

Supplementary Material

Oligoyne-bridged boron subphthalocyanine dimers – synthesis and redox properties

Anne Ugleholdt Petersen,¹ Mads Georg Rasmussen,¹ Maria Cecilia Helleskov Thomsen, Aurore Ceuninck, and Mogens Brøndsted Nielsen*

Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark

Email: mbn@chem.ku.dk

¹These authors contributed equally

Table of Contents

NMR Spectroscopy.....	S2
UV-Vis Absorption Spectroscopy	S16
Electrochemistry	S18

NMR Spectroscopy

Compound 3

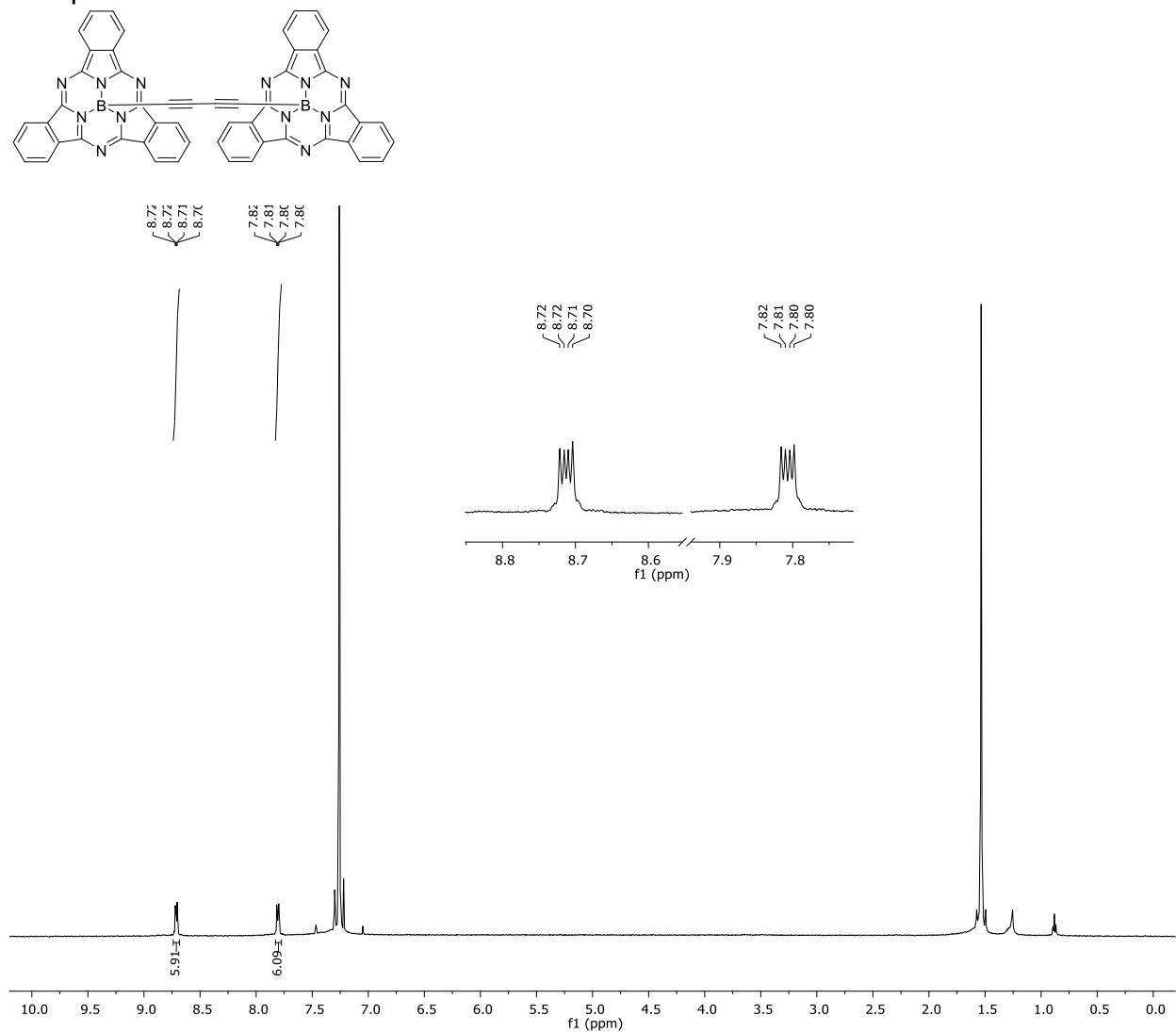


Figure S1. ¹H-NMR spectrum of compound 3 in CDCl₃.

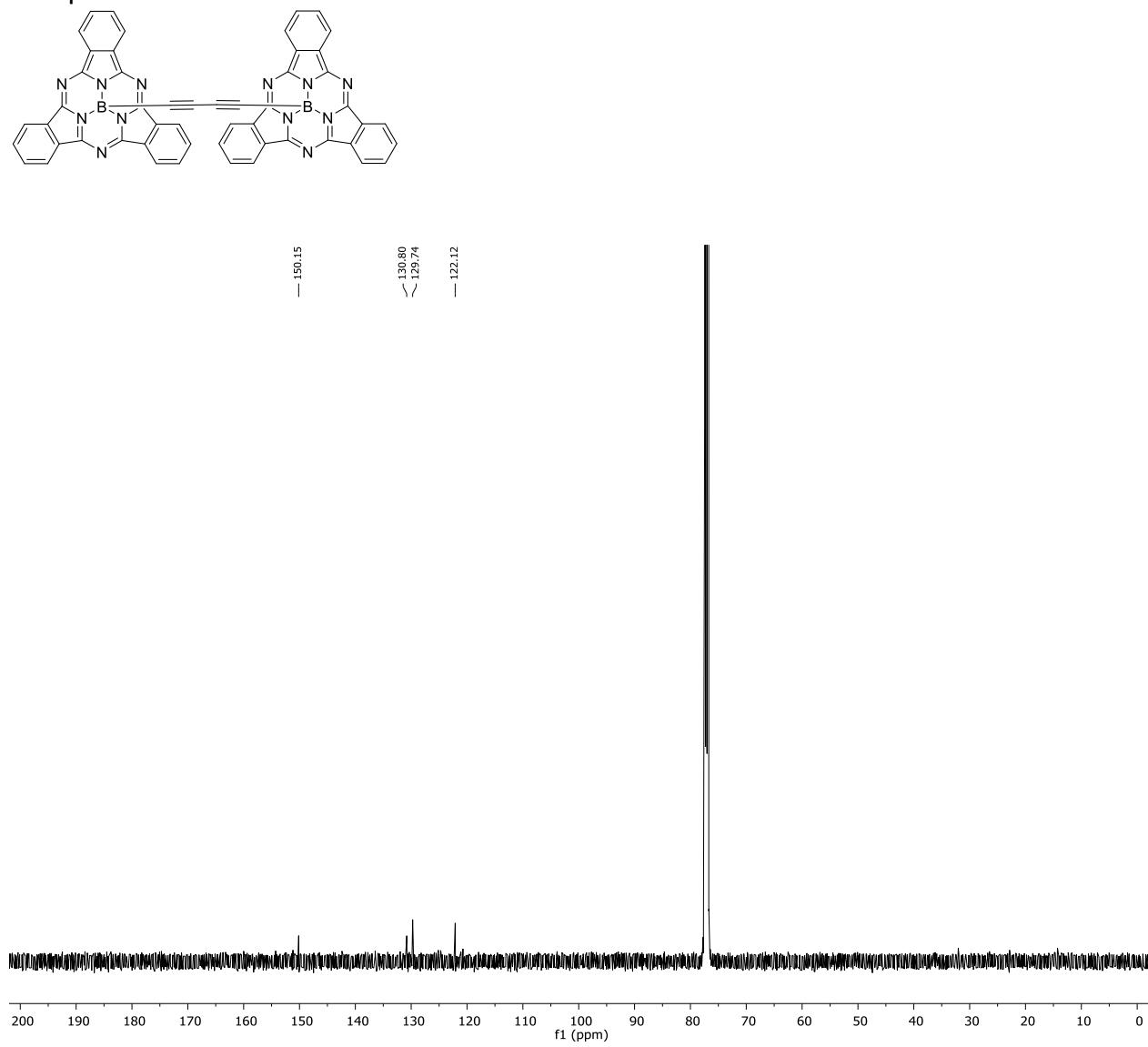
Compound 3

Figure S2. ^{13}C -NMR spectrum of compound 3 in CDCl_3 .

Compound 4

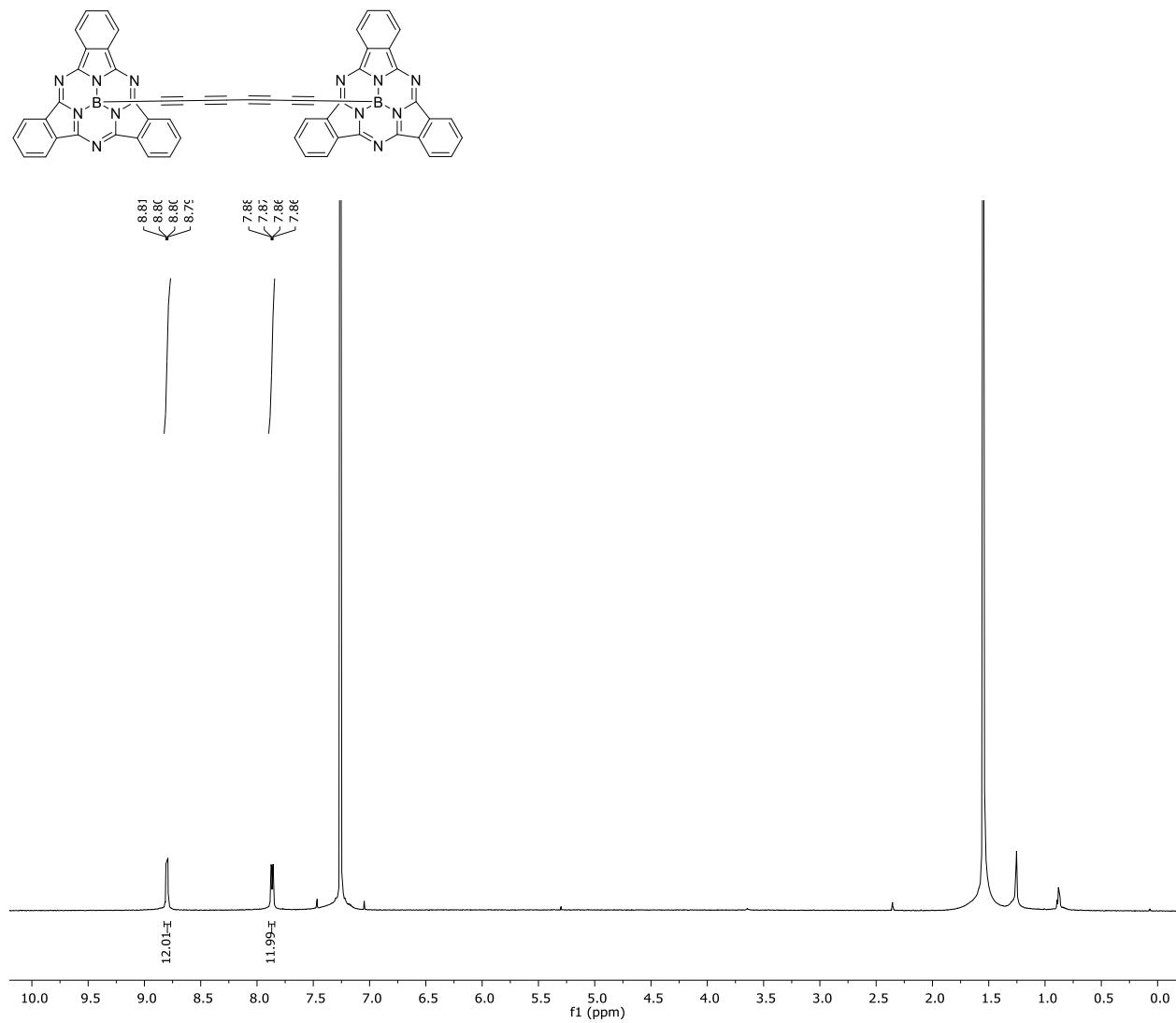


Figure S3. ^1H -NMR spectrum of compound 4 in CDCl_3 .

Compound 4

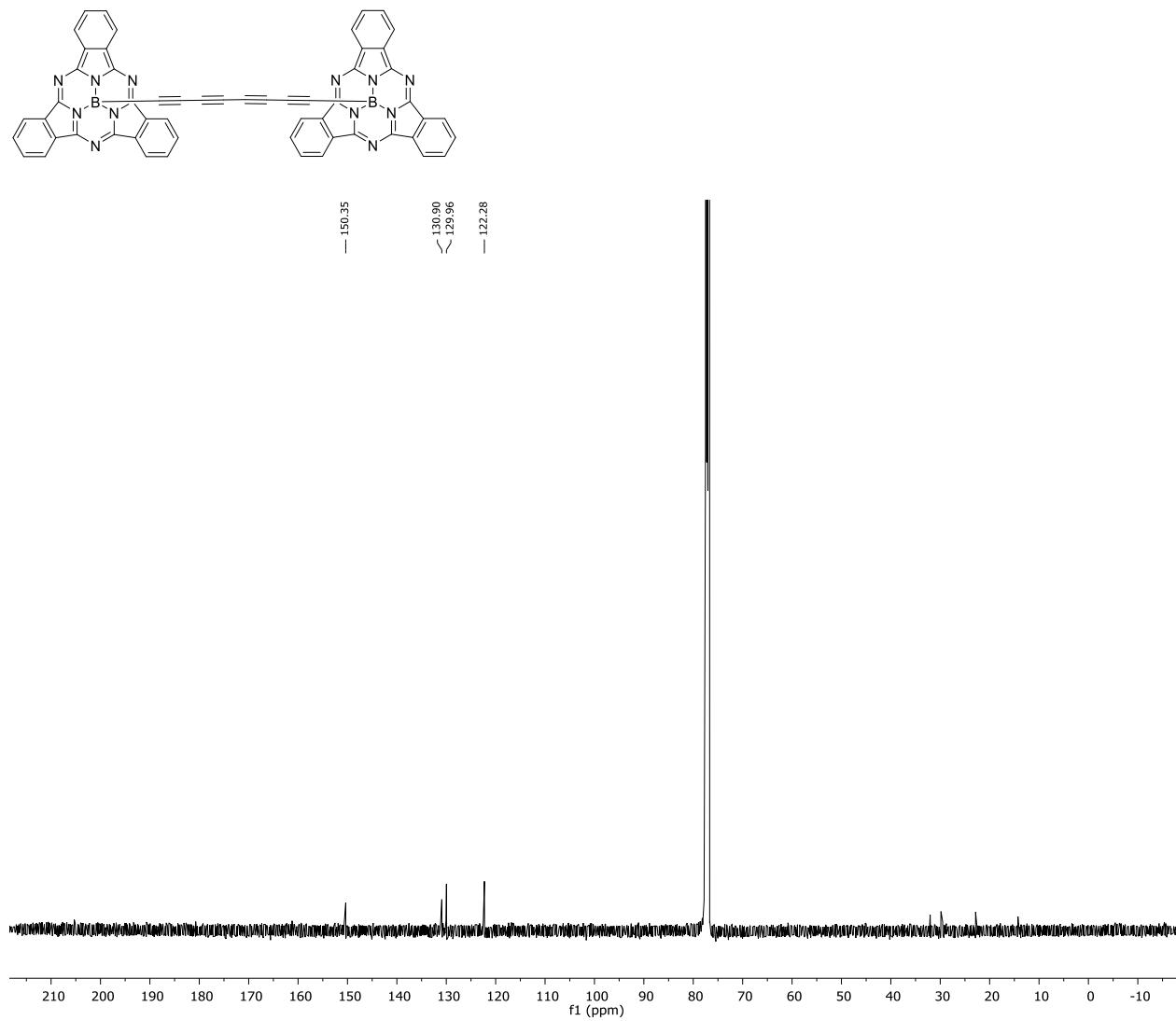
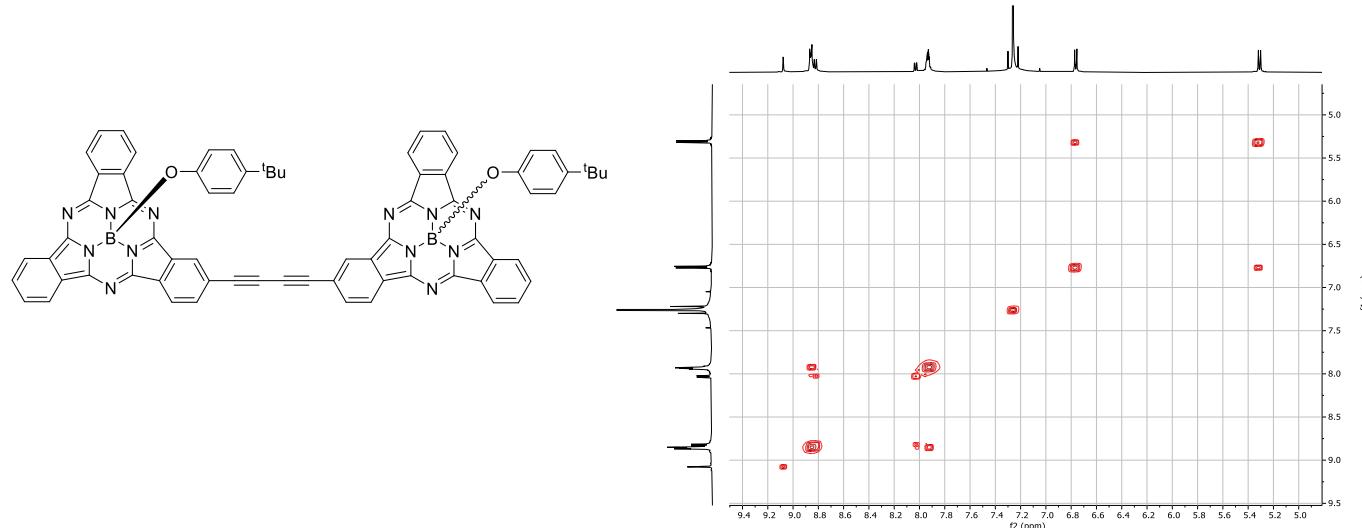
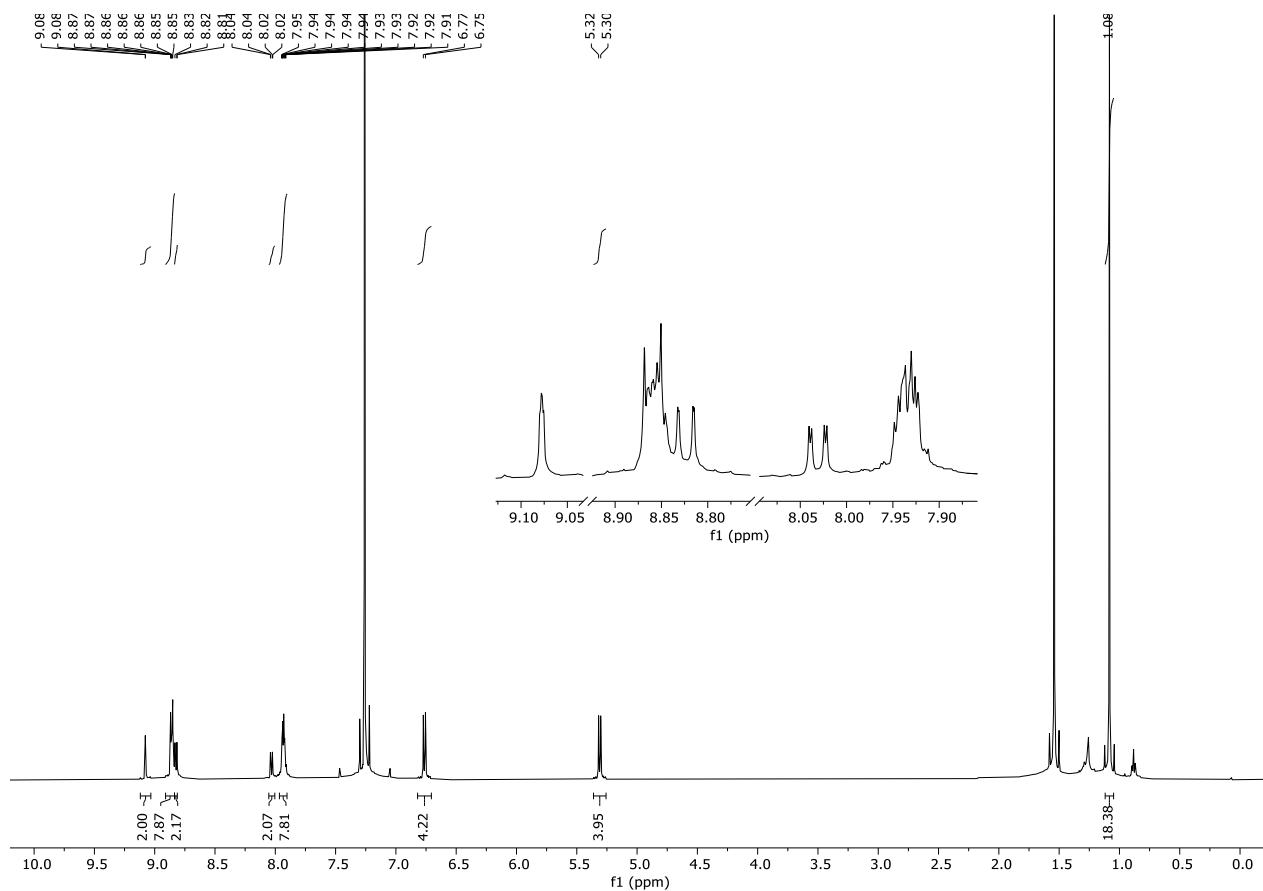


Figure S4. ^{13}C -NMR spectrum of compound 4 in CDCl_3 .

Compound 5

Figure S5. COSY spectrum of compound 5 in CDCl_3 .Figure S6. ^1H -NMR spectrum of compound 5 in CDCl_3 .

Compound 5

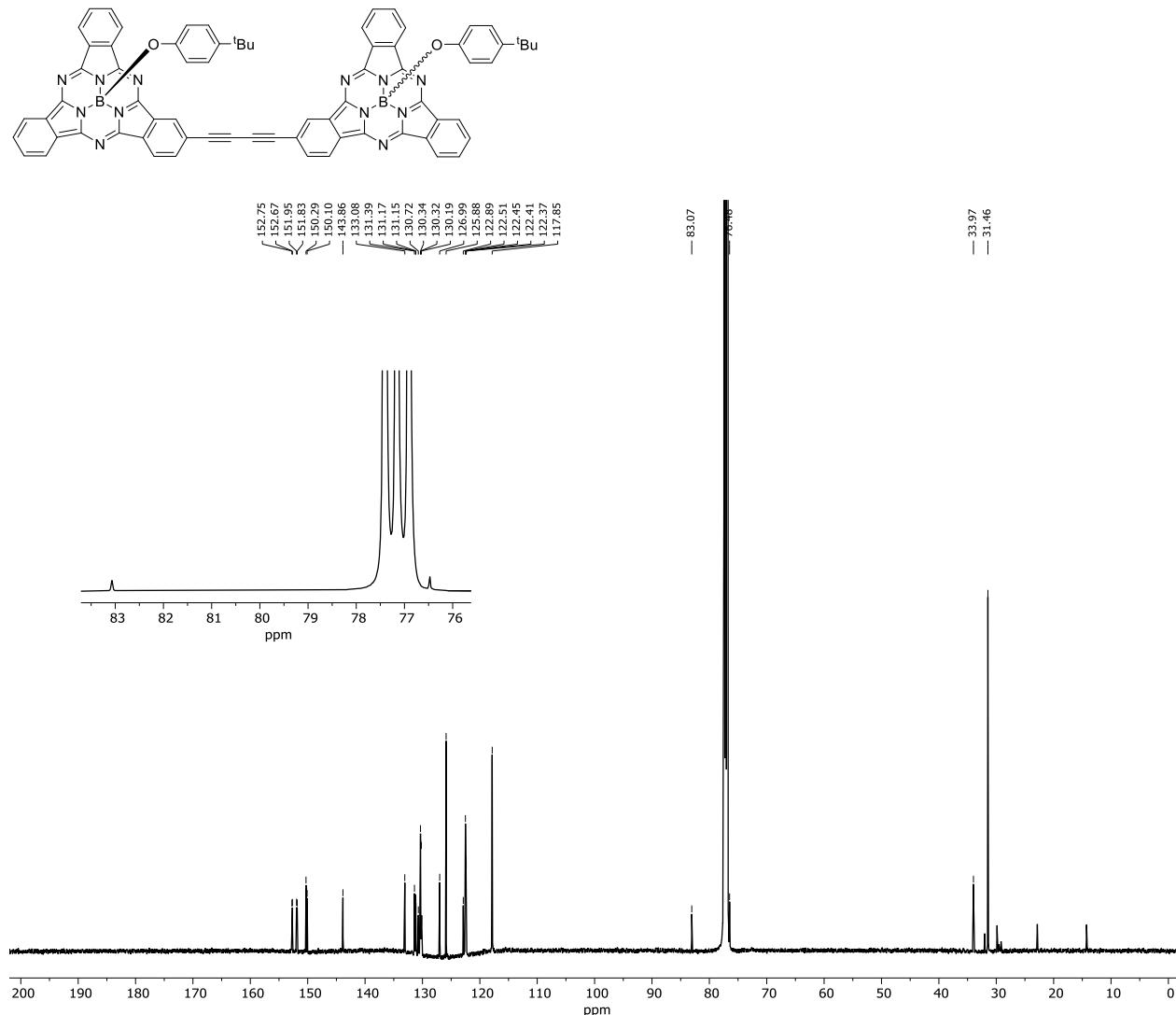
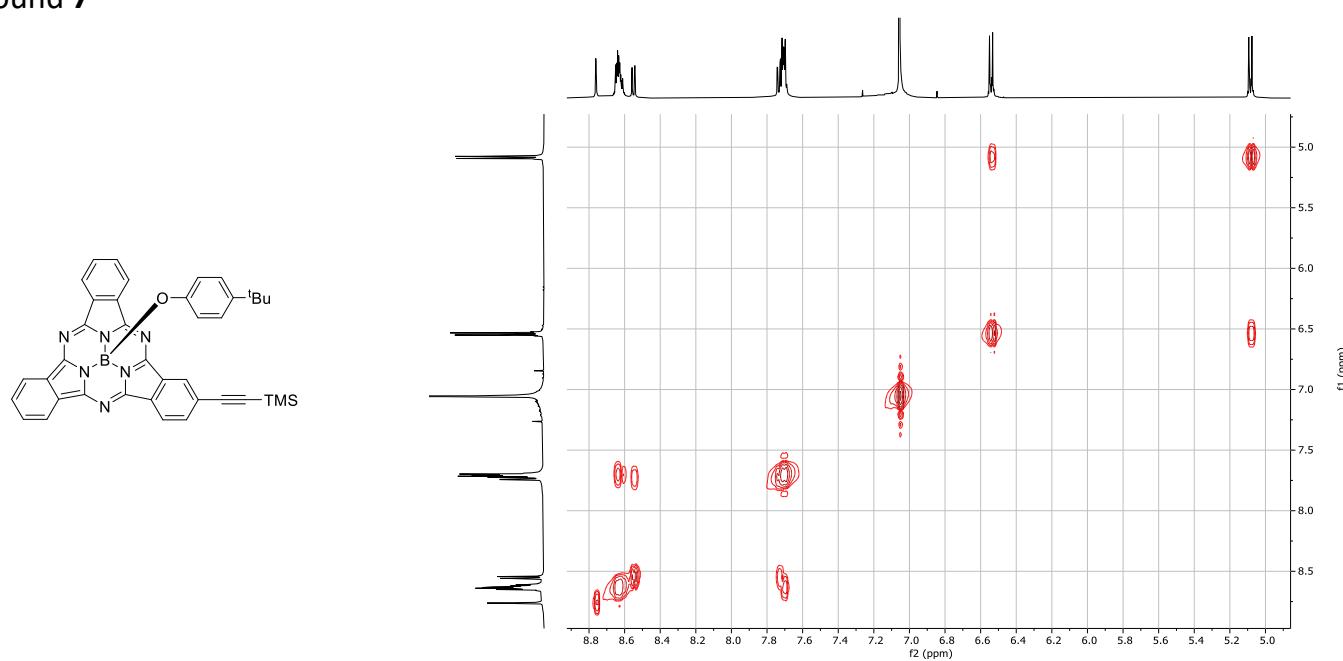
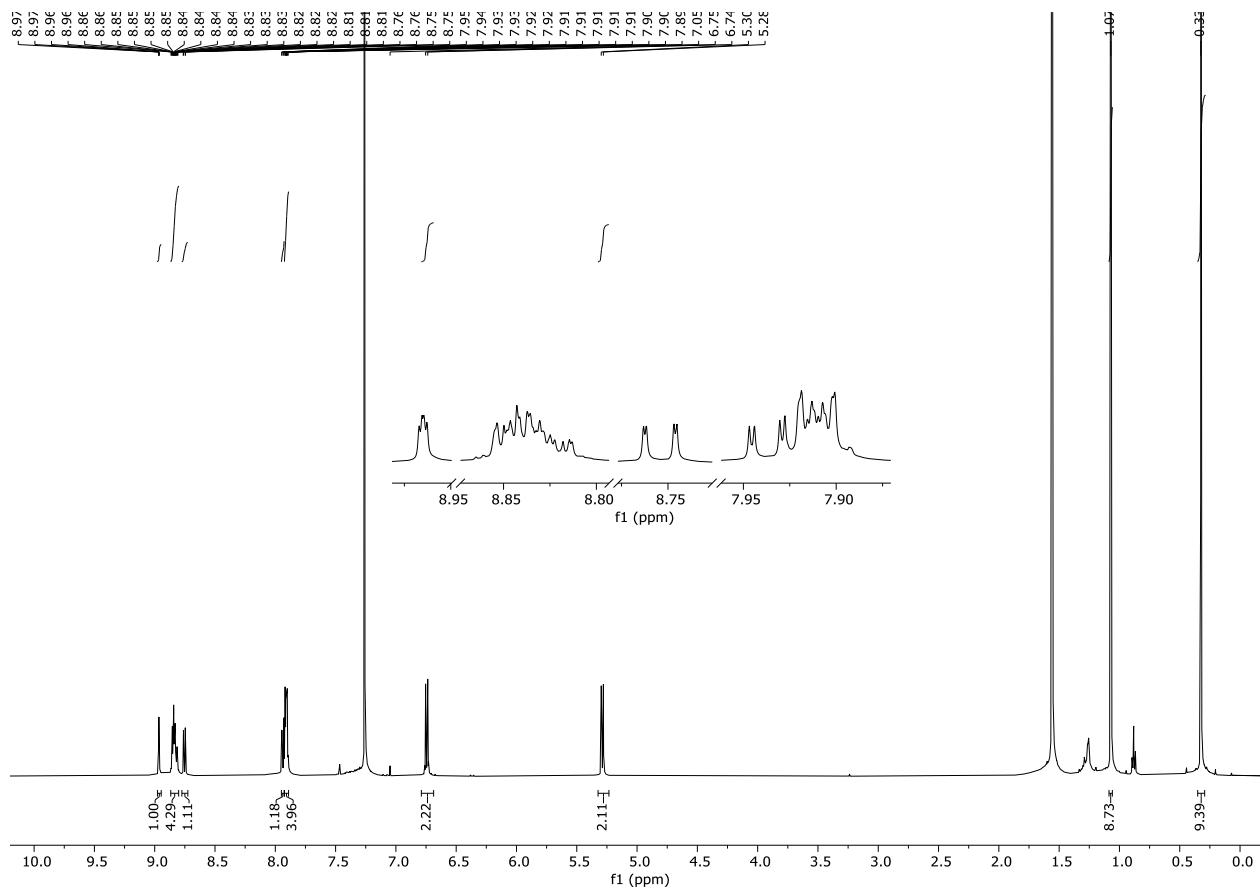


Figure S7. ^{13}C -NMR spectrum of compound 5 in CDCl_3 .

Compound 7

Figure S8. COSY spectrum of compound 7 in CDCl_3 Figure S9. ^1H -NMR spectrum of compound 7 in CDCl_3 .

Compound 7

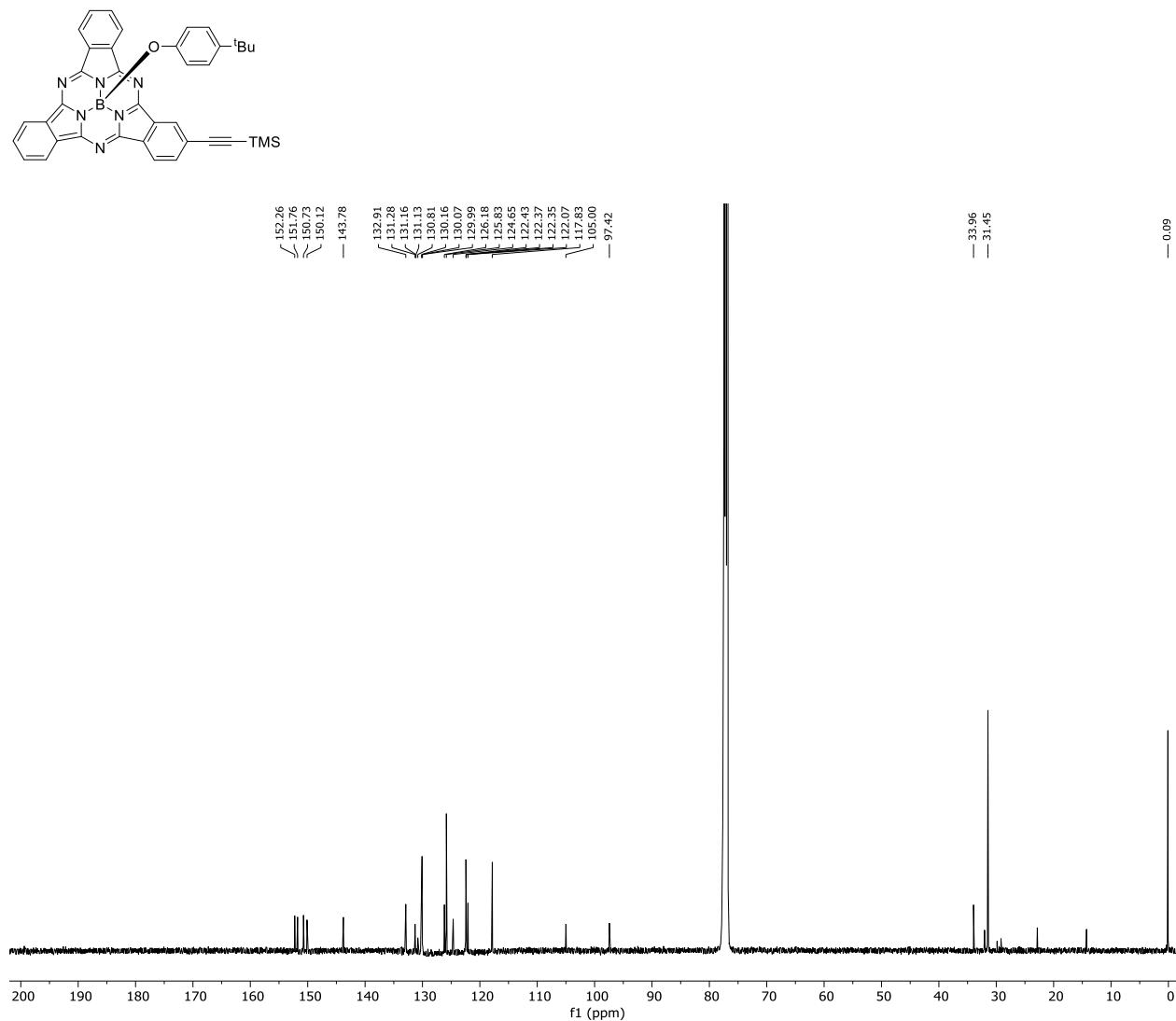


Figure S10. ^{13}C -NMR spectrum of compound 7 in CDCl_3 .

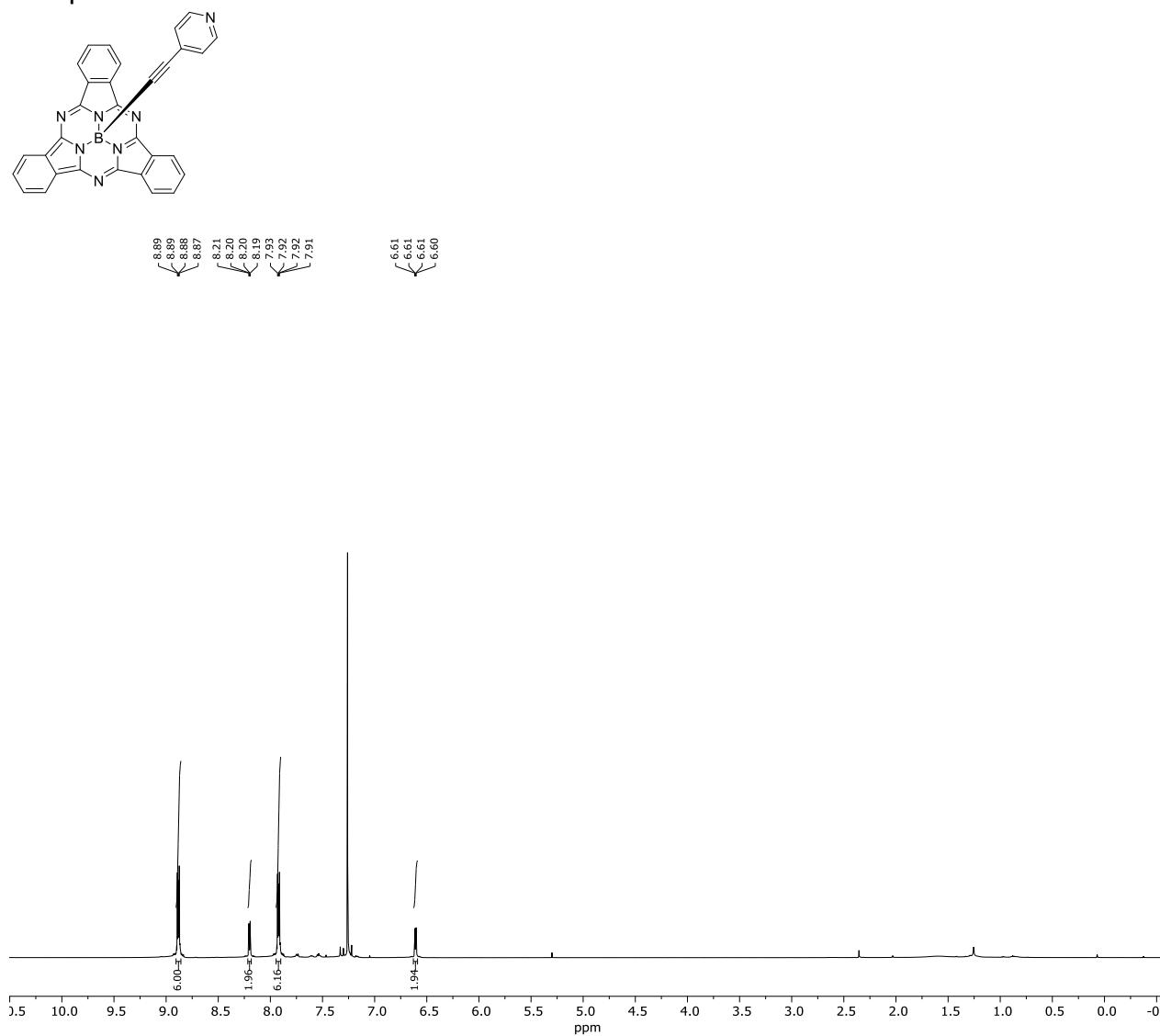
Compound 8

Figure S11. ^1H -NMR spectrum of compound 8 in CDCl_3 .

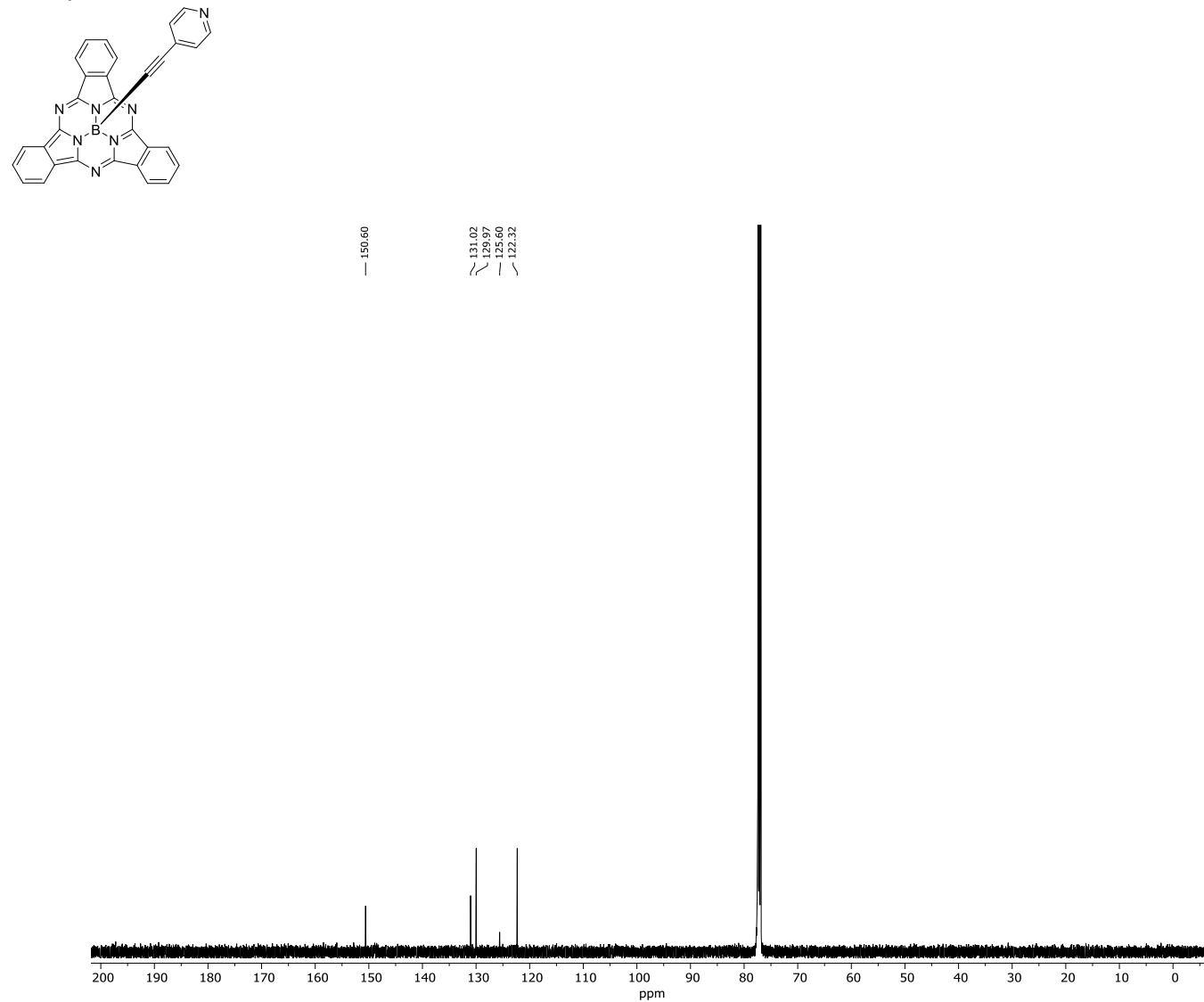
Compound 8

Figure S12. ^{13}C -NMR spectrum of compound 8 in CDCl_3 .

Compound 9

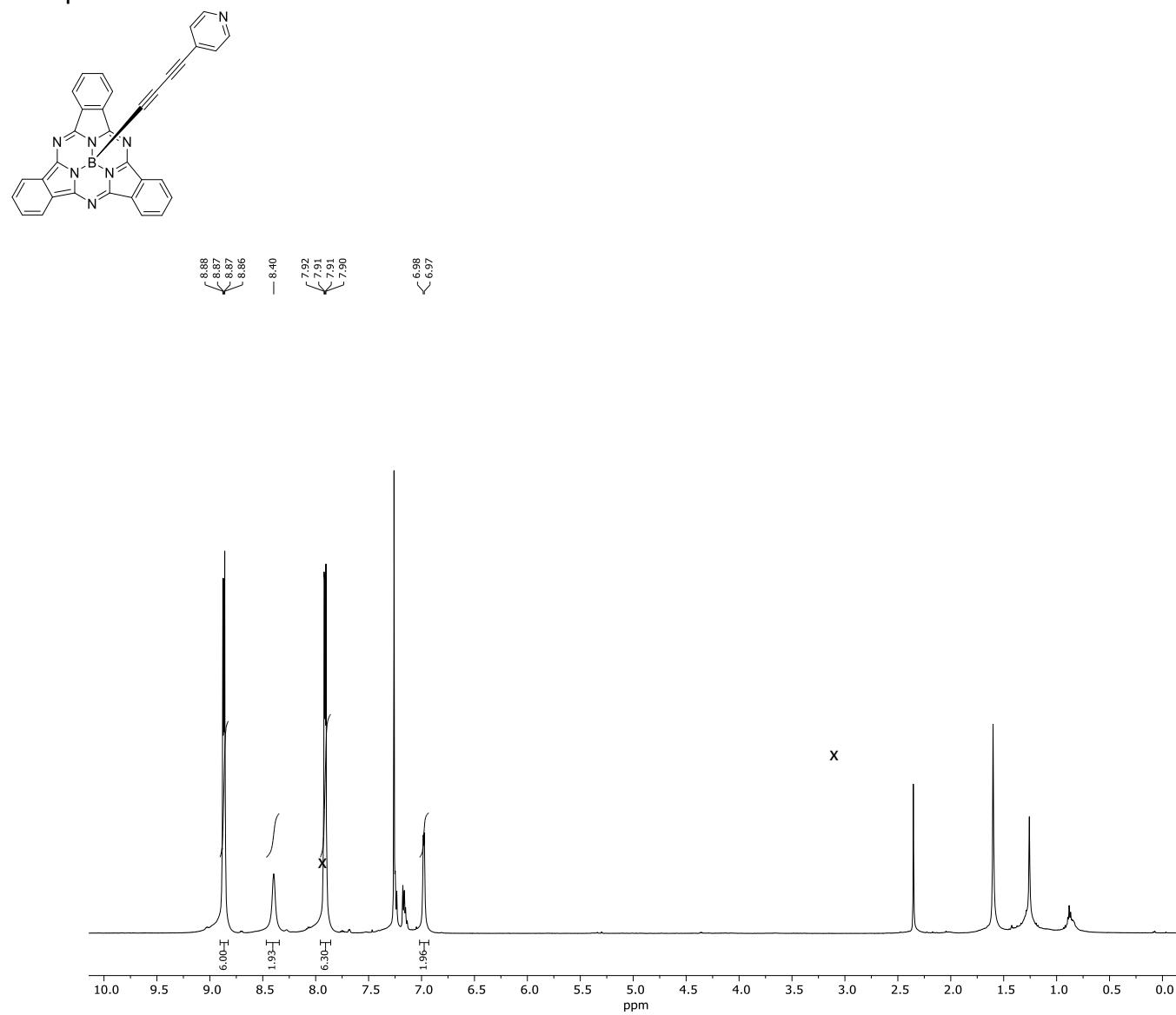


Figure S13. ¹H-NMR spectrum of compound 9 in CDCl₃. Toluene residues marked with x.

Compound 9

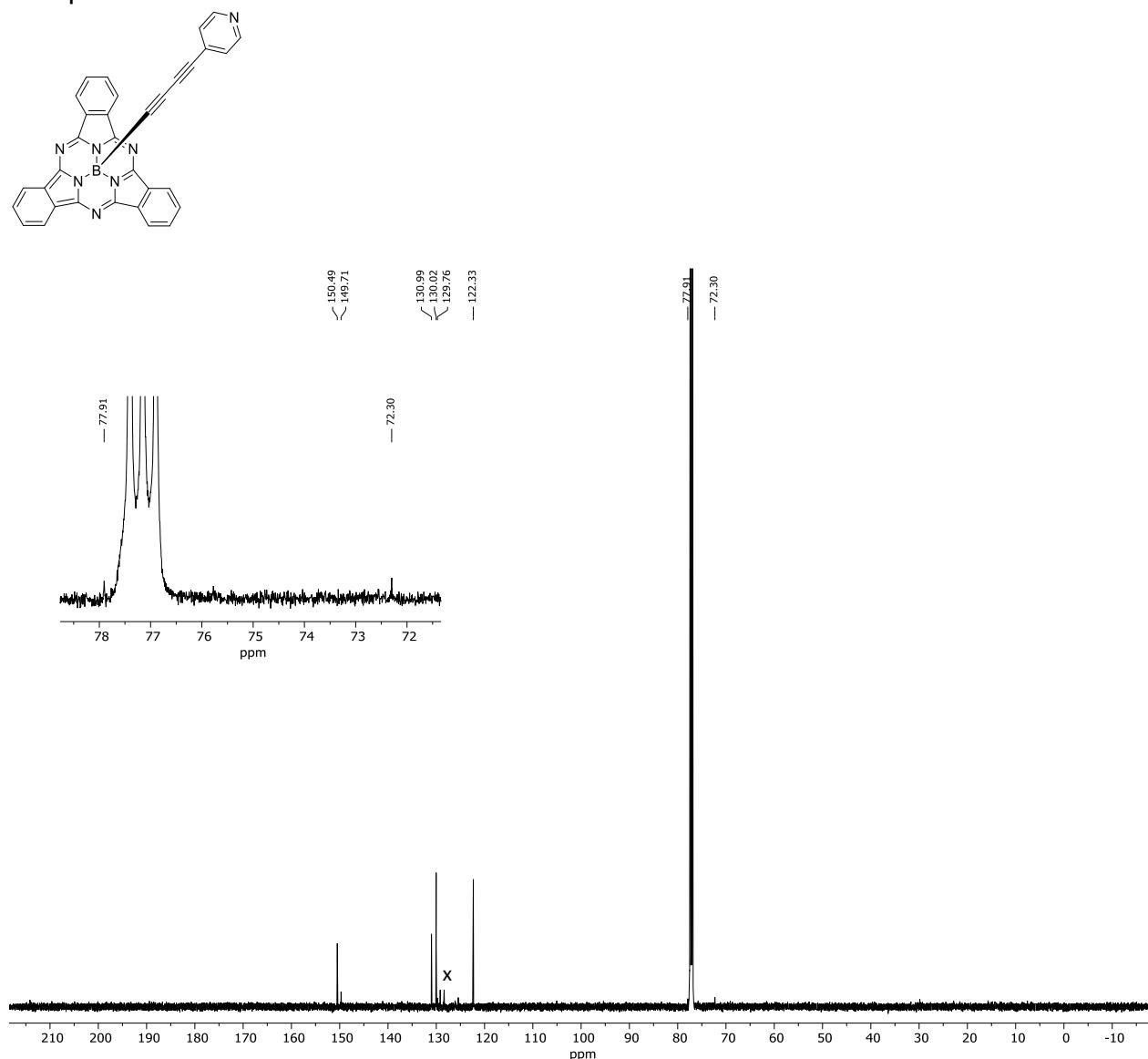
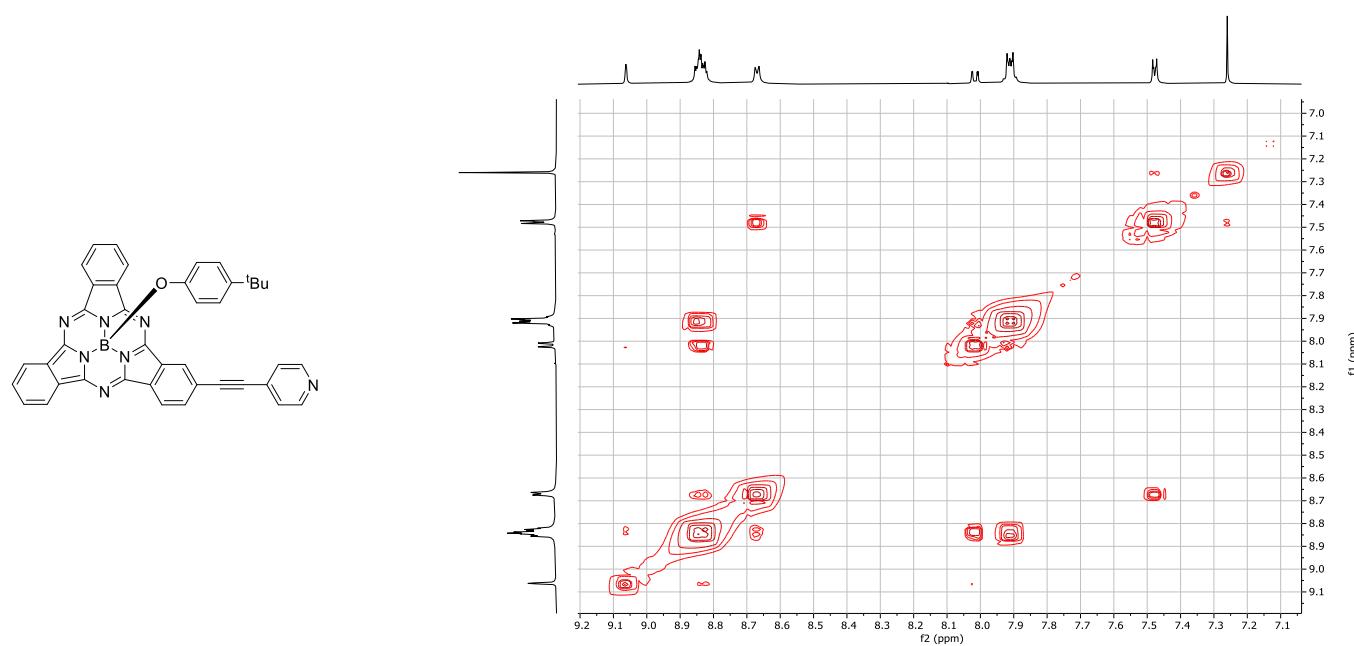
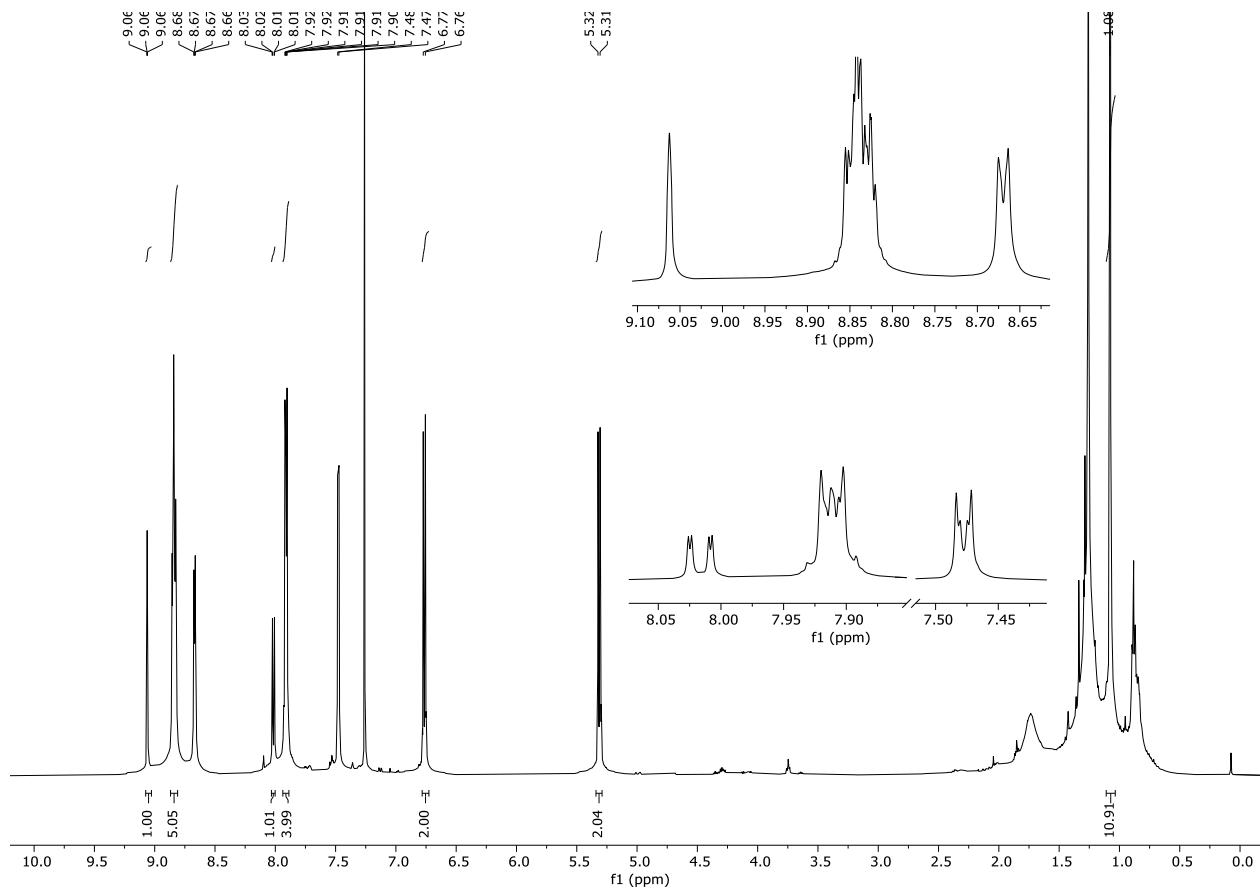


Figure S14. ^{13}C -NMR spectrum of compound 9 in CDCl_3 . Toluene residues marked with x.

Compound 10

Figure S15. COSY spectrum of compound 10 in CDCl₃Figure S16. ¹H-NMR spectrum of compound 10 in CDCl₃.

Compound 10

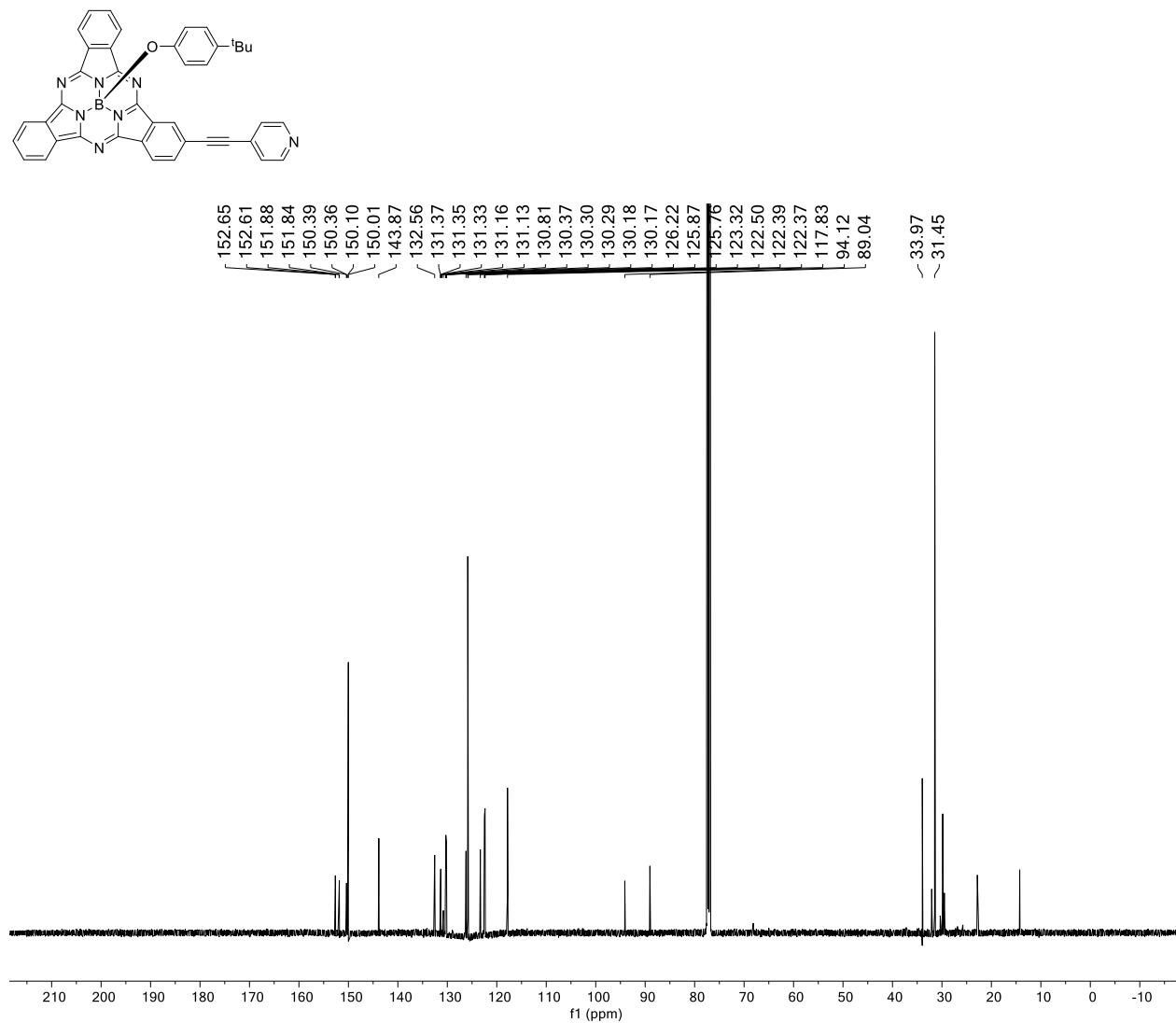


Figure S17. ^{13}C -NMR spectrum of compound 10 in CDCl_3 .

UV-Vis Absorption Spectroscopy

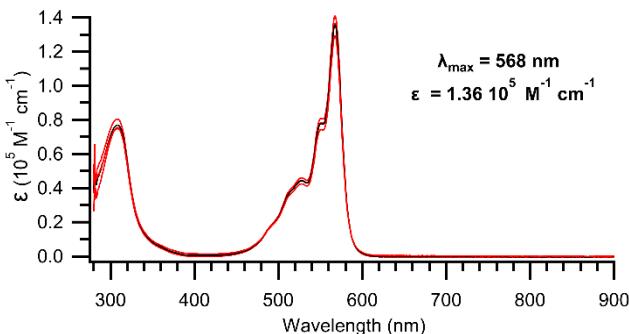


Figure S18. Absorption spectra of **3** in toluene, red lines showing the measured spectra and the black showing the average

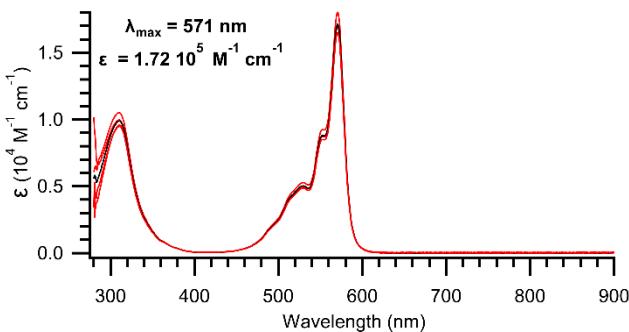
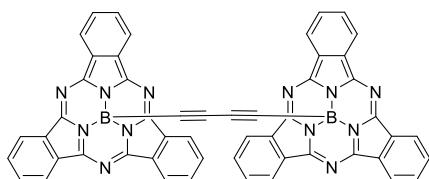


Figure S19. Absorption spectra of **4** in toluene, red lines showing the measured spectra and the black showing the average

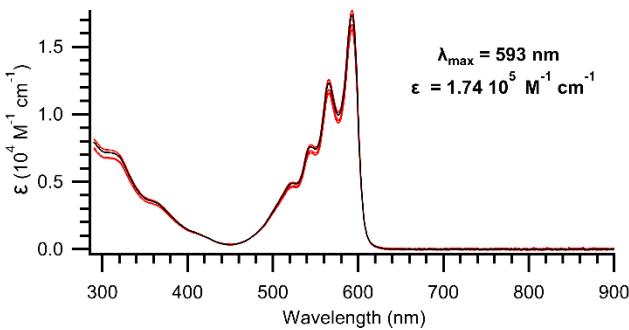
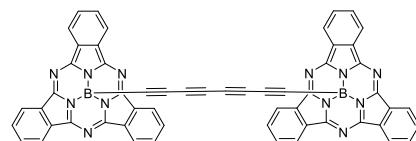
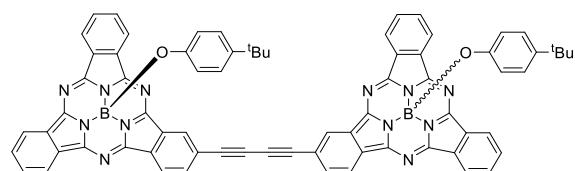
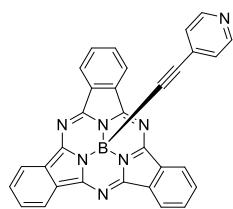
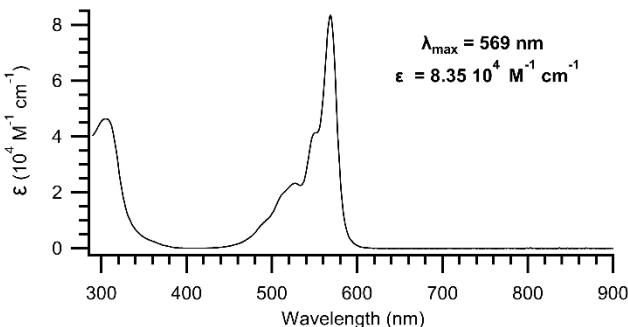
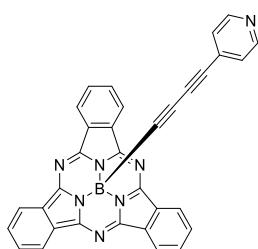
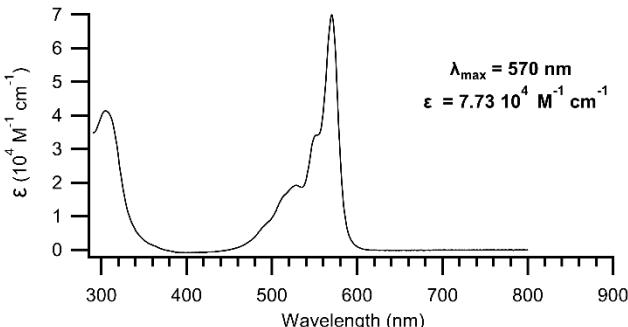
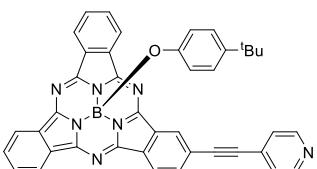
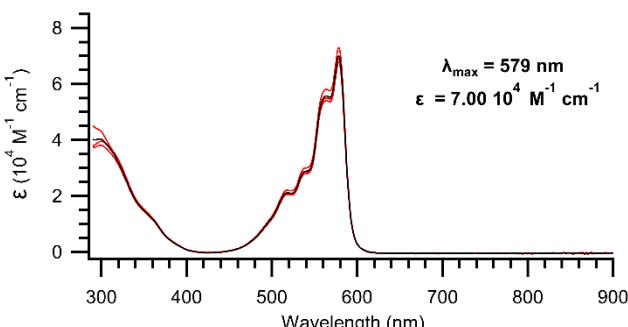


Figure S20. Absorption spectra of **5** in toluene, red lines showing the measured spectra and the black showing the average



**Figure S21.** Absorption spectrum of **8** in toluene.**Figure S22.** Absorption spectrum of **9** in toluene.**Figure S23.** Absorption spectra of **10** in toluene, red lines showing the measured spectra and the black showing the average

Electrochemistry

Compound 3

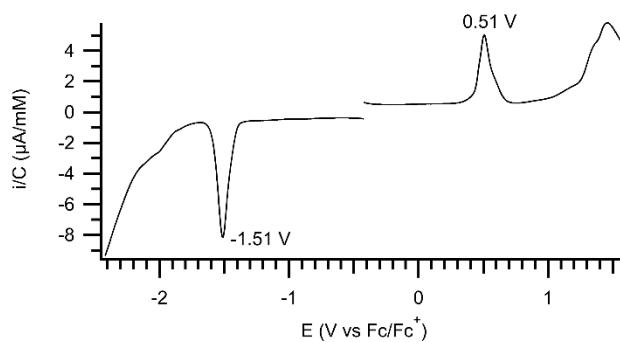
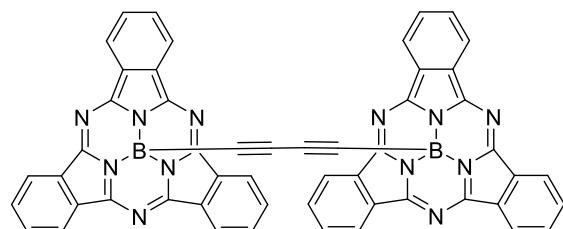


Figure S24. Differential pulse voltammogram of

compound 3 (0.24 mM) in CH_2Cl_2 (+ Bu_4NPF_6).

Reference electrode: Ag/AgCl , counter electrode: Pt wire; working electrode: glassy-carbon disc electrode (diameter 3 mm). Potentials are referenced to the ferrocene/ferrocenium (Fc/Fc^+) redox couple.

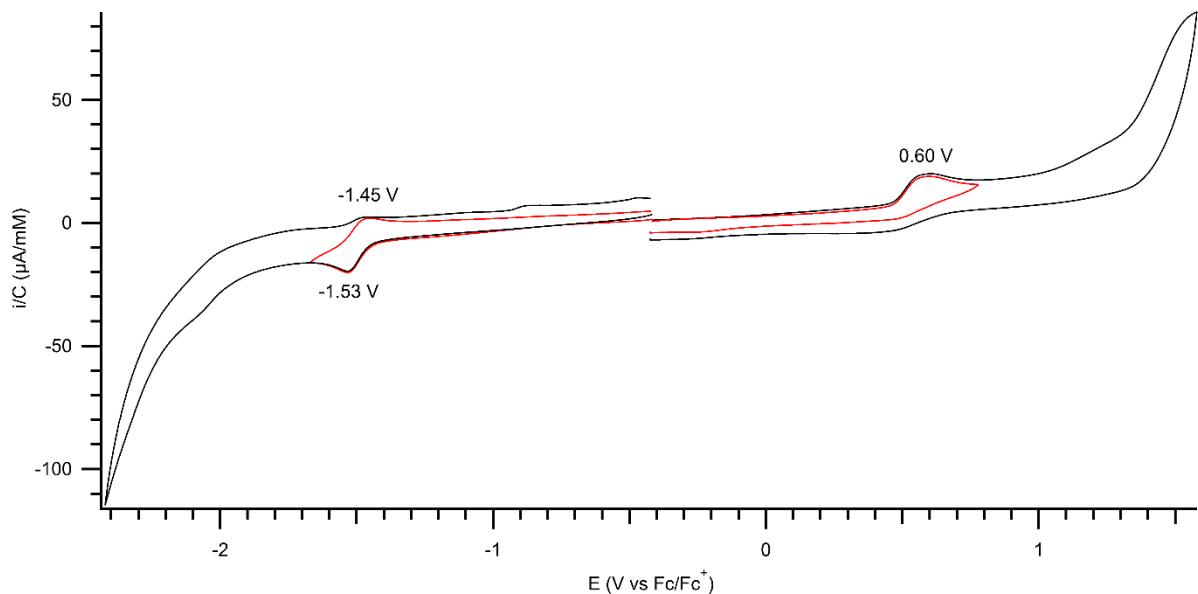


Figure S25. Cyclic voltammogram of compound 3 (0.24 mM) in CH_2Cl_2 (+ Bu_4NPF_6). Scan rate 0.1 V s^{-1} .

Reference electrode: Ag/AgCl , counter electrode: Pt wire; working electrode: glassy-carbon disc electrode (diameter 3 mm). Potentials are referenced to the ferrocene/ferrocenium (Fc/Fc^+) redox couple.

Compound 4

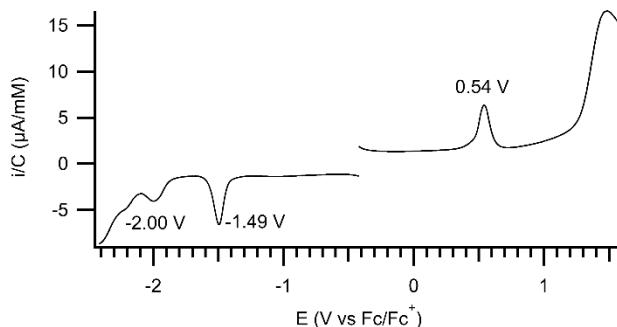
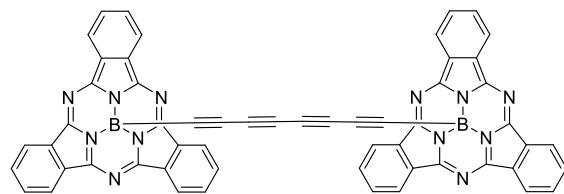


Figure S26. Differential pulse voltammogram of compound **4** (0.094 mM) in CH_2Cl_2 (+ Bu_4NPF_6).

Reference electrode: Ag/AgCl, counter electrode: Pt wire; working electrode: glassy-carbon disc electrode (diameter 3 mm). Potentials are referenced to the ferrocene/ferrocenium (Fc/Fc^+) redox couple.

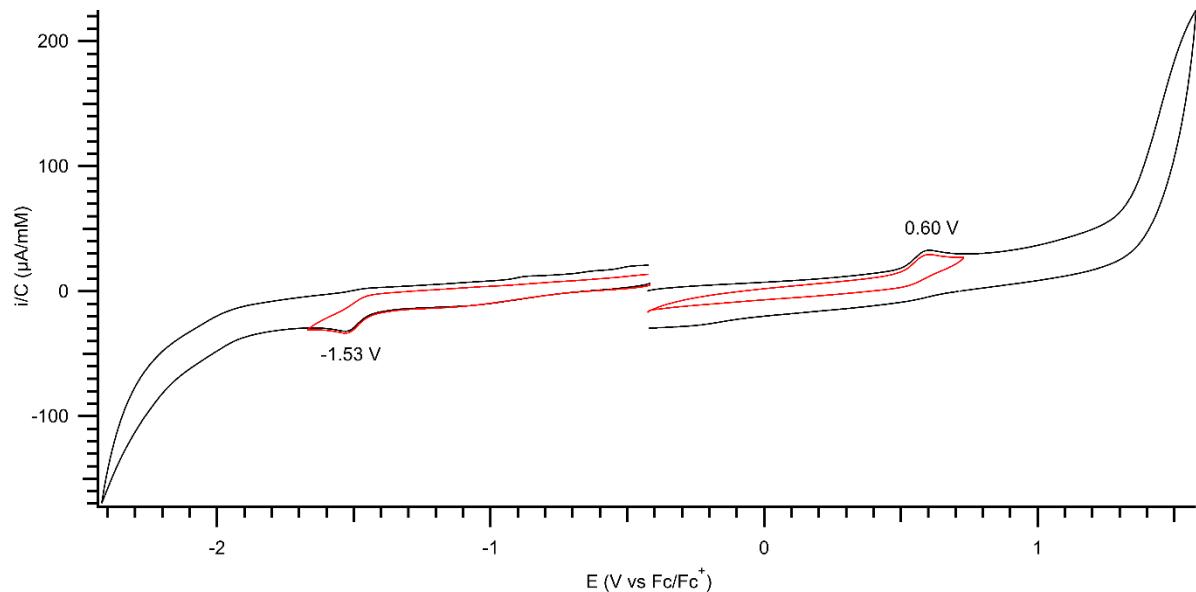


Figure S27. Cyclic voltammogram of compound **4** (0.094 mM) in CH_2Cl_2 (+ Bu_4NPF_6). Scan rate 0.1 V s^{-1} .

Reference electrode: Ag/AgCl, counter electrode: Pt wire; working electrode: glassy-carbon disc electrode (diameter 3 mm). Potentials are referenced to the ferrocene/ferrocenium (Fc/Fc^+) redox couple.

Compound 5

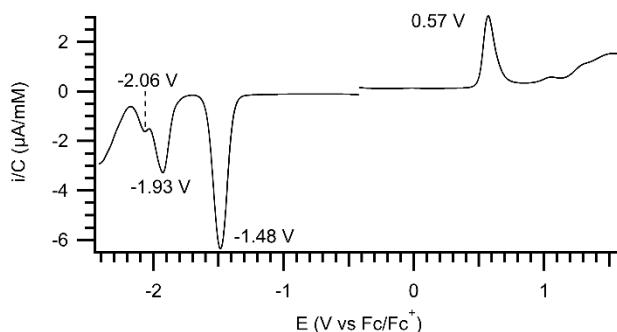
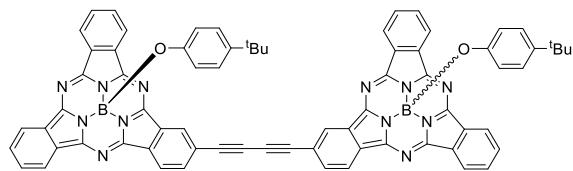


Figure S28. Differential pulse voltammogram of compound 5 (0.99 mM) in CH_2Cl_2 (+ Bu_4NPF_6).

Reference electrode: Ag/AgCl, counter electrode: Pt wire; working electrode: glassy-carbon disc electrode (diameter 3 mm). Potentials are referenced to the ferrocene/ferrocenium (Fc/Fc^+) redox couple.

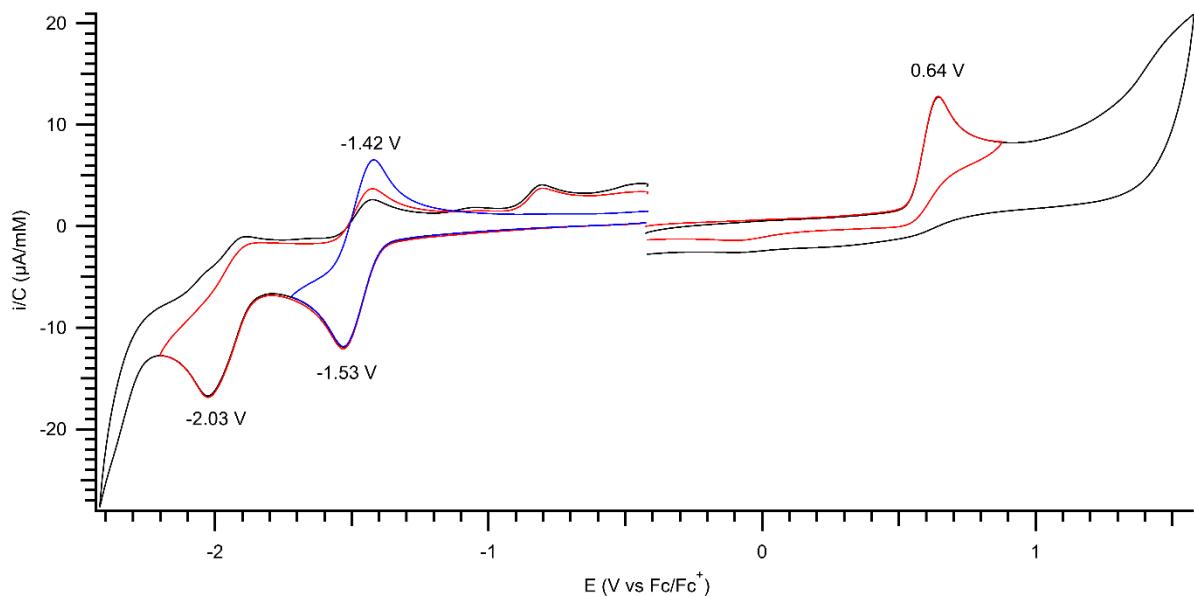


Figure S29. Cyclic voltammogram of compound 5 (0.99 mM) in CH_2Cl_2 (+ Bu_4NPF_6). Scan rate 0.1 V s^{-1} .

Reference electrode: Ag/AgCl, counter electrode: Pt wire; working electrode: glassy-carbon disc electrode (diameter 3 mm). Potentials are referenced to the ferrocene/ferrocenium (Fc/Fc^+) redox couple.