

Supporting Information for

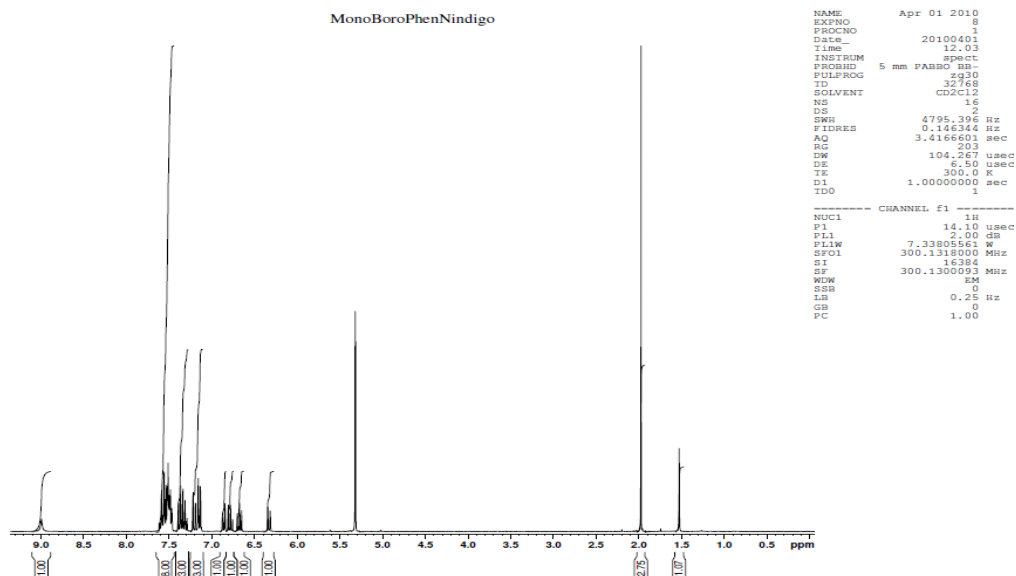
Redox-active, near-infrared dyes based on 'Nindigo' (indigo-*N,N'*-diarylimine) boron chelate complexes

Graeme Nawn,^a Simon R. Oakley,^a Marek B. Majewski,^b Robert McDonald,^c Brian O. Patrick,^b and Robin G. Hicks^{*a}

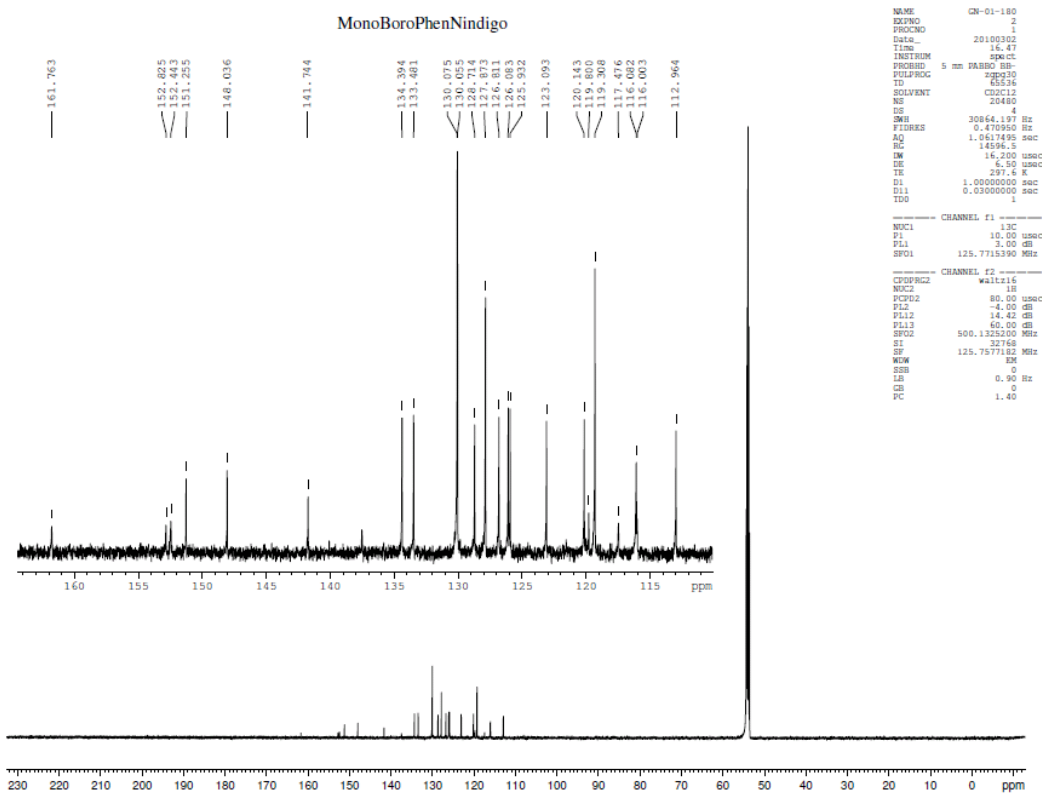
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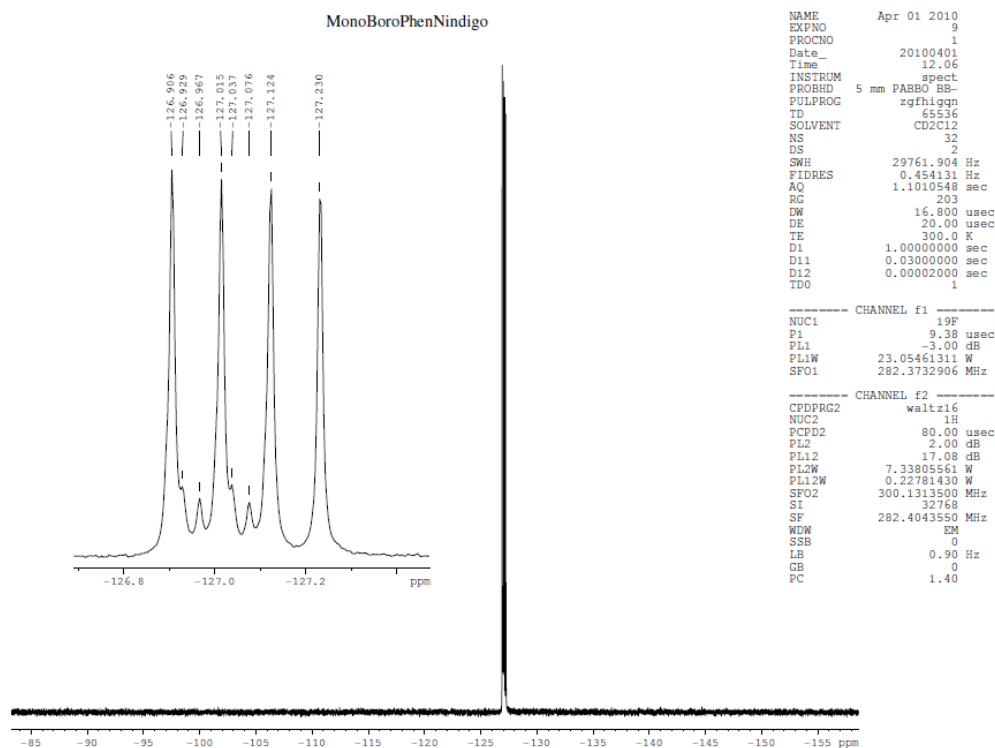
¹H NMR spectrum of **2a**. Peak at ~1.5 ppm is due to residual water and peak at ~5.2 ppm due to solvent.



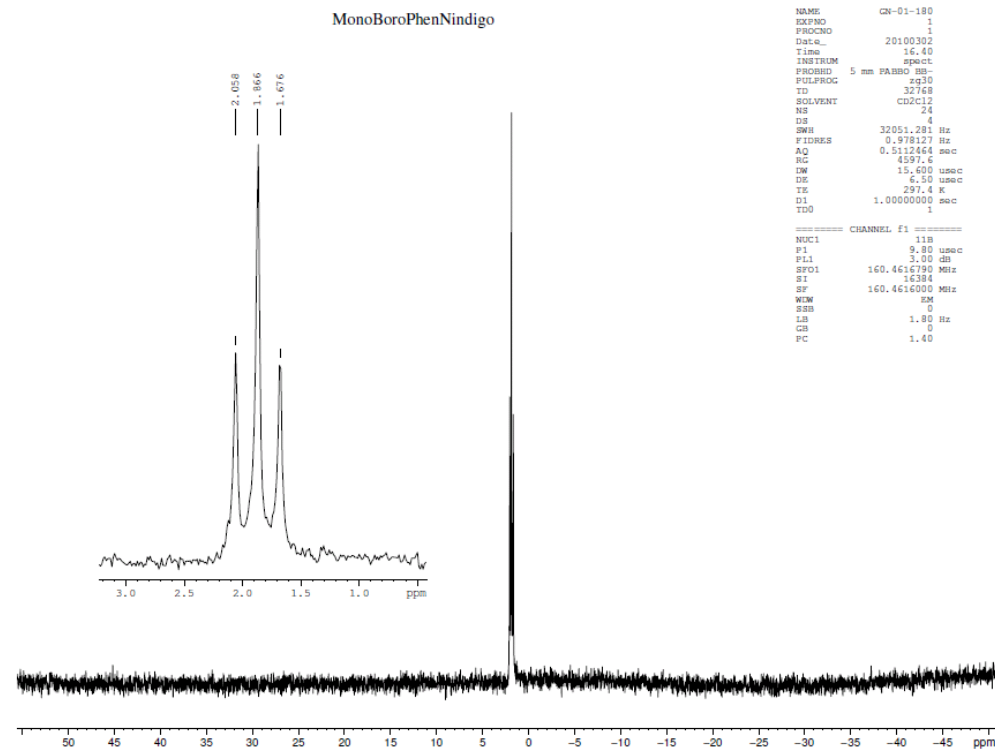
¹³C NMR spectrum of **2a**



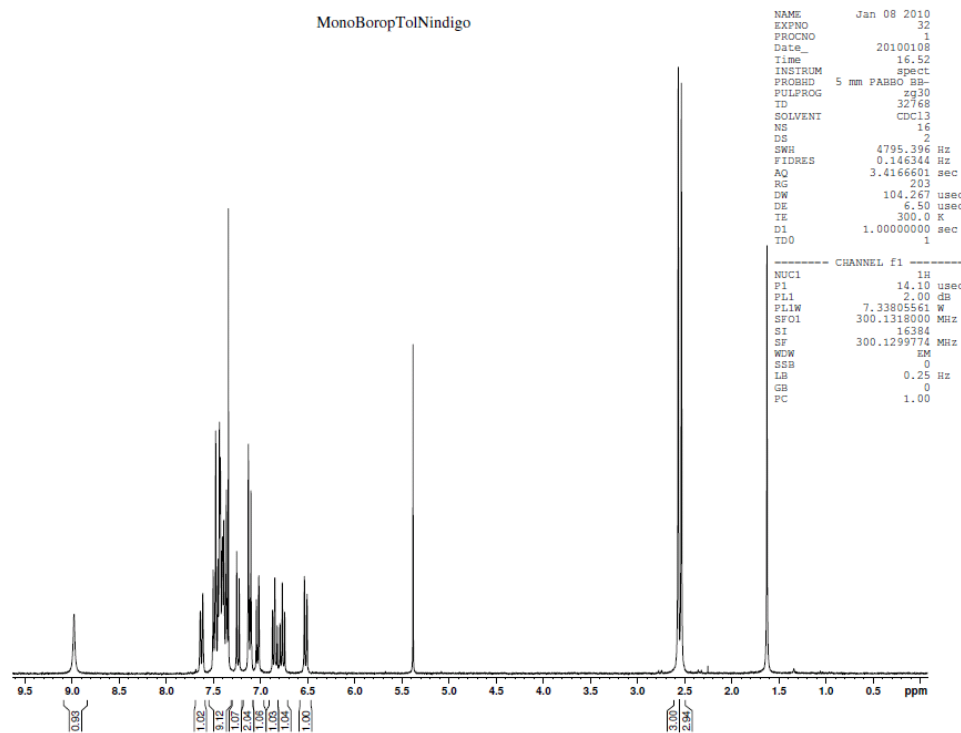
¹⁹F NMR spectrum of **2a**



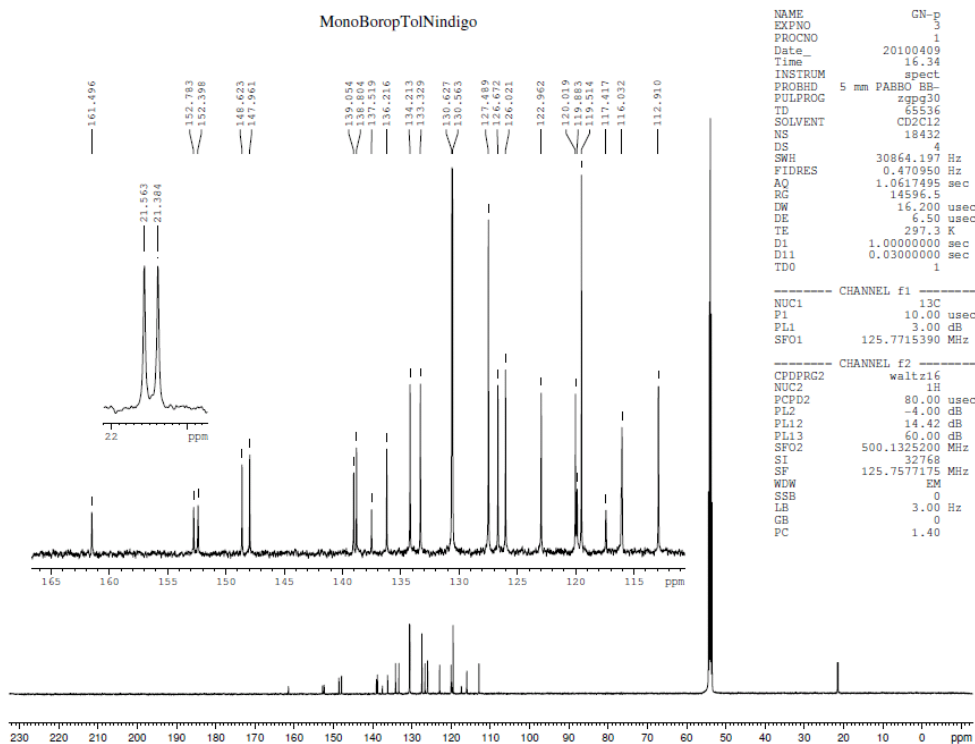
¹¹B NMR spectrum of **2a**



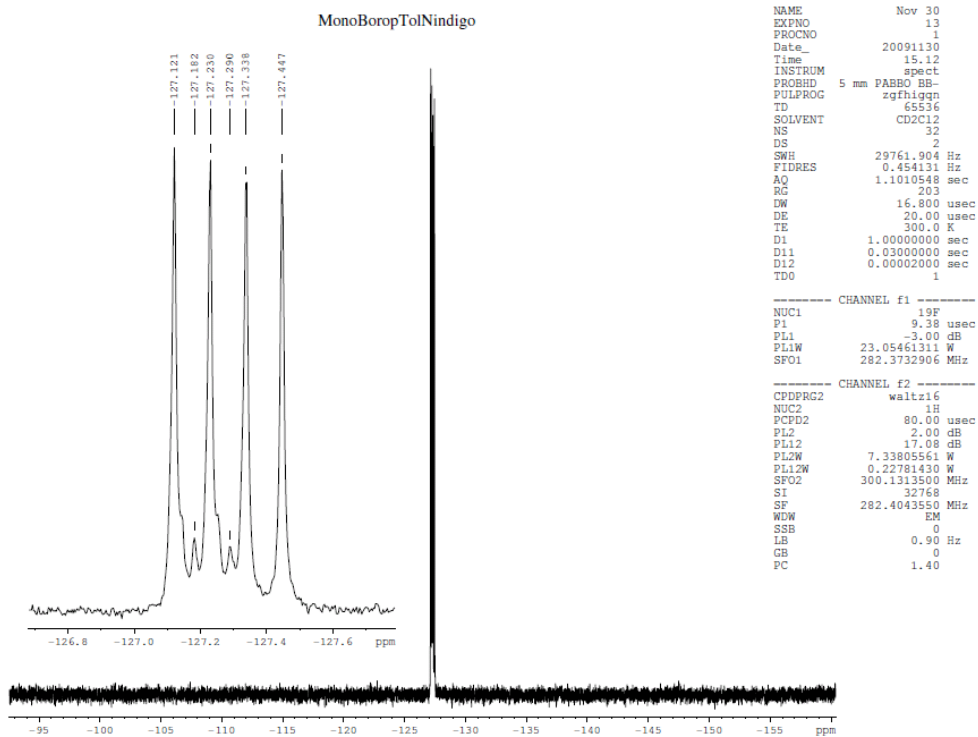
¹H NMR spectrum of **2b**. Peak at ~1.5 ppm is due to residual water and peak at ~5.2 ppm due to solvent.



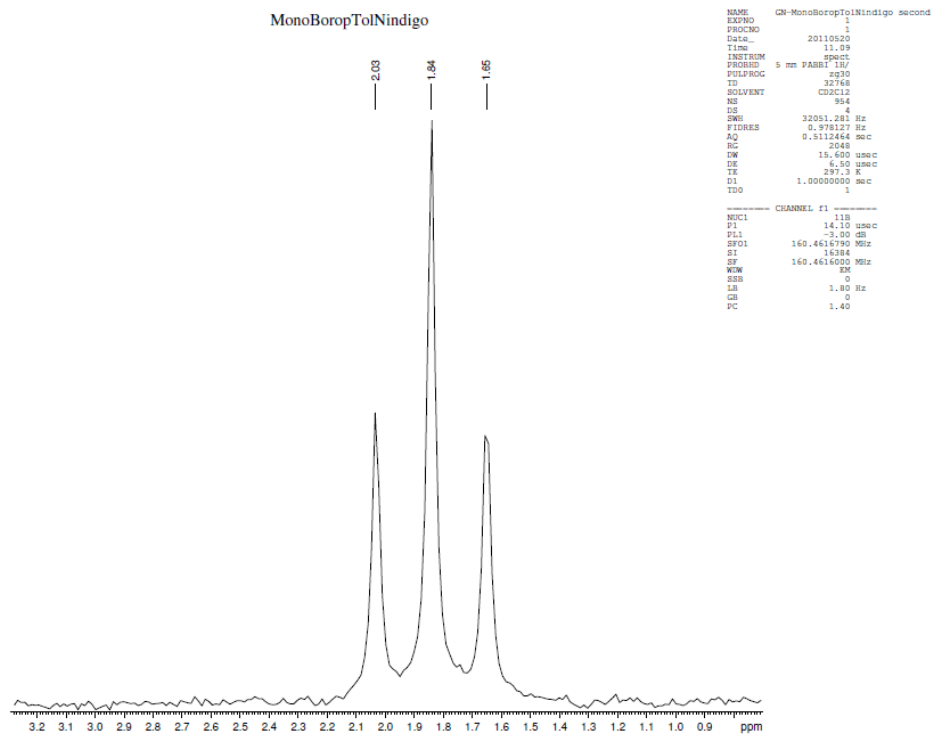
¹³C NMR spectrum of **2b**



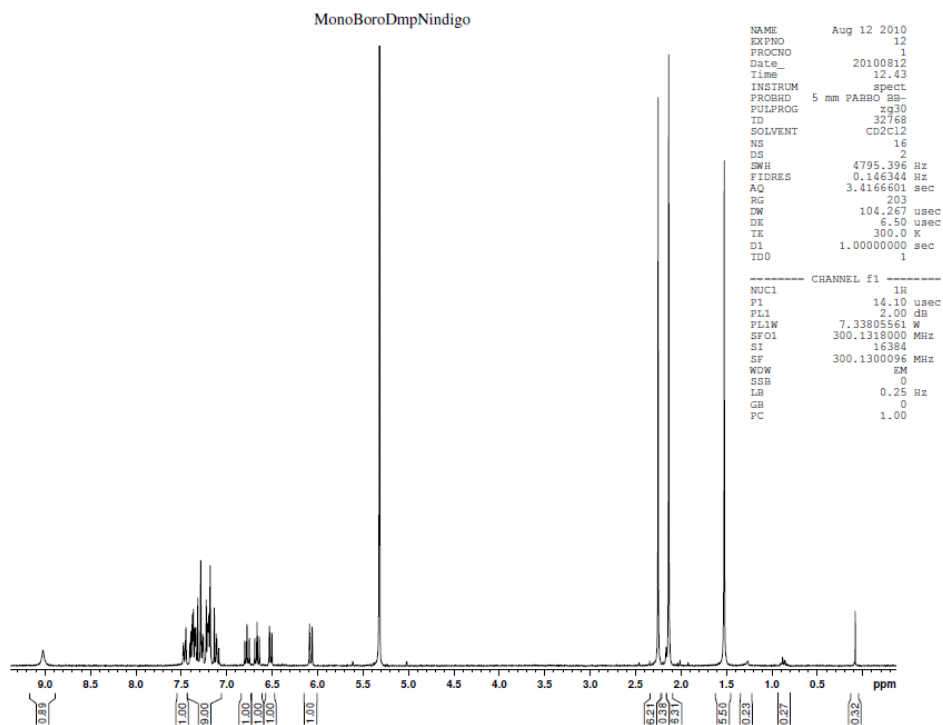
¹⁹F NMR spectrum of **2b**



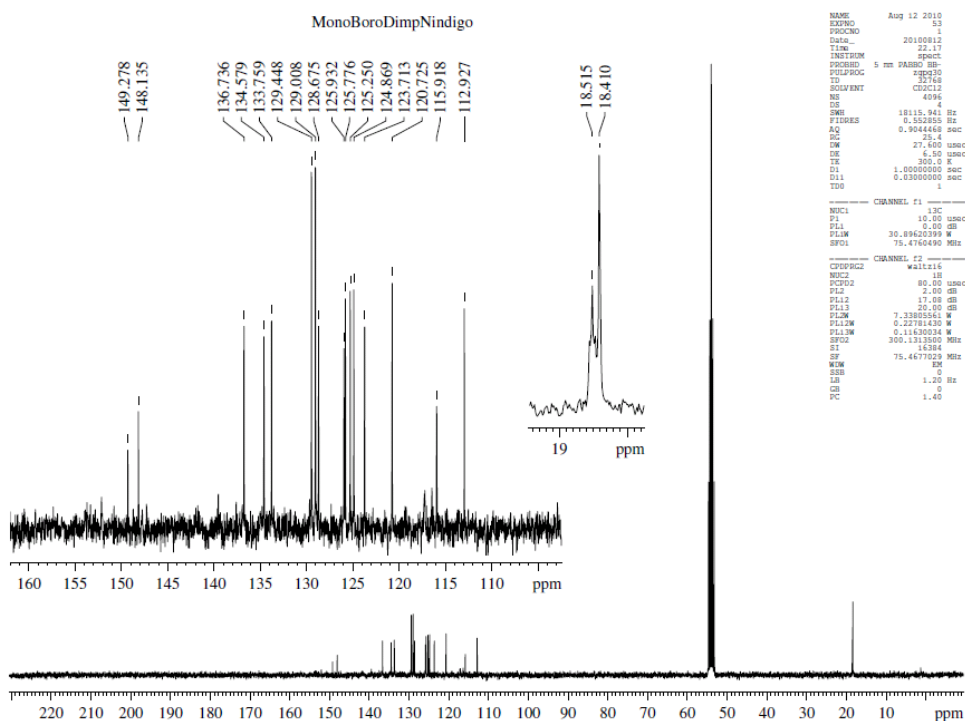
¹¹B NMR spectrum of **2b**



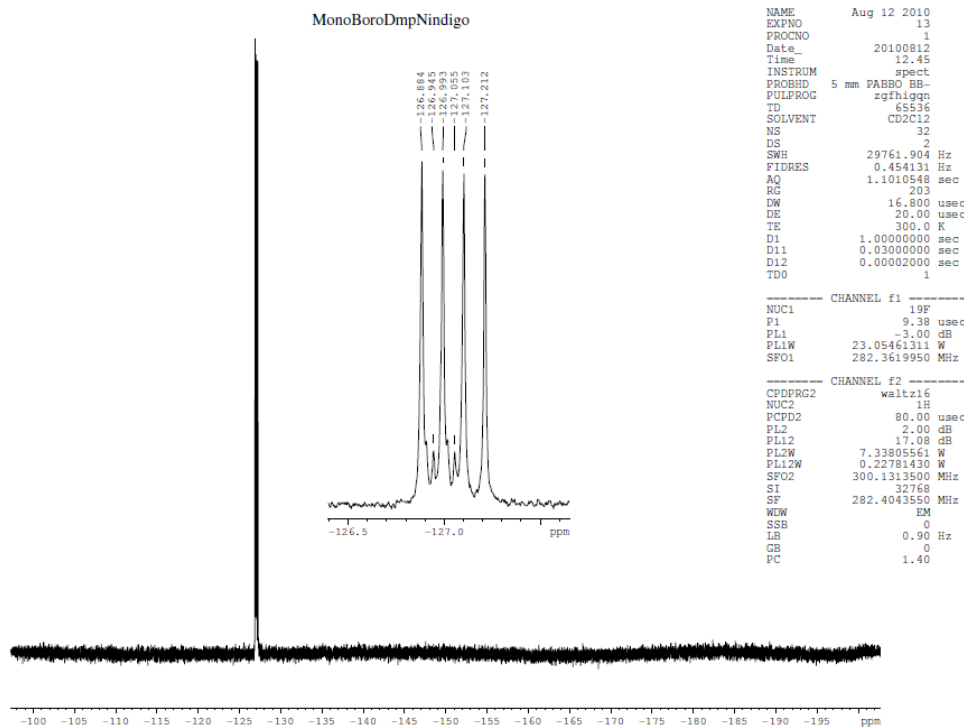
^1H NMR spectrum of **2c**. Peak at ~ 1.5 ppm is due to residual water and peak at ~ 5.2 ppm due to solvent.



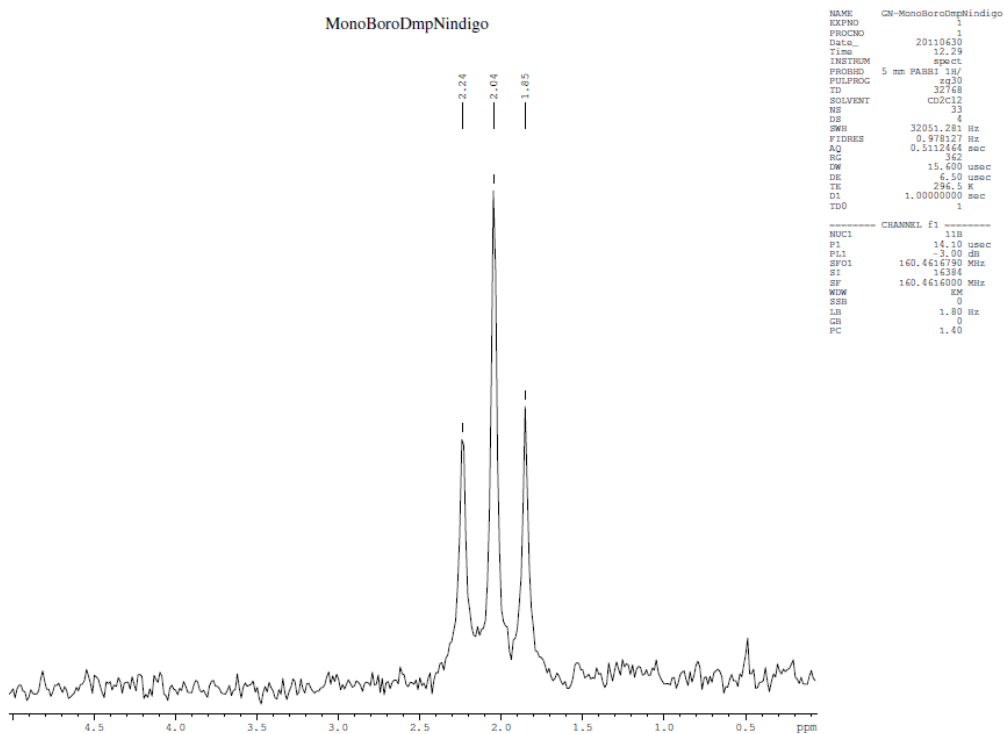
^{13}C NMR spectrum of **2c**



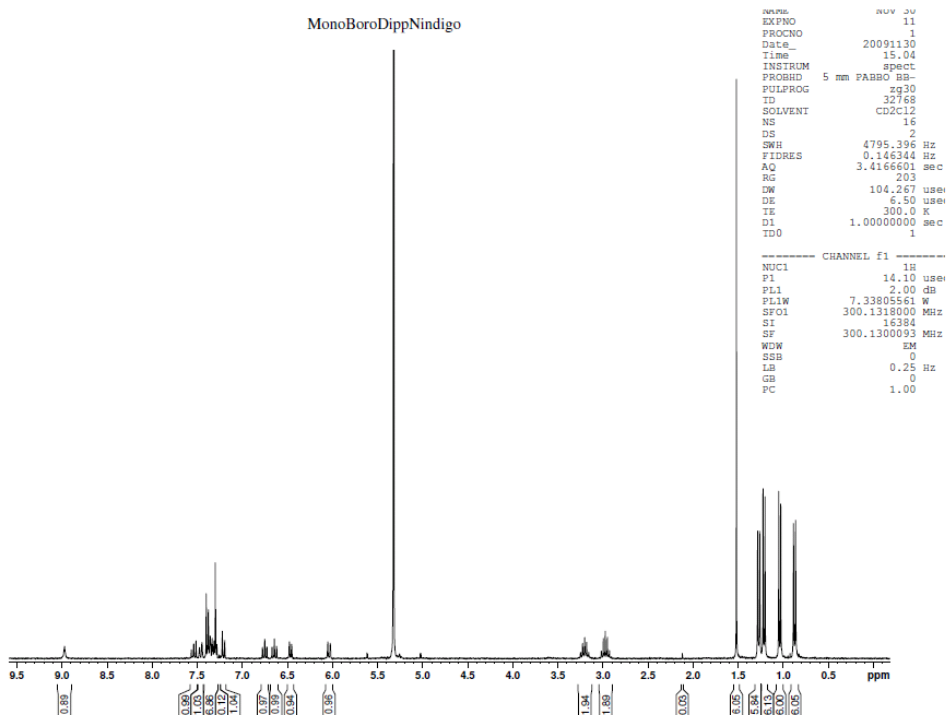
¹⁹F NMR spectrum of **2c**



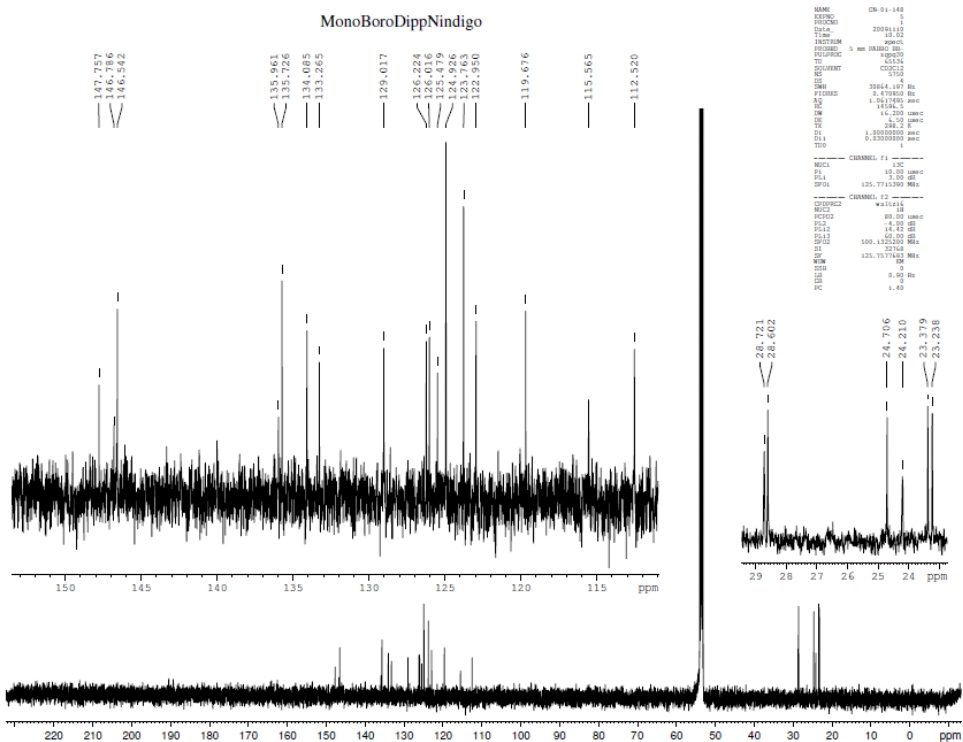
¹¹B NMR spectrum of **2c**



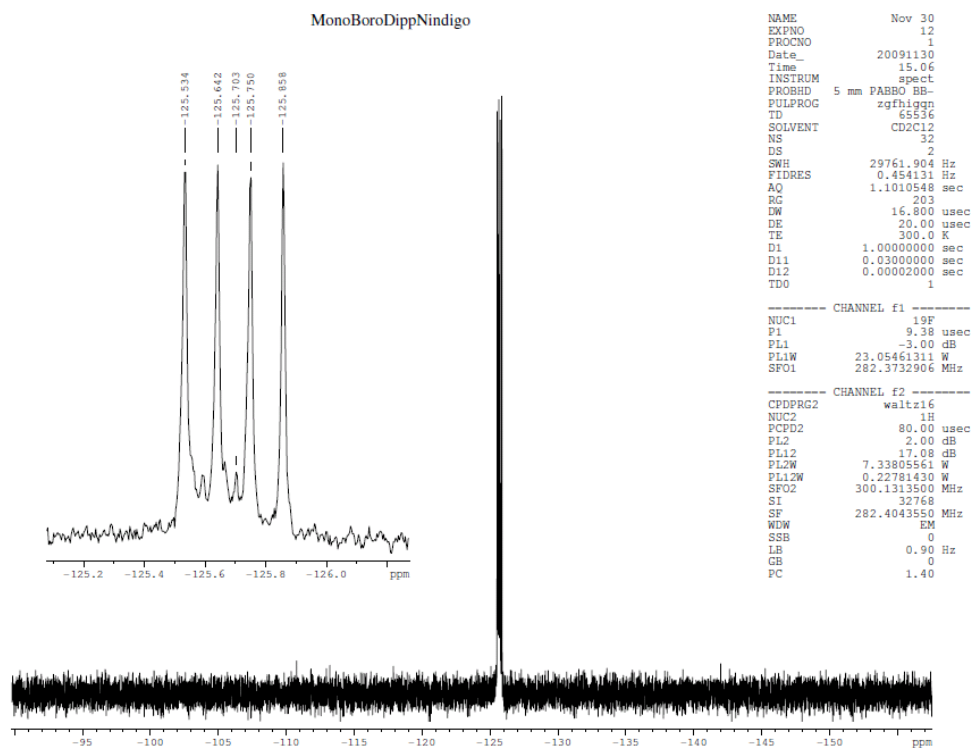
^1H NMR spectrum of **2d**. Peak at ~ 1.5 ppm is due to residual water and peak at ~ 5.2 ppm due to solvent.



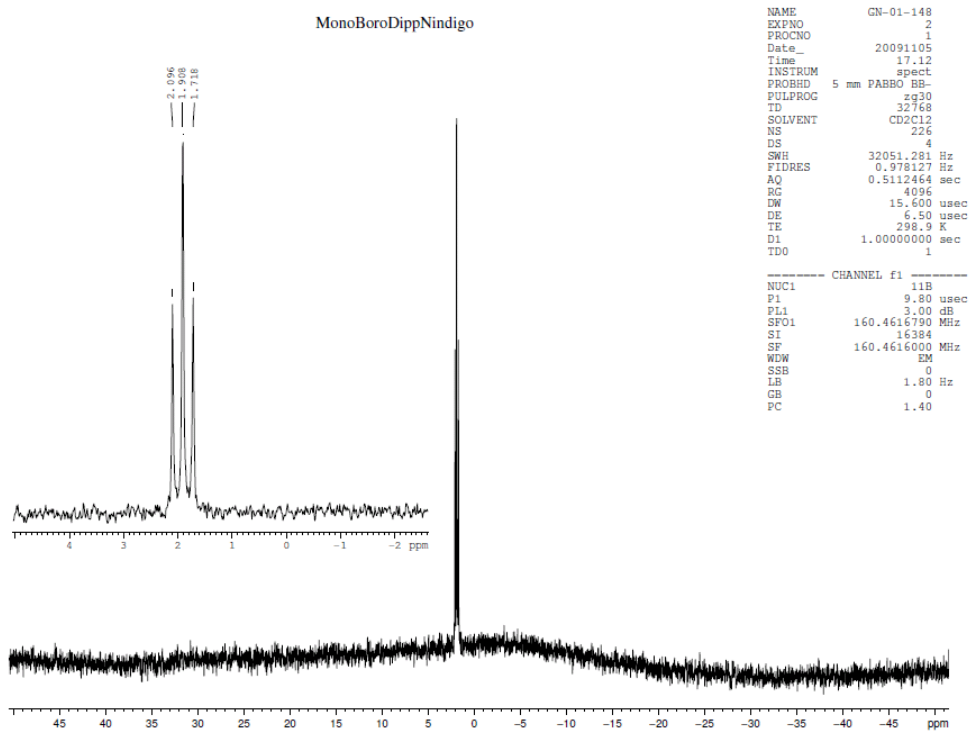
^{13}C NMR spectrum of **2d**



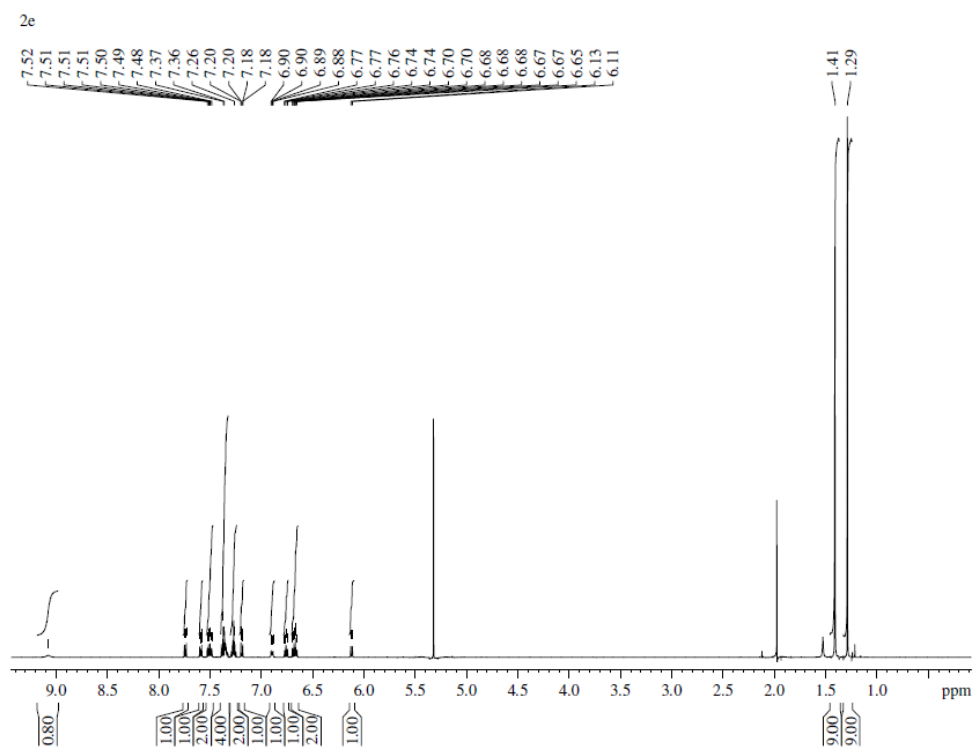
^{19}F NMR spectrum of **2d**



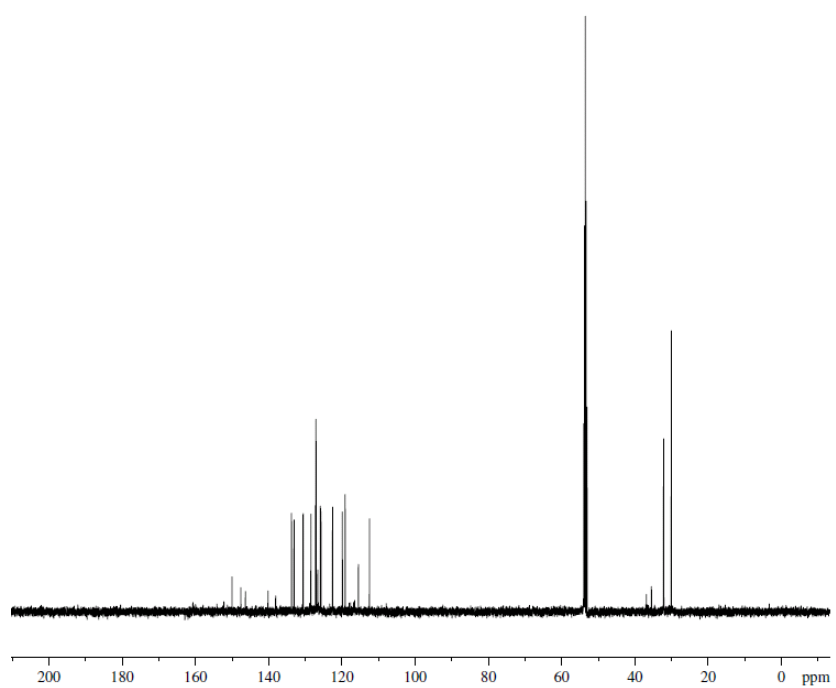
^{11}B NMR spectrum of **2d**



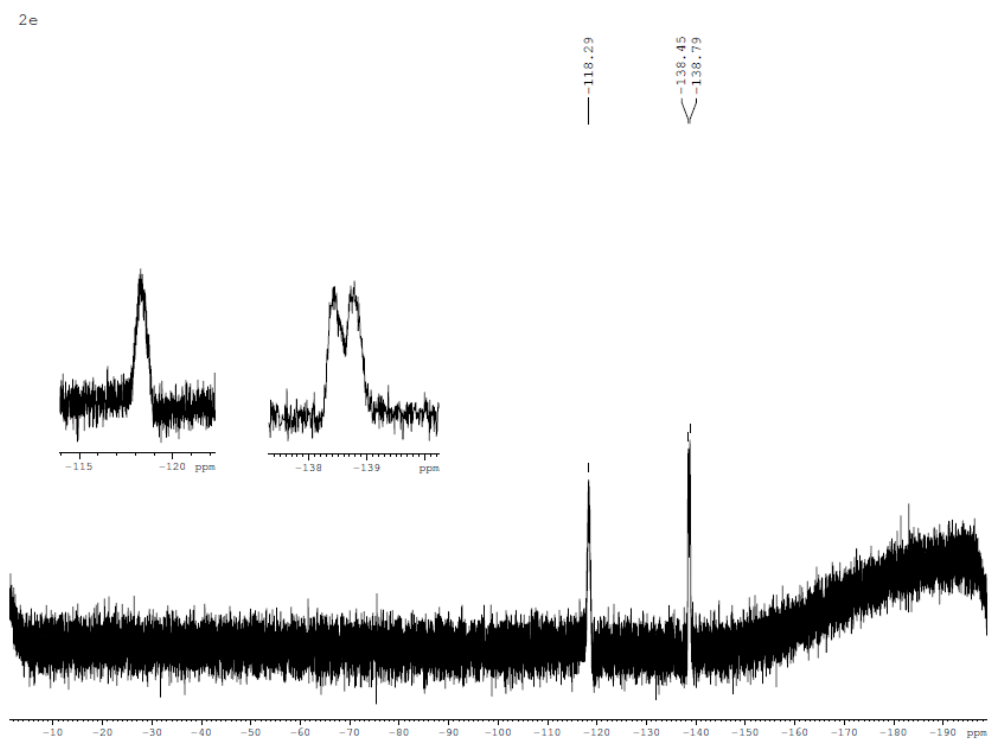
^1H NMR spectrum of **2e**



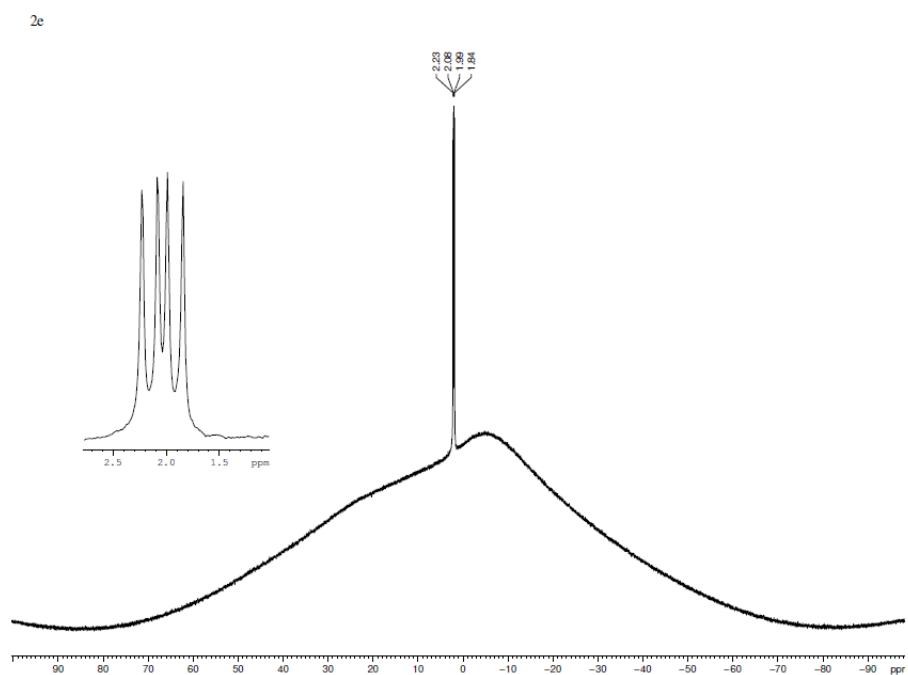
^{13}C NMR spectrum of **2e**



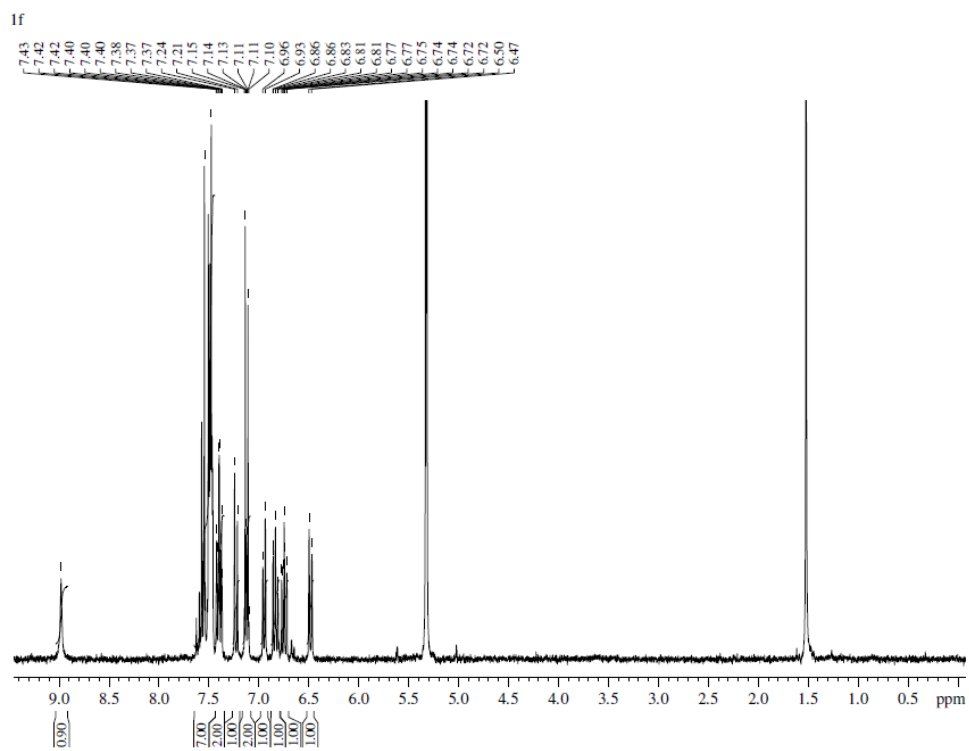
^{19}F NMR spectrum of **2e**



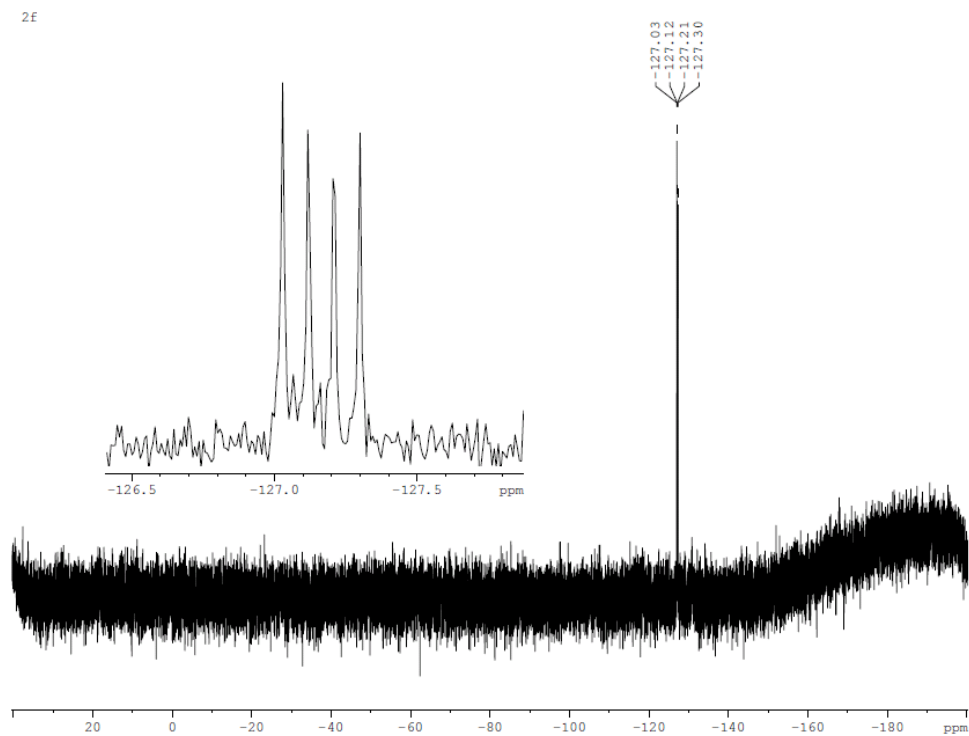
^{11}B NMR spectrum of **2e**



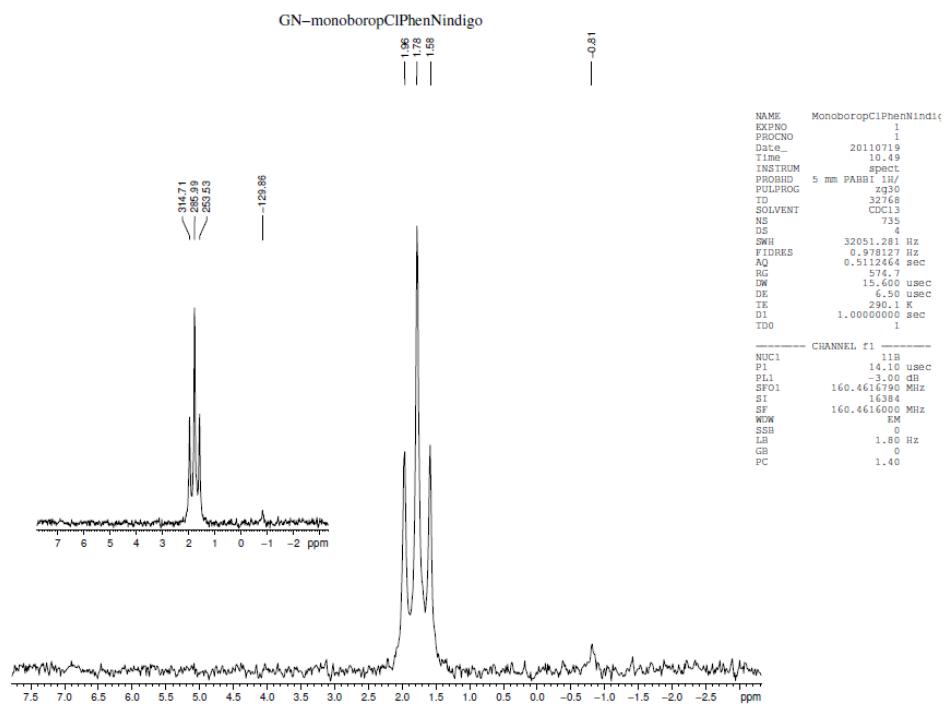
¹H NMR spectrum of **2f**



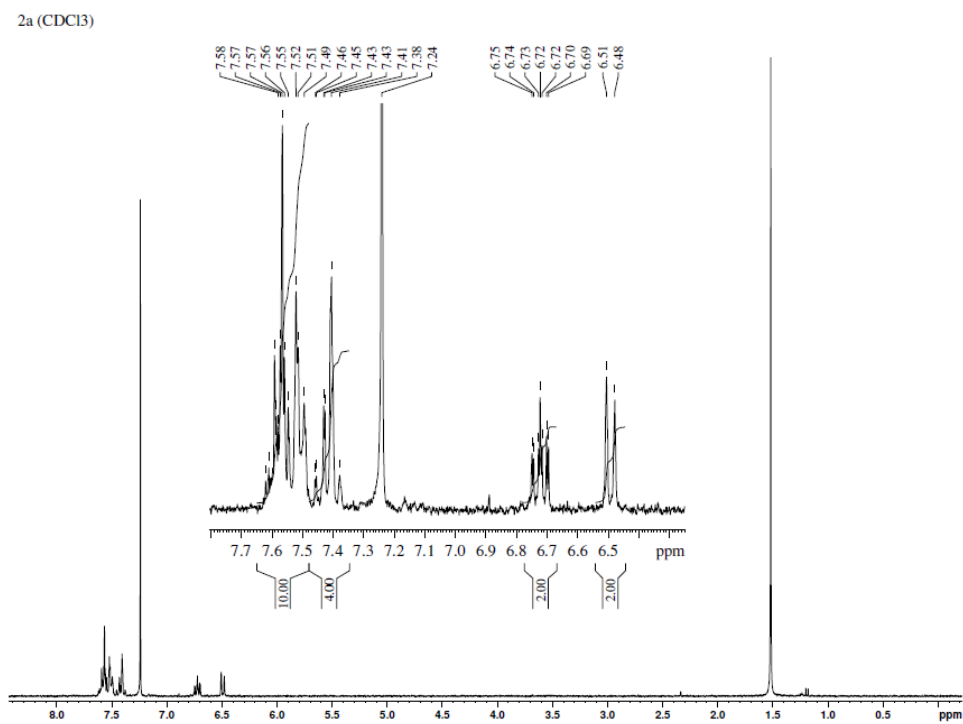
¹⁹F NMR spectrum of **2f**



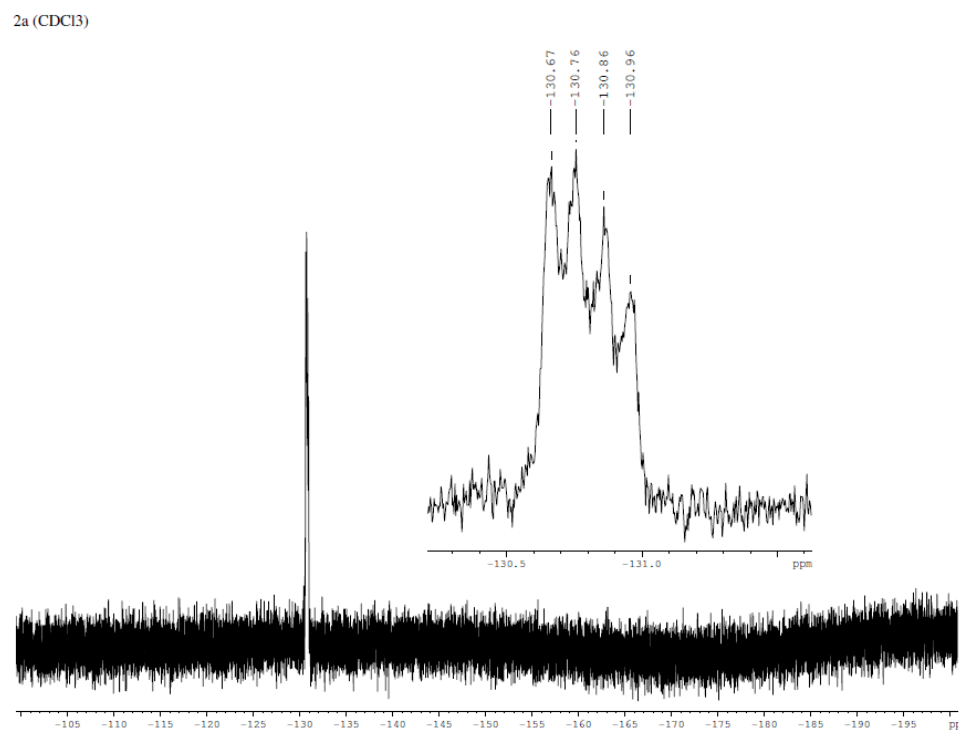
¹¹B NMR spectrum of **2f**



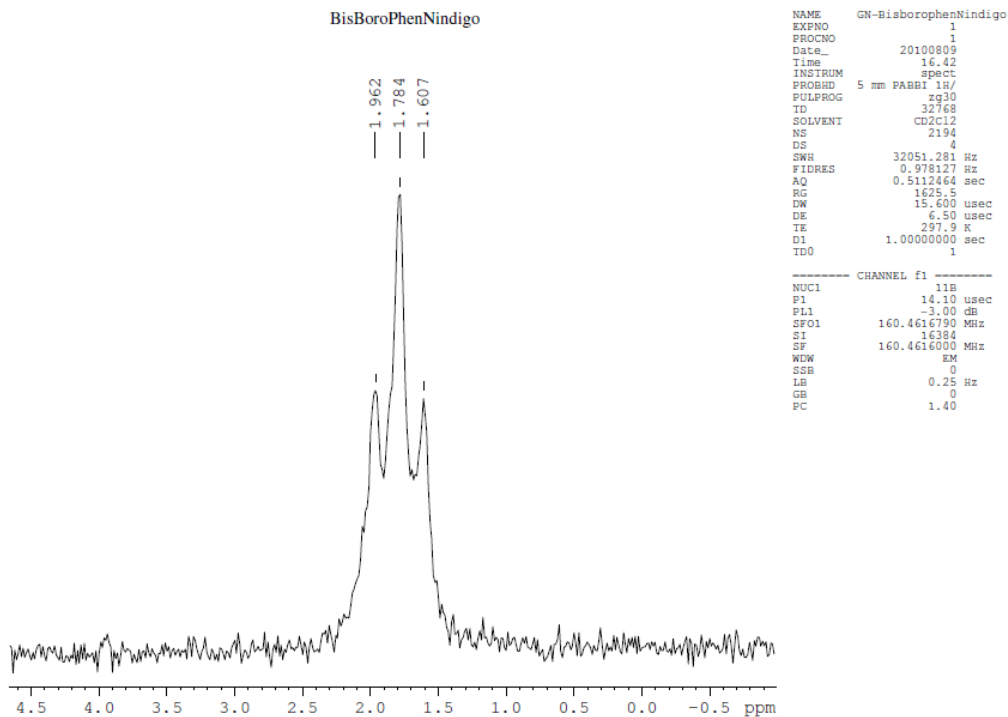
¹H NMR spectrum of **3a**



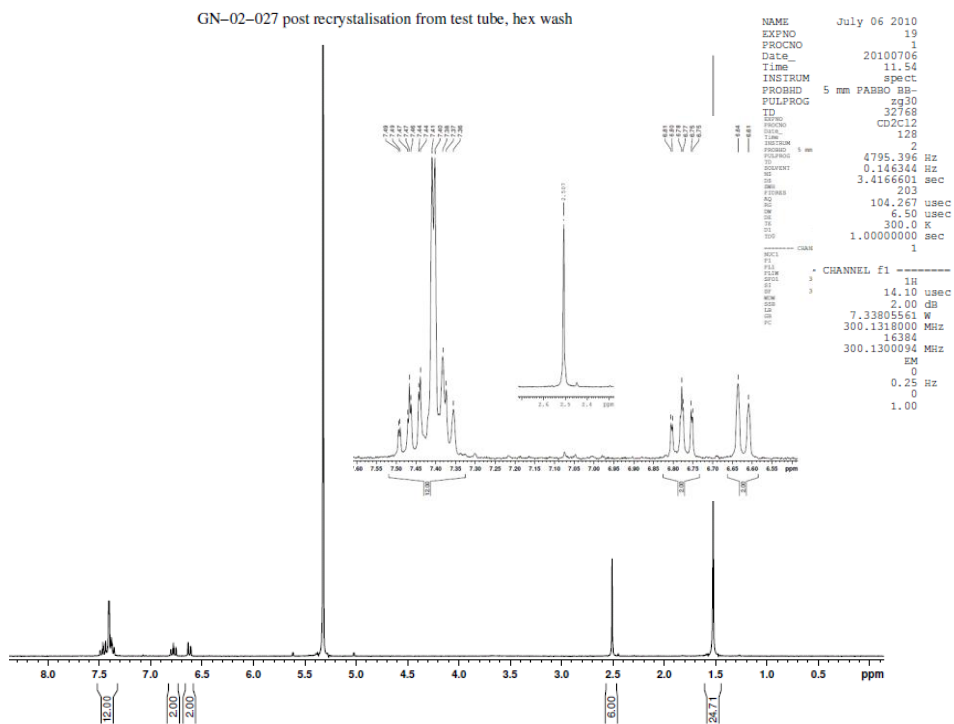
¹⁹F NMR spectrum of **3a**



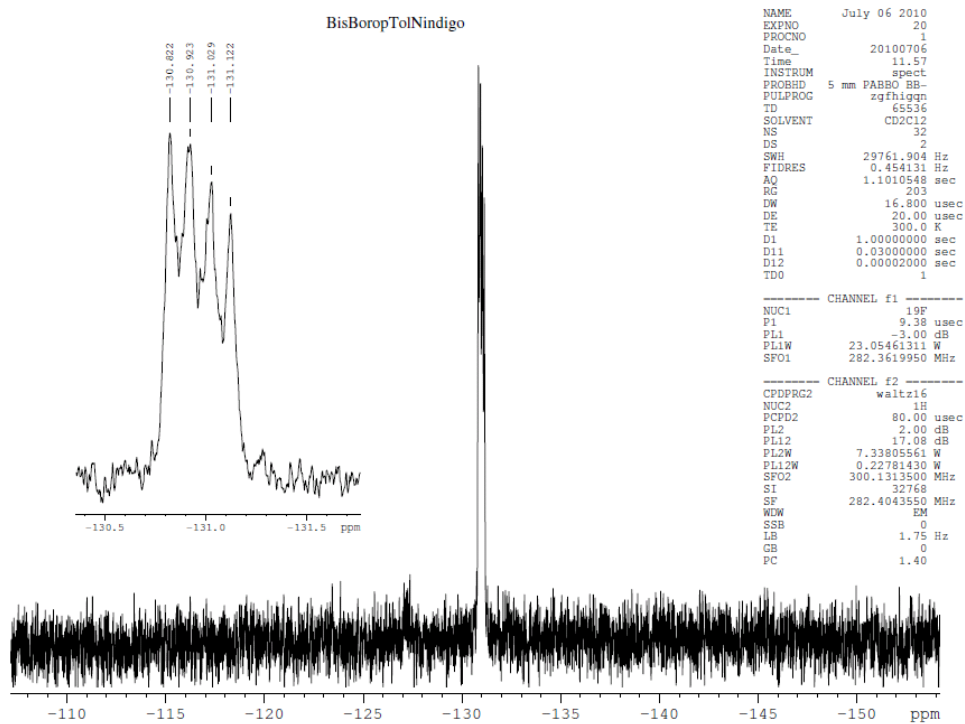
^{11}B NMR spectrum of **3a**



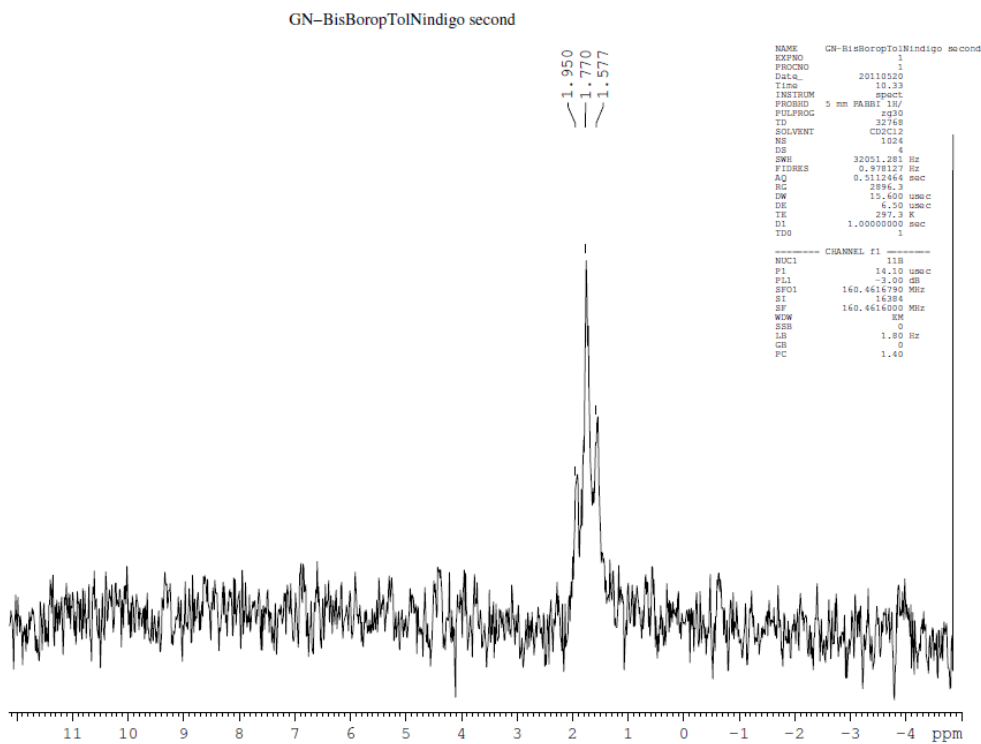
^1H NMR spectrum of **3b**



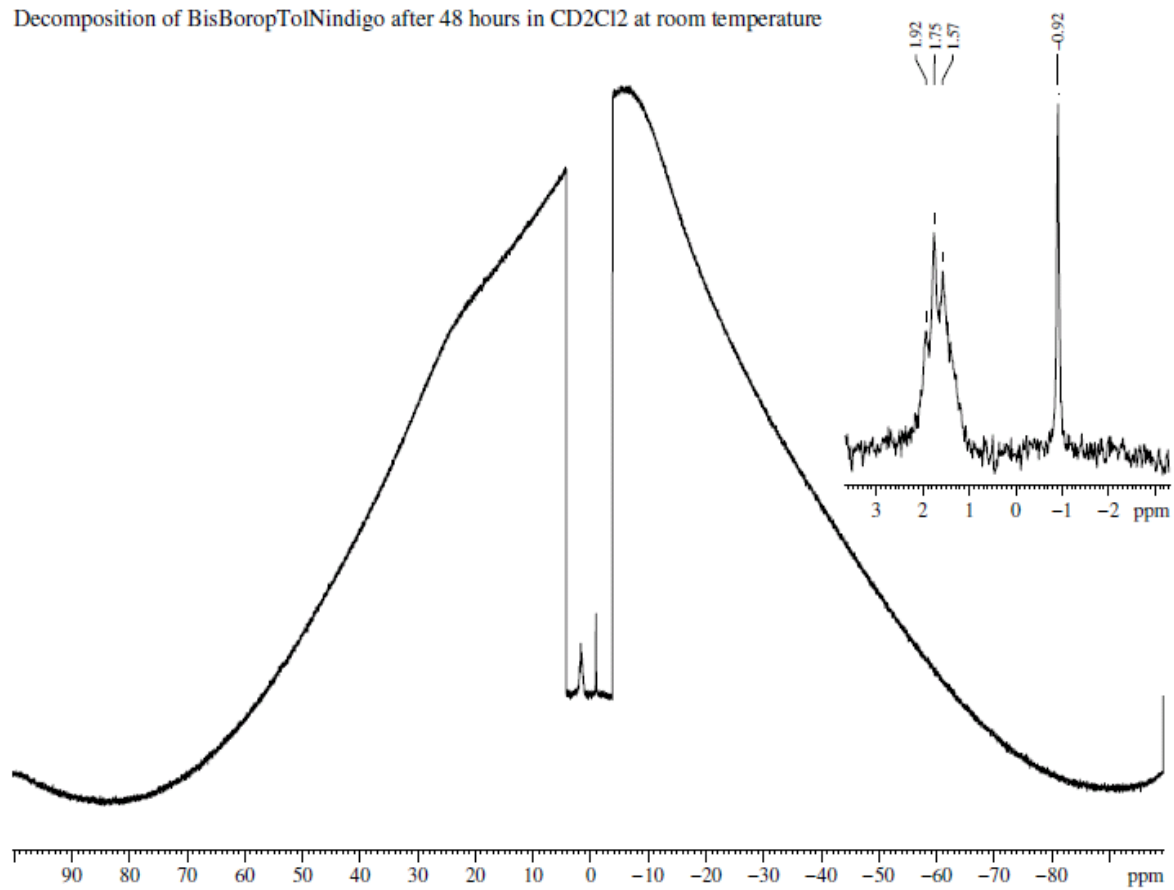
¹⁹F NMR spectrum of **3b**



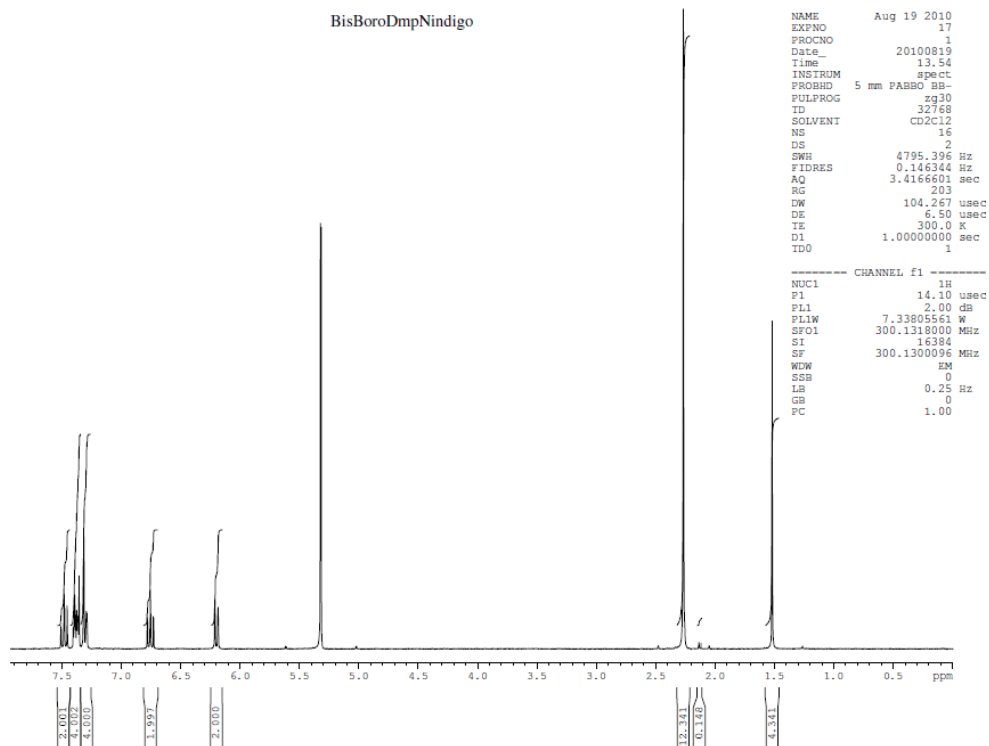
¹¹B NMR spectrum of **3b**



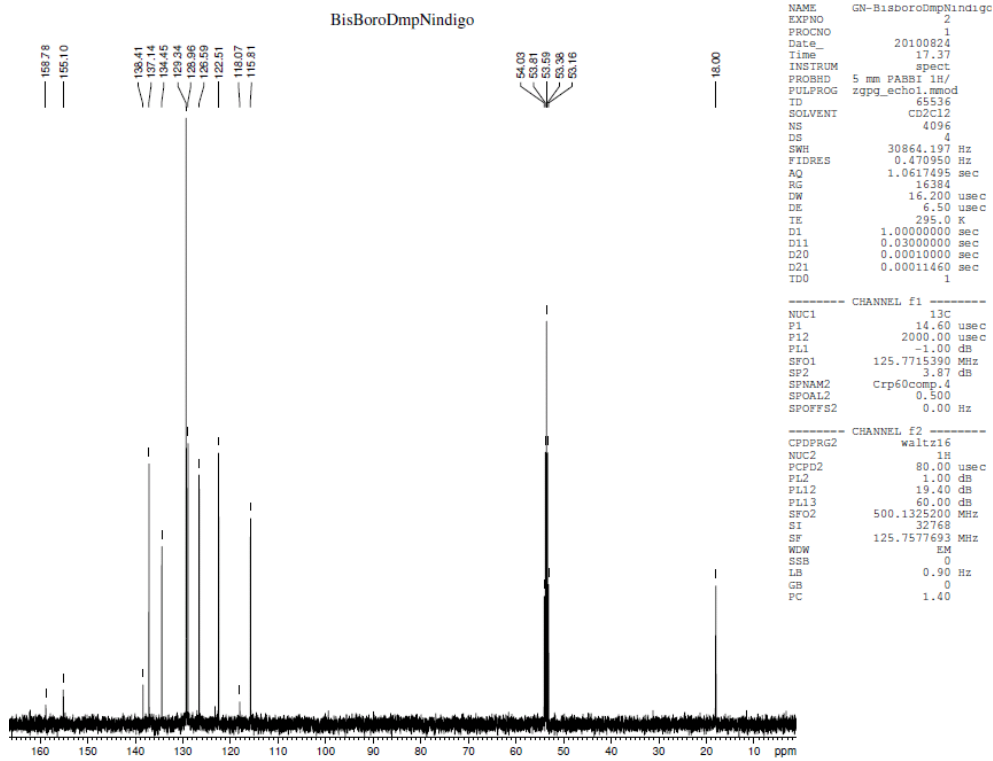
Decomposition of BisBoropTolNindigo after 48 hours in CD₂Cl₂ at room temperature



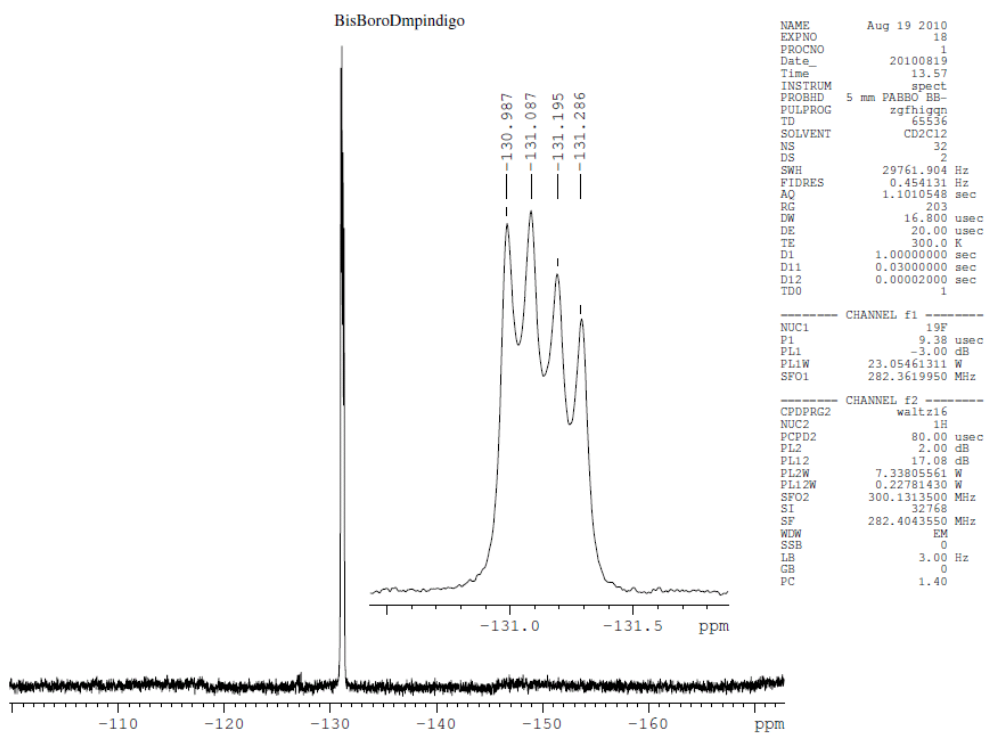
¹H NMR spectrum of **3c**



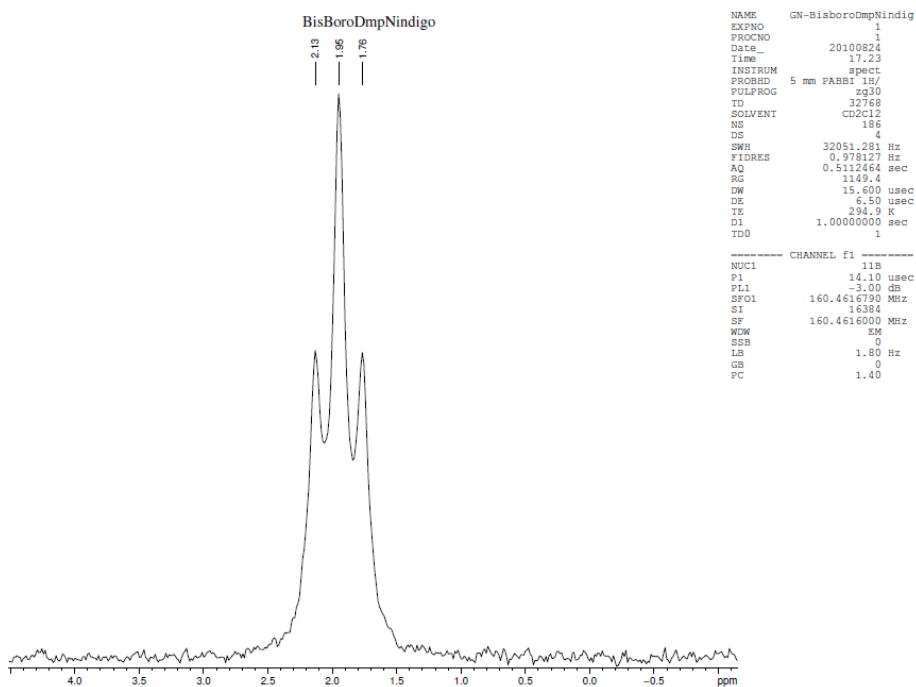
¹³C NMR spectrum of **3c**



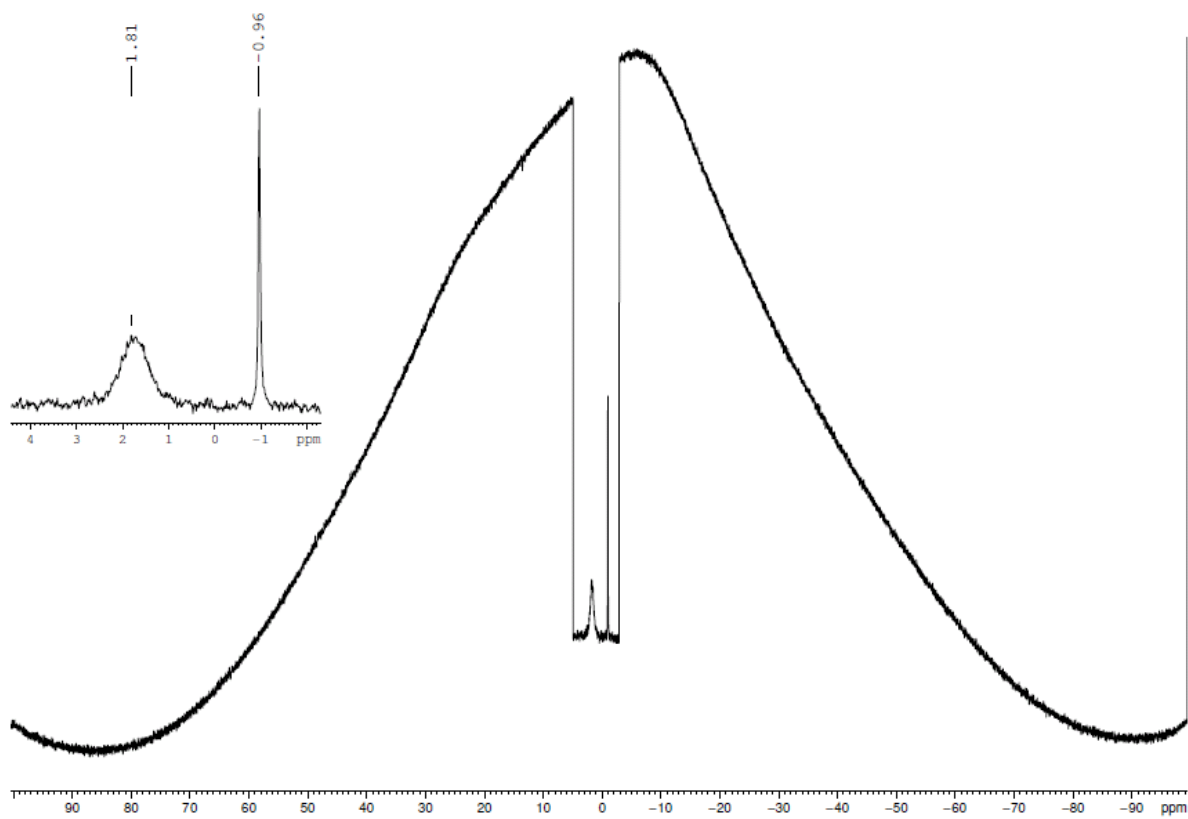
¹⁹F NMR spectrum of **3c**



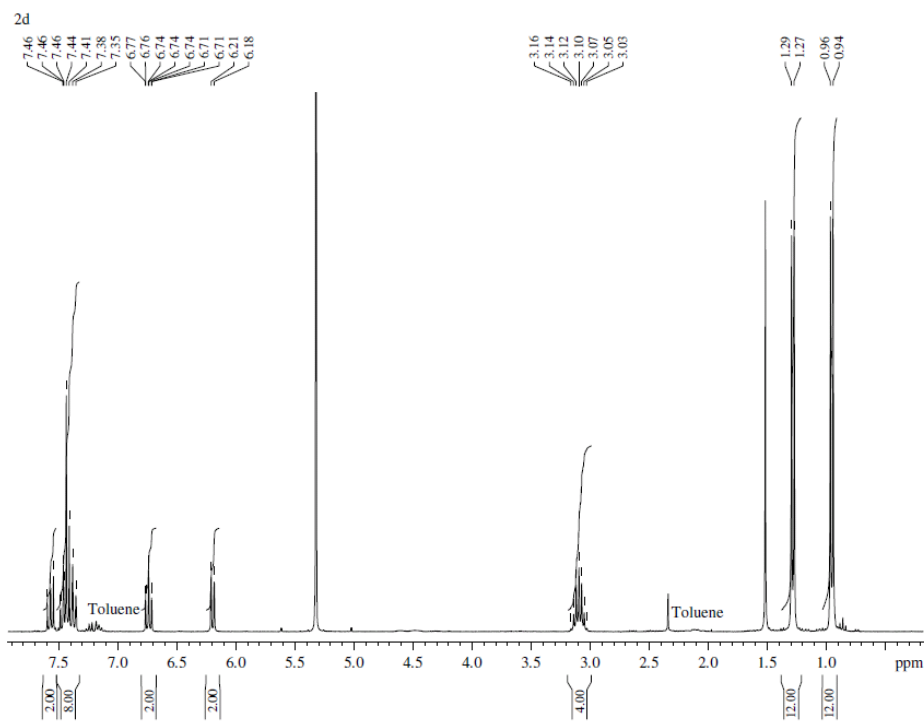
¹¹B NMR spectrum of **3c**



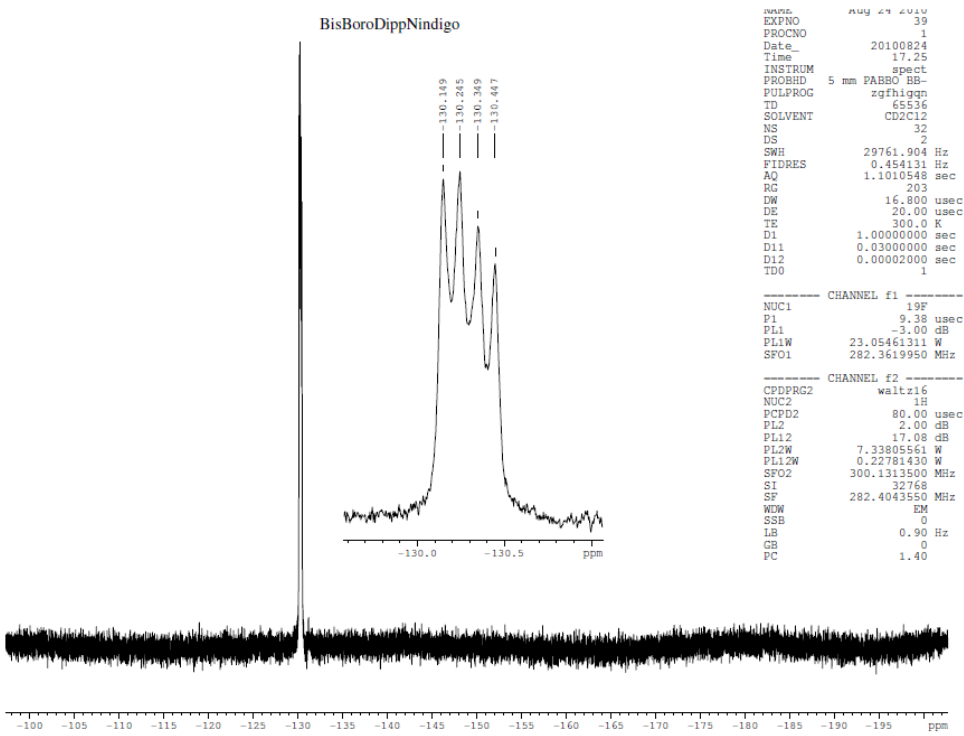
Decomposition of BisBoroDmpNindigo after 52 hours in CD₂Cl₂ at room temperature



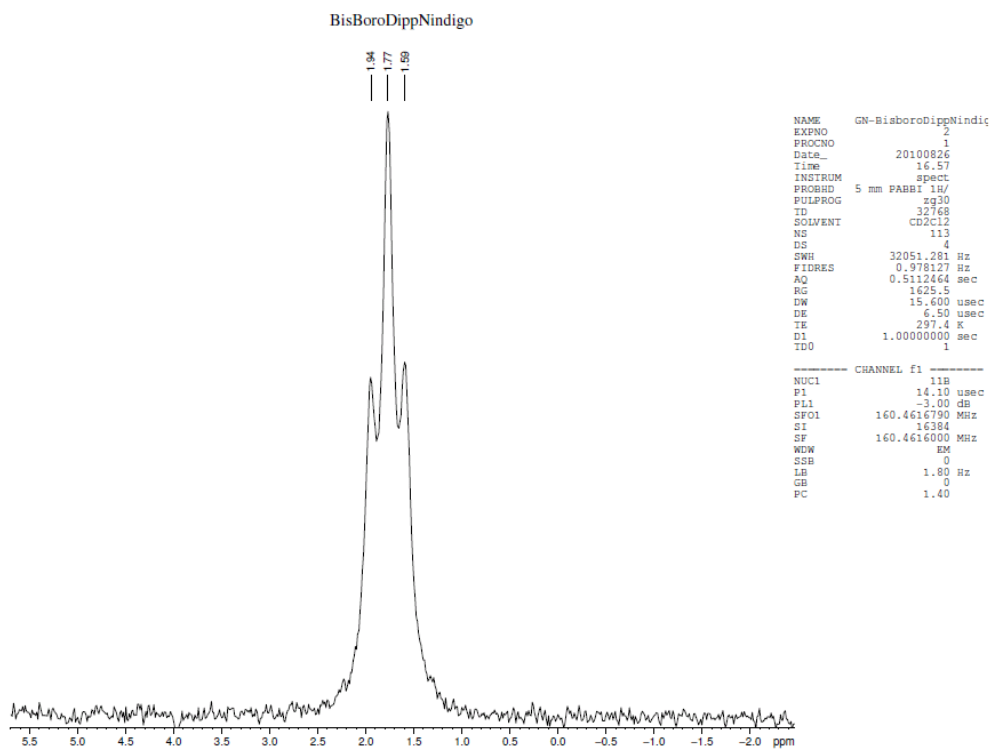
¹H NMR spectrum of **3d**



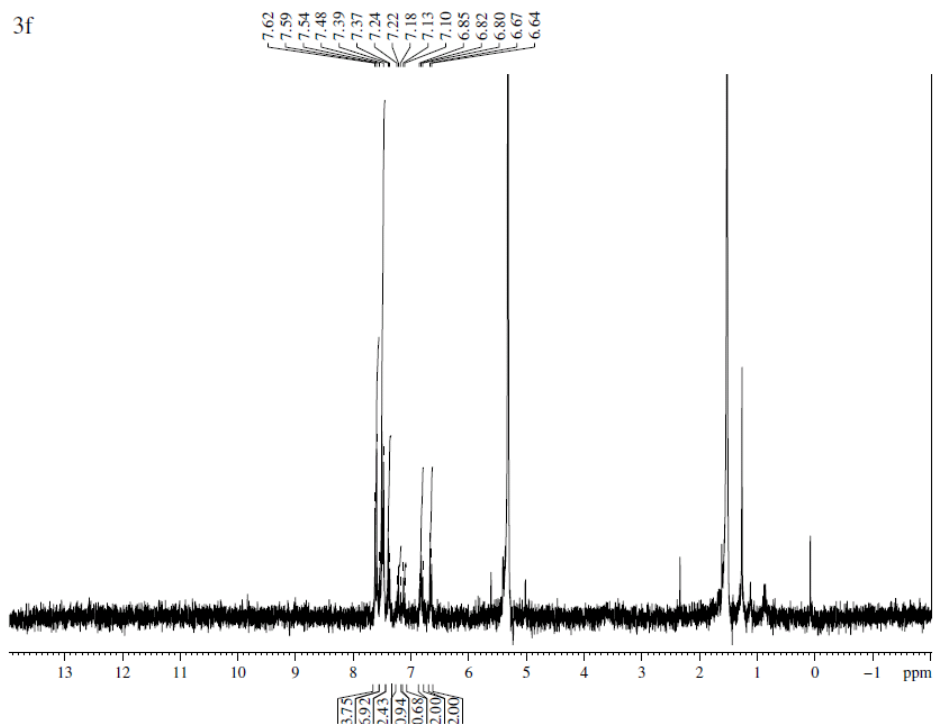
¹⁹F NMR spectrum of **3d**



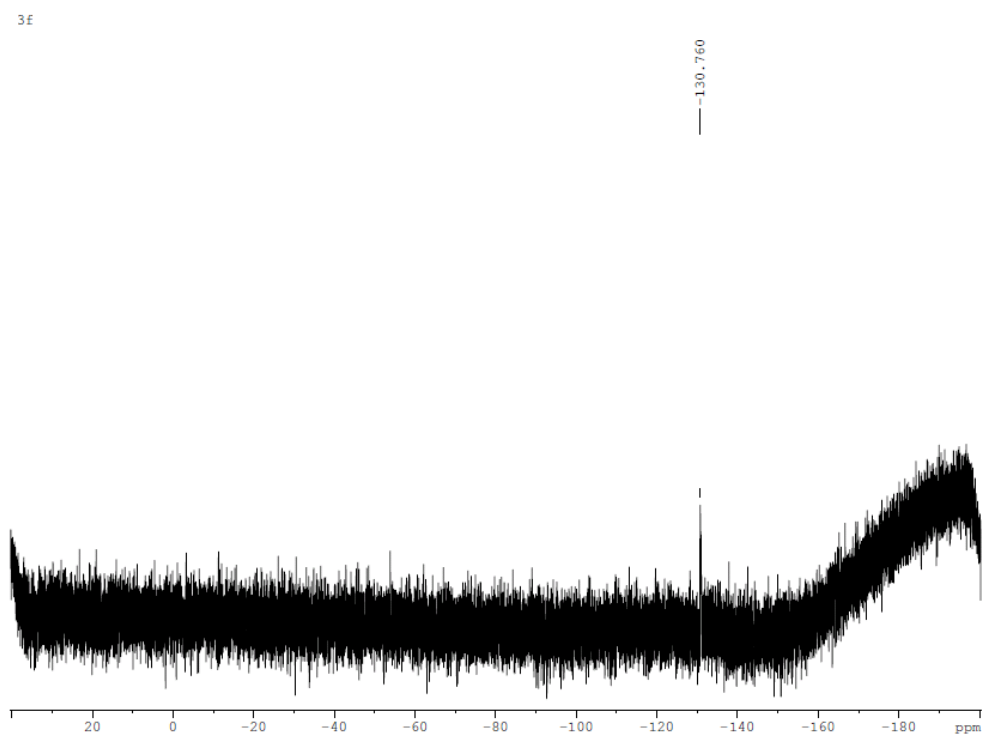
^{11}B NMR spectrum of **3d**



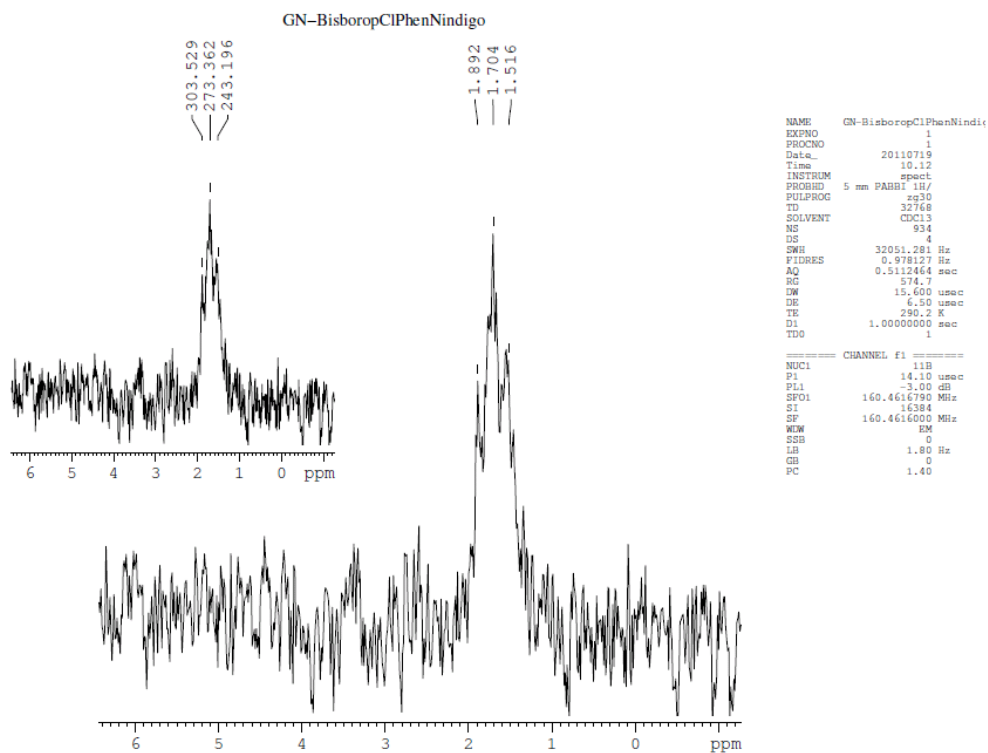
^1H NMR spectrum of **3f**



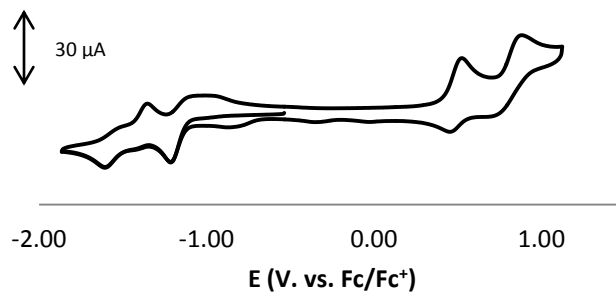
¹⁹F NMR spectrum of **3f**



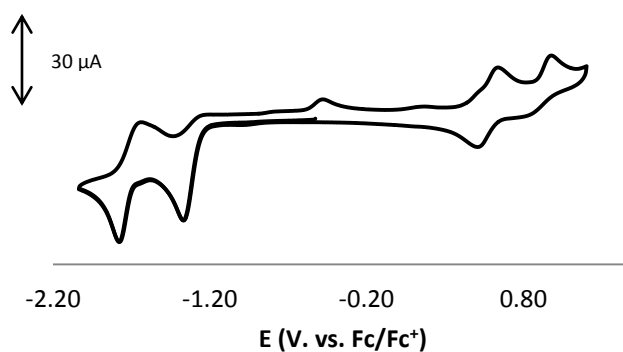
¹¹B NMR spectrum of **3f**



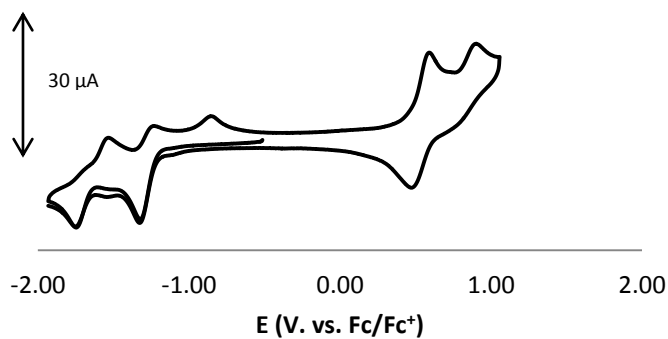
Electrochemical Data



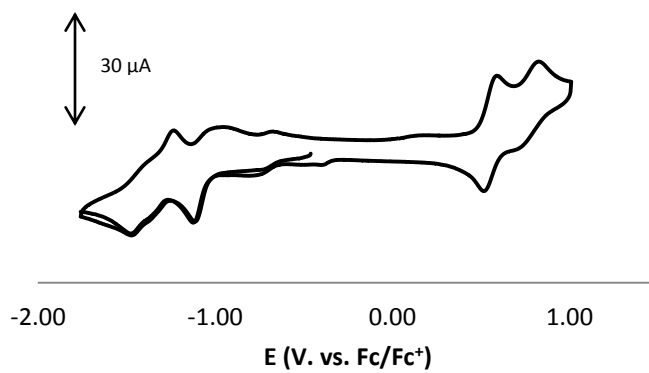
Cyclic voltammogram of 2b (CH₂Cl₂ solution, 0.1 mM Bu₄NBF₄ electrolyte and scan rate 100 mVs⁻¹)



Cyclic voltammogram of 2d (CH₂Cl₂ solution, 0.1 mM Bu₄NBF₄ electrolyte and scan rate 100 mVs⁻¹)

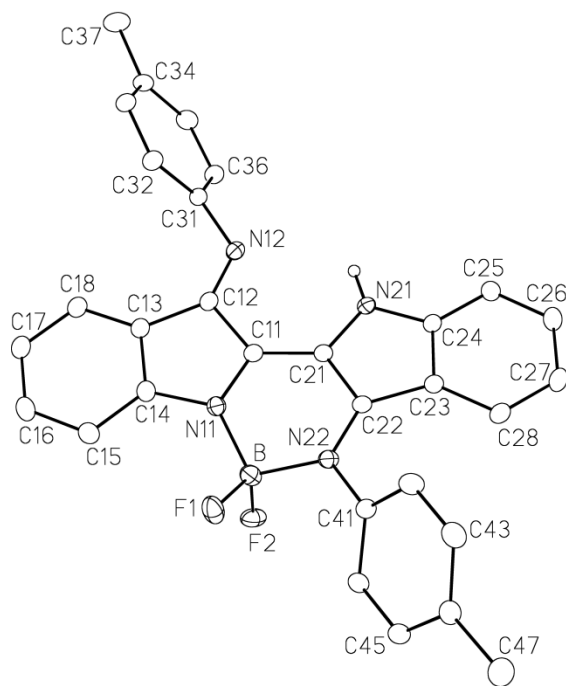


Cyclic voltammogram of 2e (CH₂Cl₂ solution, 0.1 mM Bu₄NBF₄ electrolyte and scan rate 100 mVs⁻¹)

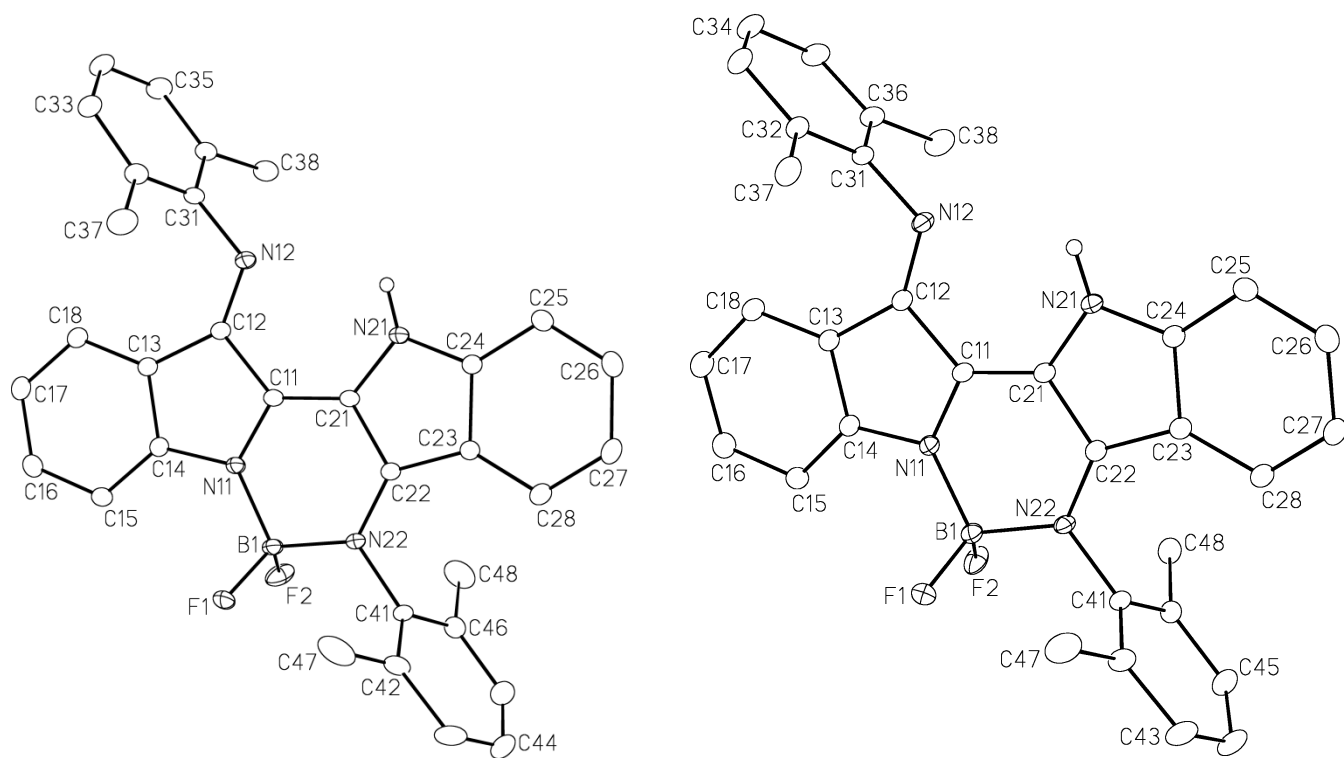


Cyclic voltammogram of 2f (CH₂Cl₂ solution, 0.1 mM Bu₄NBF₄ electrolyte and scan rate 100 mV s⁻¹)

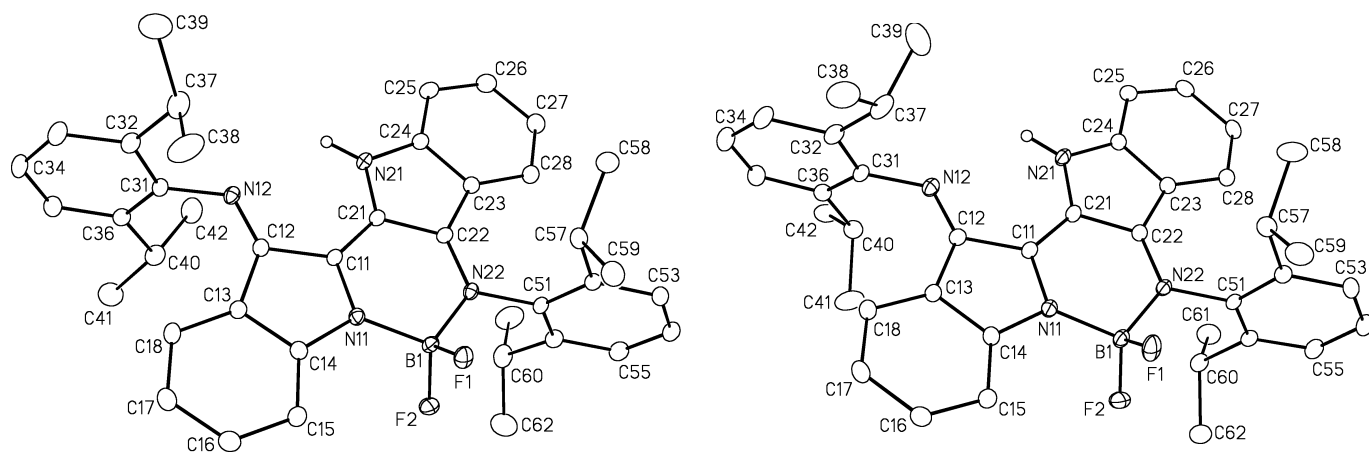
X-ray structures



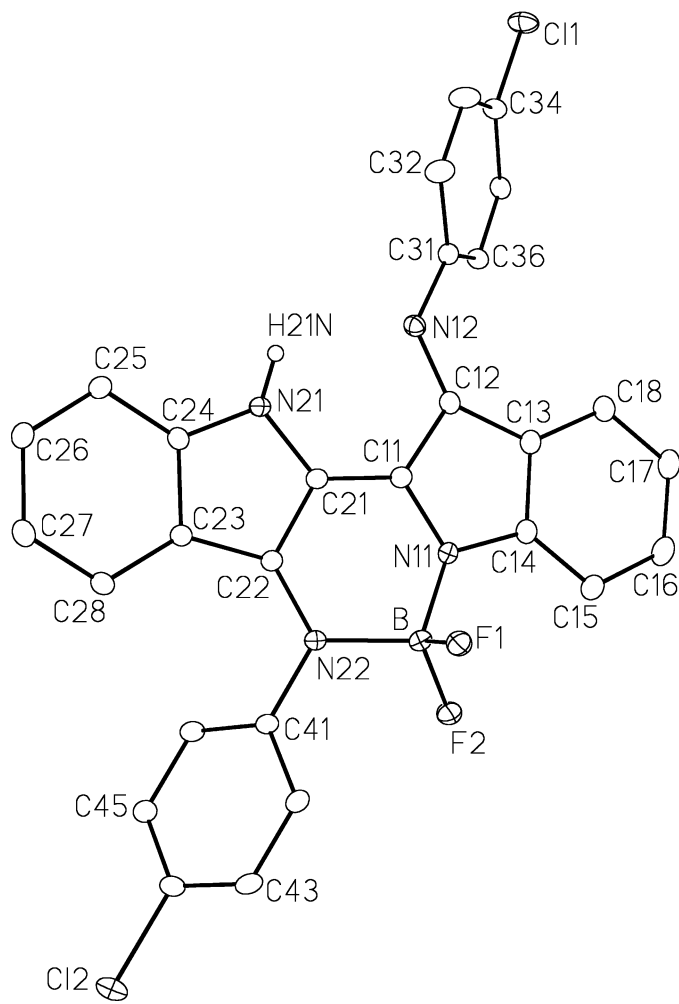
ORTEP drawing of 2b (20% probability level). Aromatic hydrogen atoms are omitted for clarity



ORTEP drawing of the two crystallographically-independent molecules of 2c (20% probability level). Aromatic hydrogen atoms are omitted for clarity



ORTEP drawing of the two crystallographically-independent molecules of 2d (20% probability level). Aromatic hydrogen atoms are omitted for clarity



ORTEP drawing of 2f (20% probability level). Aromatic hydrogen atoms are omitted for clarity