NMR DATA

CHAPTER 2

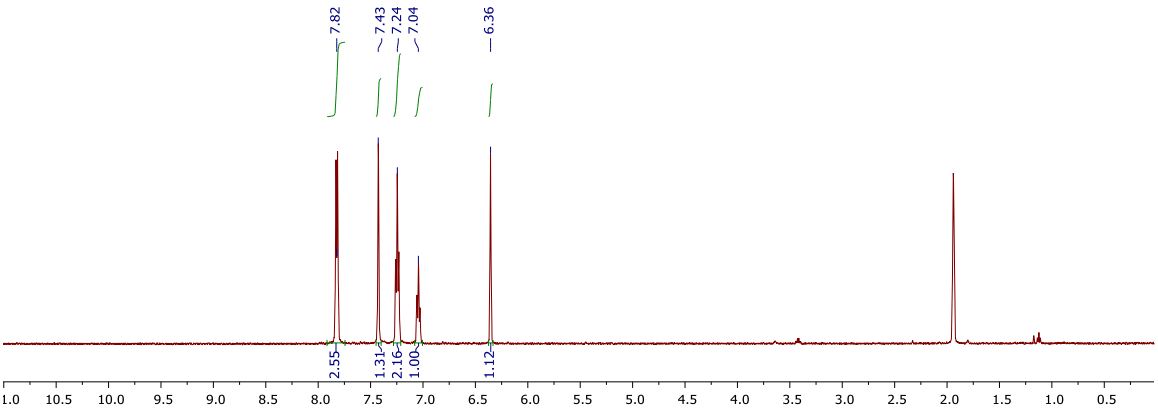

Figure 1. ^{1}H NMR spectrum (300 MHz) of potassium 3-phenyl pyrazolate in CD_3CN.

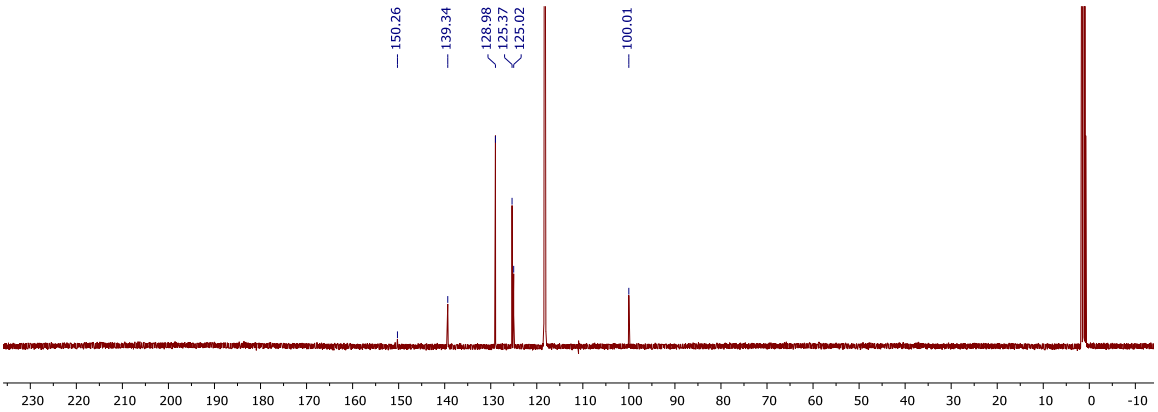

Figure 2. ^{13}C {^{1}H} NMR spectrum (300 MHz) of potassium 3-phenyl pyrazolate in CD_3CN.

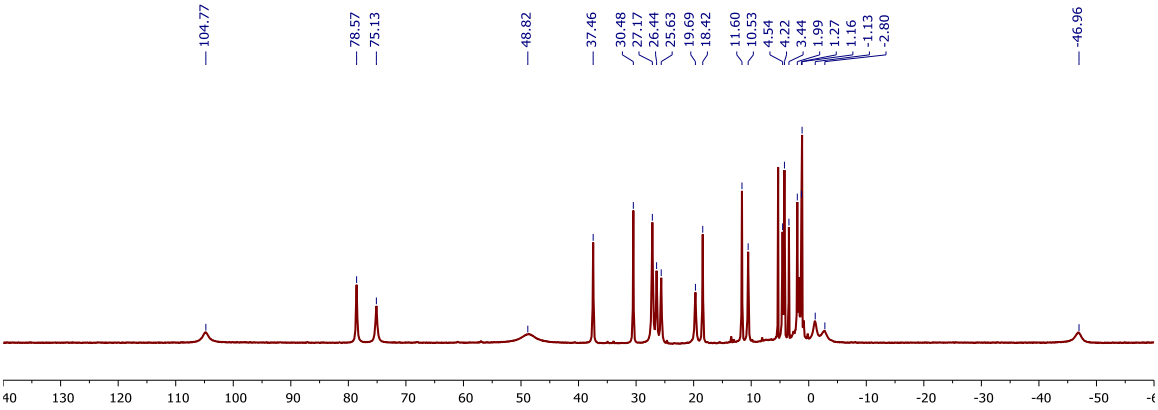

Figure 3. ^{1}H NMR spectrum (300 MHz) of $[LFe_3F(PhPz)_3Fe][OTf]$ (**1**) in CD_2Cl_2.

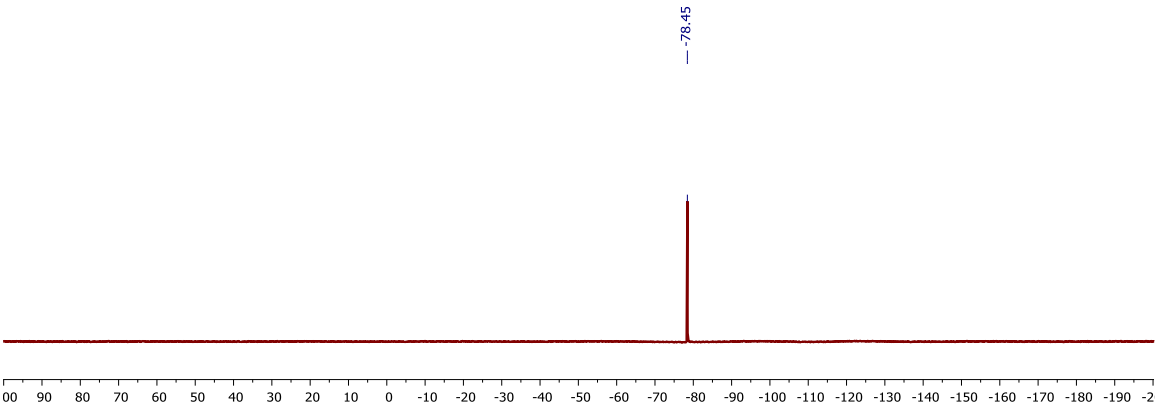

Figure 4. ^{19}F NMR spectrum (300 MHz) of $[LFe_3F(PhPz)_3Fe][OTf]$ (**1**) in CD_2Cl_2.

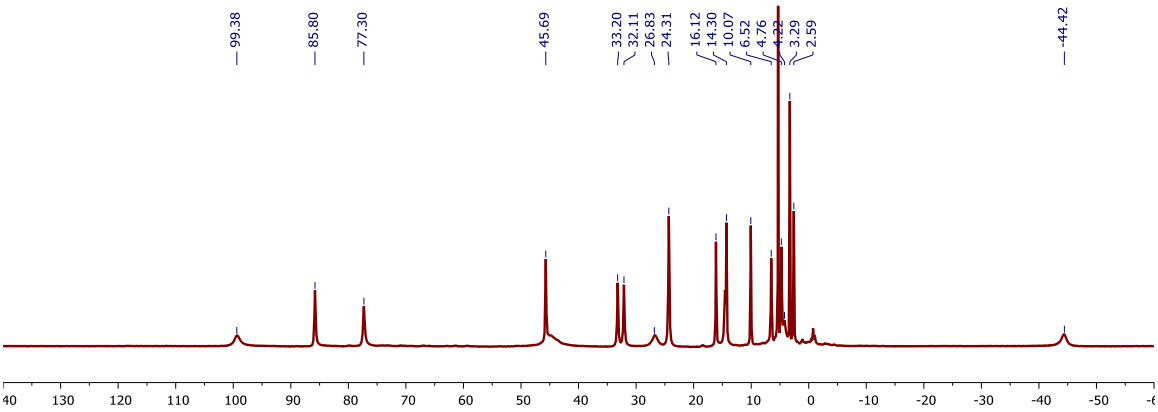

Figure 5. ^{1}H NMR spectrum (300 MHz) of $[LFe_3F(PhPz)_3Fe][OTf]_2$ (**2**) in CD_2Cl_2.

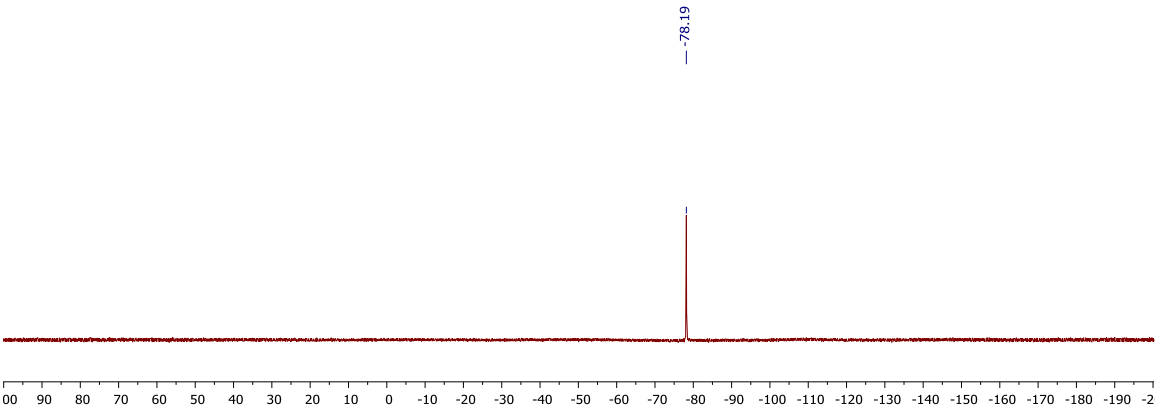

Figure 6. ^{19}F NMR spectrum (300 MHz) of $[LFe_3F(PhPz)_3Fe][OTf]_2$ (**2**) in CD_2Cl_2.

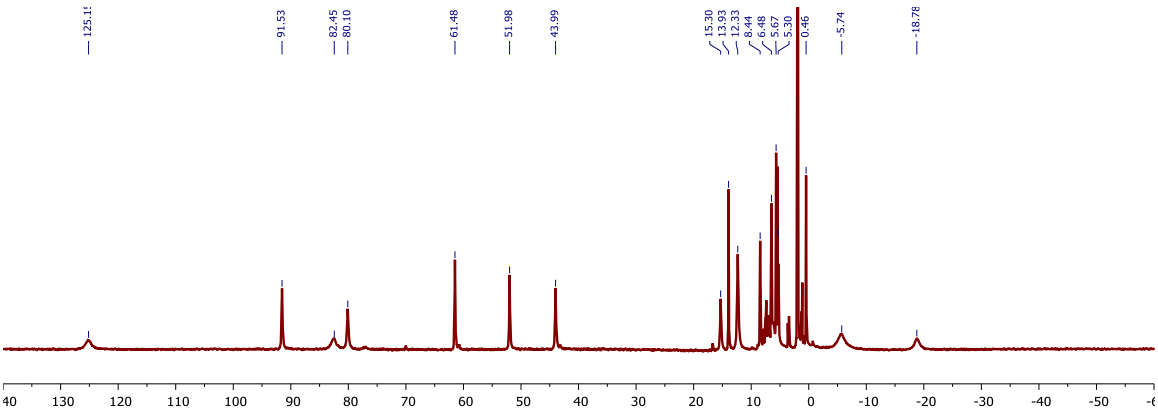

Figure 7. ^{1}H NMR spectrum (300 MHz) of $[LFe_3F(PhPz)_3Fe(CH_3CN)][OTf]_3$ (**3**) in CD_3CN.

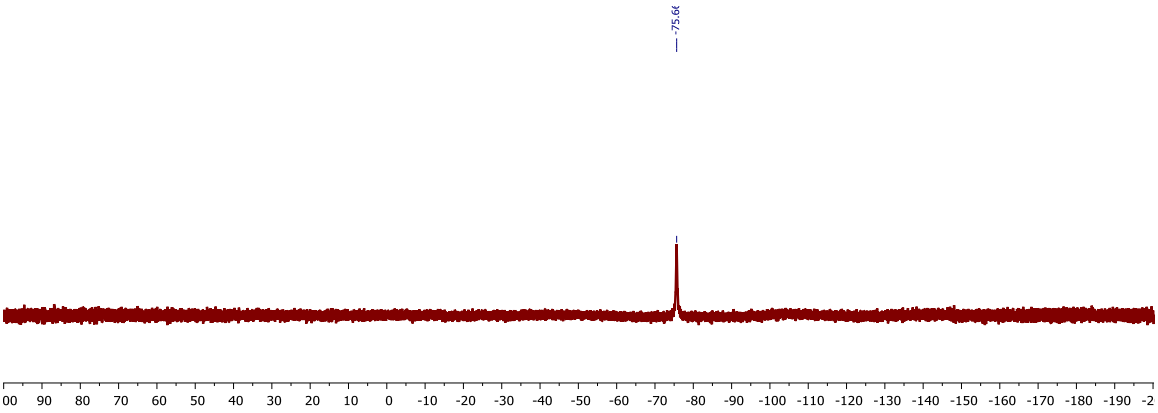

Figure 8. ^{19}F NMR spectrum (300 MHz) of $[LFe_3F(PhPz)_3Fe(CH_3CN)][OTf]_3$ (**3**) in CD_3CN.

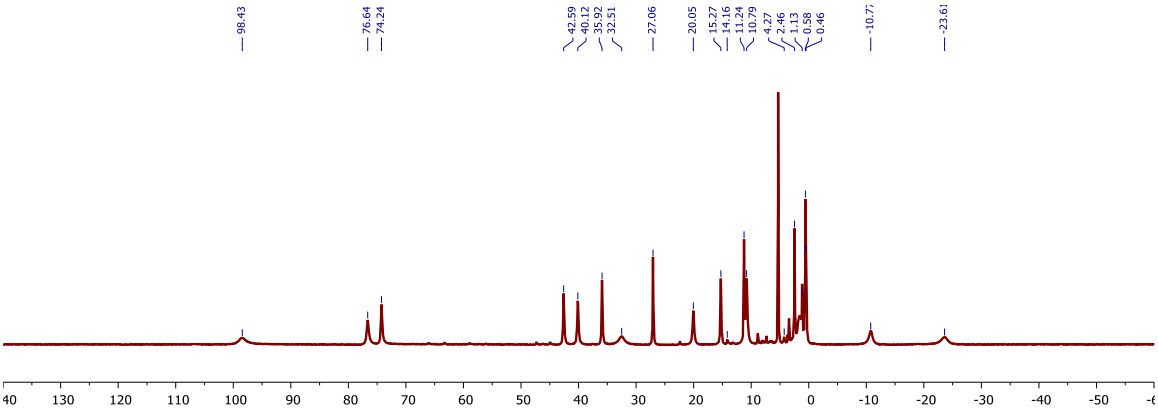

Figure 9. ^{1}H NMR spectrum (300 MHz) of $[LFe_3F(PhPz)_3Fe(NO)][OTf]$ (**1-NO**) in CD_2Cl_2.

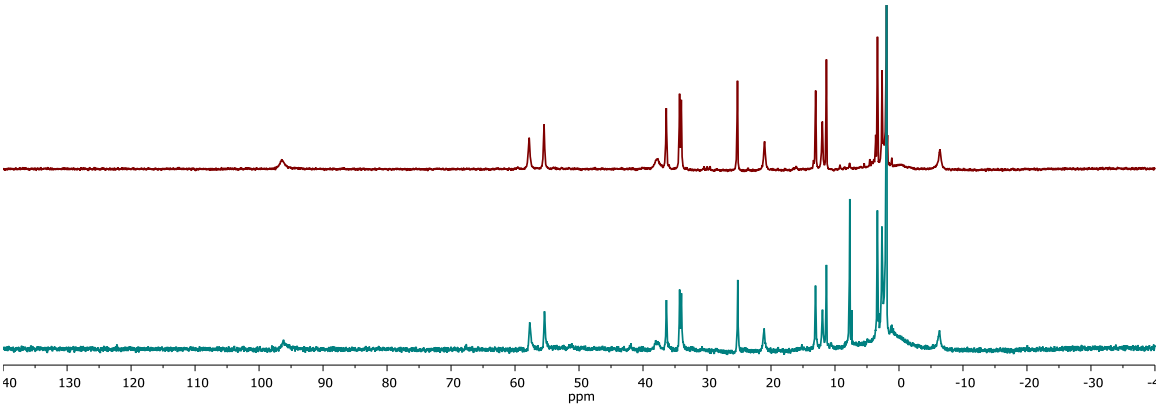

Figure 10. ^{1}H NMR spectrum (300 MHz) of [$LFe_3O(Pz)_3Mn$][OTf] (**1-[OTf]**) (top) and [$LFe_3O(Pz)_3Mn$][[BArF4]] (**1-[BAr^F_4]**; bottom) in CD_3CN.

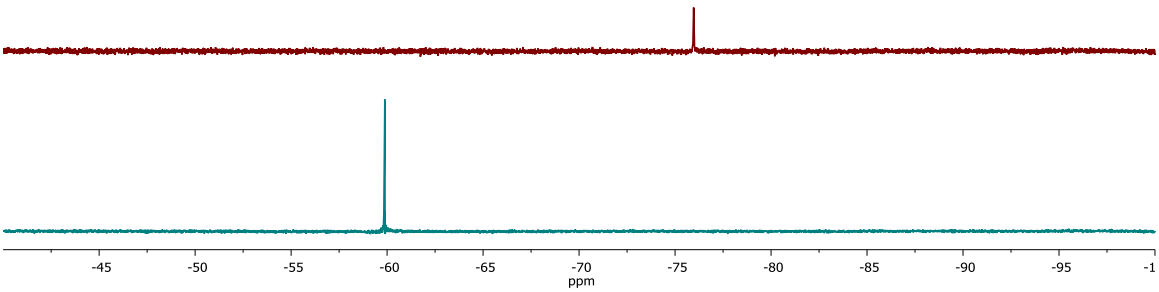

Figure 11. ^{19}F NMR spectrum (300 MHz) of [$LFe_3O(Pz)_3Mn$][OTf] (**1-[OTf]**; top) and [$LFe_3O(Pz)_3Mn$][BAr^F_4] (**1-[BAr^F_4]**; bottom) in CD_3CN.

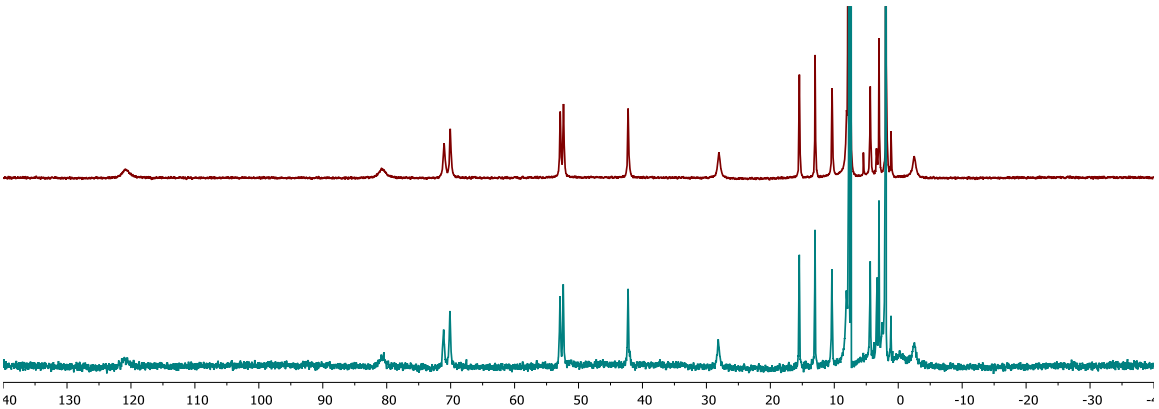

Figure 12. ^{1}H NMR spectrum (300 MHz) of [$LFe_3O(Pz)_3Mn$][OTf]$_2$ (**2-[OTf]**; top) and [$LFe_3O(Pz)_3Mn$][BAr^F_4]$_2$ (**2-[BAr^F_4]**; bottom) in CD_3CN.

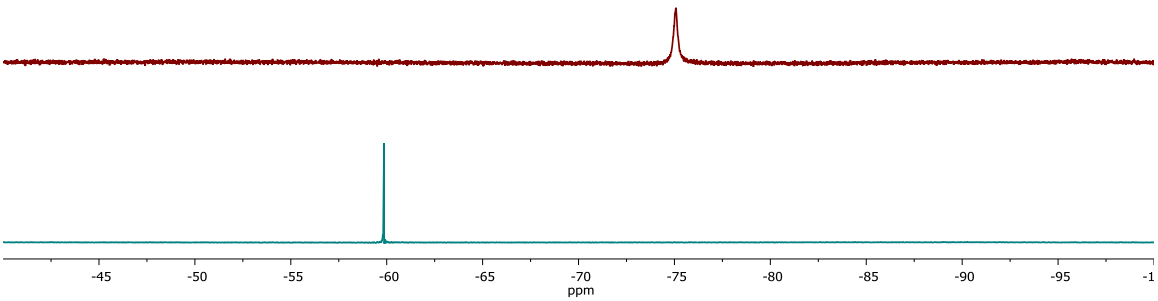

Figure 13. ^{19}F NMR spectrum (300 MHz) of $[LFe_3O(Pz)_3Mn][OTf]_2$ (**2-[OTf]**; top) and $[LFe_3O(Pz)_3Mn][BAr^F{}_4]_2$ (**2-[BAr$^F{}_4$]**; bottom) in CD_3CN.

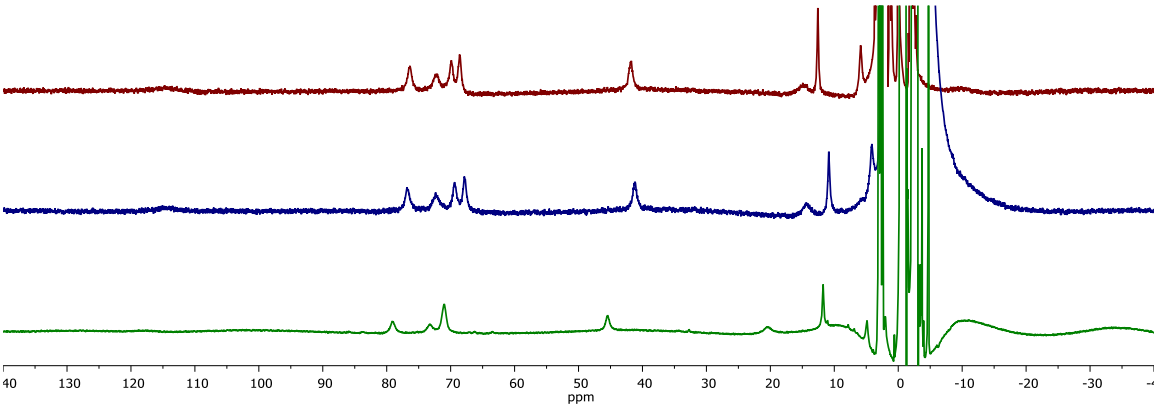

Figure 14. ^1H NMR spectrum (300 MHz) of $[LFe_3O(Pz)_3Mn][OTf]_3$ in CD_2Cl_2 (**3-[OTf]**; top), $[LFe_3O(Pz)_3Mn][BAr^F{}_4]_3$ in THF/C_6D_6 with three equivalents tetrabutylammonium trifluoromethanesulfonate (400 MHz, middle), and $[LFe_3O(Pz)_3Mn][BAr^F{}_4]_3$ in THF/C_6D_6 (500 MHz) (**3-[BAr$^F{}_4$]**; bottom).

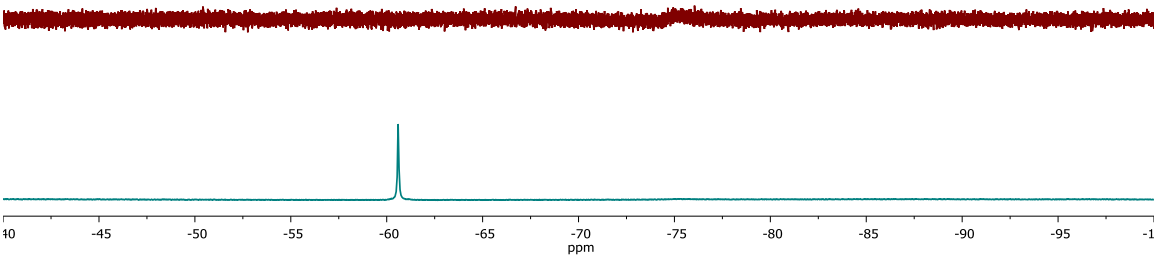

Figure 15. ^{19}F NMR spectrum (300 MHz) of $[LFe_3O(Pz)_3Mn][OTf]_3$ (**3-[OTf]**) in CD_2Cl_2 (top) and $[LFe_3O(Pz)_3Mn][BAr^F{}_4]_3$ (**3-[BAr$^F{}_4$]**; bottom) in THF/C_6D_6 (400 MHz).

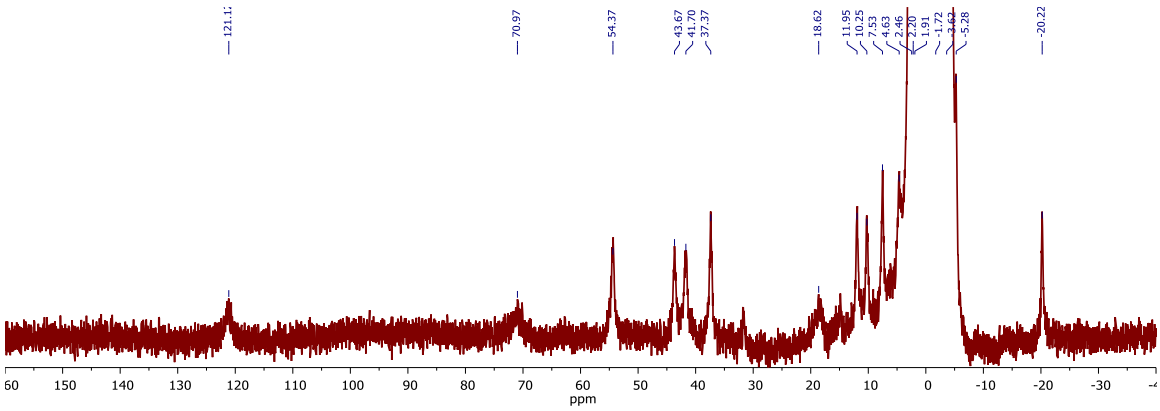

Figure 16. ^{1}H NMR spectra (400 MHz) of [$LFe_3O(Pz)_3Mn(OH)$] (**5**) in THF/C_6D_6 [250 mM H_2O].

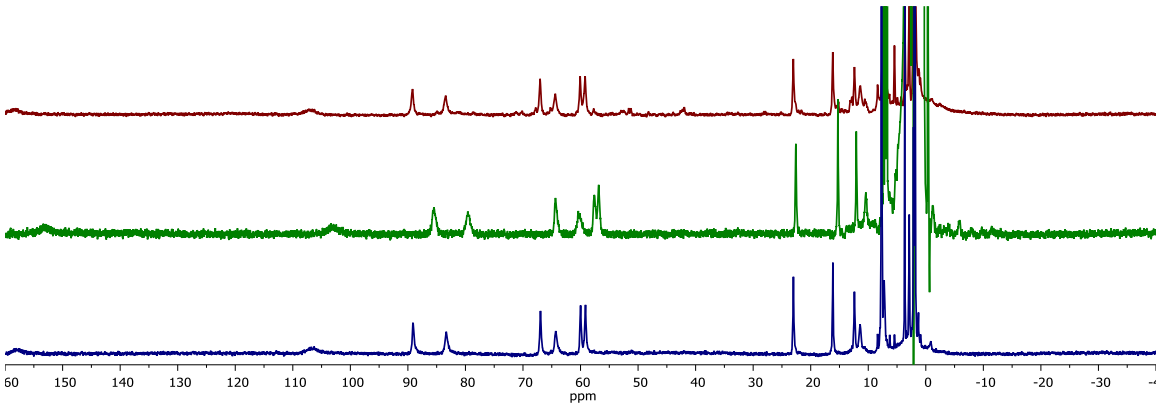

Figure 17. ^{1}H NMR spectrum (300 MHz) of [$LFe_3O(Pz)_3Mn(OH)$][OTf] (**6-[OTf]**; top) and [$LFe_3O(Pz)_3Mn(OH)$][$BAr^F{}_4$] (**6-[$BAr^F{}_4$]**; middle) in CD3CN. ^{1}H NMR spectrum (400 MHz) of [$LFe_3O(Pz)_3Mn(OH)$][$BAr^F{}_4$] (**6-[$BAr^F{}_4$]**; bottom) in THF/C_6D_6 [250 mM H_2O].

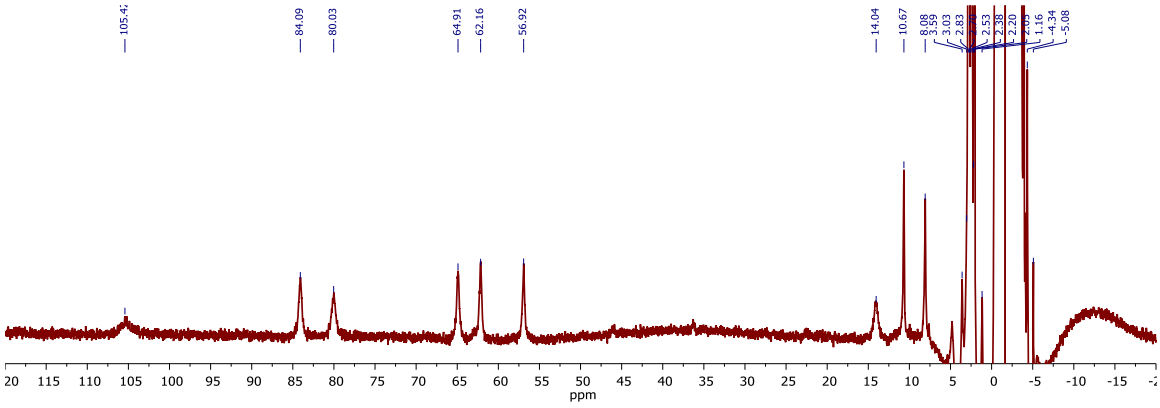

Figure 18. ^{1}H NMR spectrum (400 MHz) of [$LFe_3O(Pz)_3Mn(OH)$][$BAr^F{}_4$]$_2$ (**7-[$BAr^F{}_4$]**) in THF/C_6D_6 [250 mM H_2O].

CHAPTER 4

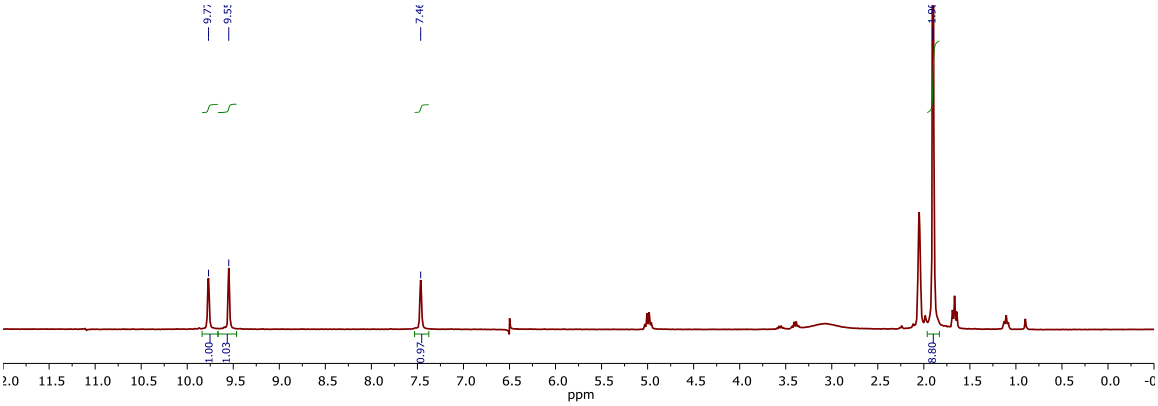

Figure 19. ^{1}H NMR spectrum (300 MHz) of 2-*tert*-butyl-isoxazolium tetrafluoroborate in $(CD_3)_2CO$.

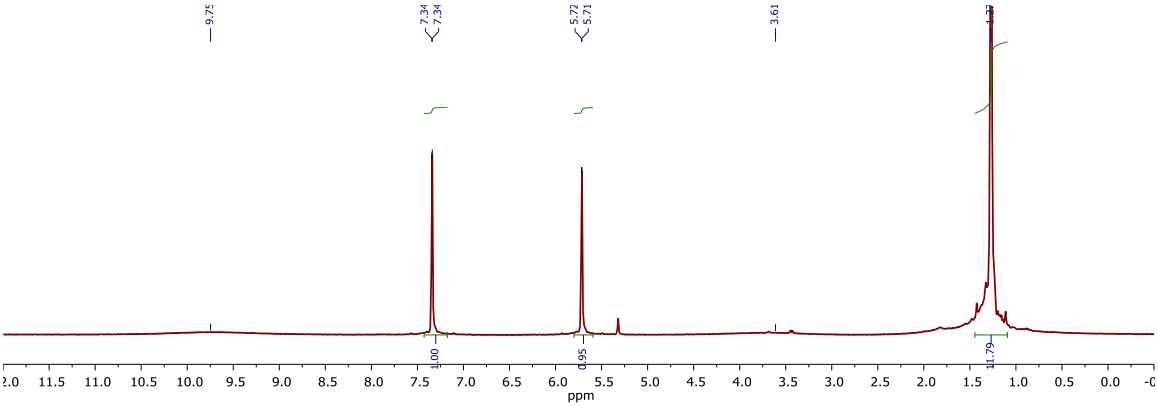

Figure 20. ^{1}H NMR spectrum (400 MHz) of *N*-*tert*-butyl-1*H*-pyrazol-3-amine in CD_2Cl_2.

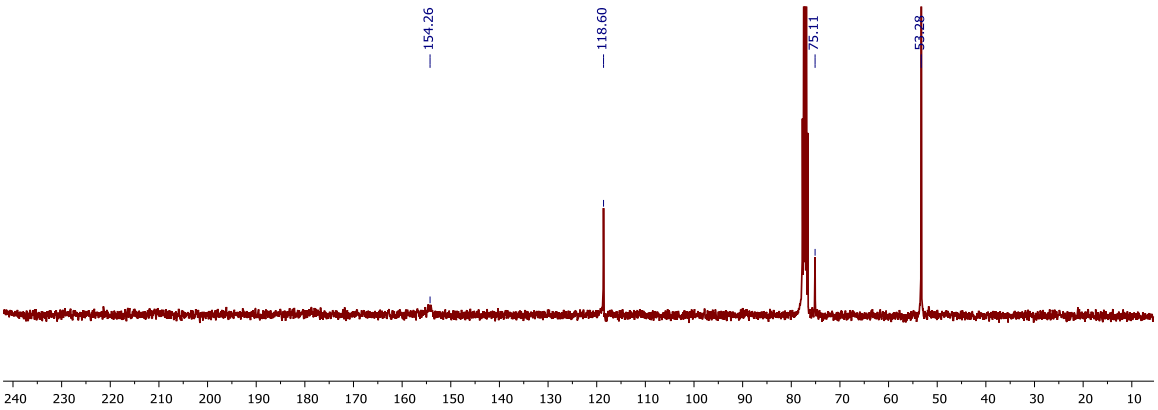

Figure 21. ^{13}C{^{1}H} NMR spectrum (100 MHz) of *N*-*tert*-butyl-1*H*-pyrazol-3-amine in CD_2Cl_2.

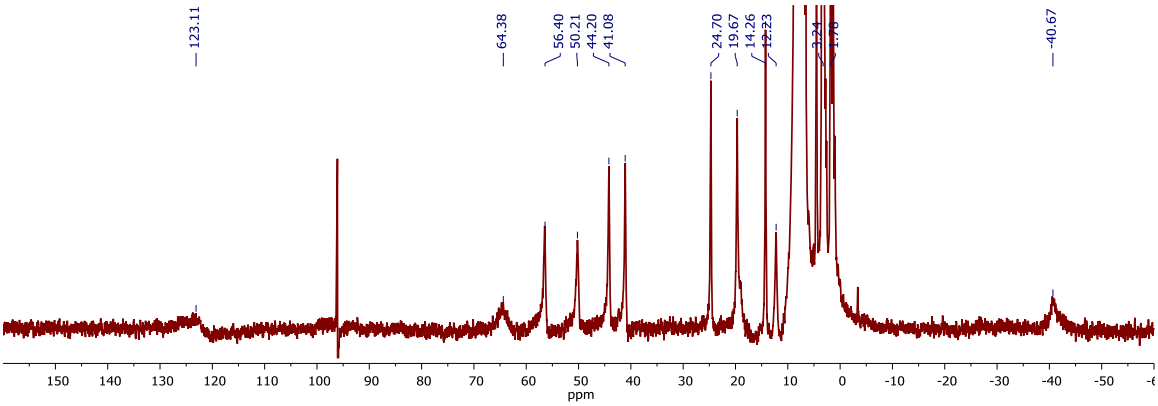

Figure 22. ^{1}H NMR spectrum (300 MHz) of $LFe_3O(PzNHtBu)_3Fe(OH)$ (**1**) in C_6D_6. The sharp signal ~ 95 ppm is a spectral artifact.

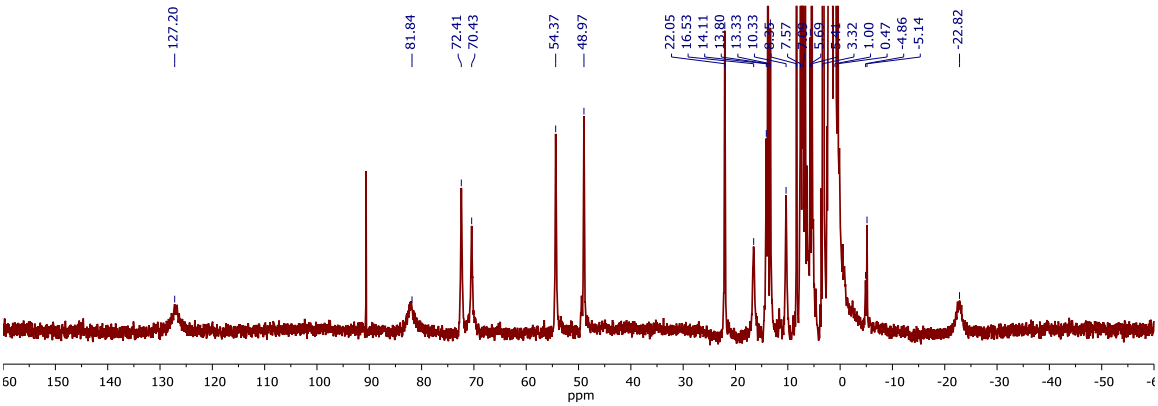

Figure 23. ^{1}H NMR spectrum (300 MHz) of $[LFe_3O(PzNHtBu)_3Fe(OH)][OTf]$ (**2**) in CD_3CN. The sharp signal ~ 90 ppm is a spectral artifact.

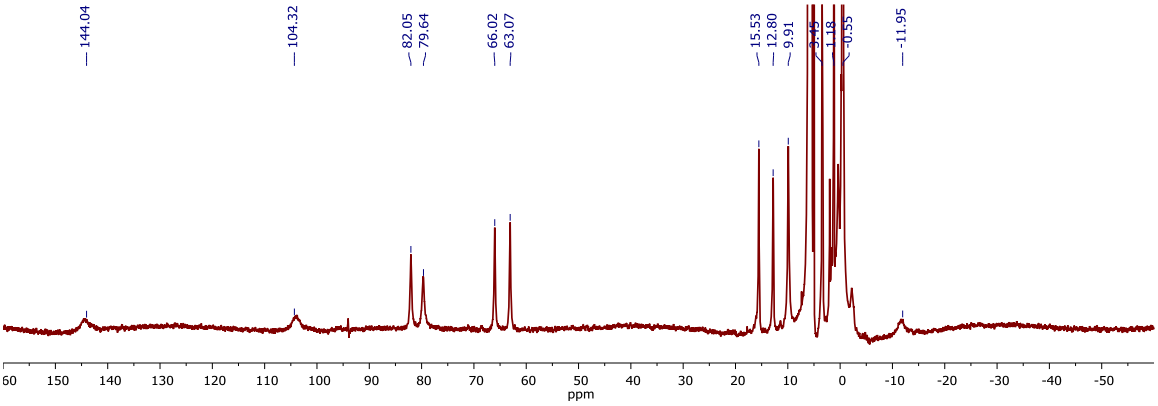

Figure 24. ^{1}H NMR spectrum (300 MHz) of $[LFe_3O(PzNHtBu)_3Fe(OH)][OTf]_2$ (**3**) in CD_2Cl_2.

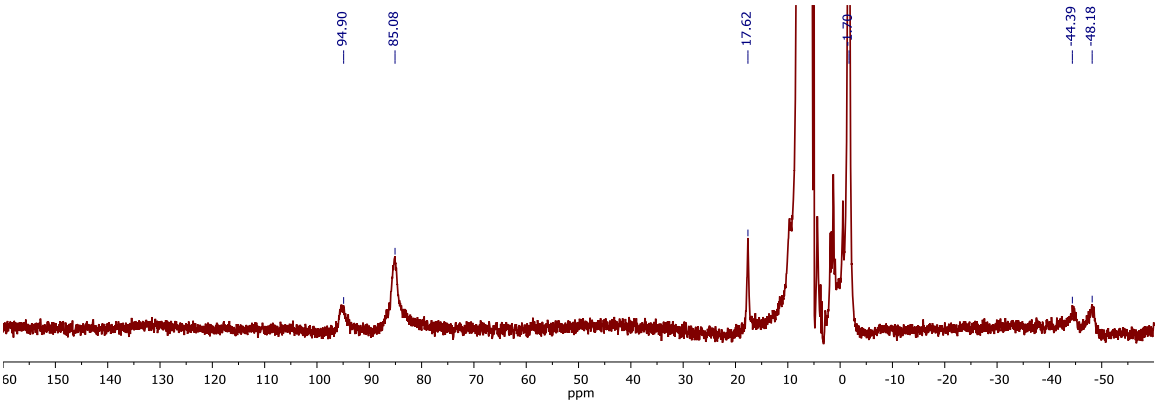

Figure 25. ^{1}H NMR spectrum (300 MHz) of [LFe$_3$O(PzNHtBu)$_3$Fe(OH)][OTf]$_3$ (**4**) in CD_2Cl_2.

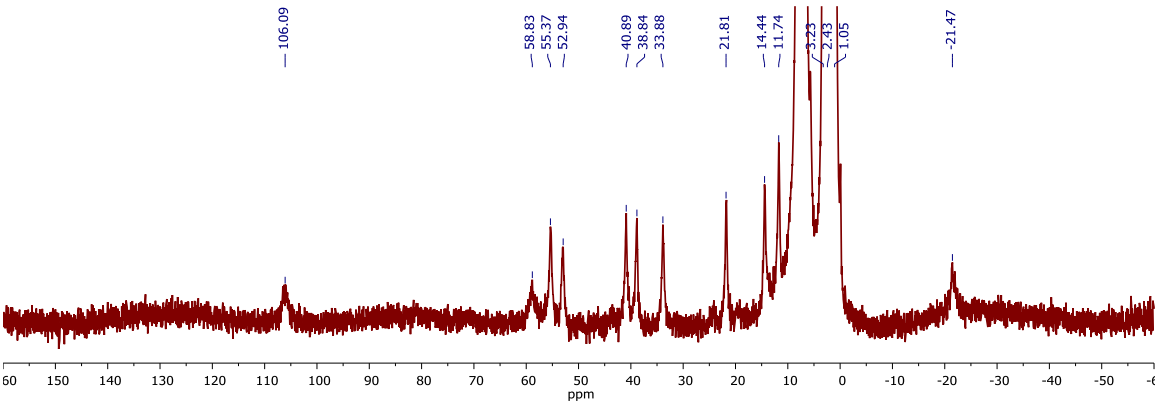

Figure 26. ^{1}H NMR spectrum (300 MHz) of LFe$_3$O(PzNHtBu)$_3$Fe(O) (**5**) in C_6D_6.

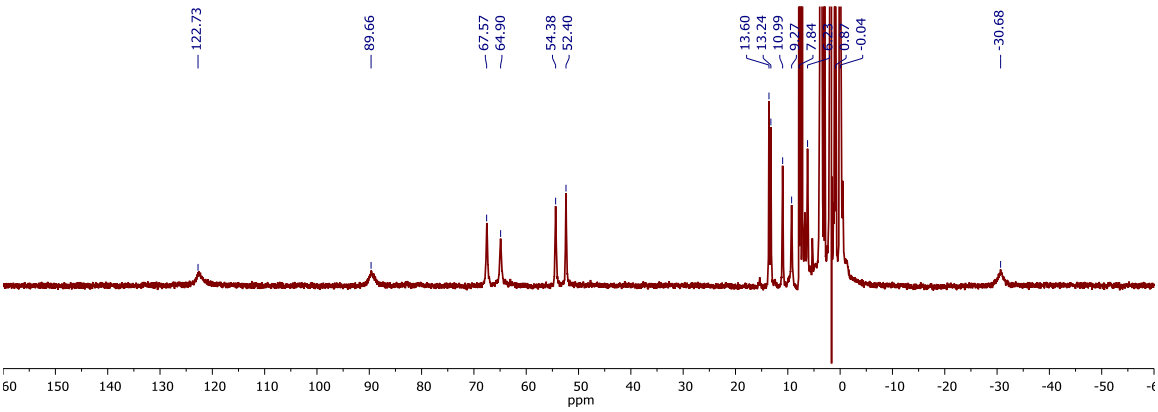

Figure 27. ^{1}H NMR spectrum (400 MHz) of [LFe$_3$O(PzNHtBu)$_3$Fe(O)][OTf] (**6**) in THF/C_6D_6.

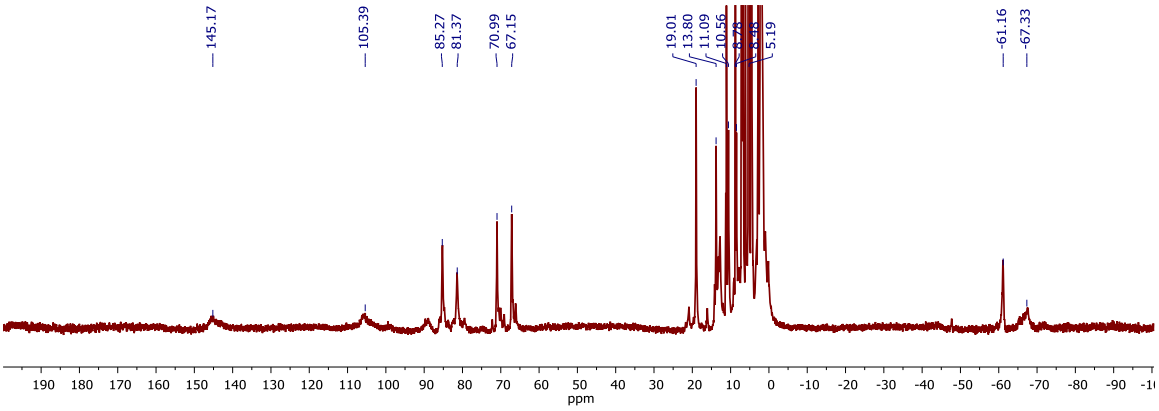

Figure 28. ^{1}H NMR spectrum (300 MHz) of [LFe$_3$O(PzNHtBu)$_3$Fe(O)][OTf]$_2$ (**7**) in 1:1 CD$_3$CN/CD$_2$Cl$_2$.

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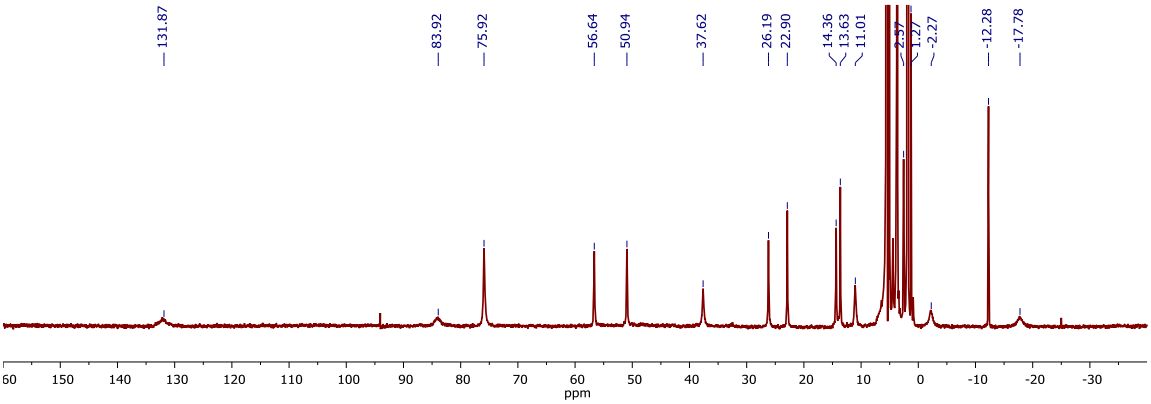

Figure 29. ^{1}H NMR spectrum (300 MHz) of [$LFe_3O(Pz)_3Fe(OAc)$][OTf] (**1**) in CD_2Cl_2.

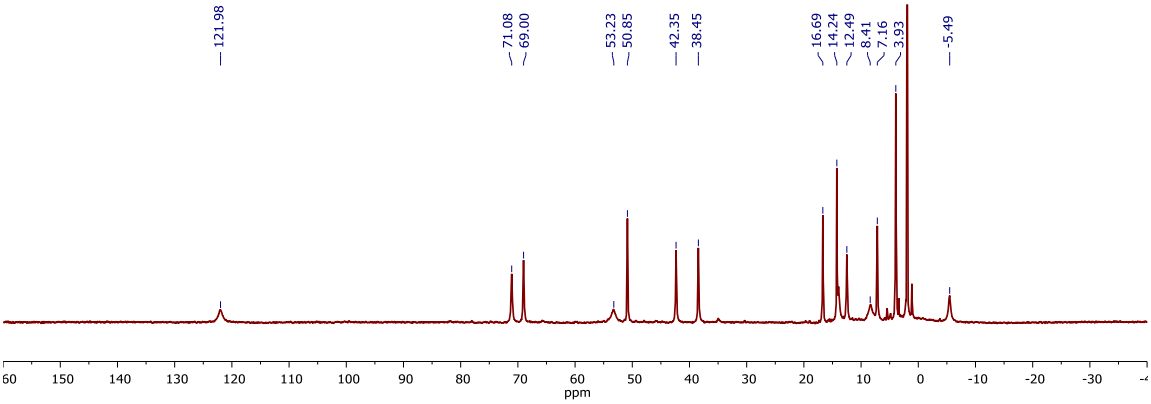

Figure 30. ^{1}H NMR spectrum (300 MHz) of [$LFe_3O(Pz)_3Fe$][OTf]$_2$ (**2**) in CD_3CN.

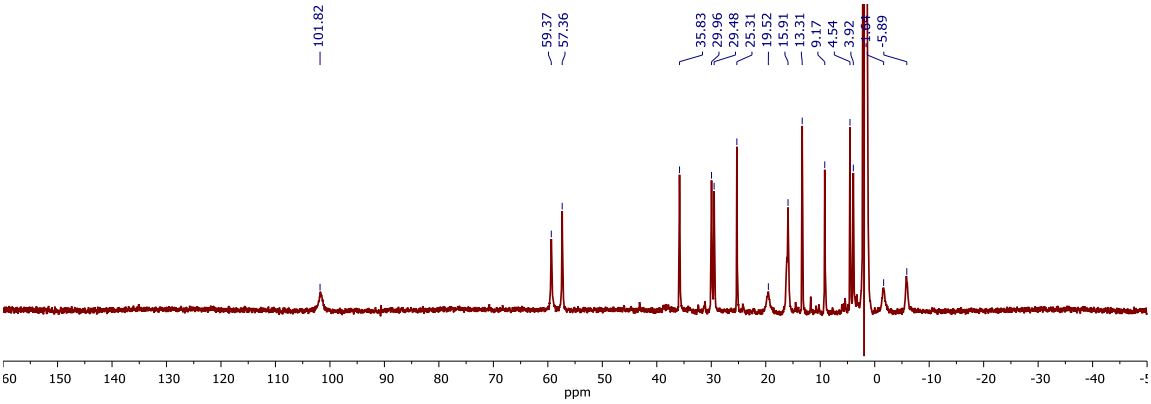

Figure 31. ^{1}H NMR spectrum (300 MHz) of [$LFe_3O(Pz)_3Fe$][OTf] (**3**) in CD_3CN.

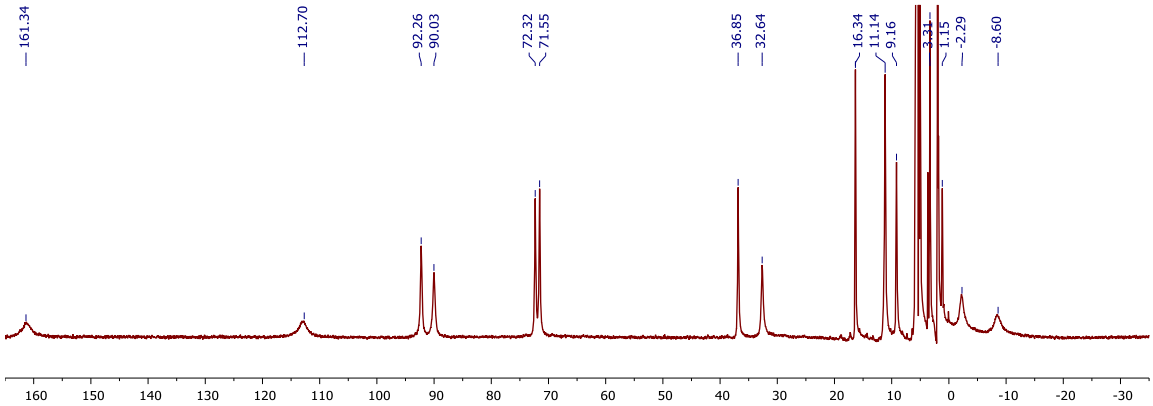

Figure 32. ^{1}H NMR spectrum (300 MHz) of $[LFe_3O(Pz)_3Fe][OTf]_3$ (**4**) in CD_2Cl_2.

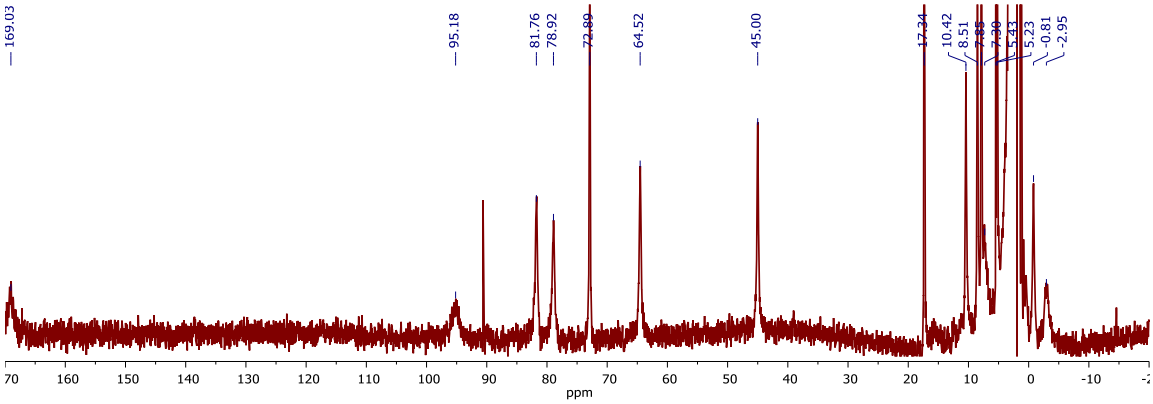

Figure 33. ^{1}H NMR spectrum (300 MHz) of $[LFe_3O(Pz)_3Fe(MeCN)][OTf]_3$ (**4-MeCN**) in CD_3CN.

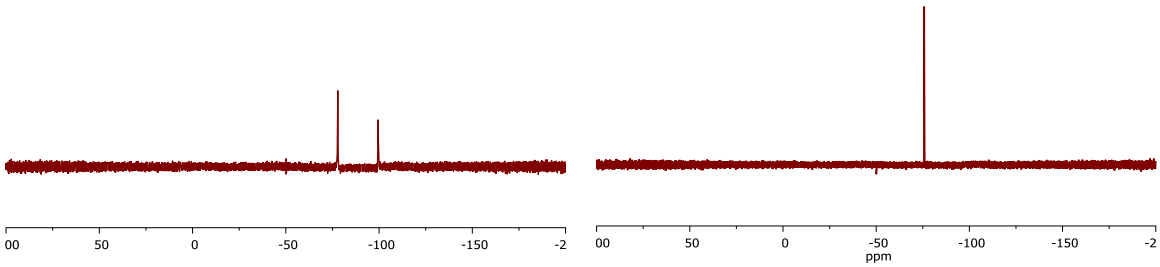

Figure 34. ^{19}F NMR spectra (300 MHz) of $[LFe_3O(Pz)_3Fe][OTf]_3$ (**4**) in CD_2Cl_2 (left) and $[LFe_3O(Pz)_3Fe(MeCN)][OTf]_3$ (**4-MeCN**) in CD_3CN (right).

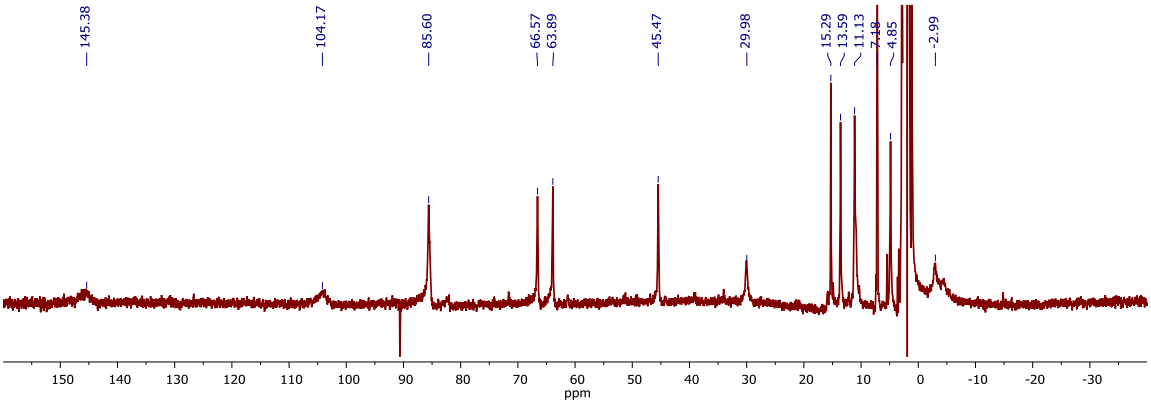

Figure 35. ^{1}H NMR spectrum (300 MHz) of $[LFe_3O(Pz)_3Fe(OH)][OTf]_2$ (**5**) in CD_3CN.

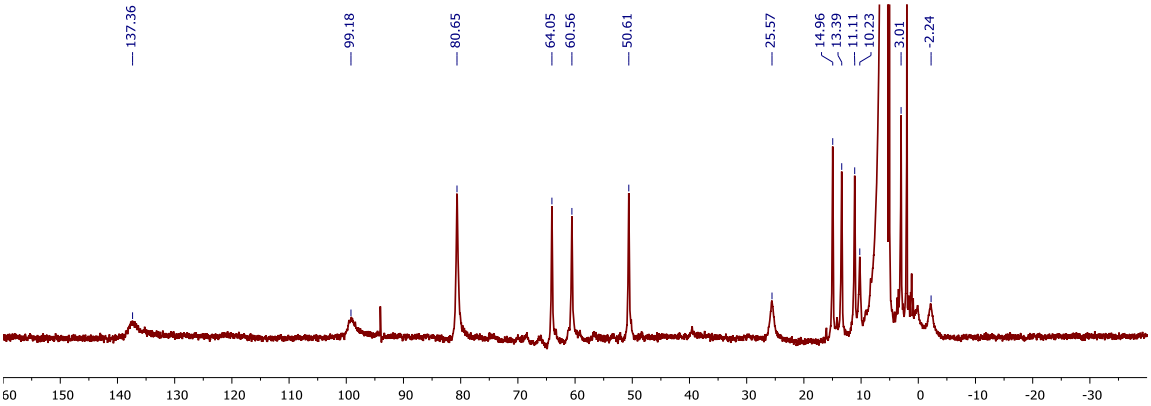

Figure 36. ^{1}H NMR spectrum (300 MHz) of $[(LFe_3O(Pz)_3Fe)_2O][OTf]_4$ (**6**) in CD_2Cl_2.

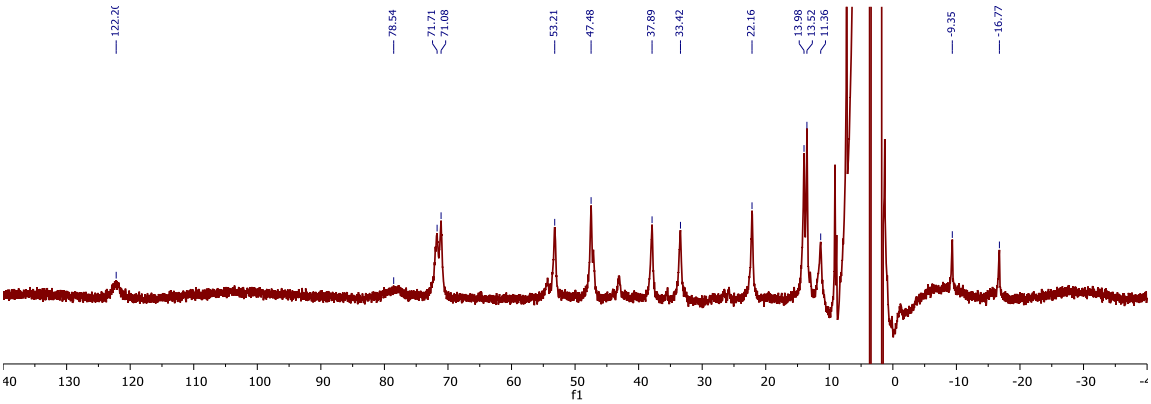

Figure 37. ^{1}H NMR spectrum (500 MHz) of $[LFe_3O(Pz)_3Fe(2\text{-phenyl-anilide})][OTf]$ (**7**) in THF/C_6D_6.

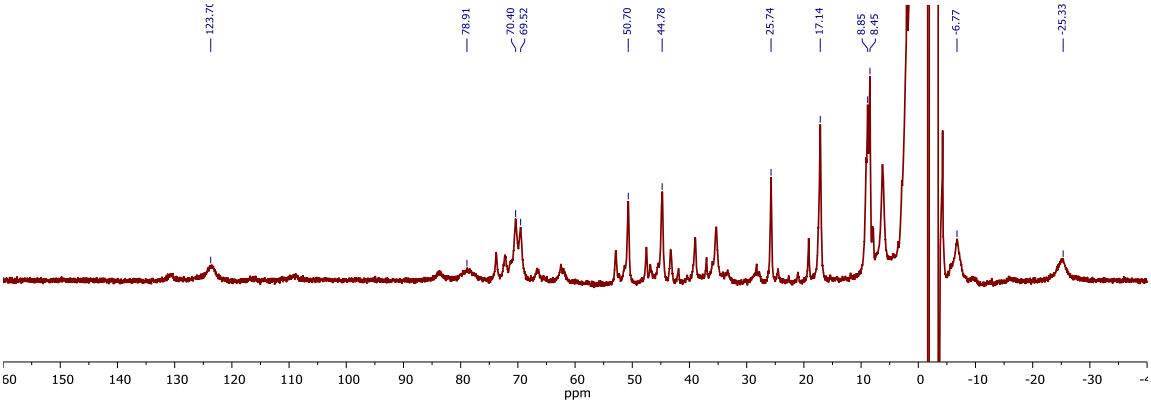

Figure 38. ^{1}H NMR spectrum (500 MHz) of reaction mixture containing [$LFe_3O(Pz)_3Fe$(3,5-trifluoromethyl-anilide)][OTf] (**8**) in THF/C_6D_6.

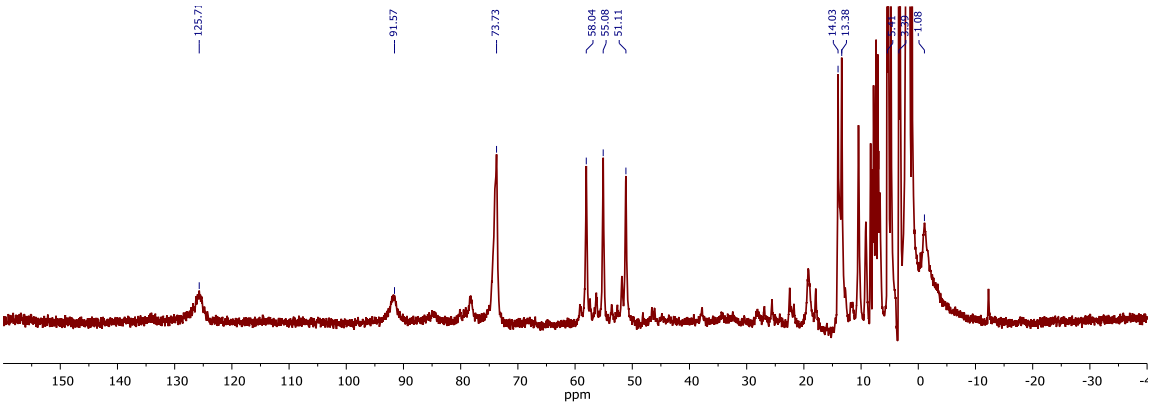

Figure 39. ^{1}H NMR spectrum (300 MHz) of [$LFe_3O(Pz)_3Fe$(para-tolylsulfonamide)][OTf] (**9**) in CD_3CN.

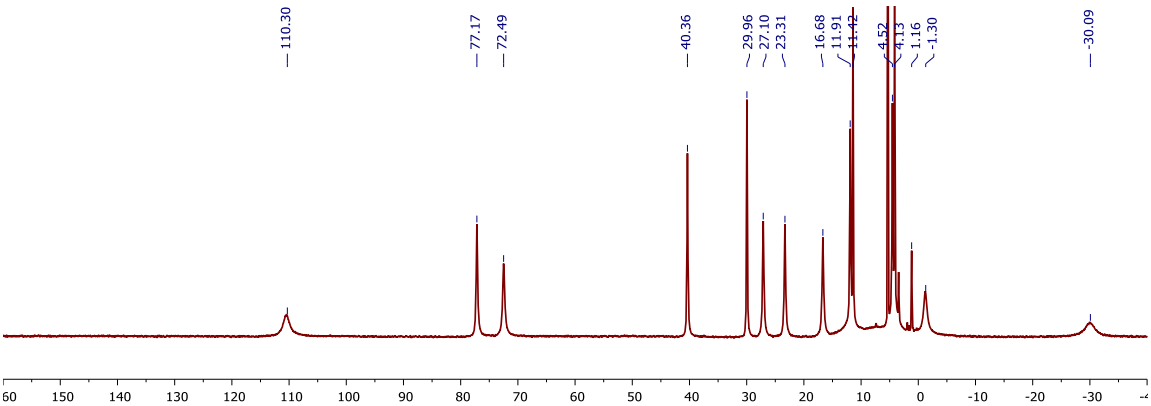

Figure 40. ^{1}H NMR spectrum (300 MHz) of [$LFe_3F(Pz)_3Fe$][OTf] (**10**) in CD_2Cl_2.

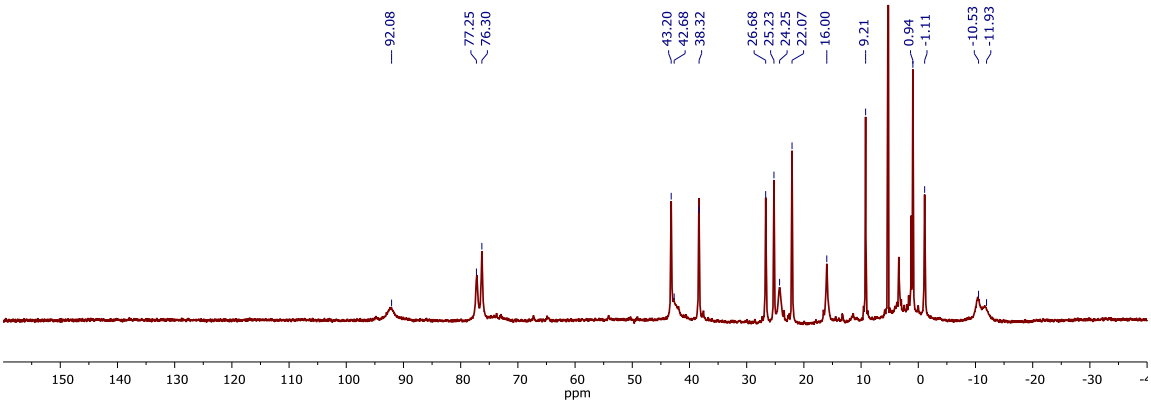

Figure 41. ^{1}H NMR spectrum (300 MHz) of $[(LFe_3F(Pz)_3Fe)_2O][OTf]_2$ (**11**) in CD_2Cl_2.

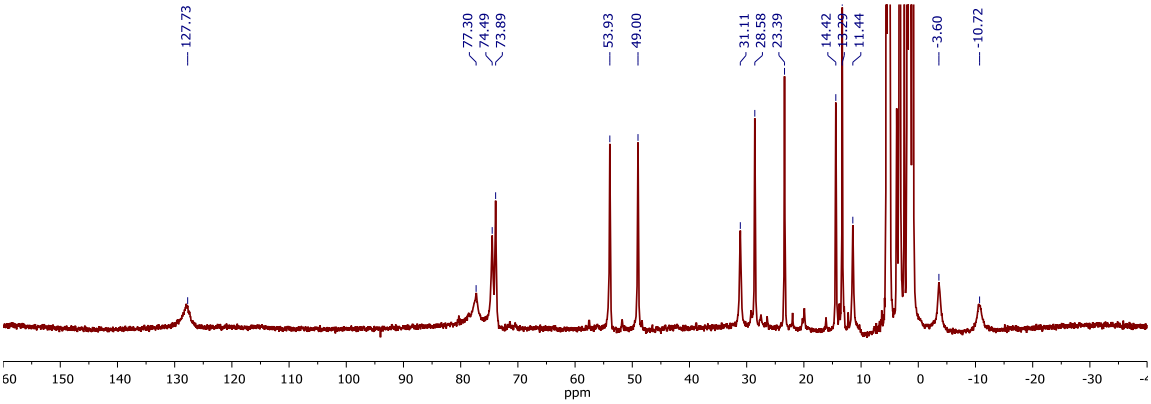

Figure 42. ^{1}H NMR spectrum (300 MHz) of $[LFe_3O(Pz)_3Fe(F)][OTf]$ (**12**) in CD_2Cl_2.

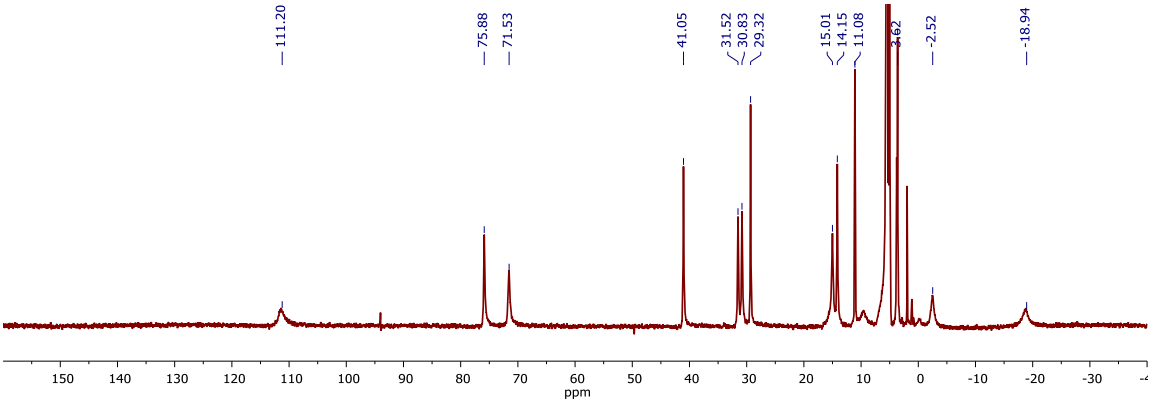

Figure 43. ^{1}H NMR spectrum (300 MHz) of $LFe_3N(Pz)_3Fe(N_3)$ (**13**) in CD_2Cl_2.