

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

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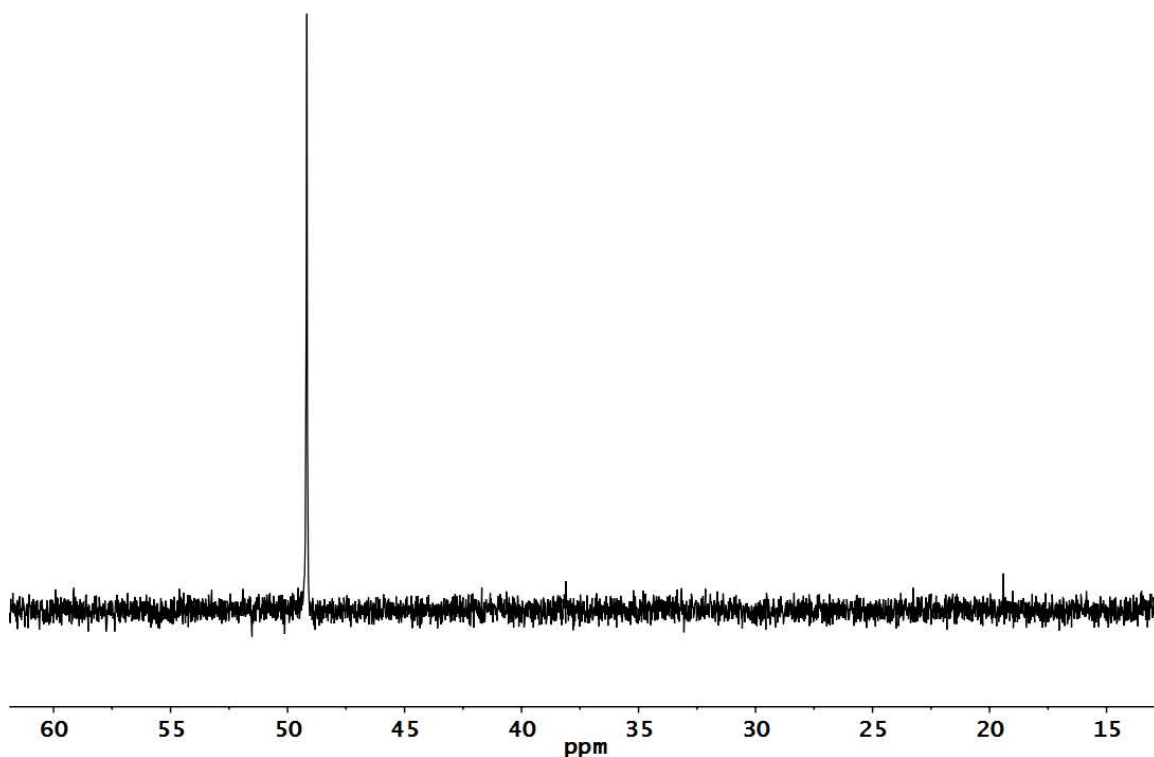


Figure 1: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[1\text{I}]\text{BF}_4$.

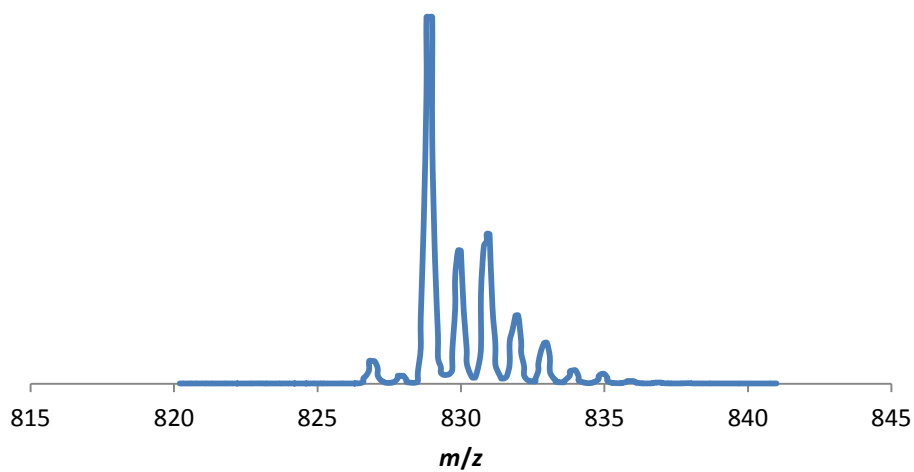


Figure 2: Positive ion ESI mass spectrum of [11]BF₄.

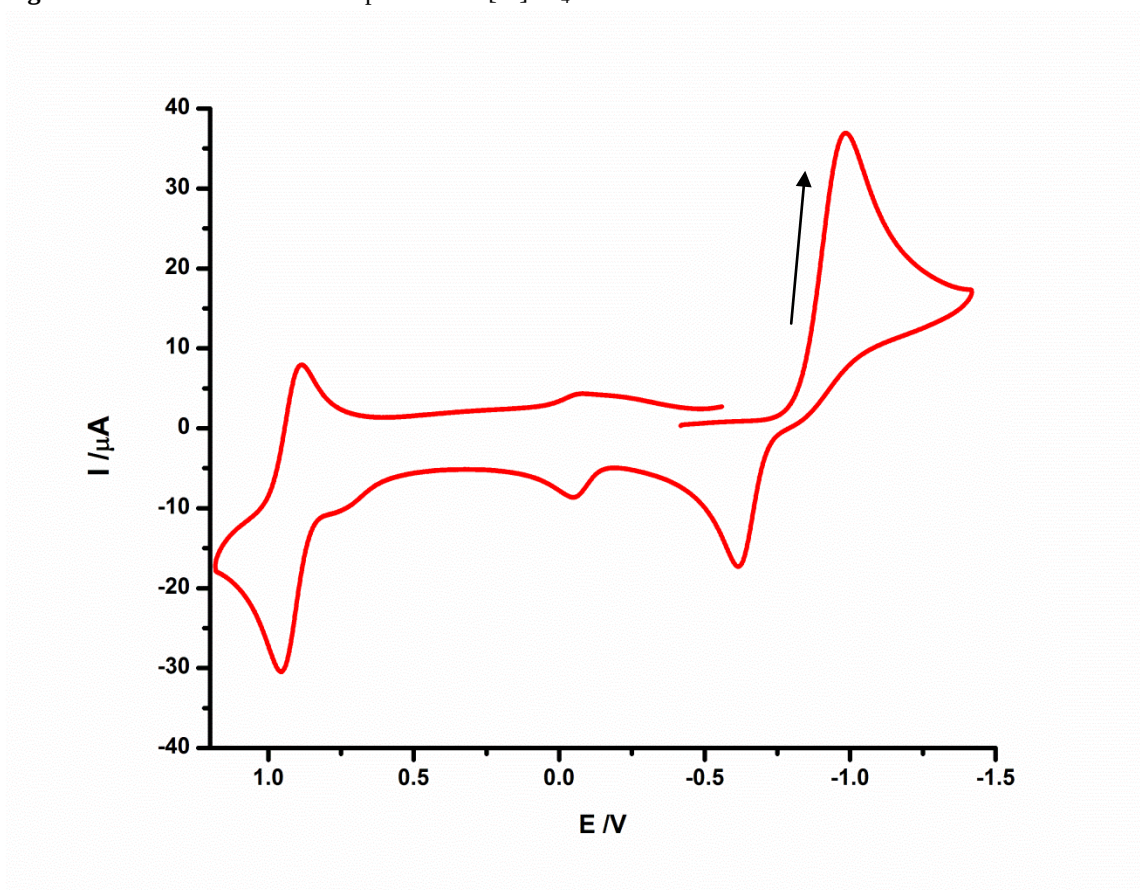


Figure 3: Cyclic voltammogram of [11]BF₄.

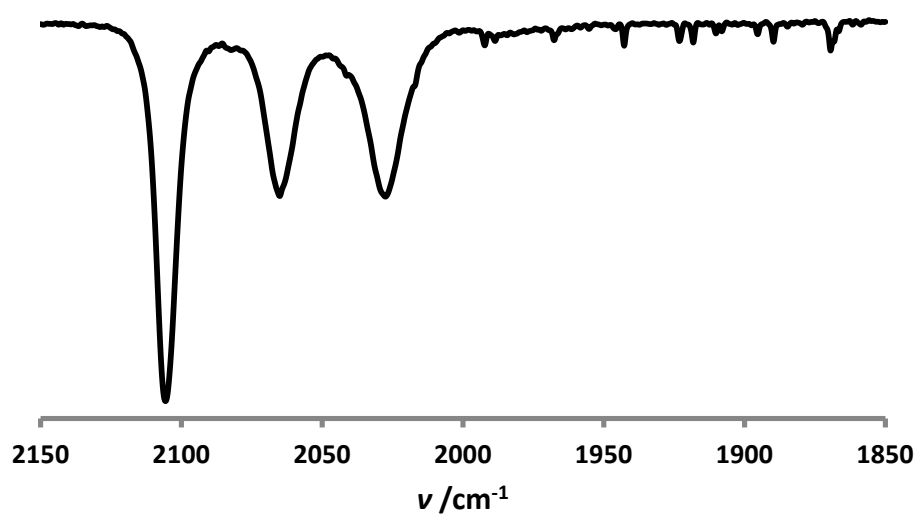


Figure 4: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1Br}]\text{BF}_4$.

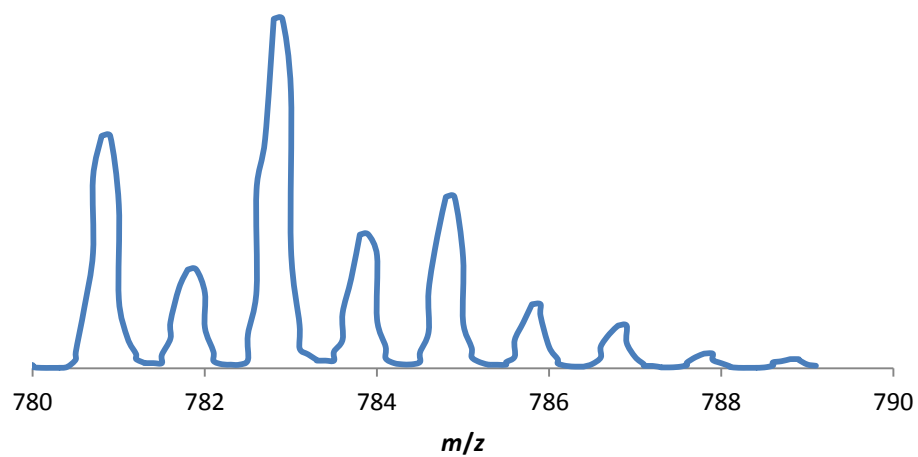


Figure 5: Positive ion ESI mass spectrum of $[\mathbf{1Br}]\text{BF}_4$.

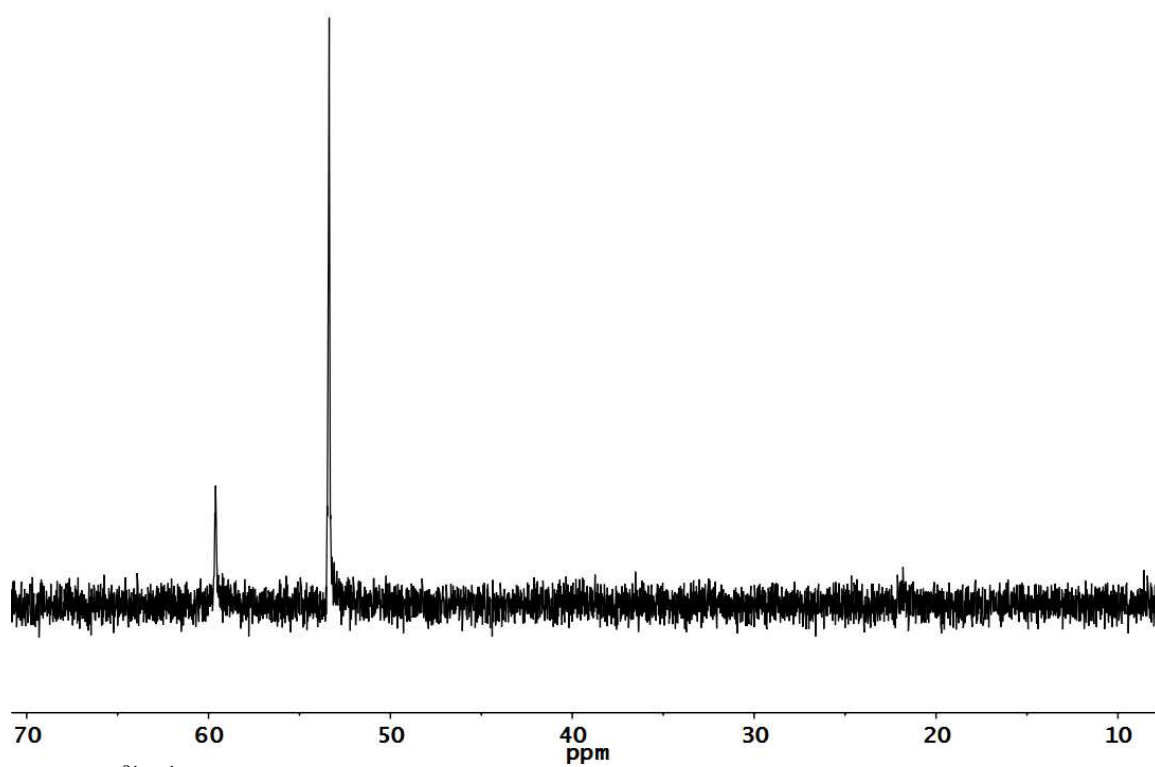


Figure 6: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\text{1Br}]\text{BF}_4$.

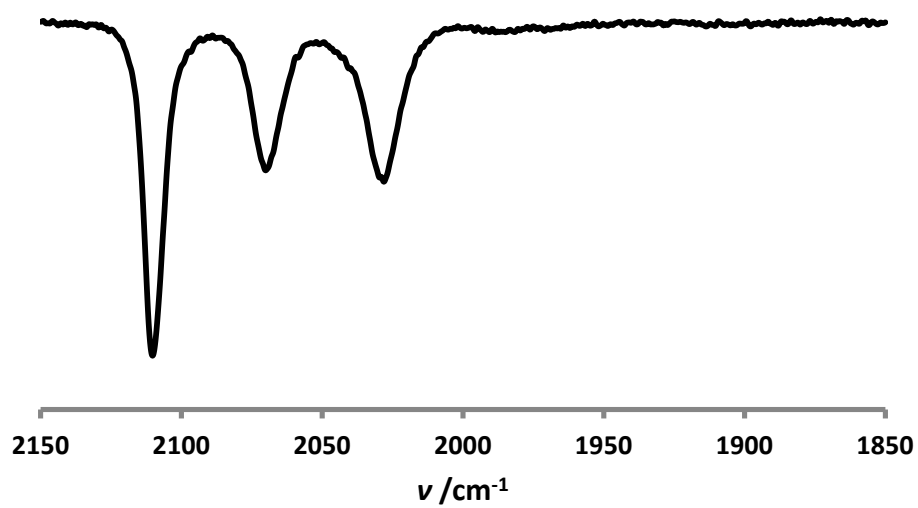


Figure 7: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\text{1Cl}]\text{BF}_4$.

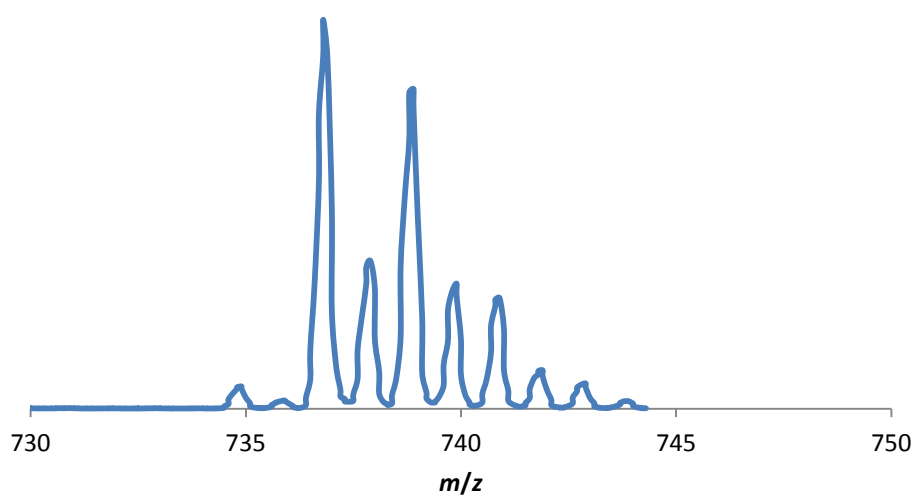


Figure 8: Positive ion ESI mass spectrum of [1Cl]BF₄.

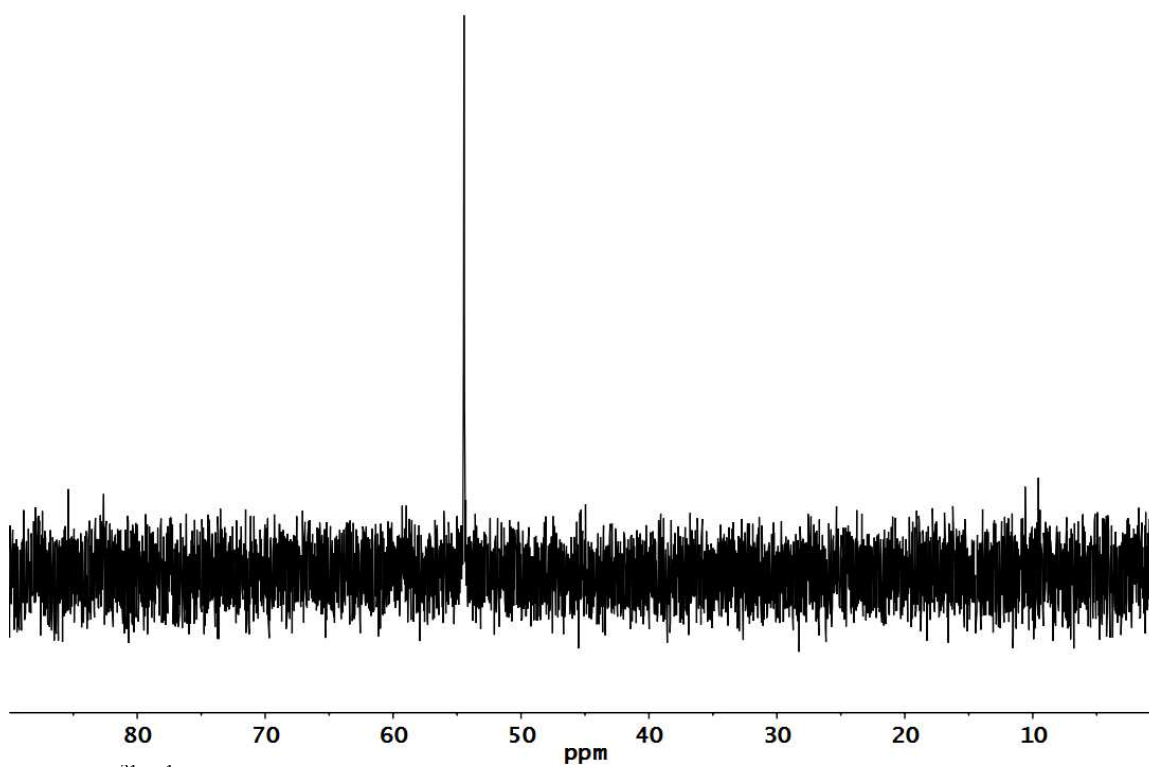


Figure 9: ³¹P{¹H} NMR spectrum (CD₂Cl₂, 202 MHz) of [1Cl]BF₄.

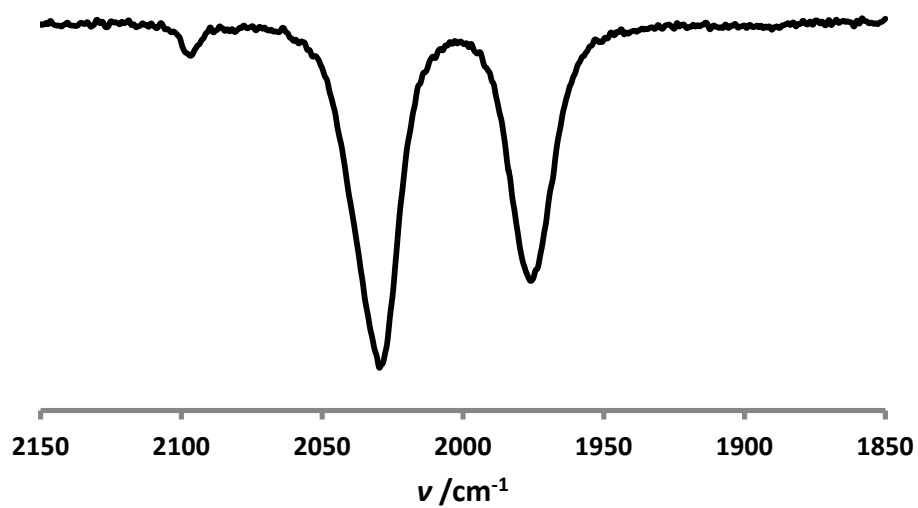


Figure 10: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1aI}]\text{BF}_4$.

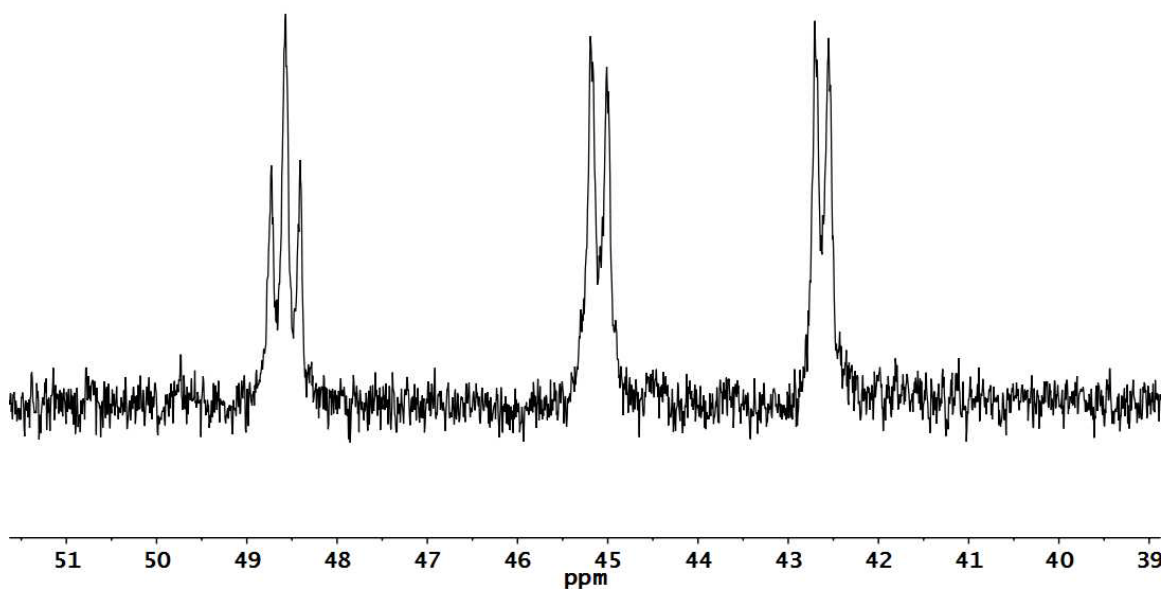


Figure 11: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\mathbf{1aI}]\text{BF}_4$.

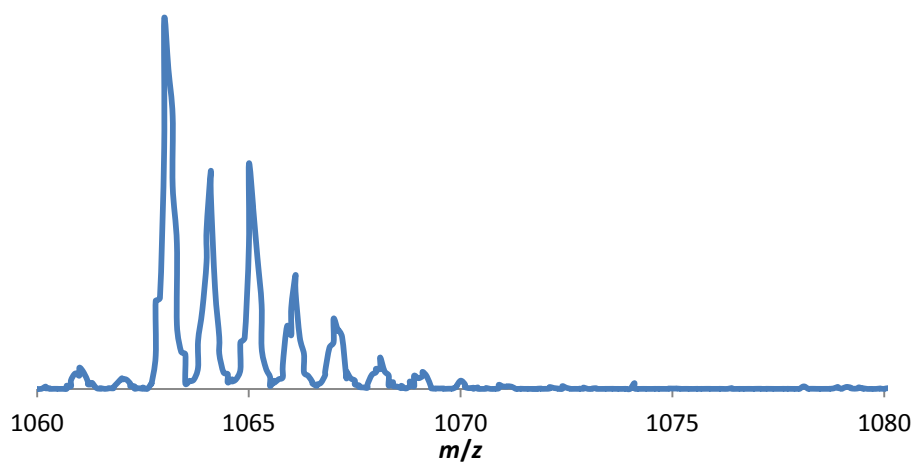


Figure 12: Positive ion ESI mass spectrum of [1aI]BF₄.

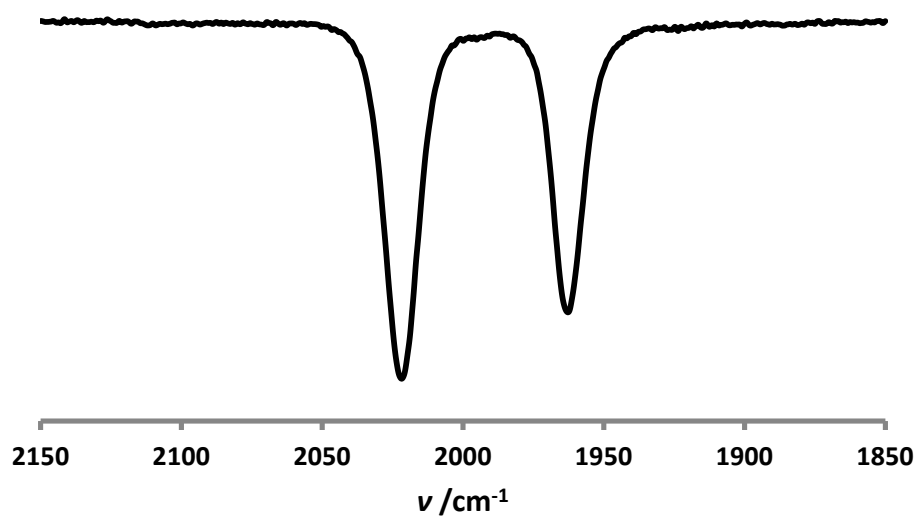


Figure 13: FT-IR spectrum (ν_{CO} region, CH₂Cl₂) of [1bI]BF₄.

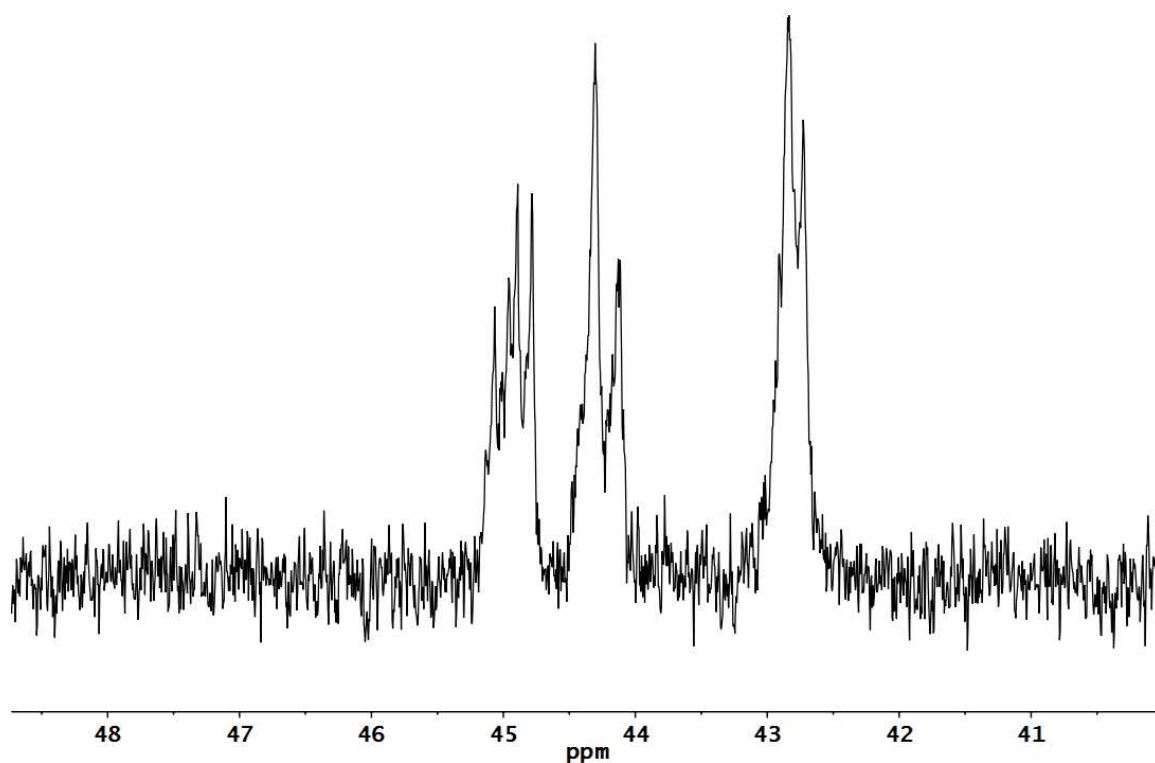


Figure 14: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\mathbf{1bI}]\text{BF}_4$.

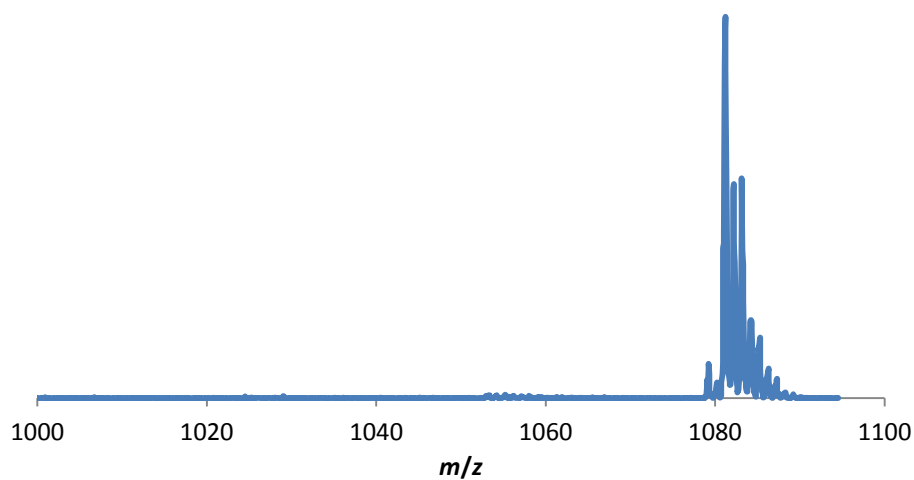


Figure 15: Positive ion ESI mass spectrum of $[\mathbf{1bI}]\text{BF}_4$.

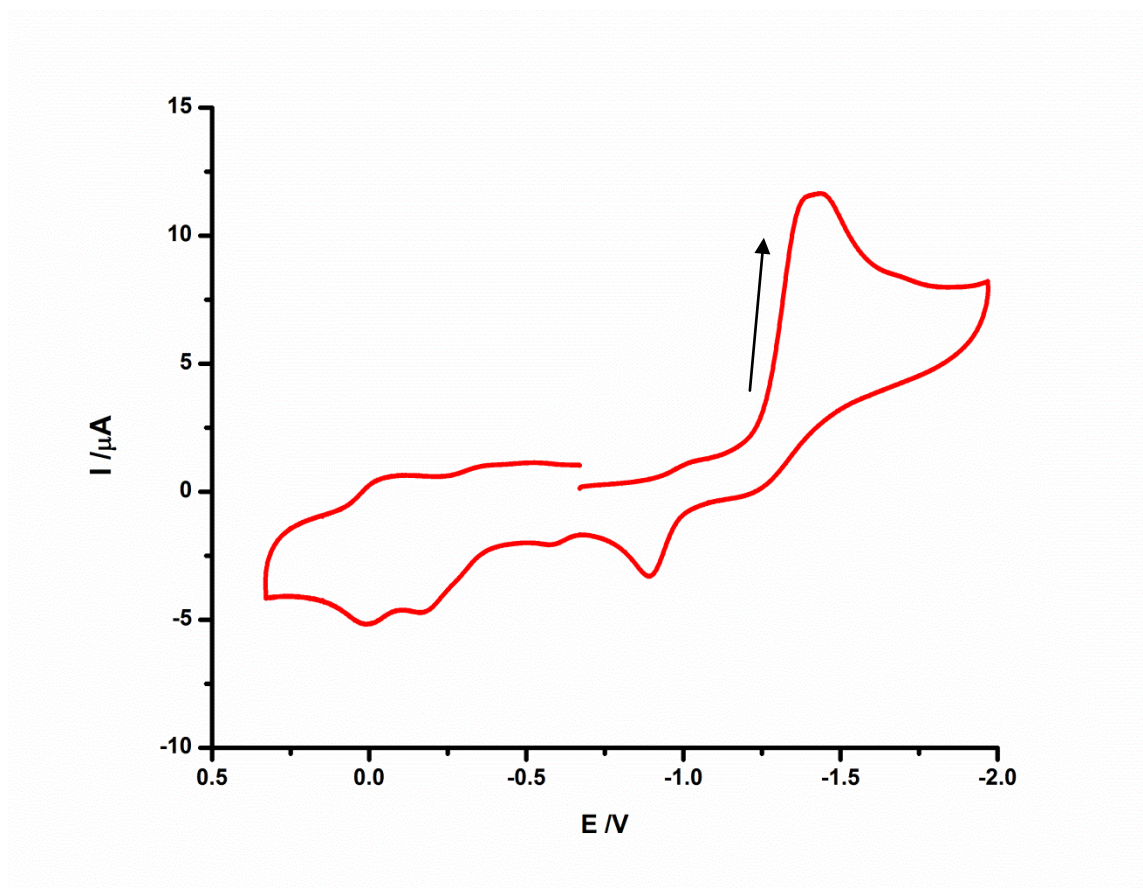


Figure 16: Cyclic voltammogram of $[1bI]BF_4$.

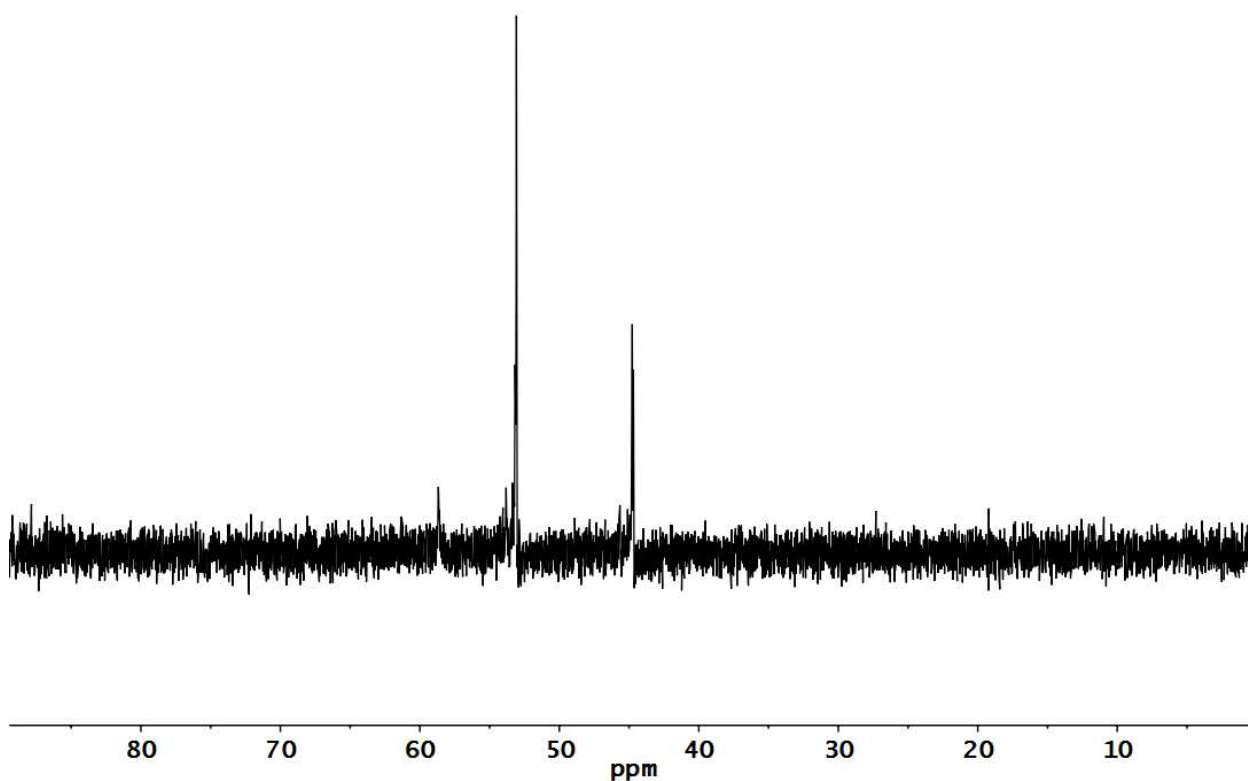


Figure 17: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\mathbf{1aCl}]\text{BF}_4$.

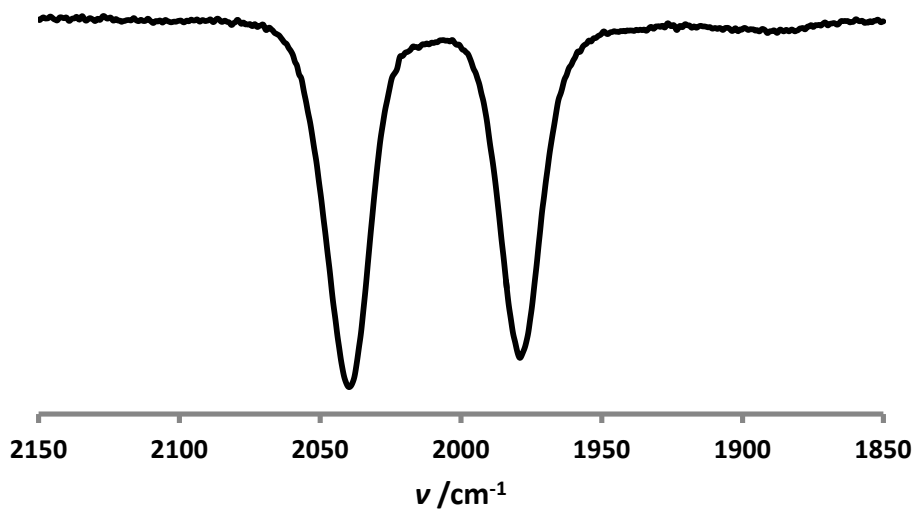


Figure 18: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1aCl}]\text{BF}_4$.

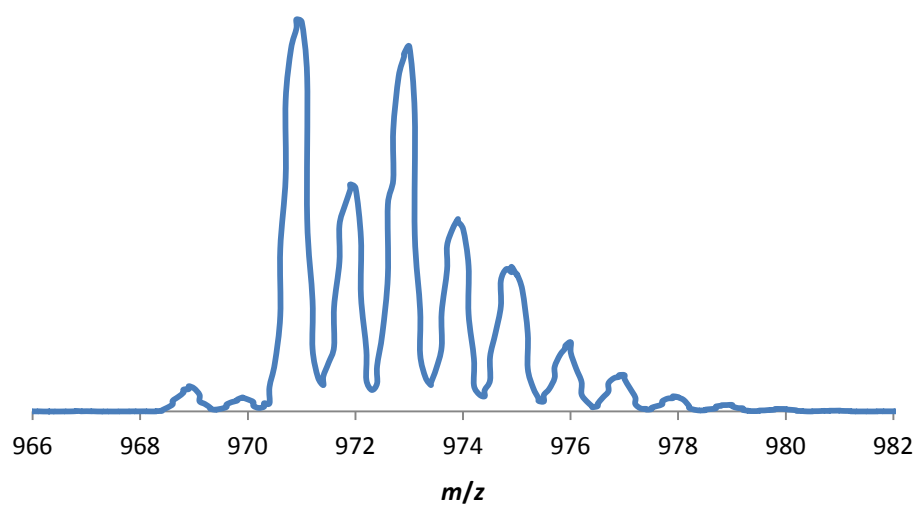


Figure 19: Positive ion ESI mass spectrum of $[1aCl]BF_4$.

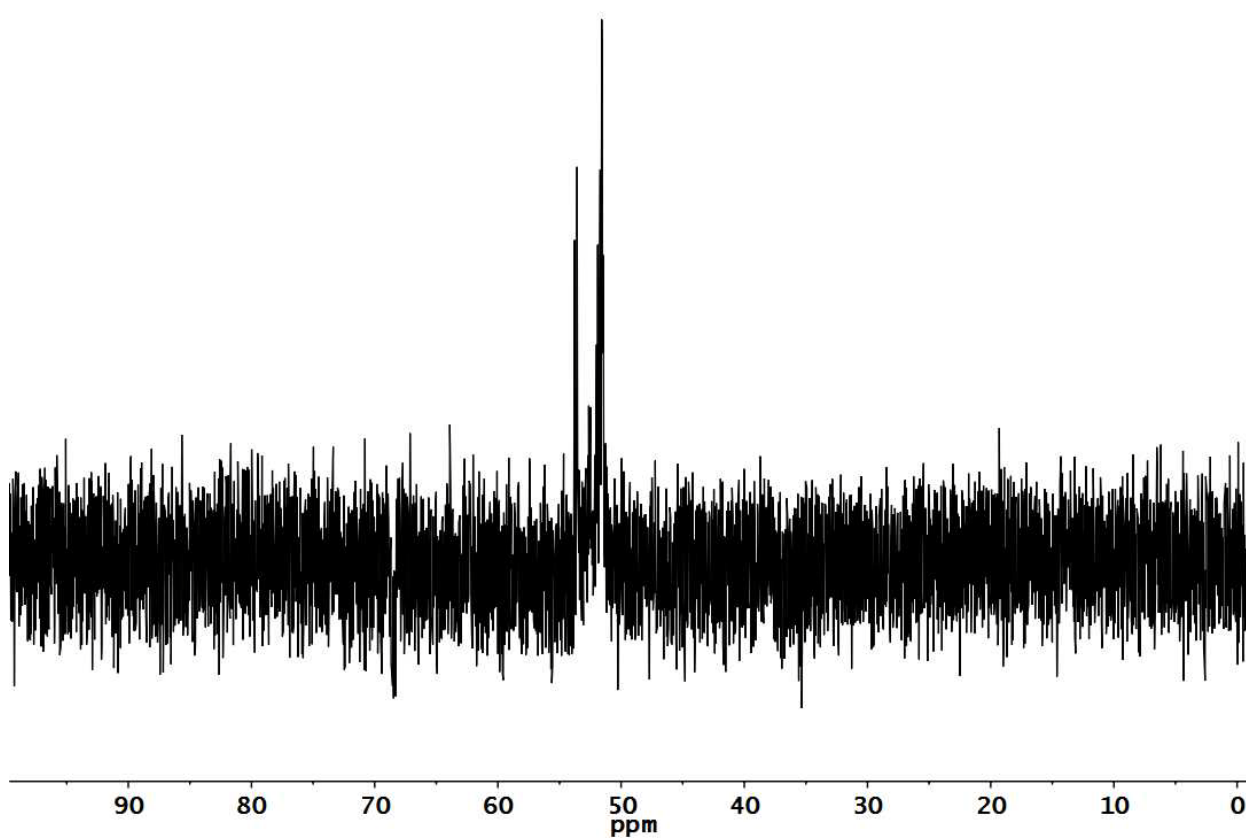


Figure 20: $^{31}P\{^1H\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[1bCl]BF_4$.

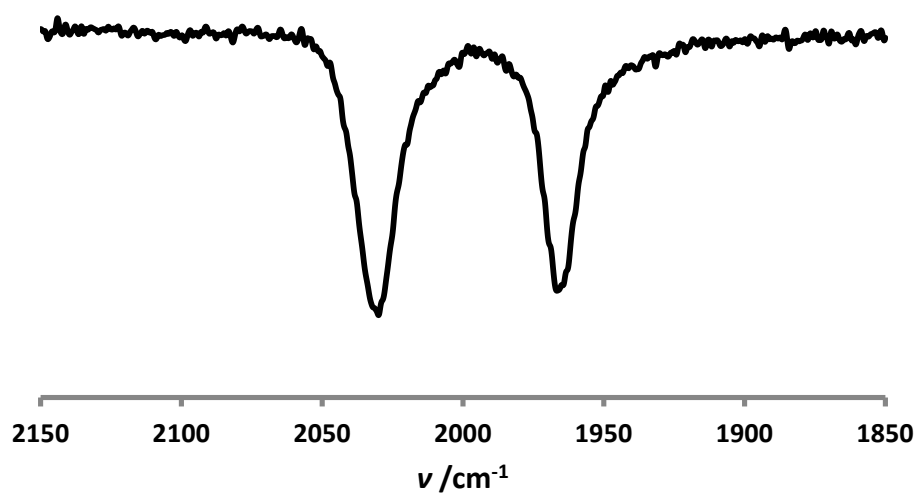


Figure 21: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1bCl}]\text{BF}_4$.

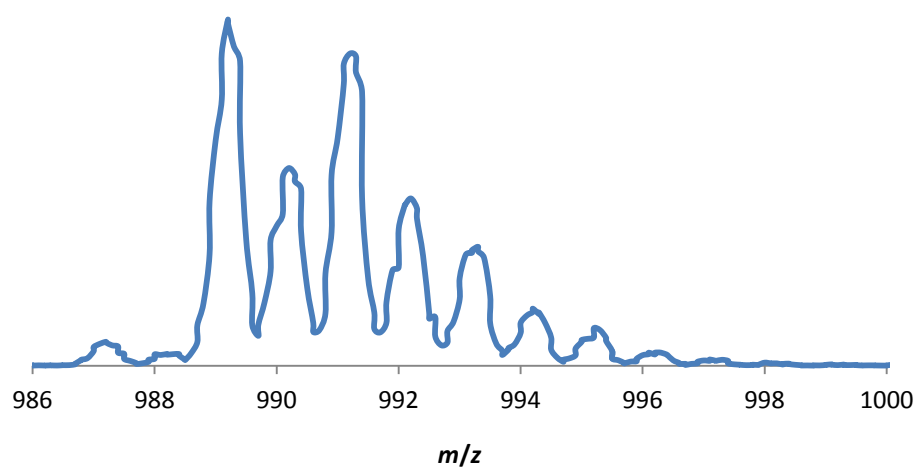


Figure 22: Positive ion ESI mass spectrum of $[\mathbf{1bCl}]\text{BF}_4$.

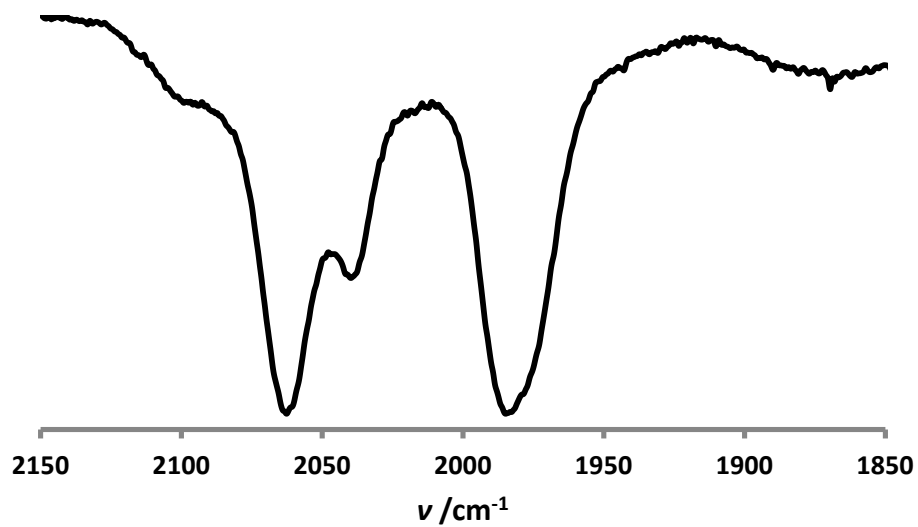


Figure 23: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1aF}]\text{BF}_4$.

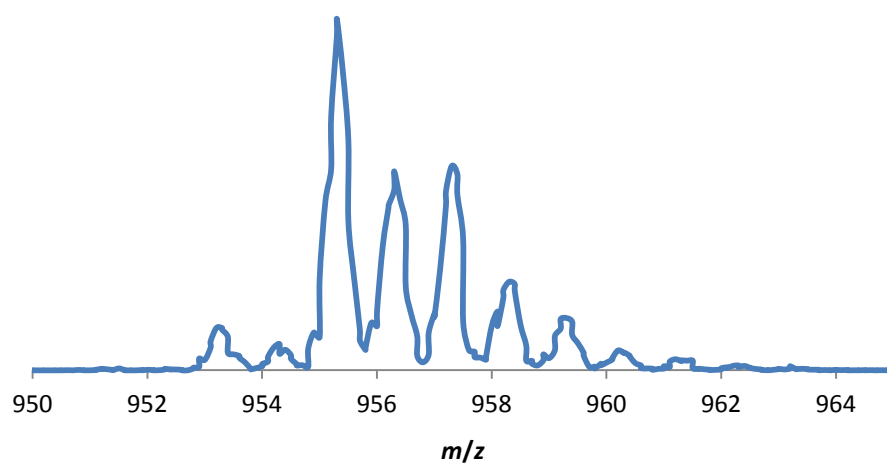


Figure 24: Positive ion ESI mass spectrum of $[\mathbf{1aF}]\text{BF}_4$.

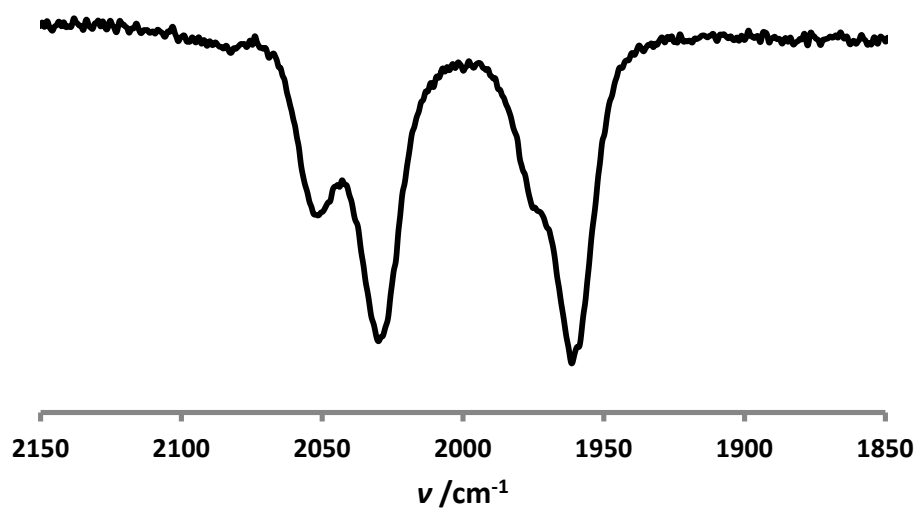


Figure 25: FT-IR spectrum (ν_{CO} region, CH_2Cl_2) of $[\mathbf{1bF}]\text{BF}_4$.

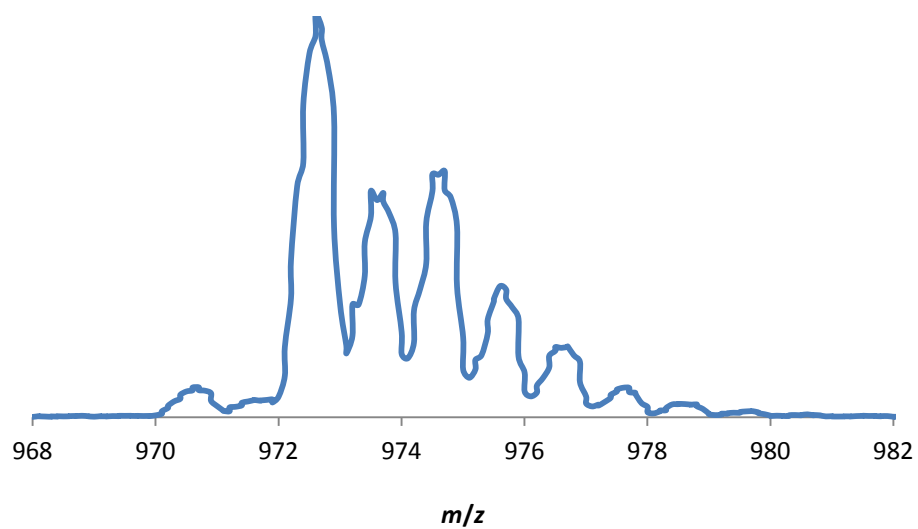


Figure 26: Positive ion ESI mass spectrum of $[\mathbf{1bF}]\text{BF}_4$.

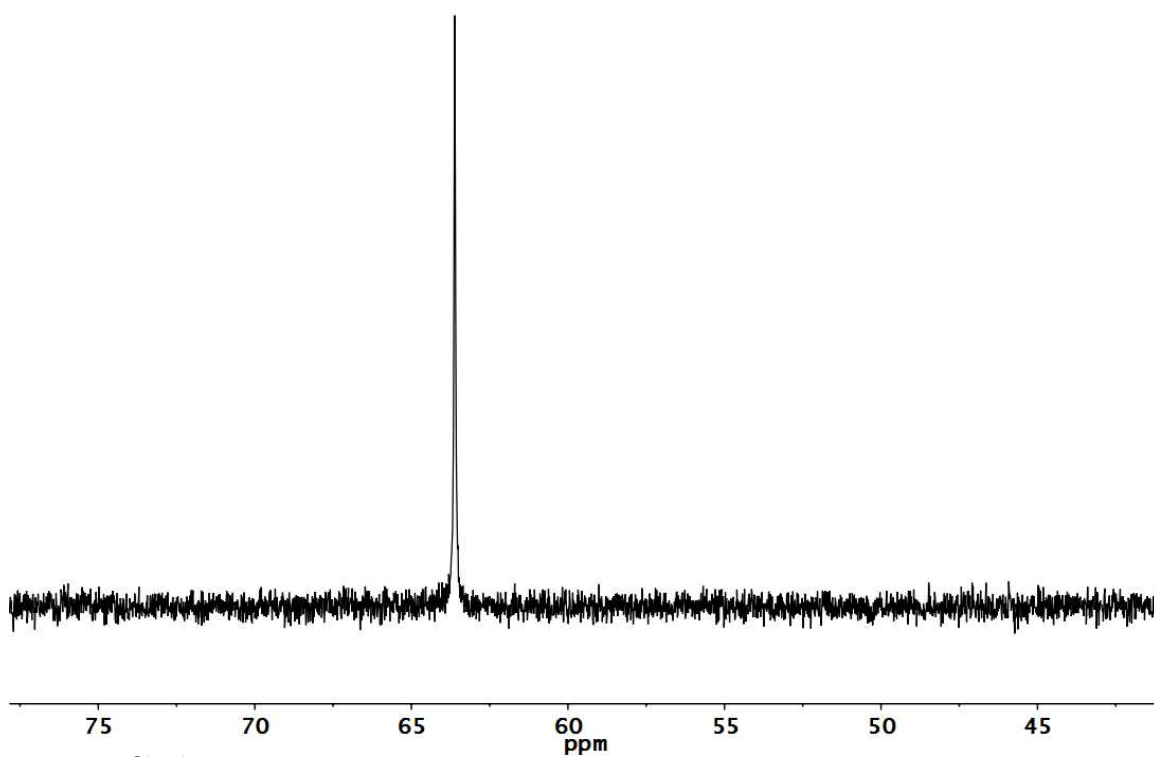


Figure 27: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2 , 202 MHz) of $[\text{2I}]\text{BF}_4$.

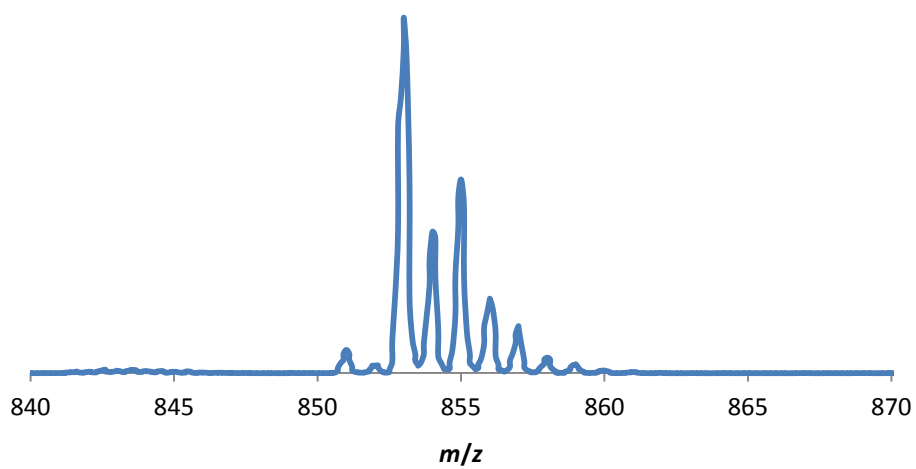


Figure 28: Positive ion ESI mass spectrum of $[\text{2I}]\text{BF}_4$.

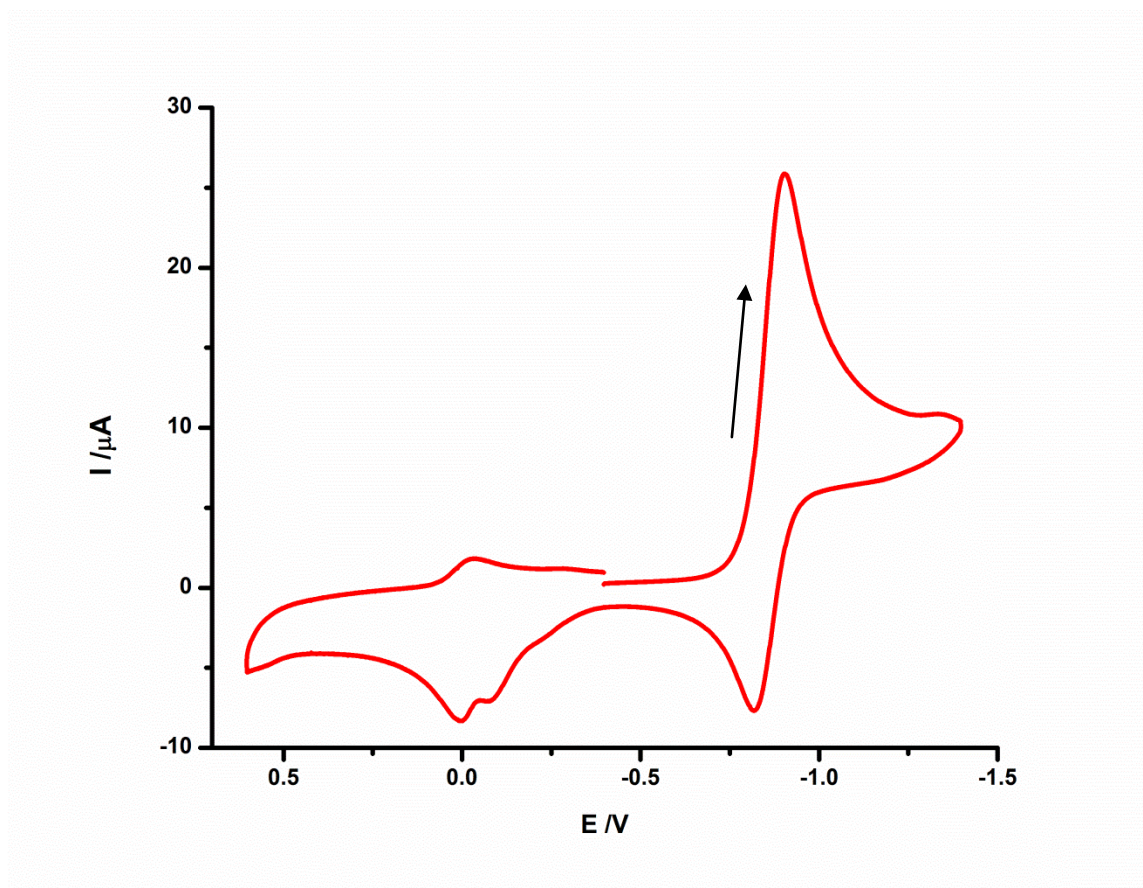


Figure 29: Cyclic voltammogram of [2I]BF₄.