Acetylenic scaffolding with subphthalocyanines – synthetic scope and elucidation of electronic interactions in dimeric structures

Henrik Gotfredsen, Line Broløs, Thomas Holmstrøm, Jacob Sørensen, Alberto Viñas Muñoz, Martin Drøhse Kilde, Anders B. Skov, Marco Santella, Ole Hammerich and Mogens Brøndsted Nielsen*

Department of Chemistry, Center for Exploitation of Solar Energy, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark

Corresponding author e-mail: mbn@chem.ku.dk

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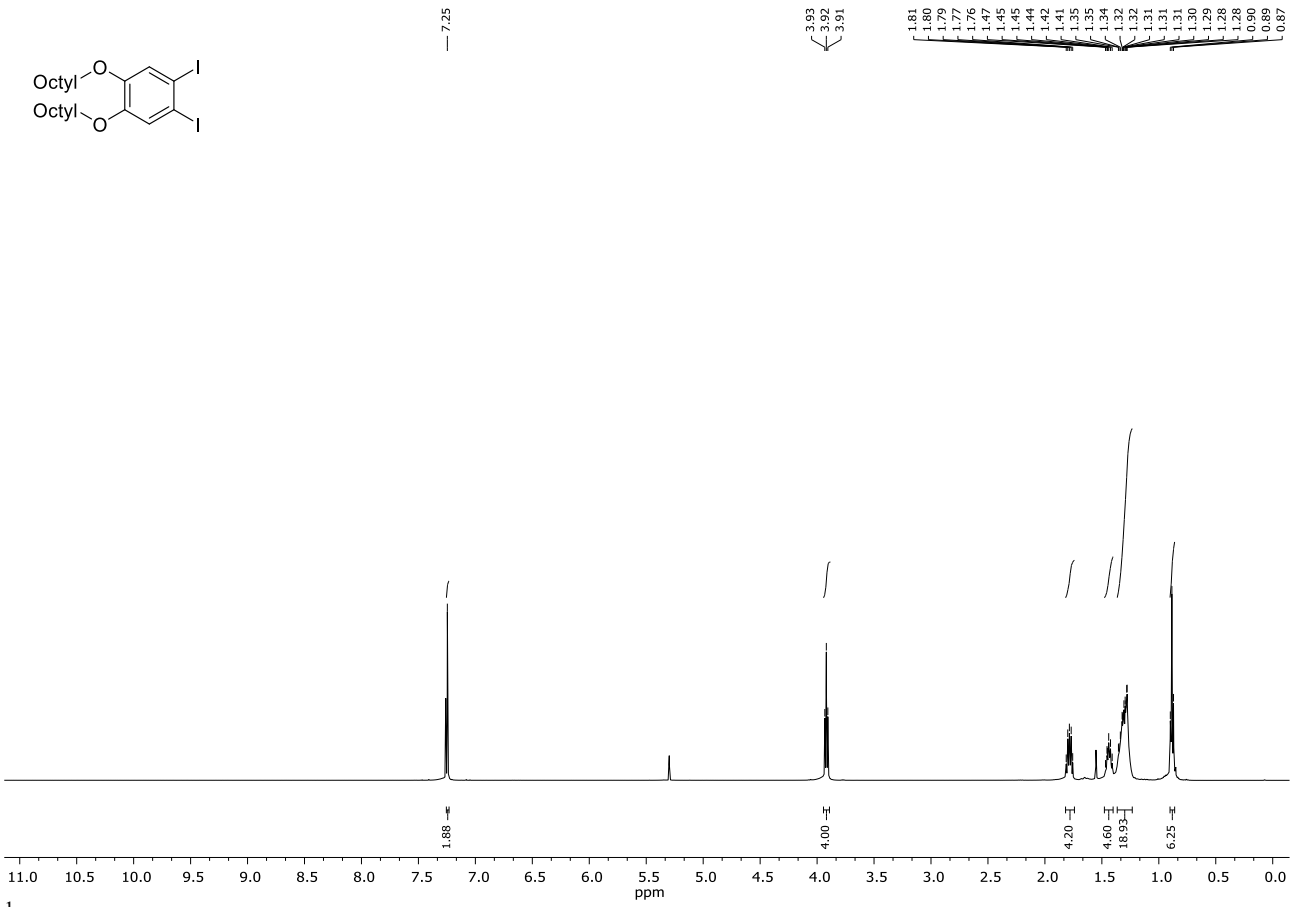
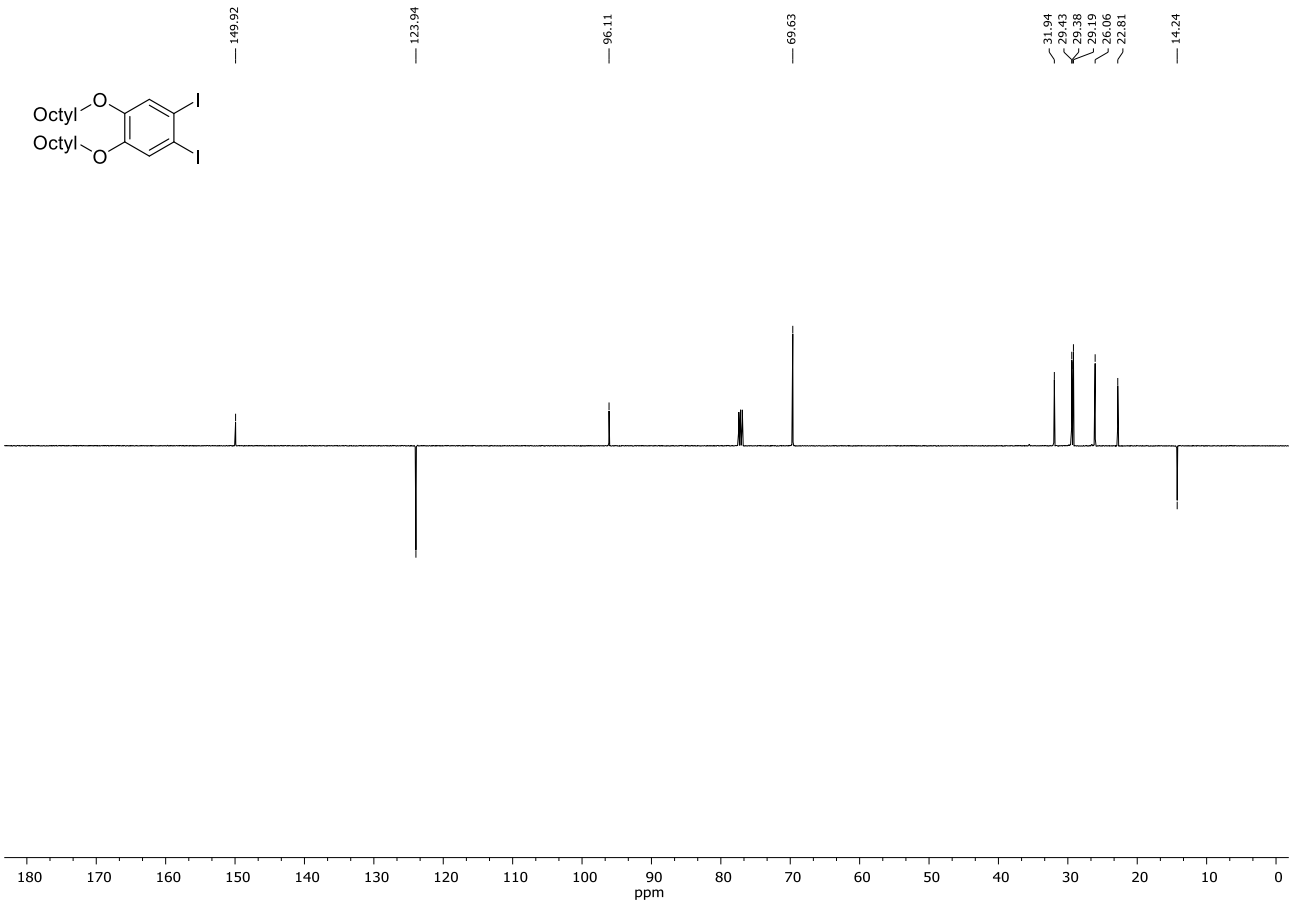
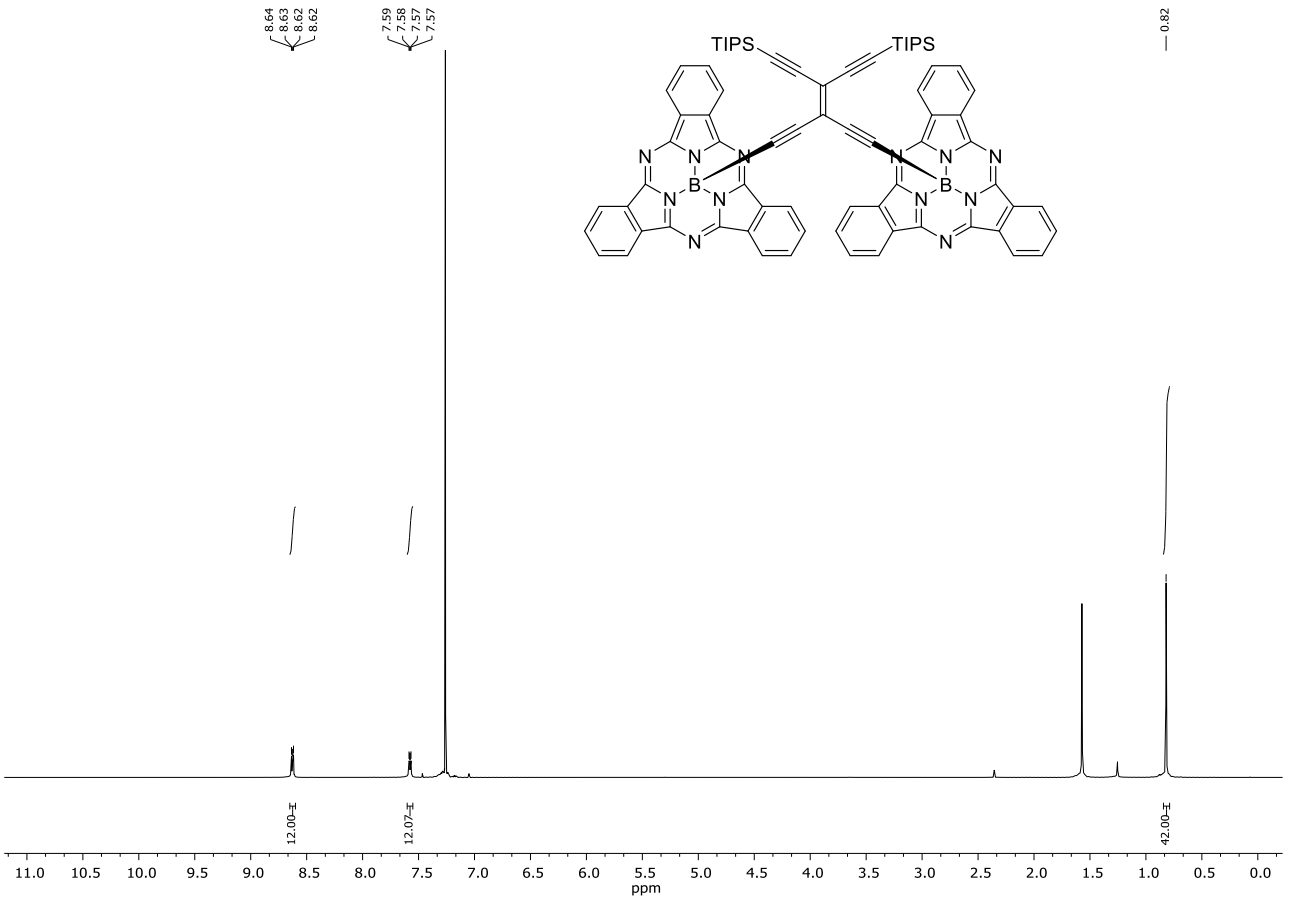


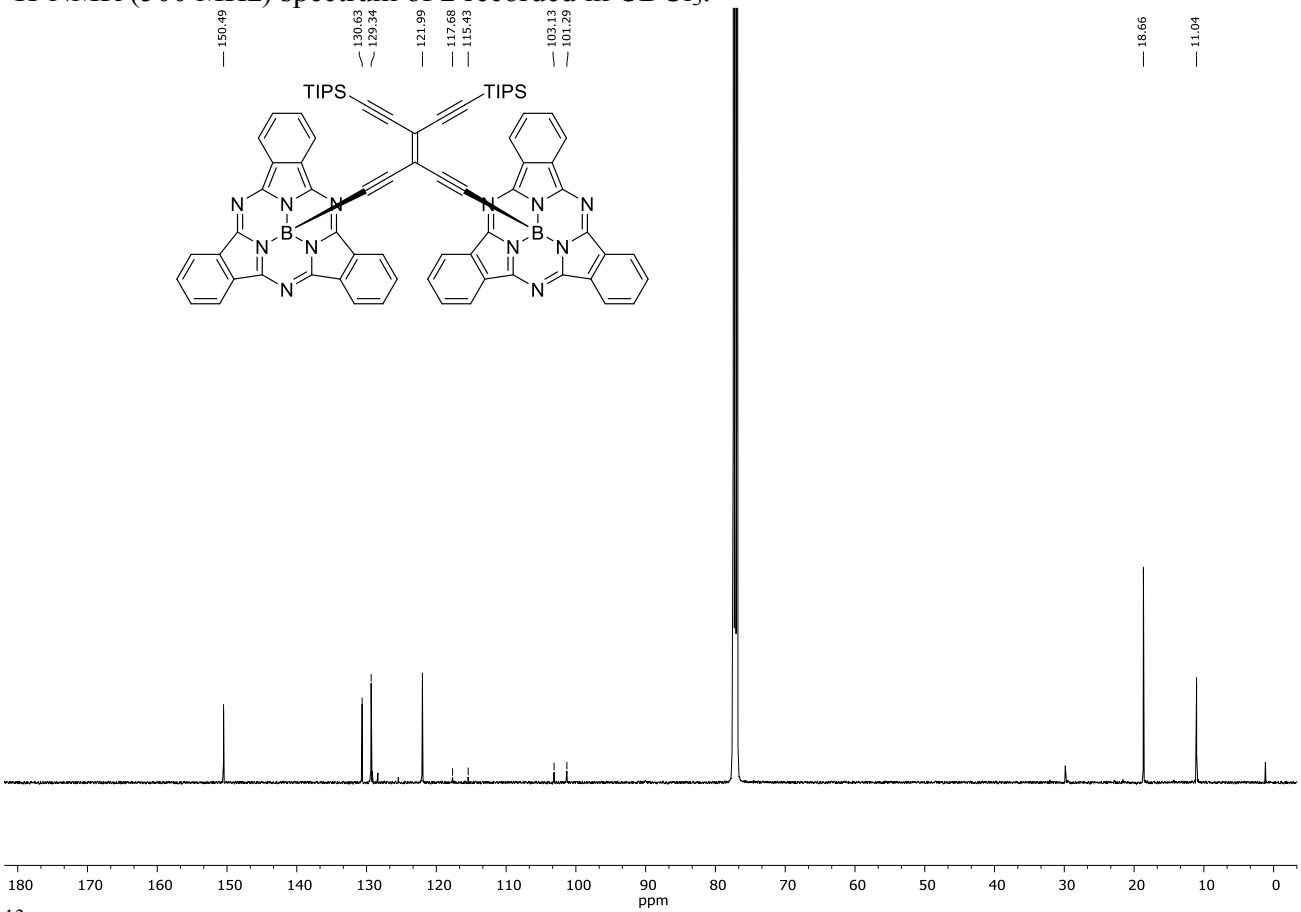
^{1}H-NMR (500 MHz) spectrum of **1,2-Dioctyloxy-4,5-diiodobenzene** recorded in $CDCl_3$.



^{13}C APT NMR (126 MHz) spectrum of **1,2-Dioctyloxy-4,5-diiodobenzene** recorded in $CDCl_3$.



^{1}H-NMR (500 MHz) spectrum of **2** recorded in $CDCl_3$.



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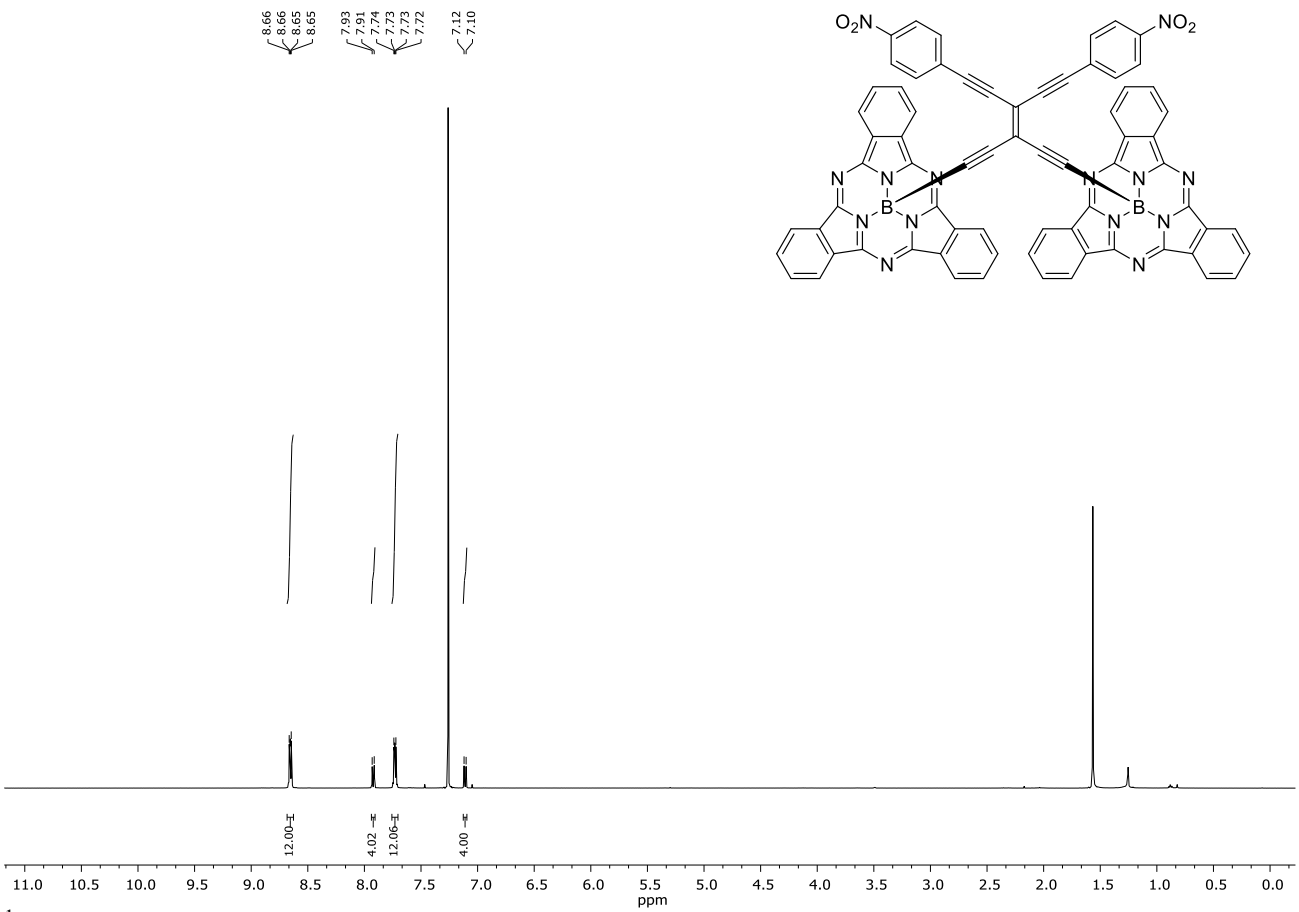
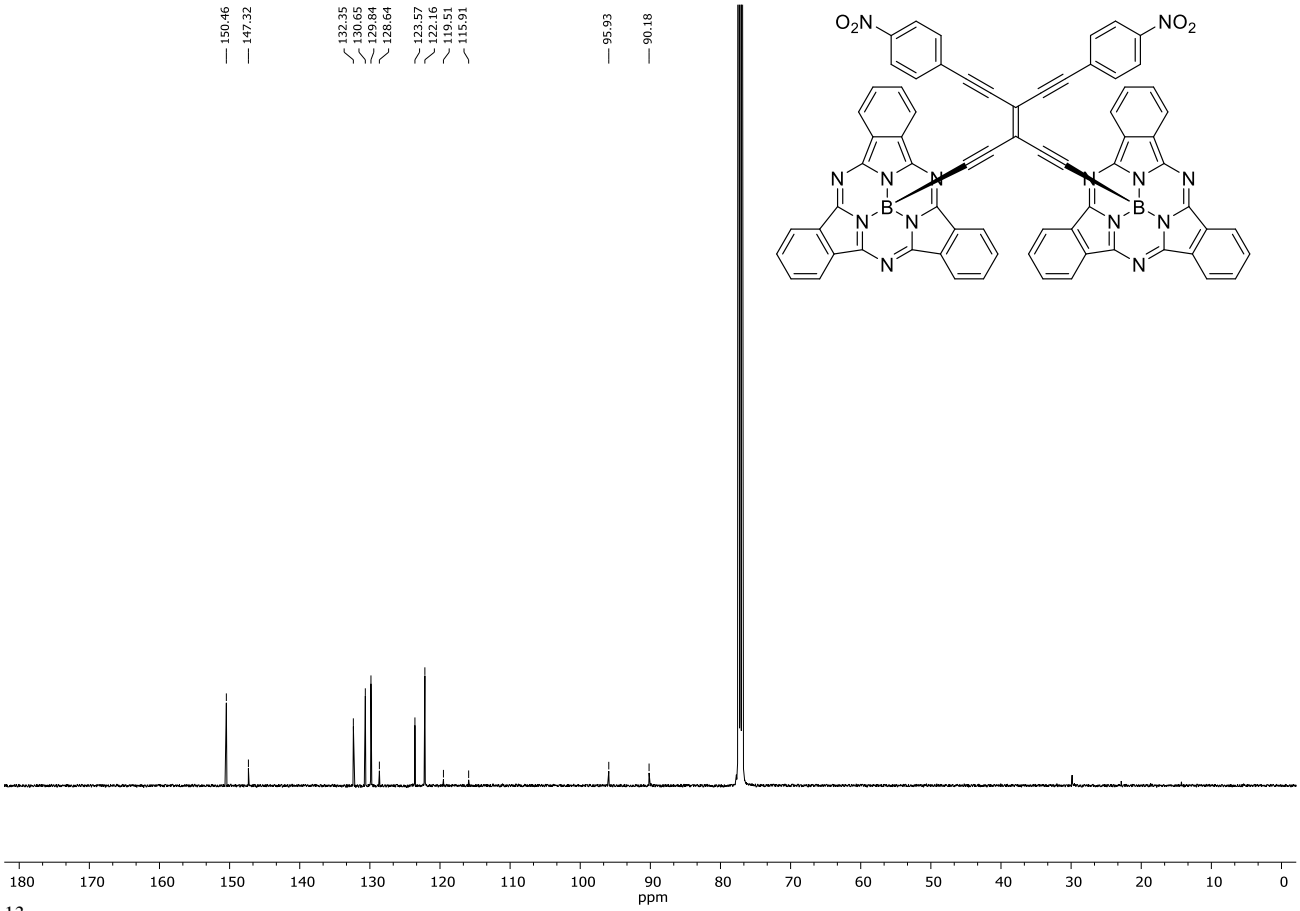
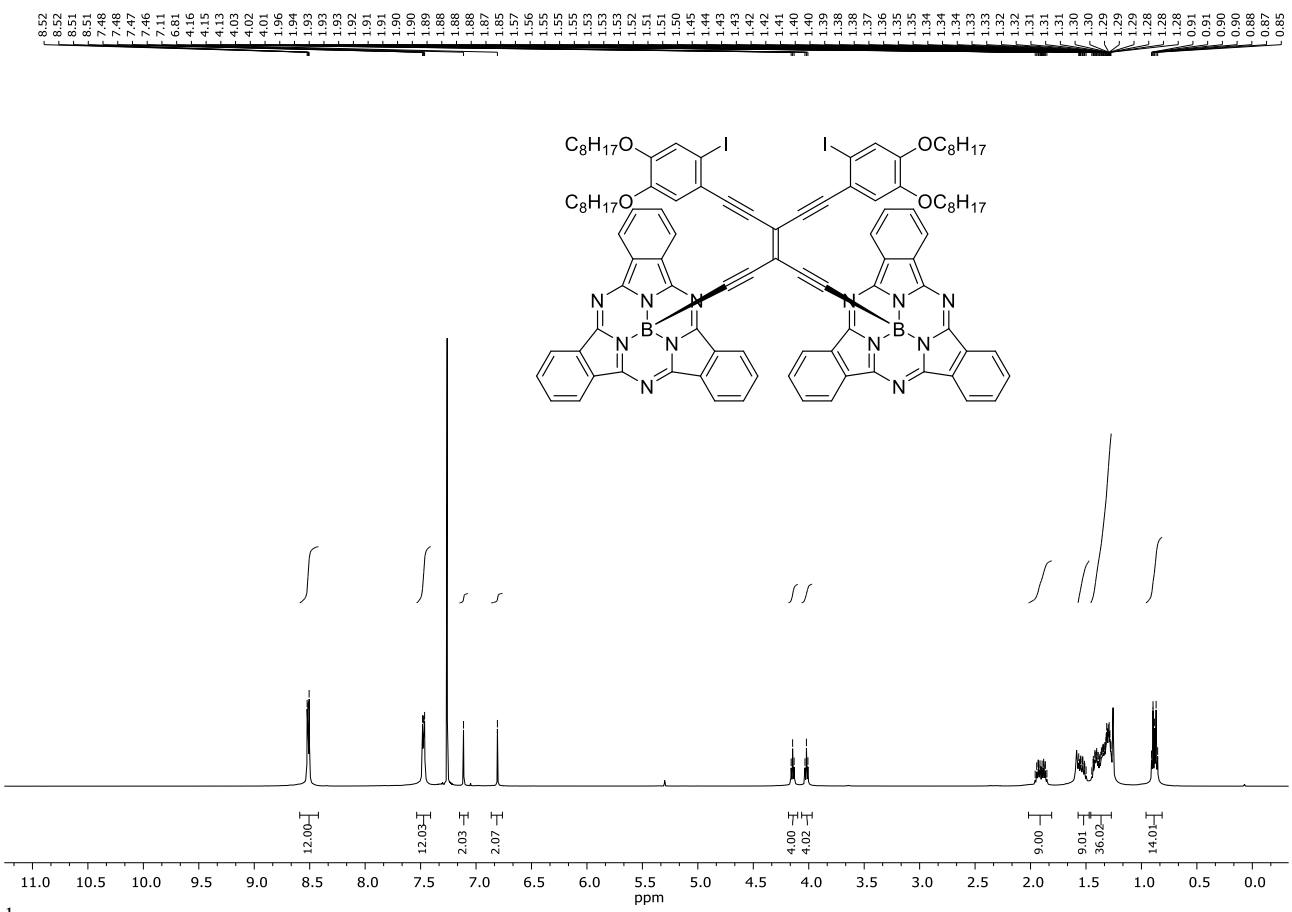


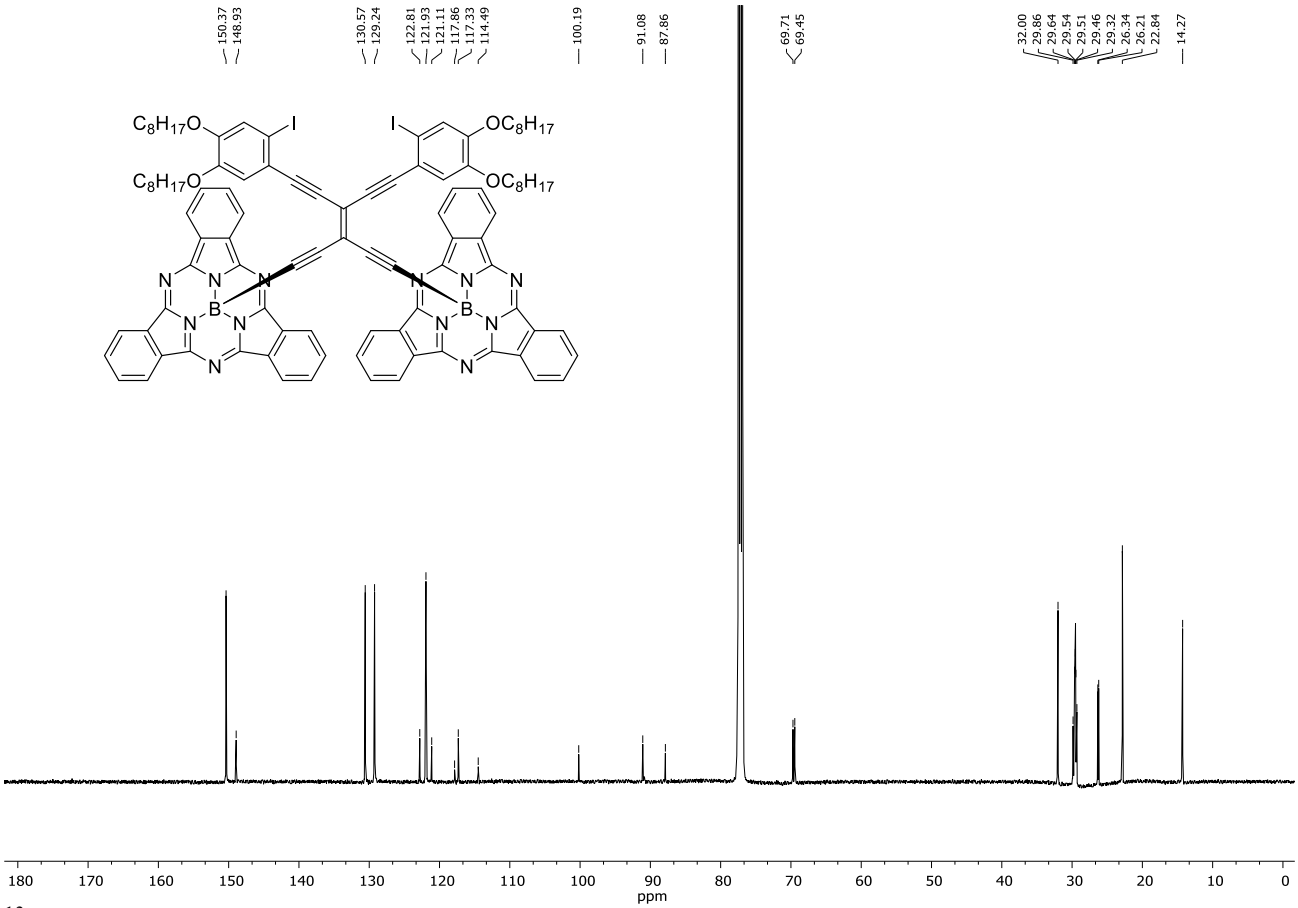
^{1}H-NMR (500 MHz) spectrum of **3** recorded in $CDCl_3$.



^{13}C-NMR (126 MHz) spectrum of **3** recorded in $CDCl_3$.



^{1}H-NMR (500 MHz) spectrum of **4** recorded in $CDCl_3$.



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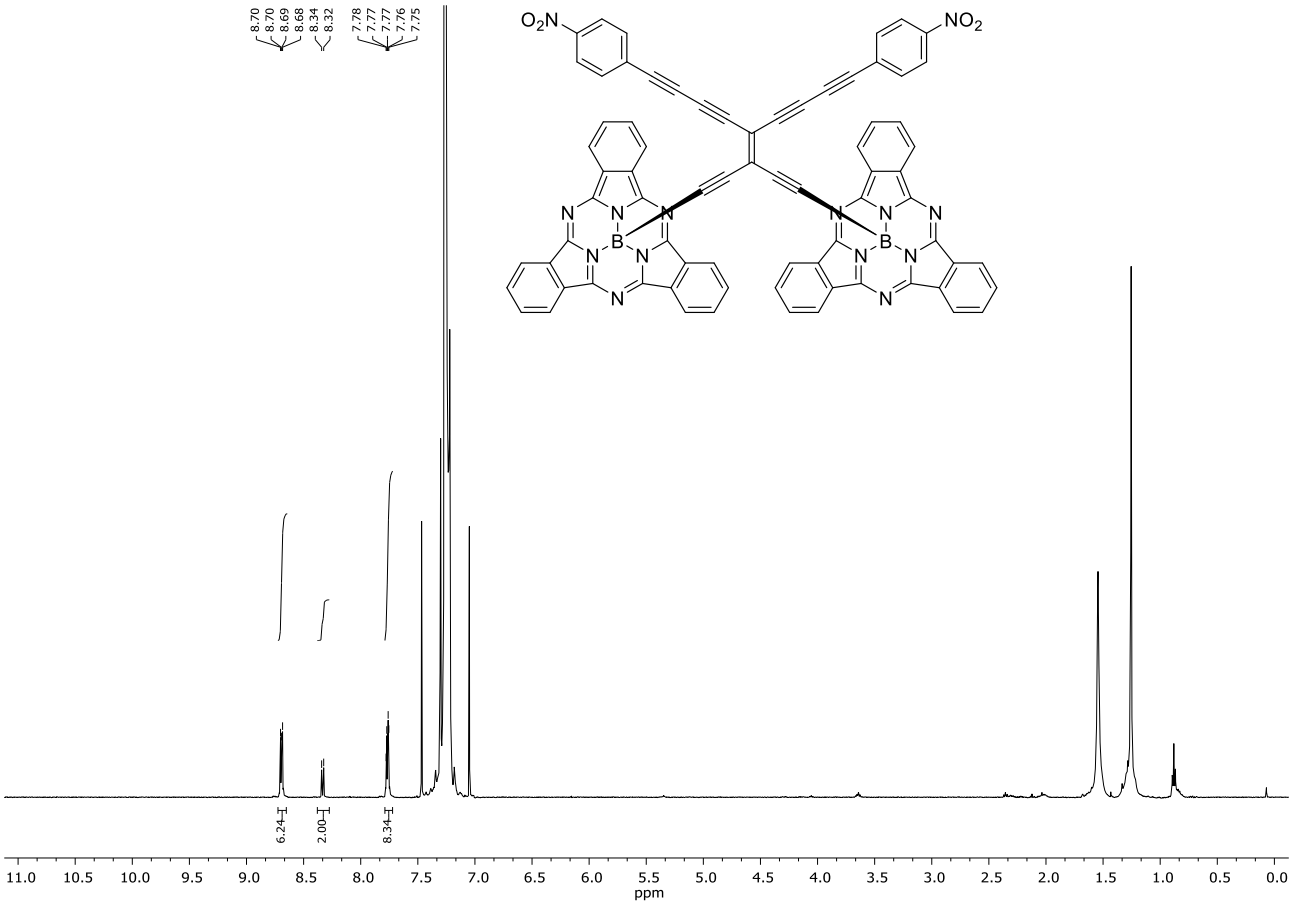

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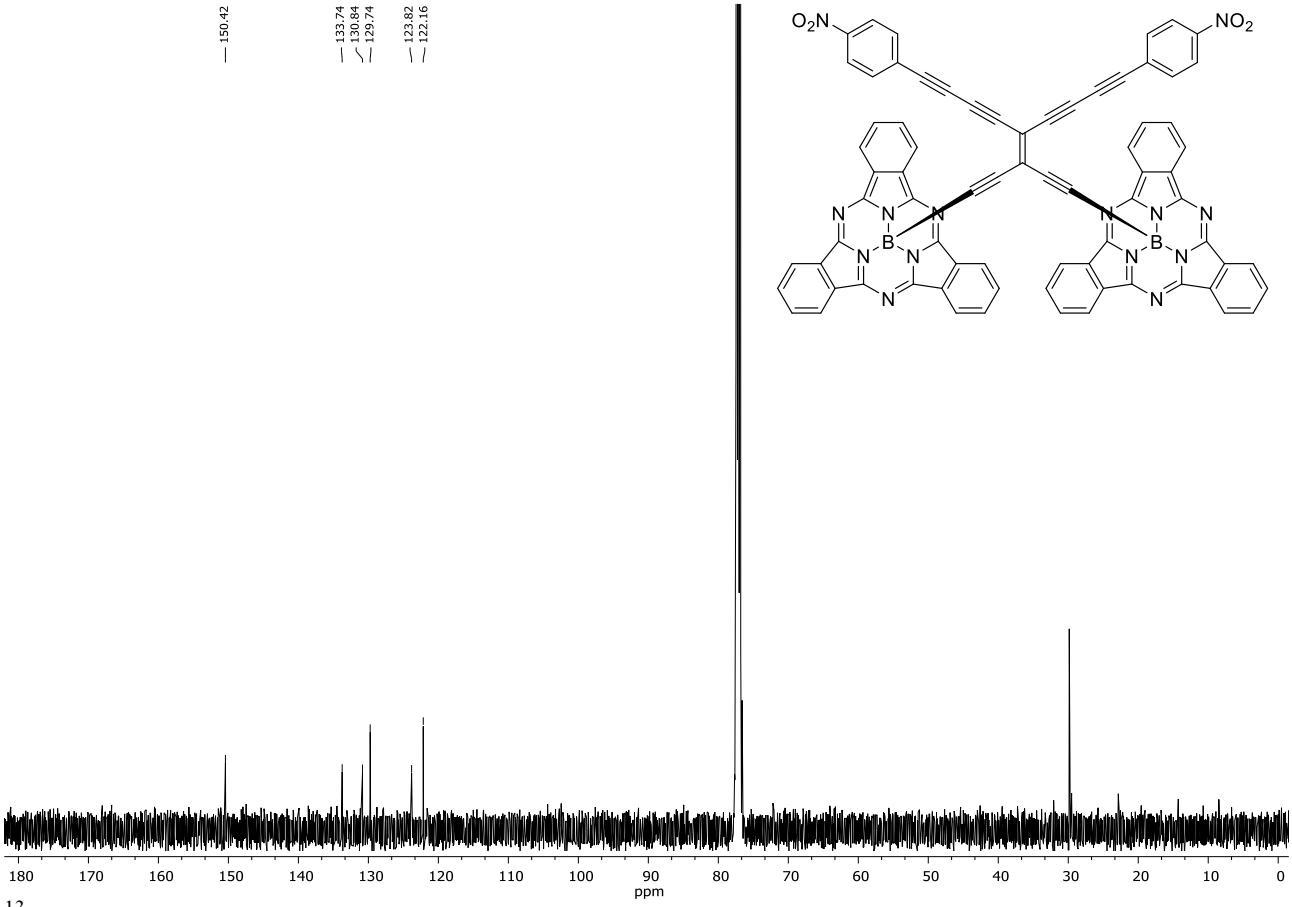

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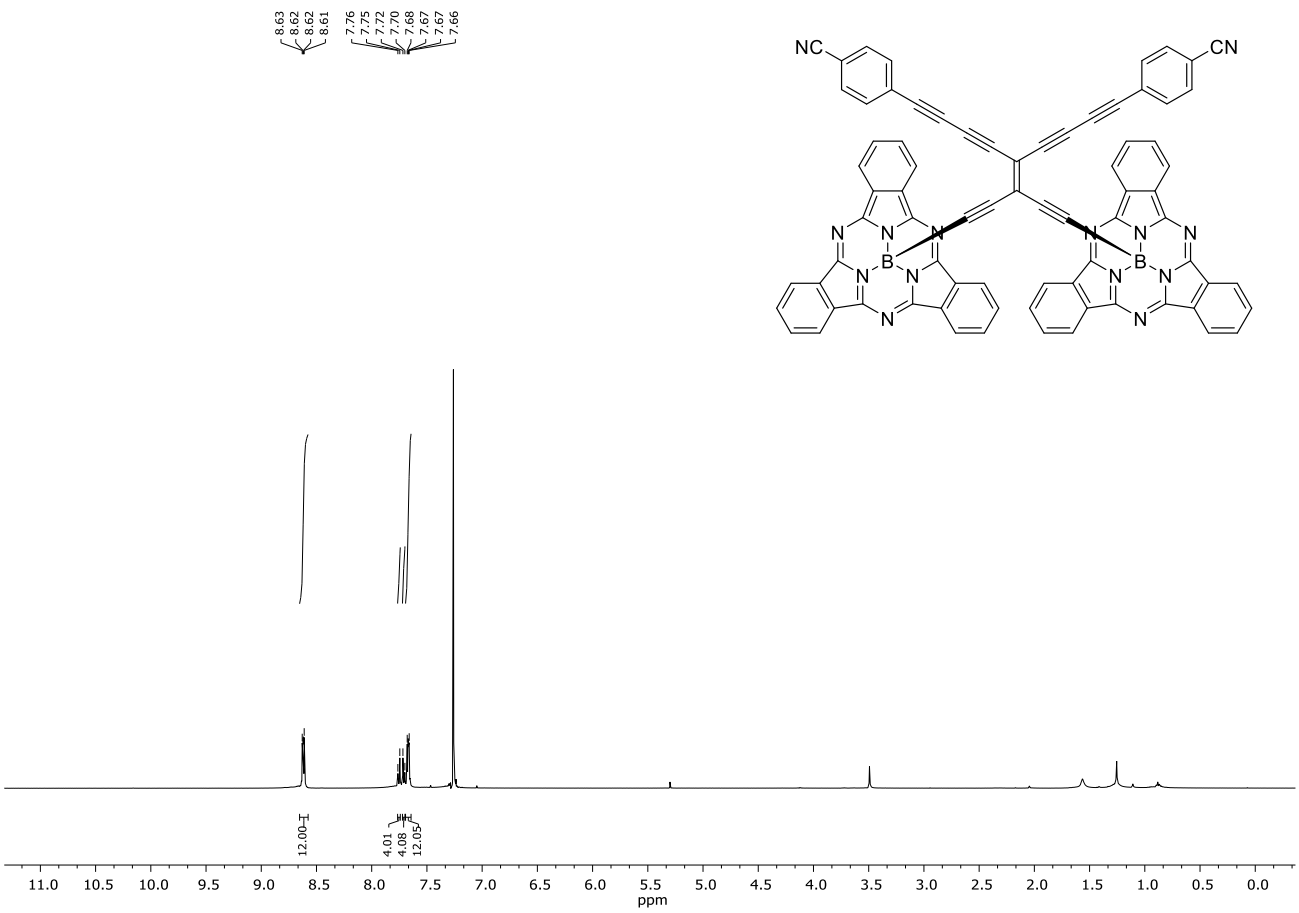
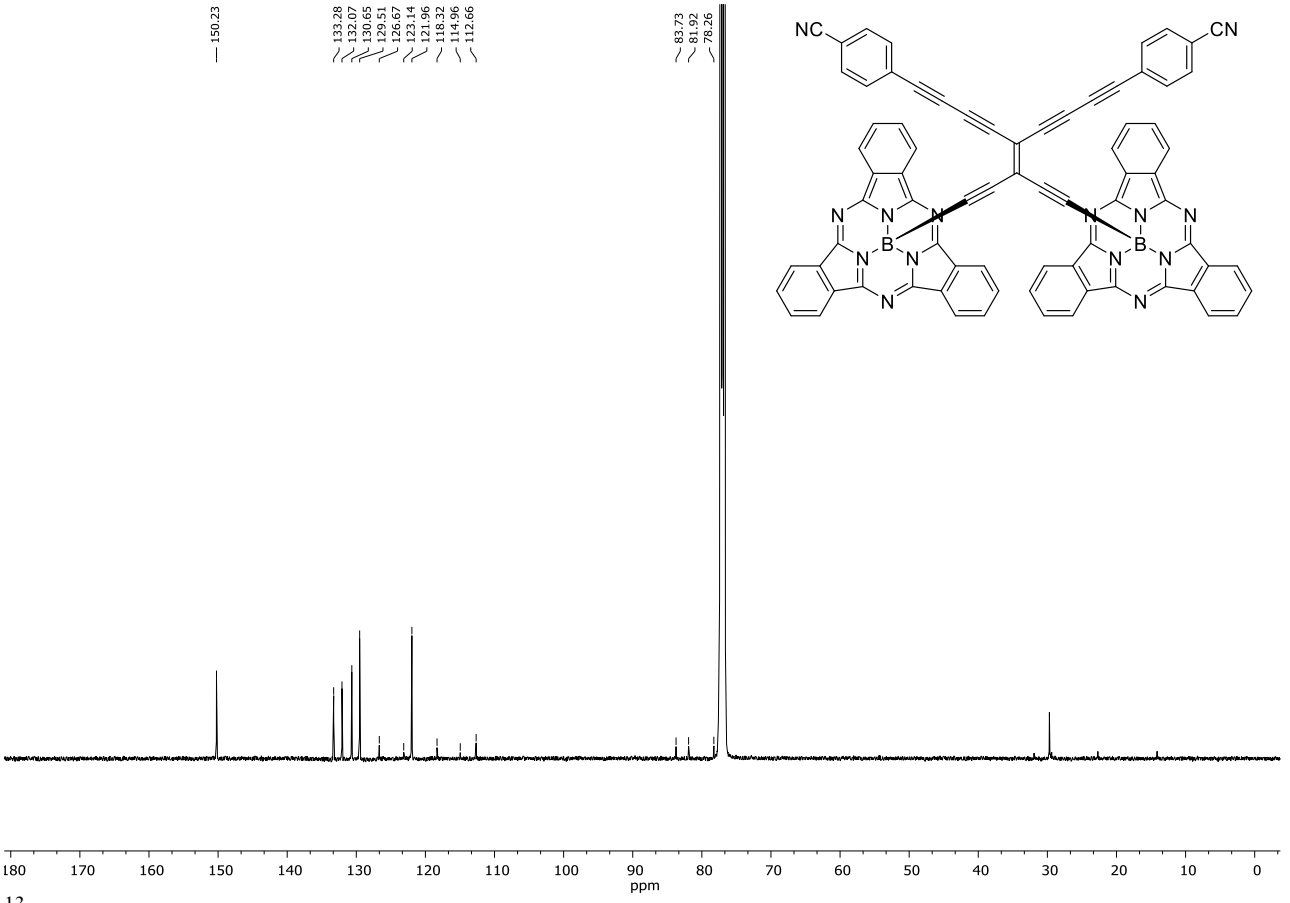


^{1}H-NMR (500 MHz) spectrum of **6** recorded in $CDCl_3$.



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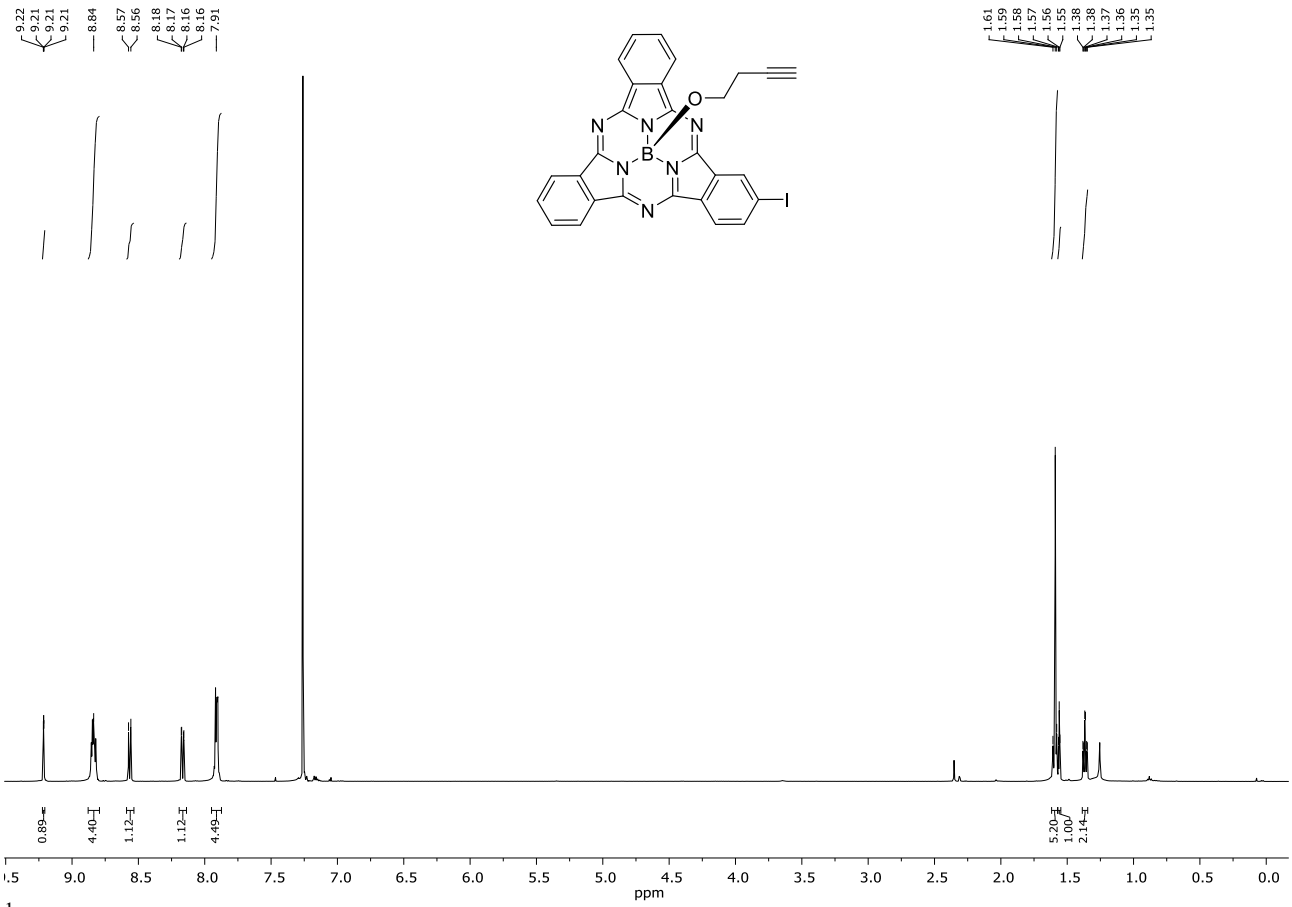
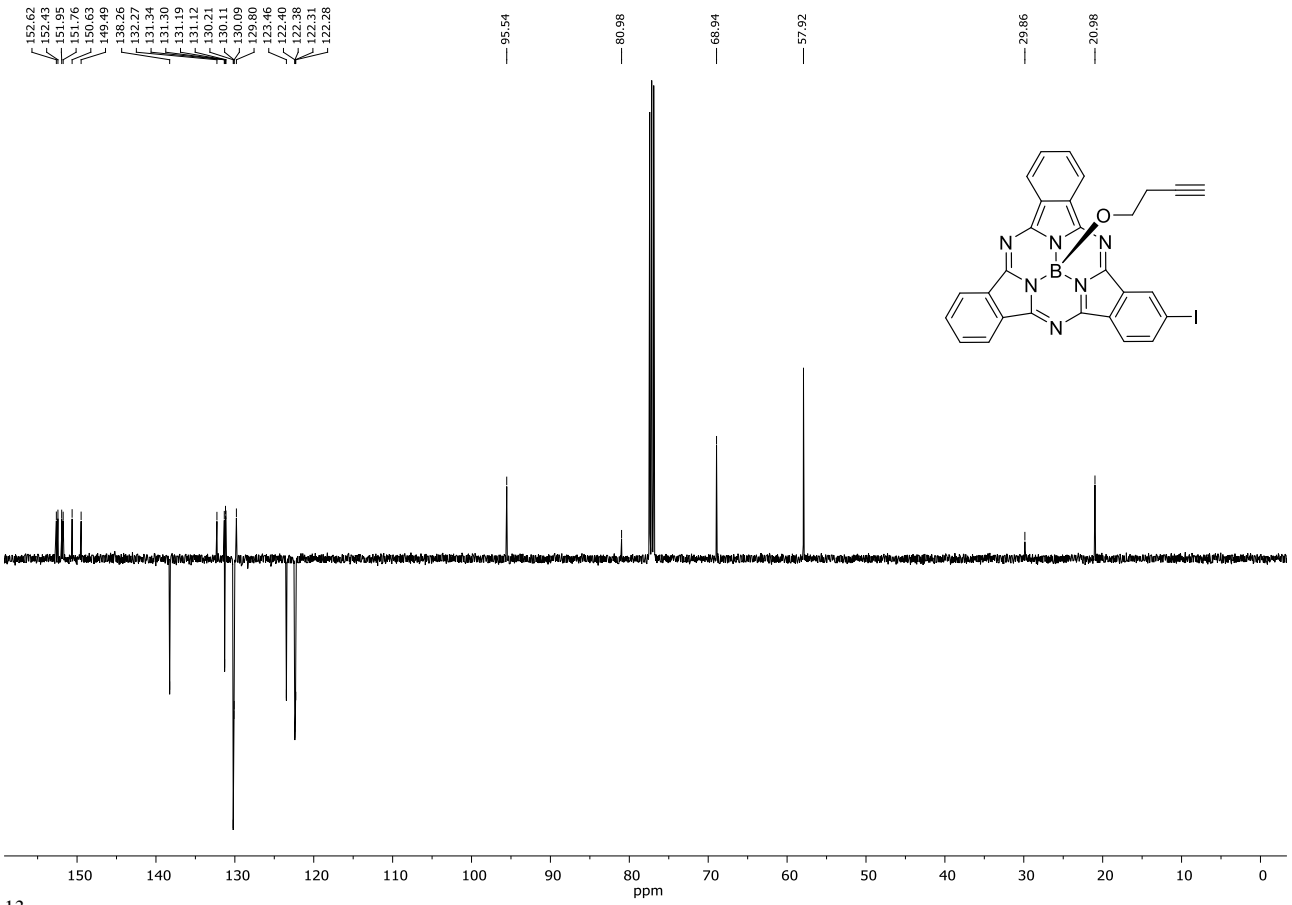
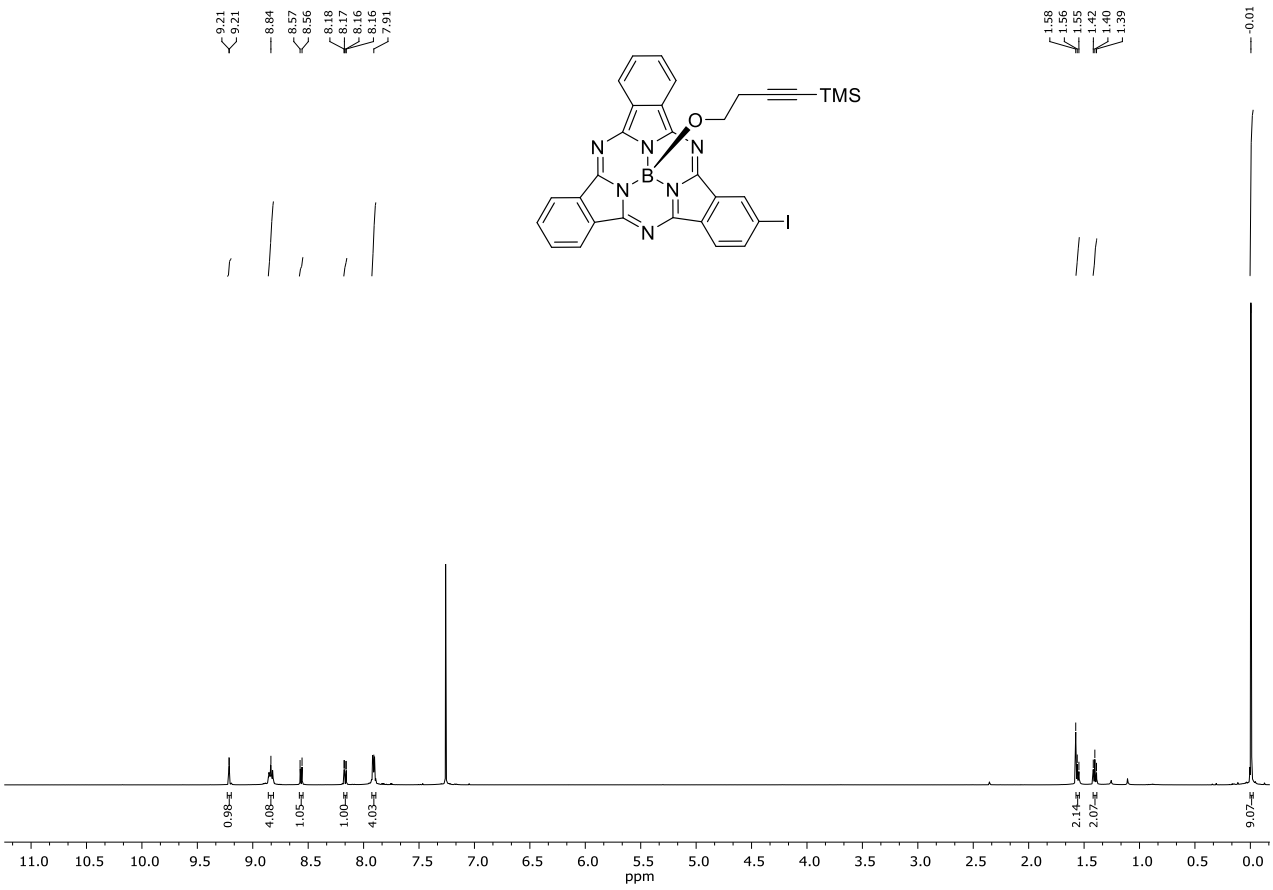


^{1}H-NMR (500 MHz) spectrum of **9** recorded in $CDCl_3$.



^{13}C APT NMR (126 MHz) spectrum of **9** recorded in $CDCl_3$.



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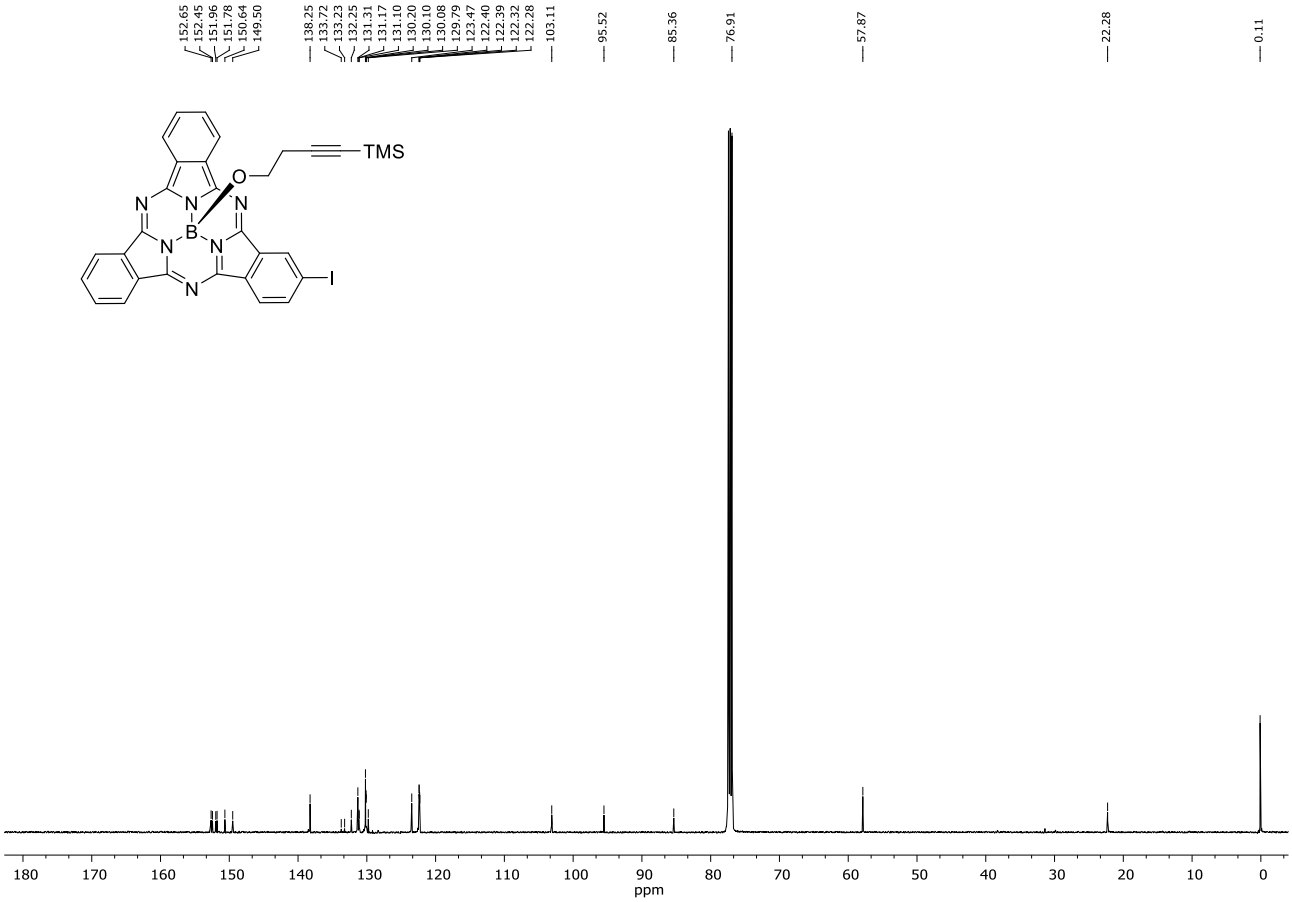

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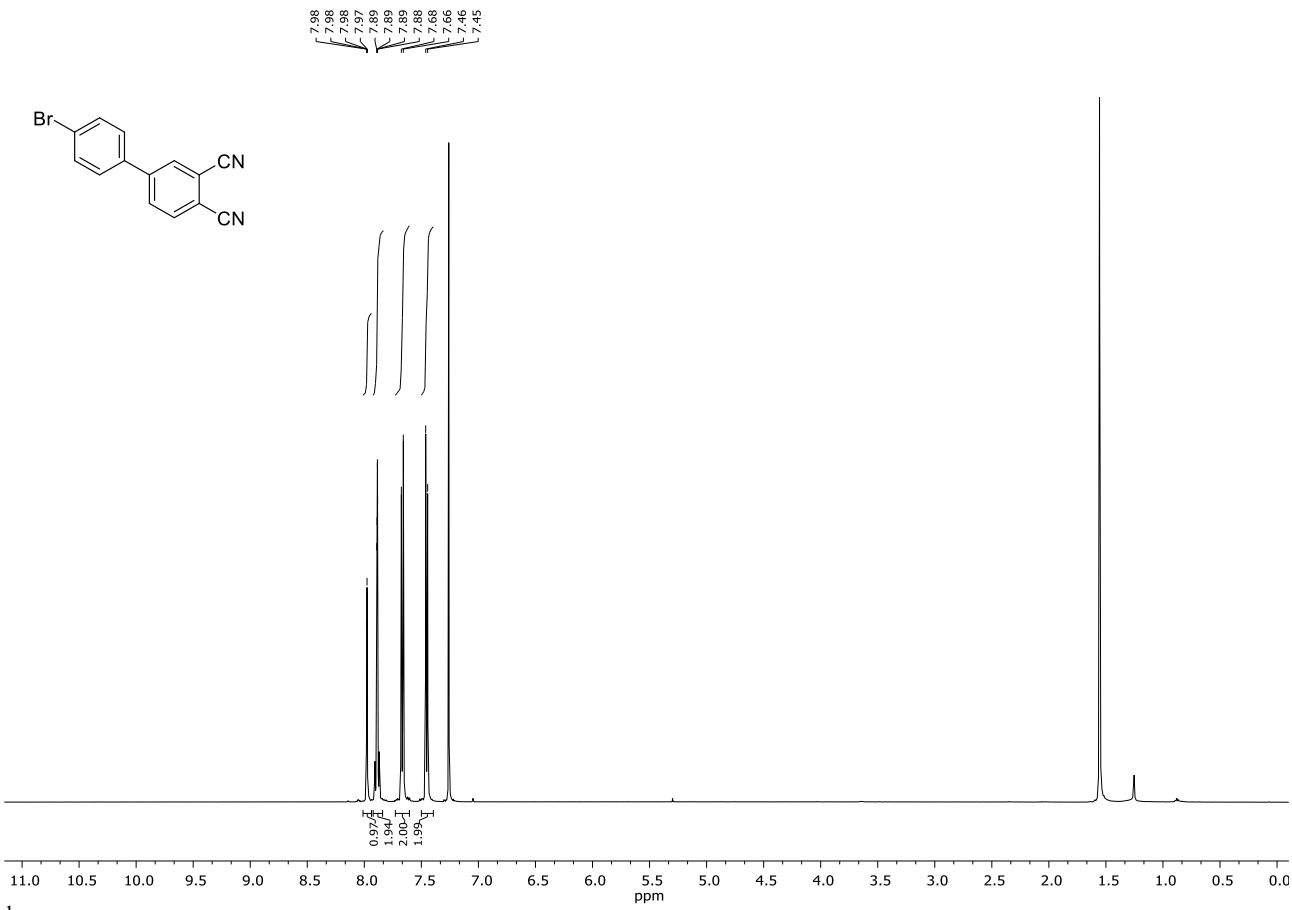
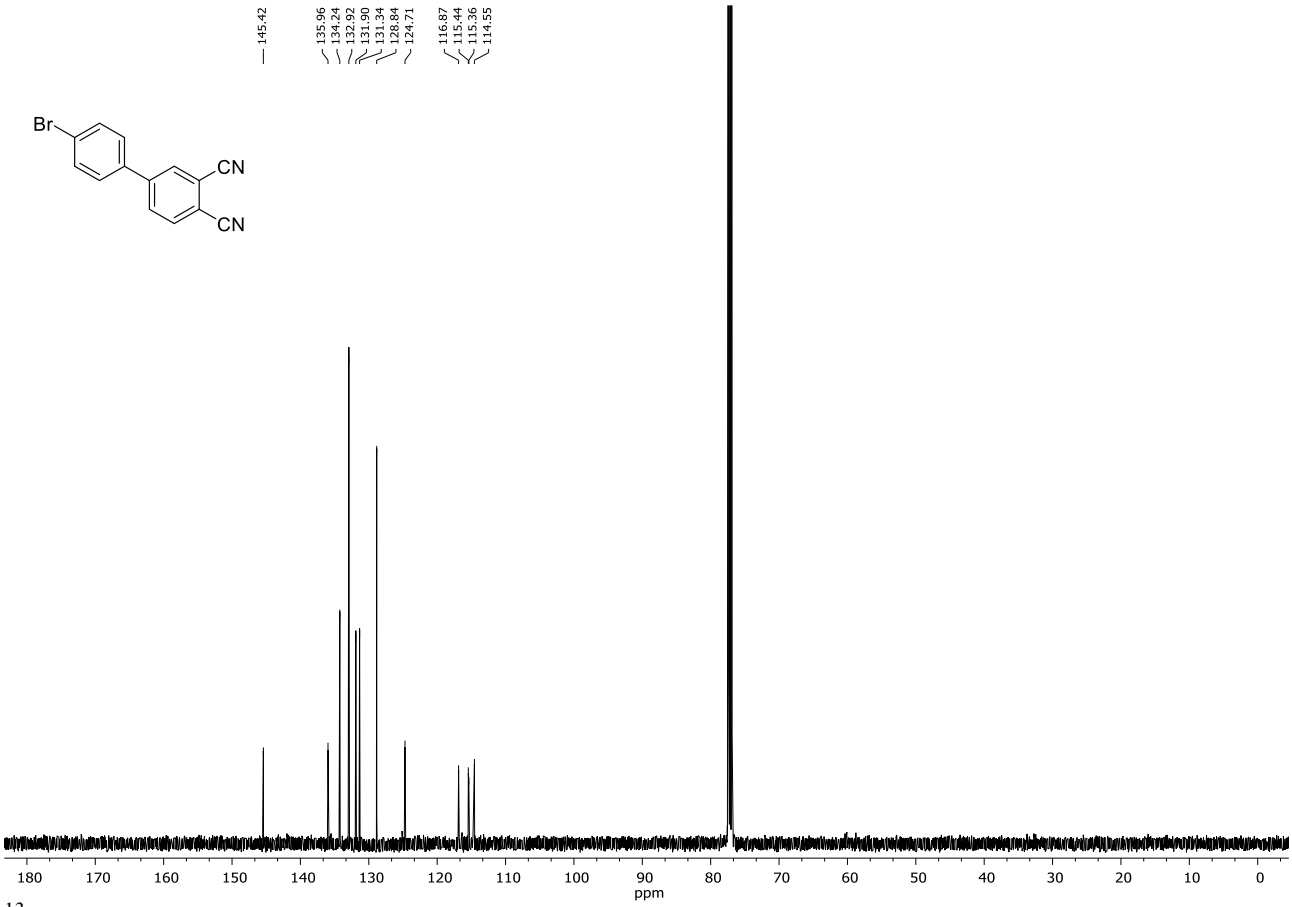


^{1}H-NMR (500 MHz) spectrum of **8** recorded in $CDCl_3$.



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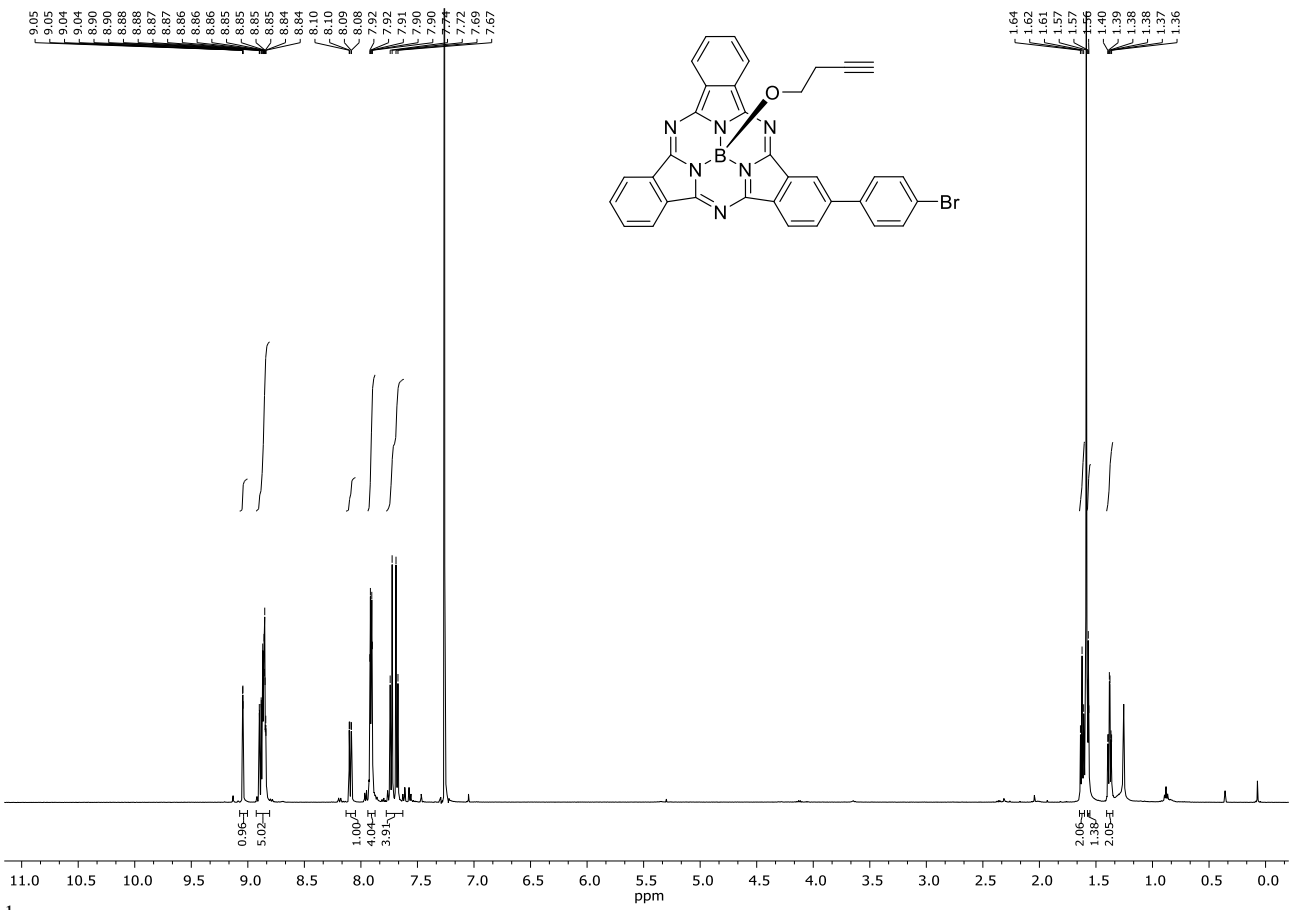

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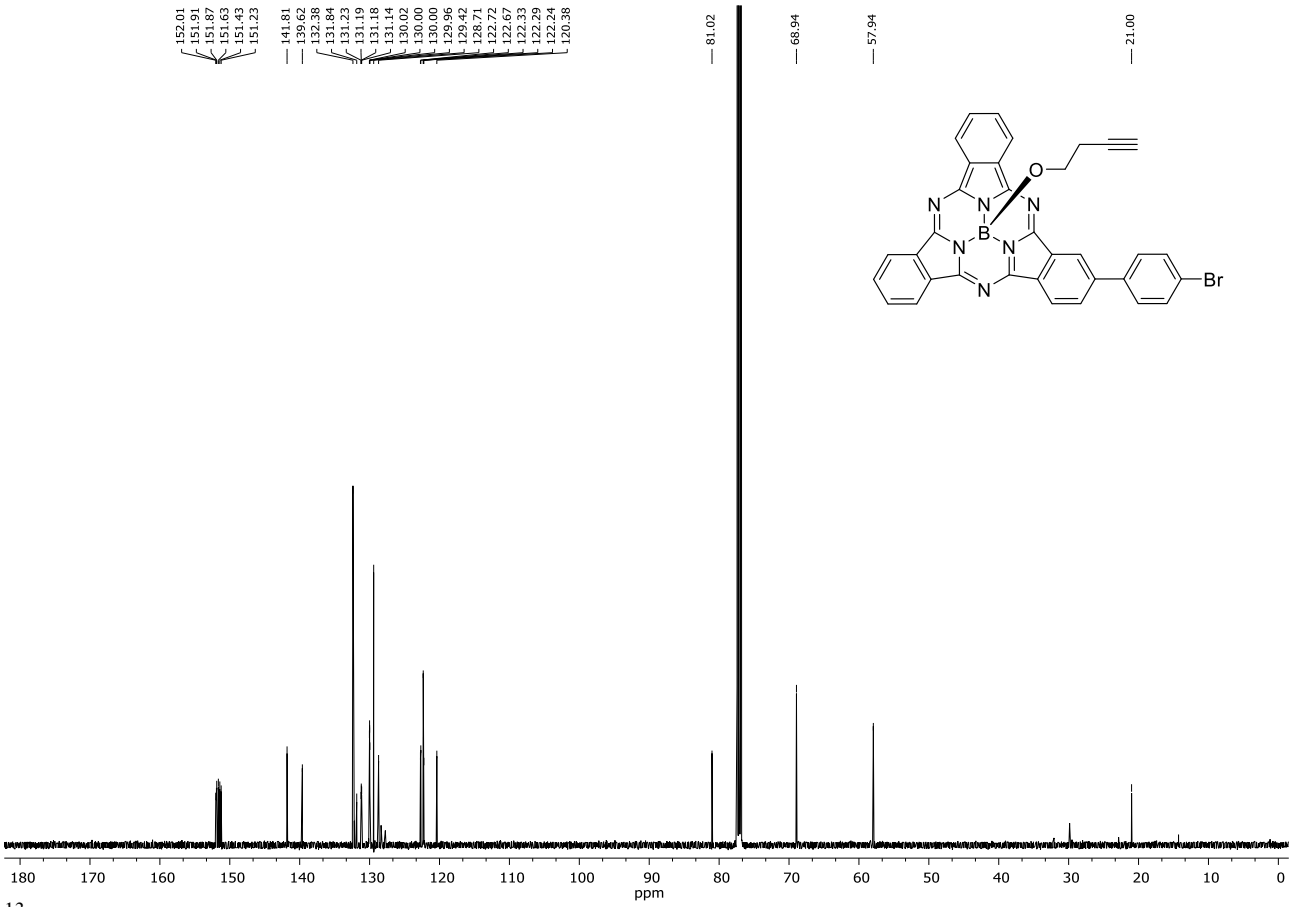
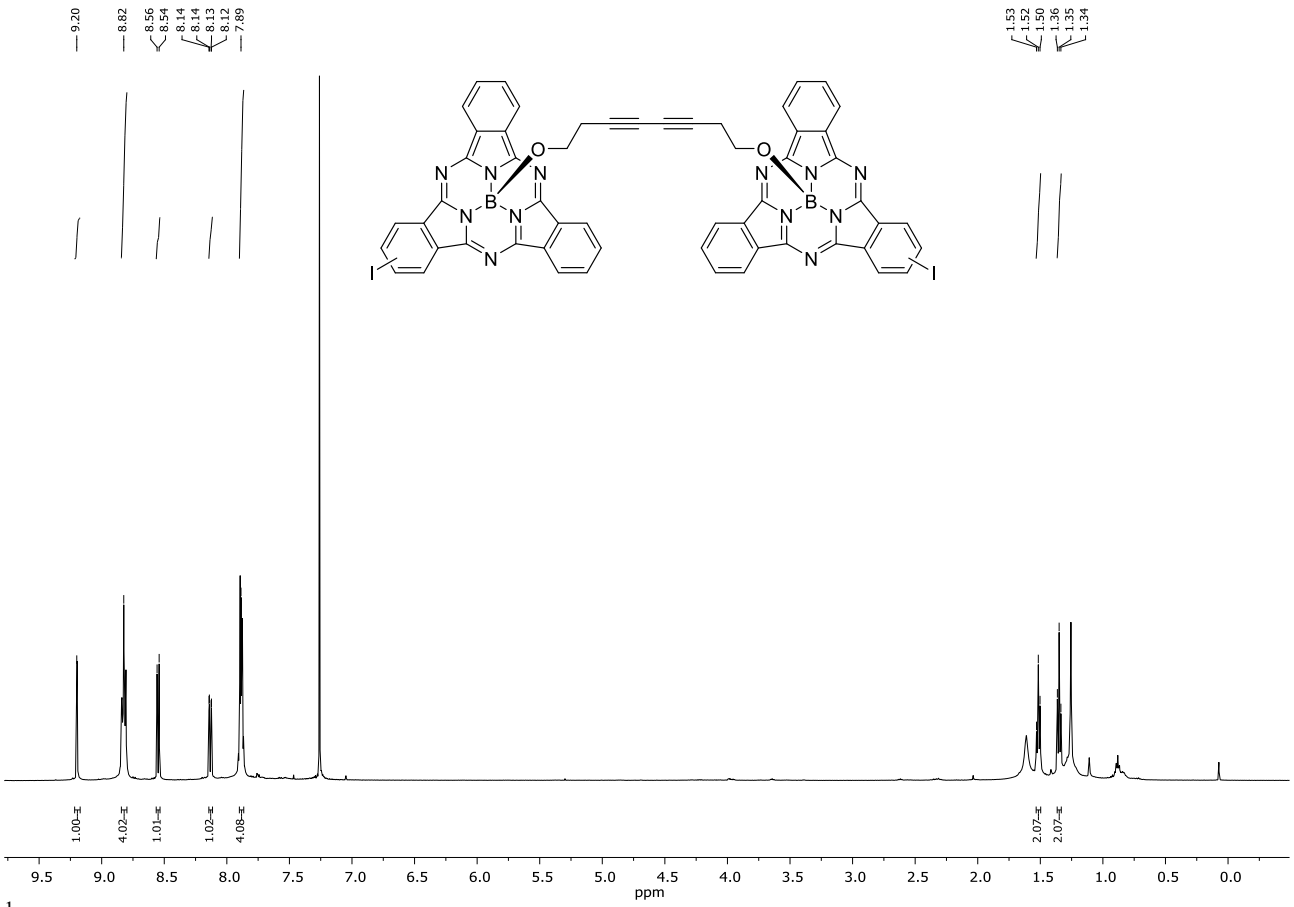
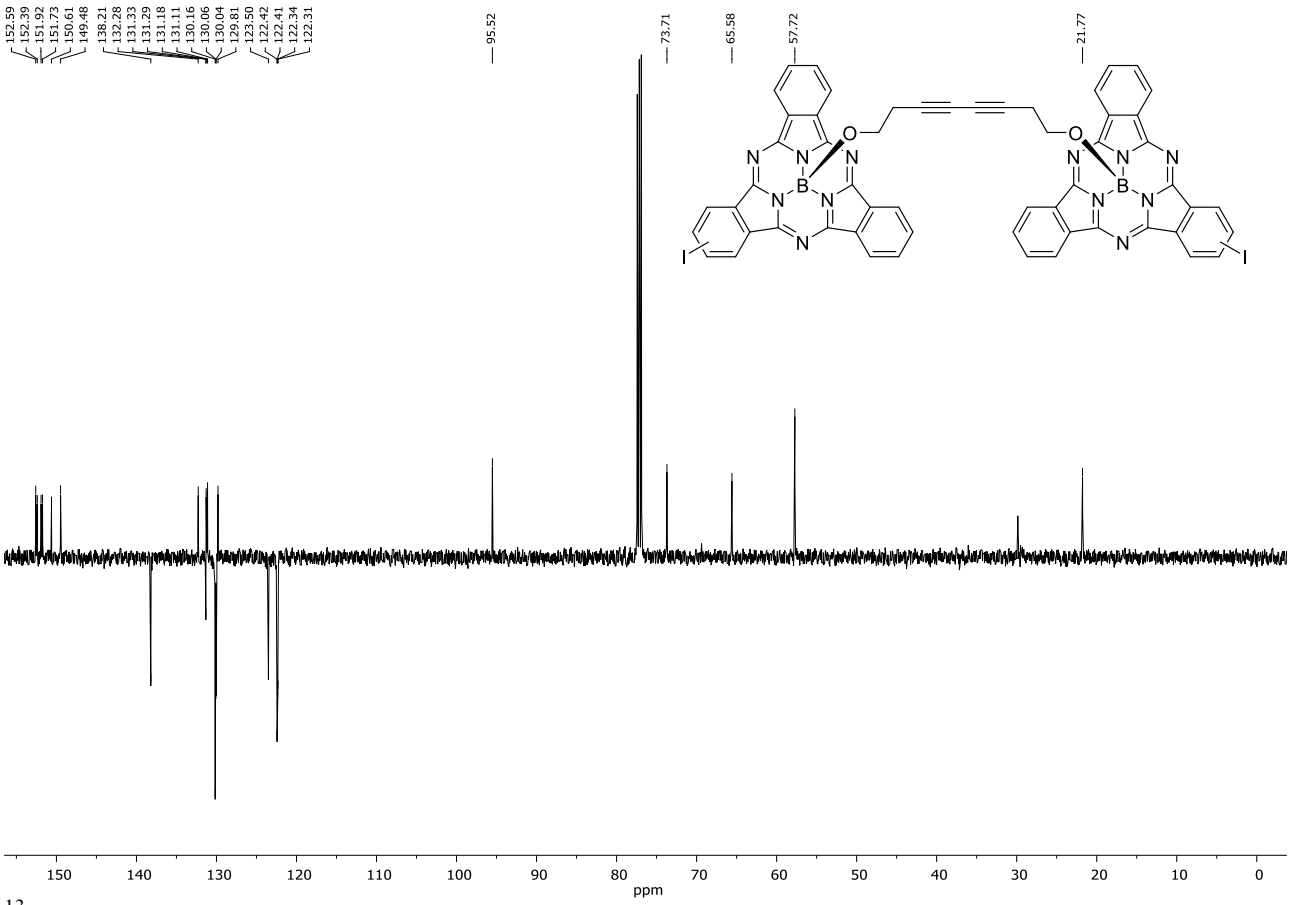


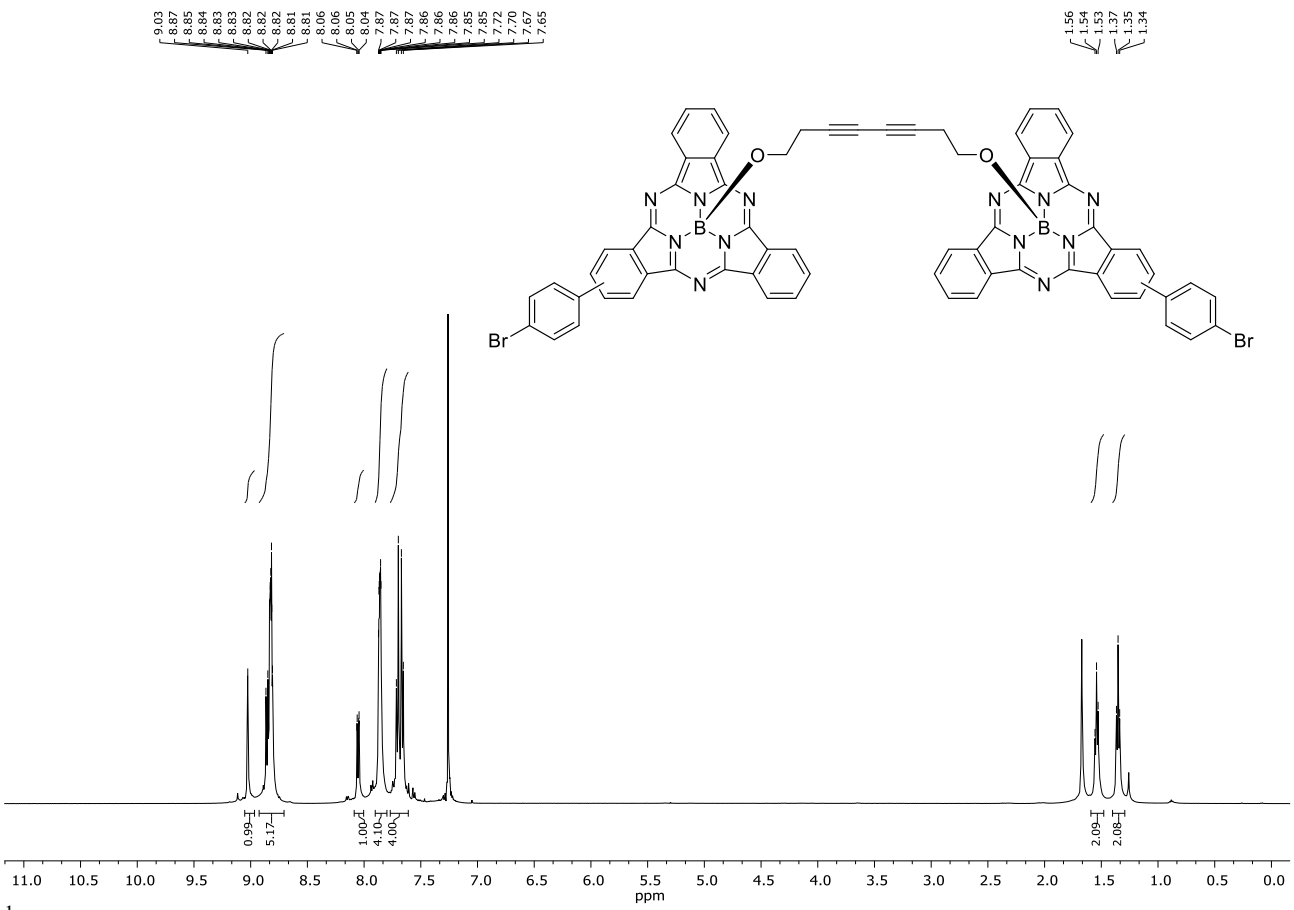
^{13}C-NMR (126 MHz) spectrum of **11** recorded in $CDCl_3$.



^{1}H-NMR (500 MHz) spectrum of **12** recorded in $CDCl_3$.



^{13}C APT NMR (126 MHz) spectrum of **12** recorded in $CDCl_3$.



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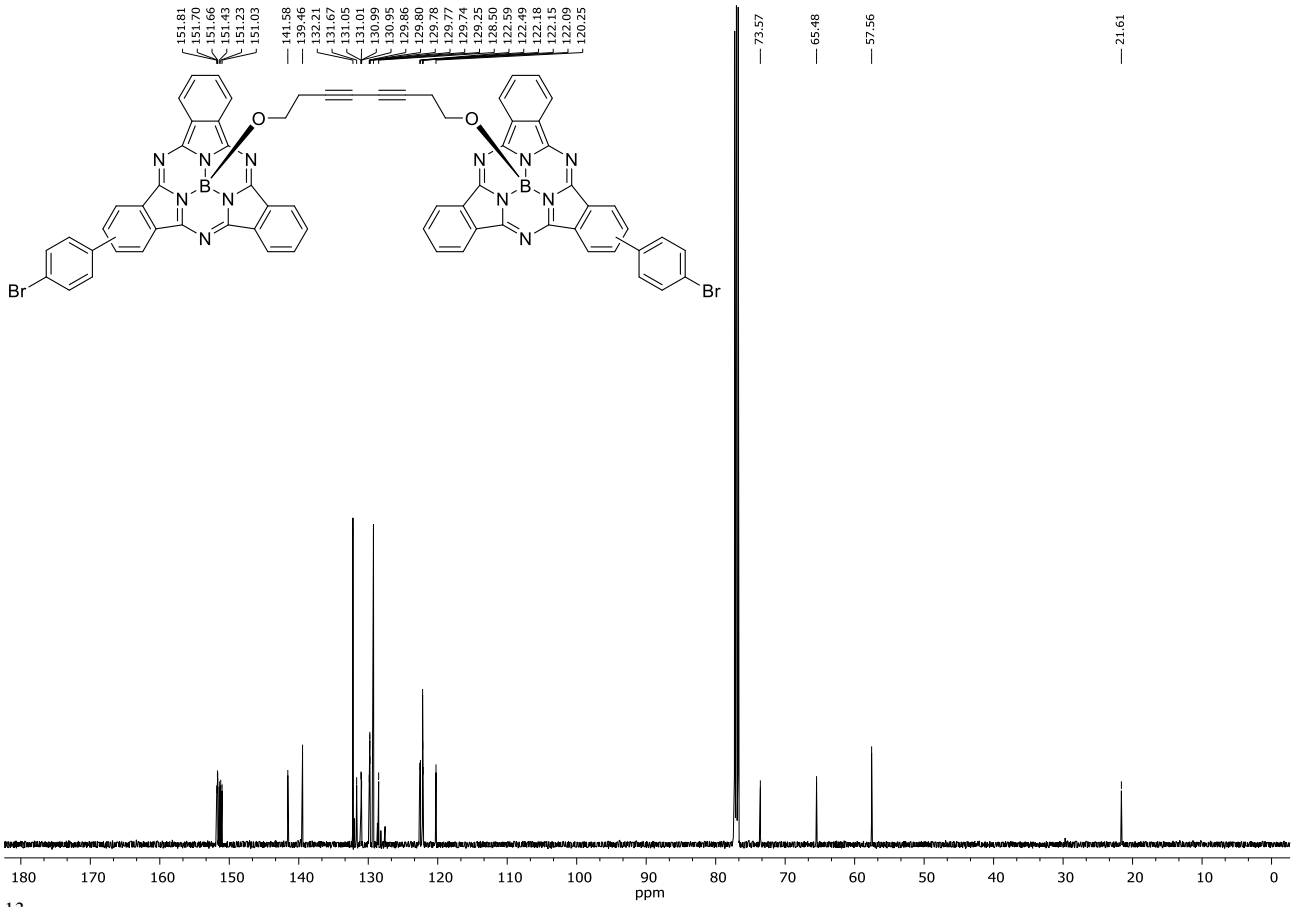
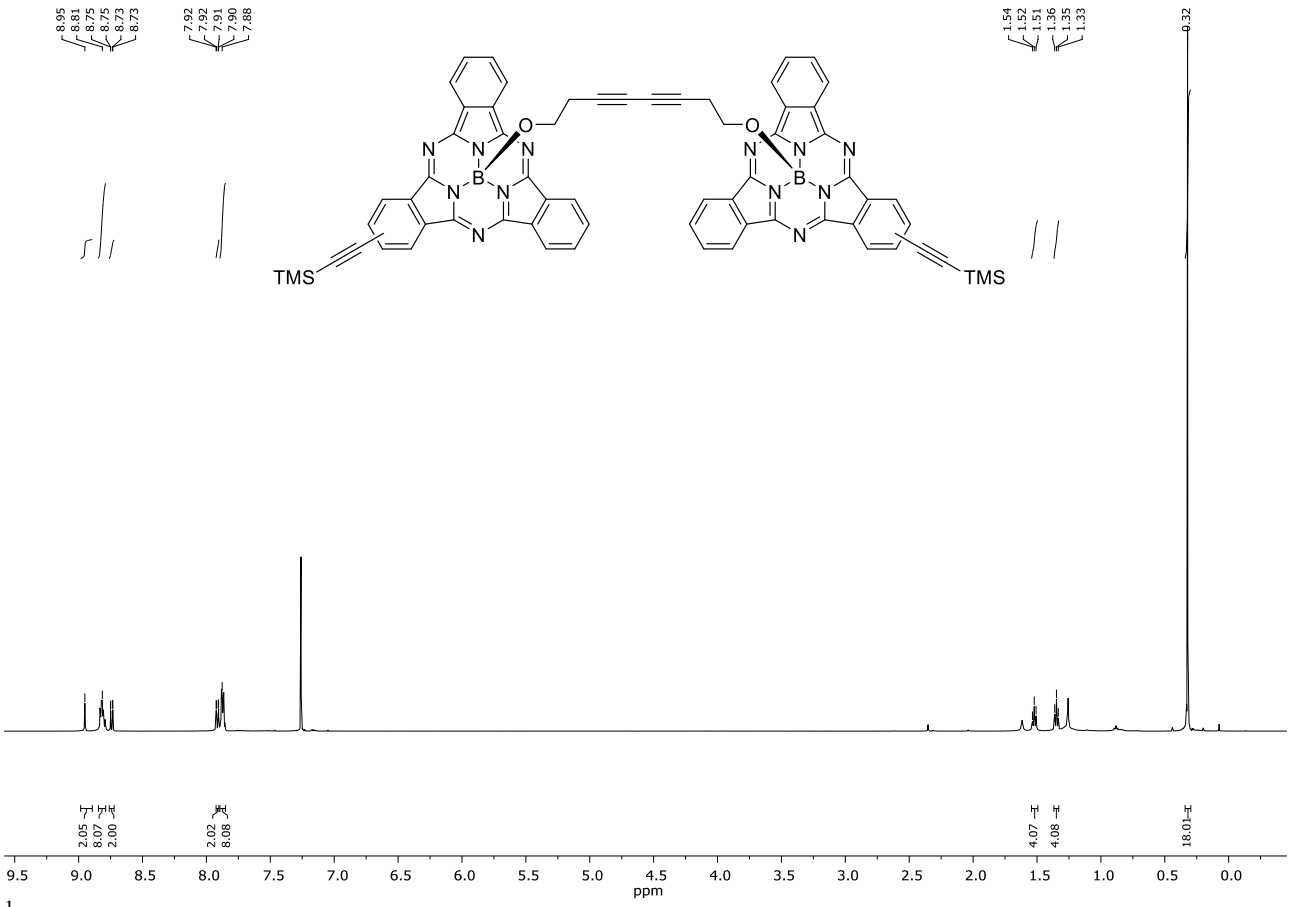
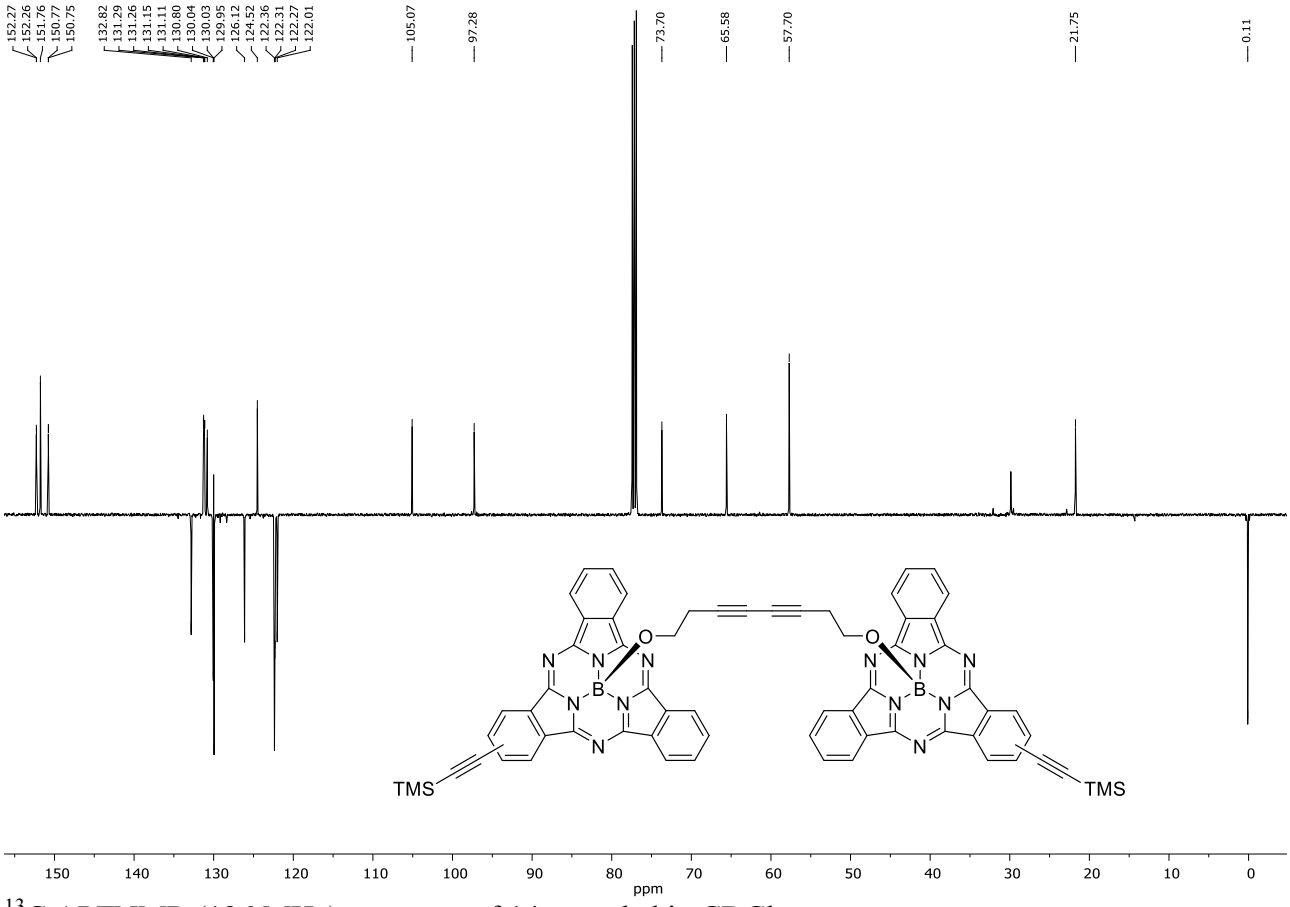


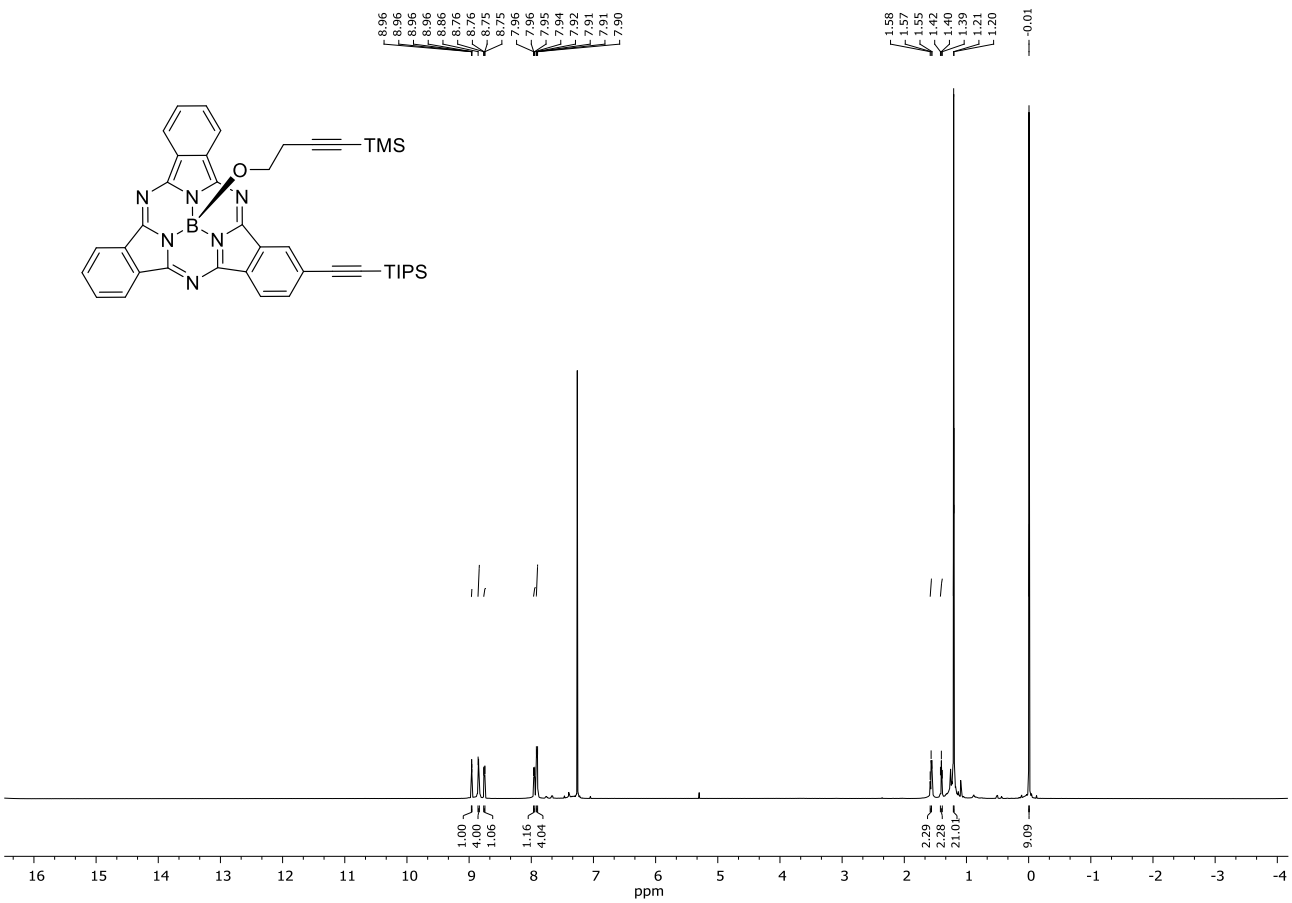
^{13}C-NMR (126 MHz) spectrum of **13** recorded in $CDCl_3$.



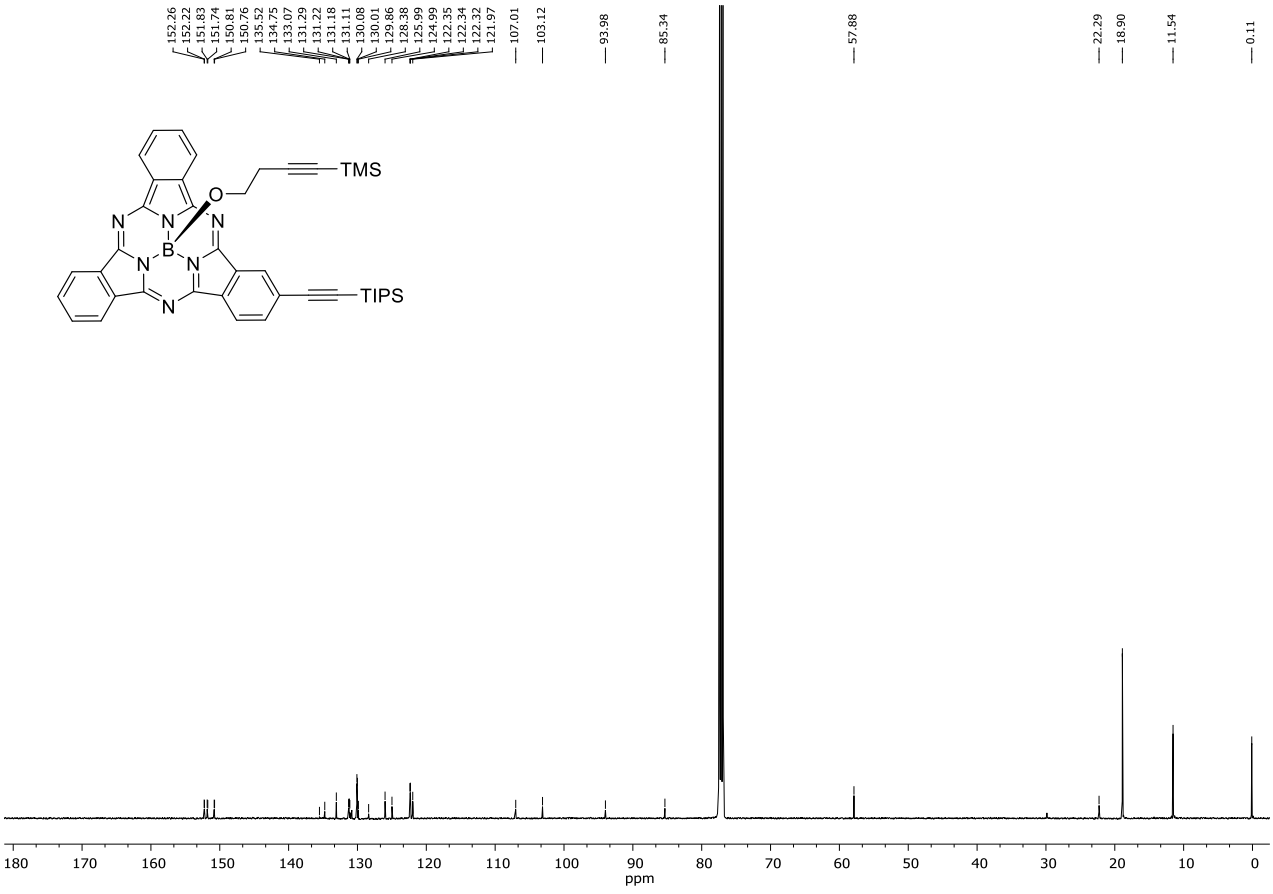
^{1}H-NMR (500 MHz) spectrum of **14** recorded in $CDCl_3$.



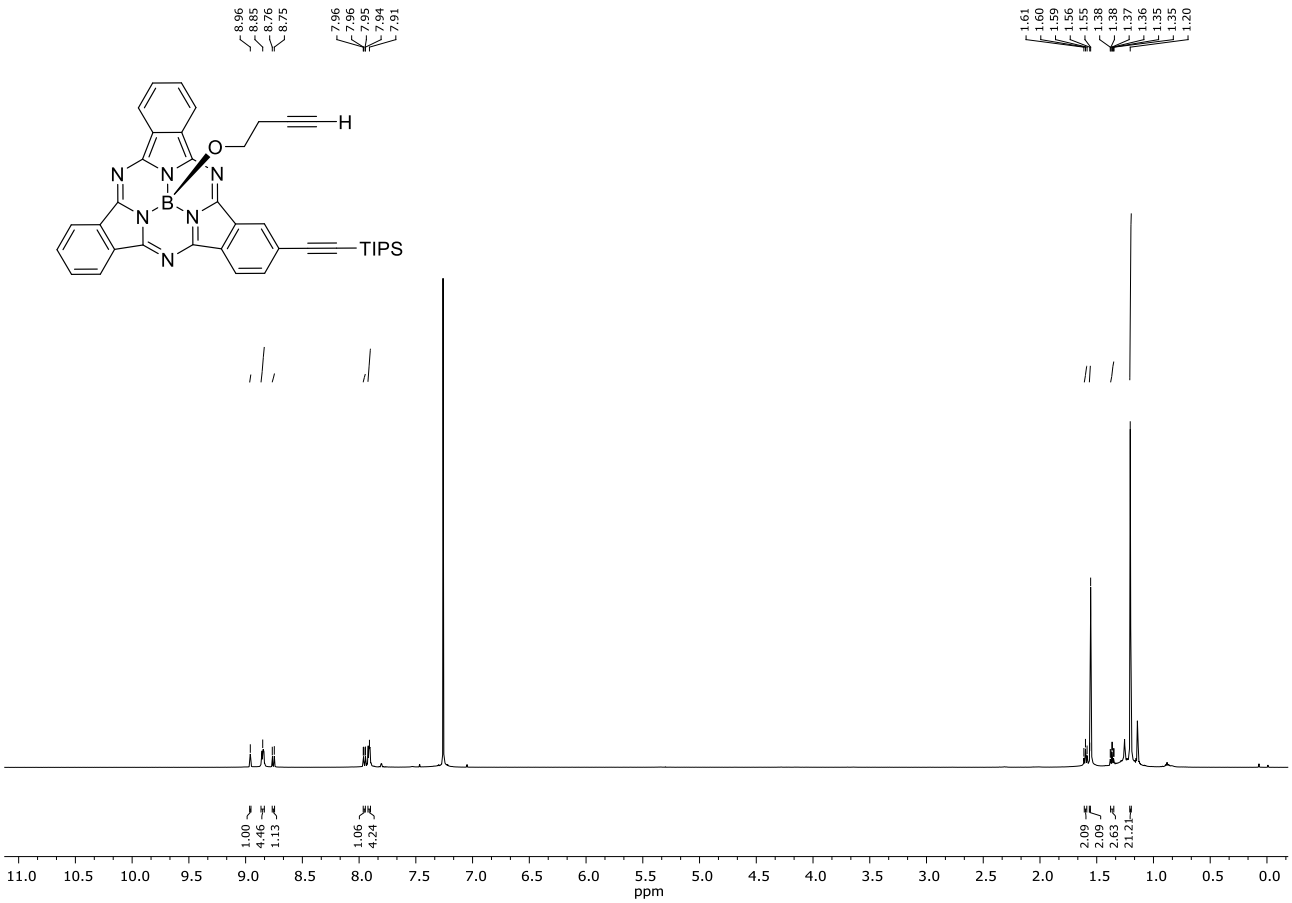
^{13}C APTNMR (126 MHz) spectrum of **14** recorded in $CDCl_3$.



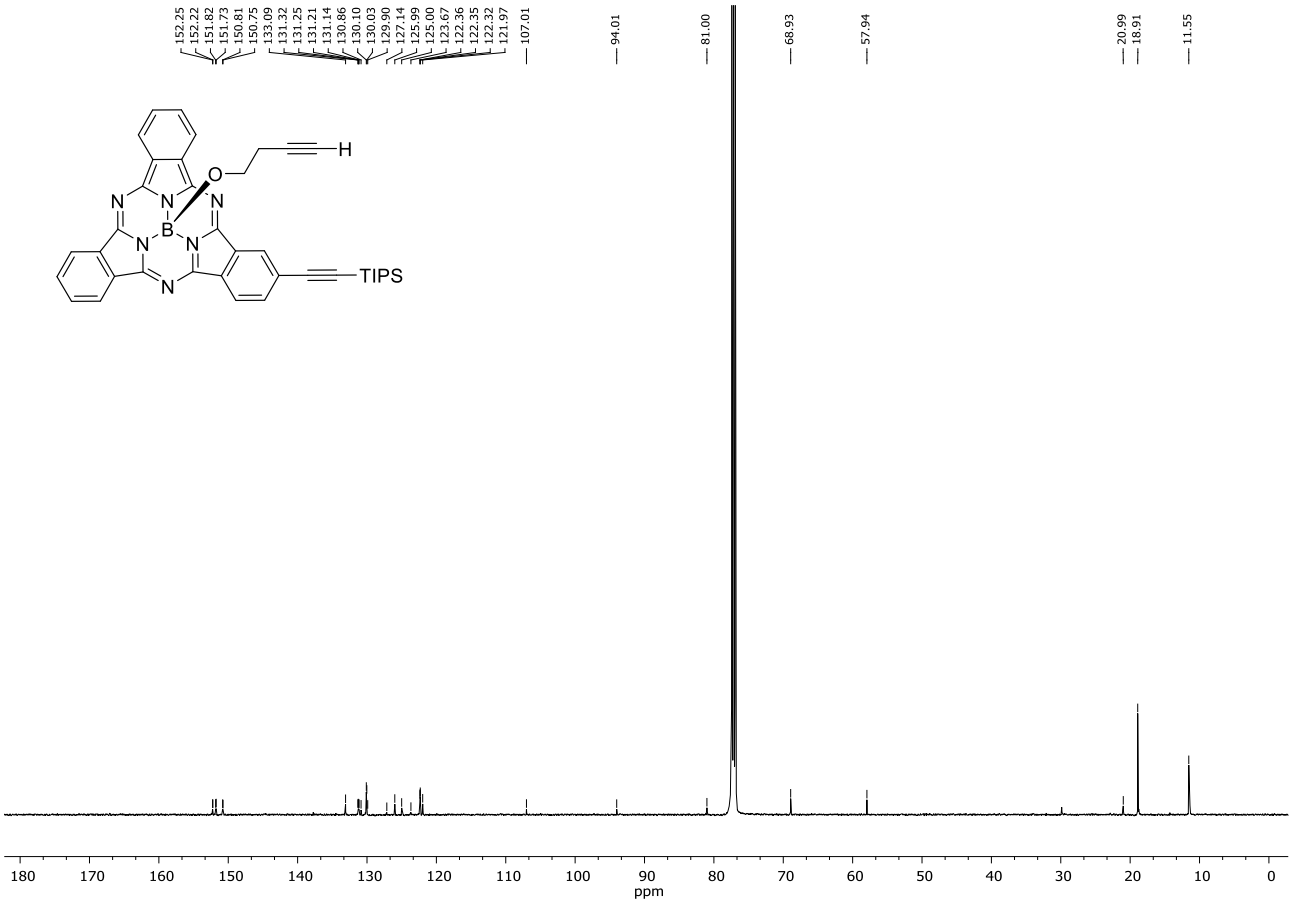
^{1}H-NMR (500 MHz) spectrum of **15** recorded in $CDCl_3$.



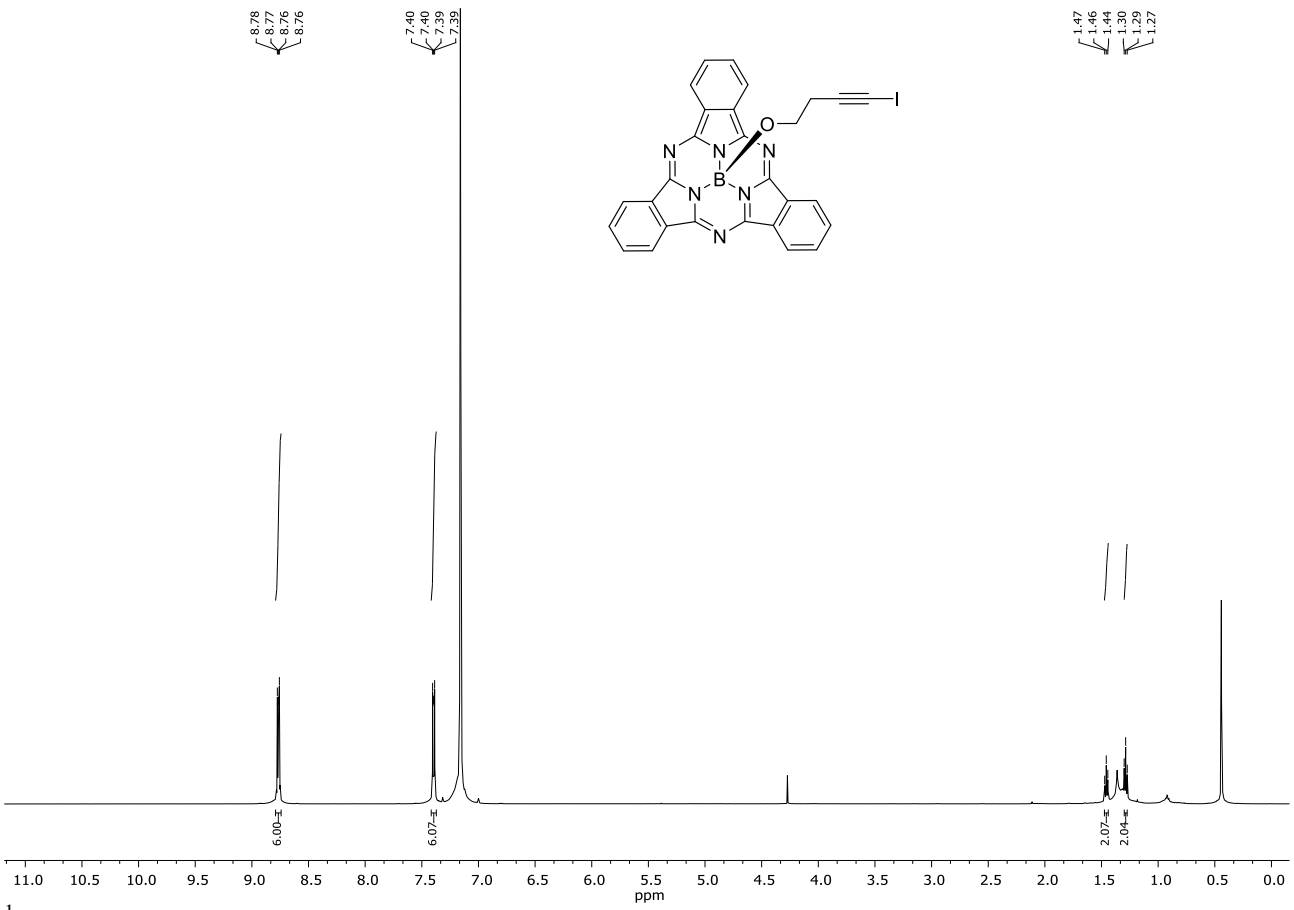
^{13}C-NMR (126 MHz) spectrum of **15** recorded in $CDCl_3$.



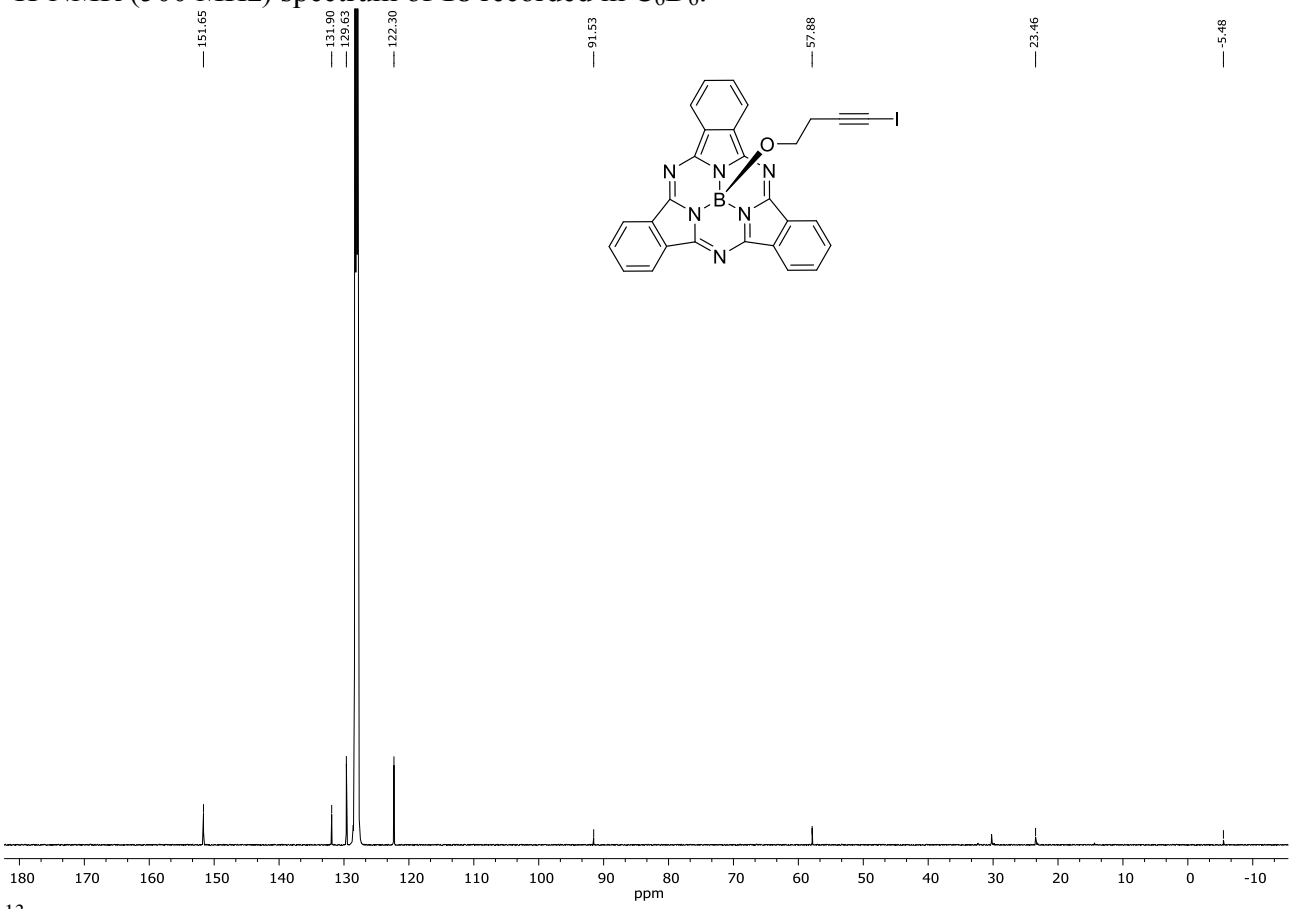
^{1}H-NMR (500 MHz) spectrum of **16** recorded in $CDCl_3$.



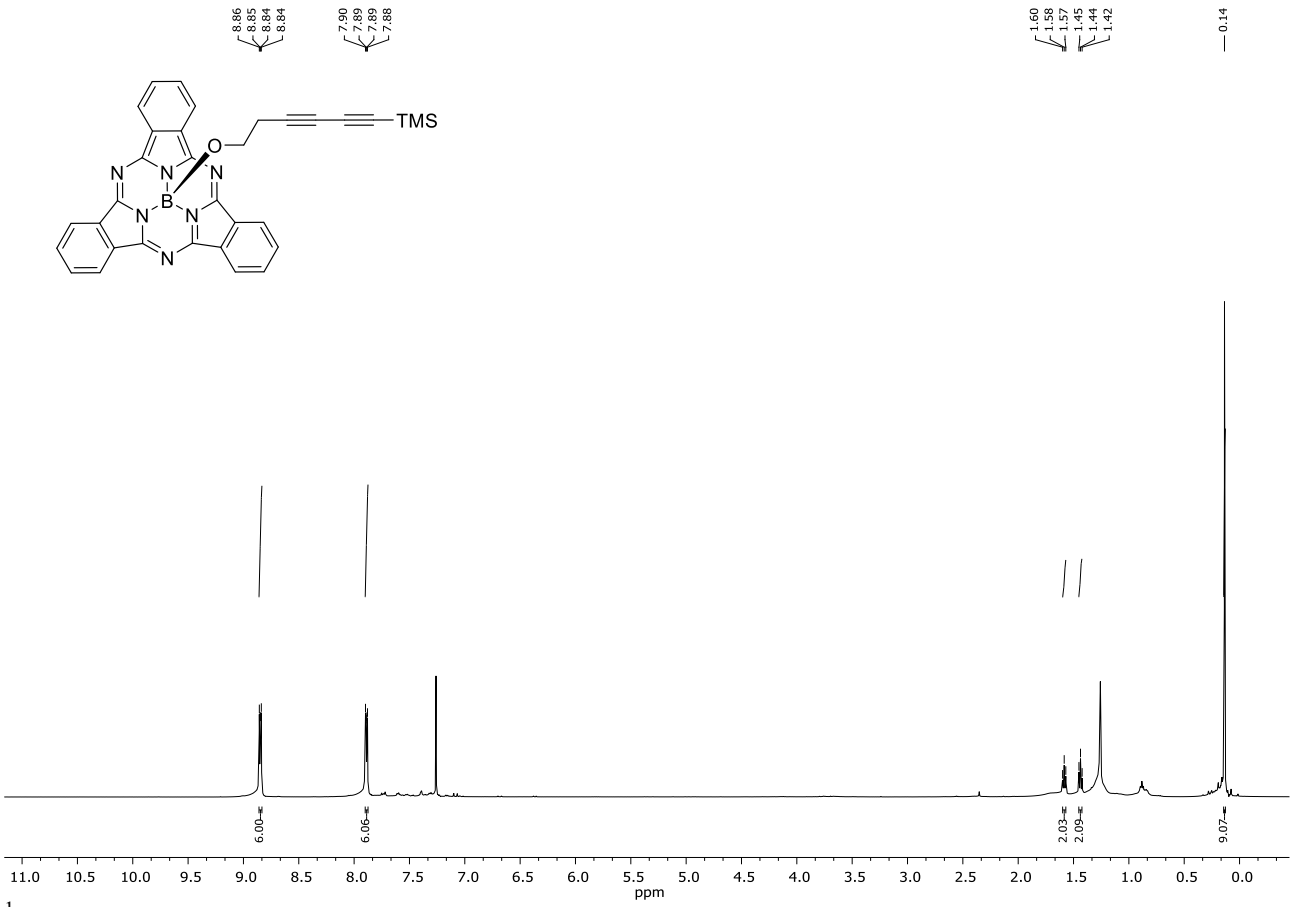
^{13}C-NMR (126 MHz) spectrum of **16** recorded in $CDCl_3$.



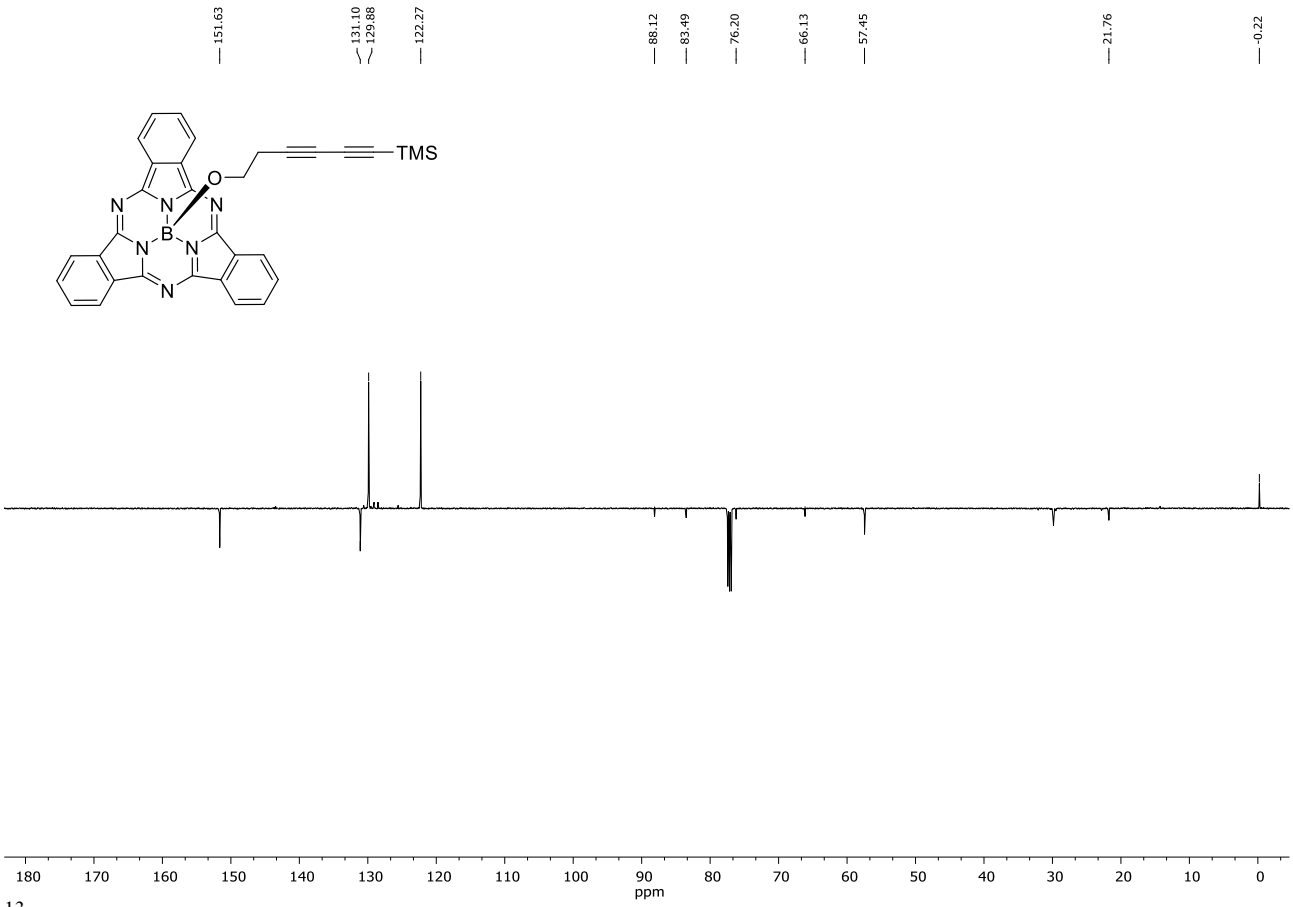
^{1}H-NMR (500 MHz) spectrum of **18** recorded in C_6D_6.



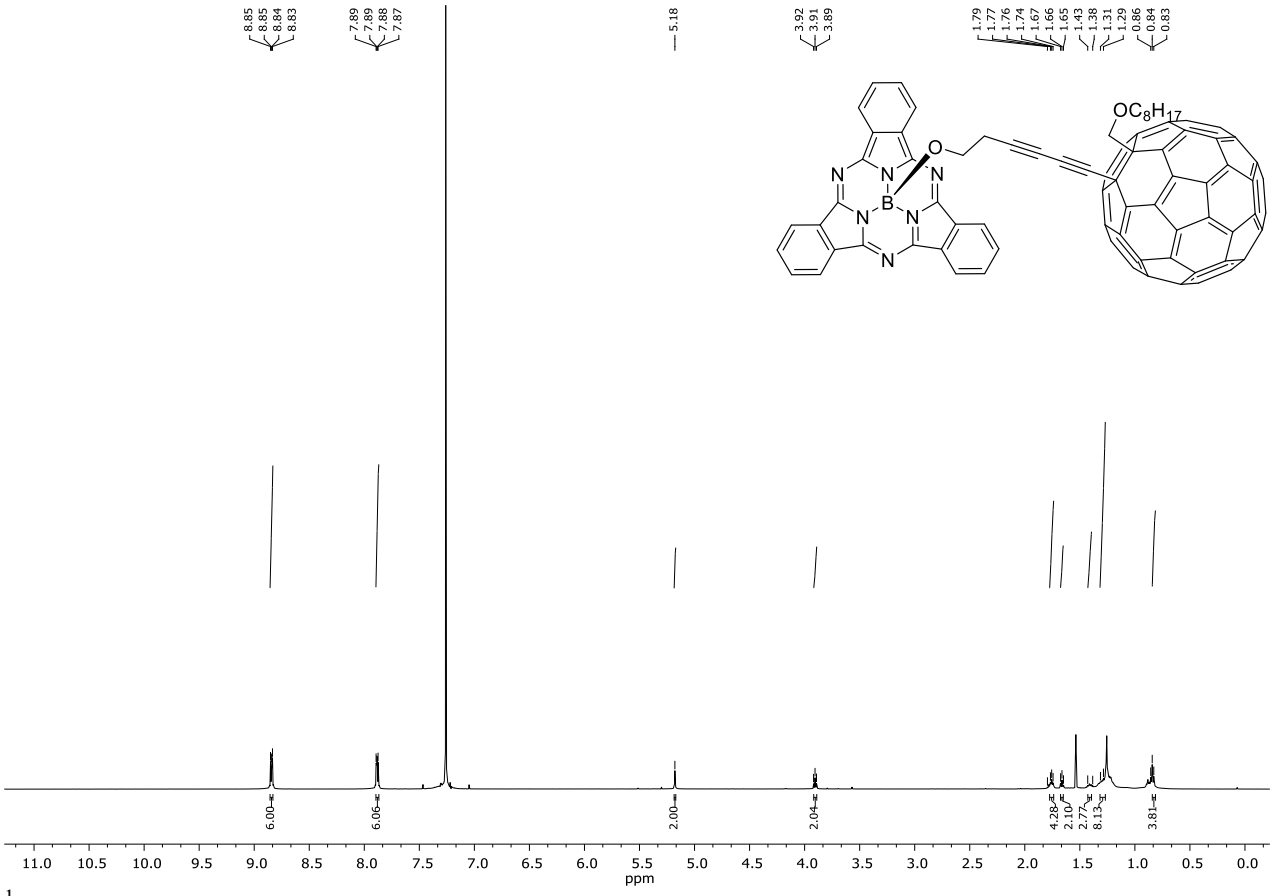
^{13}C-NMR (126 MHz) spectrum of **18** recorded in C_6D_6.



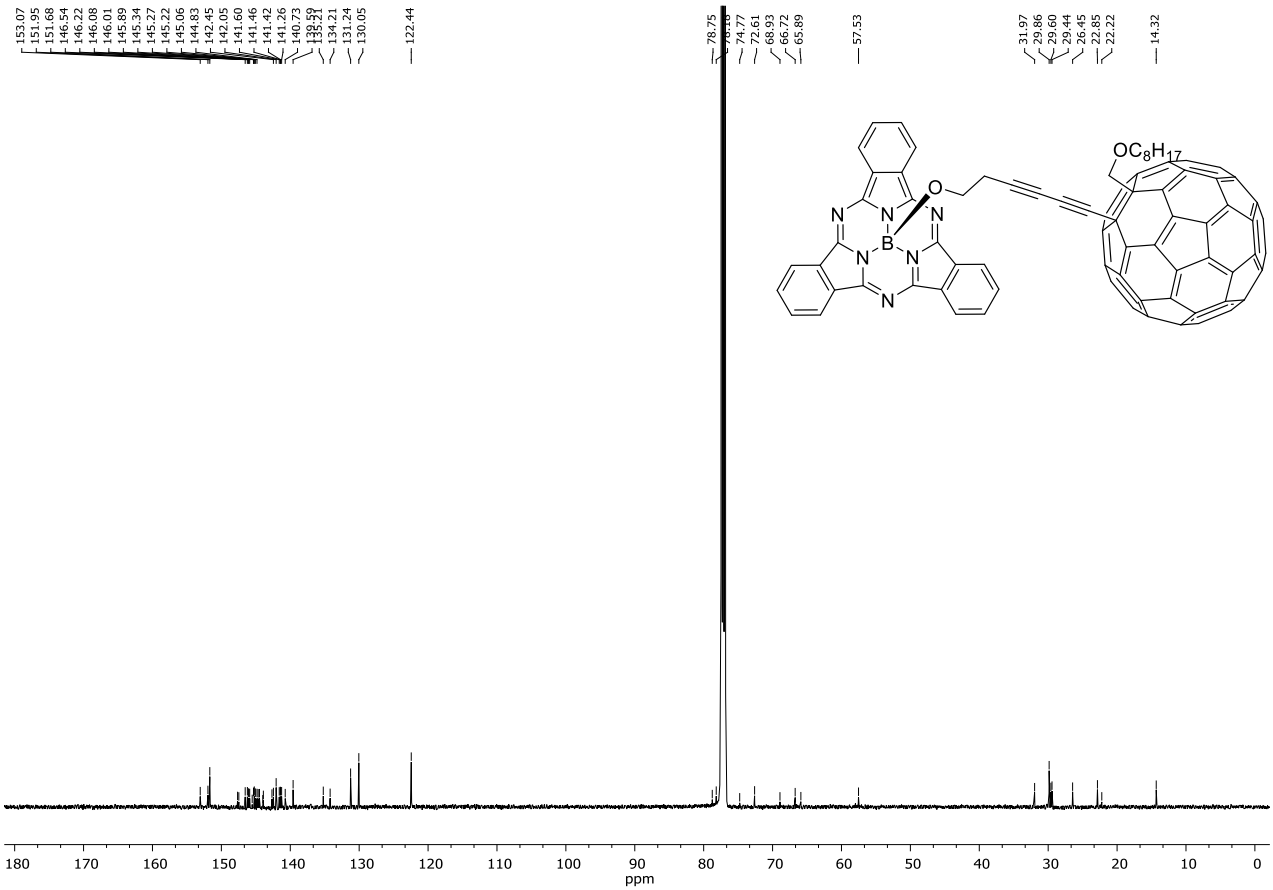
^{1}H-NMR (500 MHz) spectrum of **19** recorded in $CDCl_3$.



^{13}C APT NMR (126 MHz) spectrum of **19** recorded in $CDCl_3$.

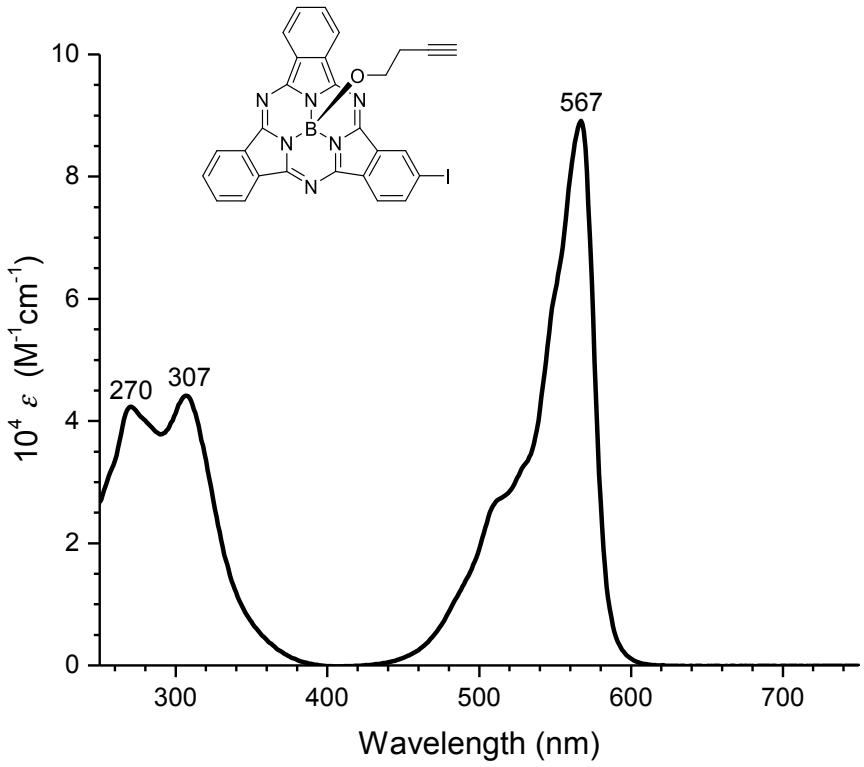


^{1}H-NMR (500 MHz) spectrum of **21** recorded in $CDCl_3$.

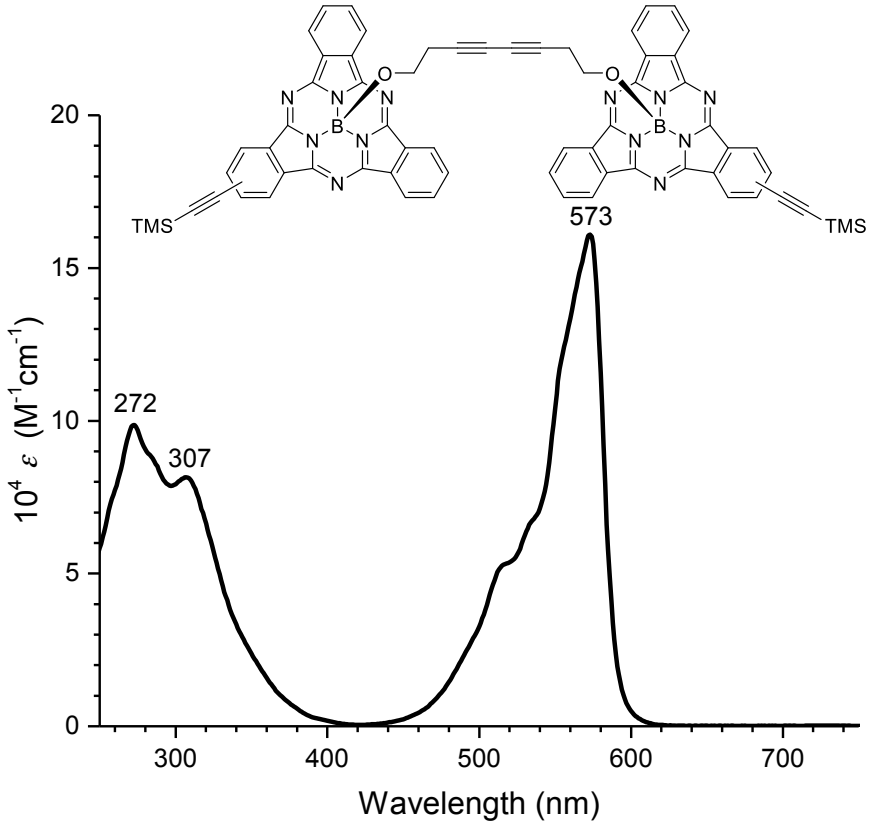


^{13}C-NMR (126 MHz) spectrum of **21** recorded in $CDCl_3$.

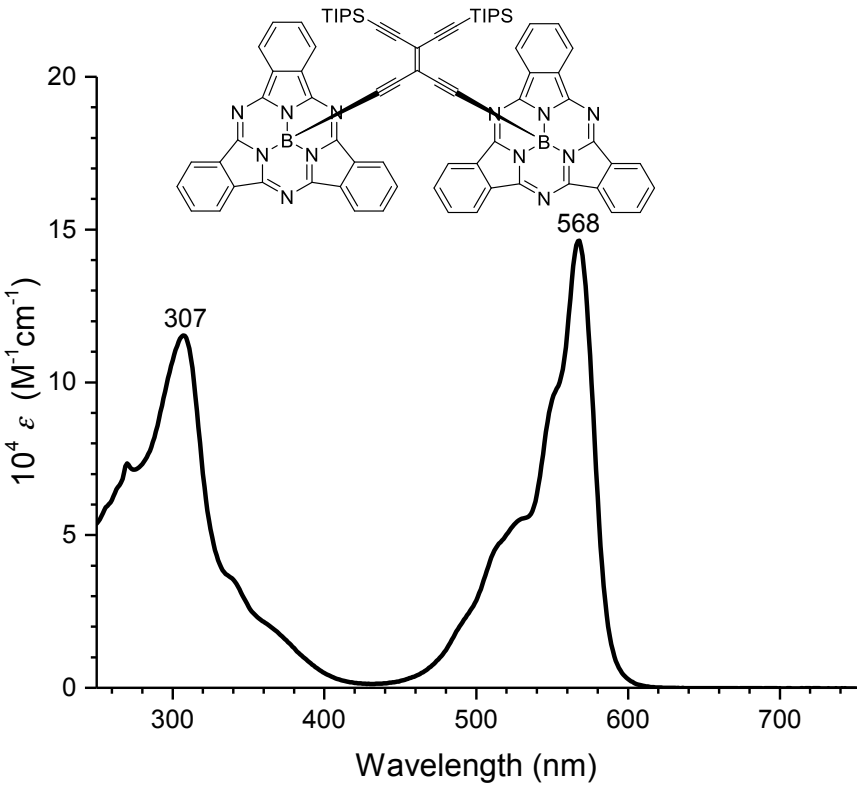
UV-Vis Absorption Spectra



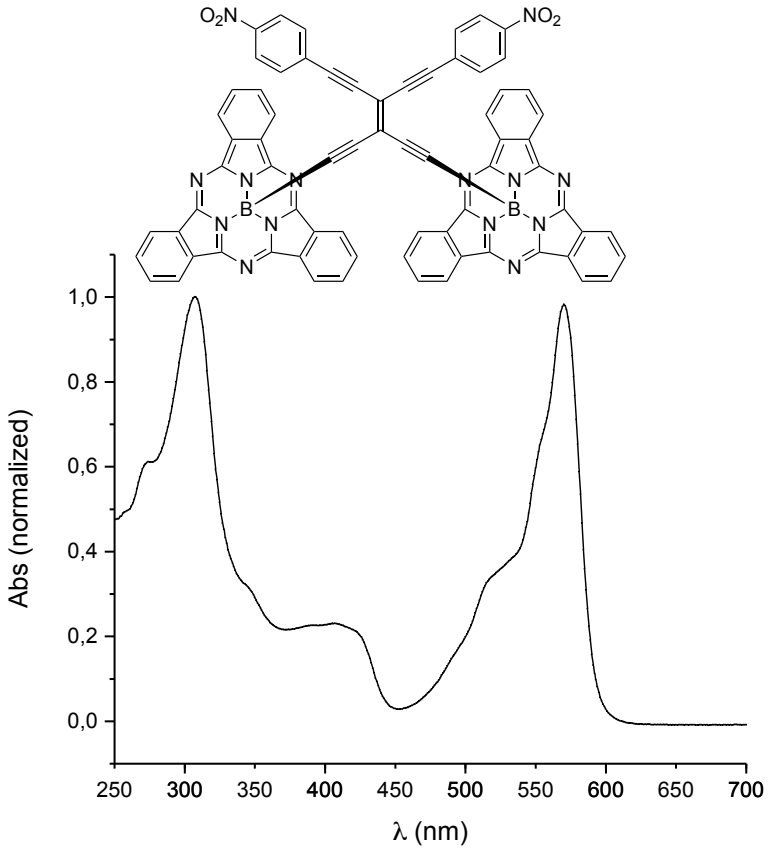
UV-Vis absorption spectrum of **9** recorded in chloroform.



UV-Vis absorption spectrum of **12** recorded in chloroform.



UV-Vis absorption spectrum of **2** recorded in chloroform.



UV-Vis absorption spectrum of **3** (normalized) recorded in chloroform.

Fluorescence Data

Determination of Fluorescence Quantum Yields

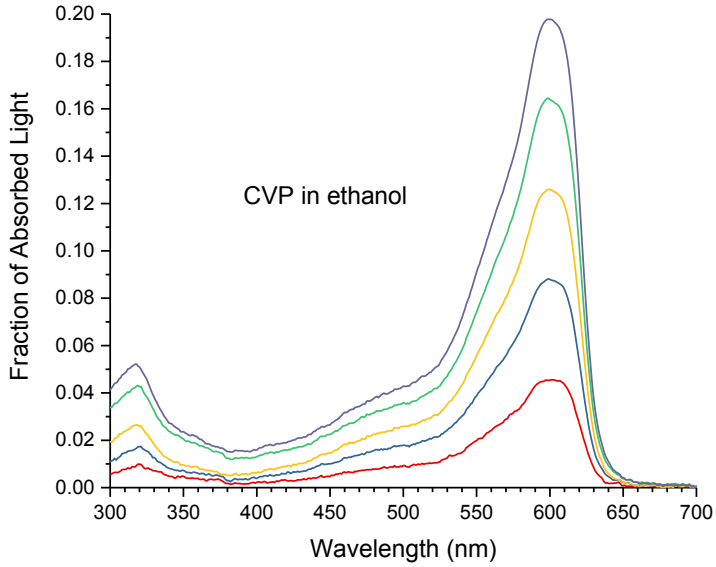
All fluorescence quantum yields (QYs) were measured using a Lambda 1050 (PerkinElmer) instrument for absorption measurements and a Fluotime 300 (PicoQuant) instrument for fluorescence measurements. For all quantum yield determinations, cresyl violet perchlorate in absolute ethanol was used as reference dye (R. Sems and K. H. Drexhage, *J. Lumin.*, 1981, **24-25**, 709-712).

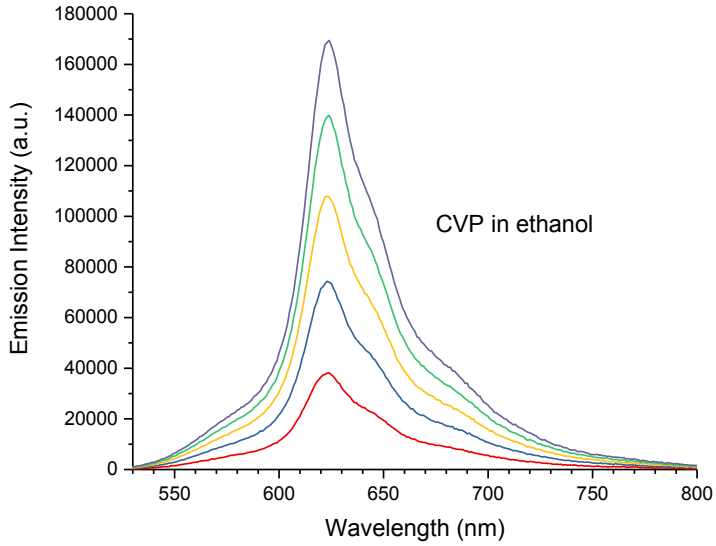
The quantum yields (Φ_F) were determined using the relative method according to the following formula (C. Würt, M. Grabolle, J. Pauli, M. Spieles and U. Resch-Genger, *Nat. Protoc.*, 2013, **8**, 1535-1550).

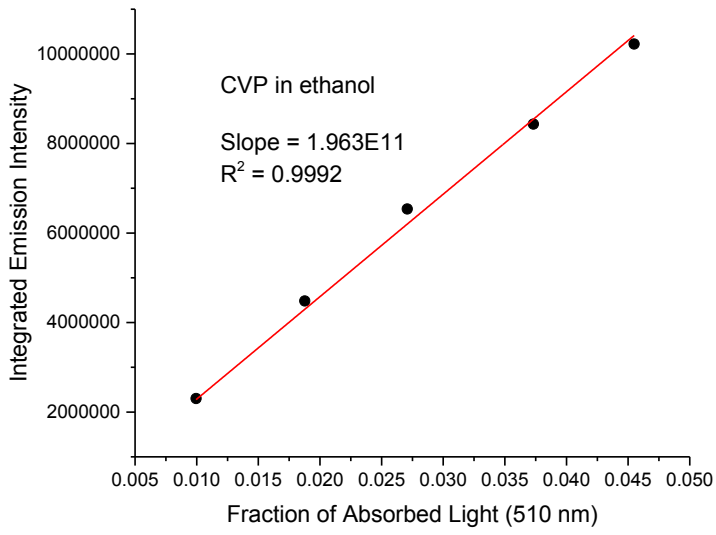
$$\Phi_F = \Phi_{F,ref} \frac{\alpha \cdot n^2}{\alpha_{ref} \cdot n_{ref}^2}$$

The subscript *ref* designates the reference dye (cresyl violet perchlorate or CVP, $\Phi_{F,ref}$ = 0.56 in ethanol), n the refractive index of the solvent and α the slope obtained from a linear-fit to a set of data points (I_{int} vs. f_a). Here I_{int} refers to the integrated emission intensity and f_a to the fraction of absorbed light ($f_a = 1\text{-}10^{-A}$, A being the absorbance measured at the wavelength of excitation). For all QY determinations five or more data points were collected with a measured absorbance below 0.1 for the longest wavelength absorption.

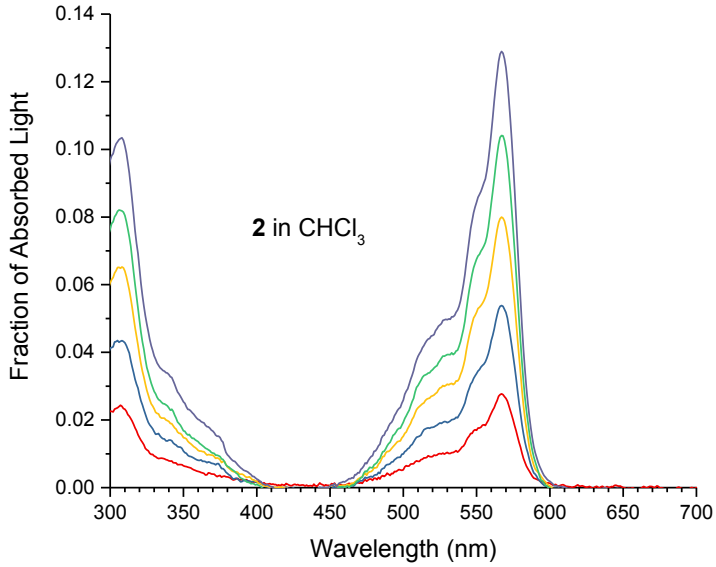
Reference dye – CVP

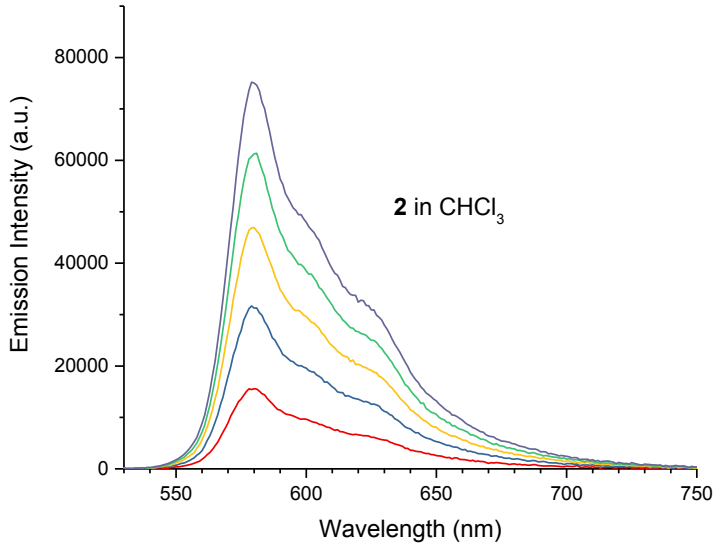


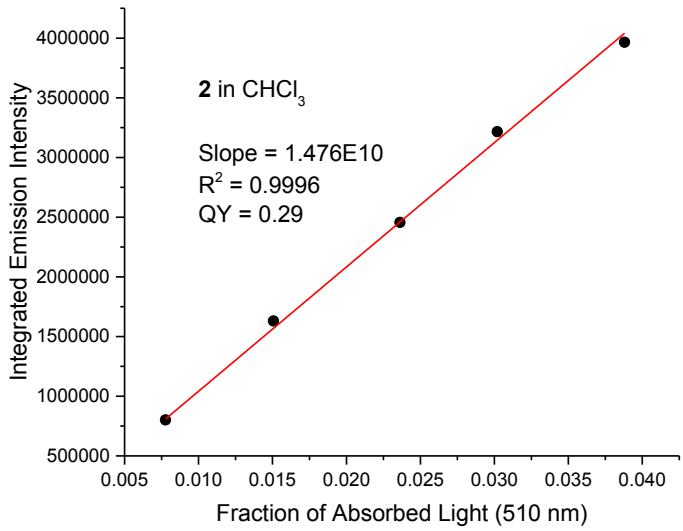




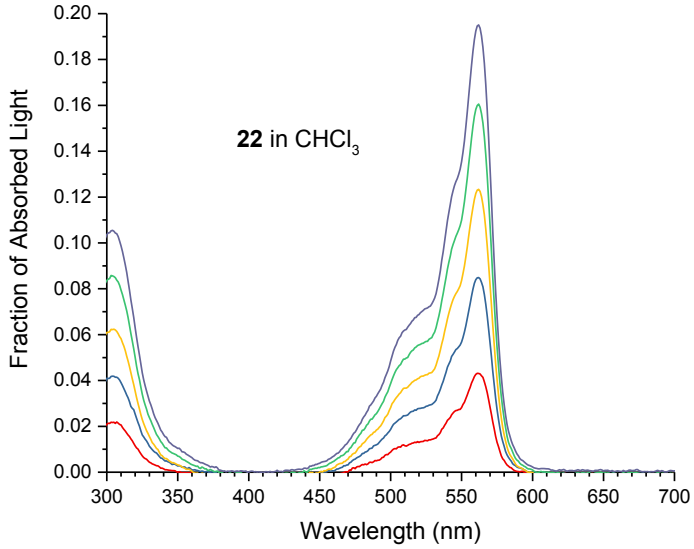
Compound 2

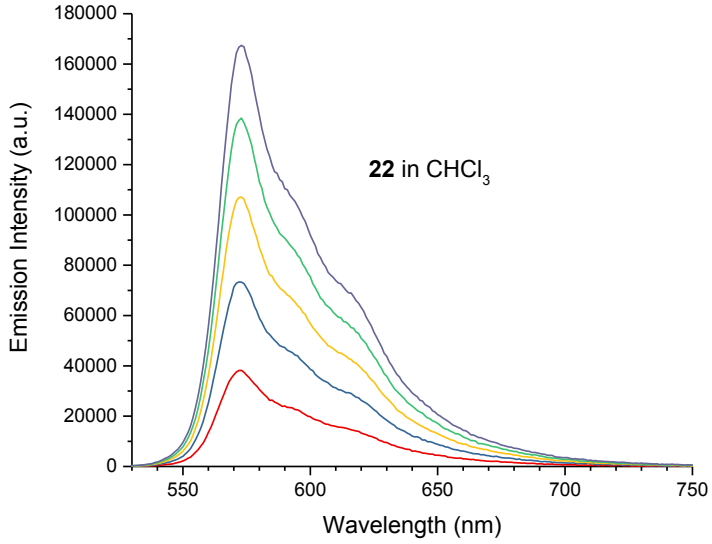

Fraction of Absorbed Light
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
2 in CHCl3
300
350
400
450
500
550
600
650
700
Wavelength (nm)

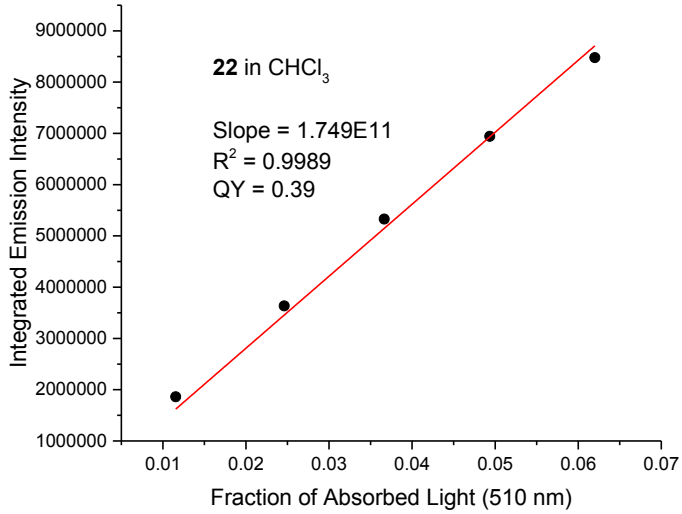

Emission Intensity (a.u.)
80000
60000
40000
20000
0
2 in CHCl3
550
600
650
700
750
Wavelength (nm)


Integrated Emission Intensity
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
2 in CHCl3
Slope = 1.476E10
R2 = 0.9996
QY = 0.29
0.005
0.010
0.015
0.020
0.025
0.030
0.035
0.040
Fraction of Absorbed Light (510 nm)

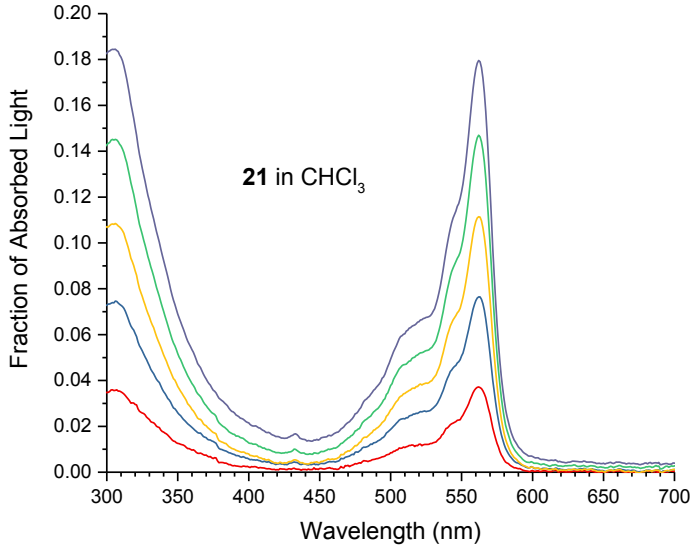
Compound 22


22 in CHCl3
Fraction of Absorbed Light
Wavelength (nm)
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
0.20
300
350
400
450
500
550
600
650
700


22 in CHCl3
Emission Intensity (a.u.)
Wavelength (nm)
0
20000
40000
60000
80000
100000
120000
140000
160000
180000
550
600
650
700
750


22 in CHCl3
Slope = 1.749E11
R2 = 0.9989
QY = 0.39
Integrated Emission Intensity
Fraction of Absorbed Light (510 nm)
1000000
2000000
3000000
4000000
5000000
6000000
7000000
8000000
9000000
0.01
0.02
0.03
0.04
0.05
0.06
0.07

Compound 21


Fraction of Absorbed Light
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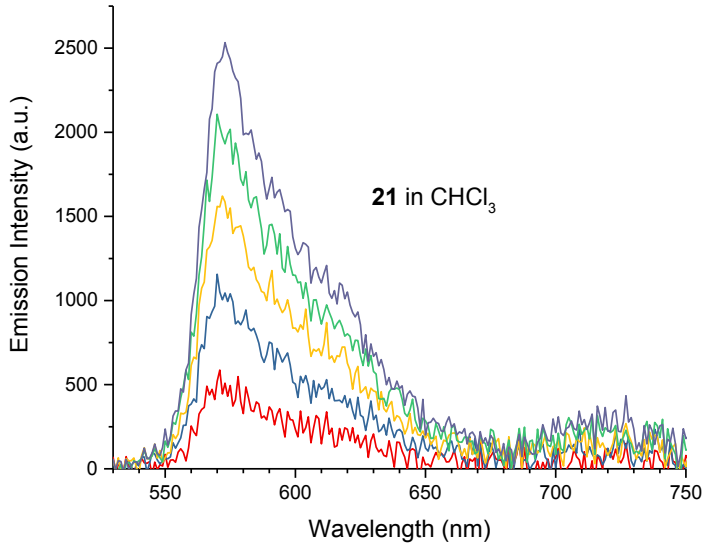
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
300
350
400
450
500
550
600
650
700
Wavelength (nm)
21 in CHCl3


Emission Intensity (a.u.)
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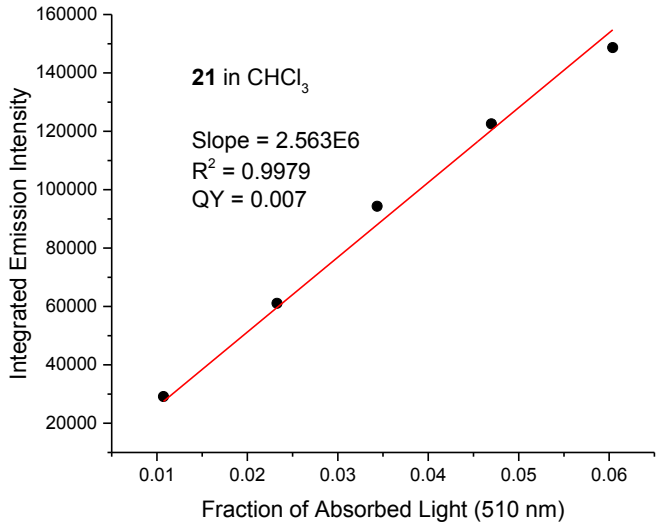
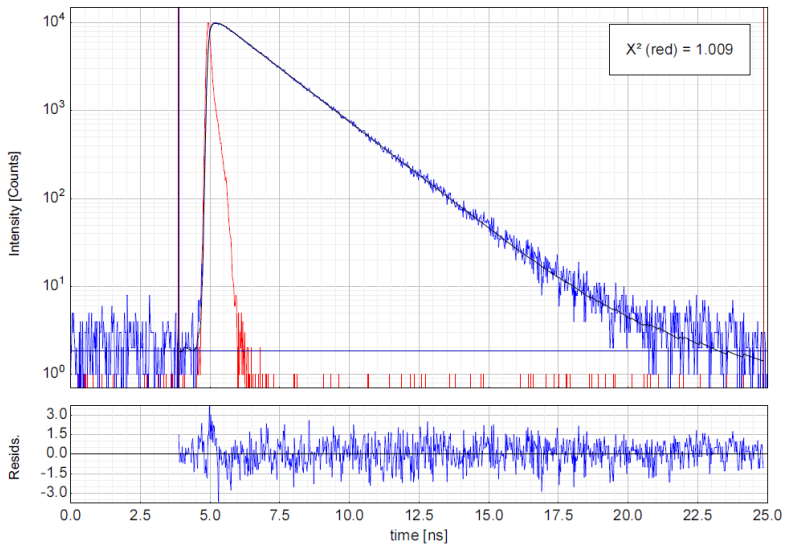
2000
1500
1000
500
0
550
600
650
700
750
Wavelength (nm)
21 in CHCl3


Integrated Emission Intensity
160000
140000
120000
100000
80000
60000
40000
20000
0.01
0.02
0.03
0.04
0.05
0.06
Fraction of Absorbed Light (510 nm)
21 in CHCl3
Slope = 2.563E6
R2 = 0.9979
QY = 0.007

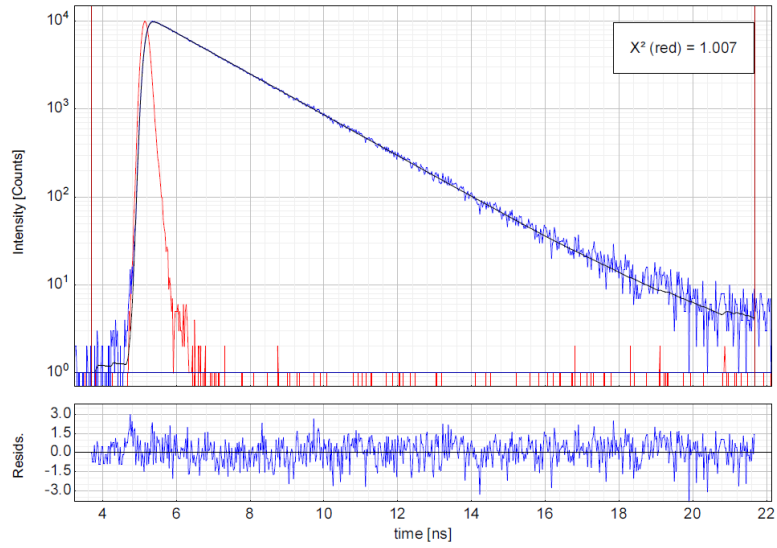
Determination of Fluorescence Lifetimes

Compound 2



Time-resolved emission decay profile of **2** in $CHCl_3$. τ = 1.8 ns

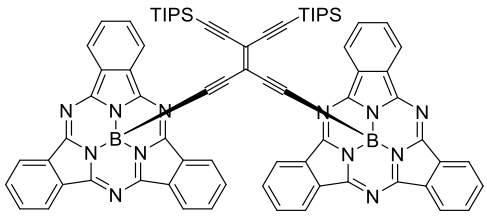
Compound 22



Time-resolved emission decay profile of **22** in $CHCl_3$. τ = 1.9 ns

X-Ray Crystal Structure Data

X-Ray crystal structure data for compound **2**:



Crystal System	Triclinic
Space Group	P-1
a (Å)	13.474
b (Å)	14.769
c (Å)	19.430
α (º)	86.11°
β (º)	73.45°
γ (º)	87.49°
Volume ($Å^3$)	3696.8
Z	2
Calculated Density (g/cm3)	1.1006
X-ray radiation	Mo Kα (0.71073 Å)
Total Reflections	84253
Unique Reflections	12889
Number of parameters	829
R_{int}	0.0878
R1 (Fo>4σ(Fo))	9.35 %
wR2 (All data)	0.2717
Goodness-of-fit	0.840
Completeness	99%
Mean I/σ	12.18
Resolution (d_{min}) (Å)	0.84
Number of constraints	0
Number of restraints	0

In solving the crystal structure, the solvent has been masked and hydrogen atoms have been omitted due to disorder.

Computational Data

G09 output

Compound 22

```
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Jul-2
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 \C,-7.200815,-2.981105,3.731817\C,-7.18601,-2.433287,2.444425\C,-
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0.365335\H,
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Compound 2

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Jul-
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