

Supporting Information for
Nickel-Iron Dithiolates Related to the Deactivated [NiFe]-Hydrogenases

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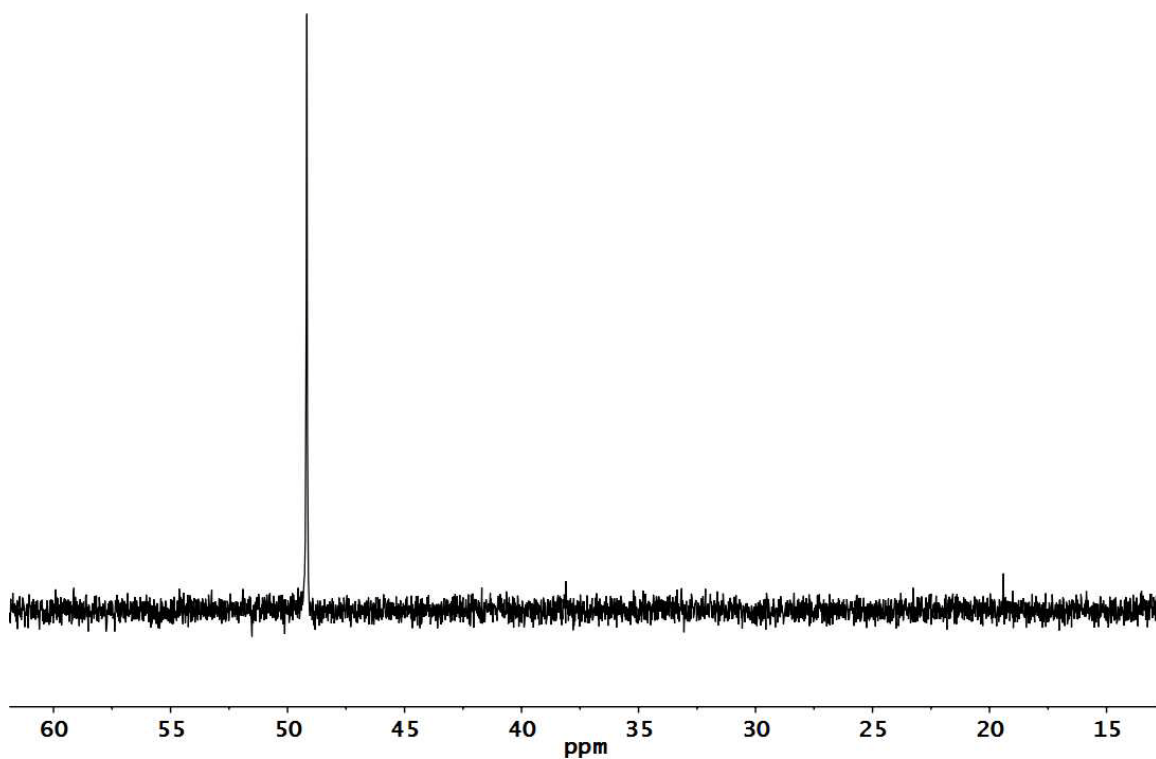


Figure 1: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\text{1I}]\text{BF}_4$.

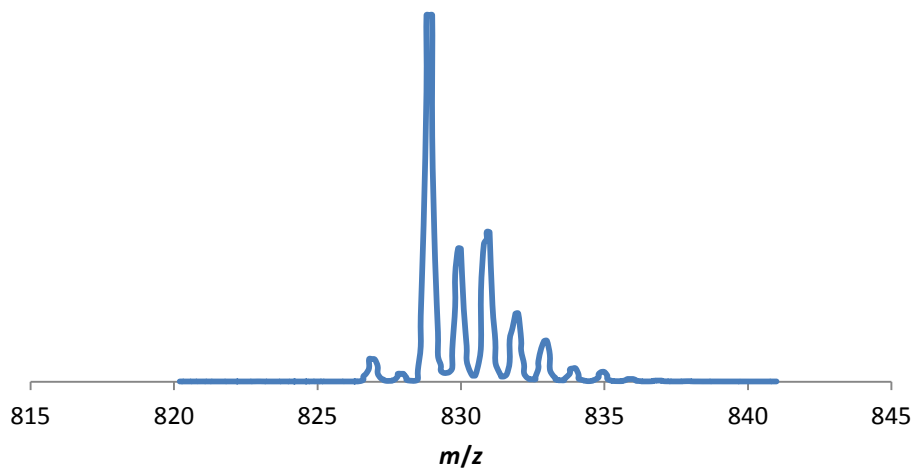


Figure 2: Positive ion ESI mass spectrum of $[11]BF_4$.

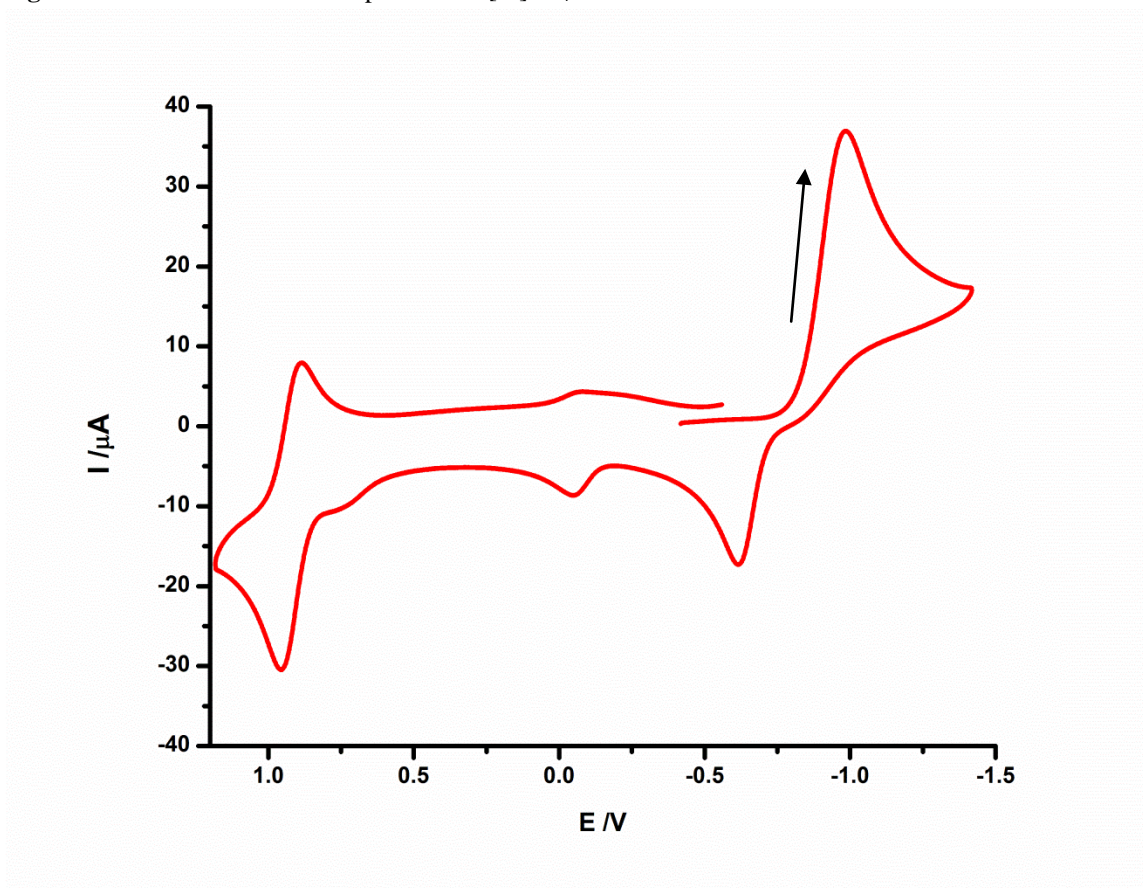


Figure 3: Cyclic voltammogram of $[11]BF_4$.

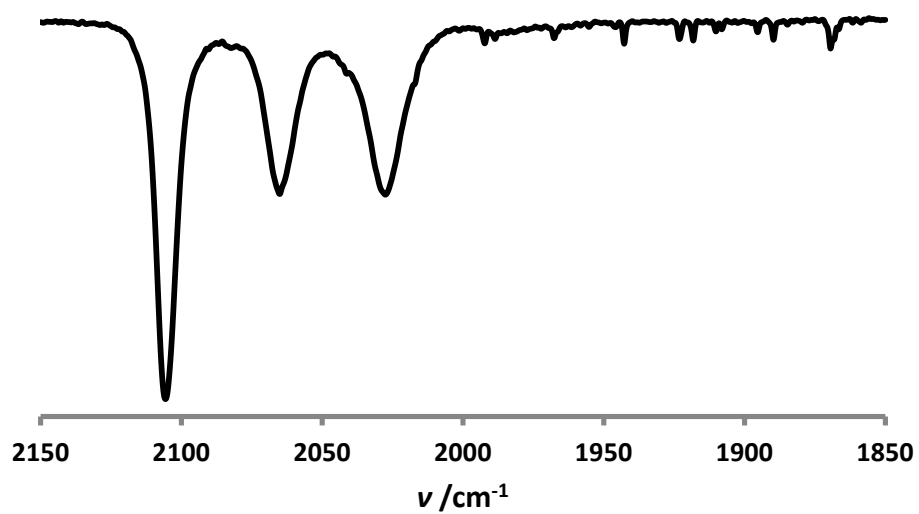


Figure 4: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1Br}]\text{BF}_4$.

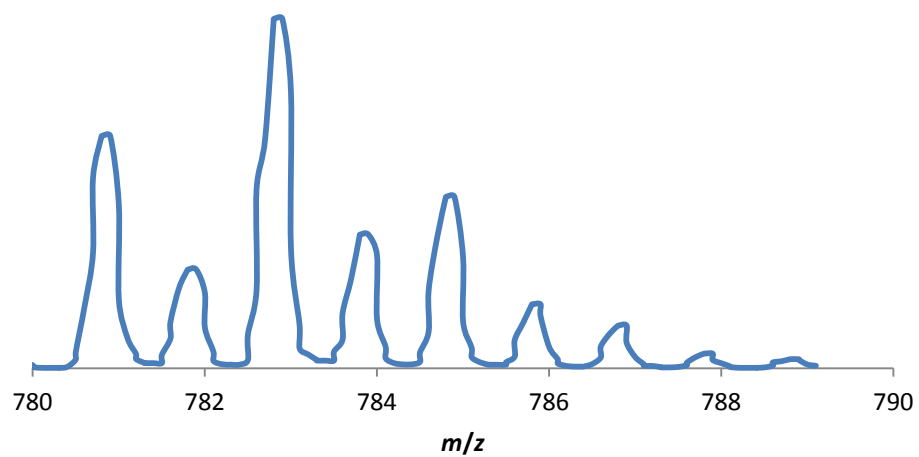


Figure 5: Positive ion ESI mass spectrum of $[\mathbf{1Br}]\text{BF}_4$.

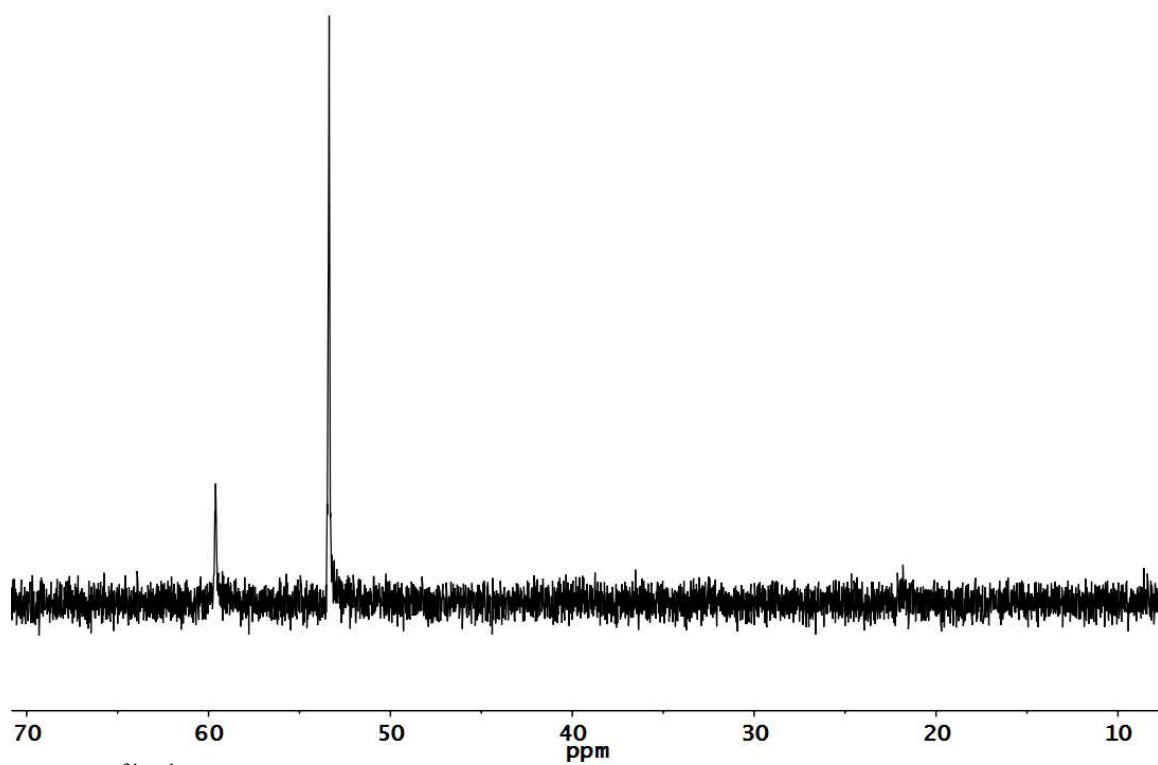


Figure 6: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\mathbf{1Br}]\text{BF}_4$.

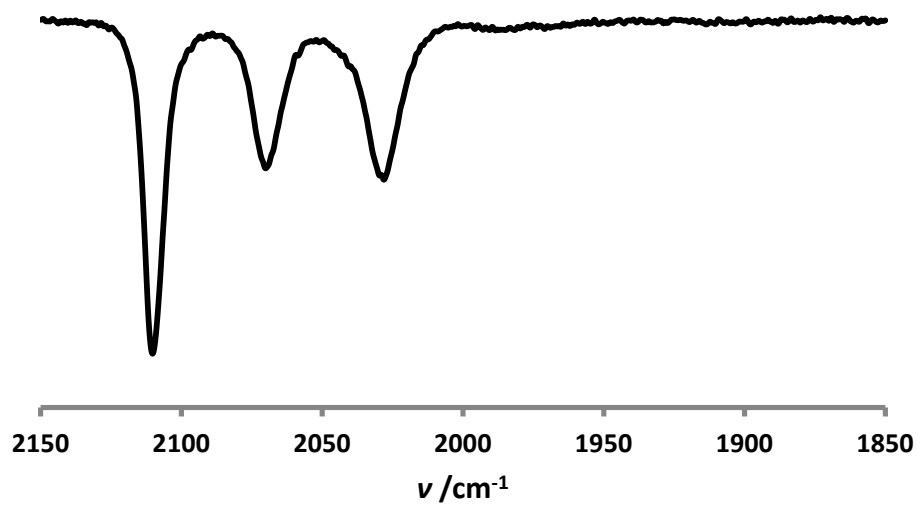


Figure 7: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1Cl}]\text{BF}_4$.

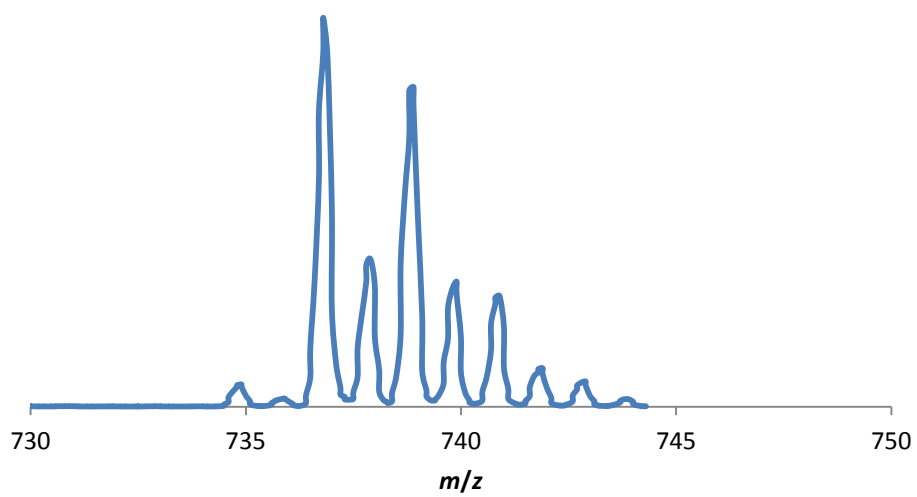


Figure 8: Positive ion ESI mass spectrum of $[1\text{Cl}]\text{BF}_4$.

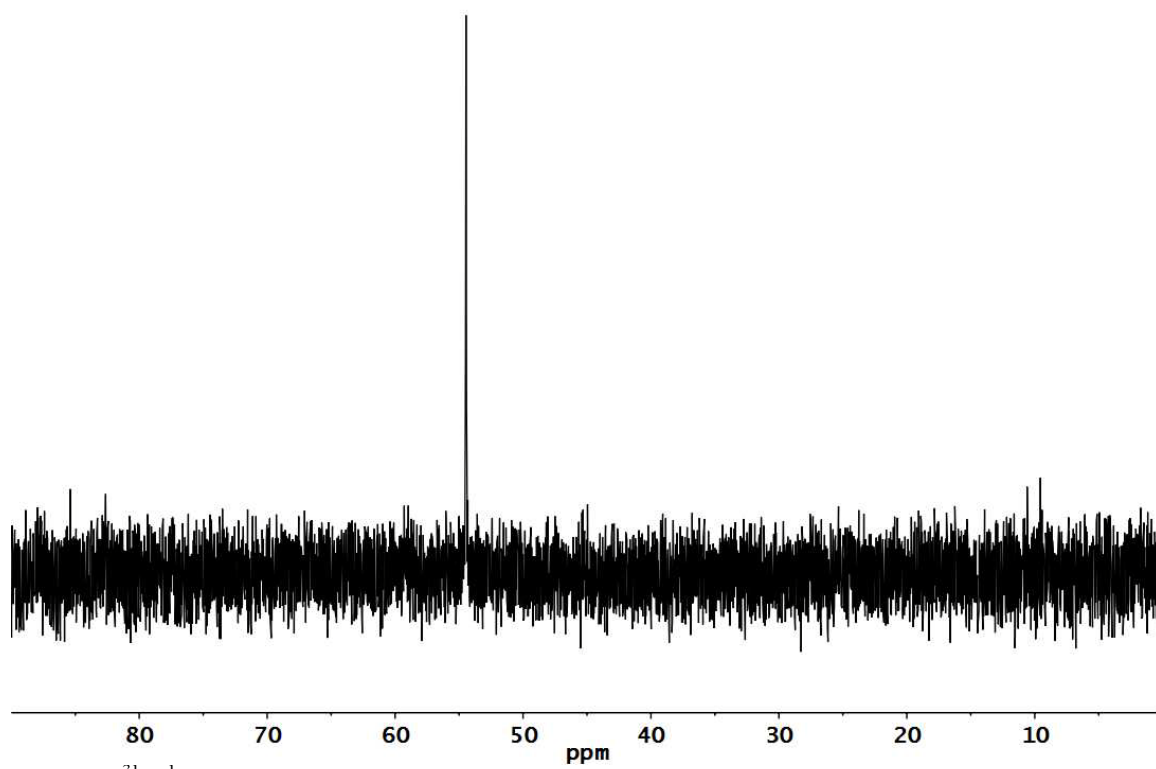


Figure 9: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[1\text{Cl}]\text{BF}_4$.

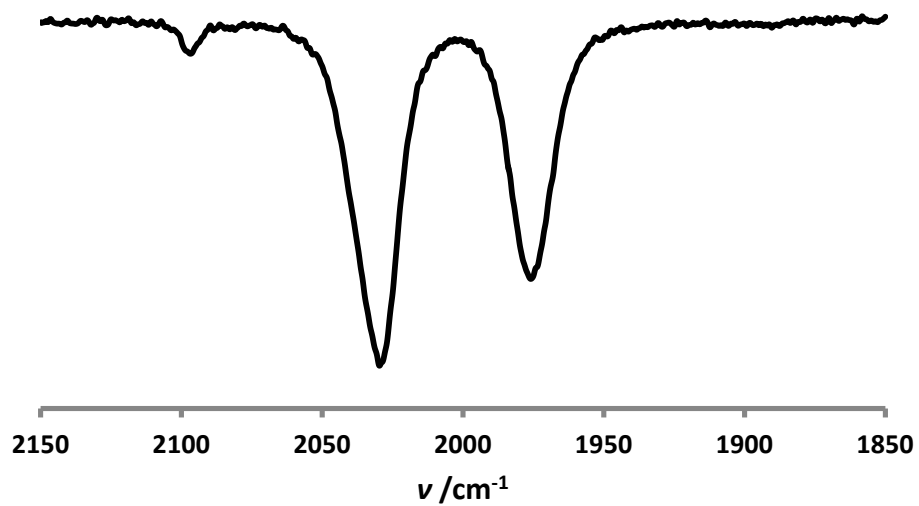


Figure 10: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1aI}]\text{BF}_4$.

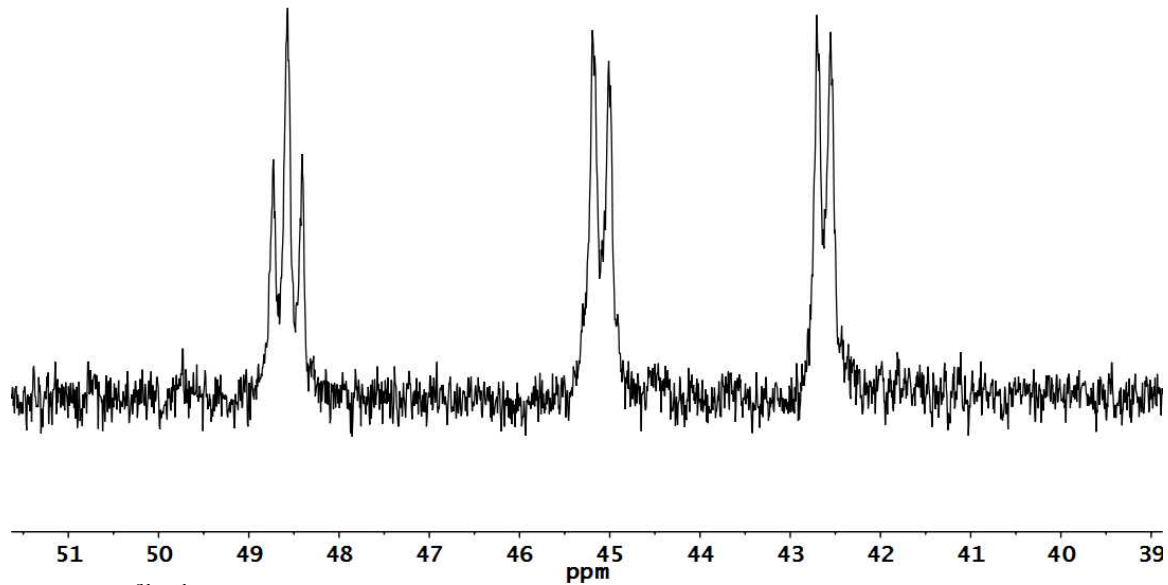


Figure 11: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\mathbf{1aI}]\text{BF}_4$.

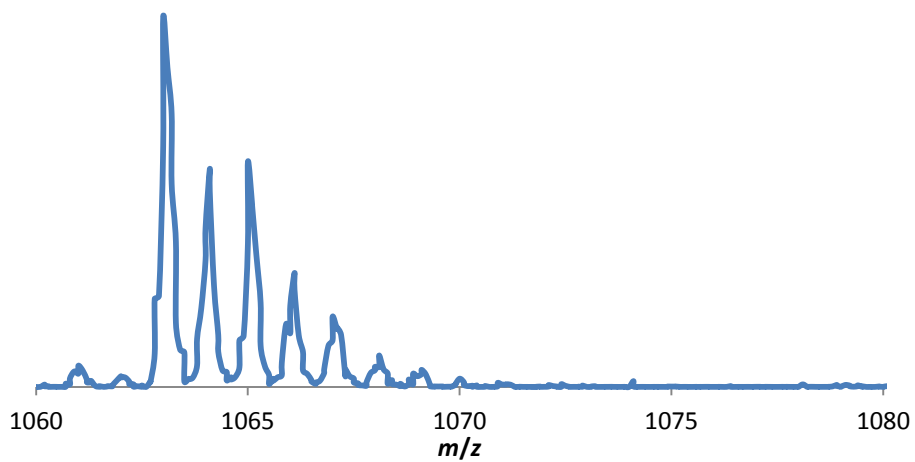


Figure 12: Positive ion ESI mass spectrum of $[1aI]BF_4$.

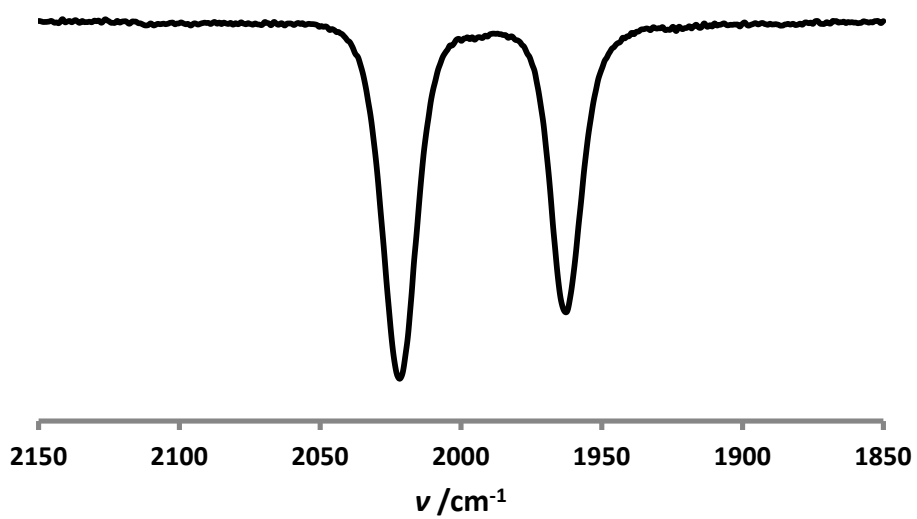


Figure 13: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[1bI]BF_4$.

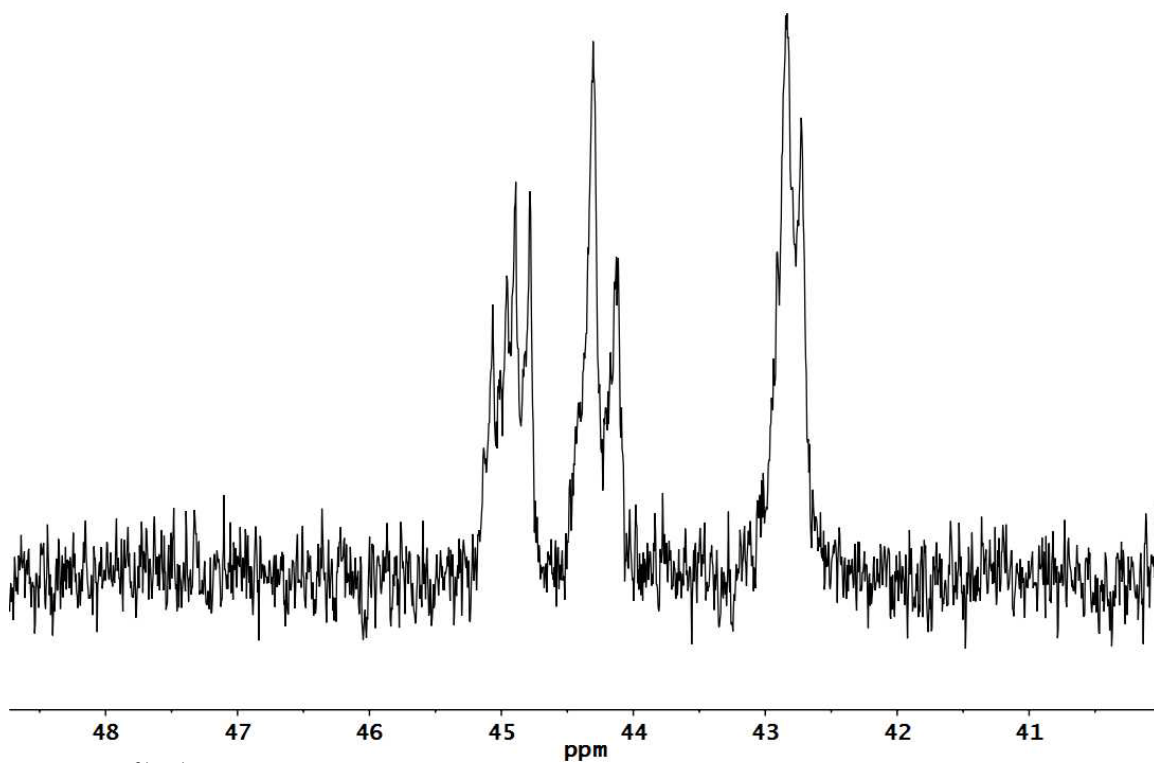


Figure 14: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\mathbf{1bI}]\text{BF}_4$.

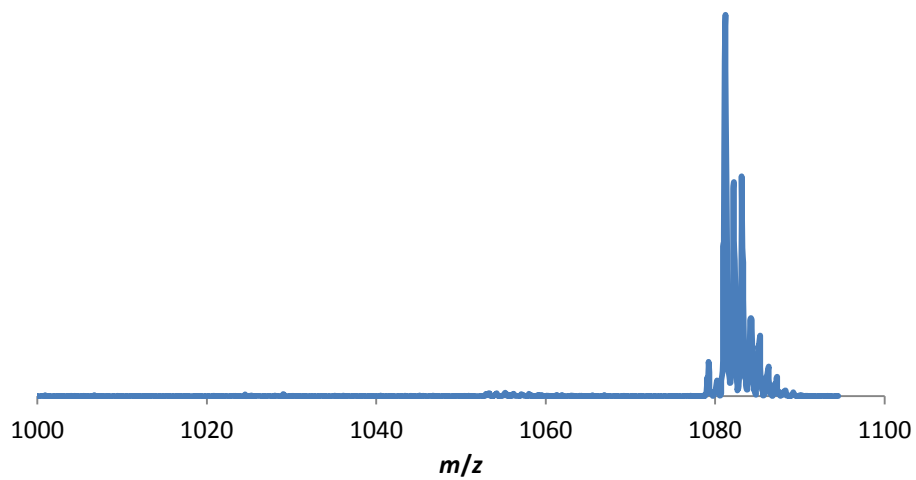


Figure 15: Positive ion ESI mass spectrum of $[\mathbf{1bI}]\text{BF}_4$.

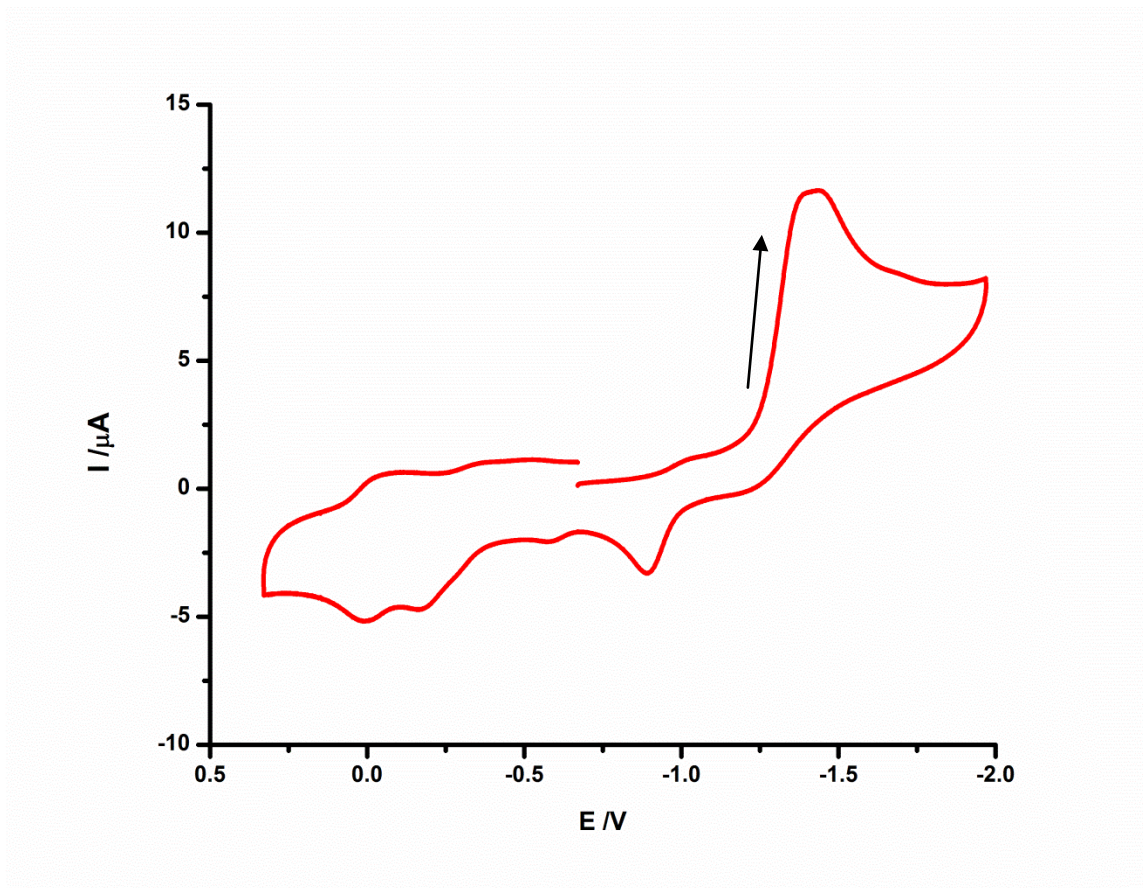


Figure 16: Cyclic voltammogram of [1bI]BF₄.

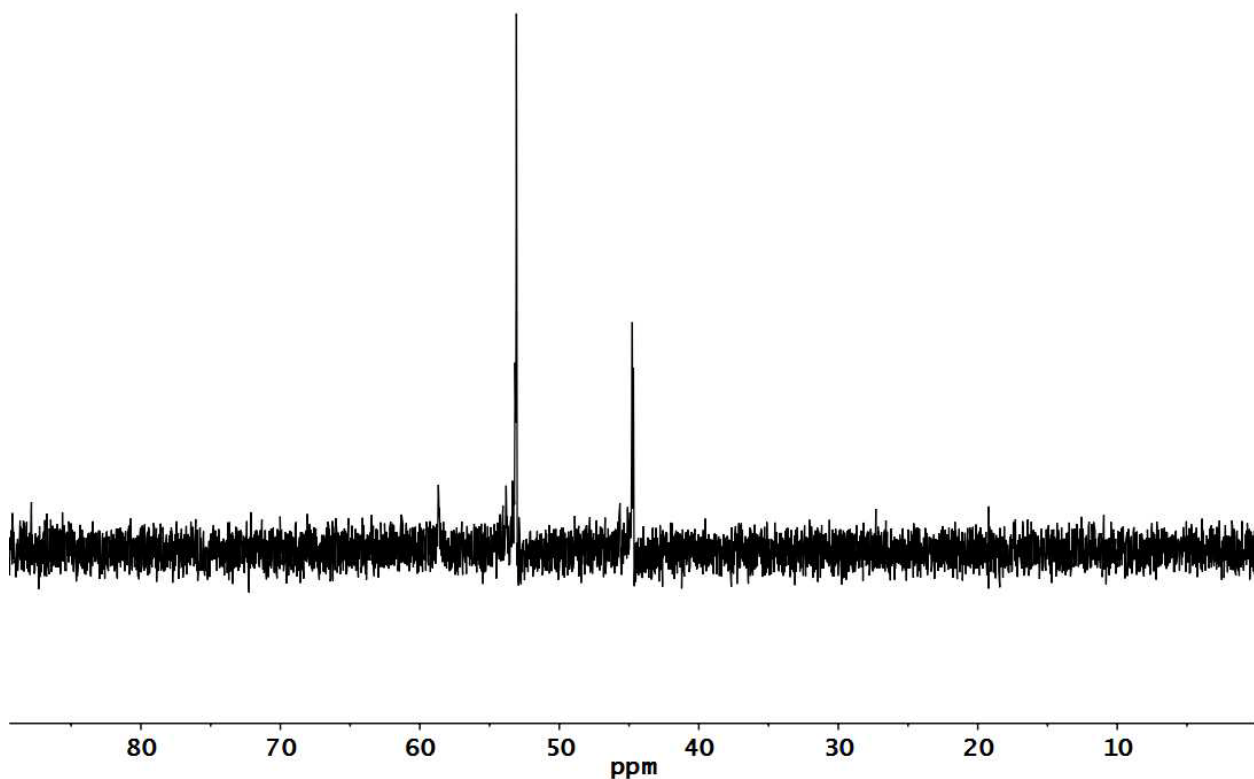


Figure 17: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\mathbf{1aCl}]\text{BF}_4$.

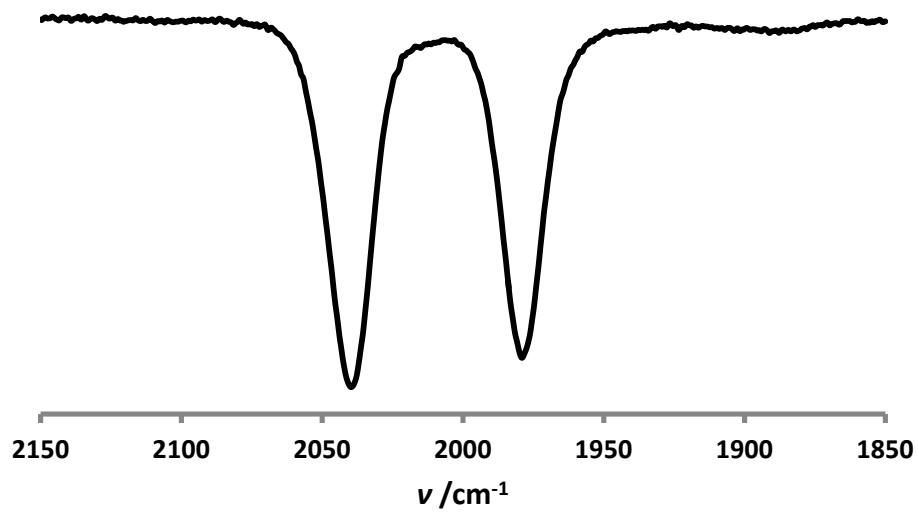


Figure 18: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1aCl}]\text{BF}_4$.

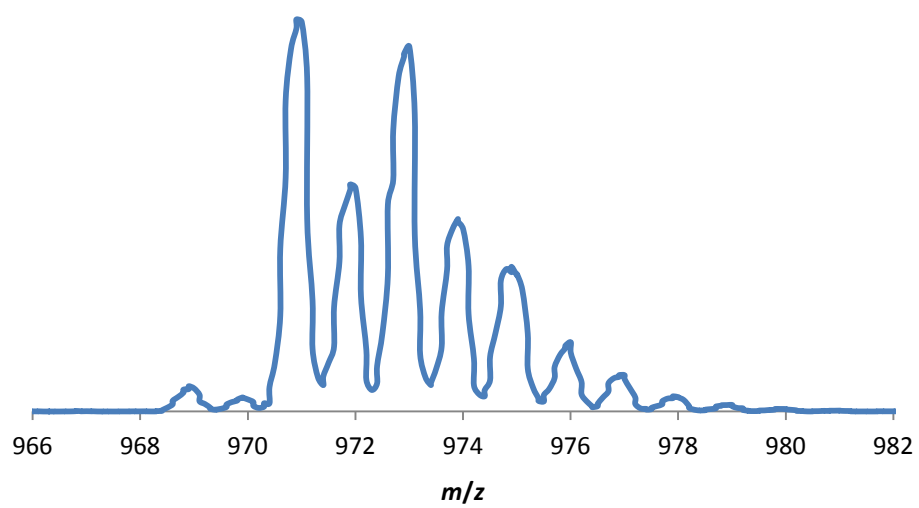


Figure 19: Positive ion ESI mass spectrum of $[1aCl]BF_4$.

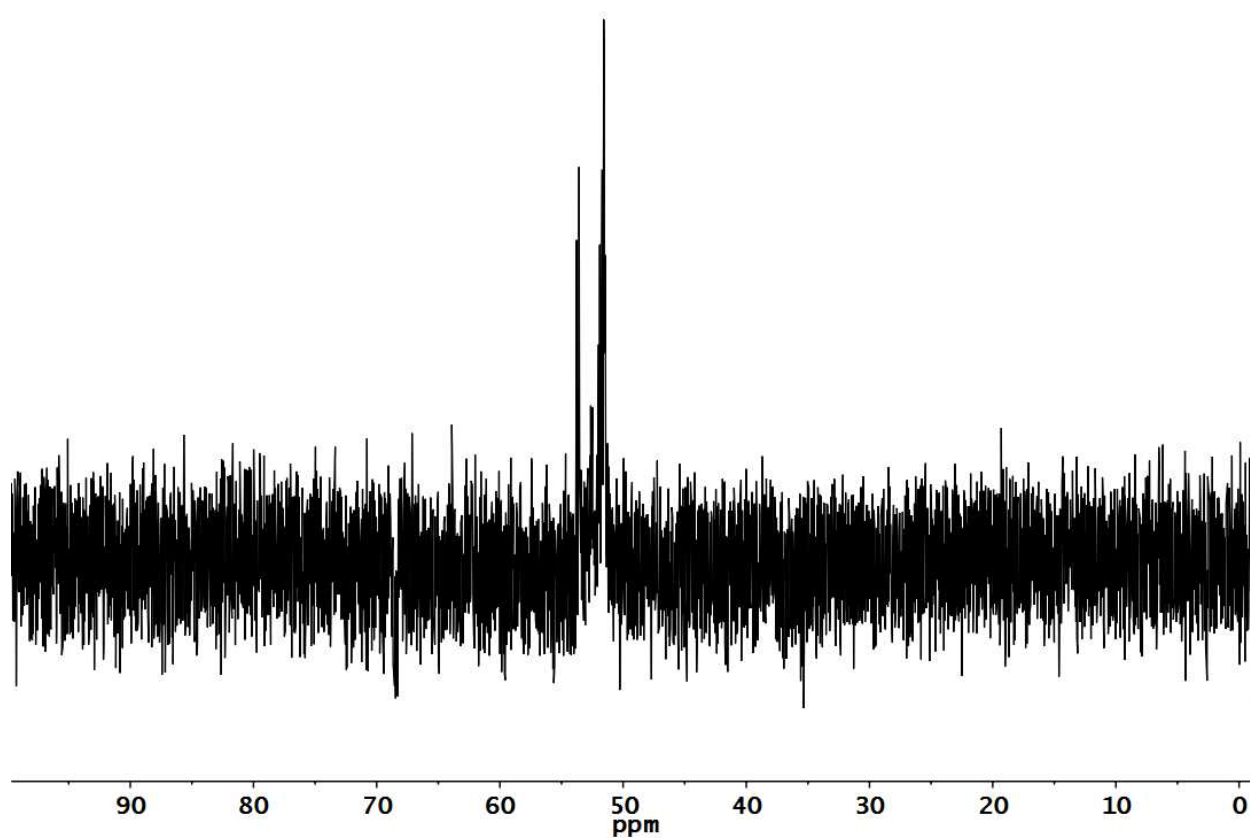


Figure 20: $^{31}P\{^1H\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[1bCl]BF_4$.

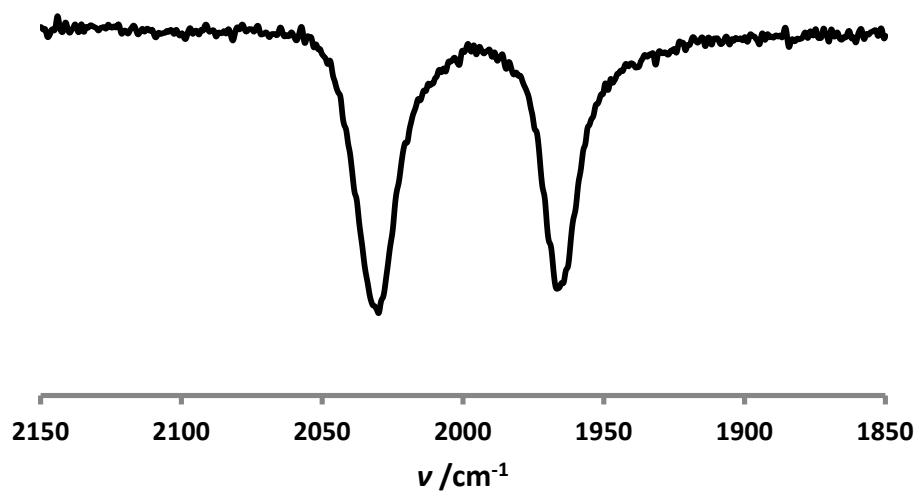


Figure 21: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1bCl}]\text{BF}_4$.

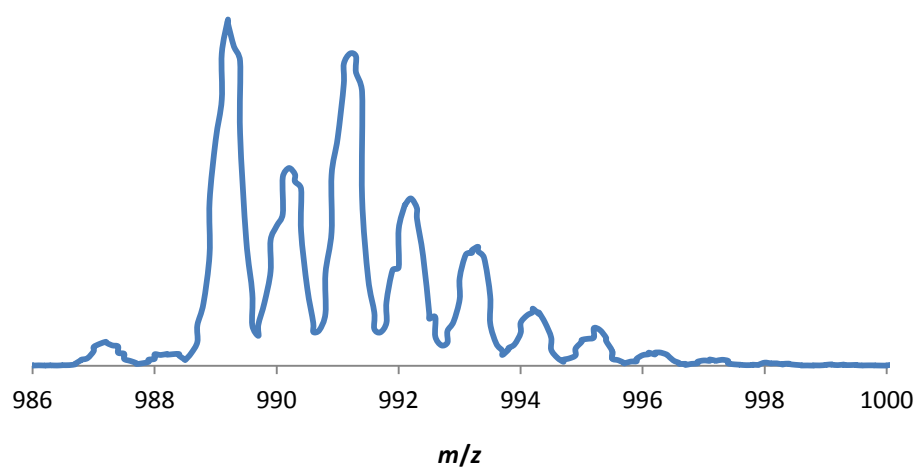


Figure 22: Positive ion ESI mass spectrum of $[\mathbf{1bCl}]\text{BF}_4$.

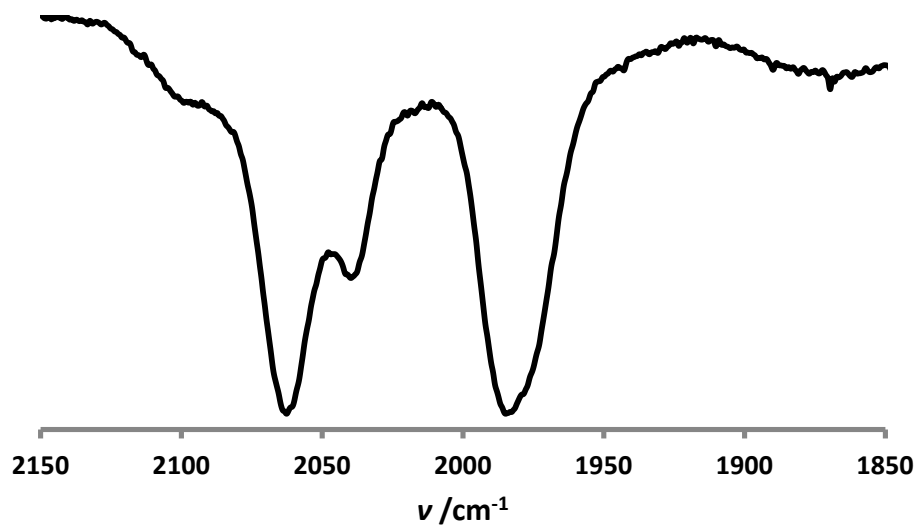


Figure 23: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1aF}]\text{BF}_4$.

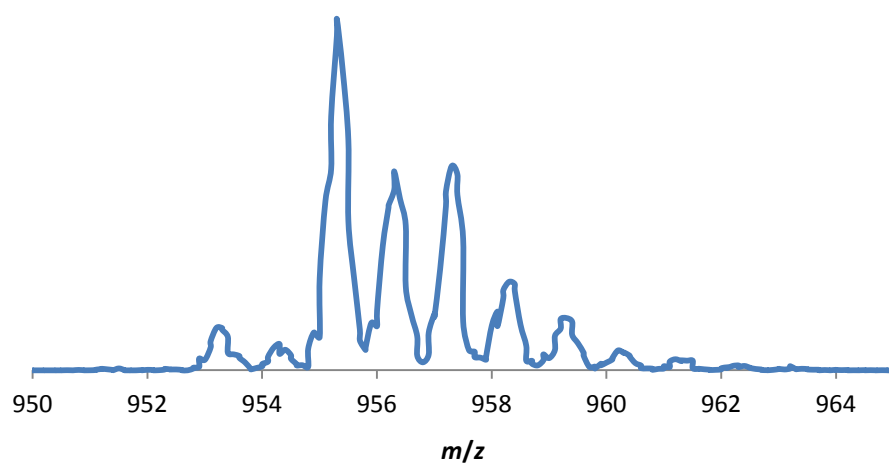


Figure 24: Positive ion ESI mass spectrum of $[\mathbf{1aF}]\text{BF}_4$.

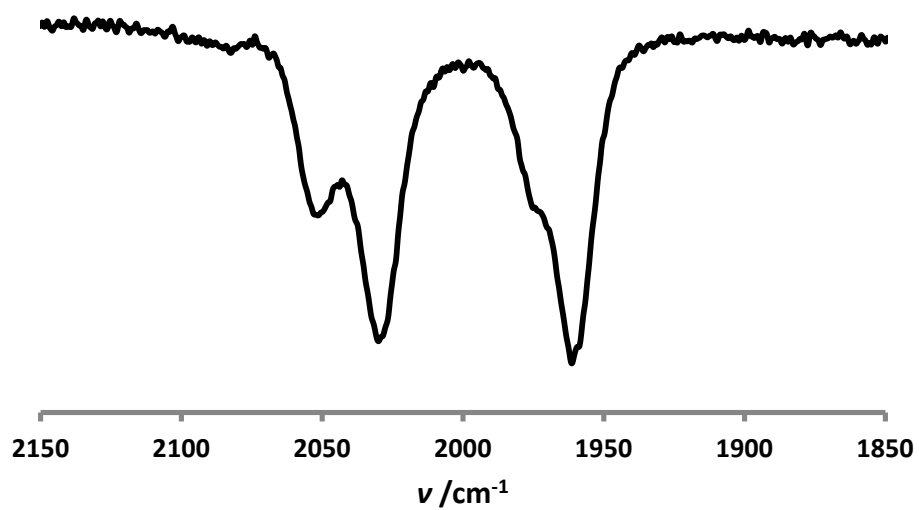


Figure 25: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of **[1bF]BF₄**.

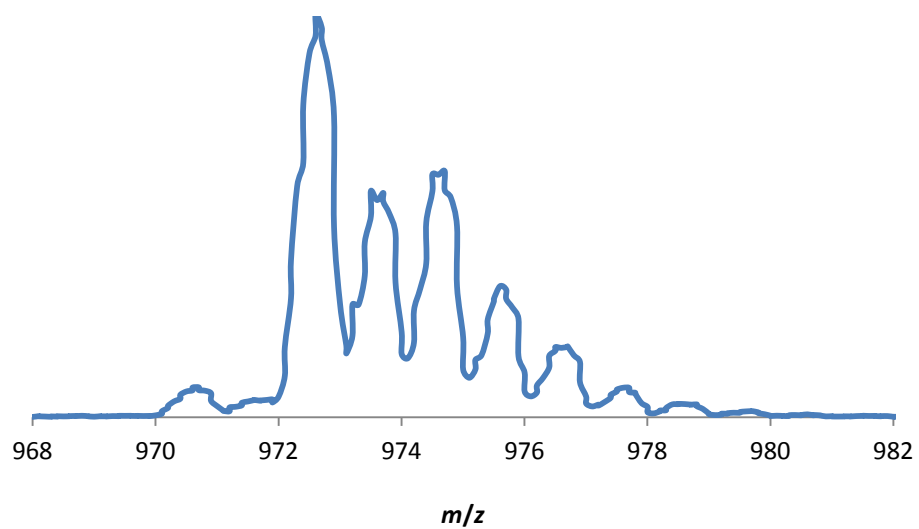


Figure 26: Positive ion ESI mass spectrum of **[1bF]BF₄**.

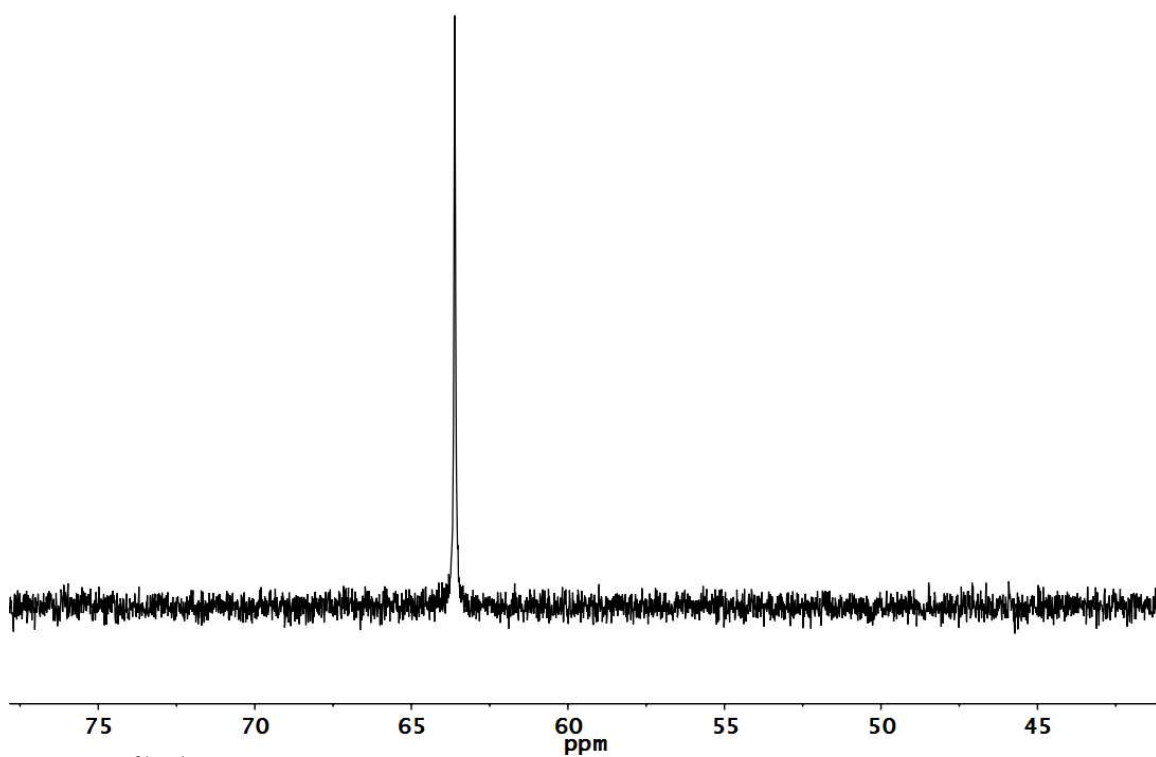


Figure 27: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\mathbf{2I}]\text{BF}_4$.

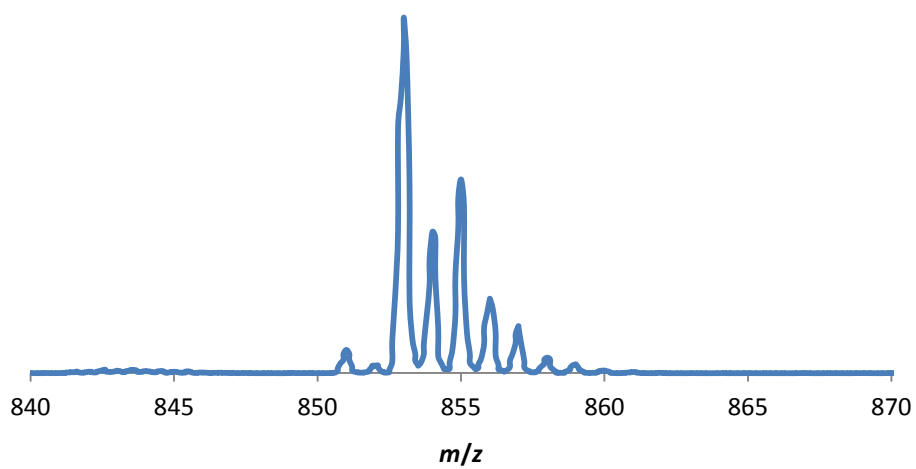


Figure 28: Positive ion ESI mass spectrum of $[\mathbf{2I}]\text{BF}_4$.

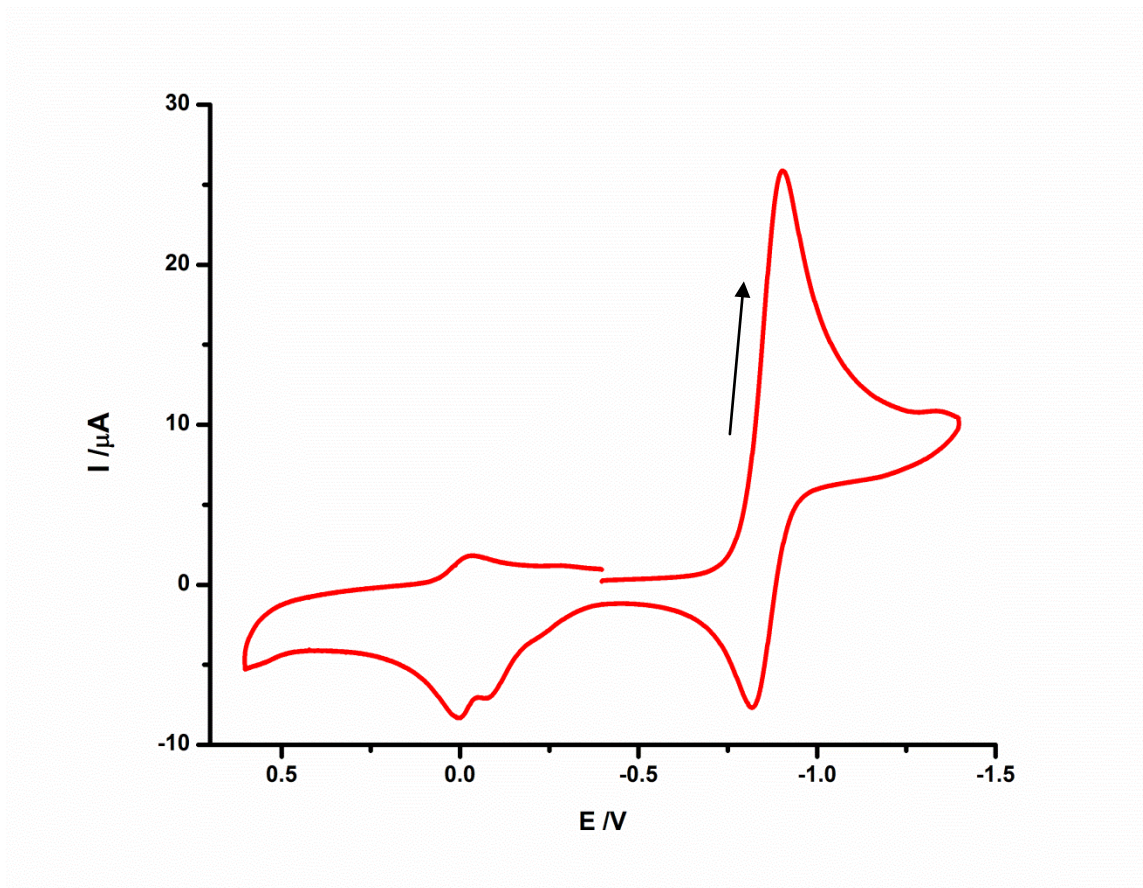


Figure 29: Cyclic voltammogram of [2I]BF₄.