

Towards novel thieno-fused subporphyrazines via functionalized thiophene precursors

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Supporting Information

Contents

NMR Spectra.....	2
Infrared Spectra.....	13
X-Ray crystallography	15

NMR Spectra

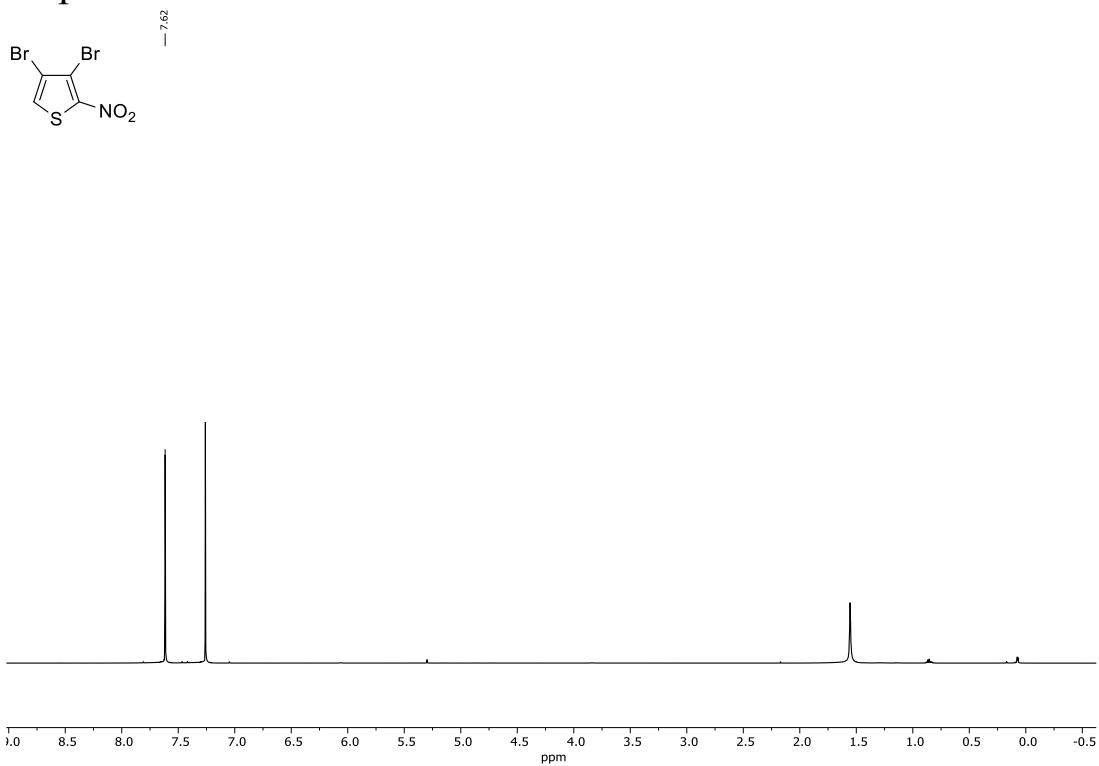


Figure S1: ¹H NMR (500 MHz, CDCl₃) spectrum of **4**.

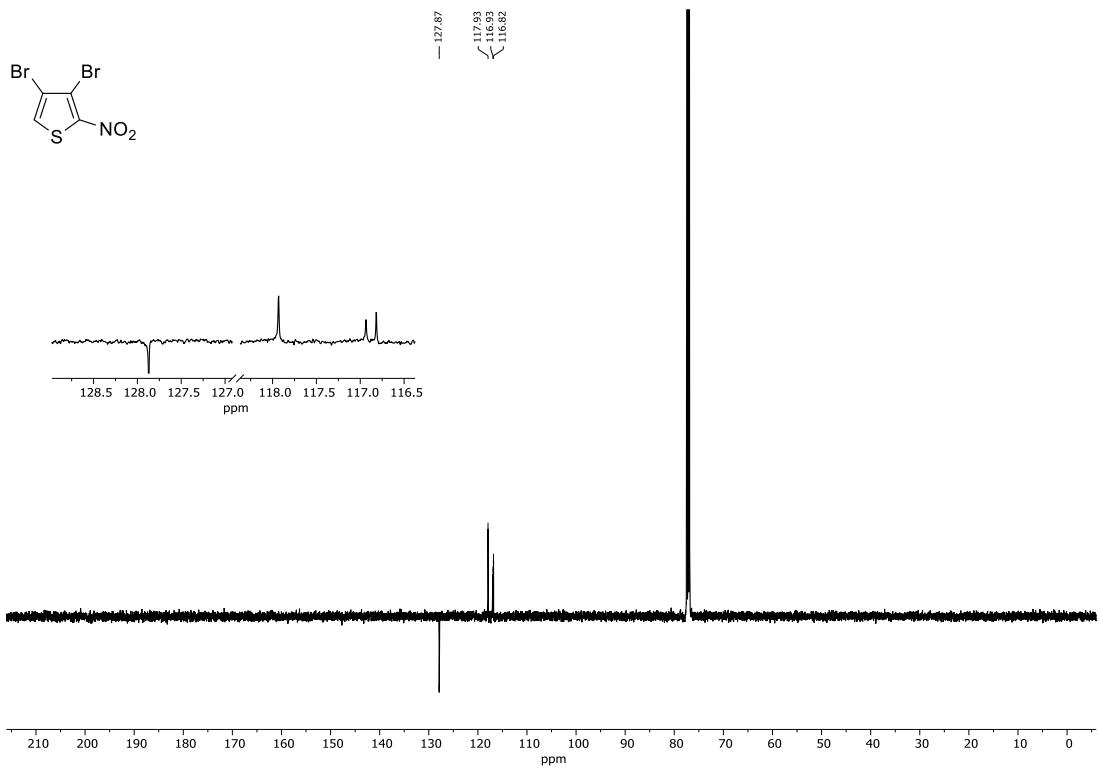


Figure S2: ¹³C NMR APT (126 MHz, CDCl₃) spectrum of **4**.

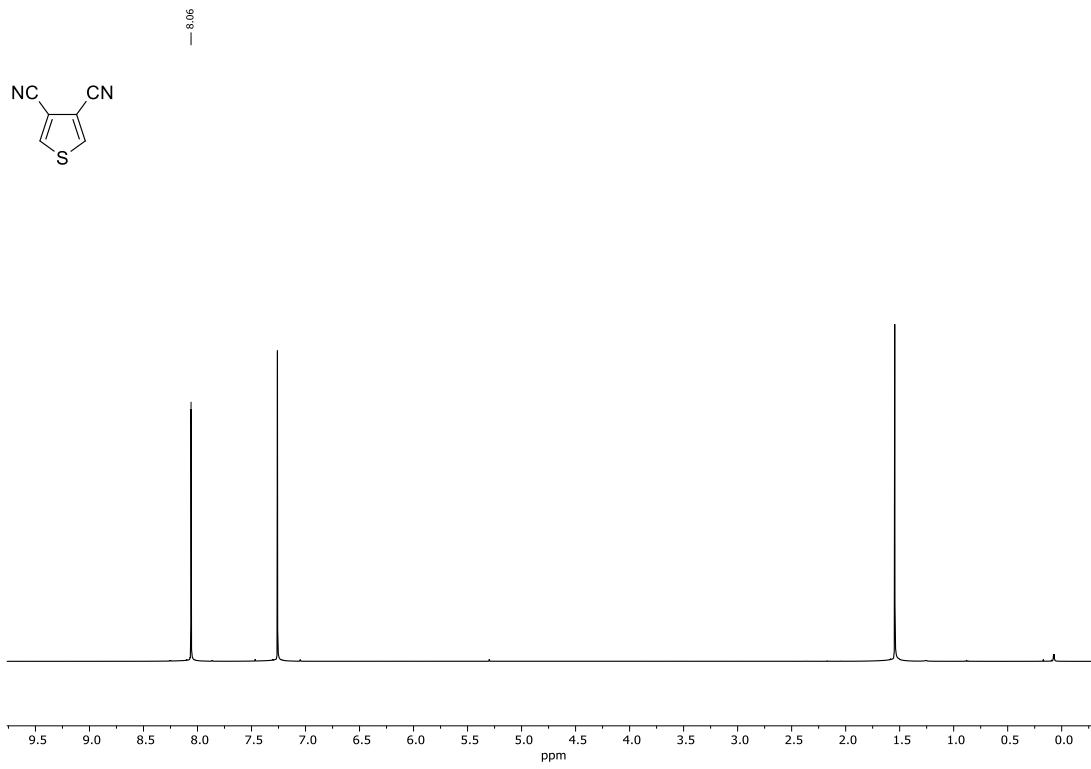


Figure S3: ^1H NMR (500 MHz, CDCl_3) spectrum of **6**.

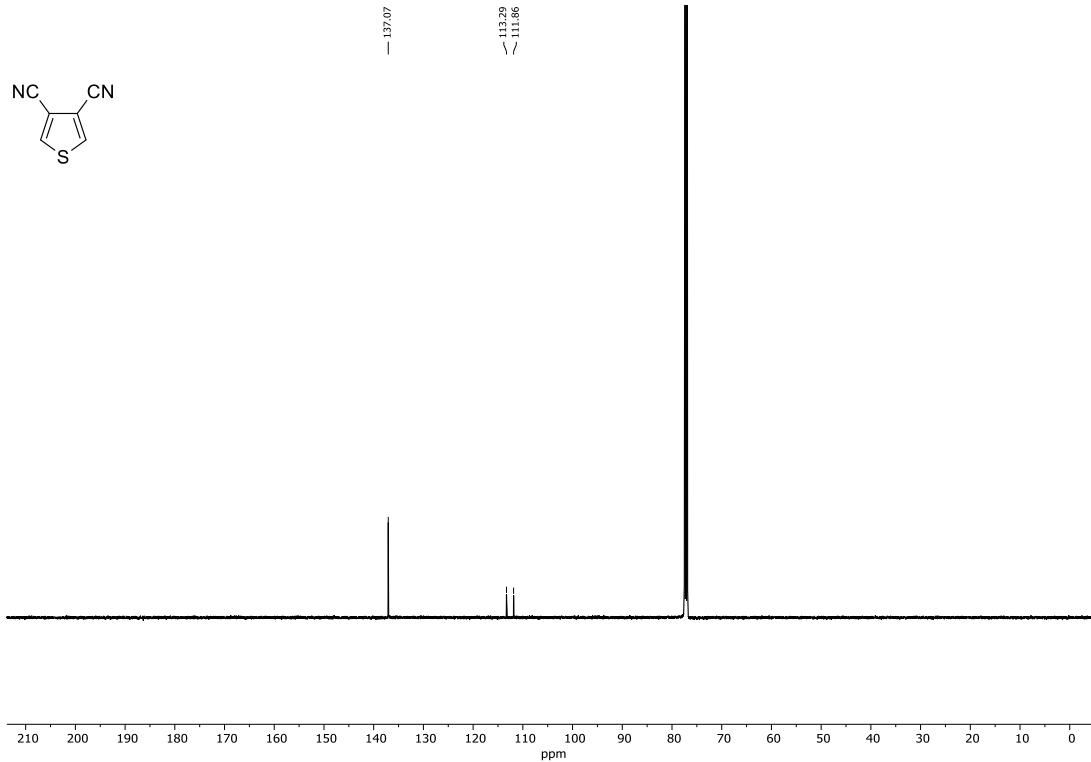


Figure S4: ^{13}C NMR (126 MHz, CDCl_3) spectrum of **6**.

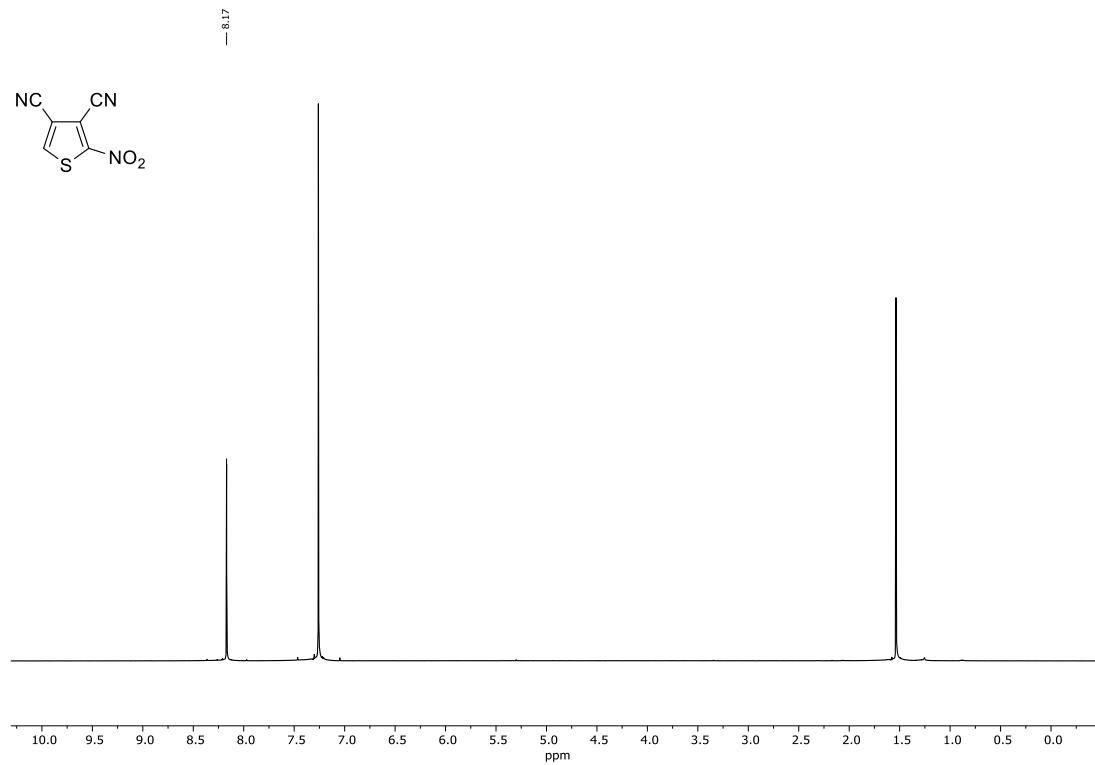


Figure S5: ^1H NMR (500 MHz, CDCl_3) spectrum of **5**.

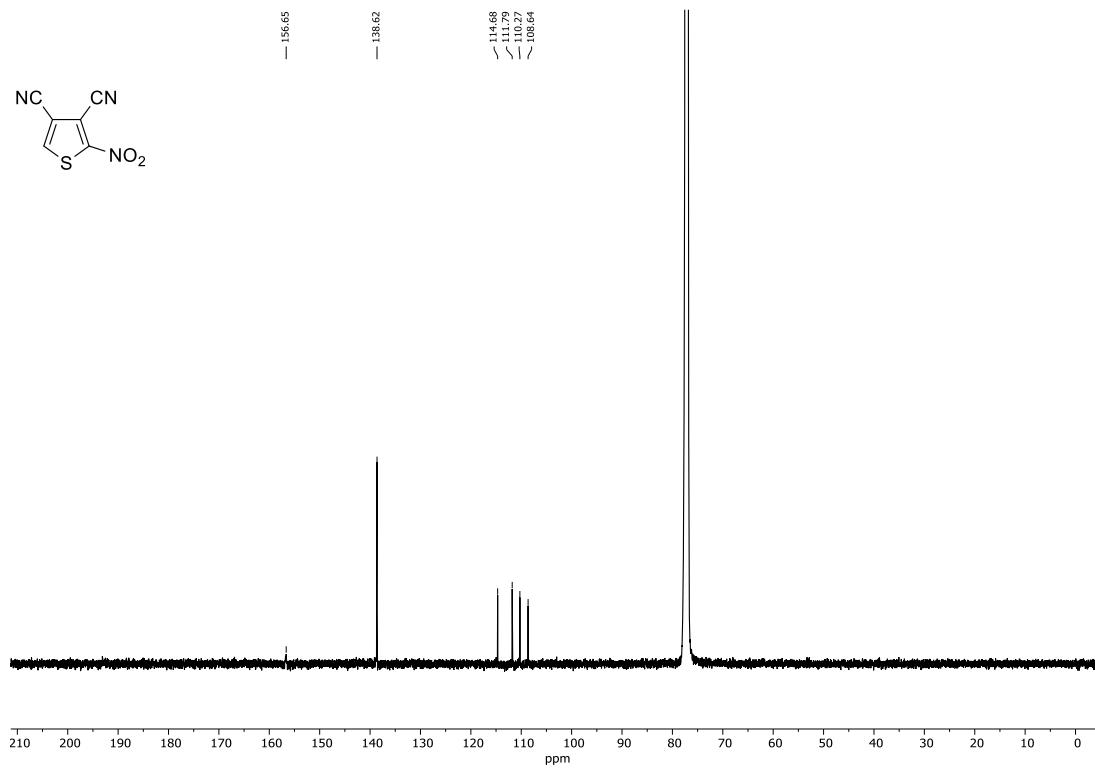


Figure S6: ^{13}C -NMR (126 MHz, CDCl_3) spectrum of **5**.

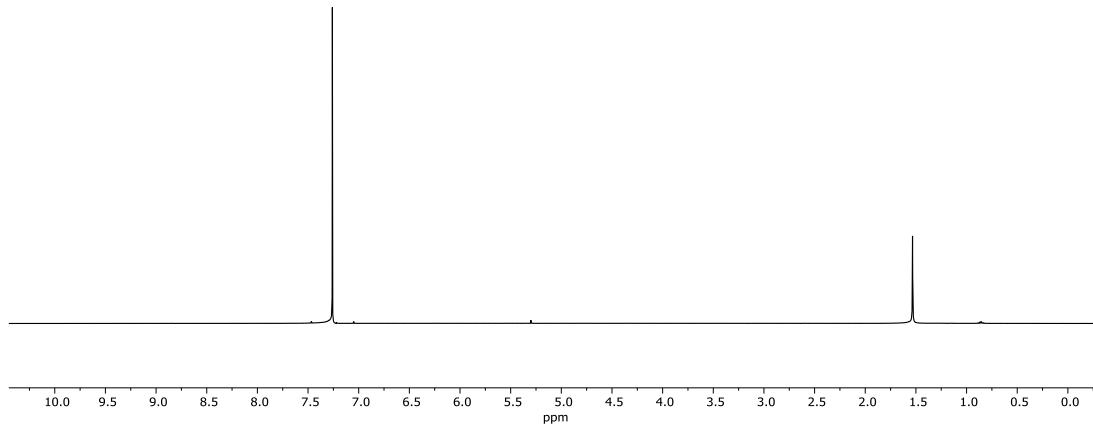
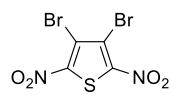


Figure S7: ¹H NMR (500 MHz, CDCl₃) spectrum of **2**.

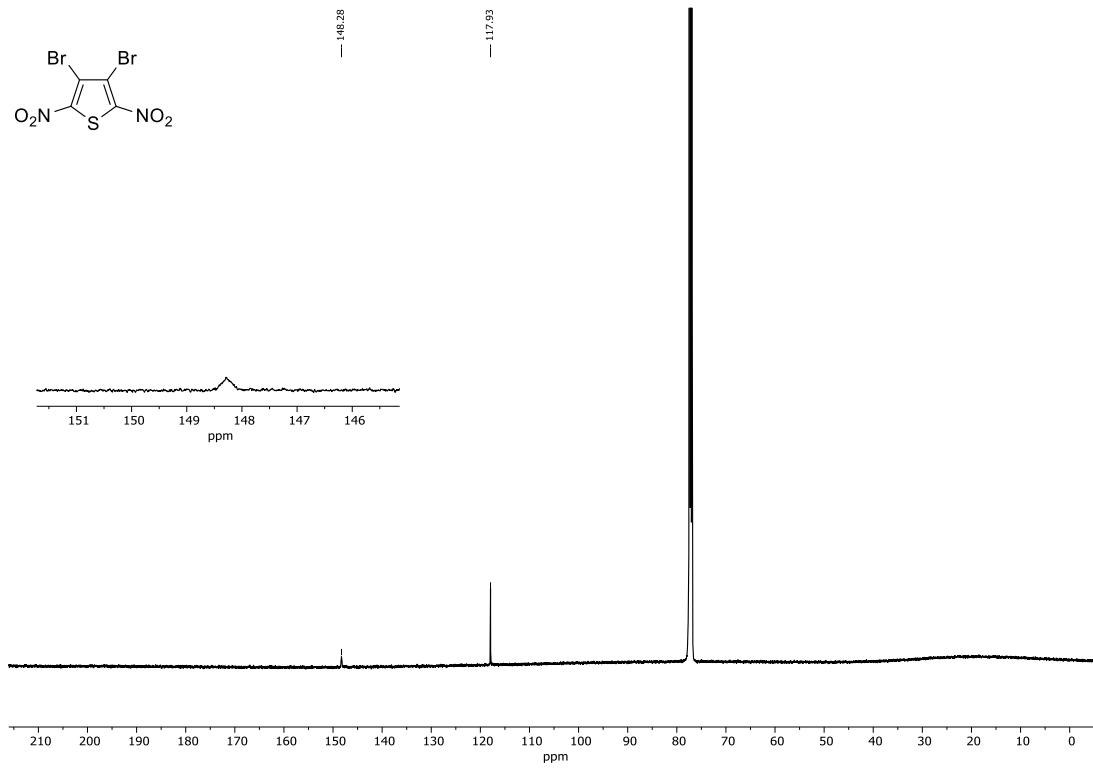


Figure S8: ¹³C NMR (126 MHz, CDCl₃) spectrum of **2**, with zoom between 151–146 ppm.

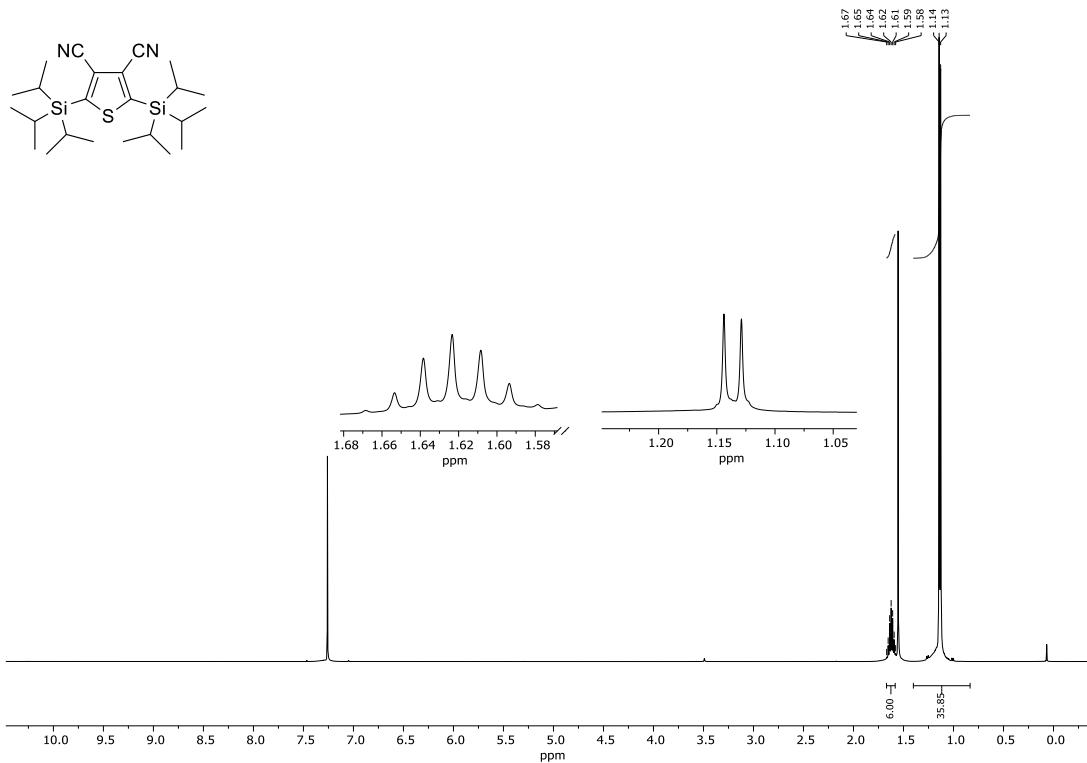


Figure S9: ^1H NMR (500 MHz, CDCl_3) spectrum **7a**, with zooms between 1.68– 1.58 and 1.25–1.05 ppm.

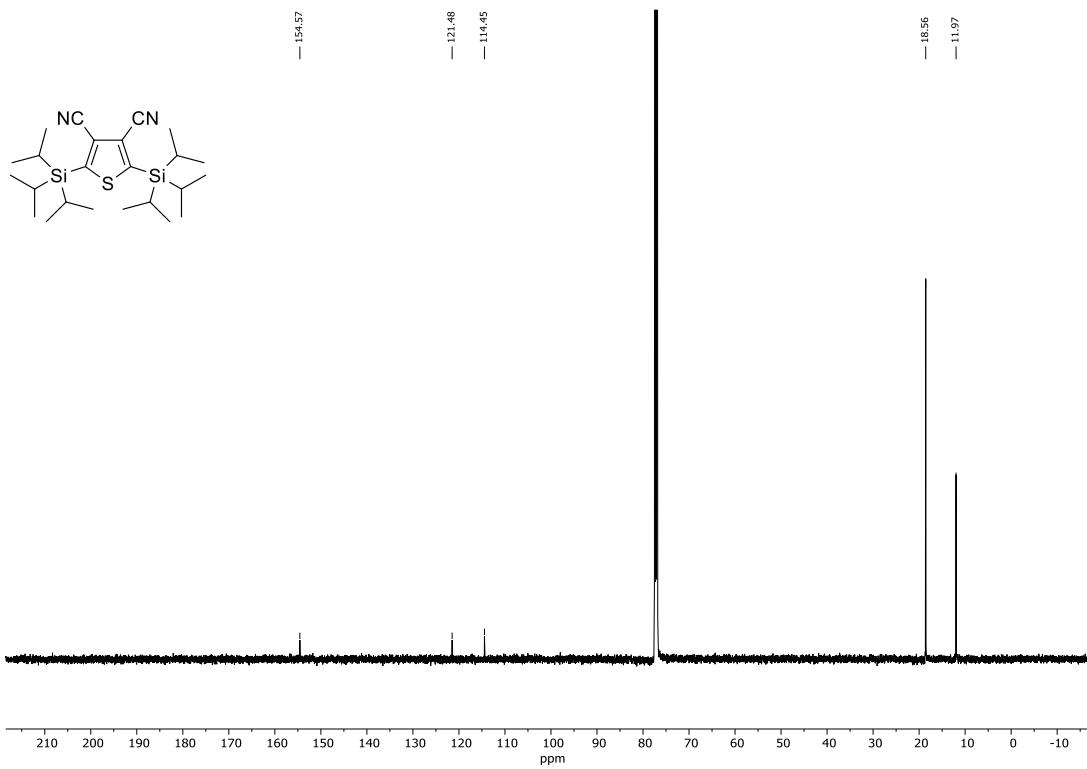


Figure S10: ^{13}C NMR (126 MHz, CDCl_3) spectrum of **7a**.

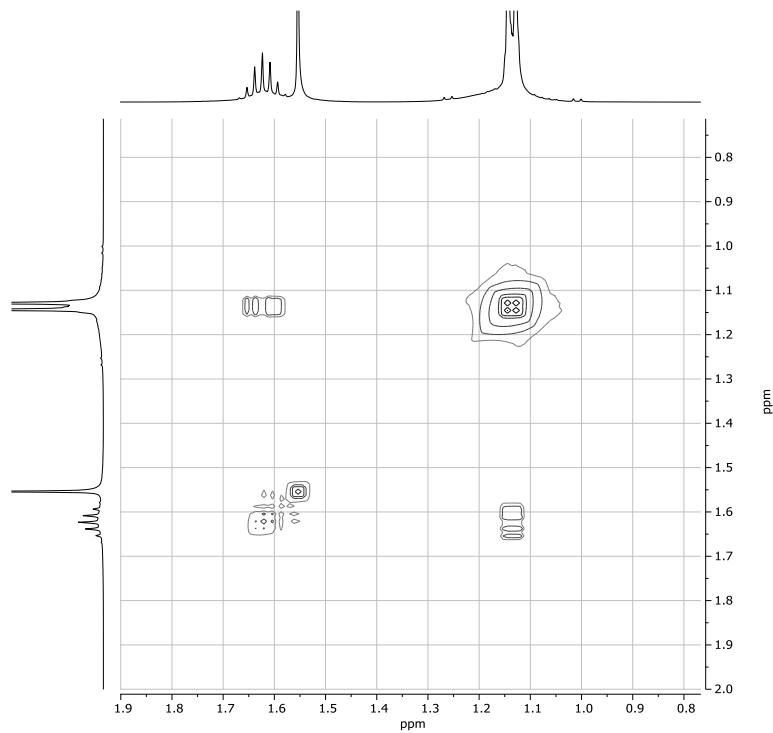


Figure S11: COSY (500 MHz, CDCl_3) spectrum of **7a**.

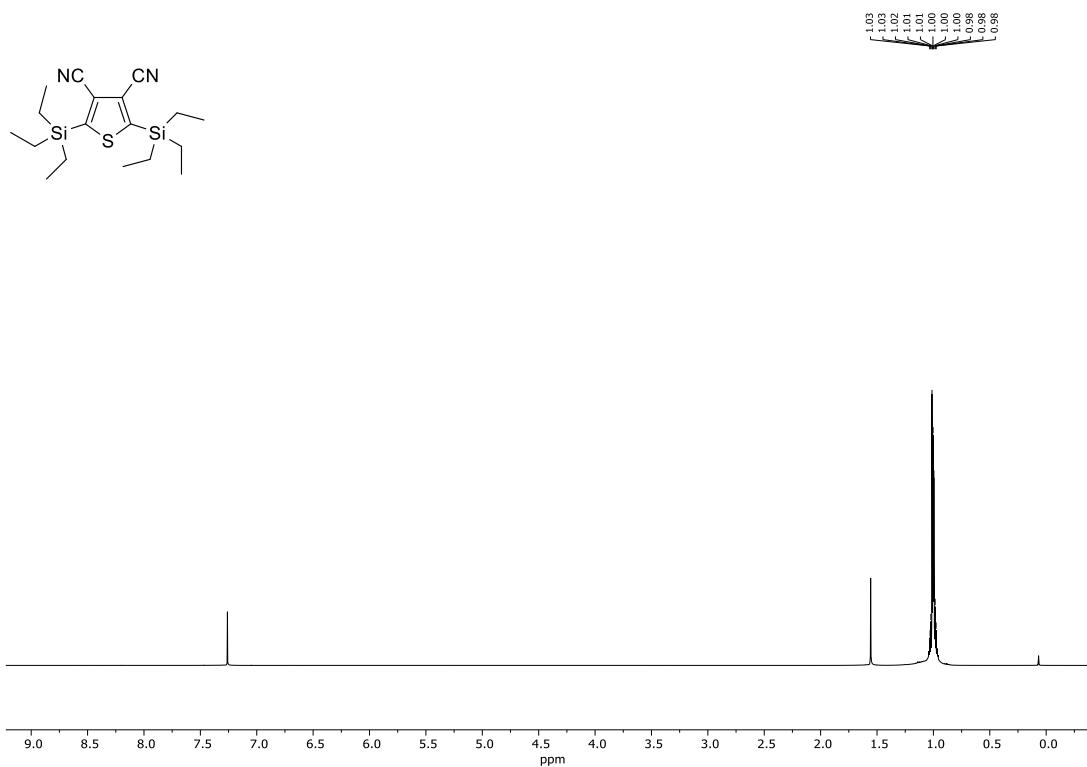


Figure S12: ¹H NMR (500 MHz, CDCl₃) spectrum of 7b.

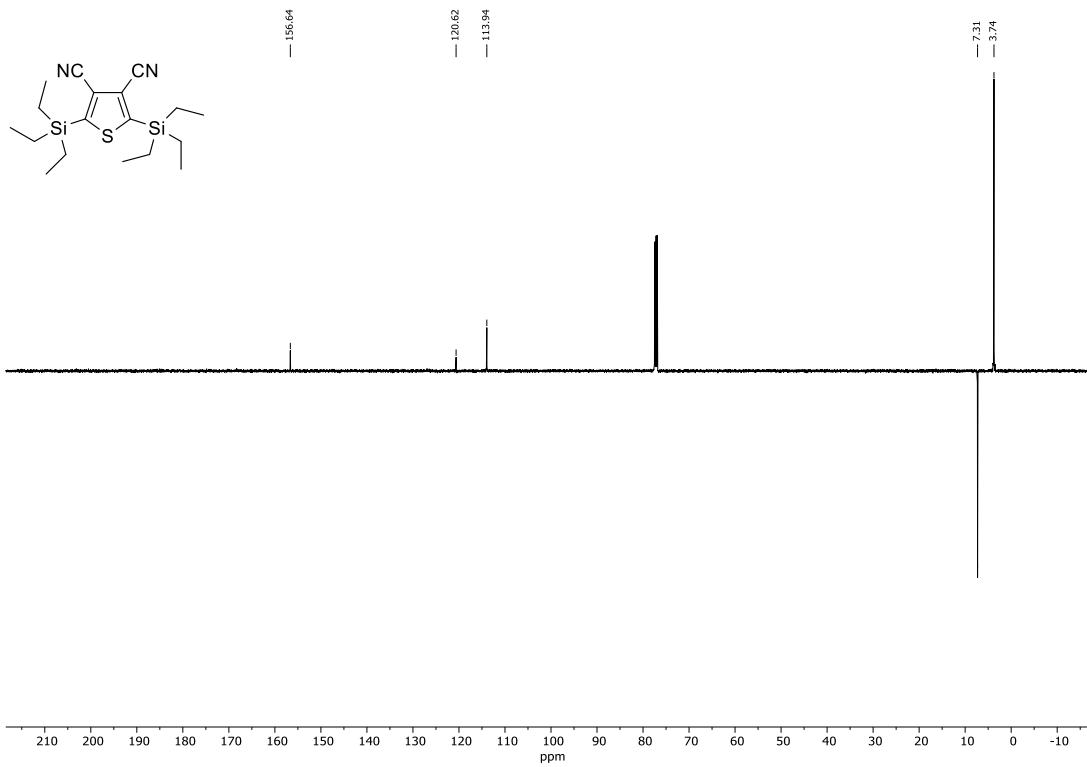


Figure S13: ¹³C NMR APT (126 MHz, CDCl₃) spectrum of 7b.

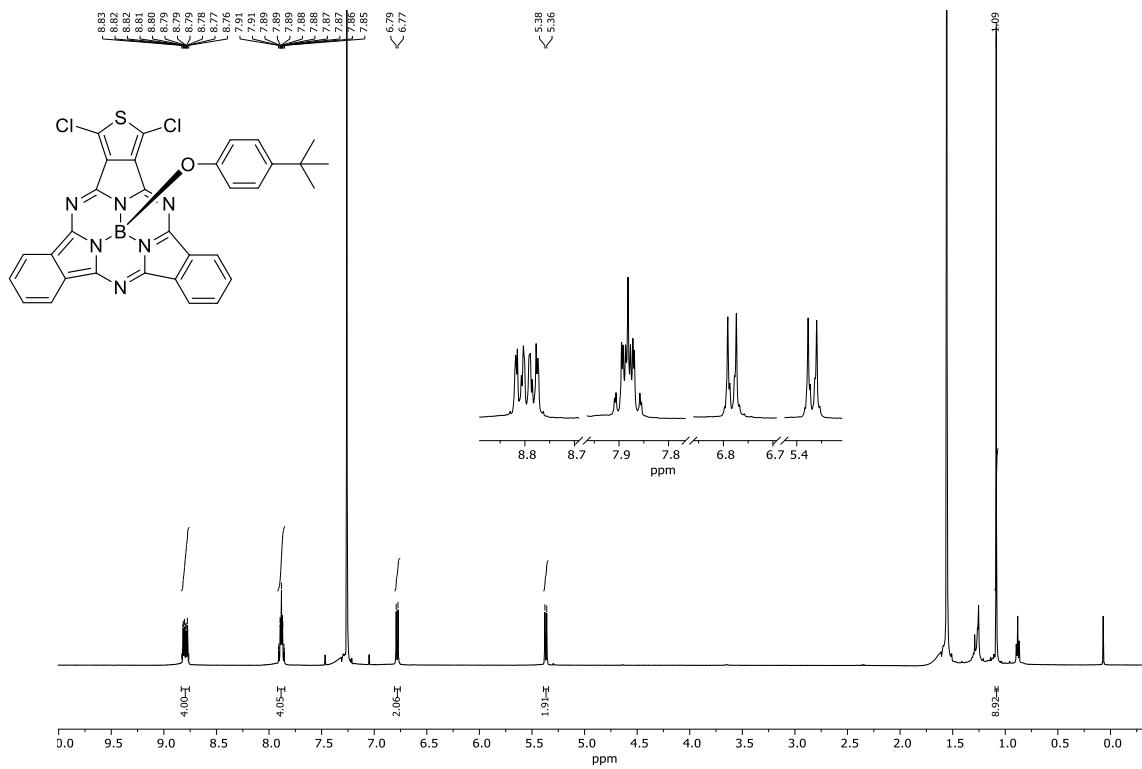


Figure S14: ^1H NMR (500 MHz, CDCl_3) spectrum of $\text{TPCl}_2\text{-Ar}$ with zoom between 8.9–5.3 ppm.

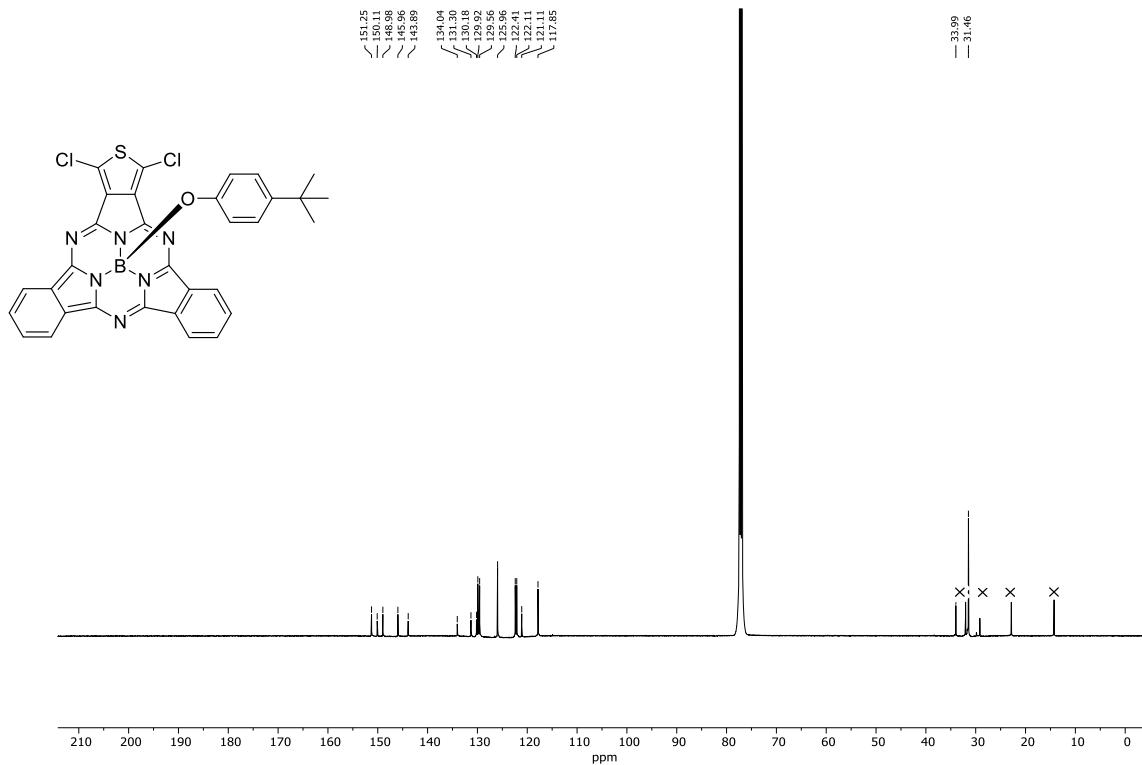


Figure S15: ^{13}C NMR (126 MHz, CDCl_3) spectrum of $\text{TPCl}_2\text{-Ar}$. Peaks originating from *n*-grease marked with x.

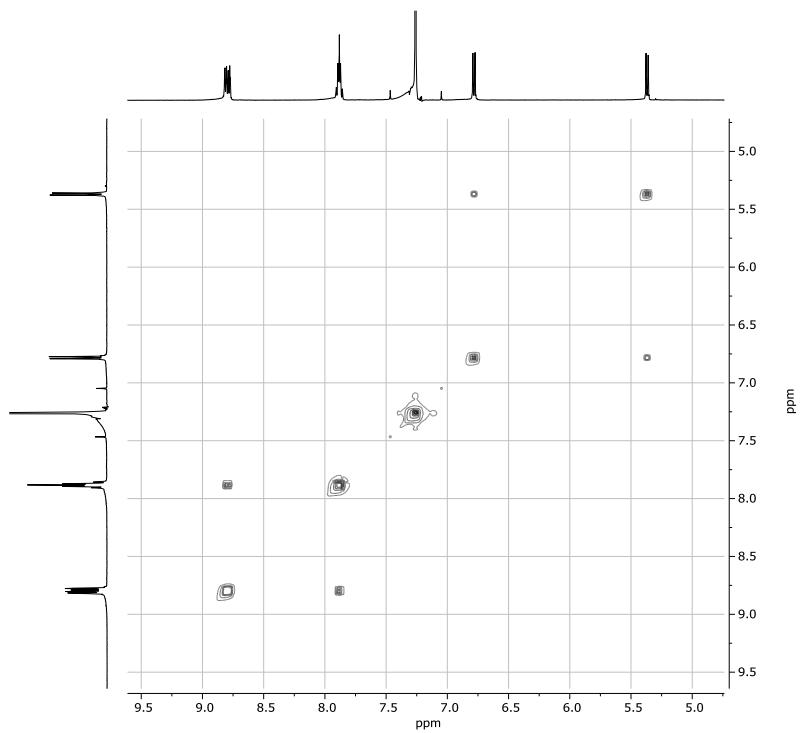


Figure S16: COSY (500 MHz, CDCl₃) spectrum of TP(Cl₂)-Ar.

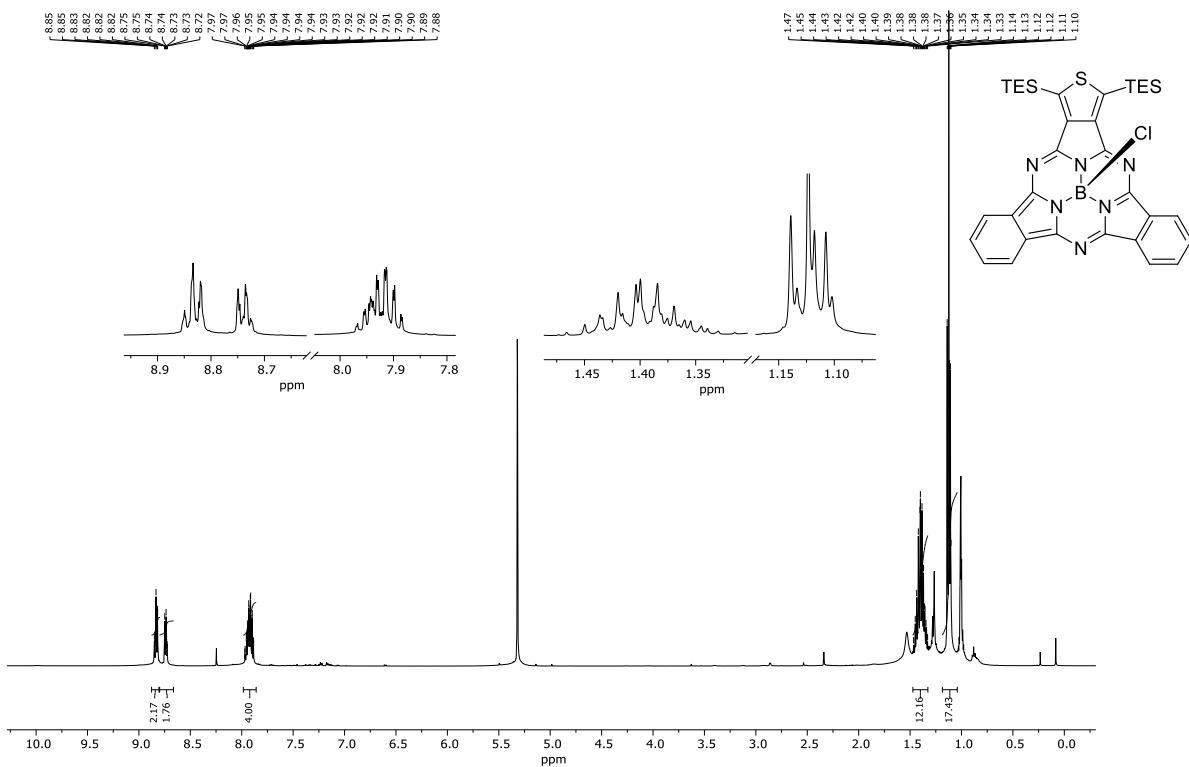


Figure S17: ^1H NMR (500 MHz, CD_2Cl_2) spectrum of **10** with trace contamination of **11**.

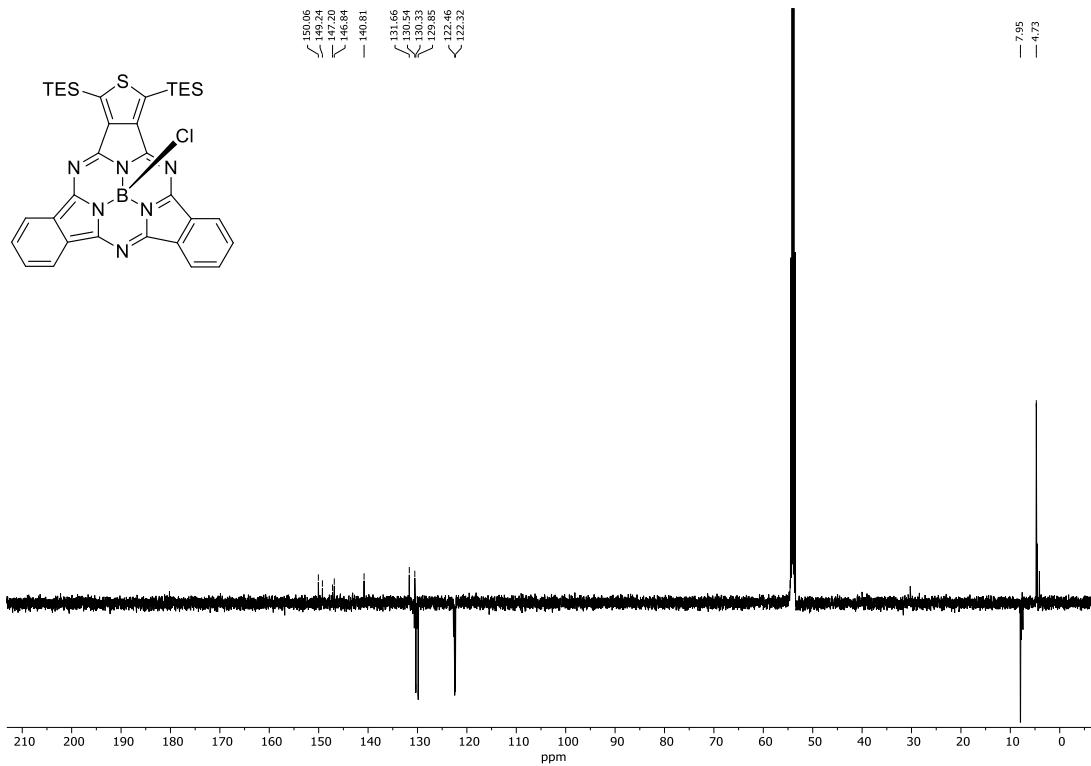


Figure S18: ^{13}C NMR APT (126 MHz, CD_2Cl_2) spectrum of **10** with trace contamination of **11**.

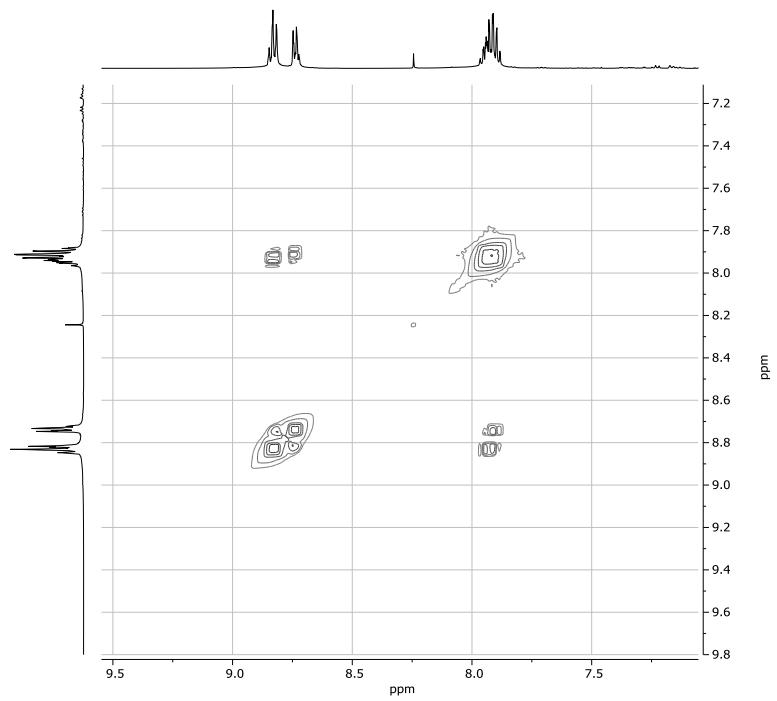


Figure S19: COSY (500 MHz, CD_2Cl_2) spectrum of **10** with trace contamination of **11**.

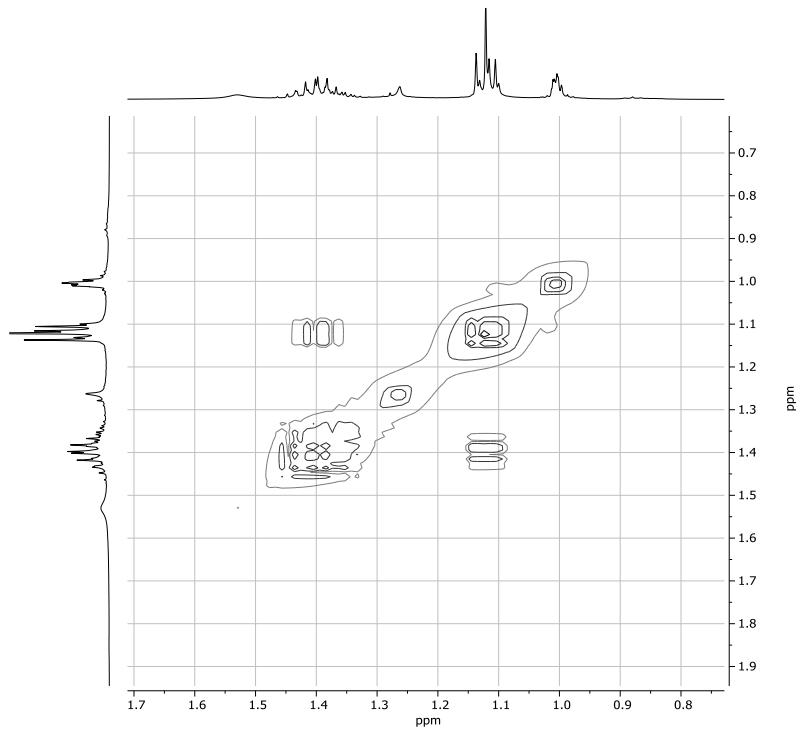


Figure S20: COSY (500 MHz, CD_2Cl_2) spectrum of **10** with trace contamination of **11**.

Infrared Spectra

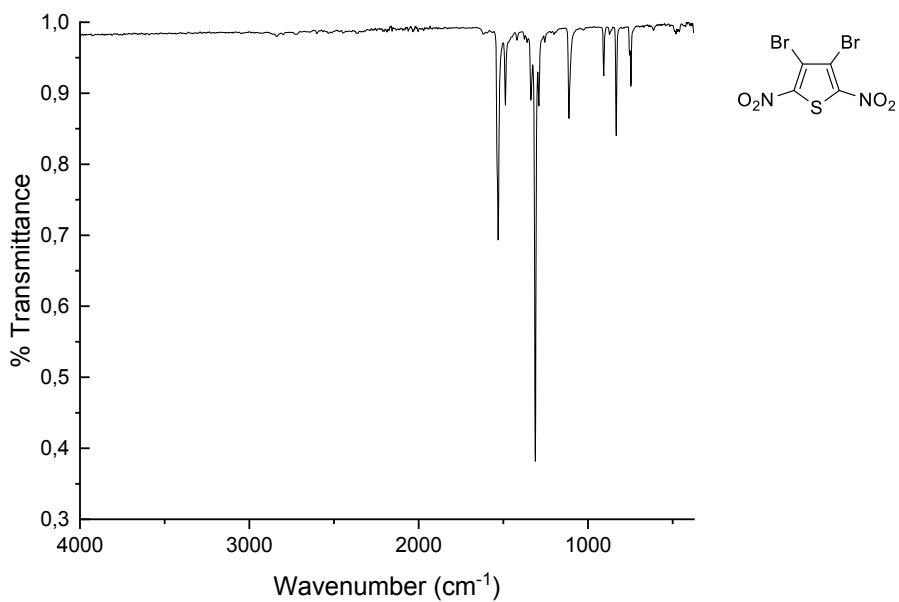


Figure S21: (ATR, neat) IR-Spectrum of 2.

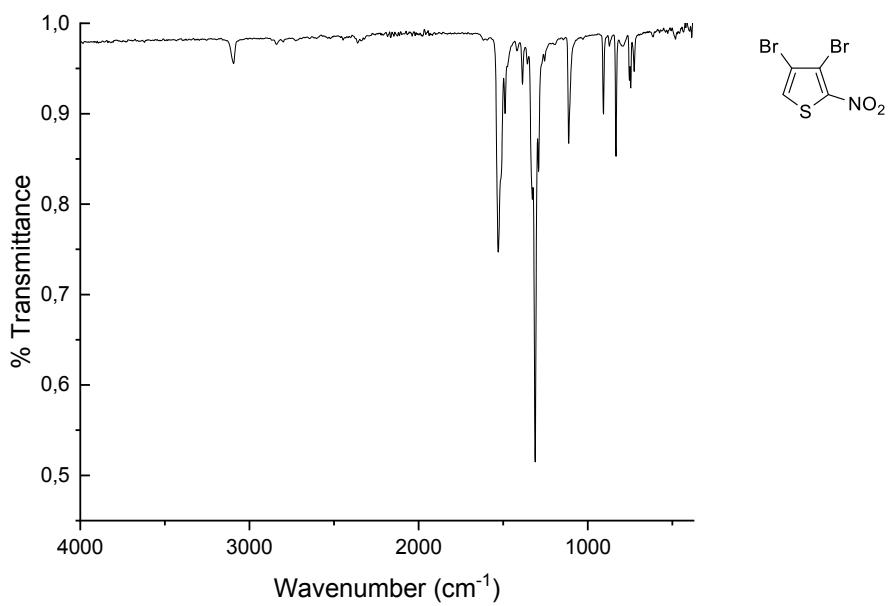


Figure S22: (ATR, neat) IR-Spectrum of 4.

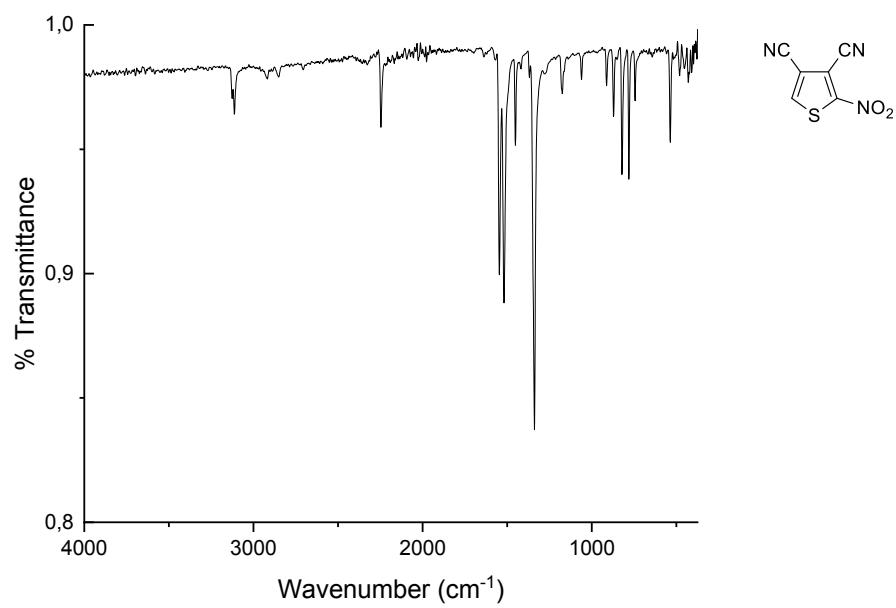


Figure S23: (ATR, neat) IR-Spectrum of **5**.

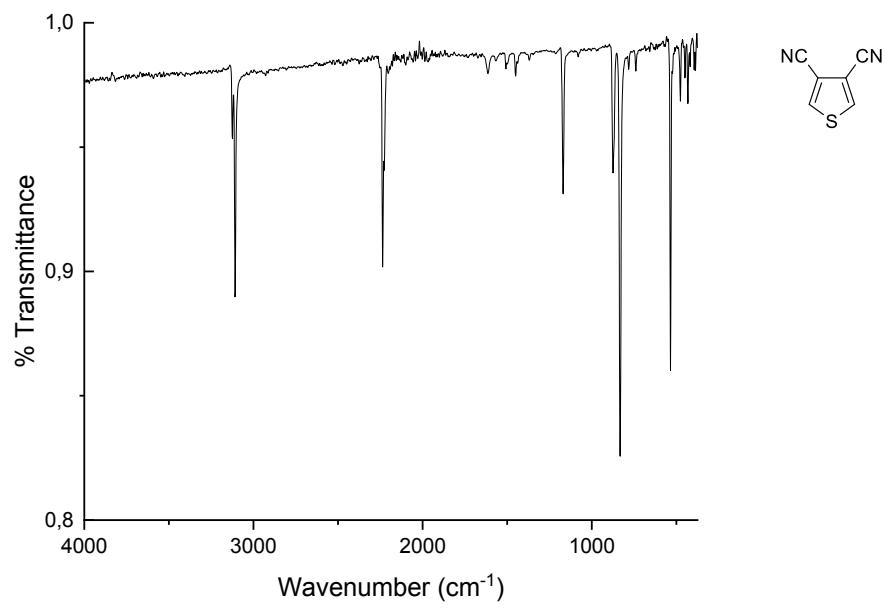


Figure S24: (ATR, neat) IR-Spectrum of **6**.

X-Ray crystallography

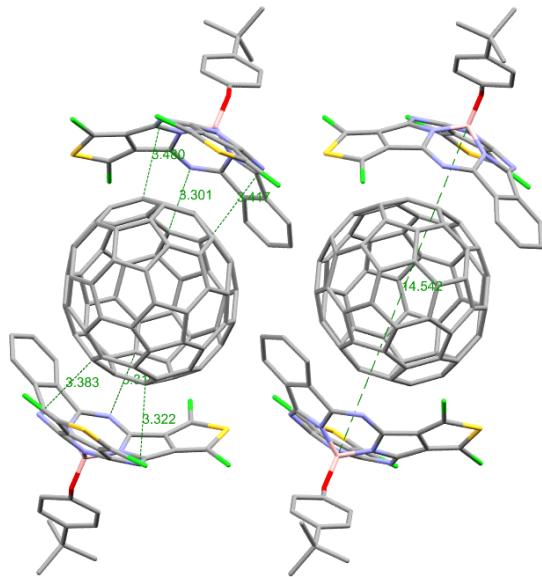


Figure S25: Unit cell of 2:1 complex of $(TPCl_2)_2\text{-Ar}$ and C_{70} viewed along the a-axis. Average distance of 3.4 Å between the π -systems is displayed, in addition to inter boron distance. Hydrogen atoms and toluene molecules have been omitted for clarity.

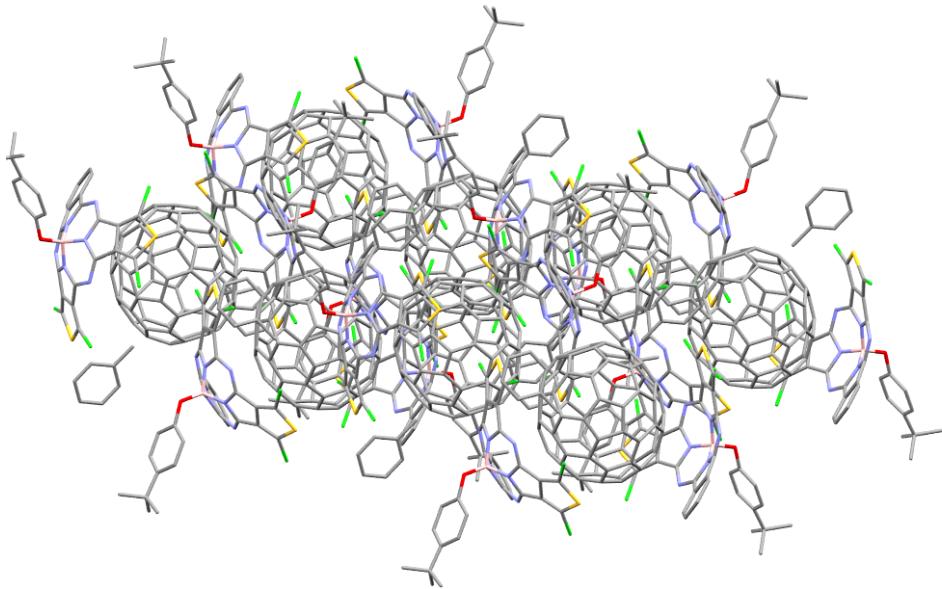


Figure S26: Crystal packing top view of 2:1 $(TPCl_2)_2\text{-Ar}$ and C_{70} . Hydrogen atoms have been omitted for clarity.