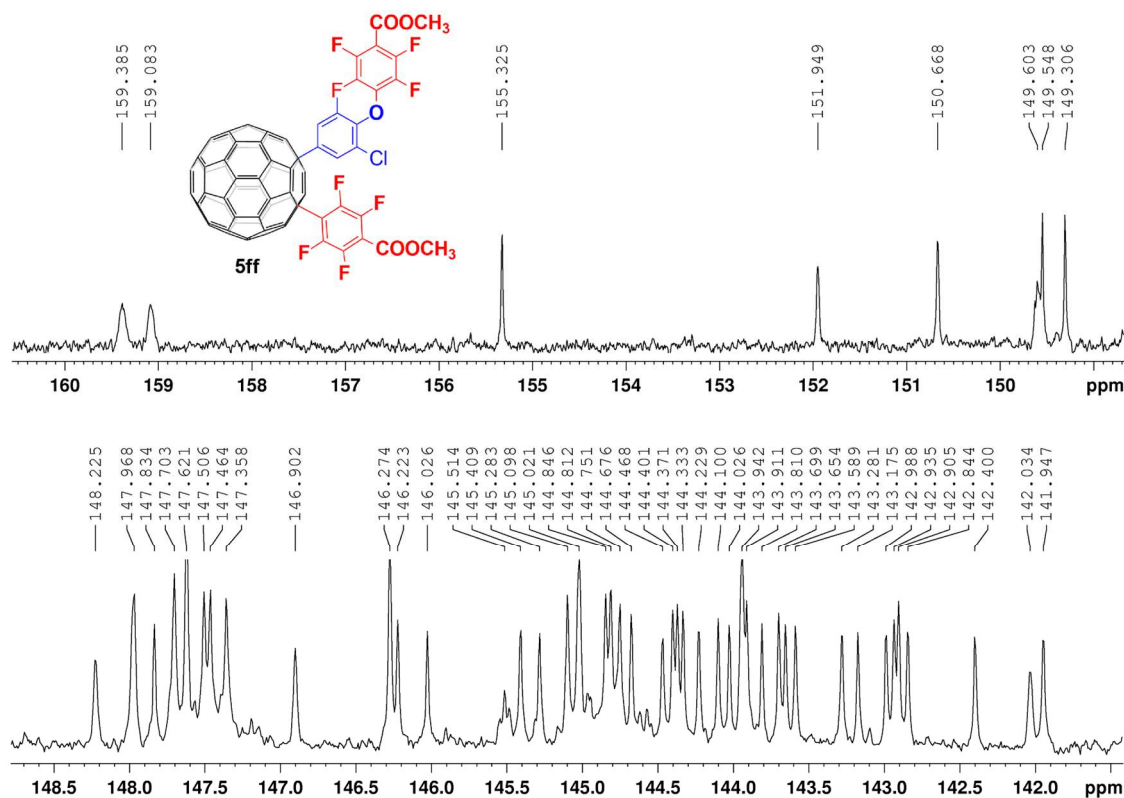
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 5ff



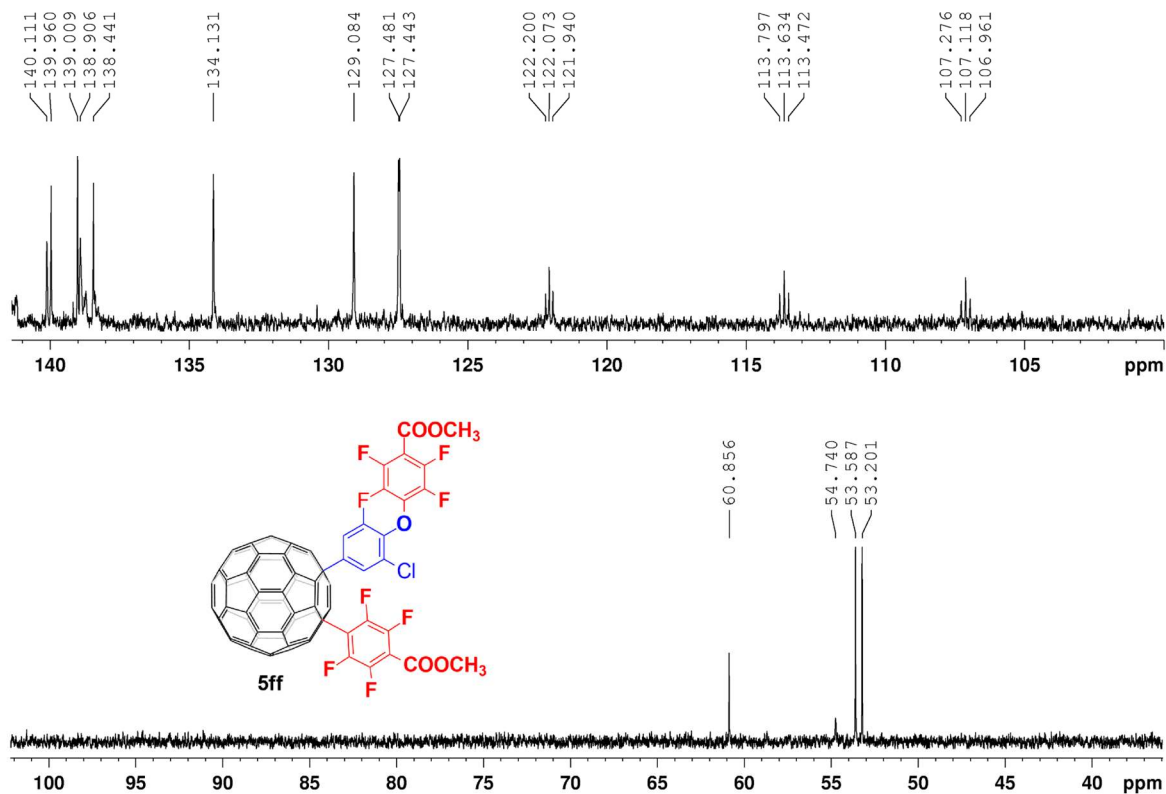
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5ff



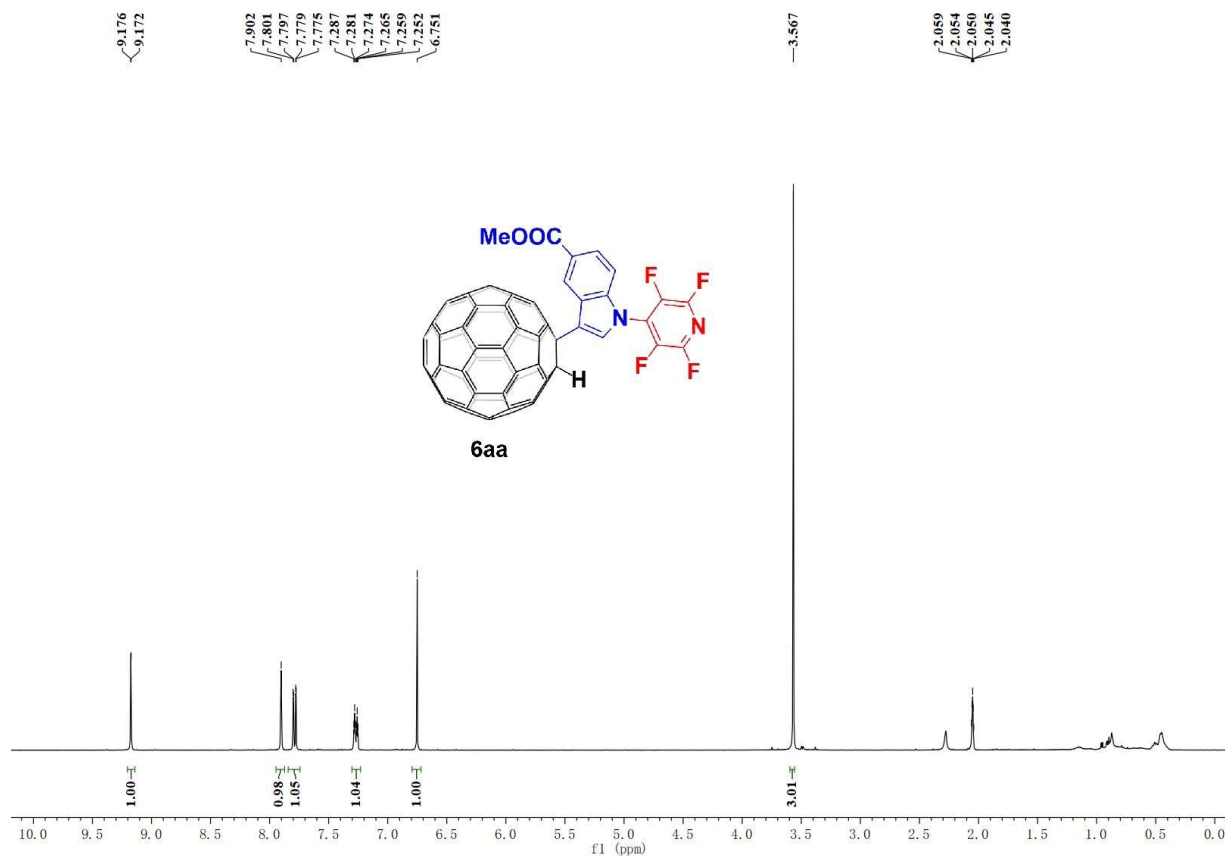
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5ff



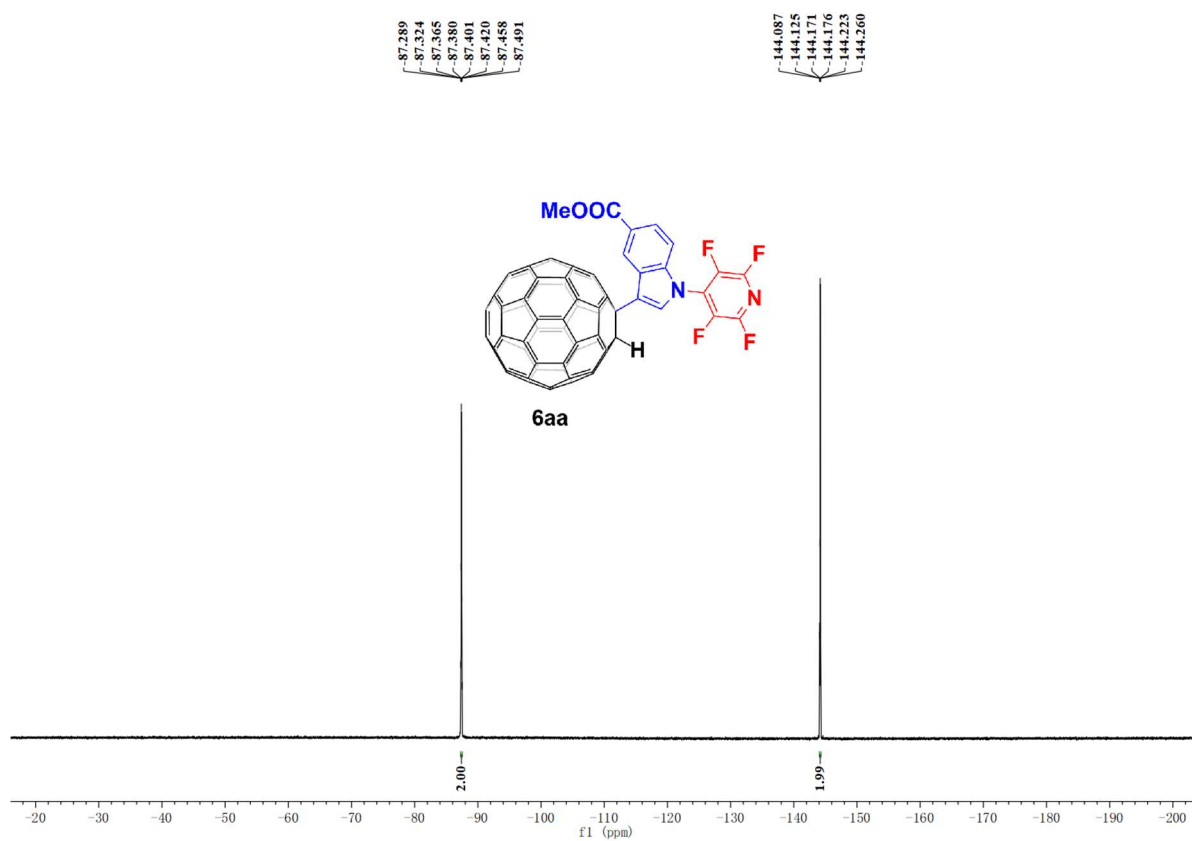
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 5ff



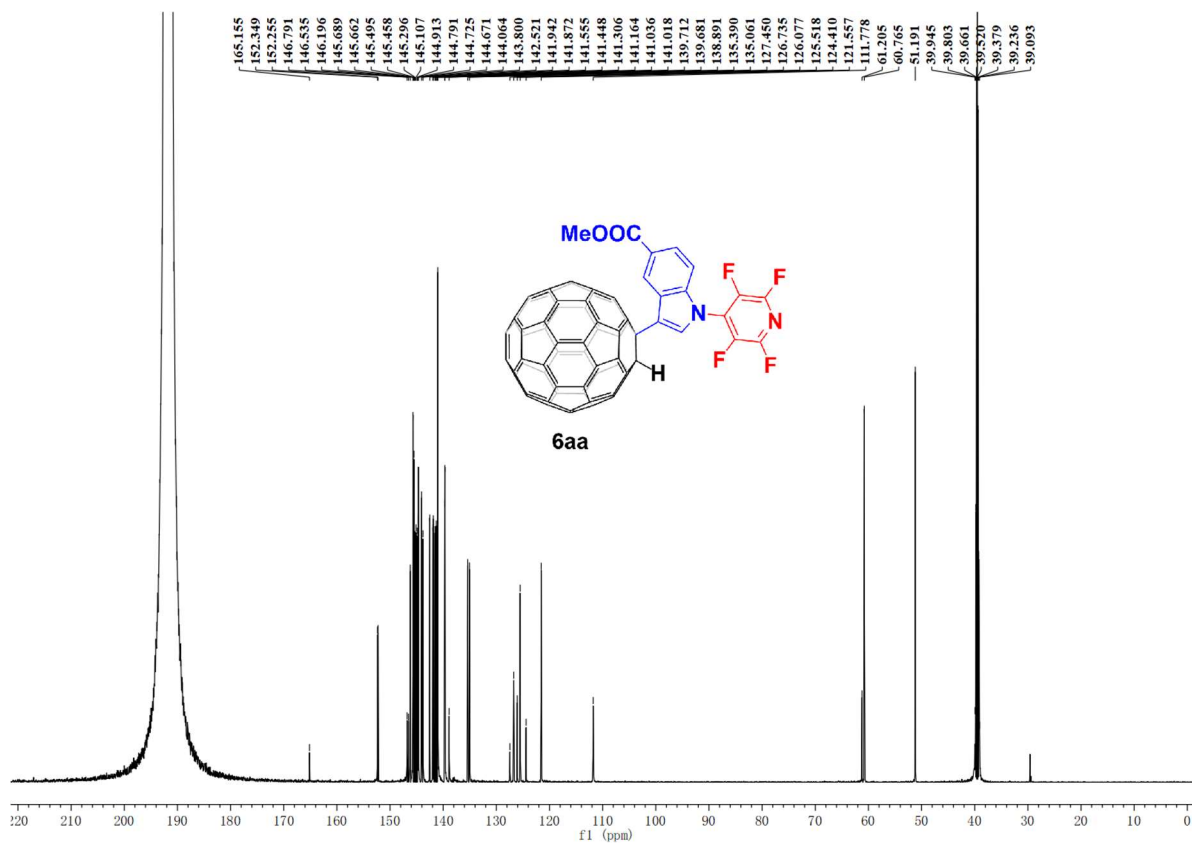
^1H NMR (400 MHz, CS_2/d_6 -DMSO) of compound 6aa



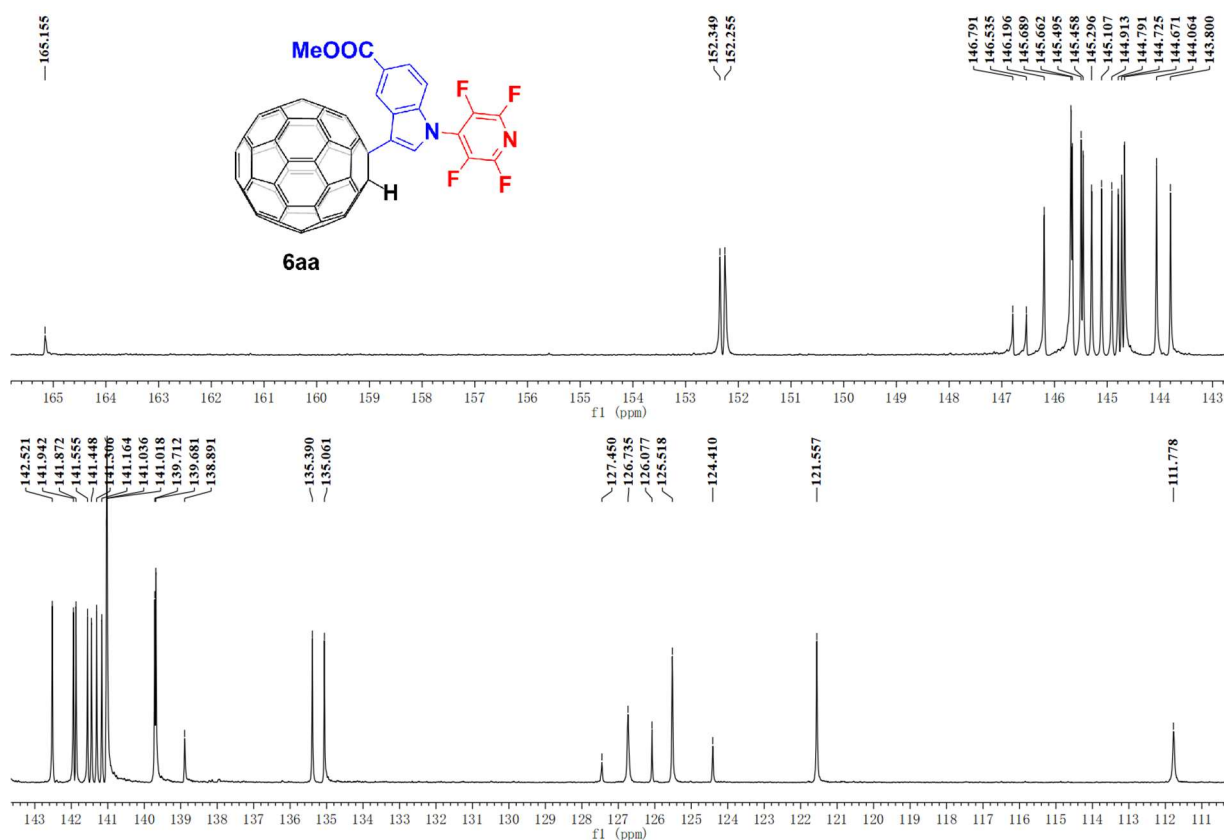
^{19}F NMR (376 MHz, CS_2/d_6 -DMSO) of compound 6aa



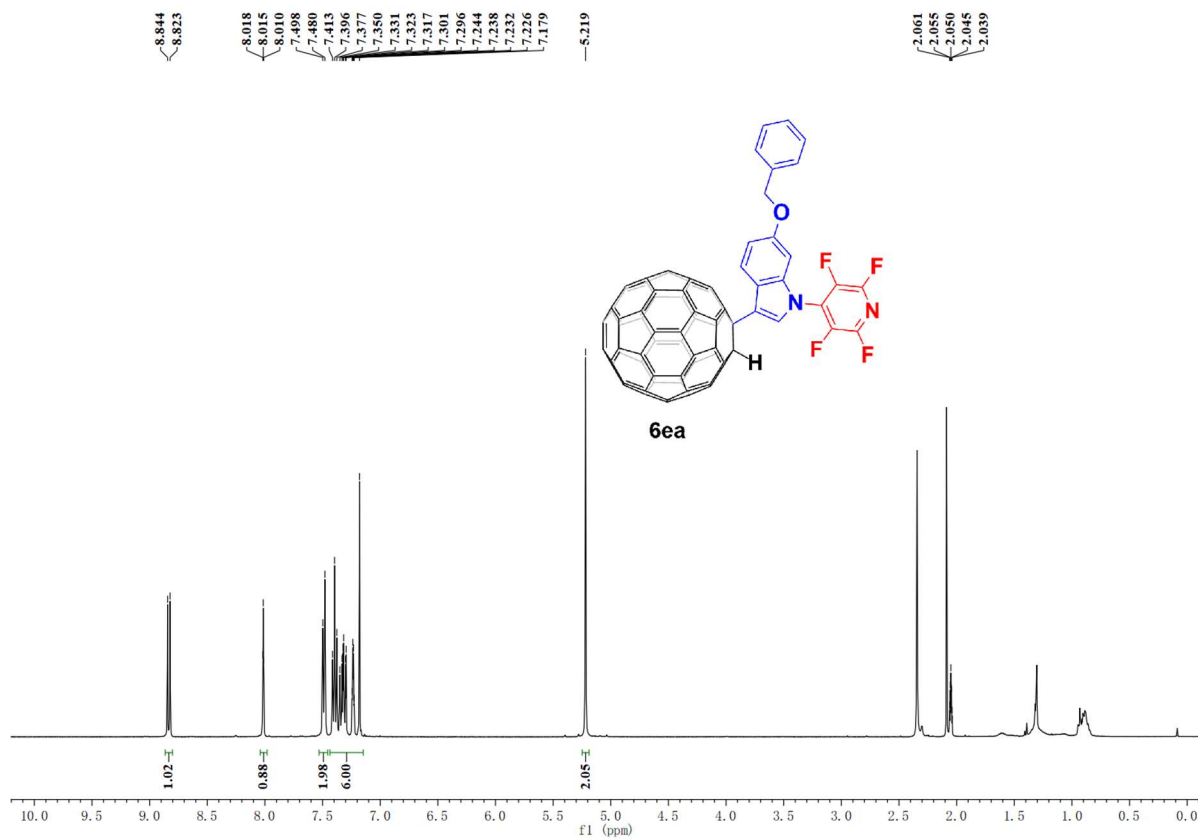
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -DMSO) of compound 6aa



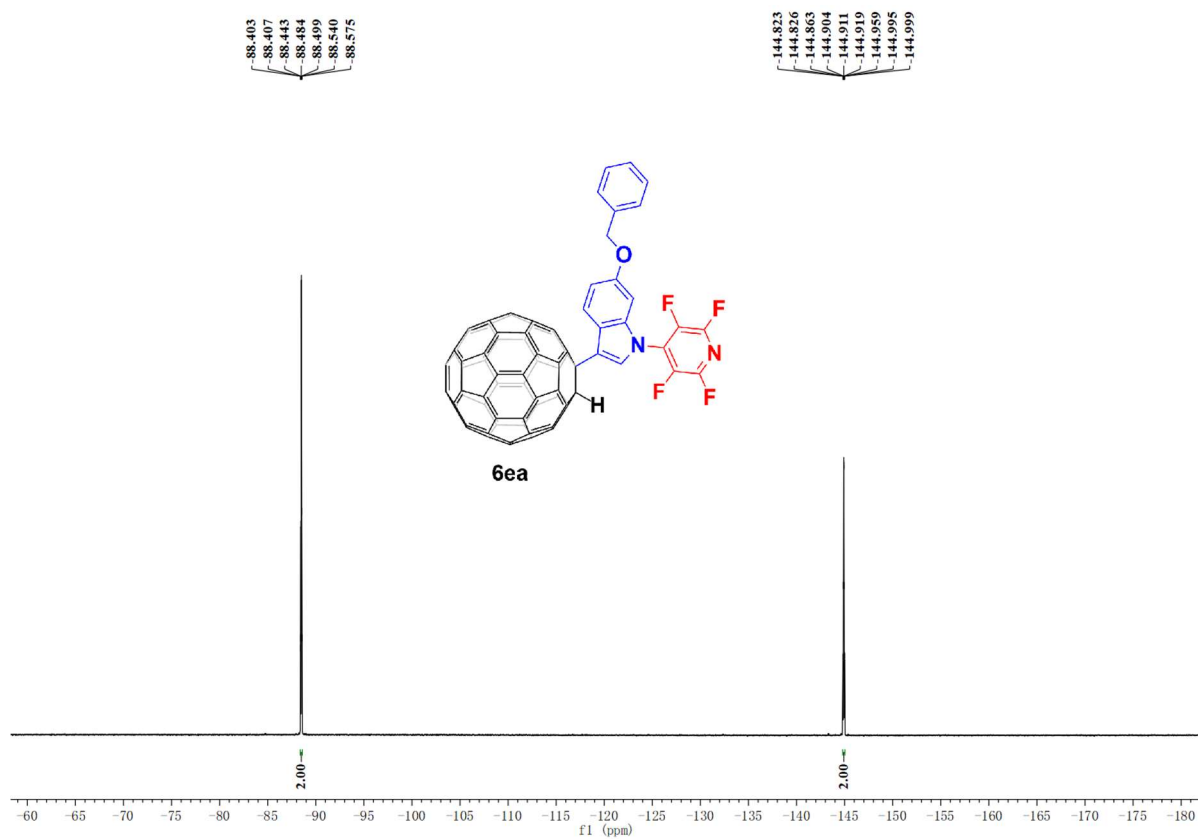
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -DMSO) of compound 6aa



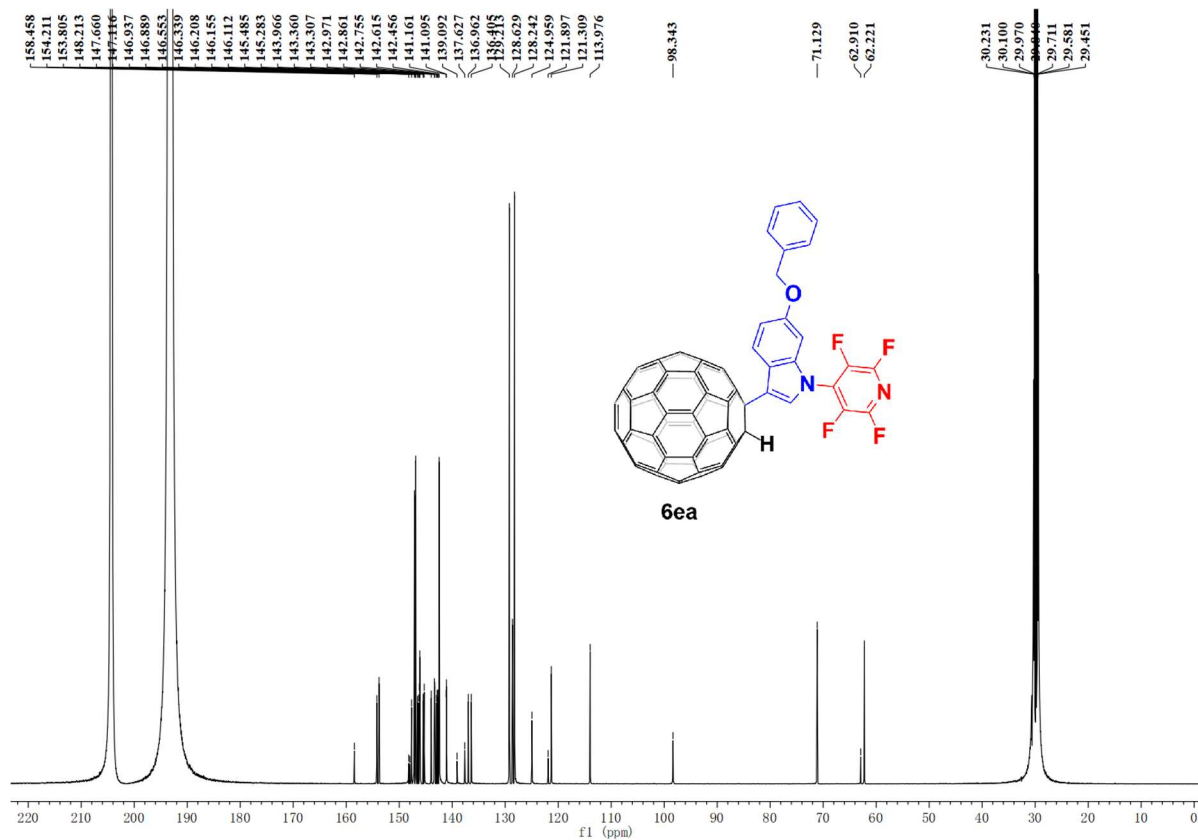
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 6ea



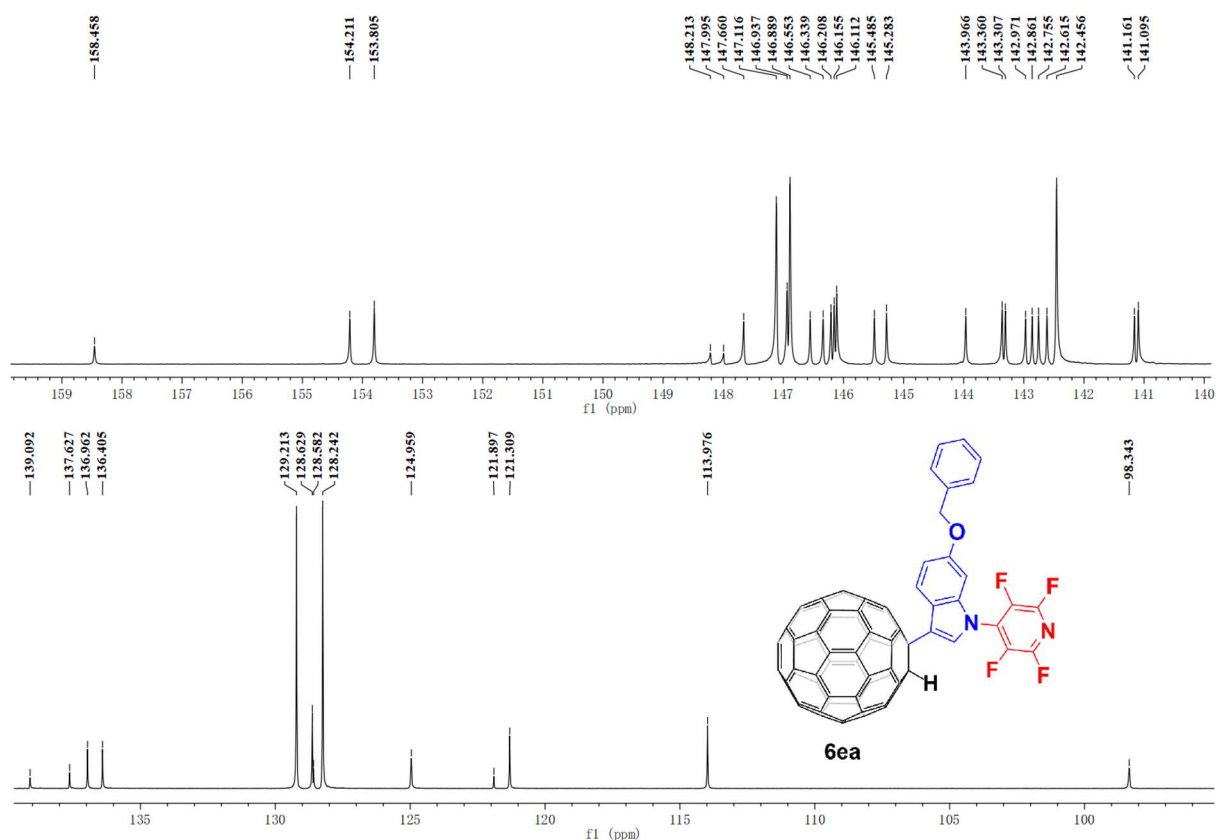
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 6ea



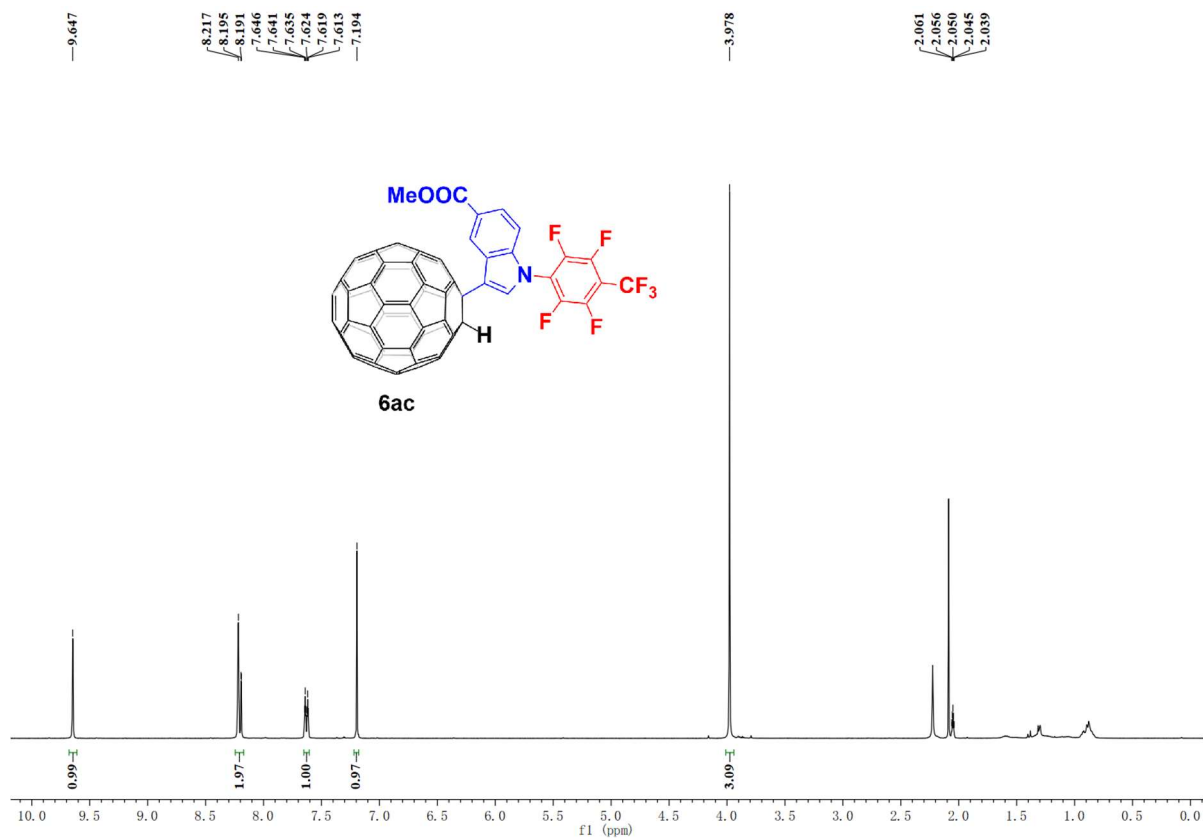
$^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound 6ea



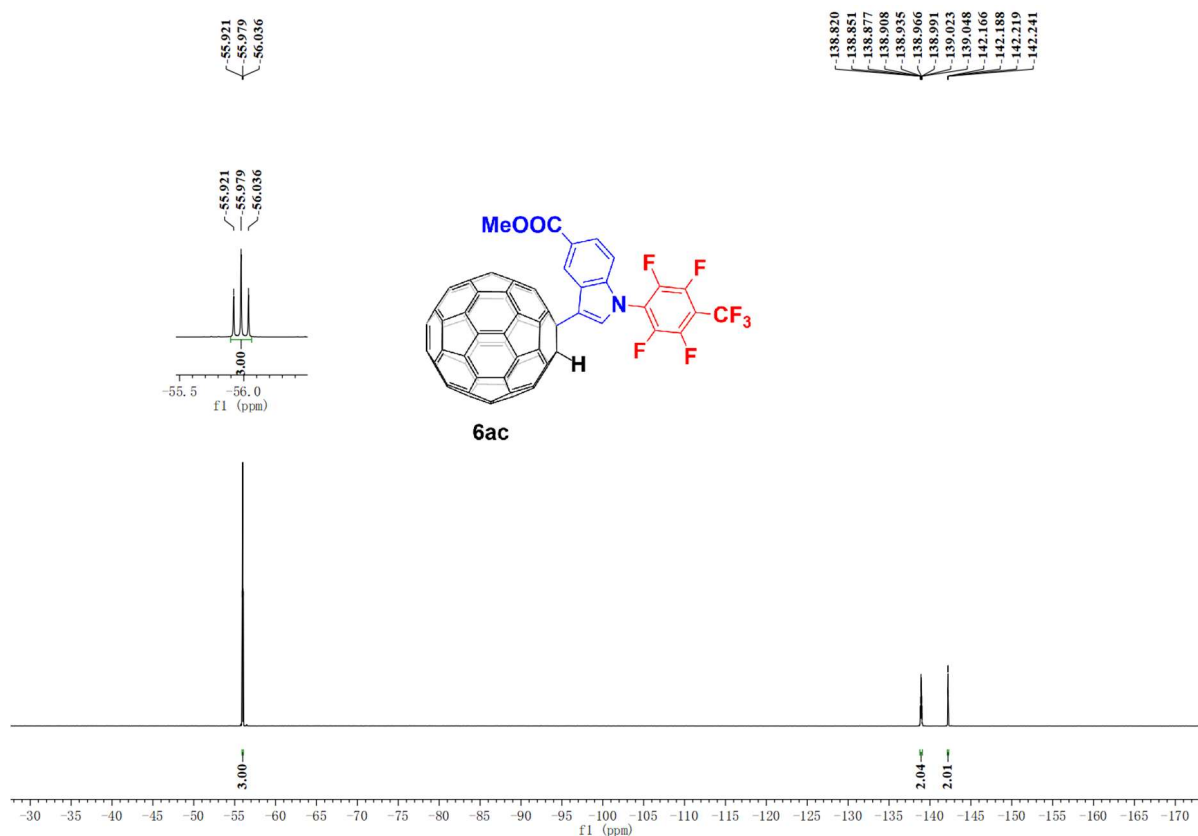
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound 6ea



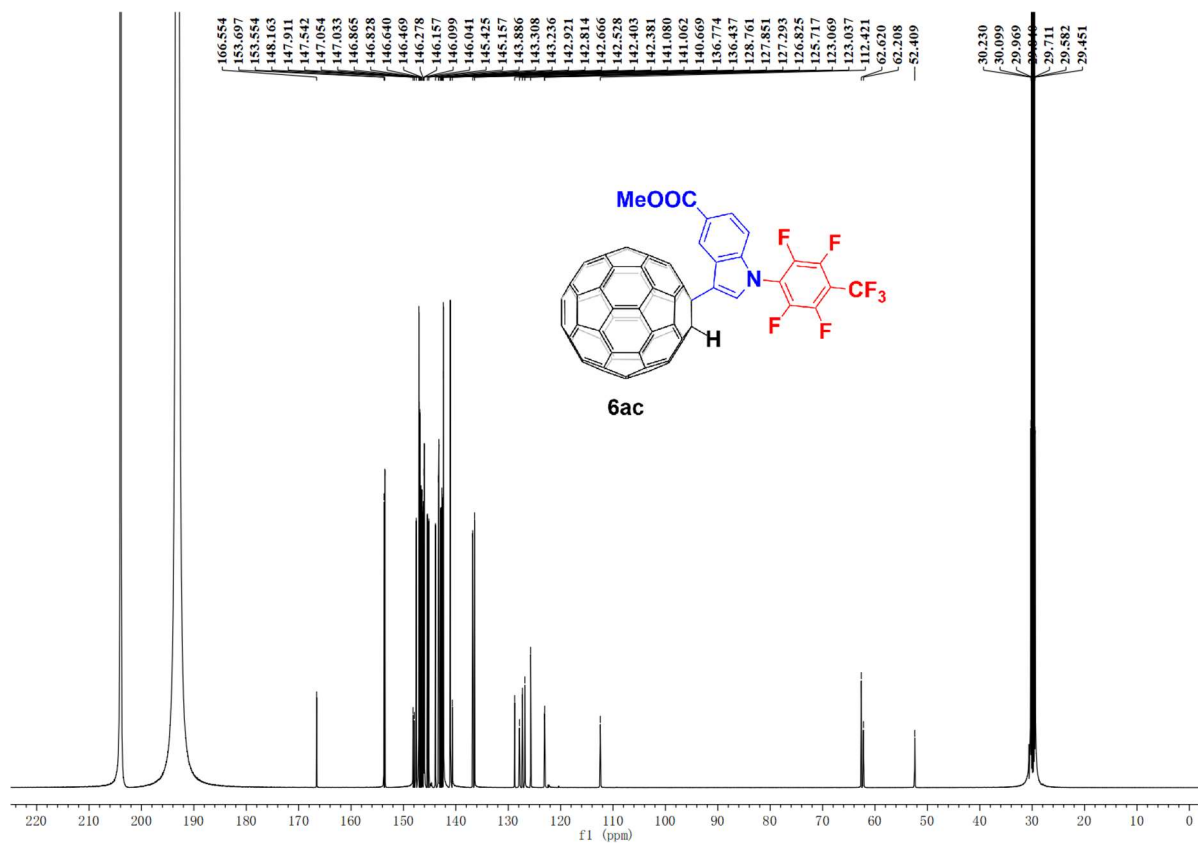
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound 6ac



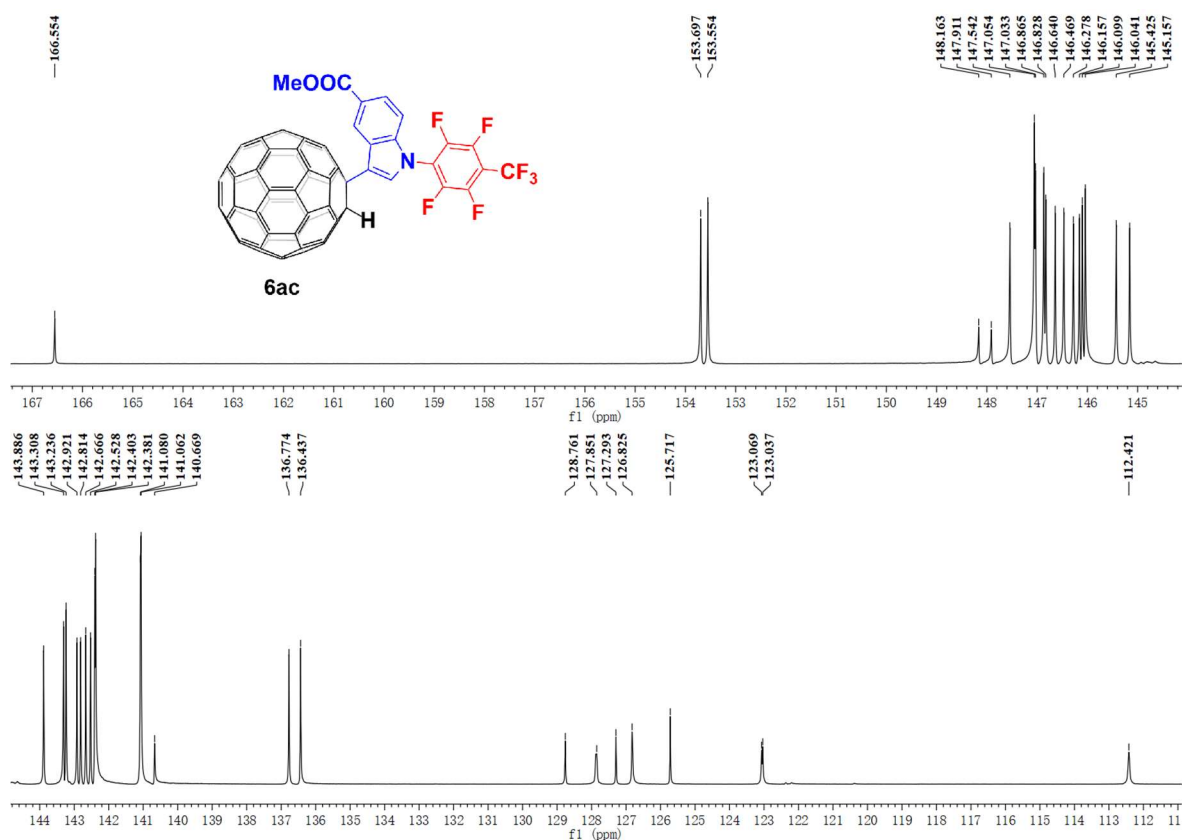
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 6ac



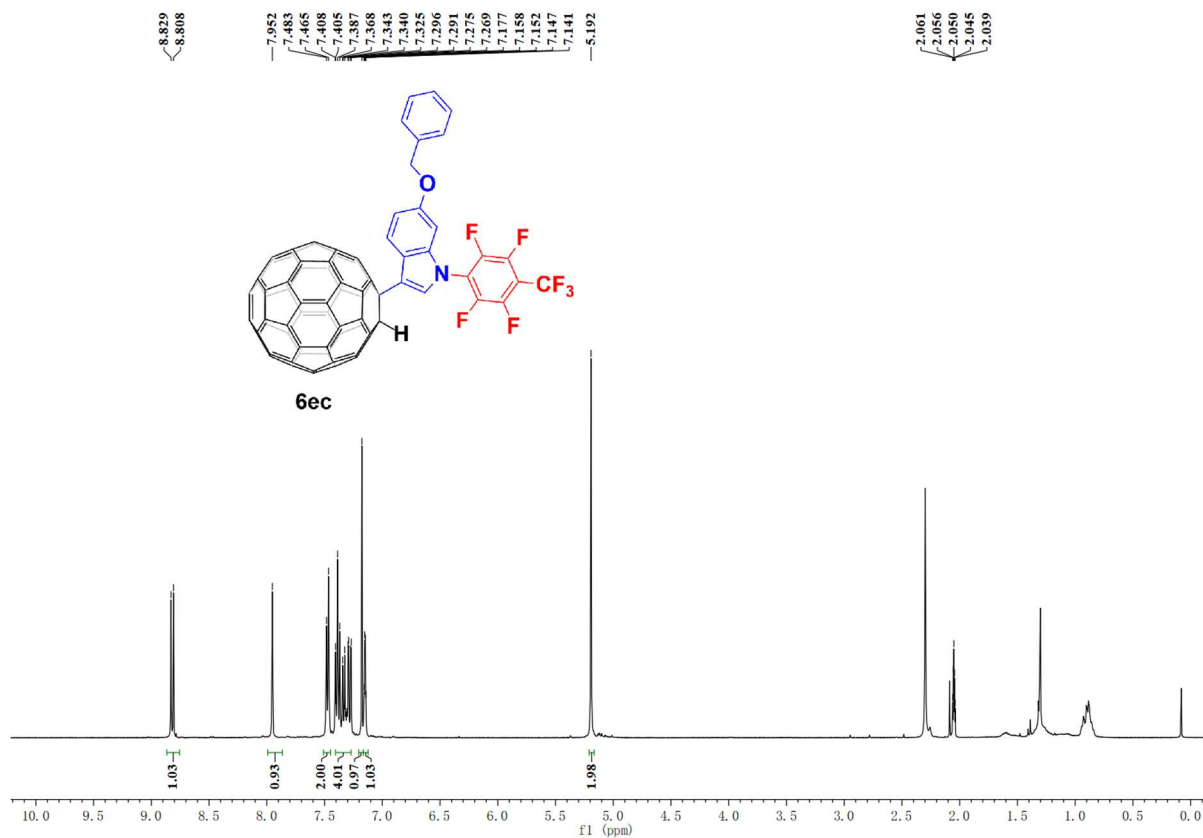
$^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound 6ac



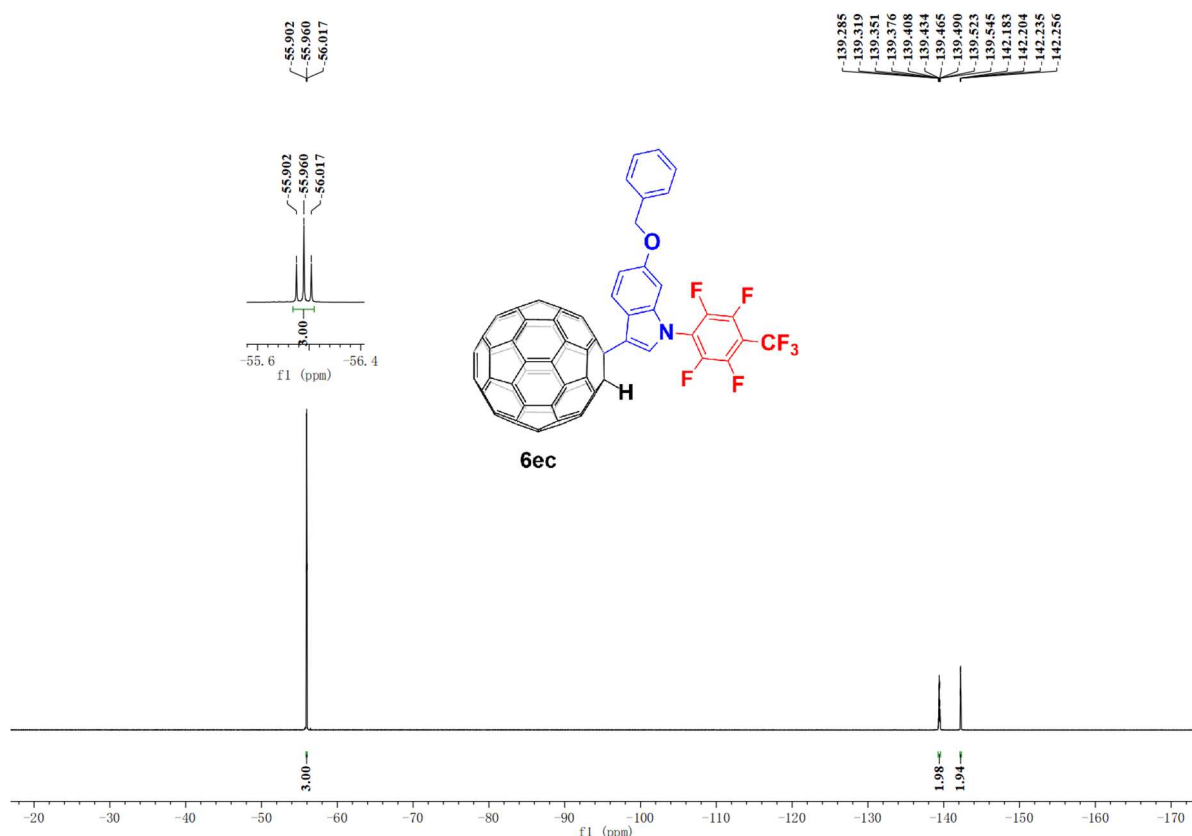
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CS_2/d_6 -acetone) of compound **6ac**



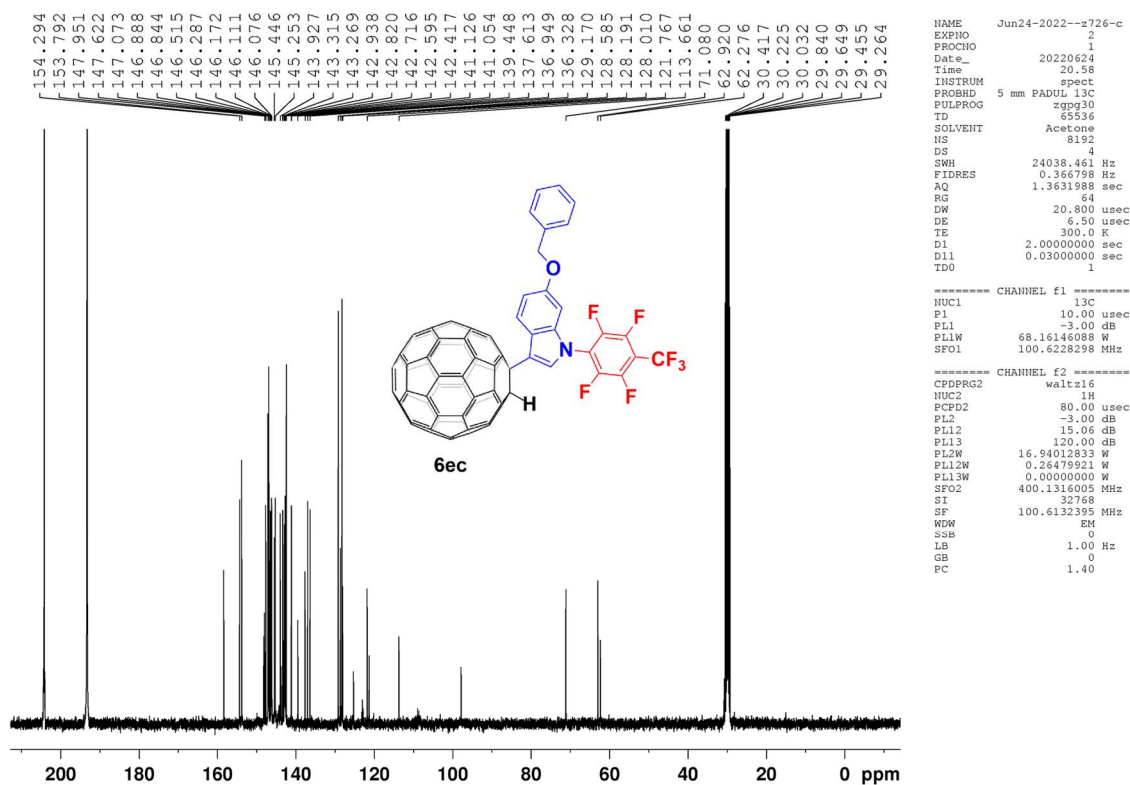
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **6ec**



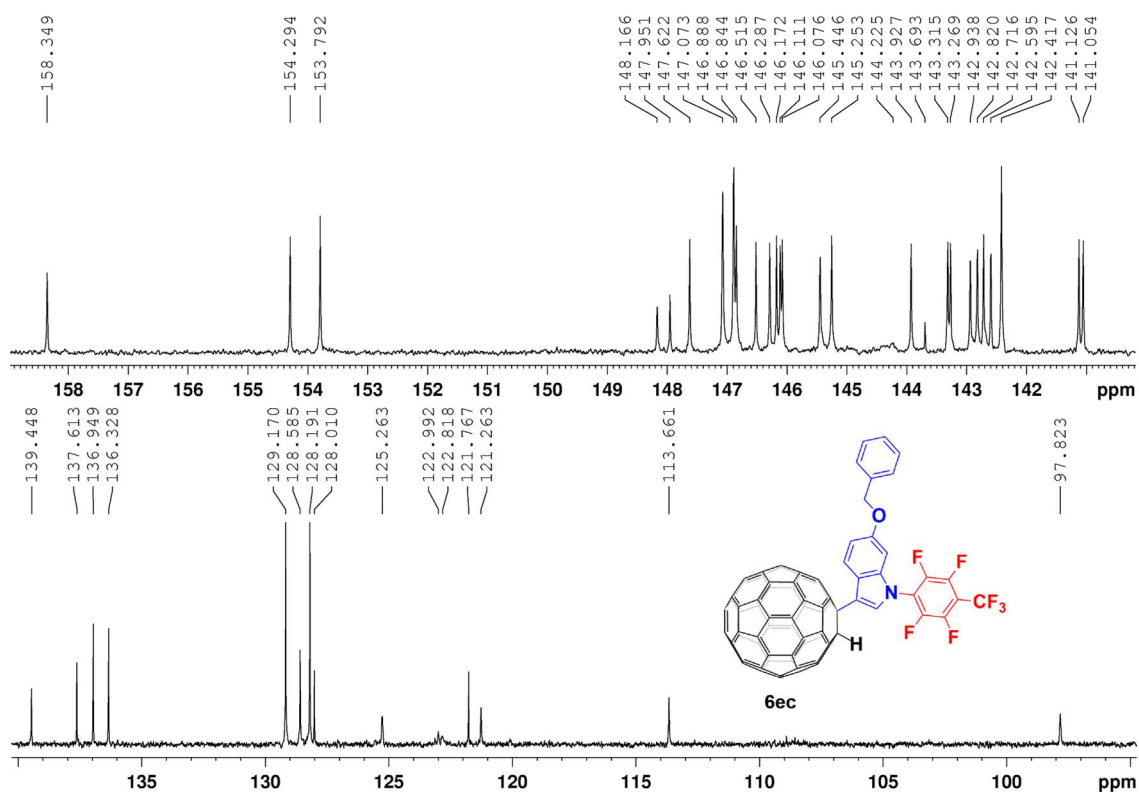
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound 6ec



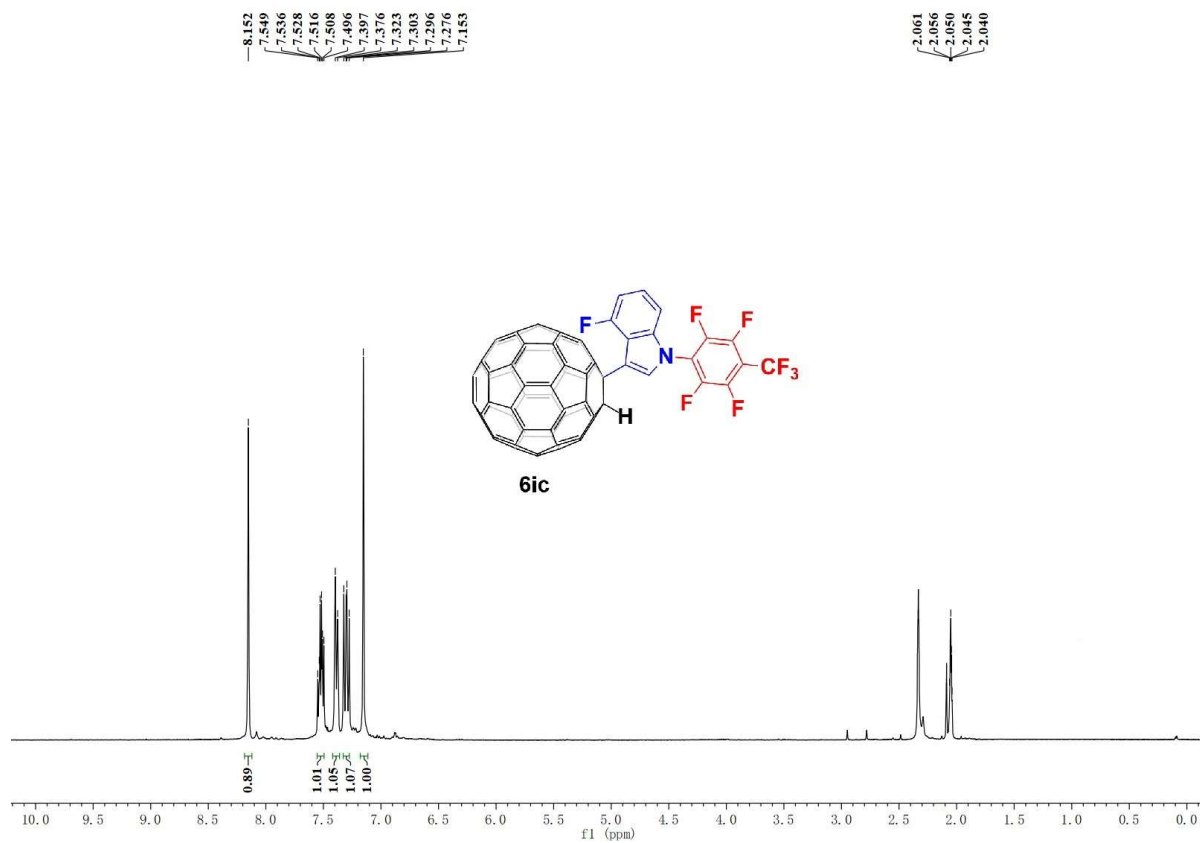
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound 6ec



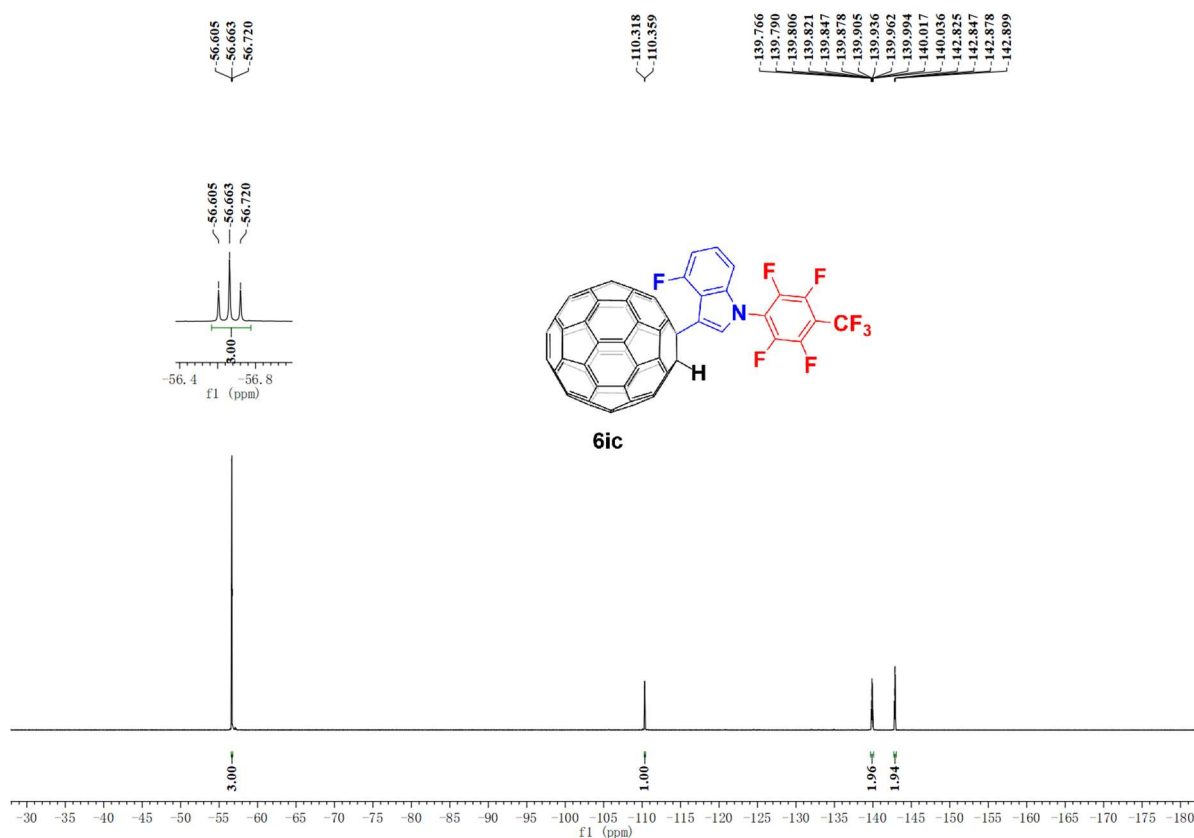
Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **6ec**



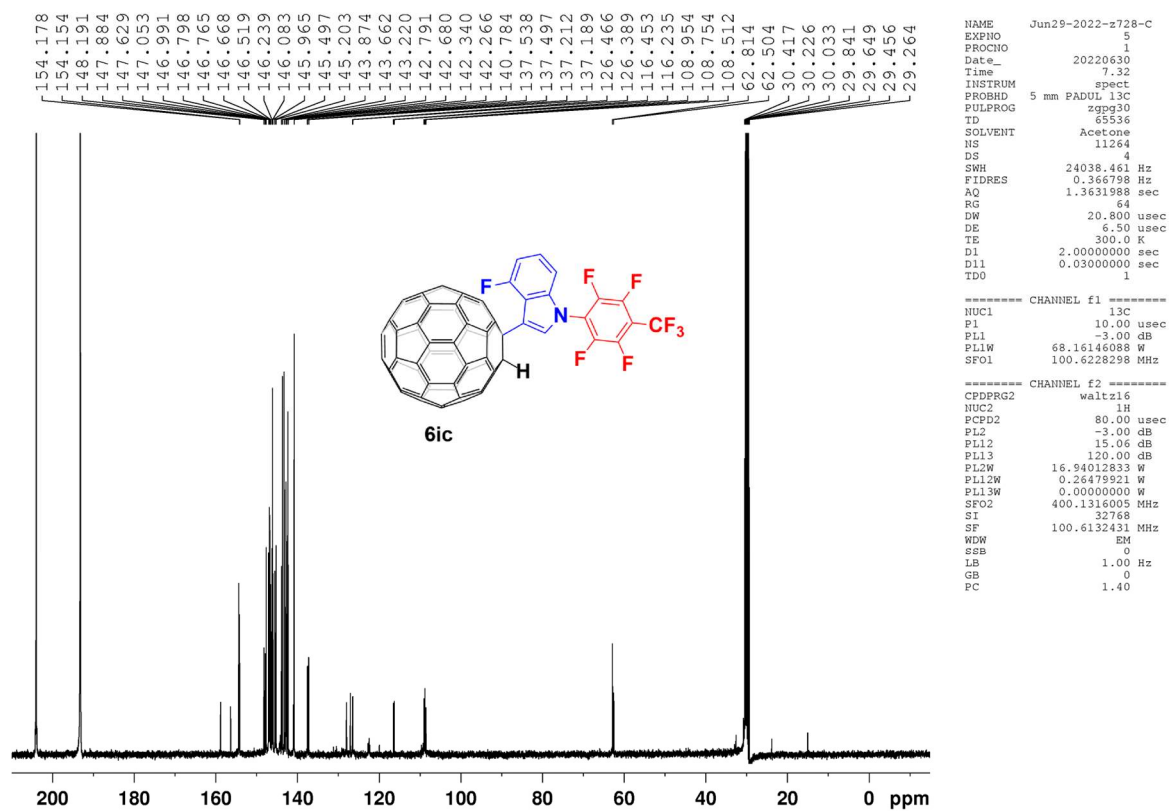
^1H NMR (400 MHz, CS_2/d_6 -acetone) of compound **6ic**



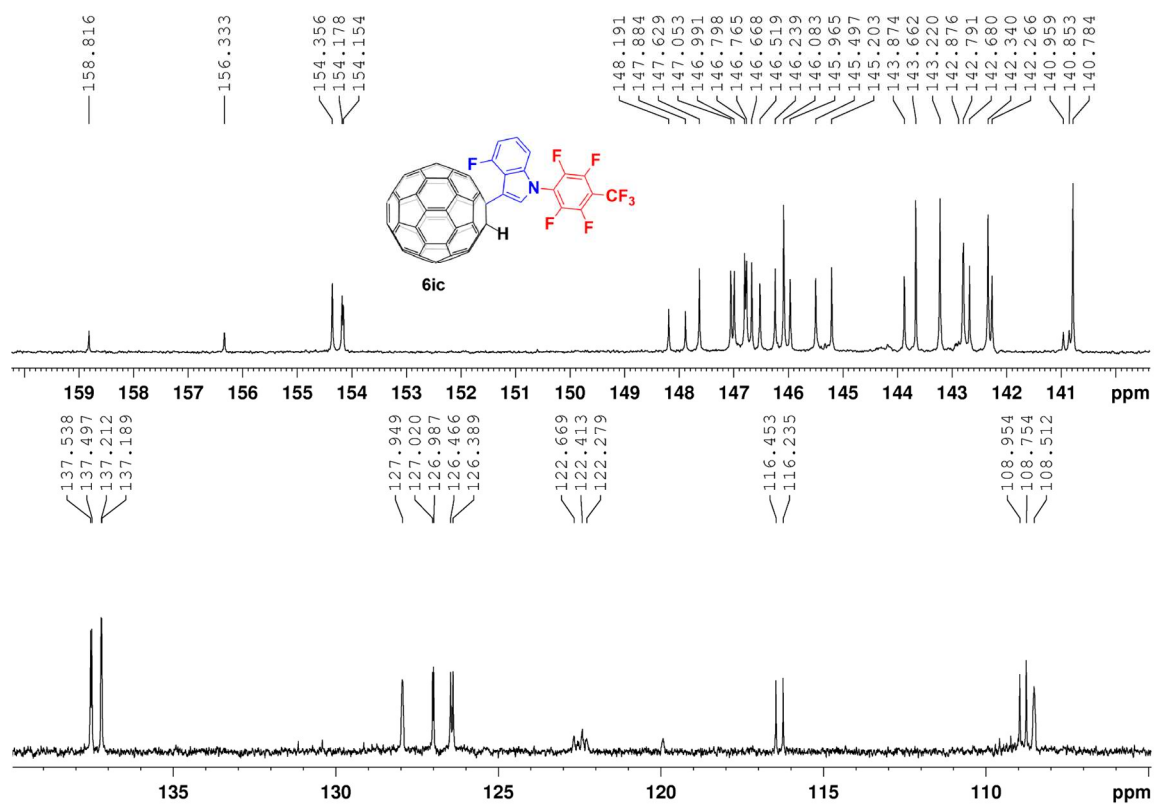
^{19}F NMR (376 MHz, CS_2/d_6 -acetone) of compound **6ic**



$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **6ic**



Expanded $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CS_2/d_6 -acetone) of compound **6ic**



2. Single-Crystal X-Ray Crystallography of 3ca, 3af, and 5ba

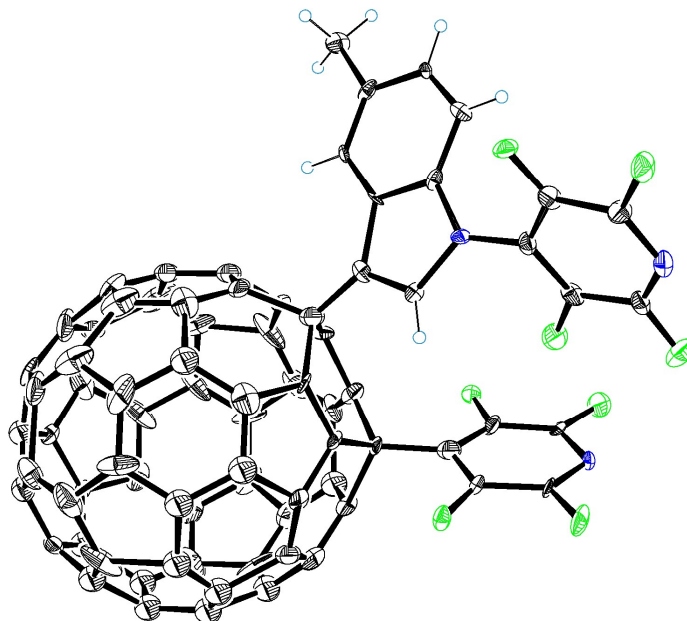


Figure S1 ORTEP diagrams of **3ca** with 30% thermal ellipsoids.

Black block crystals of **3ca** suitable for X-ray diffraction were obtained from isopropyl alcohol diffusion into its CS₂ solution. Single-crystal X-ray diffraction data were collected on a diffractometer (DECTRIS PILATUS 300K, STOE & Cie GmbH) equipped with a CCD area detector using graphite-monochromated Cu K α radiation ($\lambda = 1.54184 \text{ \AA}$) in the scan range $9.172^\circ < 2\theta < 124.998$. The structure was solved with direct methods using SHELXS-97 and refined with full-matrix least-squares refinement using the SHELXL-97 program within OLEX2. Crystallographic data have been deposited in the Cambridge Crystallographic Data Centre as deposition number CCDC 2177898.

Table S1 Crystal data and structure refinement for 3ca	
Identification code	3ca
Empirical formula	C ₇₉ H ₇ F ₈ N ₃
Formula weight	1149.88
Temperature/K	120
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	10.156
b/Å	30.702
c/Å	14.665
α /°	90
β /°	90.66

$\gamma/^\circ$	90
Volume/ \AA^3	4572.1
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.671
μ/mm^{-1}	1.016
F(000)	2296.0
Crystal size/ mm^3	$0.03 \times 0.02 \times 0.015$
Radiation	CuK α ($\lambda = 1.54186$)
2Θ range for data collection/ $^\circ$	9.172 to 124.998
Index ranges	$-9 \leq h \leq 11, -35 \leq k \leq 34, -12 \leq l \leq 16$
Reflections collected	13186
Independent reflections	6994 [$R_{\text{int}} = 0.0299, R_{\text{sigma}} = 0.0263$]
Data/restraints/parameters	6994/0/620
Goodness-of-fit on F^2	1.158
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.1015, wR_2 = 0.2380$
Final R indexes [all data]	$R_1 = 0.1186, wR_2 = 0.2650$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	0.54/-0.46

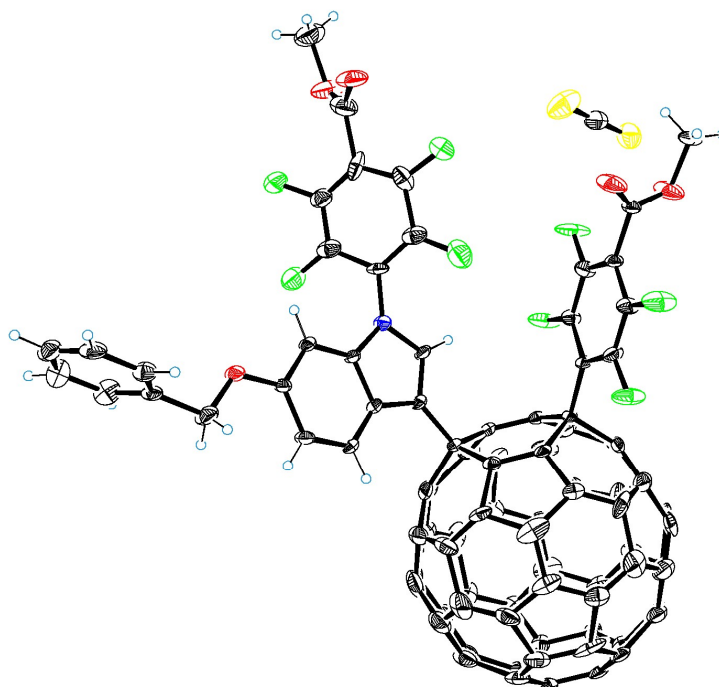


Figure S2 ORTEP diagrams of **3af** with 30% thermal ellipsoids.

Black block crystals of **3af** suitable for X-ray diffraction were obtained from acetonitrile diffusion into its CS₂ solution. Single-crystal X-ray diffraction data were collected on a diffractometer (DECTRIS PILATUS 300K, STOE & Cie GmbH) equipped with a CCD area detector using graphite-monochromated Cu K α radiation ($\lambda = 1.54184 \text{ \AA}$) in the scan range $11.584^\circ < 2\theta < 139.068$. The structure was solved with direct methods using SHELXS-97 and refined with full-matrix least-squares refinement using the SHELXL-97 program within OLEX2. Crystallographic data have been deposited in the Cambridge Crystallographic Data Centre as deposition number CCDC 2177886.

Table S2 Crystal data and structure refinement for 3af	
Identification code	3af
Empirical formula	C ₉₂ H ₁₇ F ₈ NO ₅ S ₂
Formula weight	1432.19
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.7362(7)
b/Å	17.4371(13)
c/Å	17.4852(12)
$\alpha/^\circ$	118.369(5)
$\beta/^\circ$	93.833(6)
$\gamma/^\circ$	94.424(6)
Volume/Å ³	2851.6(4)
Z	2
$\rho_{\text{calc}}/\text{cm}^3$	1.668
μ/mm^{-1}	1.676
F(000)	1440.0
Crystal size/mm ³	0.17 × 0.15 × 0.10
Radiation	CuK α ($\lambda = 1.54186$)
2 Θ range for data collection/ $^\circ$	11.584 to 139.068
Index ranges	-12 ≤ h ≤ 11, -14 ≤ k ≤ 20, -20 ≤ l ≤ 12
Reflections collected	16586
Independent reflections	10089 [R _{int} = 0.0482, R _{sigma} = 0.0484]
Data/restraints/parameters	10089/0/969
Goodness-of-fit on F ²	1.092
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.1001, wR ₂ = 0.2474
Final R indexes [all data]	R ₁ = 0.1224, wR ₂ = 0.2726
Largest diff. peak/hole / e Å ⁻³	0.92/-0.48

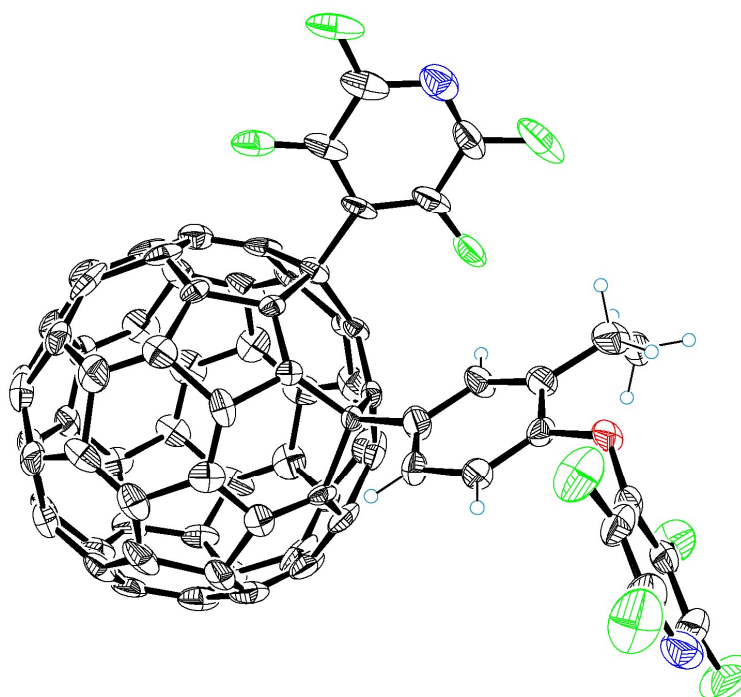


Figure S3 ORTEP diagrams of **5ba** with 30% thermal ellipsoids.

Black block crystals of **5ba** suitable for X-ray diffraction were obtained from slow evaporation of its solution in a mixture of CS₂, d₆-acetone and iso-propyl alcohol at room temperature. Single-crystal X-ray diffraction data were collected on a diffractometer (DECTRIS PILATUS 300K, STOE & Cie GmbH) equipped with a CCD area detector using graphite-monochromated Cu K α radiation ($\lambda = 1.54184 \text{ \AA}$) in the scan range $9.23^\circ < 2\theta < 139.01$. The structure was solved with direct methods using SHELXS-97 and refined with full-matrix least-squares refinement using the SHELXL-97 program within OLEX2. Crystallographic data have been deposited in the Cambridge Crystallographic Data Centre as deposition number CCDC 2177889.

Table S3 Crystal data and structure refinement for 5ba	
Identification code	5ba
Empirical formula	C ₇₈ H ₈ F ₈ N ₂ O
Formula weight	1140.86
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	21.6590(9)
b/Å	10.0799(4)
c/Å	20.0636(8)
α /°	90

$\beta/^\circ$	99.028(3)
$\gamma/^\circ$	90
Volume/ \AA^3	4326.0(3)
Z	4
$\rho_{\text{calc}}/\text{g}/\text{cm}^3$	1.752
μ/mm^{-1}	1.077
F(000)	2280.0
Crystal size/ mm^3	$0.3 \times 0.2 \times 0.1$
Radiation	CuK α ($\lambda = 1.54186$)
2Θ range for data collection/ $^\circ$	9.23 to 139.008
Index ranges	$-26 \leq h \leq 24, -12 \leq k \leq 10, -16 \leq l \leq 23$
Reflections collected	15740
Independent reflections	7644 [$R_{\text{int}} = 0.0539, R_{\text{sigma}} = 0.0496$]
Data/restraints/parameters	7644/0/779
Goodness-of-fit on F^2	1.021
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0932, wR_2 = 0.2302$
Final R indexes [all data]	$R_1 = 0.1354, wR_2 = 0.2747$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	0.51/-0.46

3. UV-vis absorption spectra of compounds 3aa-ia, 3ab-ef, 5aa-ff, 6aa-ic

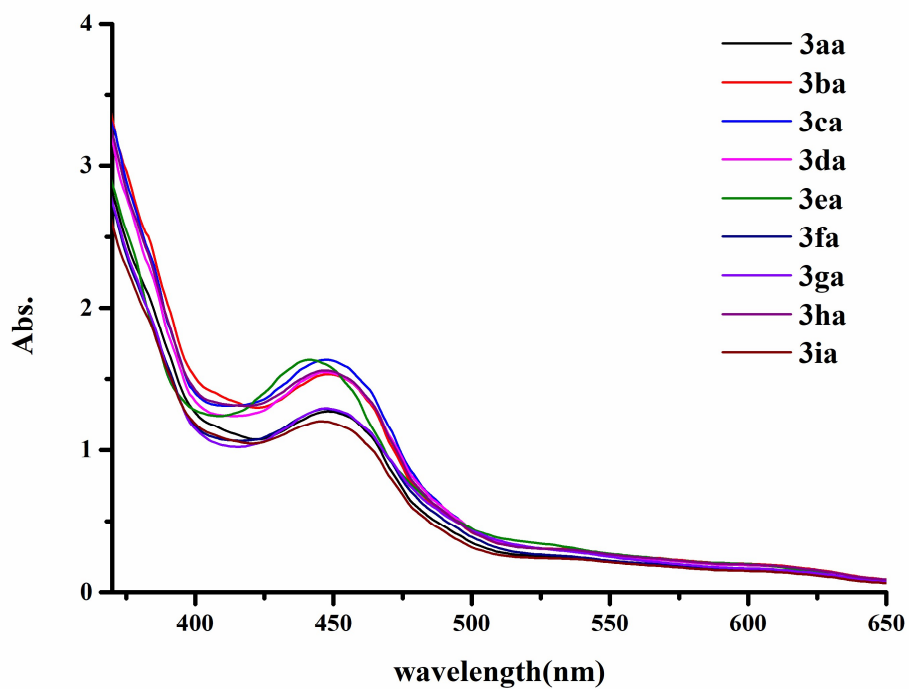


Figure S4 UV-vis spectra of 3aa-ia (solvent: CHCl₃)

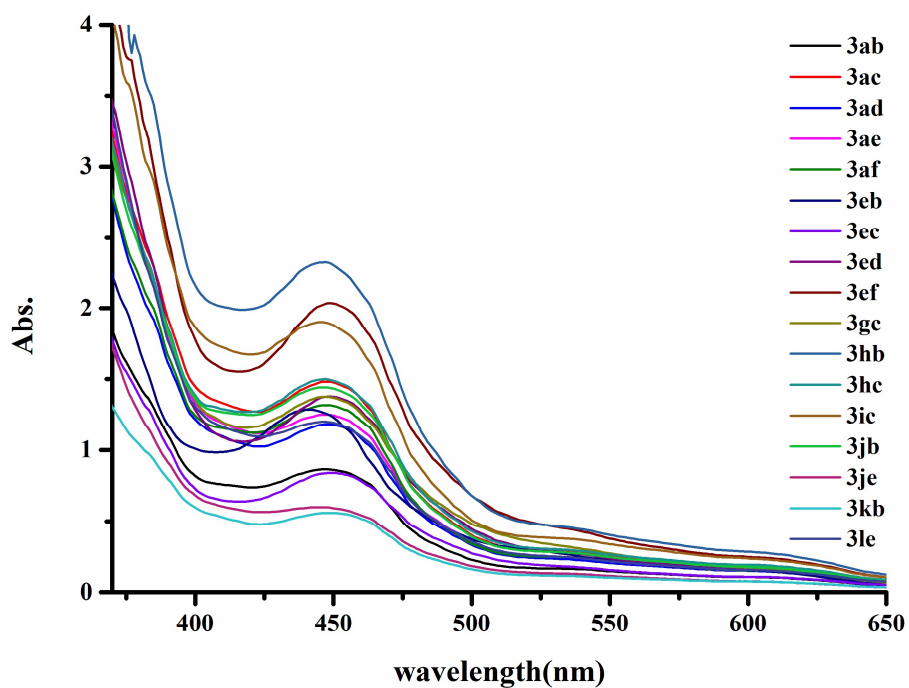


Figure S5 UV-vis spectra of 3ab-ef (solvent: CHCl₃)

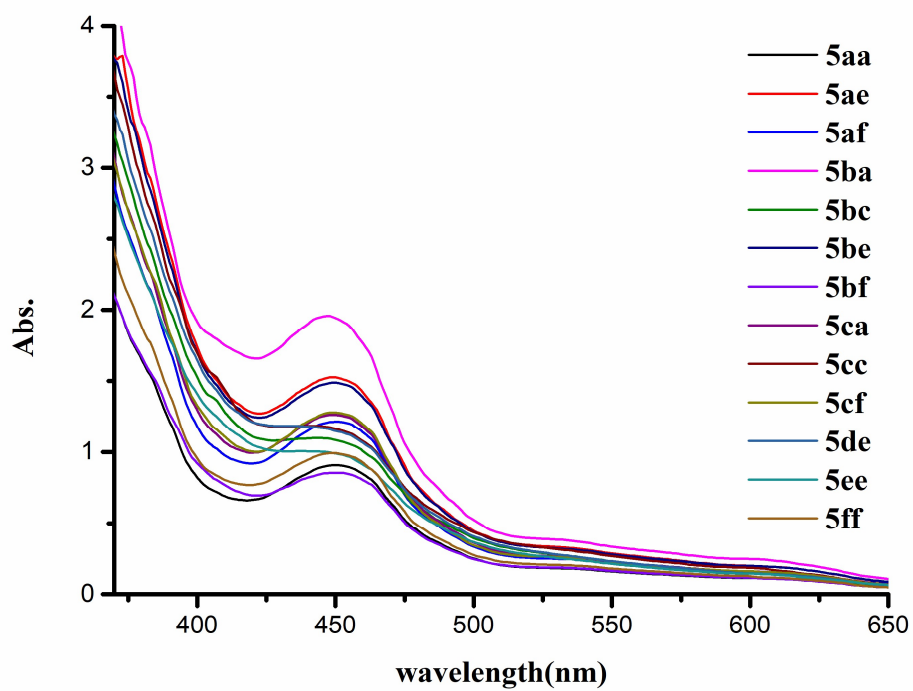


Figure S6 UV-vis spectra of **5aa-ff** (solvent: CHCl_3)

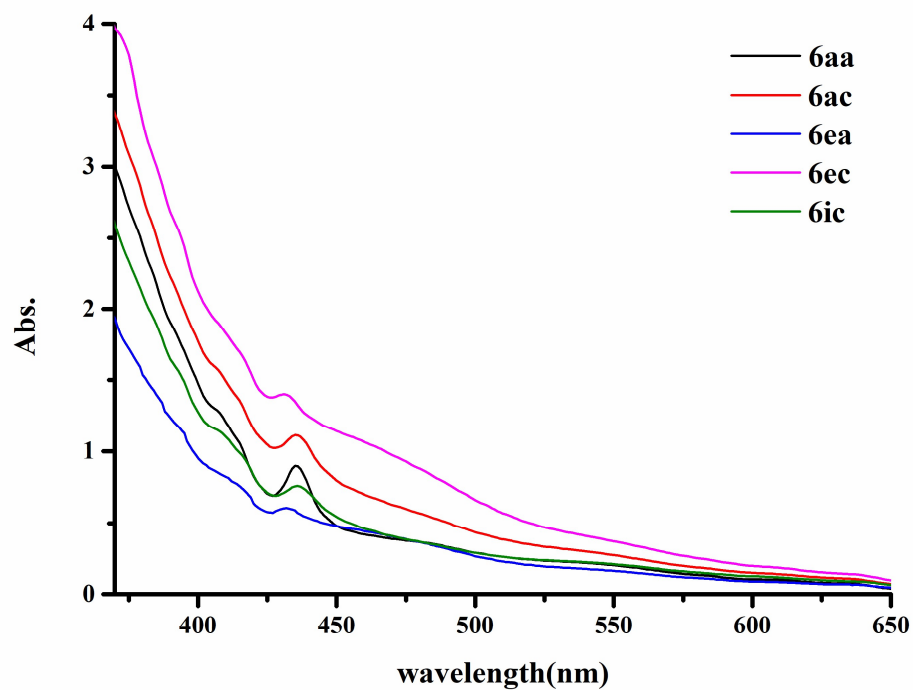


Figure S7 UV-vis spectra of **6aa-ic** (solvent: CHCl_3)