

Supplementary Materials: Synthesis, Characterization, and Electropolymerization of Extended Fused-Ring Thieno[3,4-*b*]pyrazine-Based Terthienyls

Kristine L. Konkol, Ryan L. Schwiderski and Seth C. Rasmussen

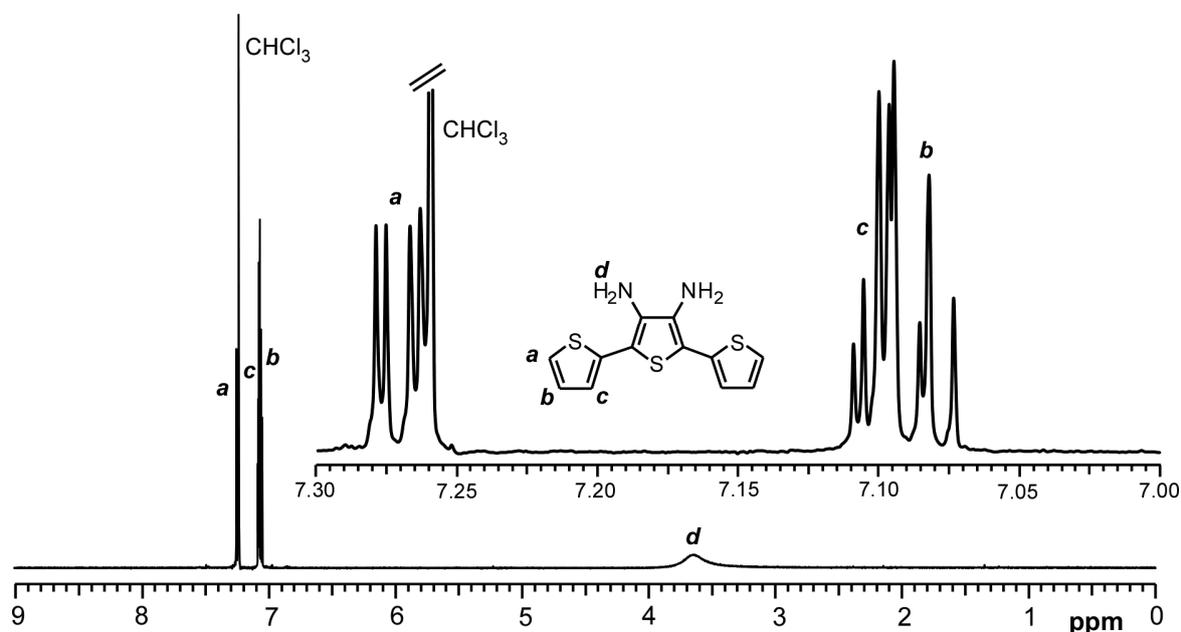


Figure S1. ¹H NMR Spectrum of Compound 10.

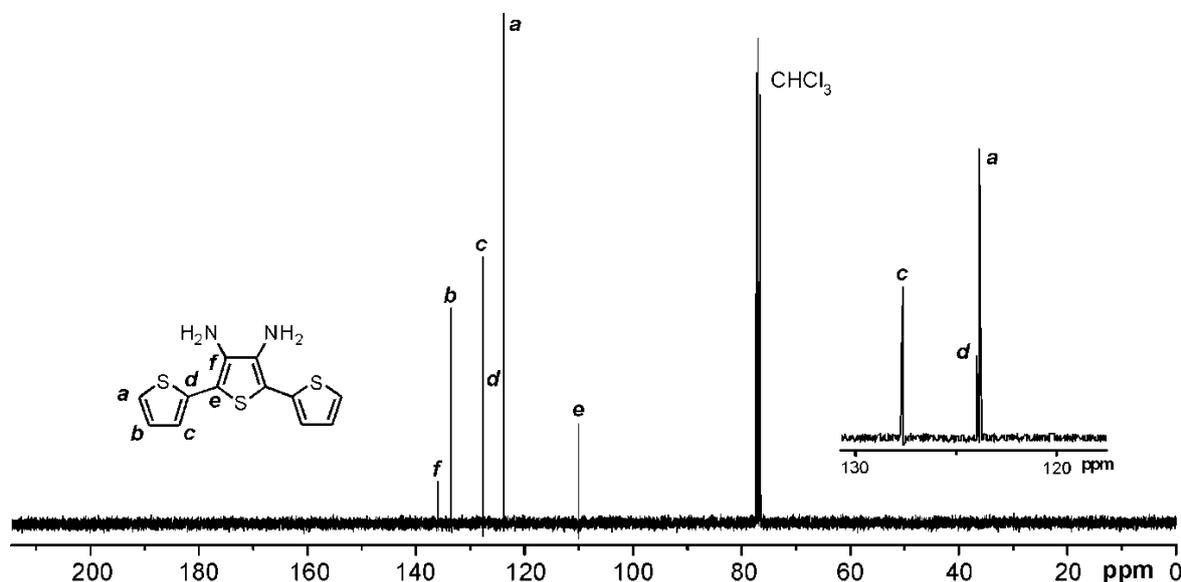


Figure S2. ¹³C NMR Spectrum of Compound 10.

Modeling of 2nd order coupling effects in Compound 10. To verify the assignment of peaks near 7.1 ppm in the ¹H NMR spectrum of compound 10 as two strongly coupled doublet-of-doublets, the experimentally determined coupling constants and chemical shifts were used to simulate the NMR spectrum. This was accomplished using a freely available NMR simulator [1] which could accurately model the 2nd order effects inherent from the close spacing of the coupled multiplets [2]. The values used for the modeling are as follows:

Spin system: ABC

delta 1 (ppm): 7.1018

delta 2 (ppm): 7.0848 J1-2 (Hz): 3.65

delta 3 (ppm): 7.2714 J1-3 (Hz): 1.44 J2-3 (Hz): 4.84

From: 7.0 to: 7.3 ppm

Field strength: 400 MHz

Line width: 0.5 Hz

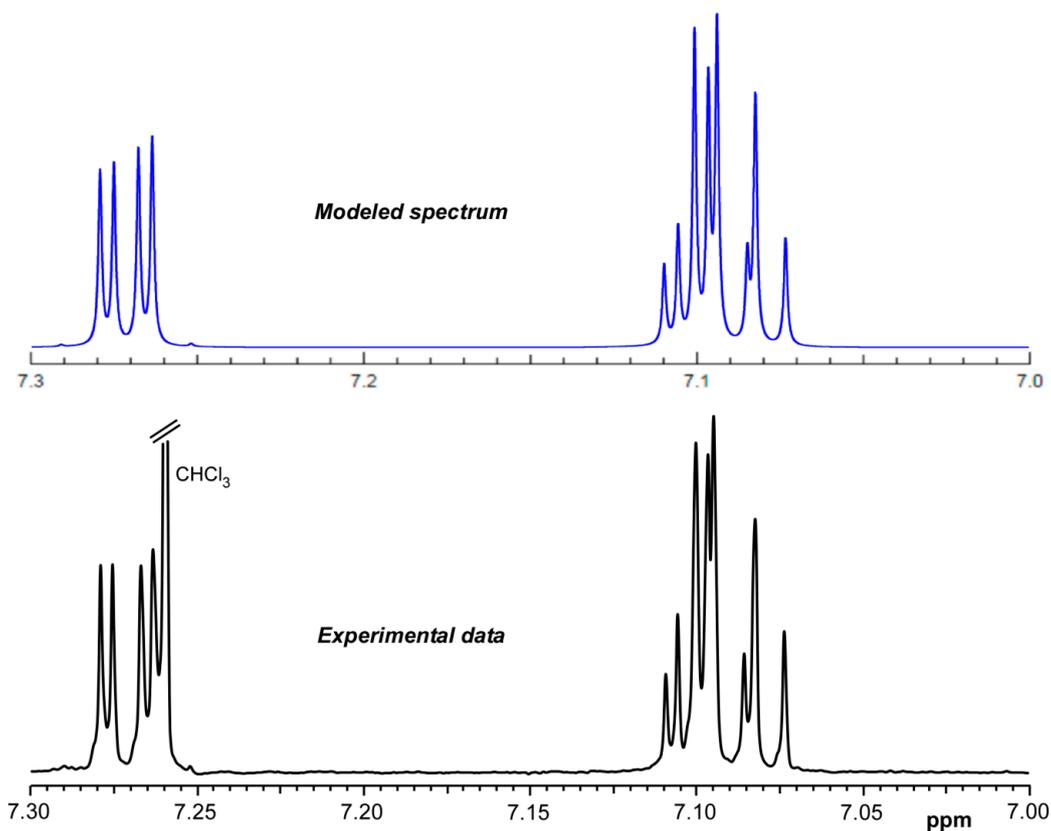


Figure S3. Comparison of results from modeling of 2nd order coupling effects in the ¹H NMR spectrum of 10.

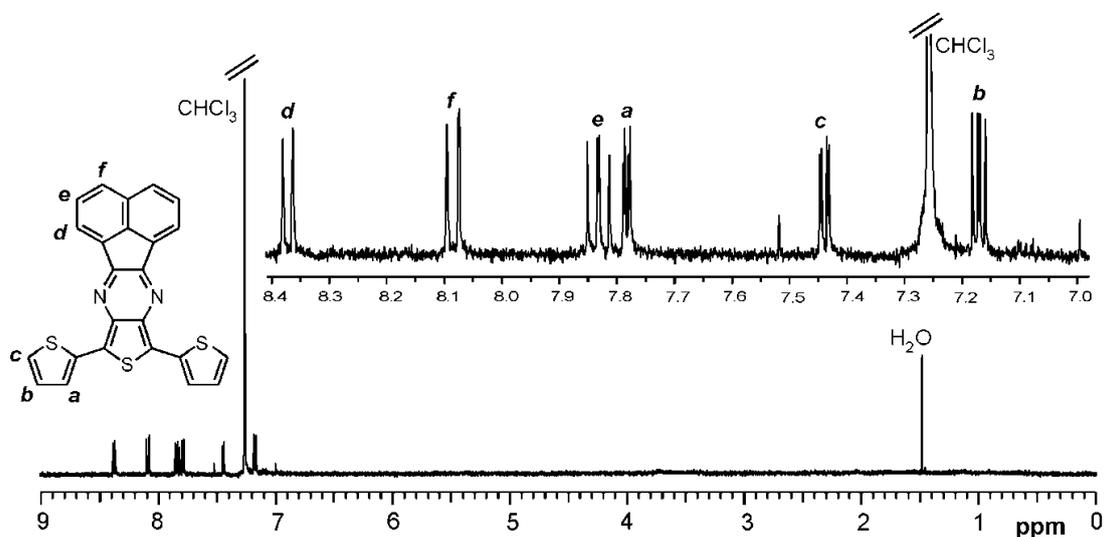


Figure S4. ¹H NMR Spectrum of Compound T3.

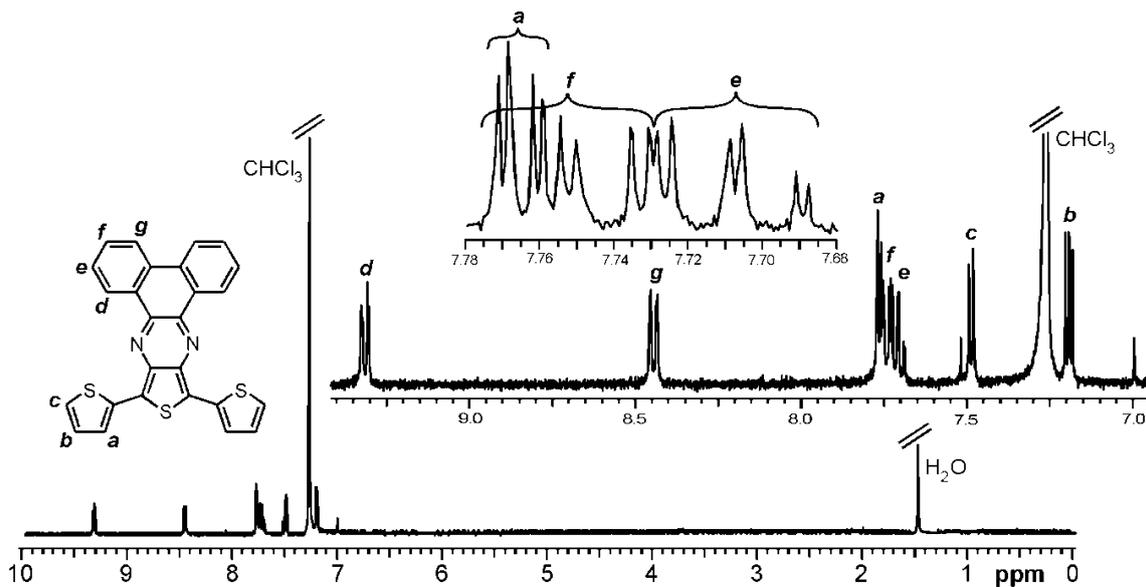


Figure S5. ¹H NMR Spectrum of Compound T4.

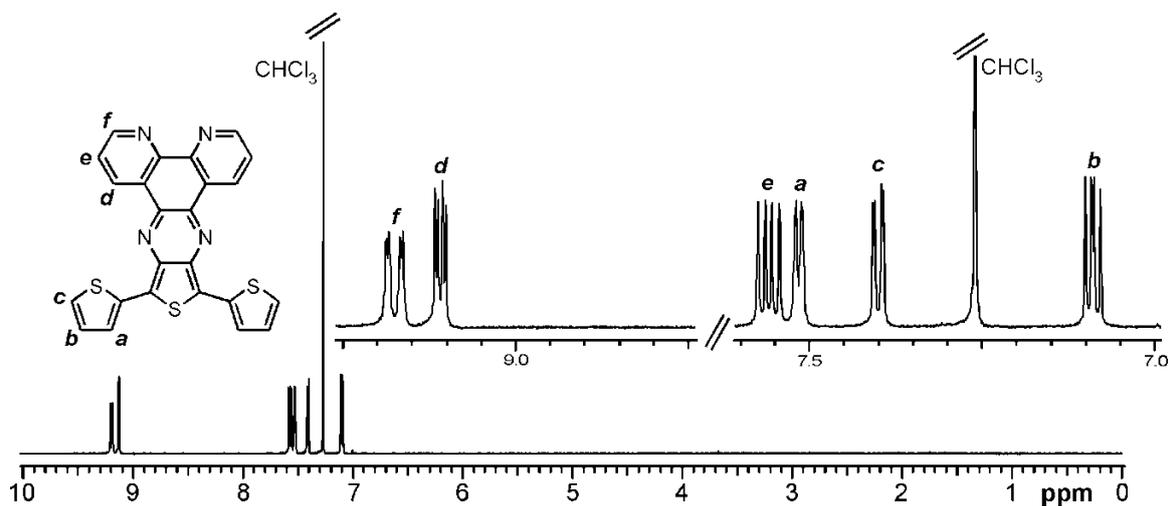


Figure S6. ¹H NMR Spectrum of Compound T5.

References

1. Institute of Chemical Sciences and Engineering. Tools for NMR Spectroscopists. Available online: <http://www.nmrdb.org/simulator/index.shtml?v=v2.34.1> (accessed on 22 April 2016).
2. Castillo, A.M.; Patiny, L.; Wist, J. Fast and accurate algorithm for the simulation of NMR for large spin systems. *J. Mag. Res.* **2011**, *209*, 123–130.