

Supplementary Materials for

Dimethyloxonium and Methoxy Derivatives of *nido*-Carborane and Metal Complexes Thereof

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Compound 10-Me₂O-7,8-C₂B₉H₁₁ (1)

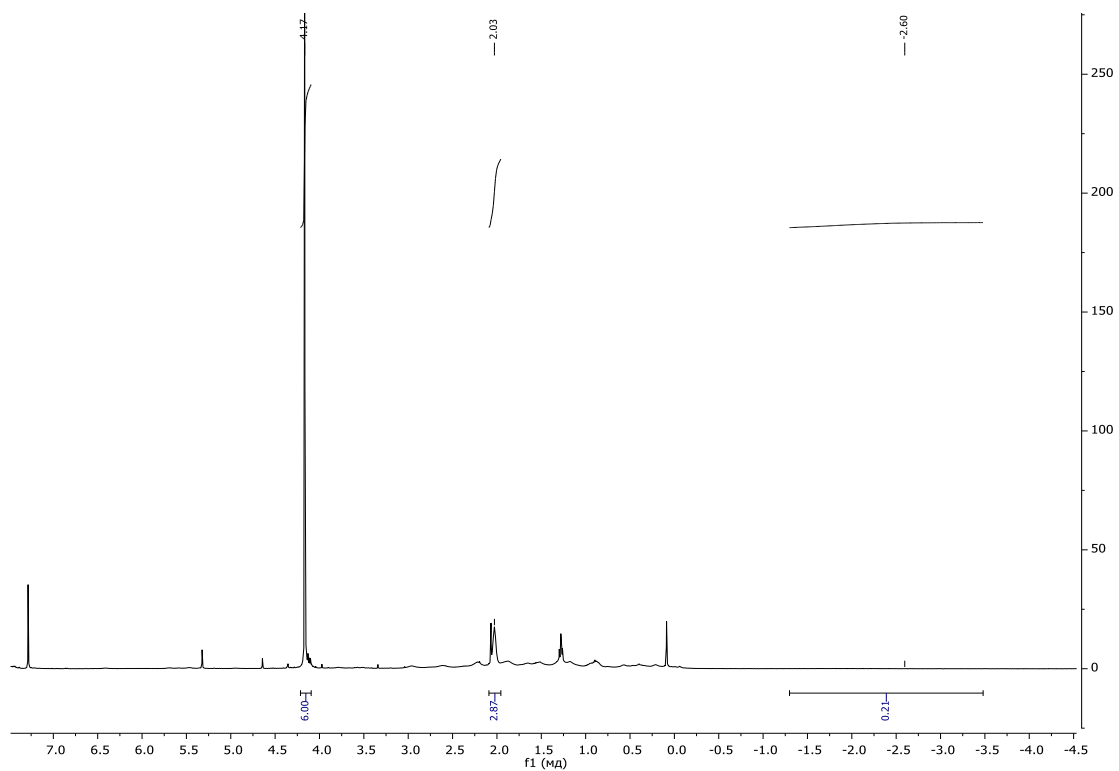


Fig. 1. ¹H NMR spectrum of 10-Me₂O-7,8-C₂B₉H₁₁ (1)

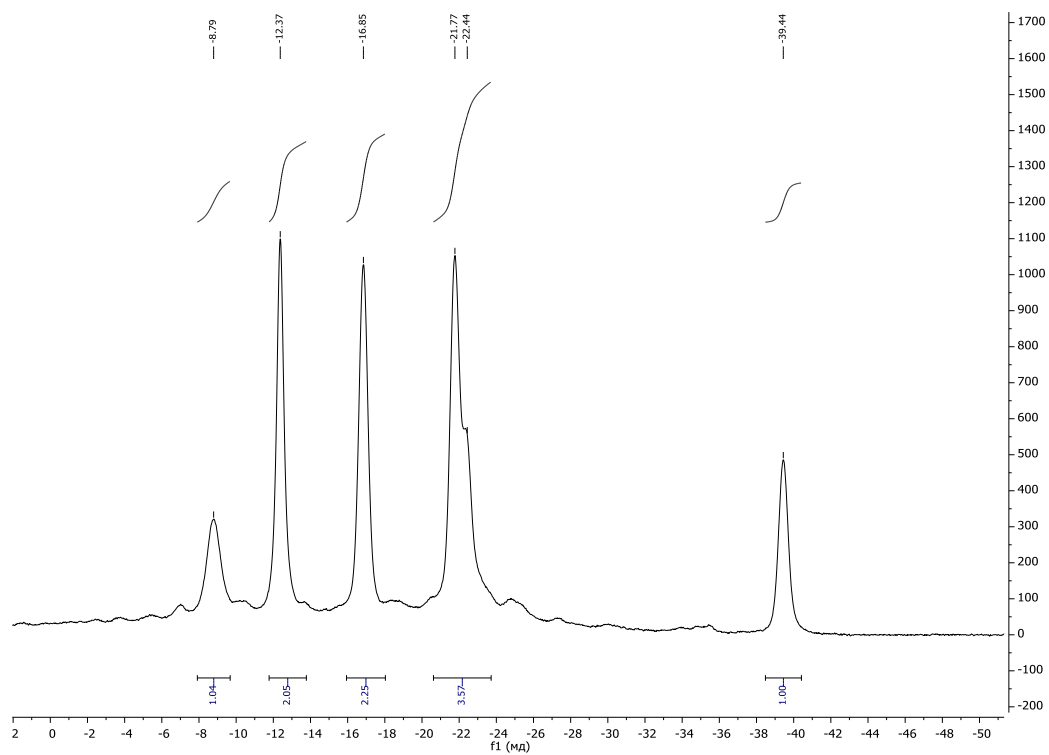


Fig. 2. ¹¹B NMR spectrum of 10-Me₂O-7,8-C₂B₉H₁₁ (1)

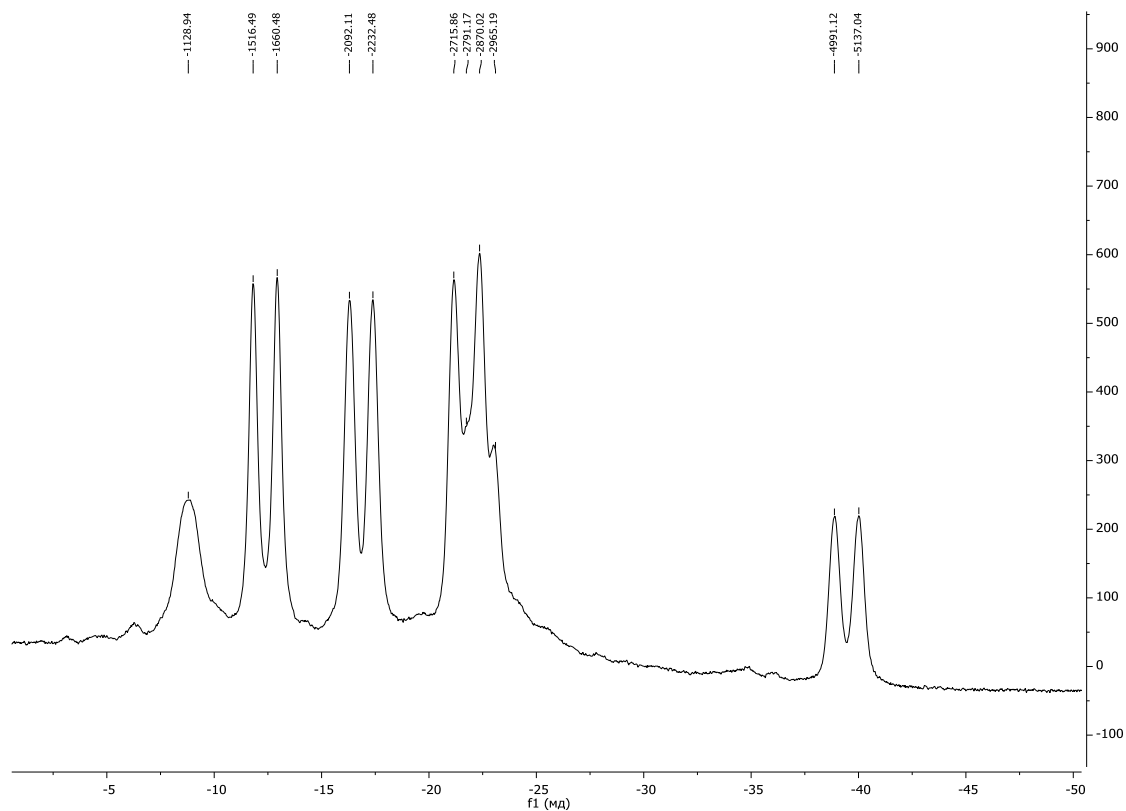


Fig. 3. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of 10-Me₂O-7,8-C₂B₉H₁₁ (**1**)

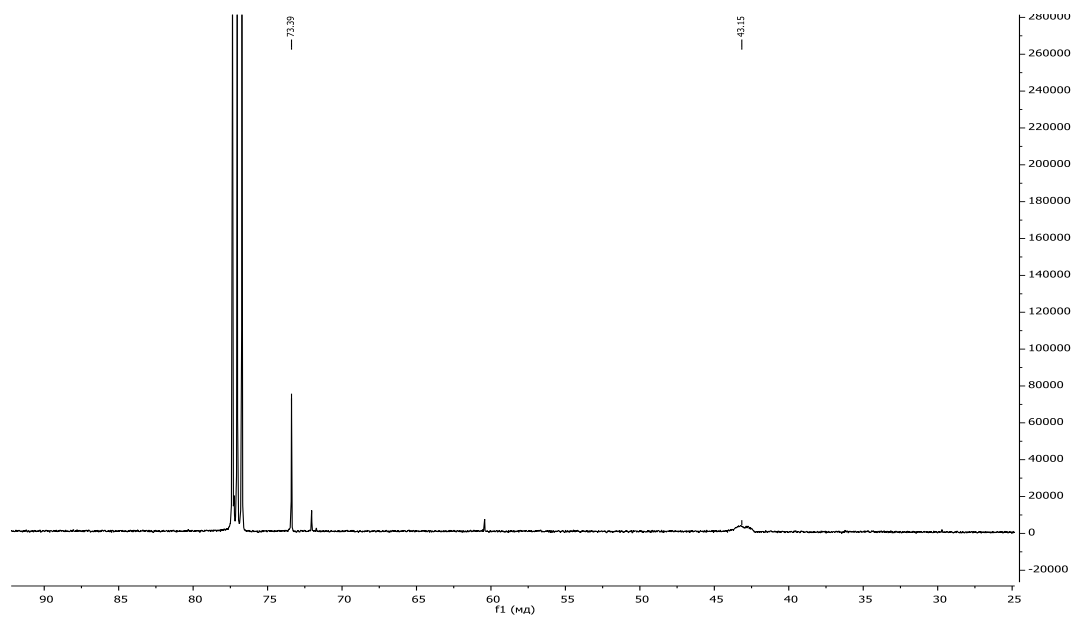


Fig. 4. ^{13}C NMR spectrum of 10-Me₂O-7,8-C₂B₉H₁₁ (**1**)

Compound 9-Me₂O-7,8-C₂B₉H₁₁ (2)

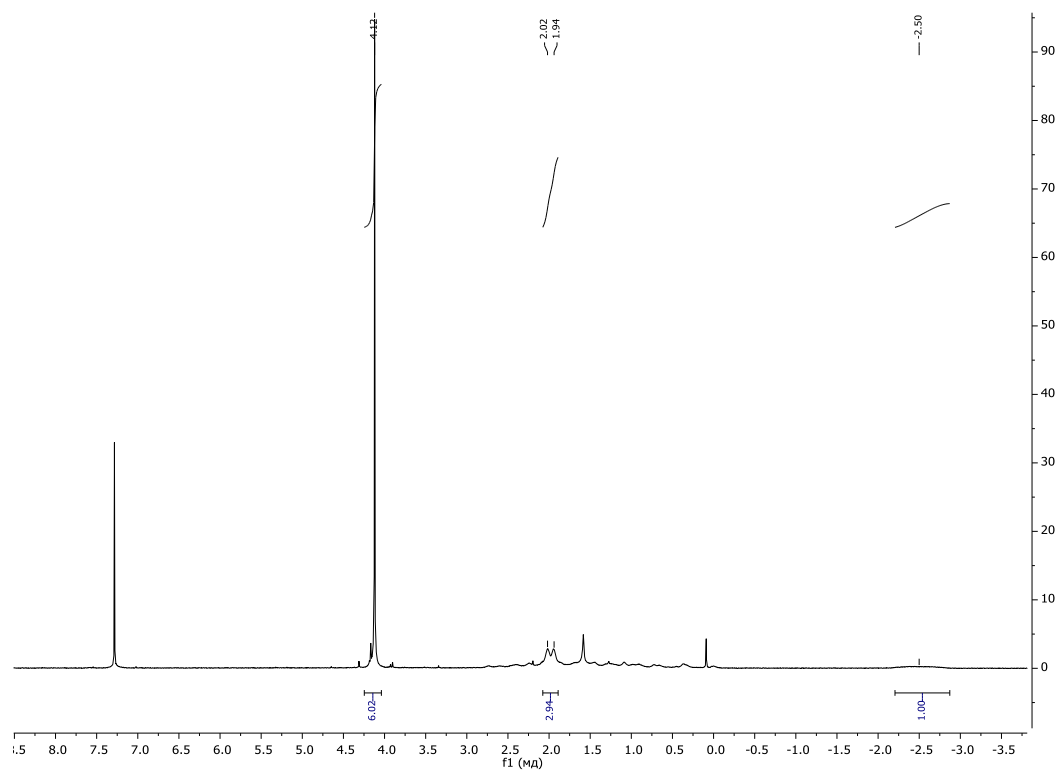


Fig. 5. ¹H NMR spectrum of 9-Me₂O-7,8-C₂B₉H₁₁ (2)

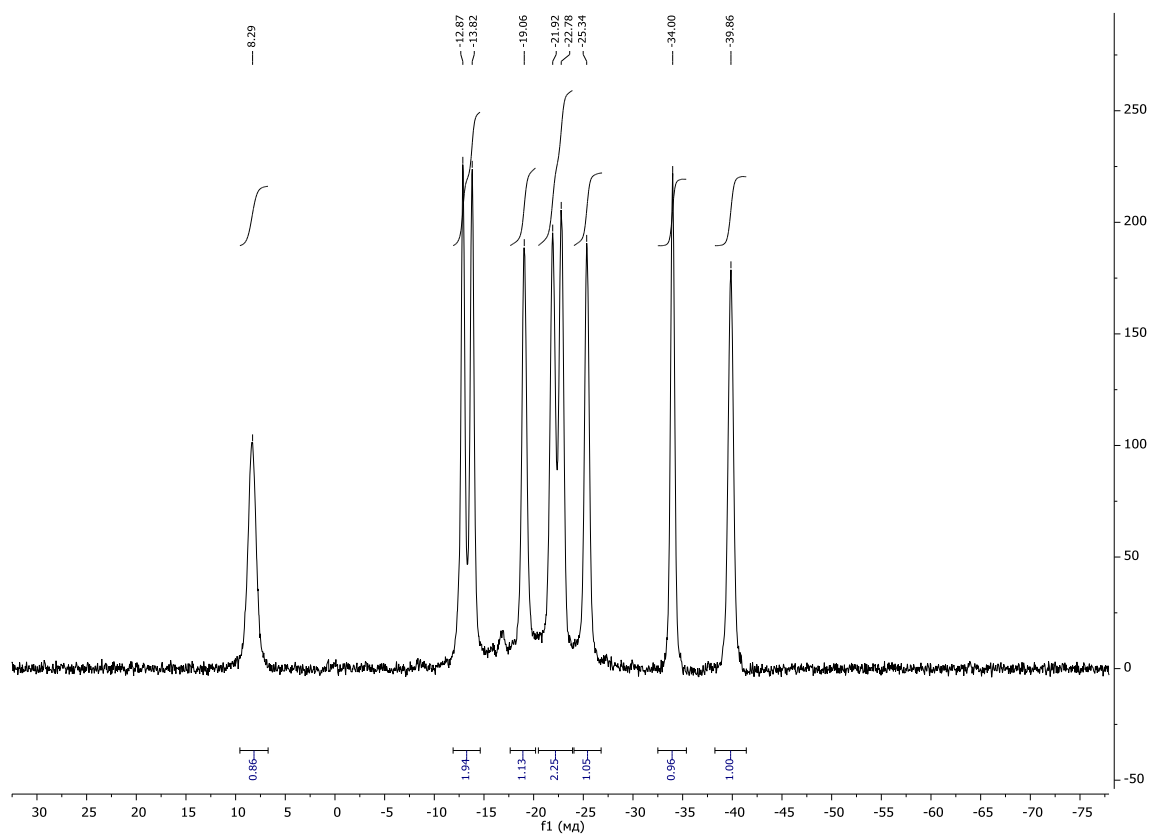


Fig. 6. ¹¹B NMR spectrum of 9-Me₂O-7,8-C₂B₉H₁₁ (2)

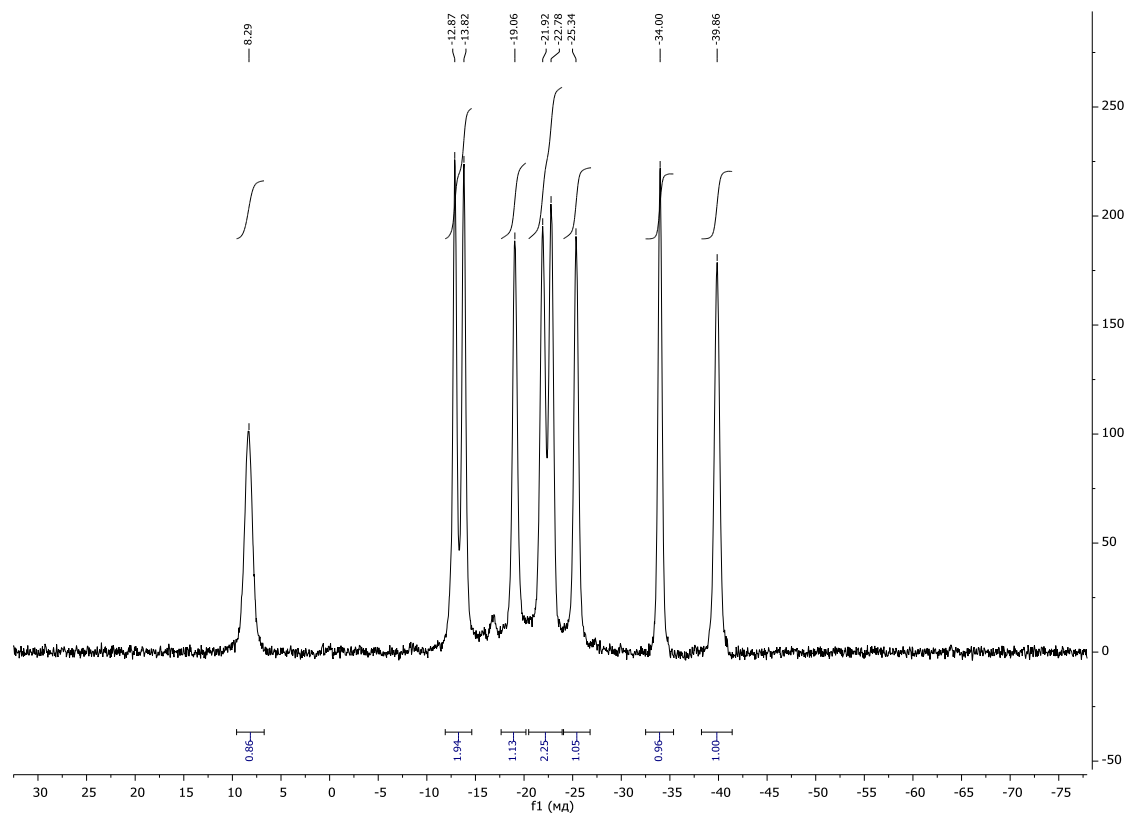


Fig. 7. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of 9-Me₂O-7,8-C₂B₉H₁₁ (**2**)

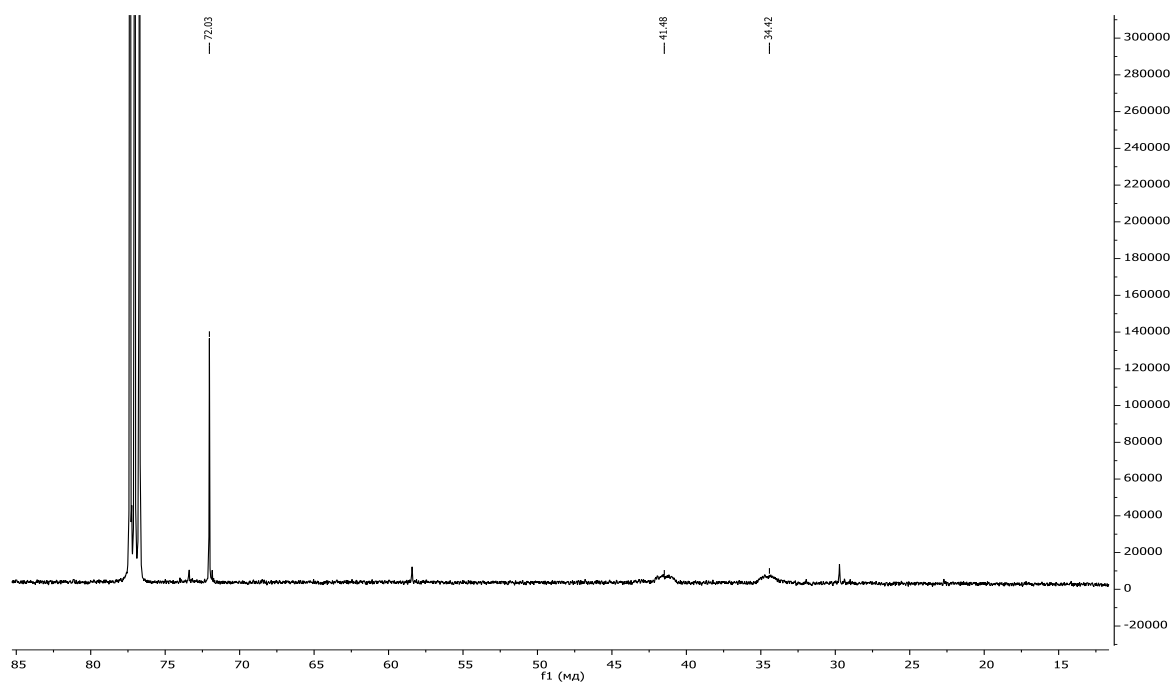


Fig. 8. ^{13}C NMR spectrum of 9-Me₂O-7,8-C₂B₉H₁₁ (**2**)

Compound K[10-MeO-7,8-C₂B₉H₁₁] (K[3])

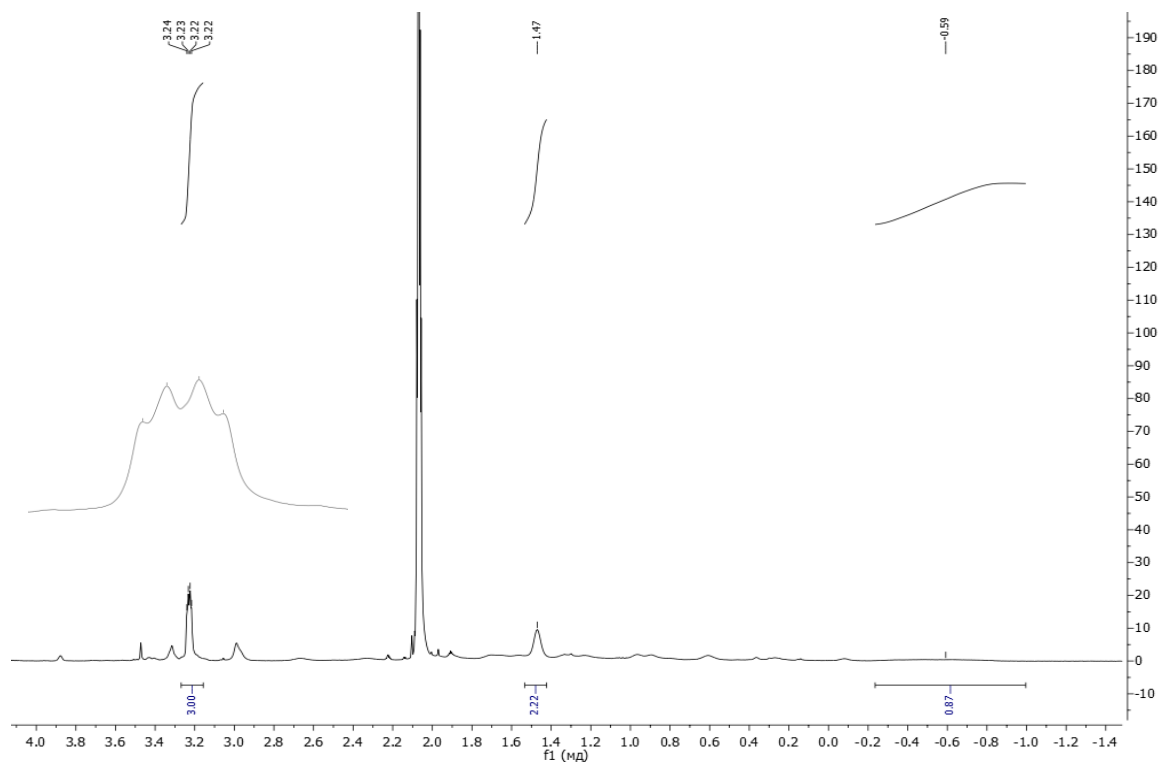


Fig. 9. ¹H NMR spectrum of K[10-MeO-7,8-C₂B₉H₁₁] (K[3])

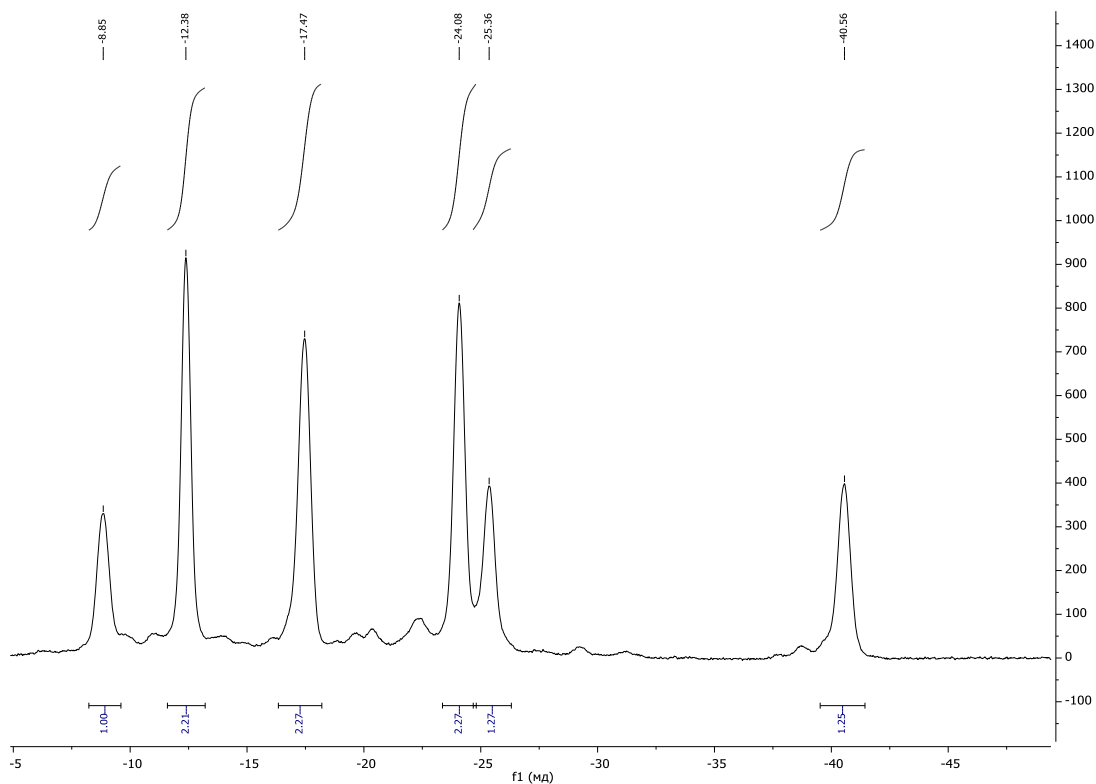


Fig. 10. ¹¹B NMR spectrum of K[10-MeO-7,8-C₂B₉H₁₁] (K[3])

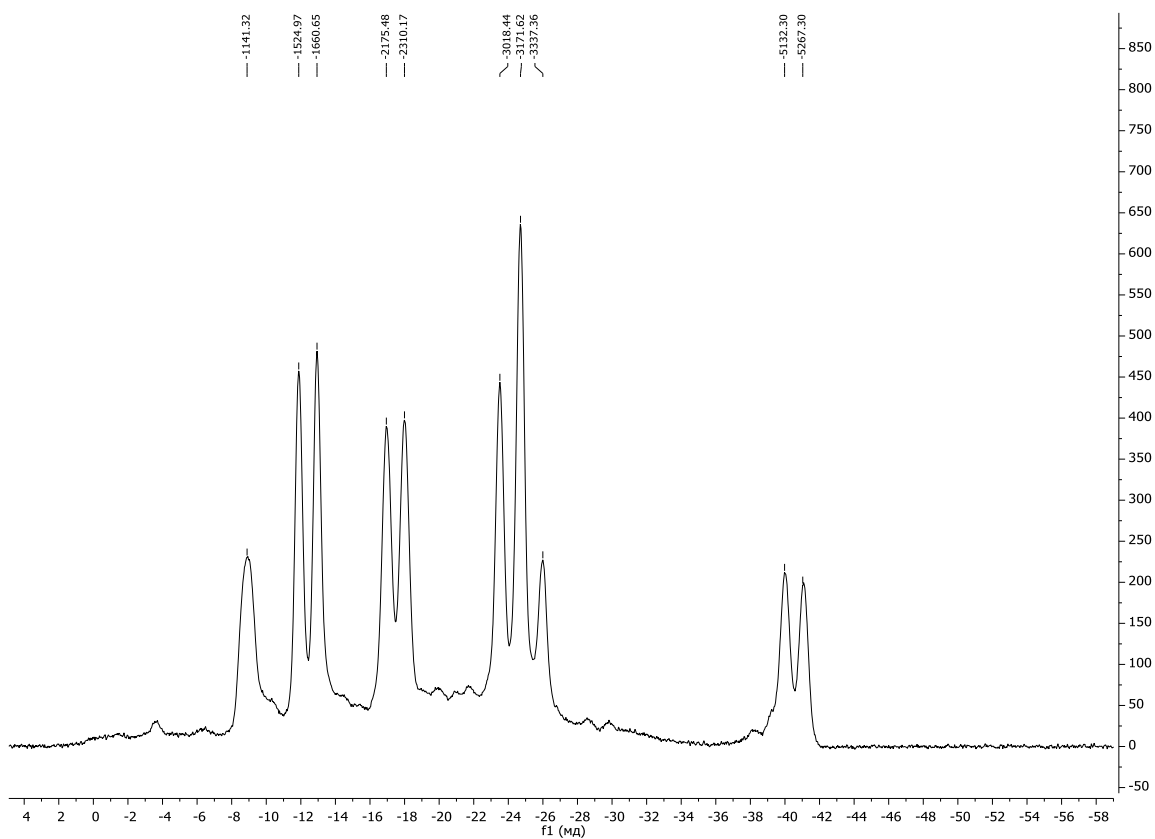


Fig. 11. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of K[10-MeO-7,8-C₂B₉H₁₁] (K[3])

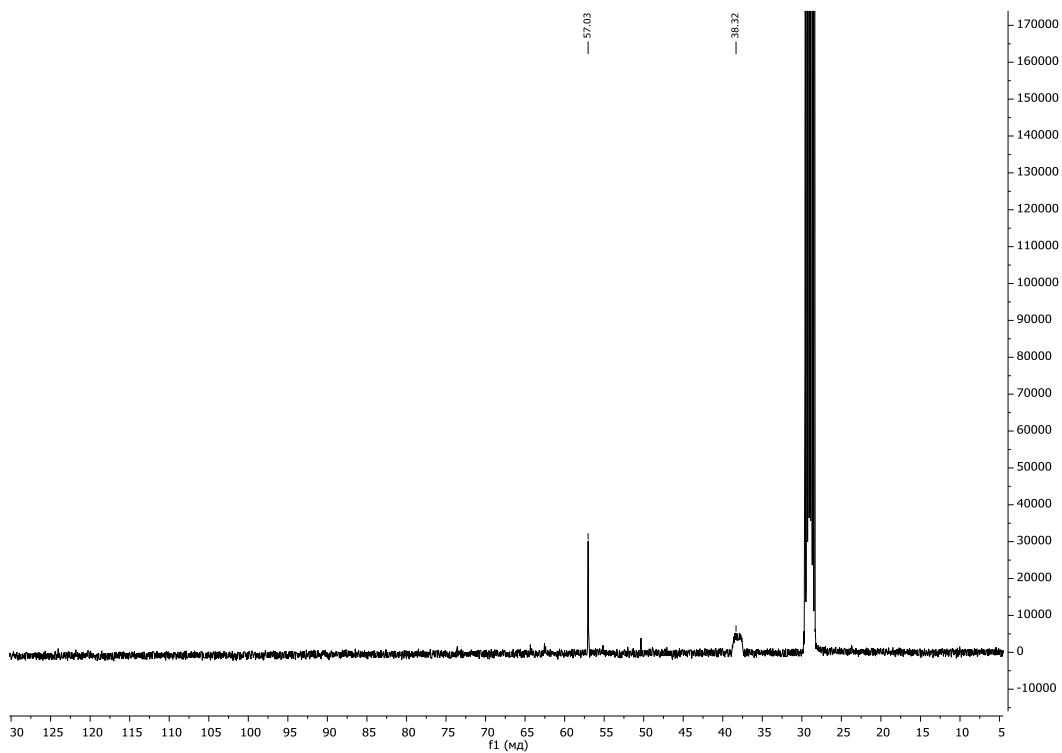


Fig. 12. ^{13}C NMR spectrum of K[10-MeO-7,8-C₂B₉H₁₁] (K[3])

Compound K[9-MeO-7,8-C₂B₉H₁₁] (K[4])

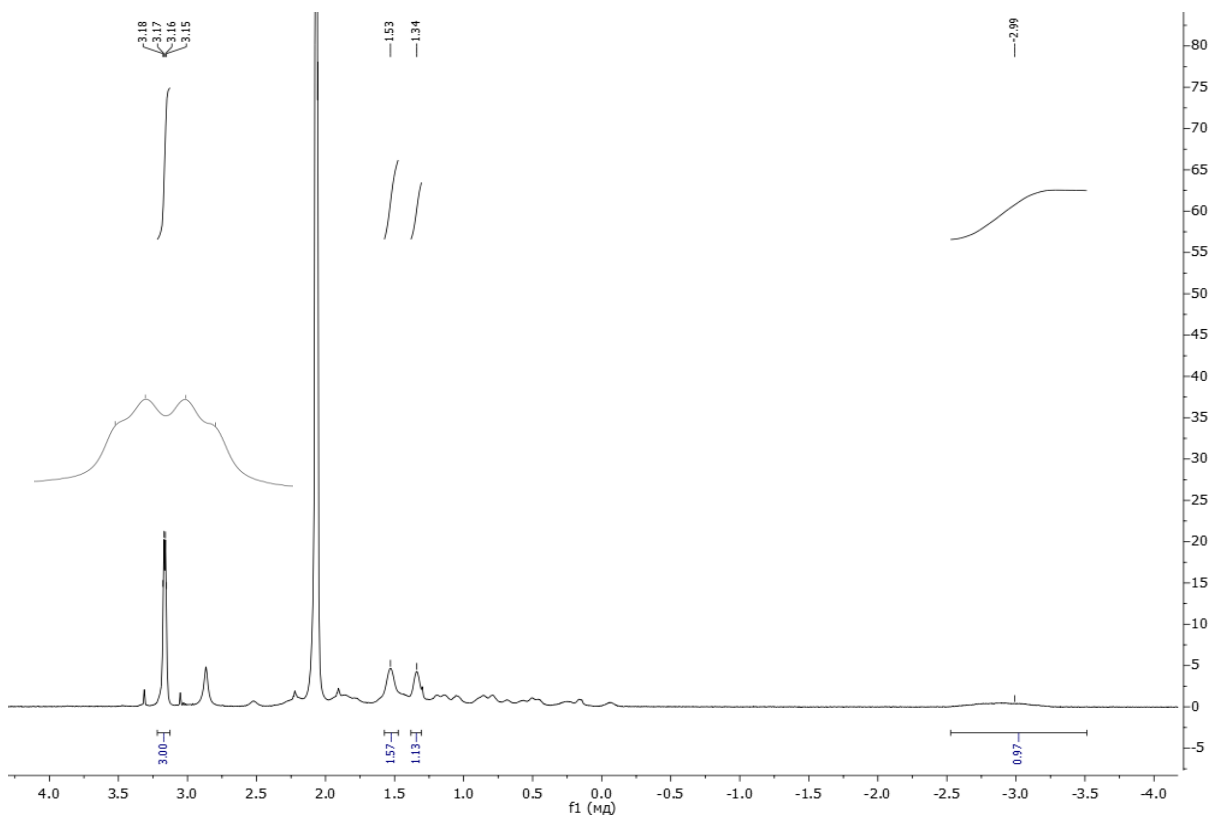


Fig. 13. ¹H NMR spectrum of K[9-MeO-7,8-C₂B₉H₁₁] (K[4])

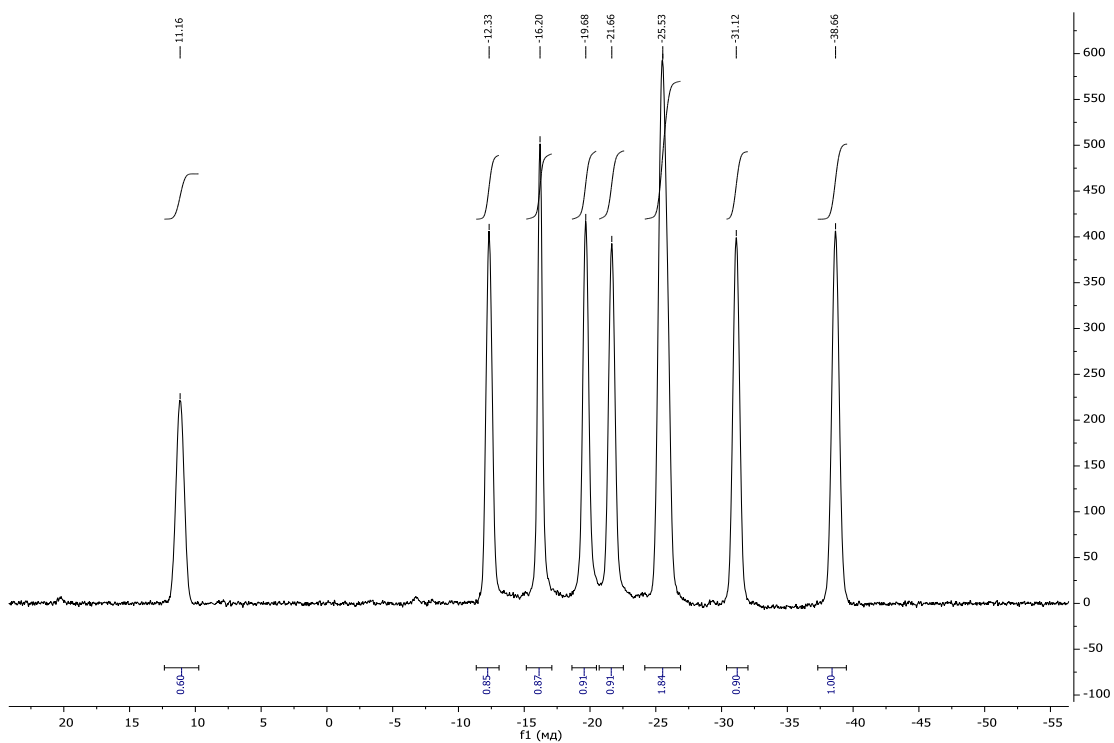


Fig. 14. ¹¹B NMR spectrum of K[9-MeO-7,8-C₂B₉H₁₁] (K[4])

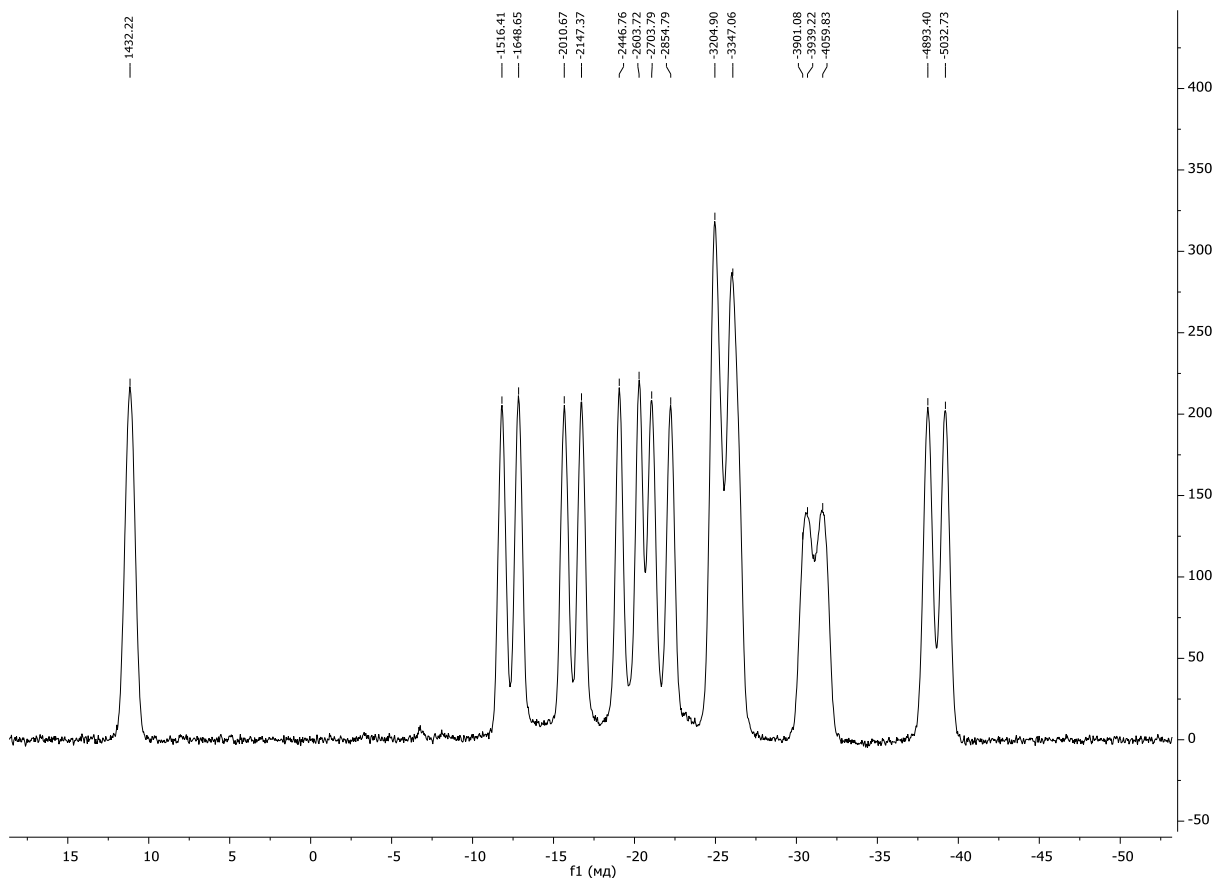


Fig. 15. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $\text{K}[9\text{-MeO-7,8-C}_2\text{B}_9\text{H}_{11}]$ (K[4])

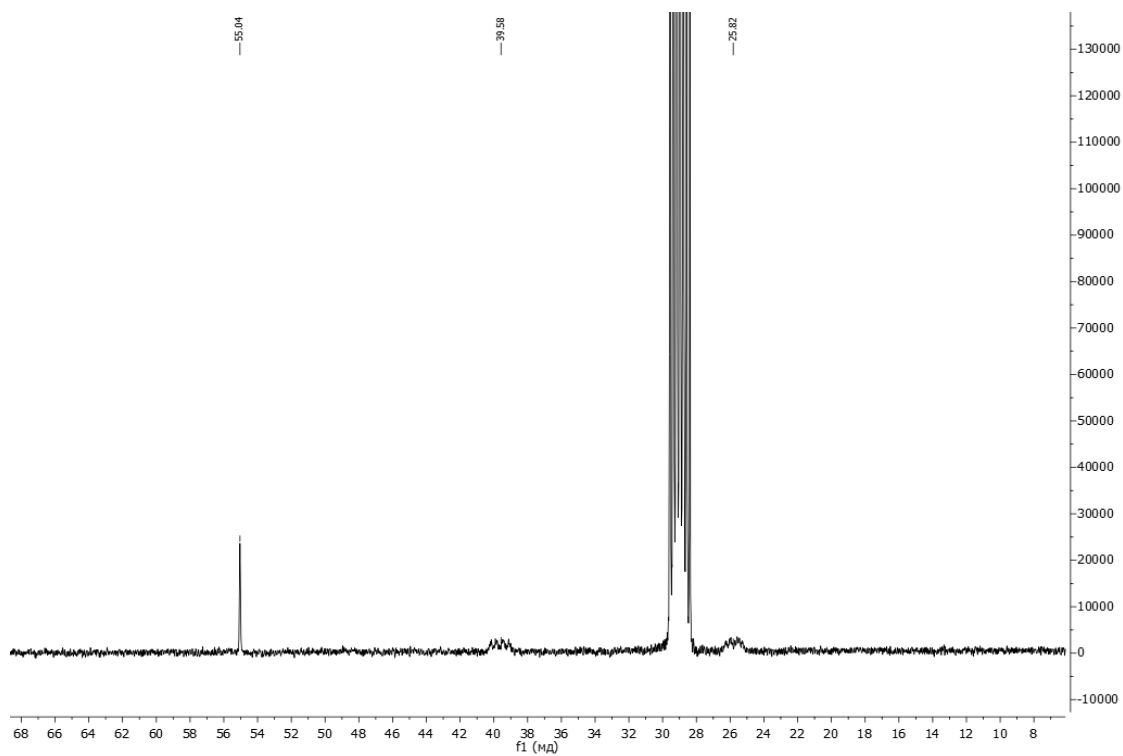


Fig. 16. ^{13}C NMR spectrum of $\text{K}[9\text{-MeO-7,8-C}_2\text{B}_9\text{H}_{11}]$ (K[4])

Compound (Et₃NMe)[10-MeO-7,8-C₂B₉H₁₁] (Et₃NMe)[3]

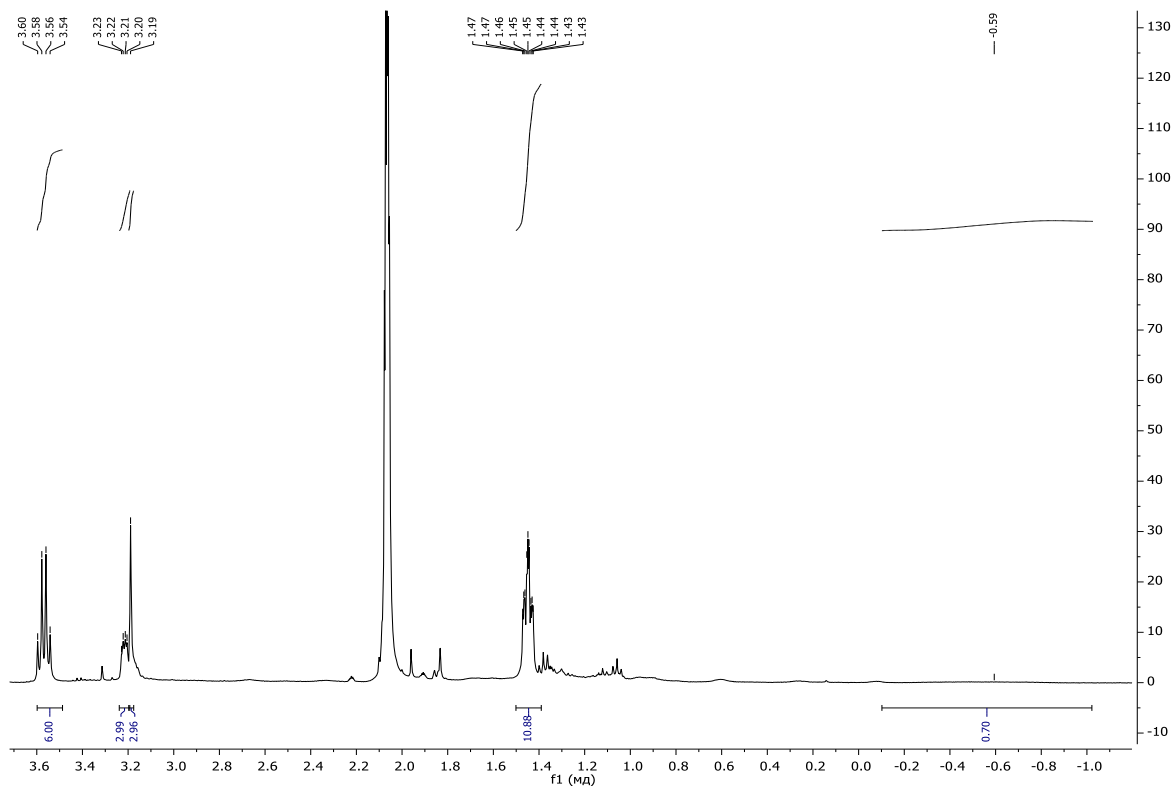


Fig. 17. ¹H NMR spectrum of (Et₃NMe)[10-MeO-7,8-C₂B₉H₁₁] (Et₃NMe)[3]

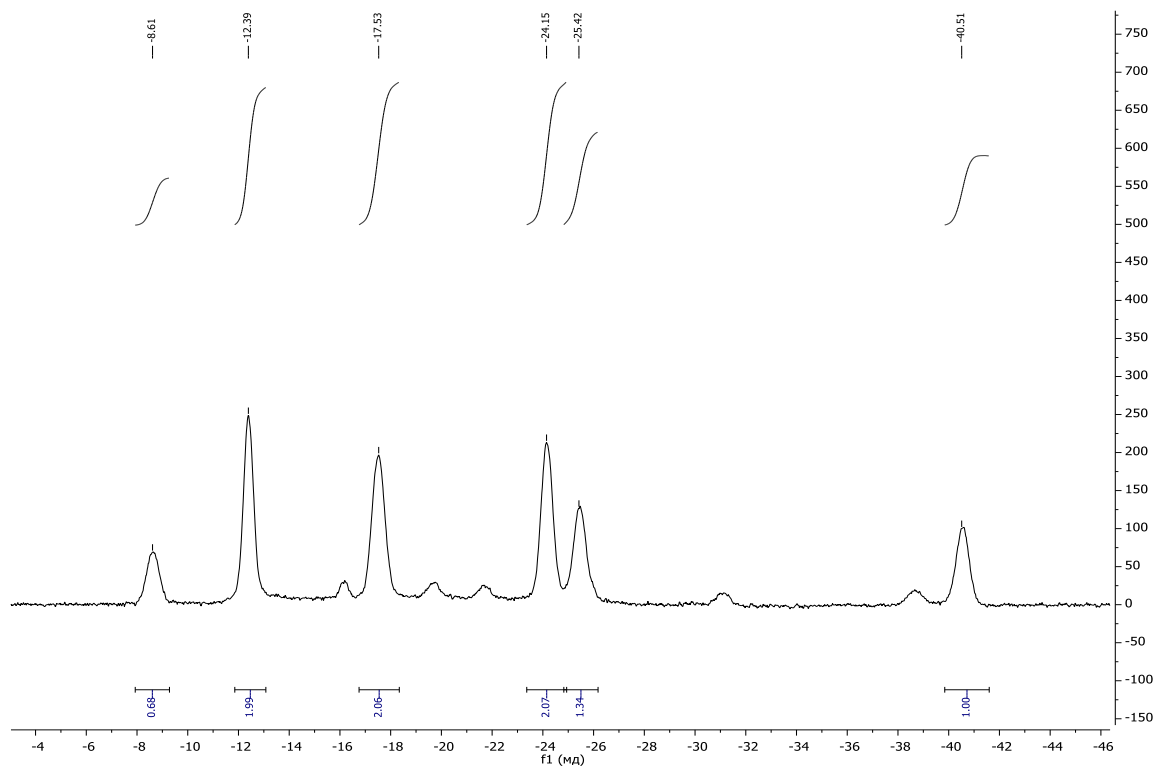


Fig. 18. ¹¹B NMR spectrum of (Et₃NMe)[10-MeO-7,8-C₂B₉H₁₁] (Et₃NMe)[3]

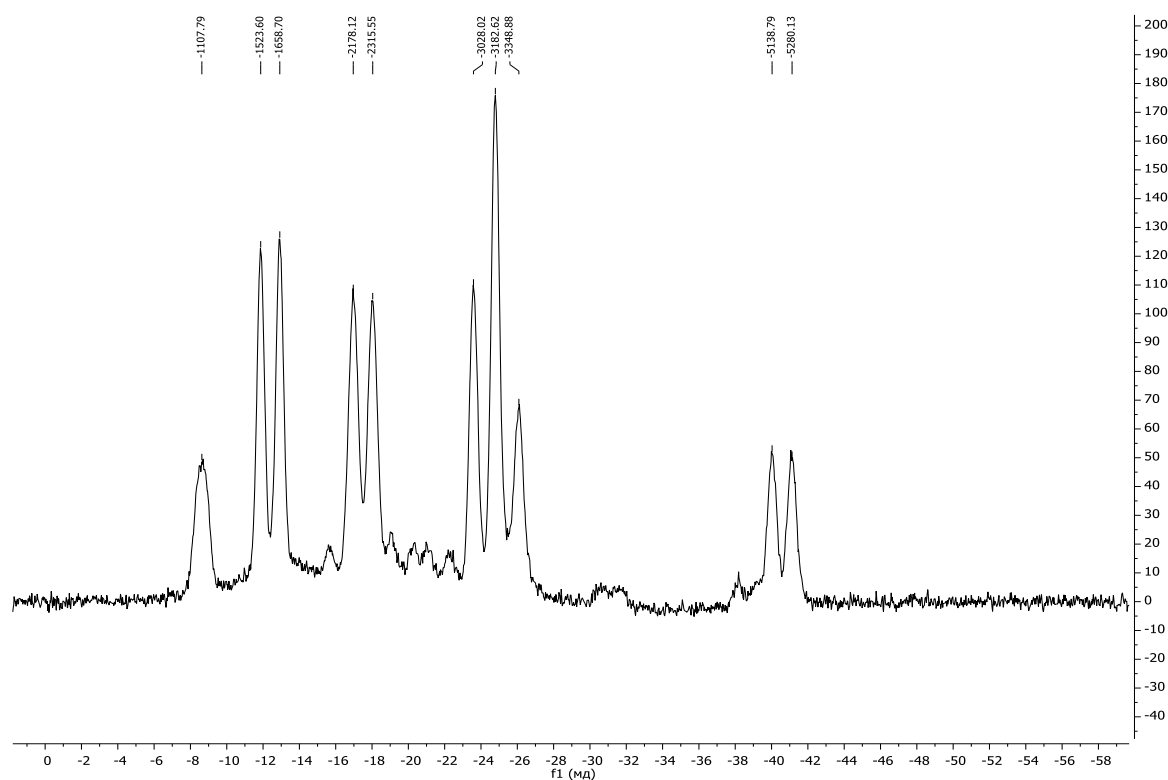


Fig. 19. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $(\text{Et}_3\text{NMe})[10\text{-MeO-}7,8\text{-C}_2\text{B}_9\text{H}_{11}] (\text{Et}_3\text{NMe})[3]$

Compound $(\text{Et}_3\text{NMe})[9\text{-MeO-}7,8\text{-C}_2\text{B}_9\text{H}_{11}] (\text{Et}_3\text{NMe})[4]$

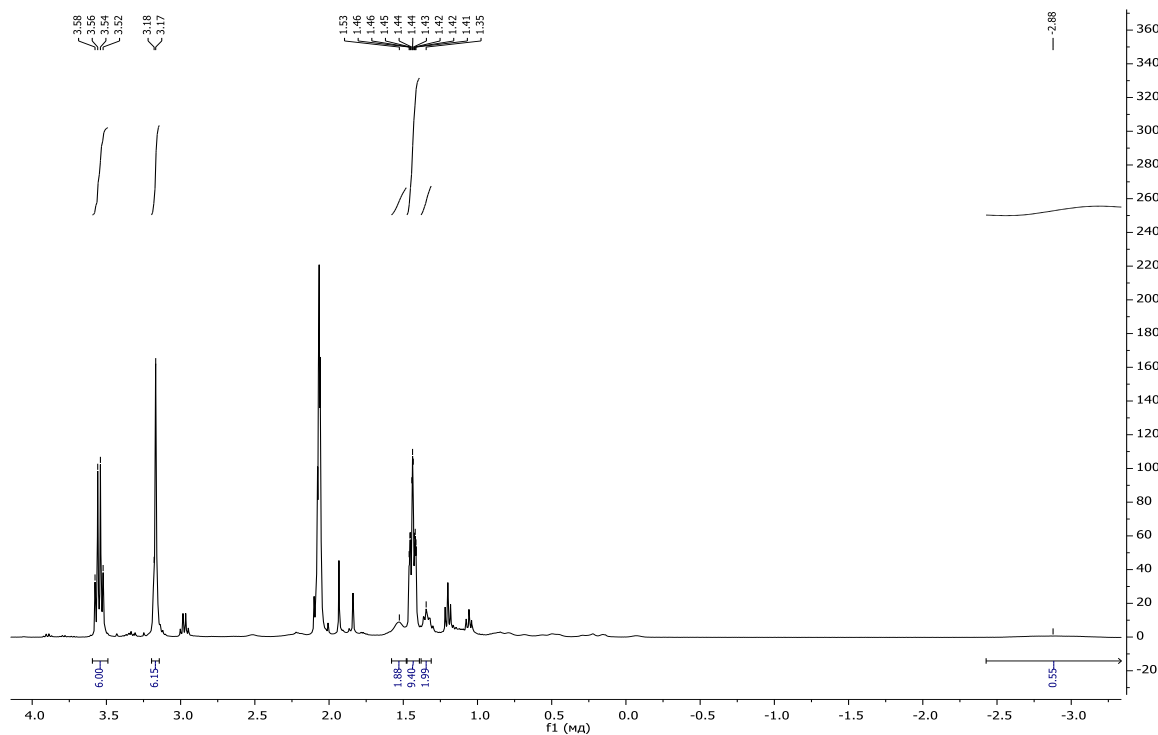


Fig. 20. ^1H NMR spectrum of $(\text{Et}_3\text{NMe})[9\text{-MeO-}7,8\text{-C}_2\text{B}_9\text{H}_{11}] (\text{Et}_3\text{NMe})[4]$

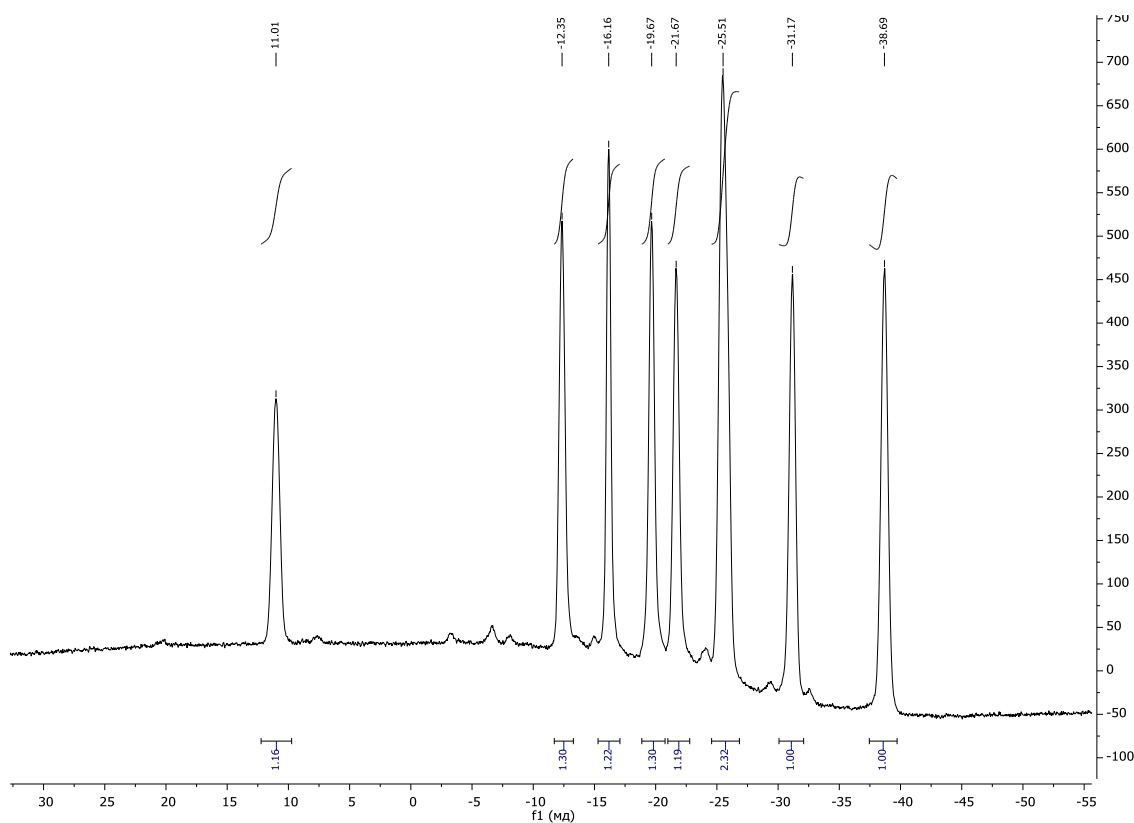


Fig. 21. ^{11}B NMR spectrum of $(\text{Et}_3\text{NMe})[9\text{-MeO-7,8-C}_2\text{B}_9\text{H}_{11}] (\text{Et}_3\text{NMe})[4]$

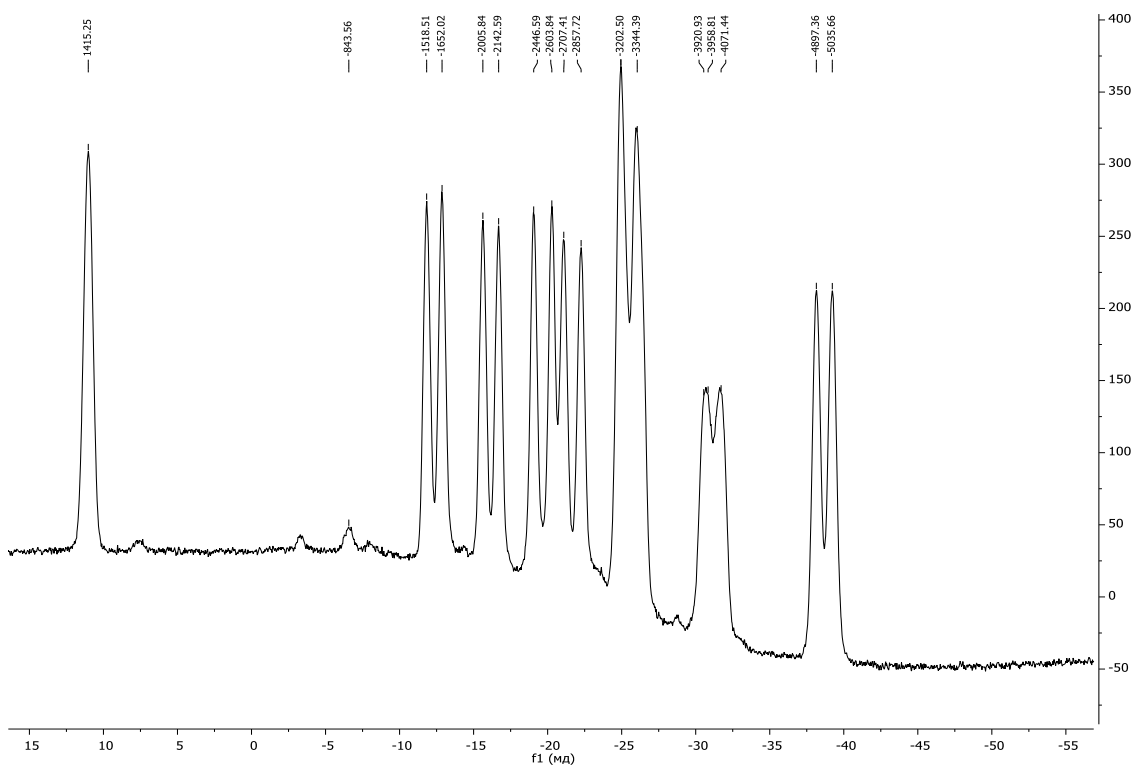


Fig. 22. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $(\text{Et}_3\text{NMe})[9\text{-MeO-7,8-C}_2\text{B}_9\text{H}_{11}] (\text{Et}_3\text{NMe})[4]$

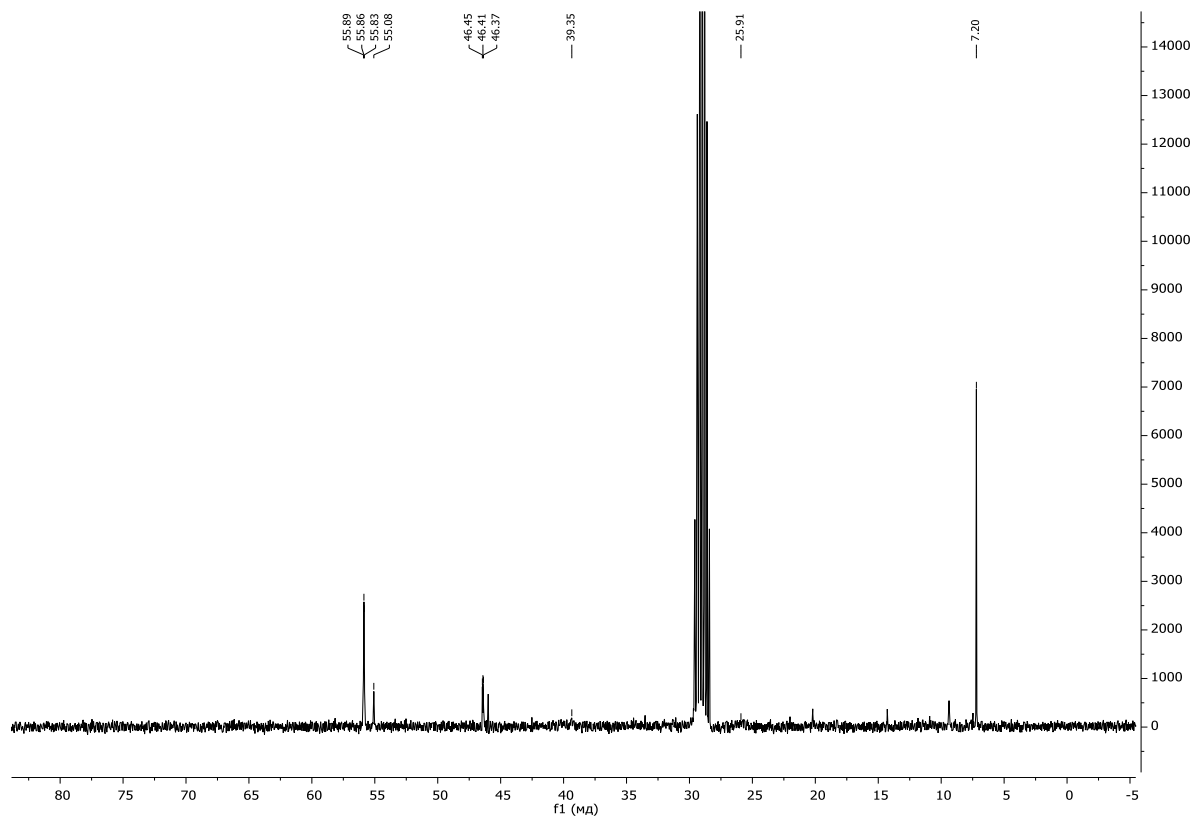


Fig. 23. ^{13}C NMR spectrum of $(\text{Et}_3\text{NMe})[9\text{-MeO-7,8-C}_2\text{B}_9\text{H}_{11}] (\text{Et}_3\text{NMe})[4]$

Compound $(\text{C}_5\text{H}_5\text{NMe})[9\text{-Me}_2\text{O-7,8-C}_2\text{B}_9\text{H}_{11}] (\text{N-MePy})[4]$

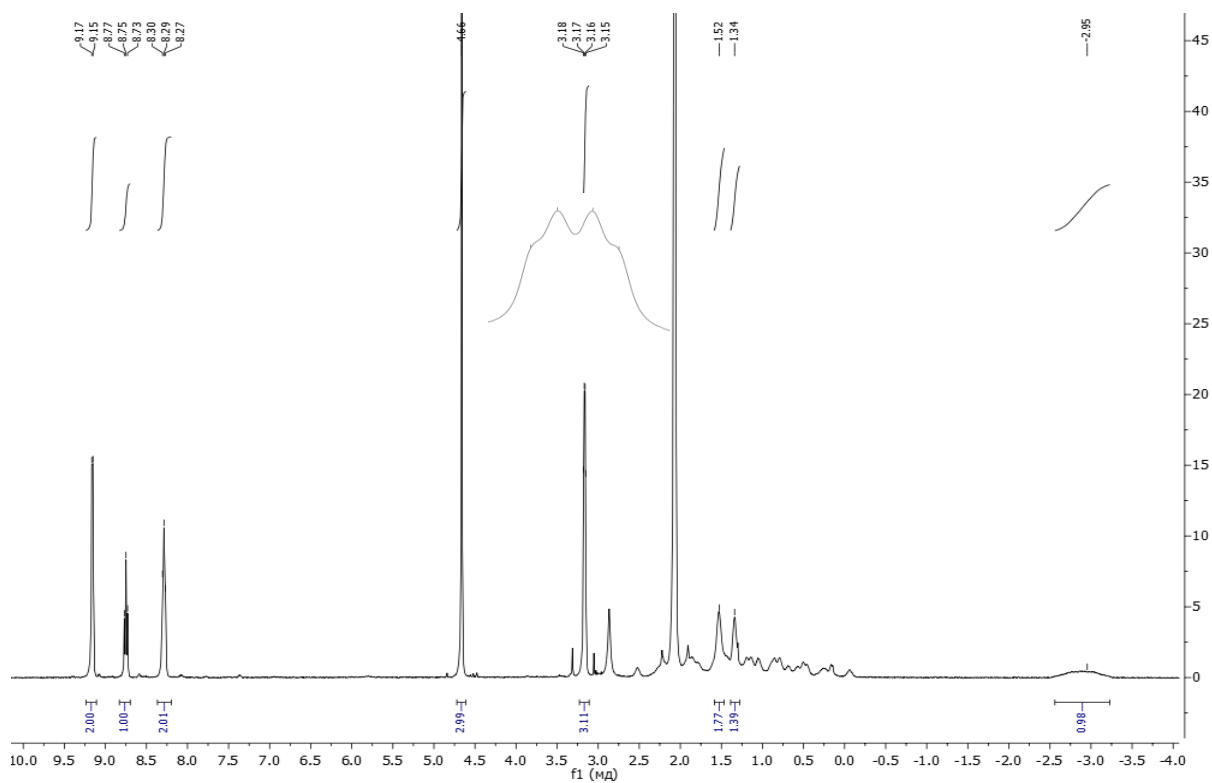


Fig. 24. ^1H NMR spectrum of $(\text{C}_5\text{H}_5\text{NMe})[9\text{-Me}_2\text{O-7,8-C}_2\text{B}_9\text{H}_{11}] (\text{N-MePy})[4]$

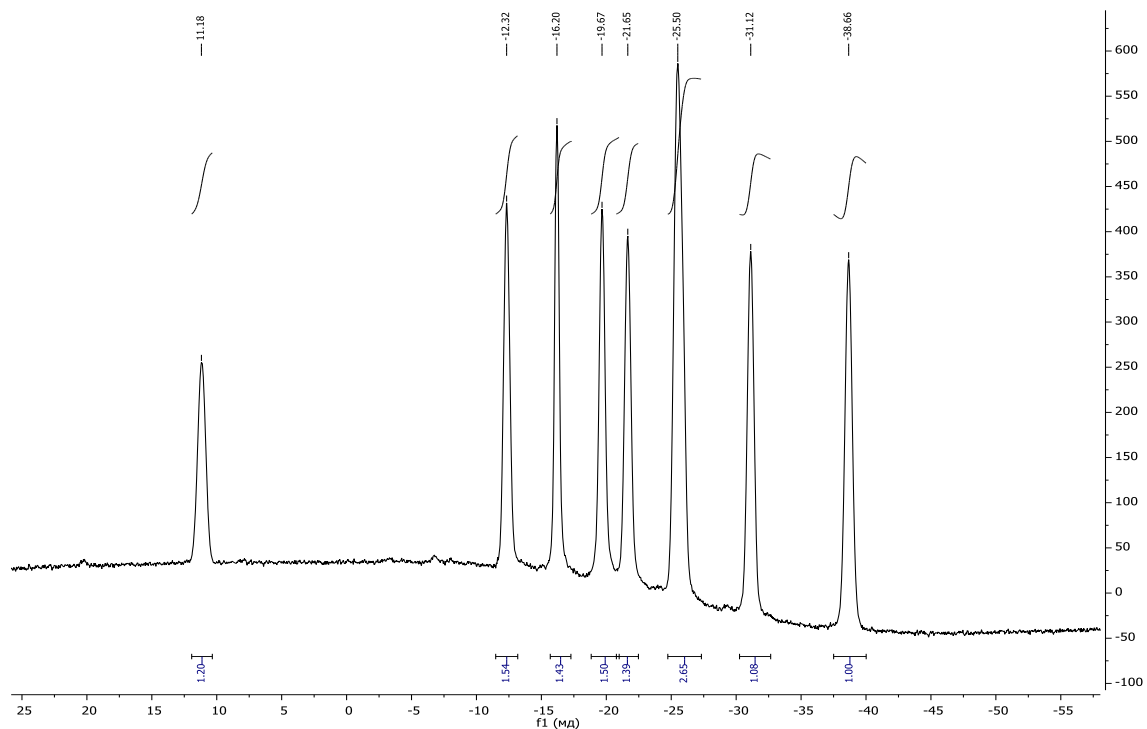


Fig. 25. ^{11}B NMR spectrum of $(\text{C}_5\text{H}_5\text{NMe})[9\text{-Me}_2\text{O-7,8-C}_2\text{B}_9\text{H}_{11}] (\text{N-MePy})[4]$

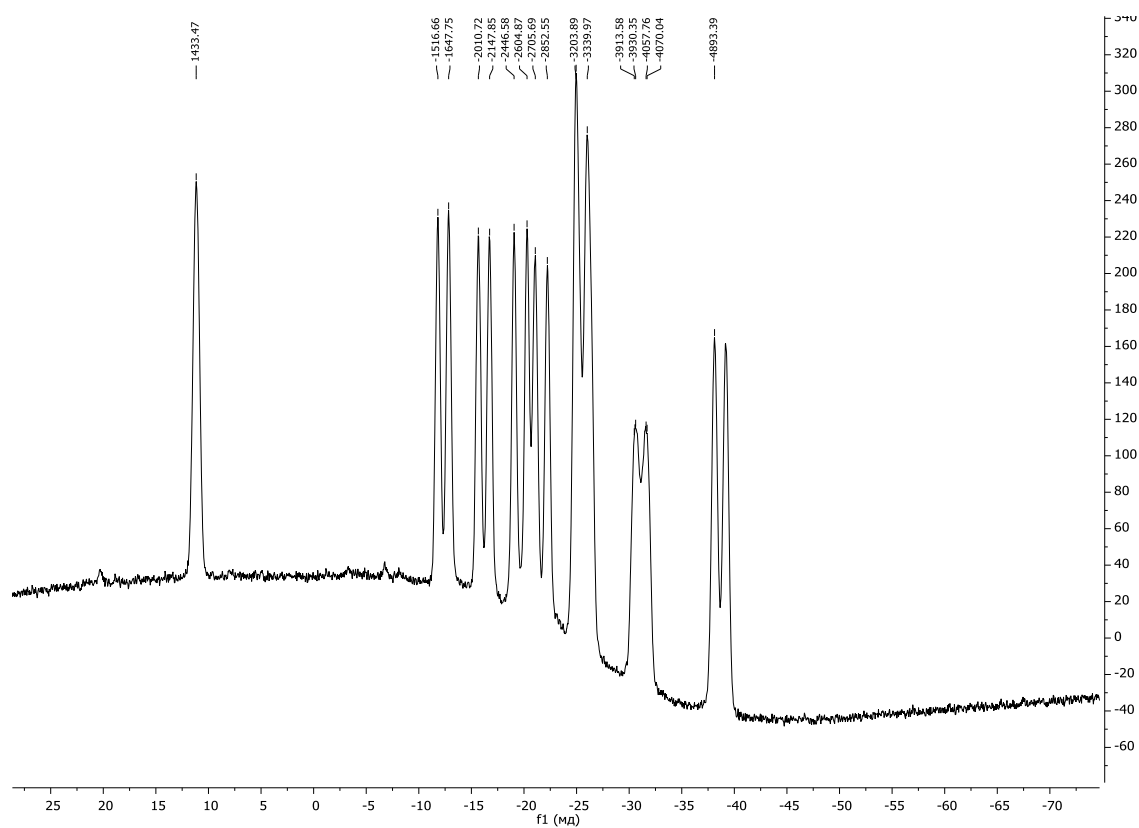


Fig. 26. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $(\text{C}_5\text{H}_5\text{NMe})[9\text{-Me}_2\text{O-7,8-C}_2\text{B}_9\text{H}_{11}] (\text{N-MePy})[4]$

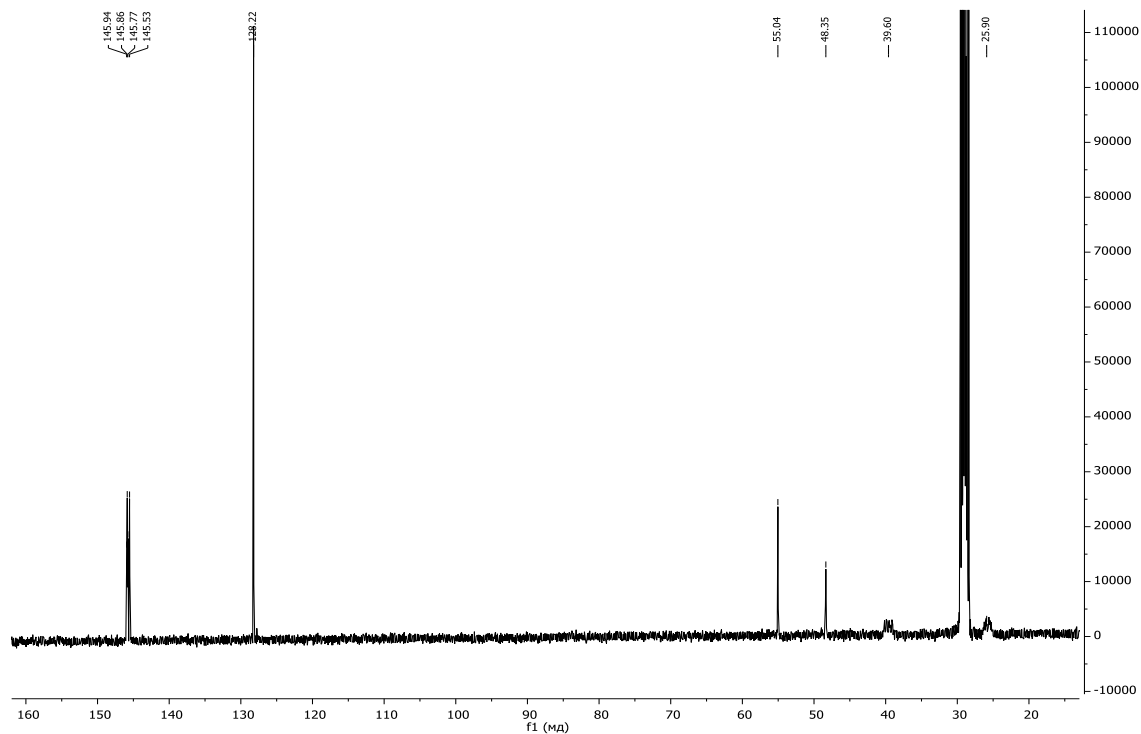


Fig. 27. ^{13}C NMR spectrum of $(\text{C}_5\text{H}_5\text{NMe})[9\text{-Me}_2\text{O-7,8-C}_2\text{B}_9\text{H}_{11}] (\text{N-MePy})[4]$

Reactions of 10-Me₂O-7,8-C₂B₉H₁₁ and 9-Me₂O-7,8-C₂B₉H₁₁ with 3-methyl-6-nitro-1H-indazole.

Compound 6

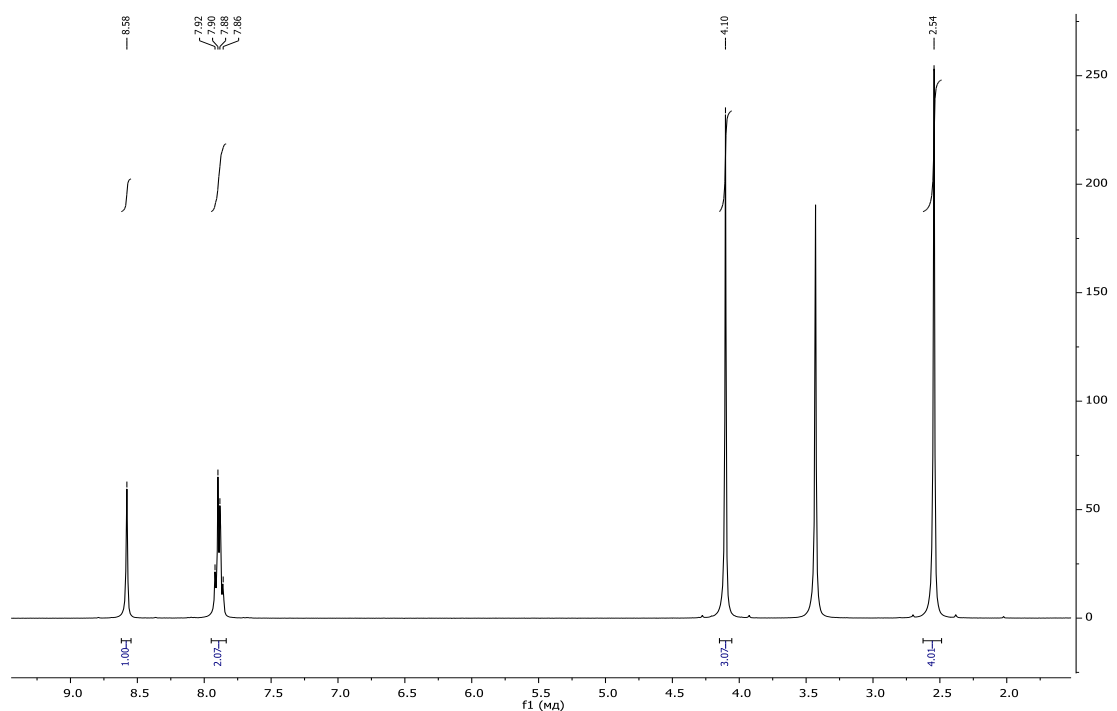


Fig. 28. ^1H NMR spectrum of Compound 6

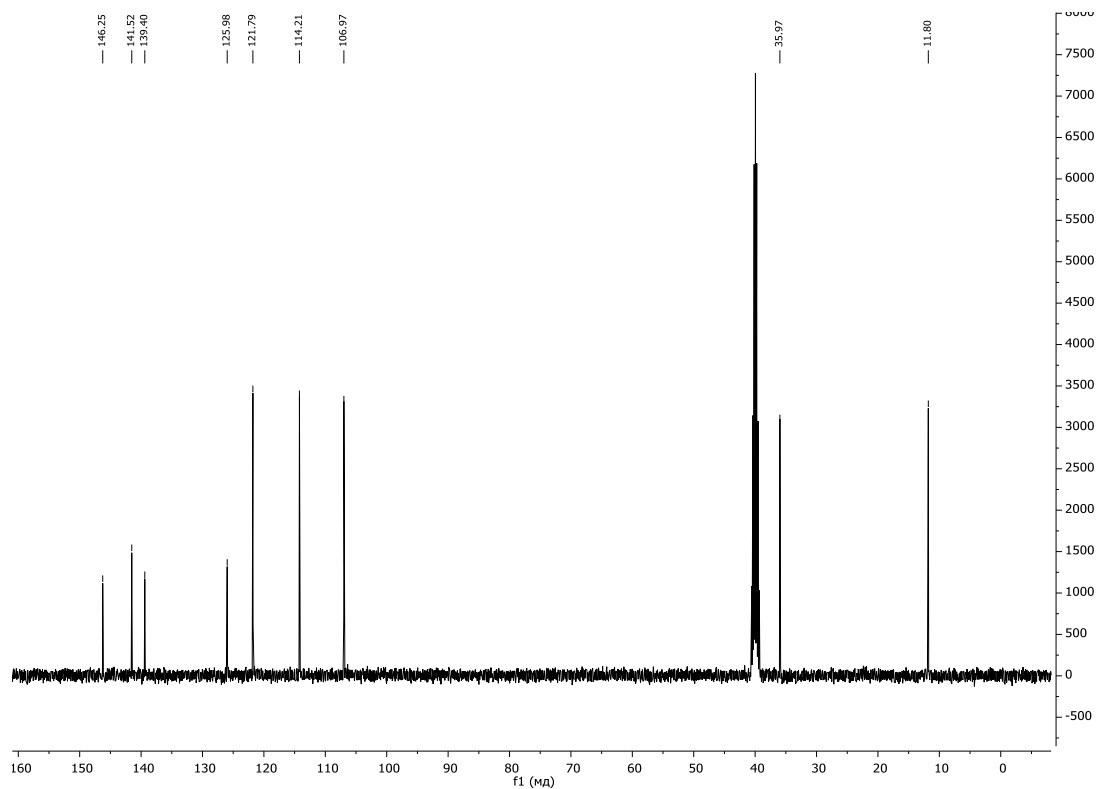


Fig. 29. ^{13}C NMR spectrum of Compound 6

Compound $\text{K}[8,8'-(\text{MeO})_2-3,3'-\text{Fe}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ (K[7])

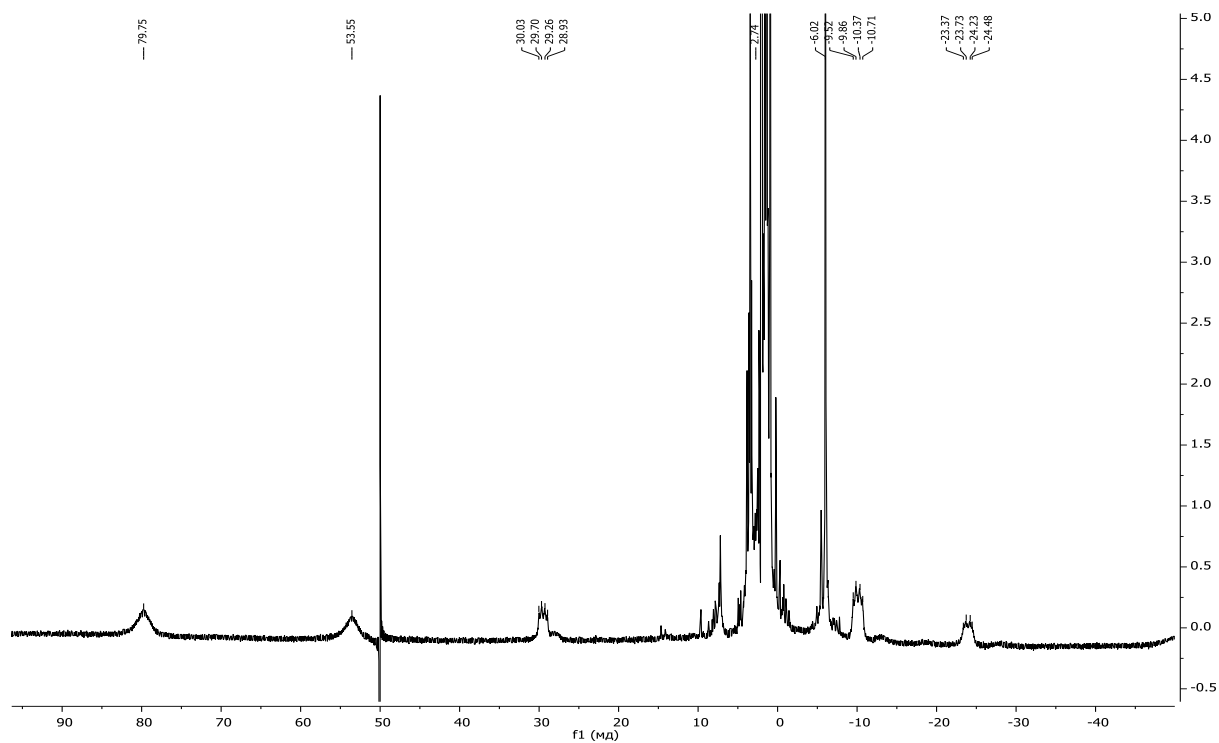


Fig. 30. ^1H NMR spectrum of $\text{K}[8,8'-(\text{MeO})_2-3,3'-\text{Fe}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ (K[7])

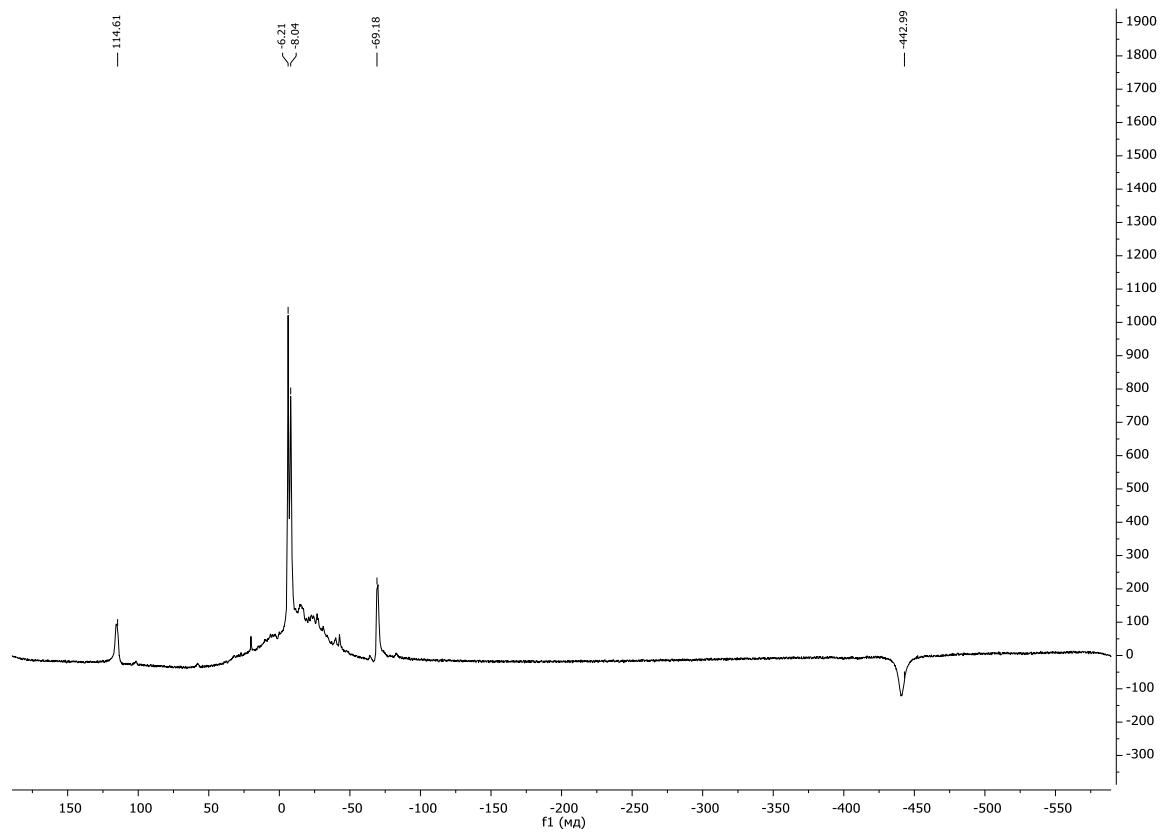


Fig. 31. ^{11}B NMR spectrum of $\text{K}[8,8'-(\text{MeO})_2-3,3'-\text{Fe}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ (**K[7]**)

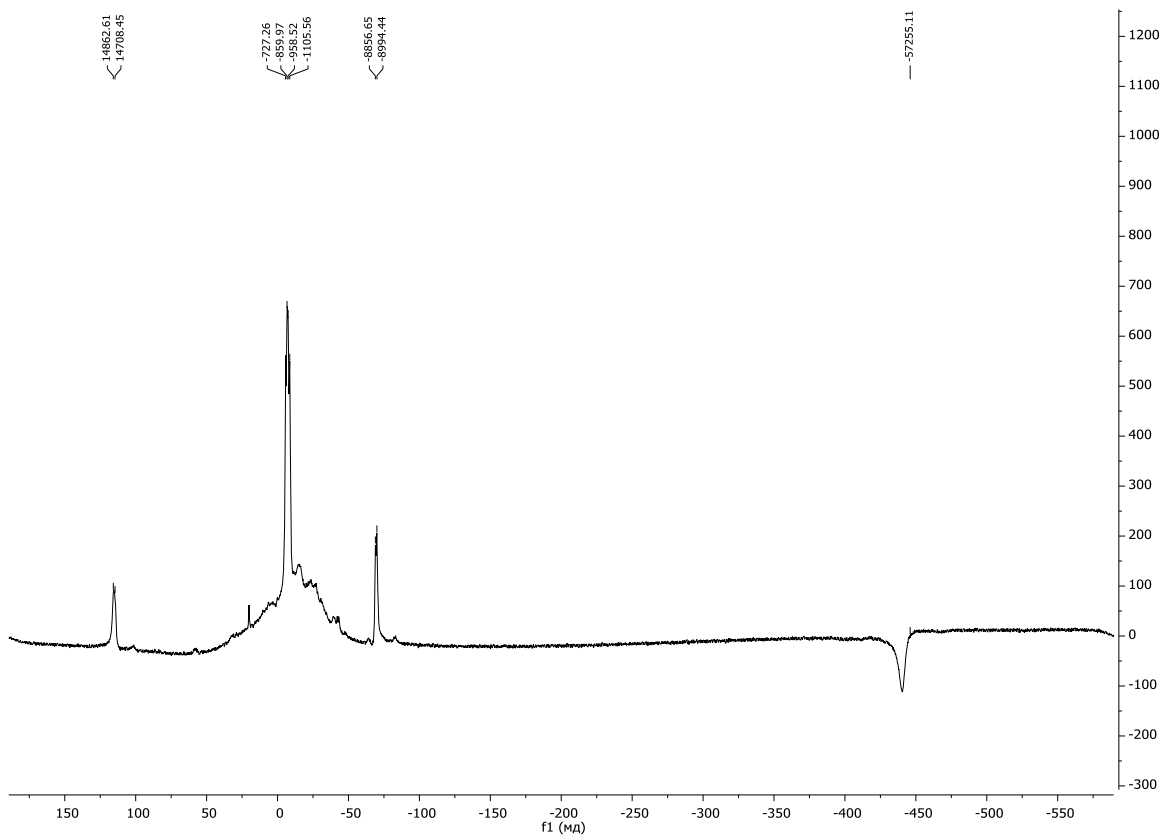


Fig. 32. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $\text{K}[8,8'-(\text{MeO})_2-3,3'-\text{Fe}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ (**K[7]**)

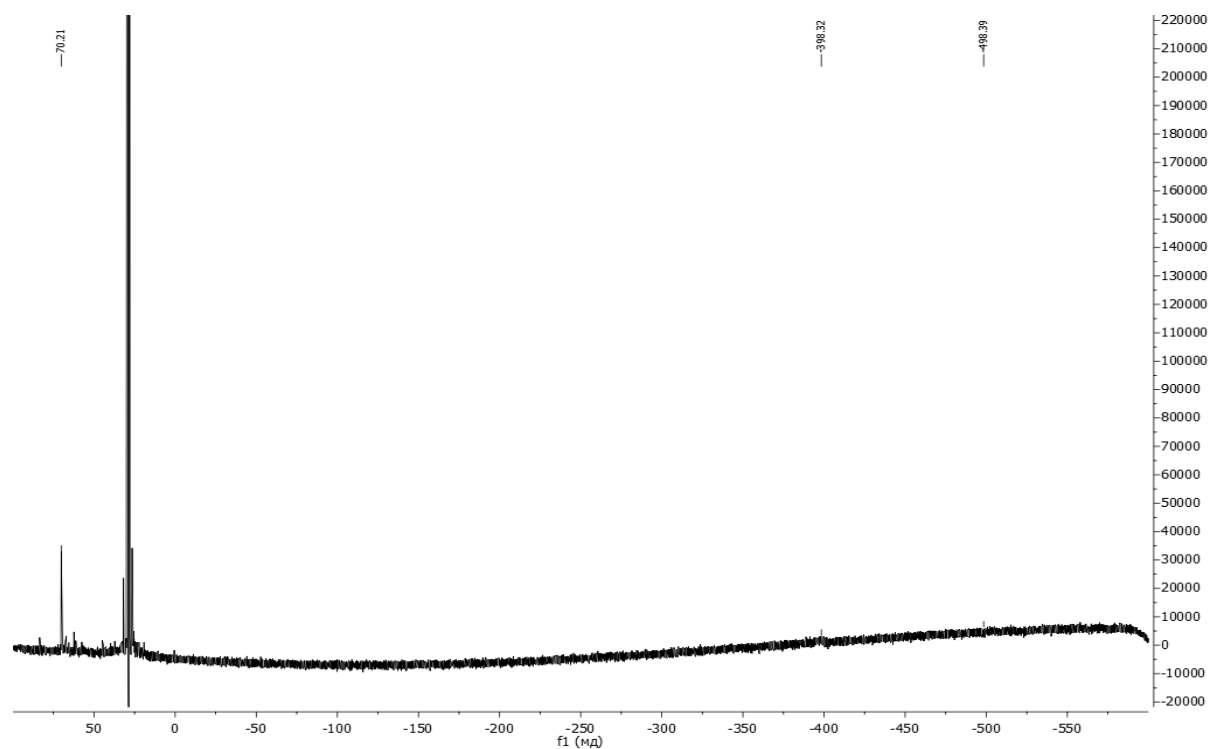


Fig. 33. ^{13}C NMR spectrum of $\text{K}[8,8'-(\text{MeO})_2-3,3'-\text{Fe}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ (K[7])

Compound $(\text{Bu}_4\text{N})[4,7'-(\text{MeO})_2-3,3'-\text{Fe}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ ((Bu₄N)[8])

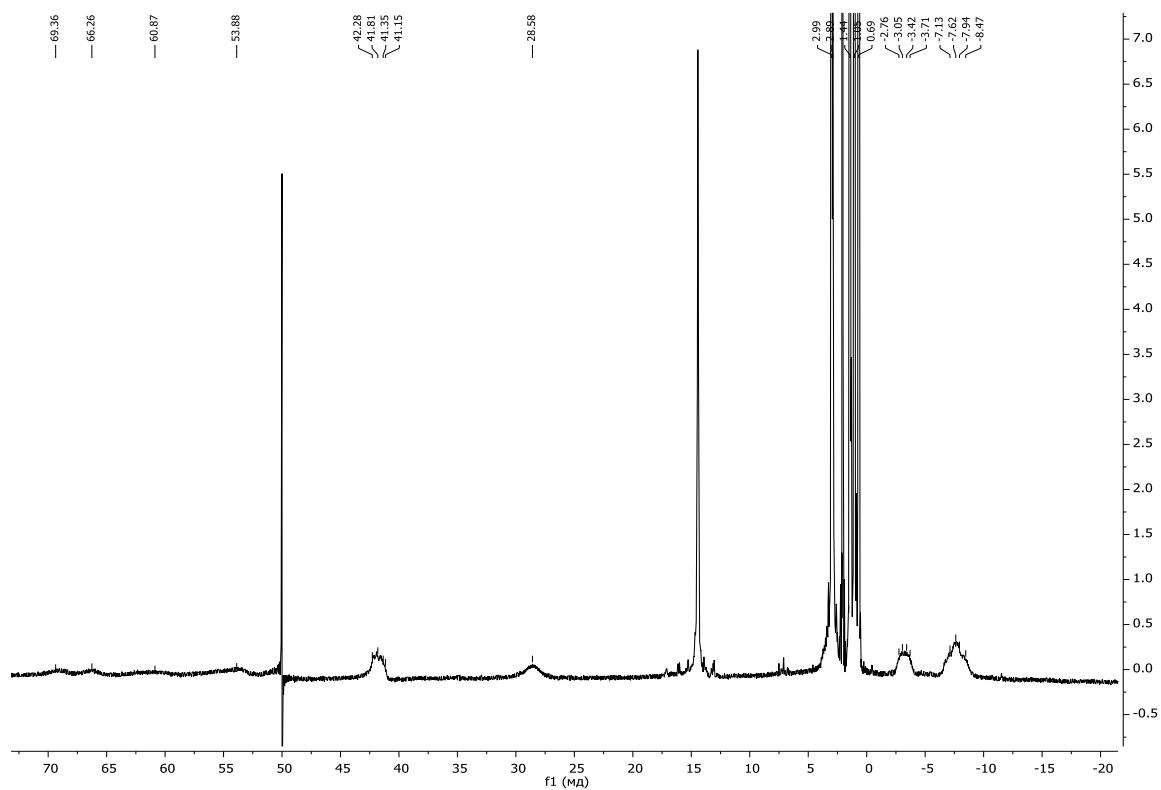


Fig. 34. ^1H NMR spectrum of $(\text{Bu}_4\text{N})[4,7'-(\text{MeO})_2-3,3'-\text{Fe}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ ((Bu₄N)[8])

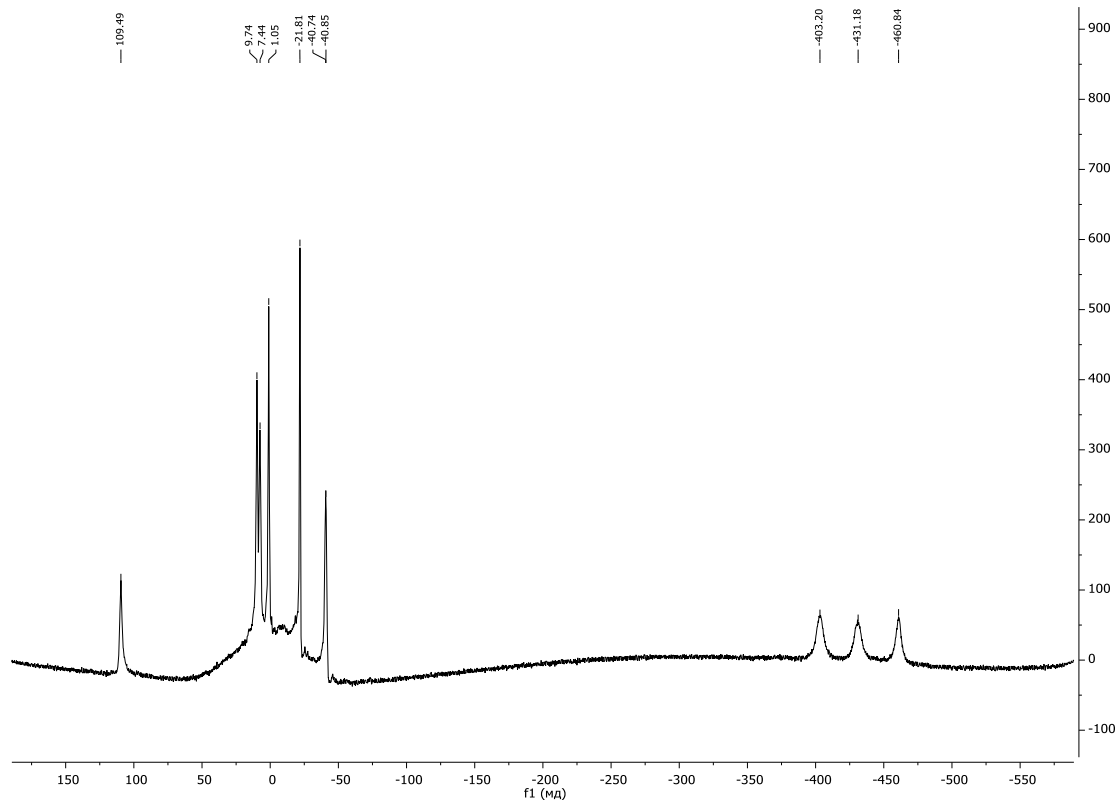


Fig. 35. ^{11}B NMR spectrum of $(\text{Bu}_4\text{N})[4,7'-(\text{MeO})_2-3,3'-\text{Fe}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ ($(\text{Bu}_4\text{N})[8]$)

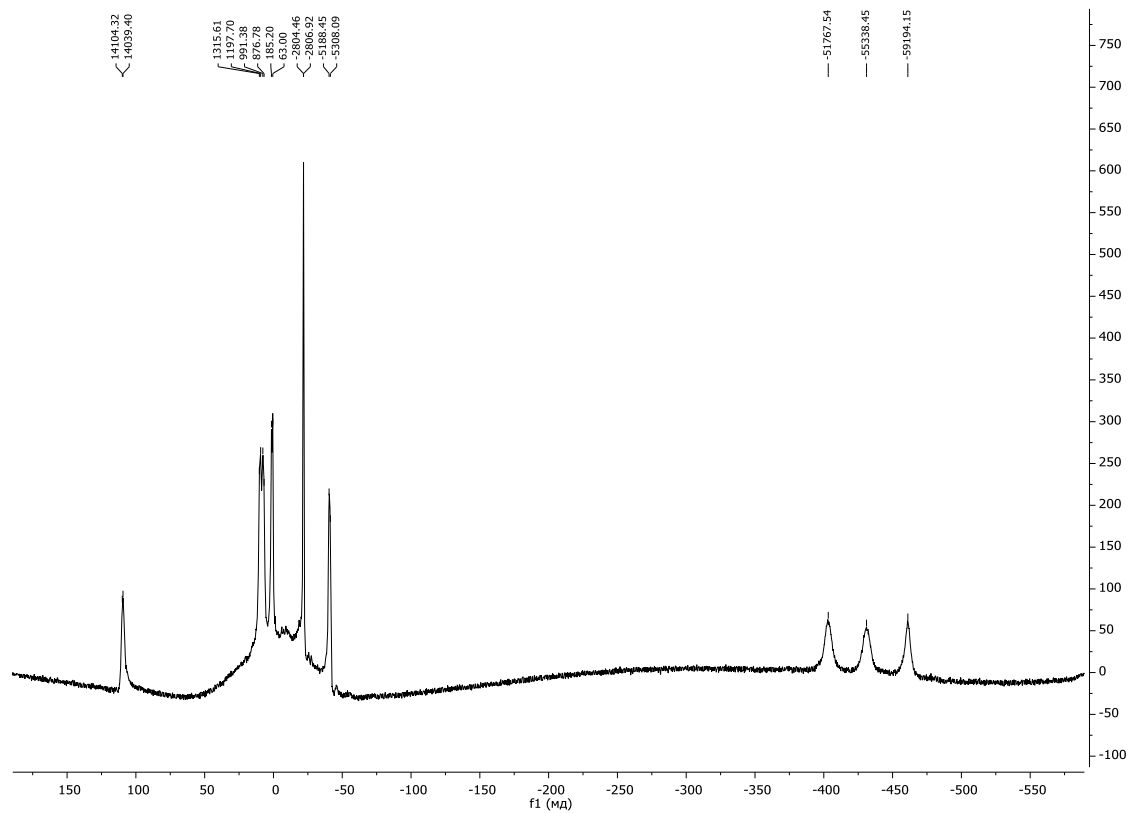


Fig. 36. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $(\text{Bu}_4\text{N})[4,7'-(\text{MeO})_2-3,3'-\text{Fe}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ ($(\text{Bu}_4\text{N})[8]$)

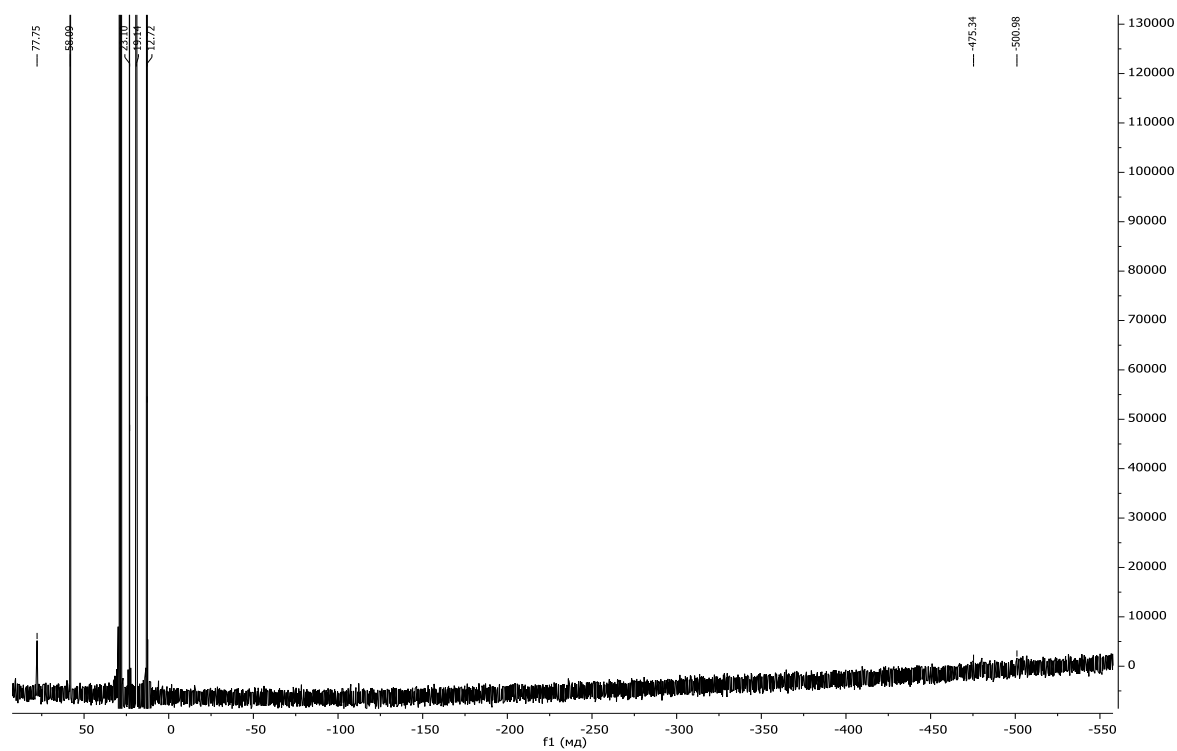


Fig. 37. ^{13}C NMR spectrum of $(\text{Bu}_4\text{N})[4,7'-(\text{MeO})_2-3,3'-\text{Fe}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ ($(\text{Bu}_4\text{N})[8]$)

Compound $(\text{Bu}_4\text{N})[4,7'-(\text{MeO})_2-3,3'-\text{Co}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ ($(\text{Bu}_4\text{N})[9]$)

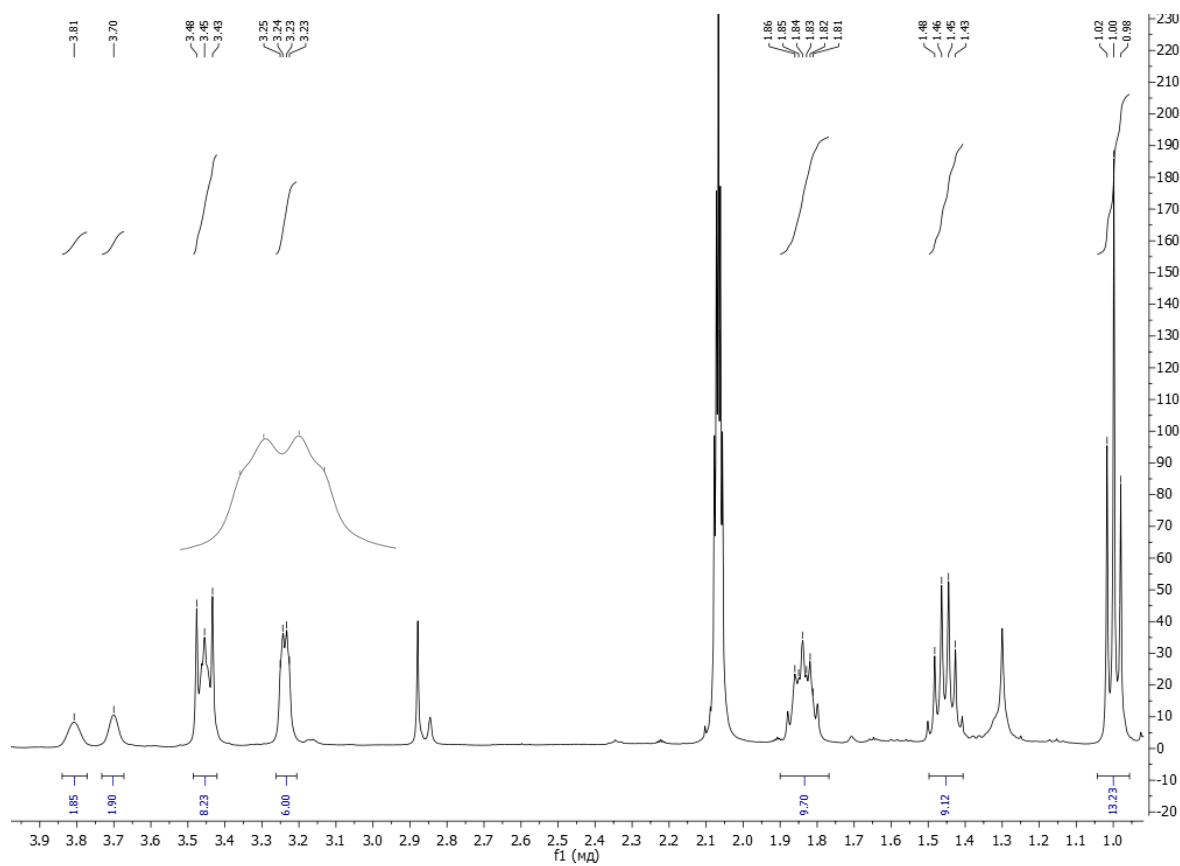


Fig. 38. ^1H NMR spectrum of $(\text{Bu}_4\text{N})[4,7'-(\text{MeO})_2-3,3'-\text{Co}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ ($(\text{Bu}_4\text{N})[9]$)

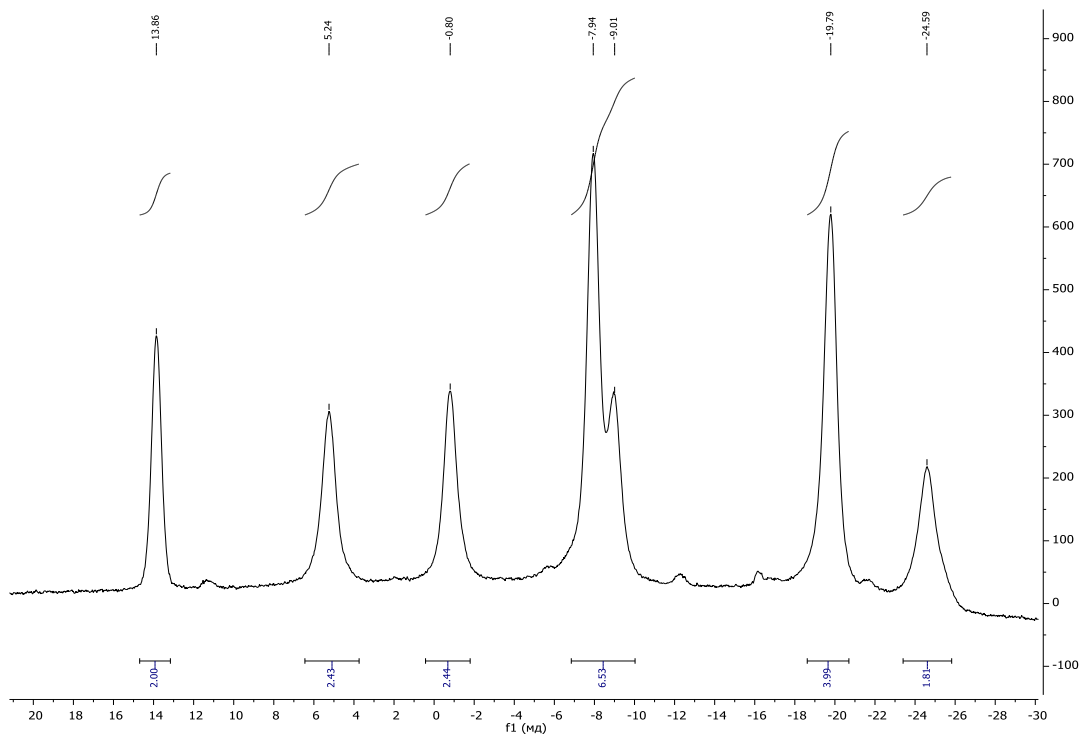


Fig. 39. ^{11}B NMR spectrum of $(\text{Bu}_4\text{N})[4,7'-(\text{MeO})_2-3,3'-\text{Co}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ ($(\text{Bu}_4\text{N})[9]$)

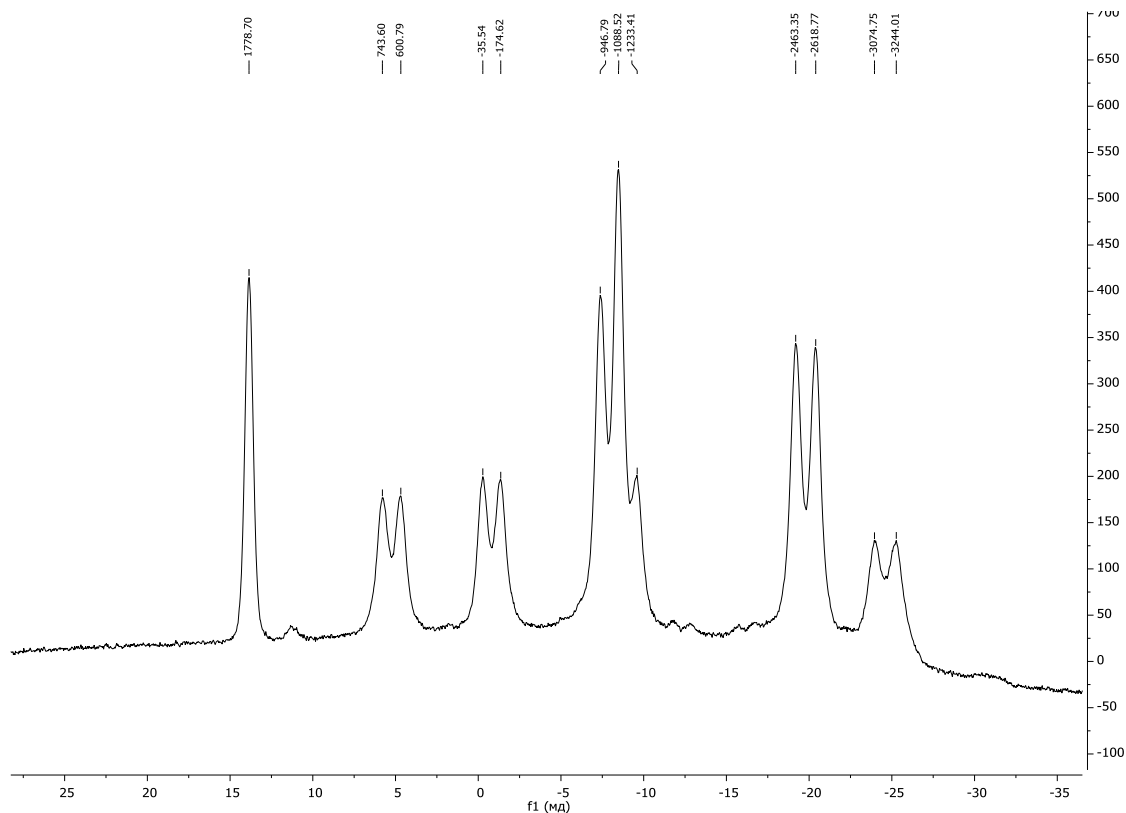


Fig. 40. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of $(\text{Bu}_4\text{N})[4,7'-(\text{MeO})_2-3,3'-\text{Co}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ ($(\text{Bu}_4\text{N})[9]$)

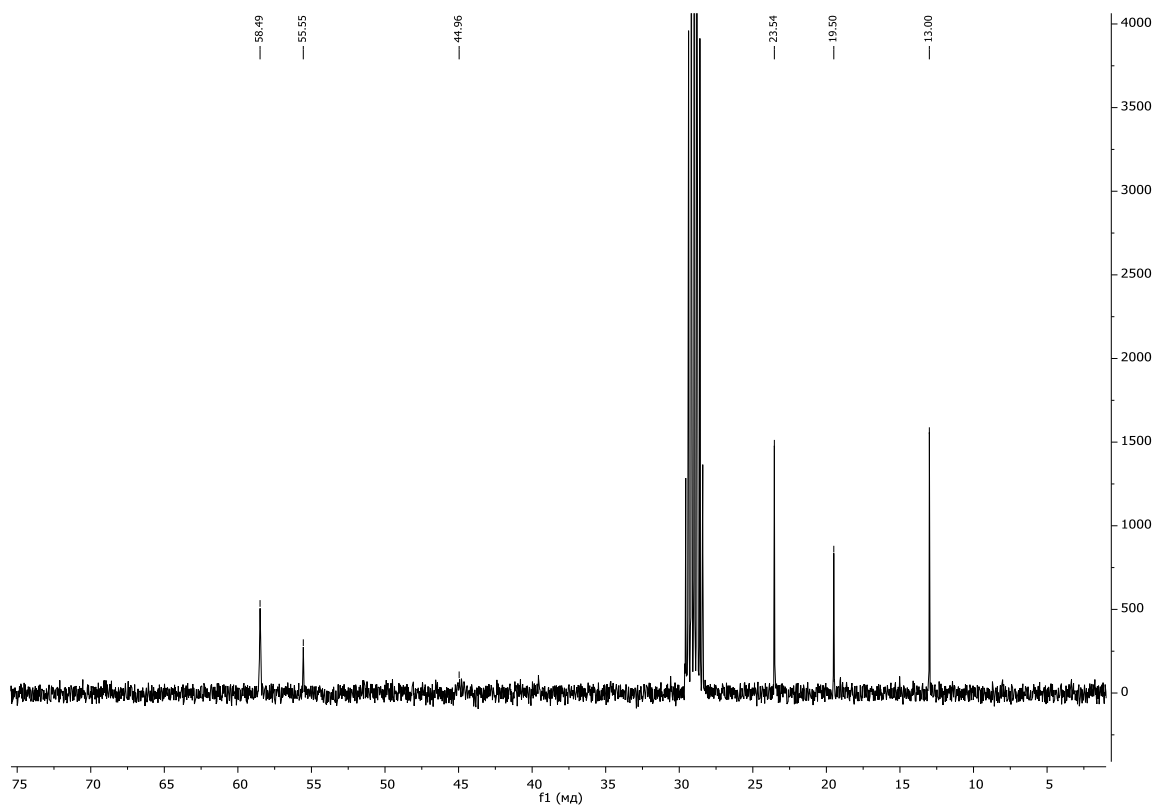


Fig. 41. ^{13}C NMR spectrum of $(\text{Bu}_4\text{N})[4,7'-(\text{MeO})_2-3,3'-\text{Co}(1,2-\text{C}_2\text{B}_9\text{H}_{10})_2]$ ($(\text{Bu}_4\text{N})[9]$)