

SUPPORTING INFORMATION

Thiophene-fused Nickel Dithiolenes: A Synthetic Scaffold for Highly Delocalized π -electron Systems

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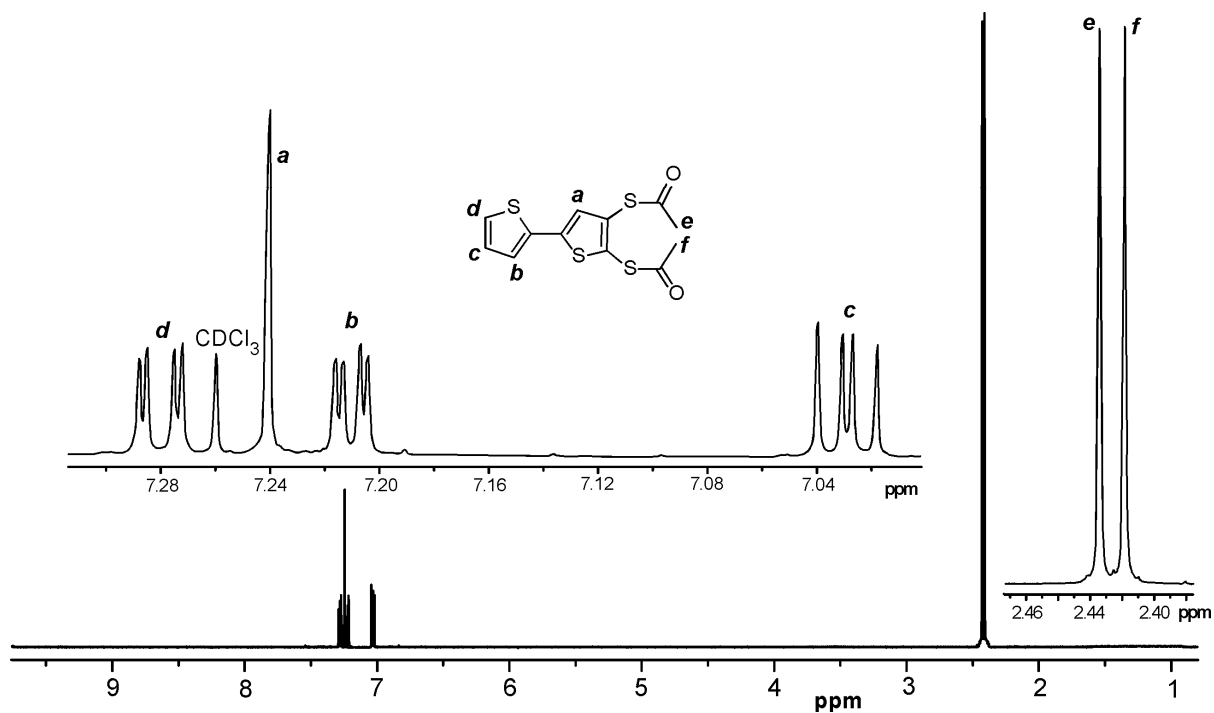


Figure S1. ^1H NMR Spectrum of Compound **5a**

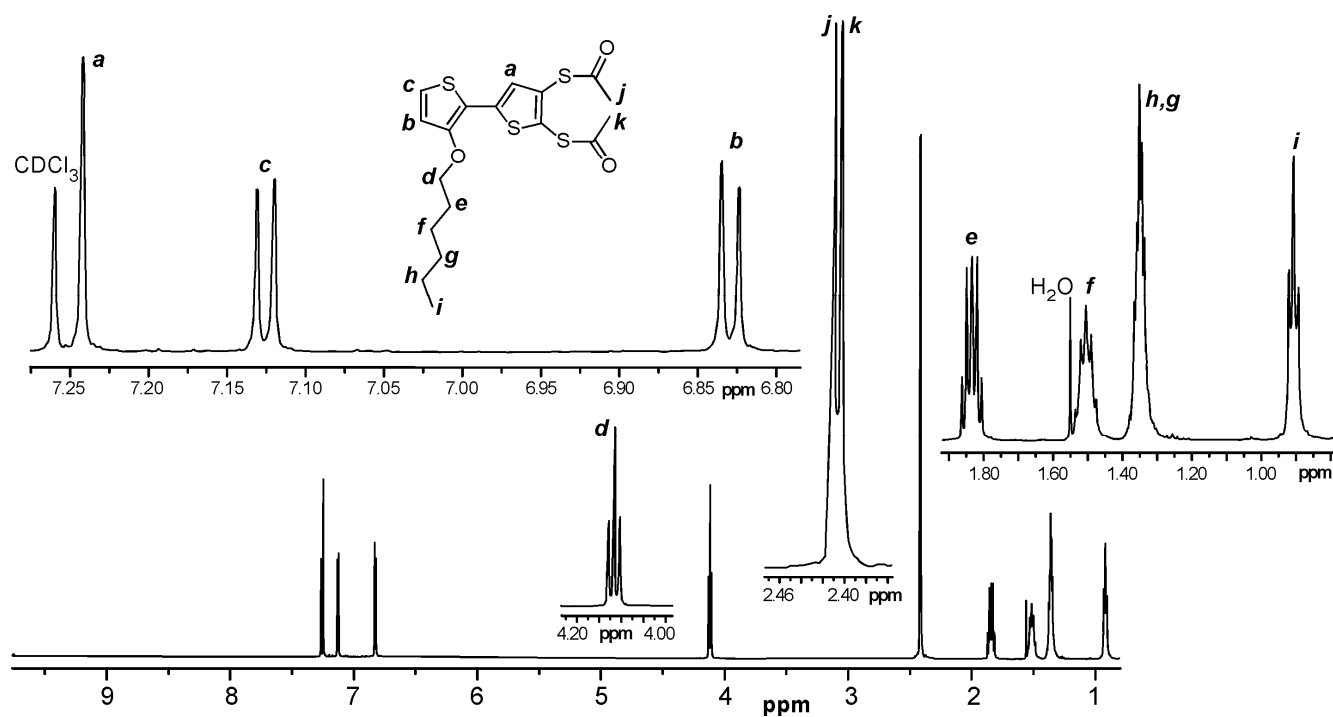


Figure S2. ^1H NMR Spectrum of Compound **5b**

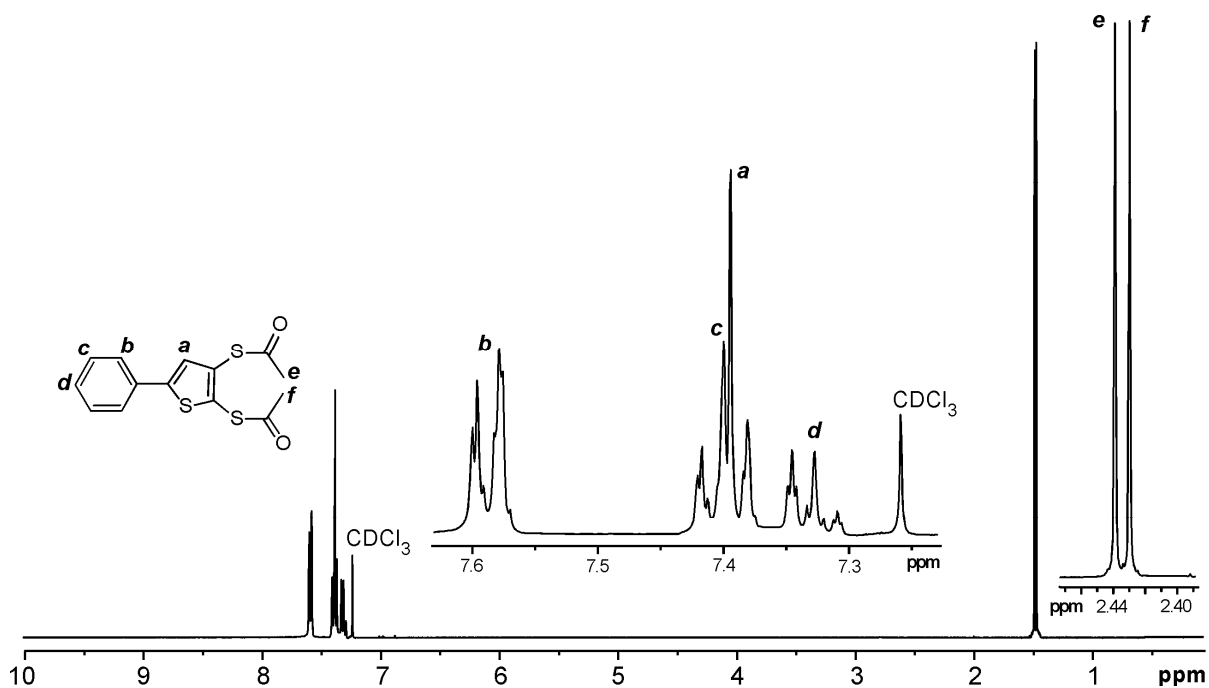


Figure S3. ^1H NMR Spectrum of Compound **5c**

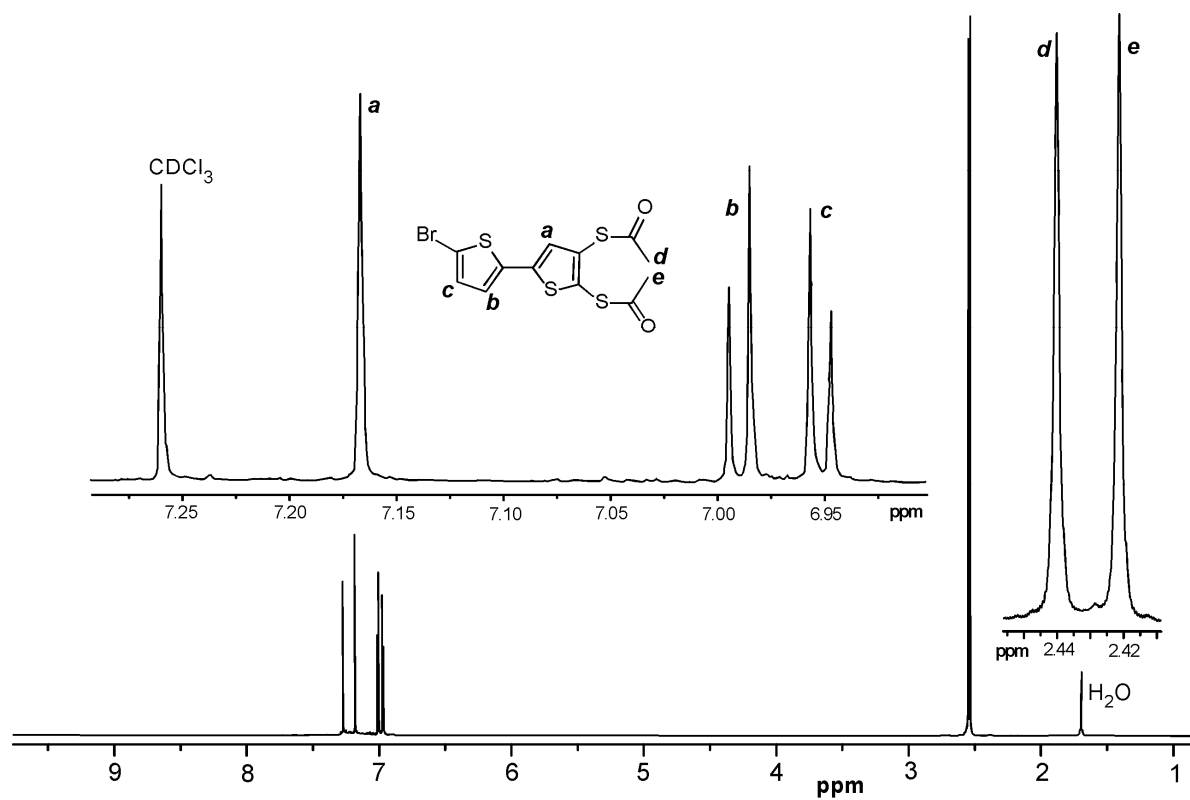


Figure S4. ¹H NMR Spectrum of Compound **5d**

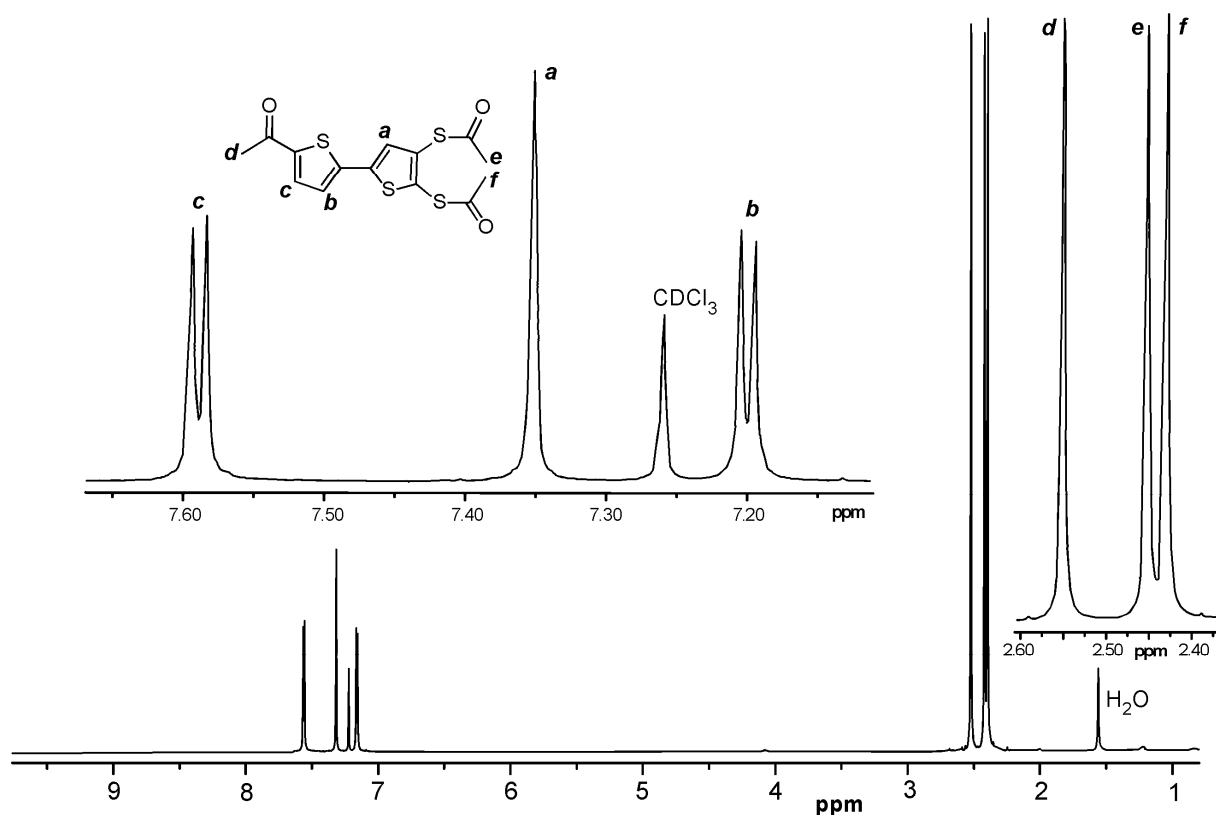


Figure S5. ¹H NMR Spectrum of Compound **5e**

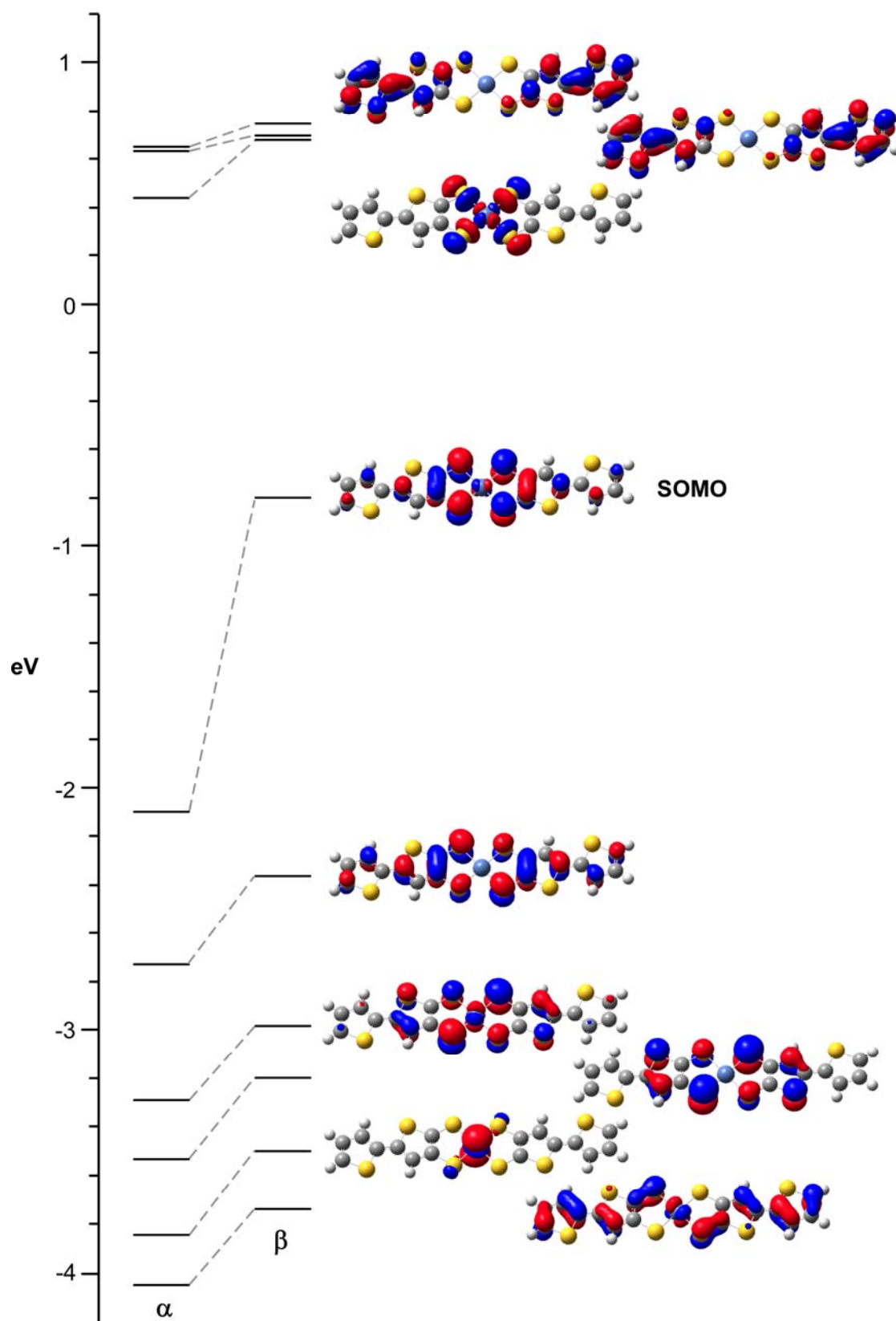


Figure S6. MOs of **6a** plotted by calculated energies

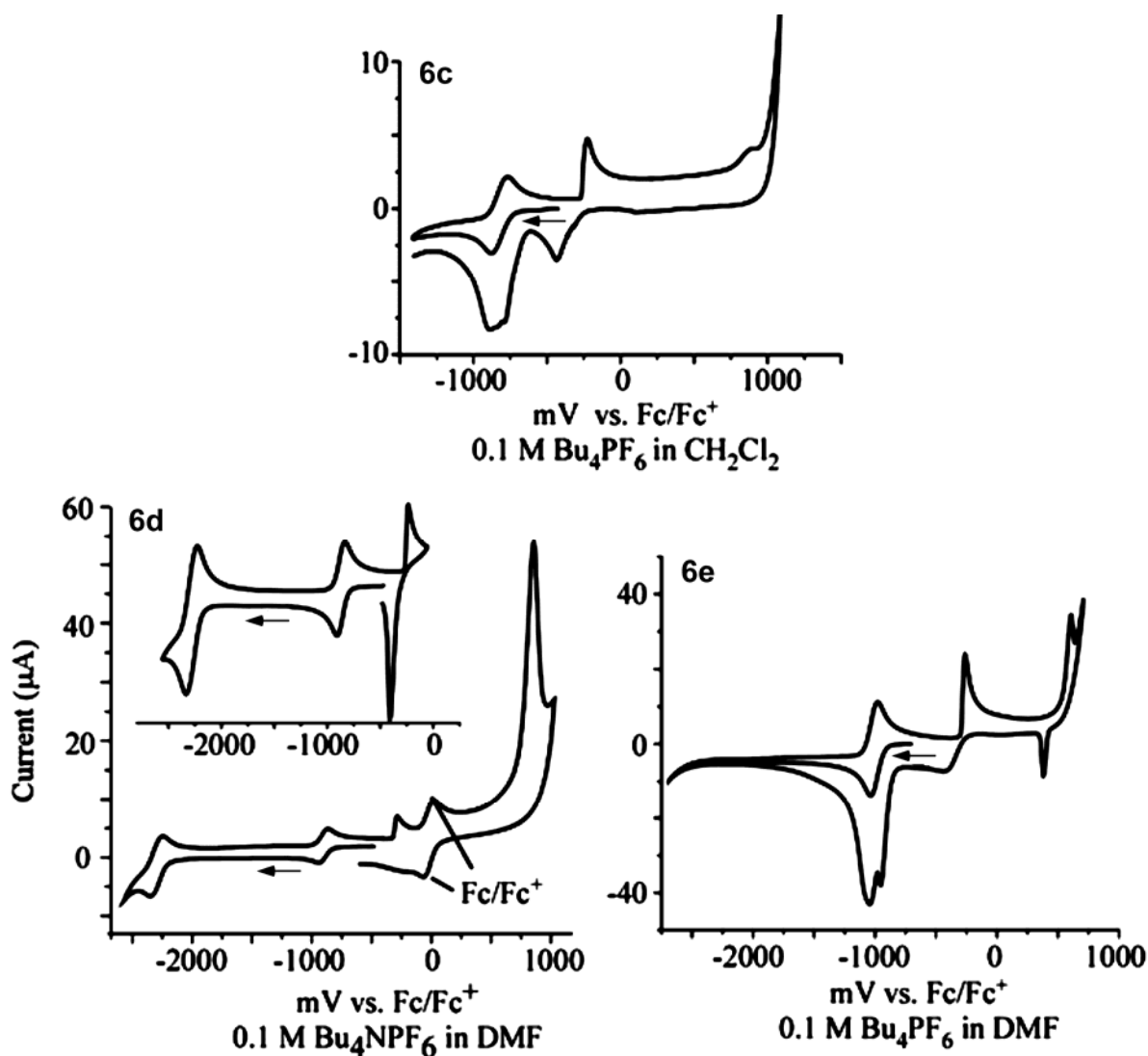


Figure S7. CVs of **6c-e**.

Additional discussion on attempted electropolymerizations

As can be seen in Figure S8, repetitive potential cycling of dithiolenes **6b** does introduce new irreversible redox waves in the region of -1500 to -750 mV, which could be the result of oxidative coupling. However, these new redox processes do not continue to grow in intensity, nor does anything deposit onto the working electrode under these conditions. This may be the result of enhanced stability of any unpaired electrons generated as a result of delocalization, rather than the typical enhanced spin density exhibited by oligothiophenes on the external thiophene α -positions. Such enhanced stability could then allow diffusion away from the working electrode to undergo further reactivity in the bulk solution. This conclusion could be somewhat supported by an increase in reversibility of the new processes by cycling at very fast scan rates.

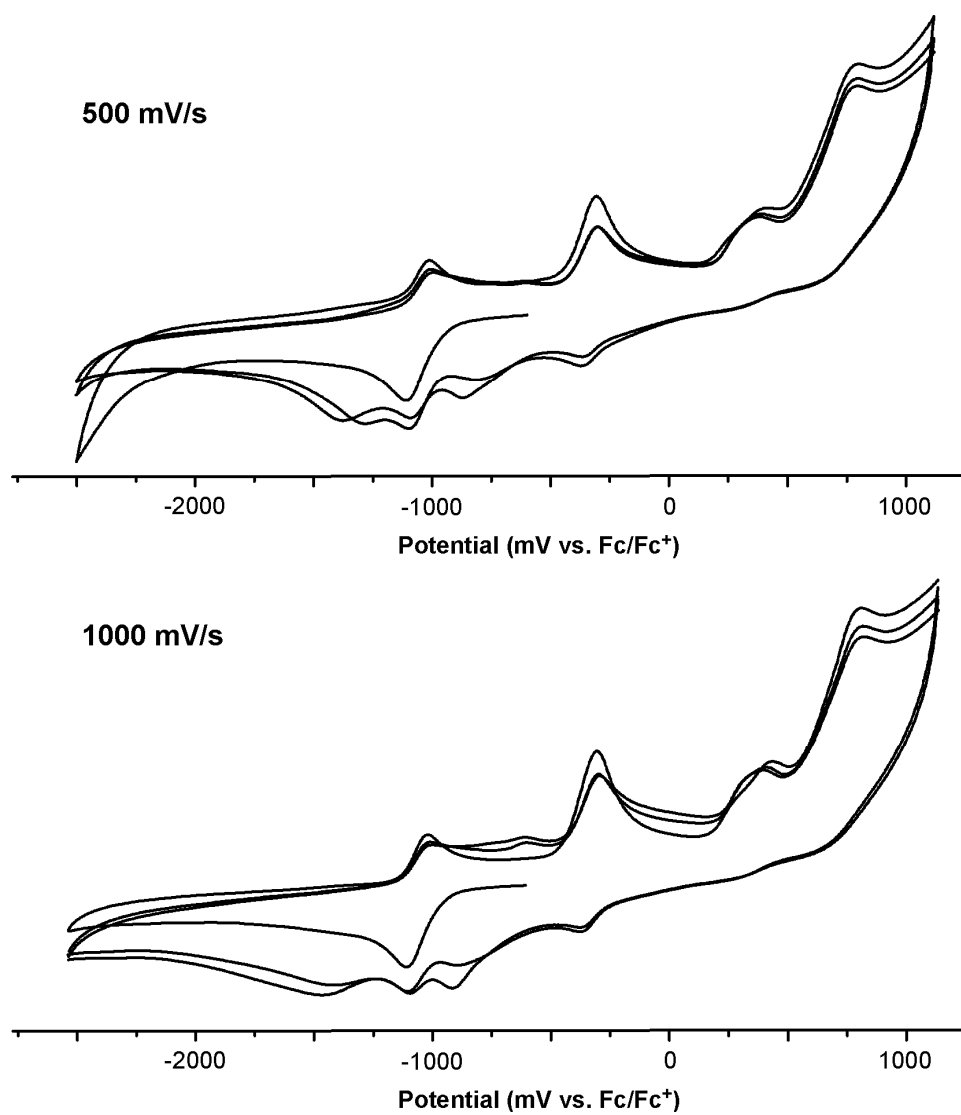


Figure S8. Multiple CV cycles of **6b** at different scan rates.