

## Synthesis and Crystal Structures of Nickel(II) and Palladium(II) Complexes with *o*-Carboranyl Amidine Ligands

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**Spectral data for 10-EtC(NHCH<sub>2</sub>CH<sub>2</sub>OMe)=HN-7,8-C<sub>2</sub>B<sub>9</sub>H<sub>11</sub> (**1a**, **1b**).**

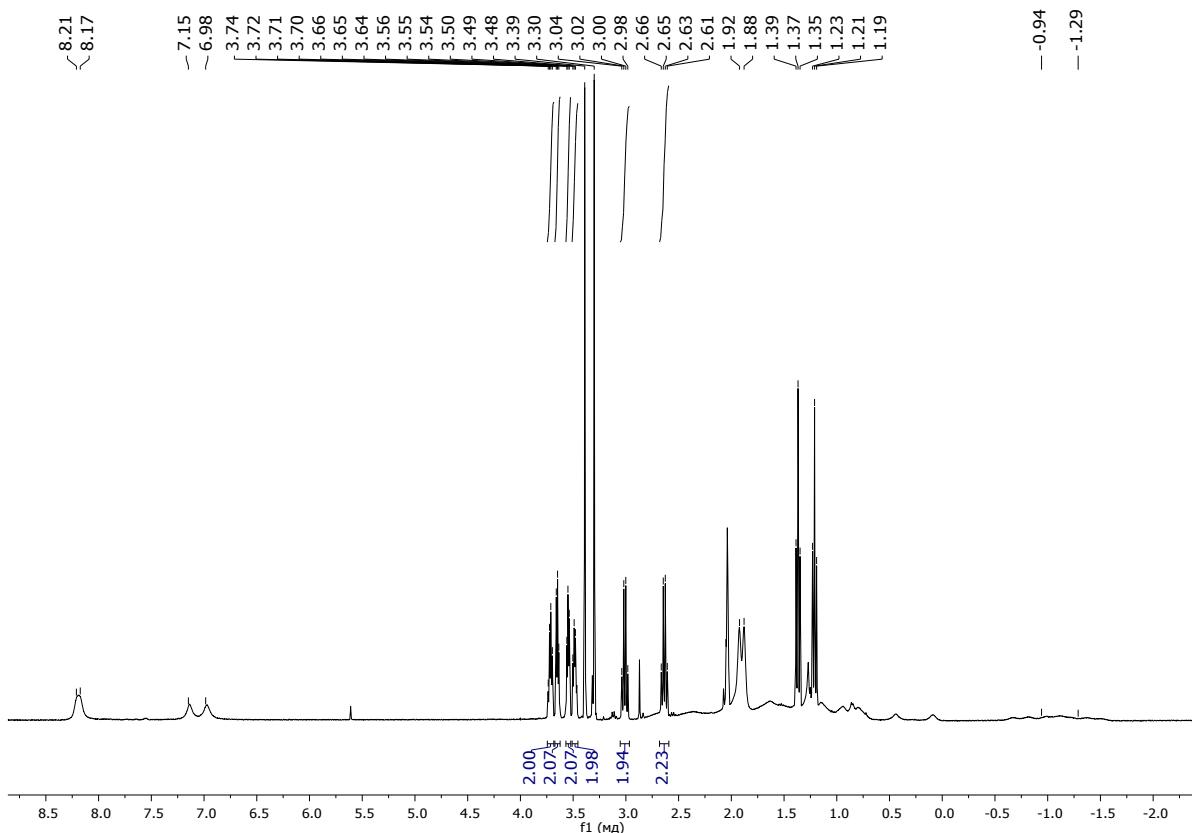


Fig. S1. <sup>1</sup>H NMR spectrum of compounds **1a** and **1b** (acetone-d<sub>6</sub>)

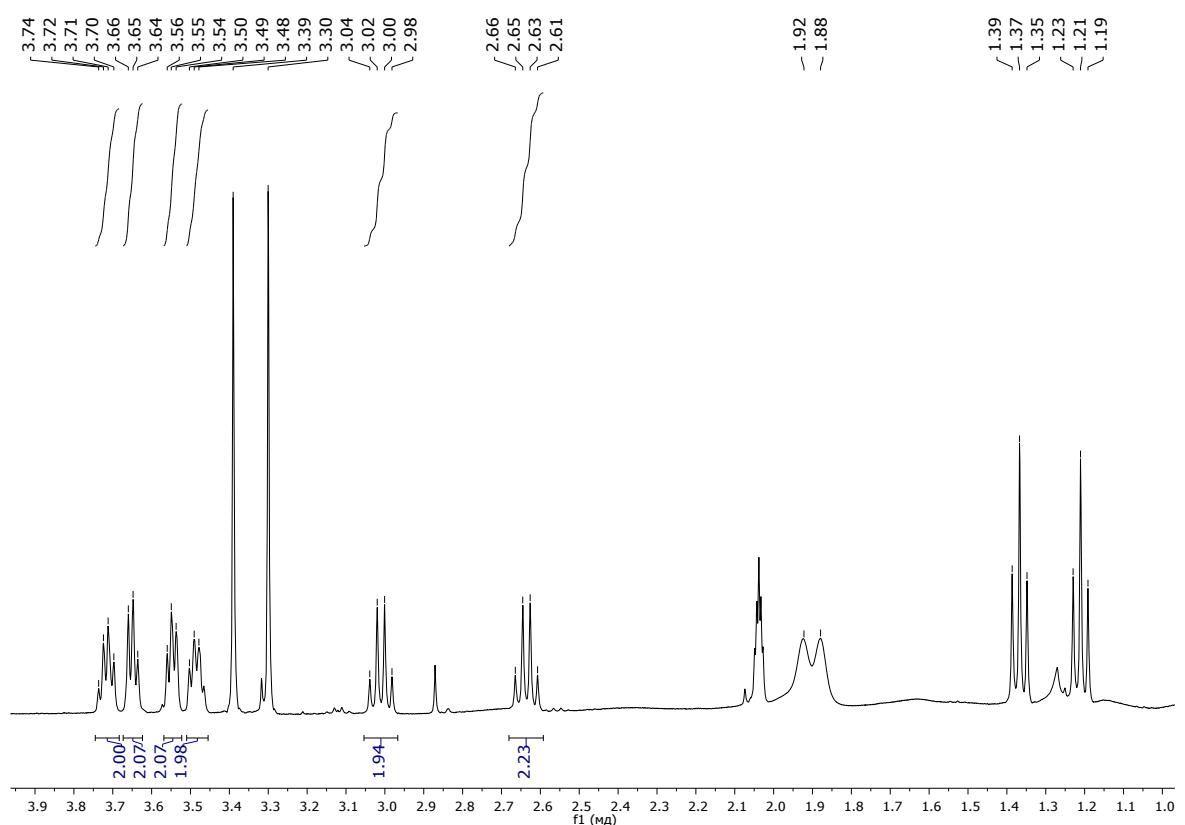


Fig. S2. The fragment of <sup>1</sup>H NMR spectrum of compounds **1a** and **1b** (acetone-d<sub>6</sub>)

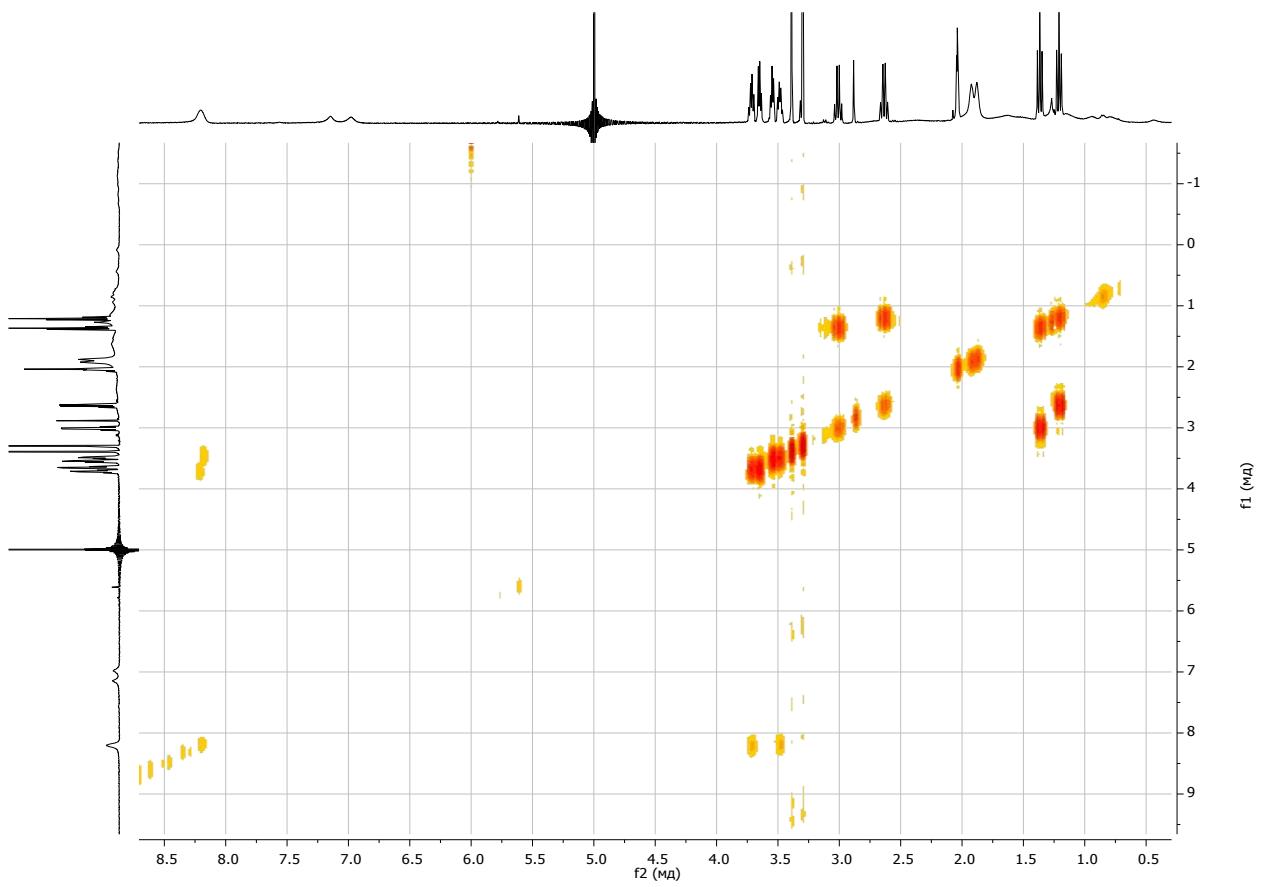


Fig. S3. (HH)gCOSY NMR spectrum of compounds **1a** and **1b** (acetone-d<sub>6</sub>)

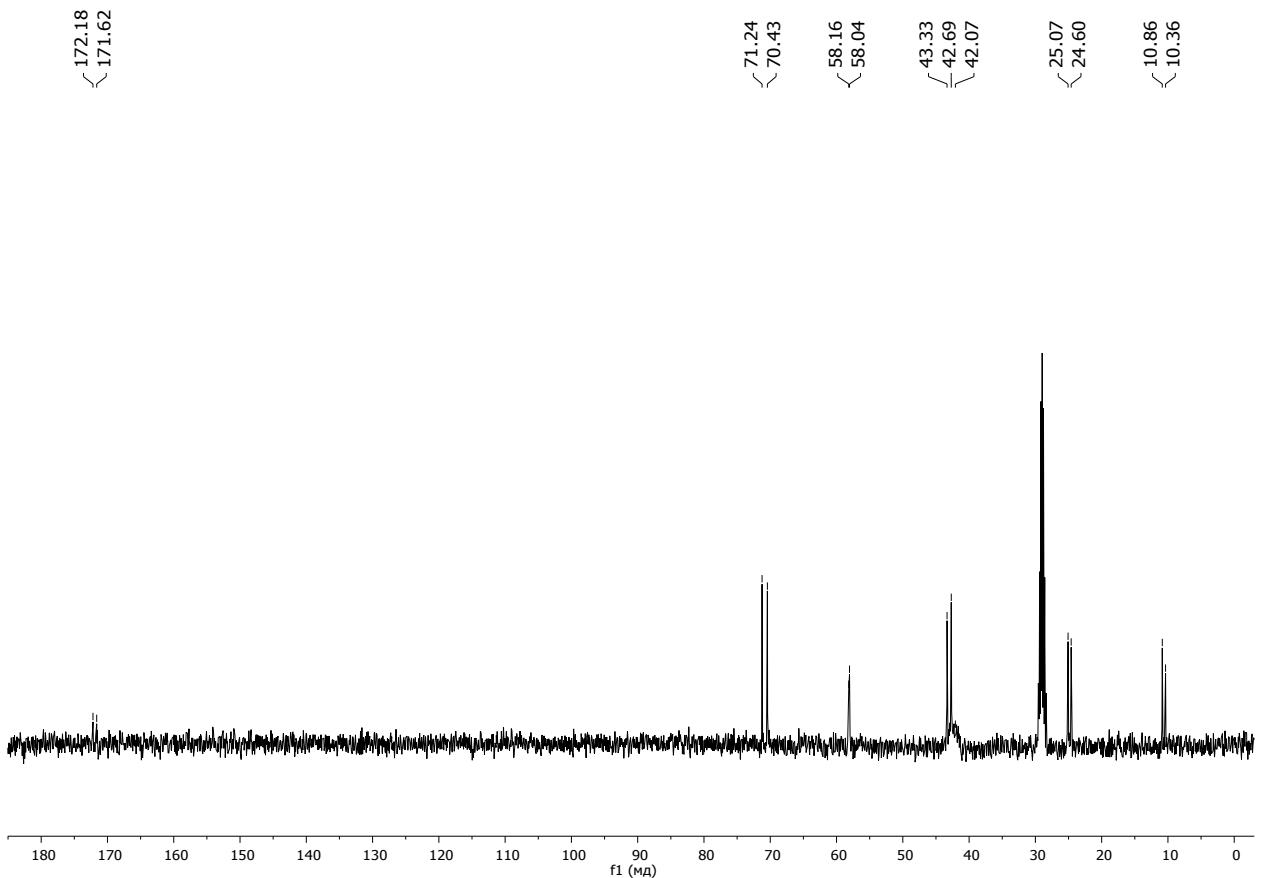


Fig. S4. <sup>13</sup>C NMR spectrum of compounds **1a** and **1b** (acetone-d<sub>6</sub>)

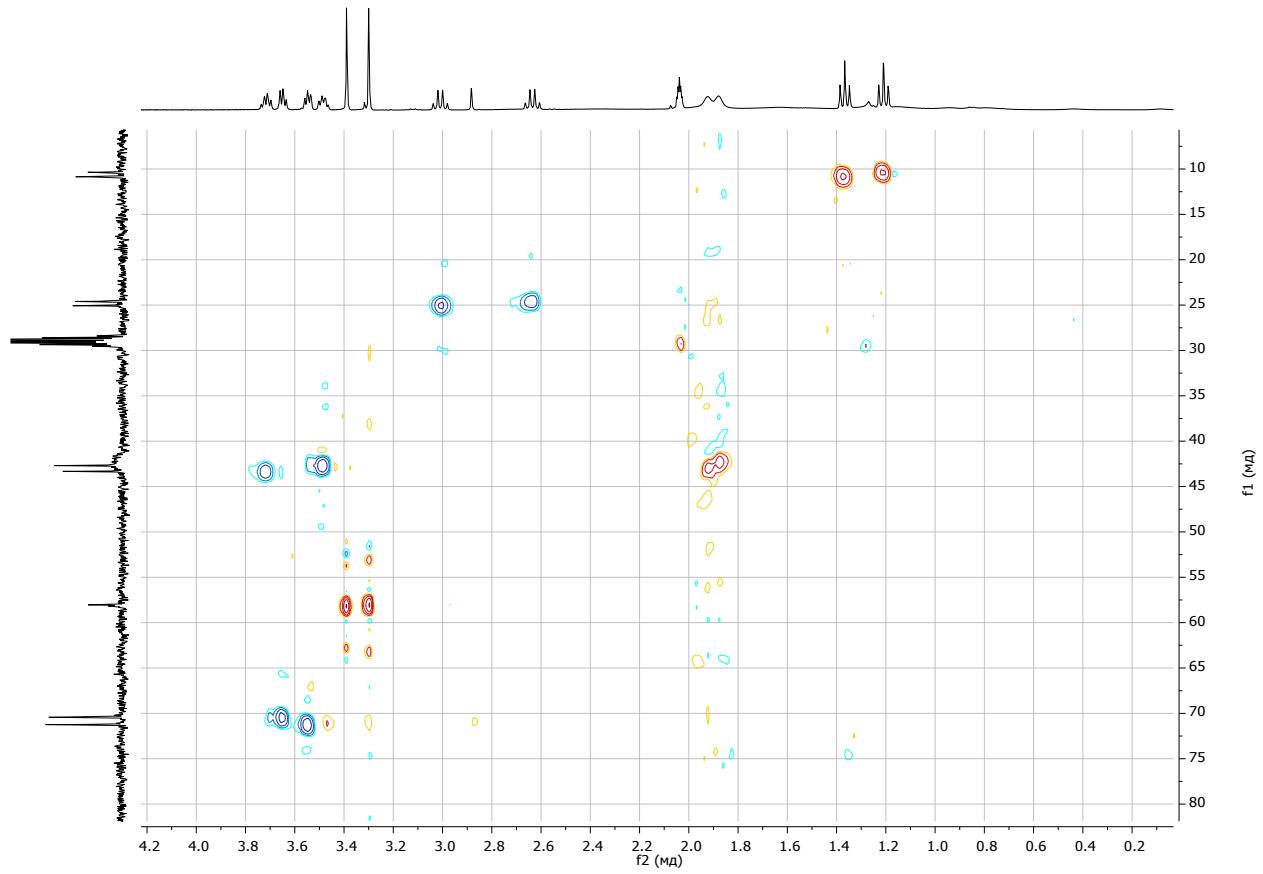


Fig. S5. (HC)HSQC NMR spectrum of compounds **1a** and **1b** (acetone-d<sub>6</sub>)

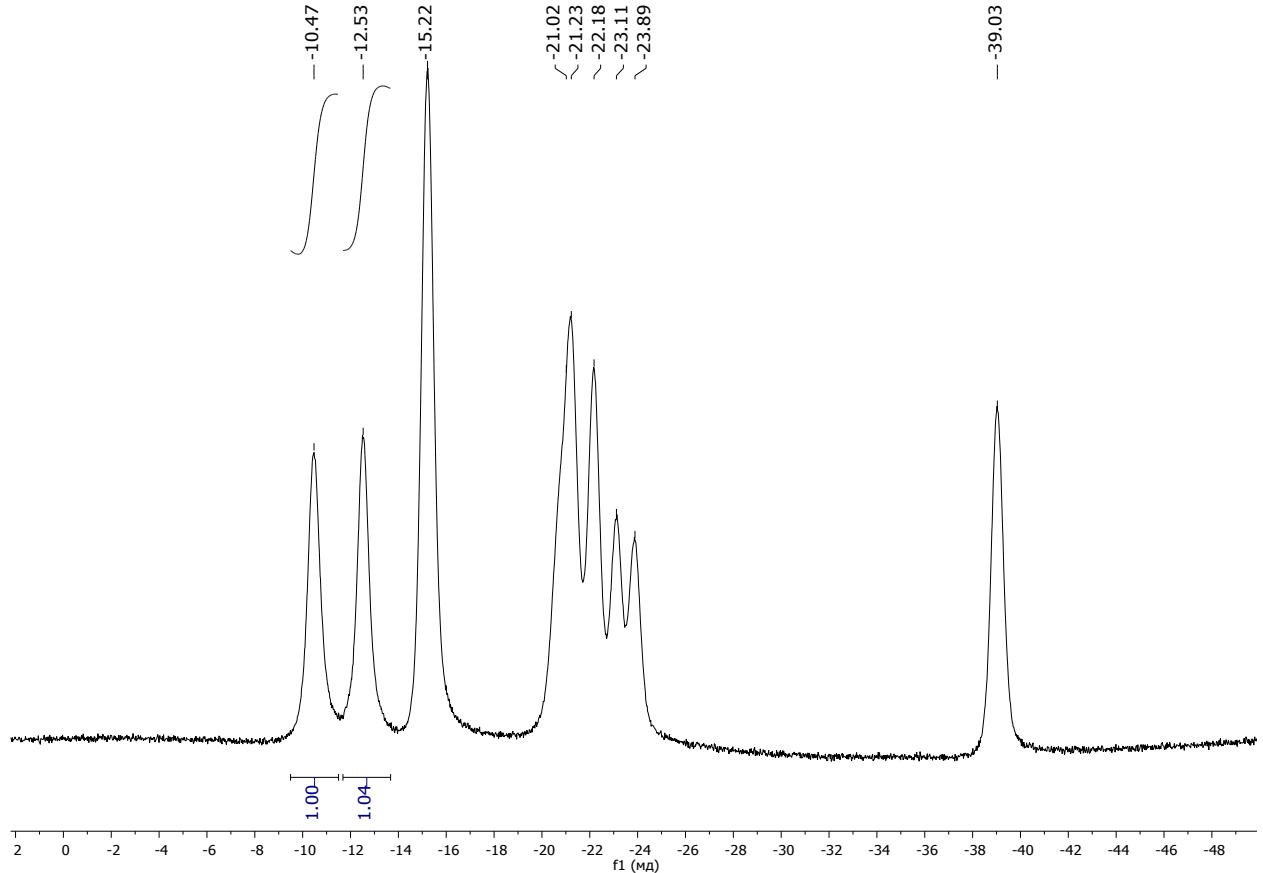


Fig. S6. <sup>11</sup>B{<sup>1</sup>H} NMR spectrum of compounds **1a** and **1b** (acetone-d<sub>6</sub>)

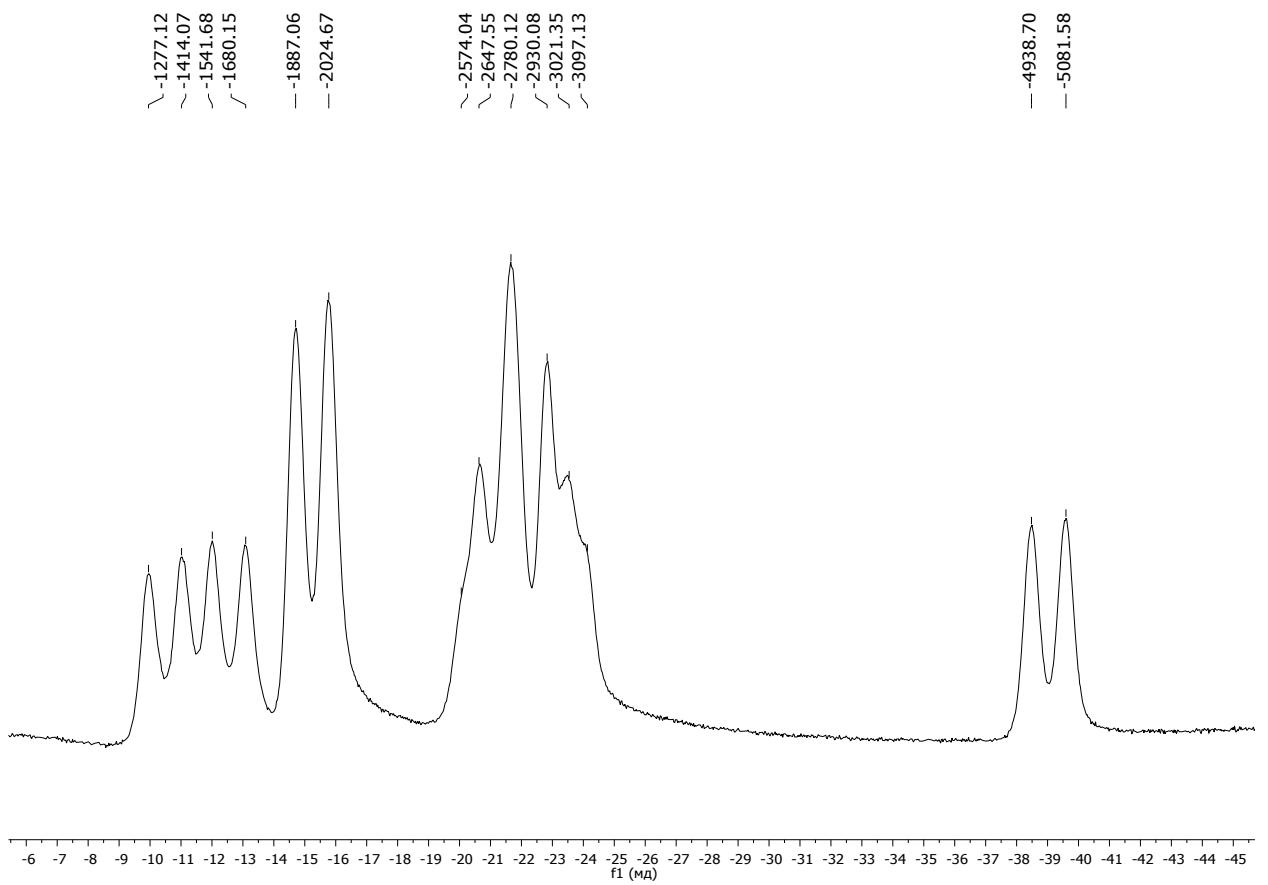


Fig. S7. <sup>11</sup>B NMR spectrum of compounds **1a** and **1b** (acetone-d<sub>6</sub>)

**Spectral data for 10-EtC(NHCH<sub>2</sub>CH<sub>2</sub>OH)=HN-7,8-C<sub>2</sub>B<sub>9</sub>H<sub>11</sub> (2a, 2b).**

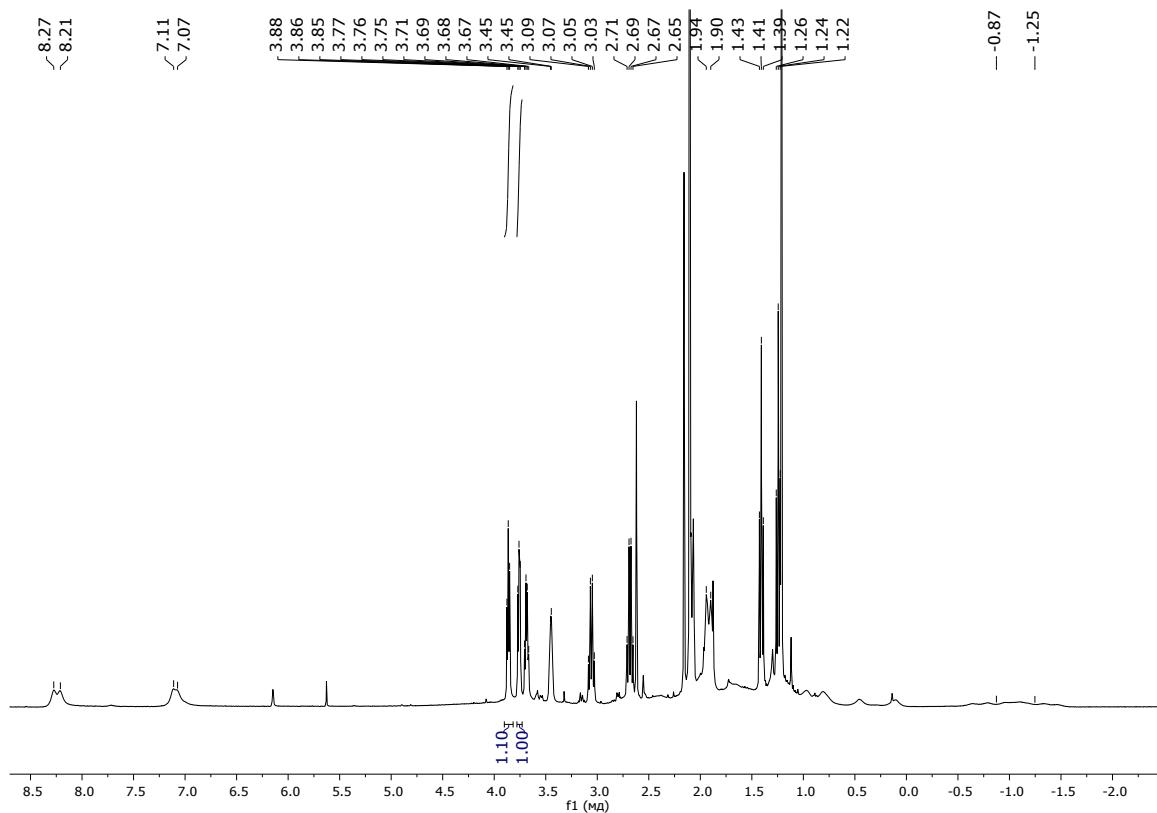


Fig. S8. <sup>1</sup>H NMR spectrum of compounds **2a** and **2b** (acetone-d<sub>6</sub>)

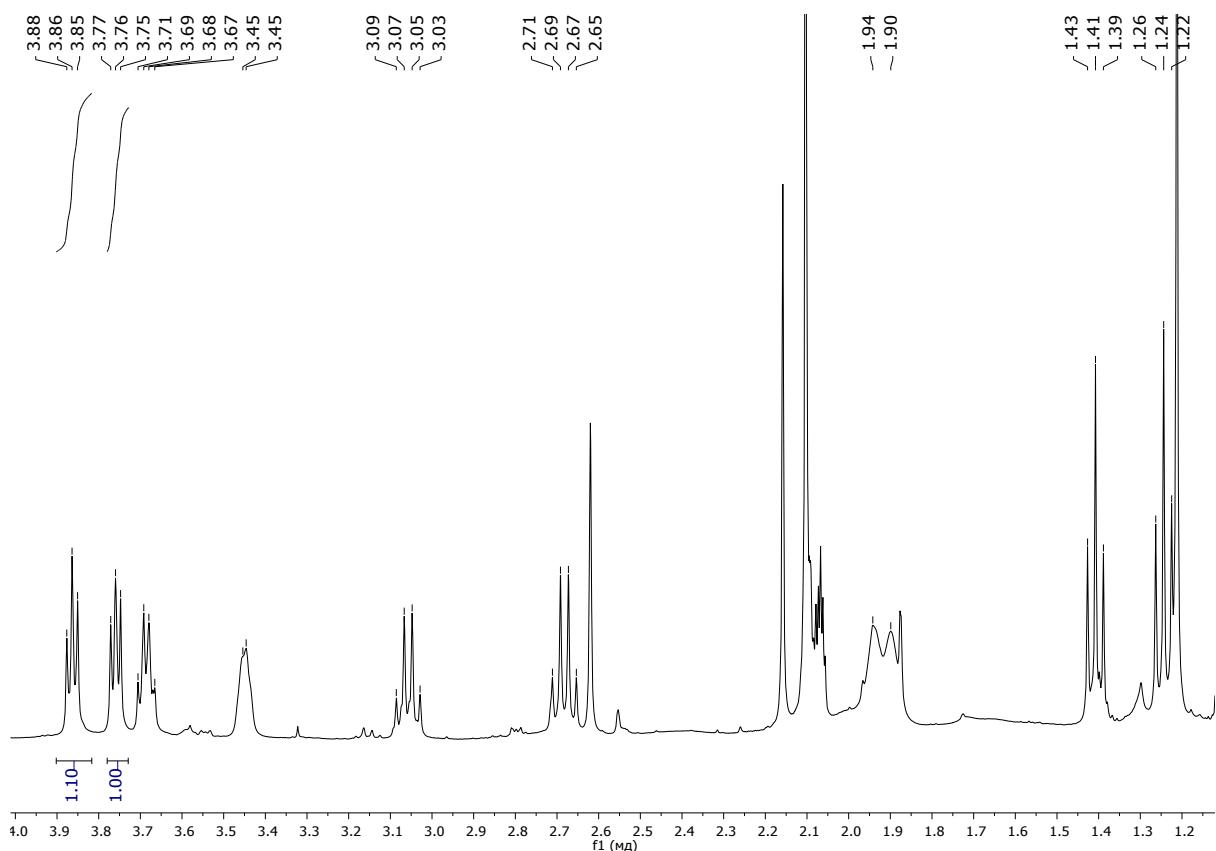


Fig. S9. The fragment of <sup>1</sup>H NMR spectrum of compounds **2a** and **2b** (acetone-d<sub>6</sub>)

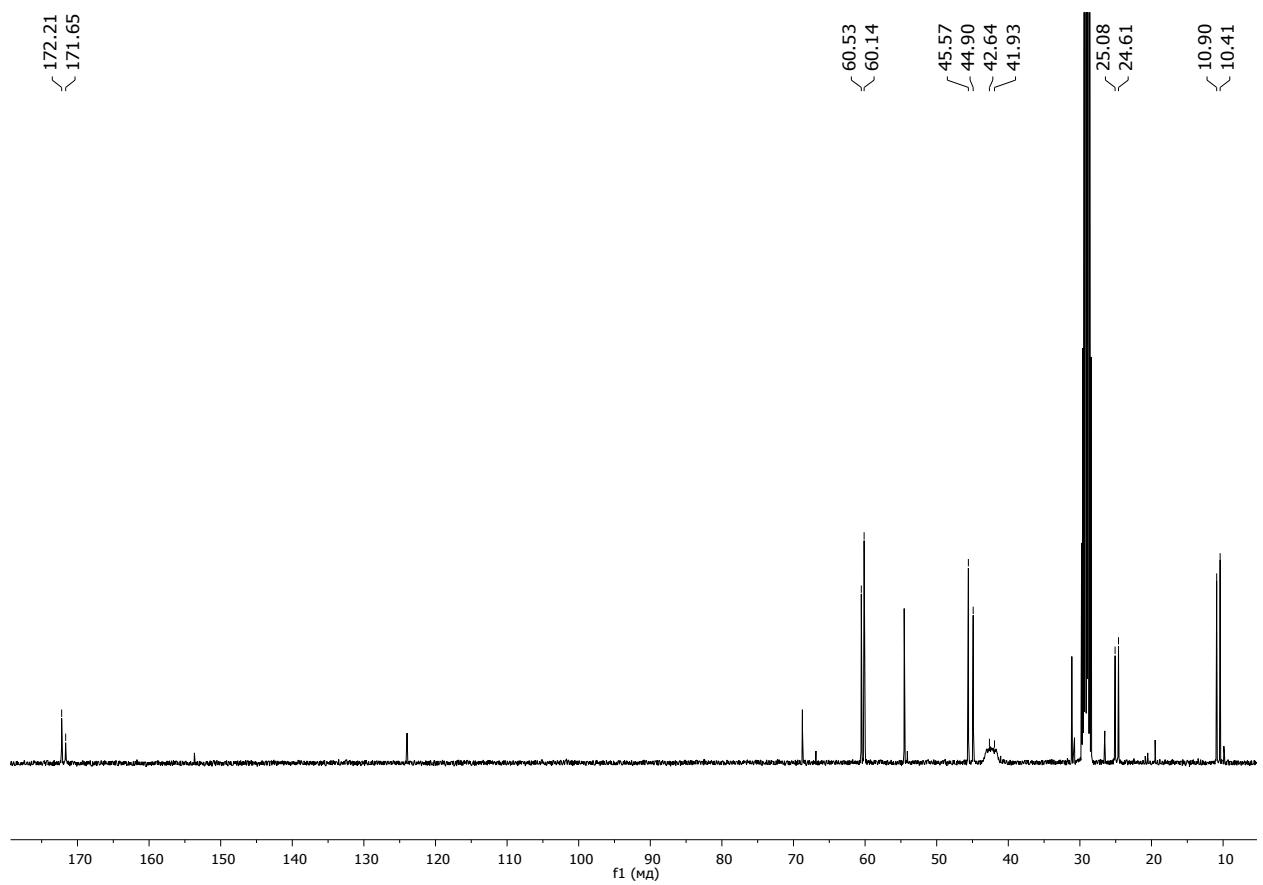


Fig. S10. <sup>13</sup>C NMR spectrum of compounds **2a** and **2b** (acetone-d<sub>6</sub>)

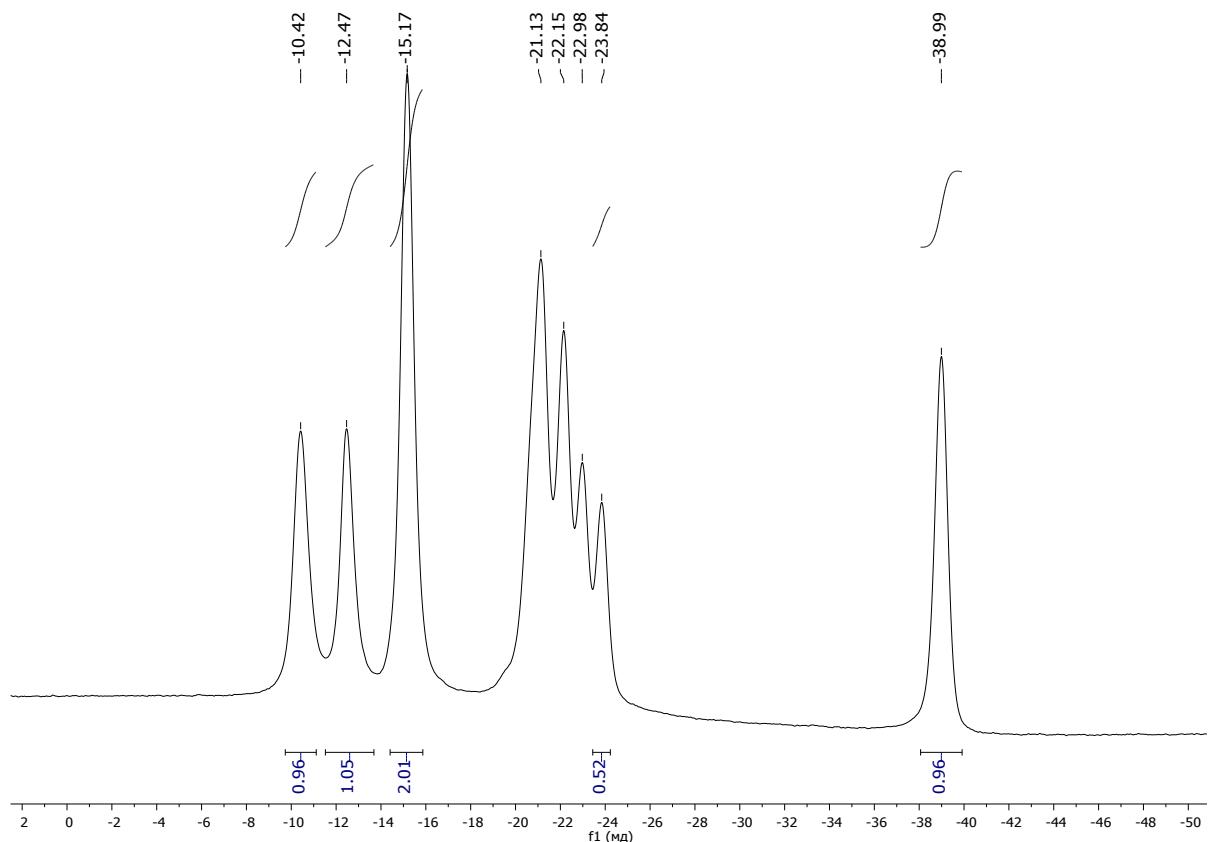


Fig. S11. <sup>11</sup>B{<sup>1</sup>H} NMR spectrum of compounds **2a** and **2b** (acetone-d<sub>6</sub>)

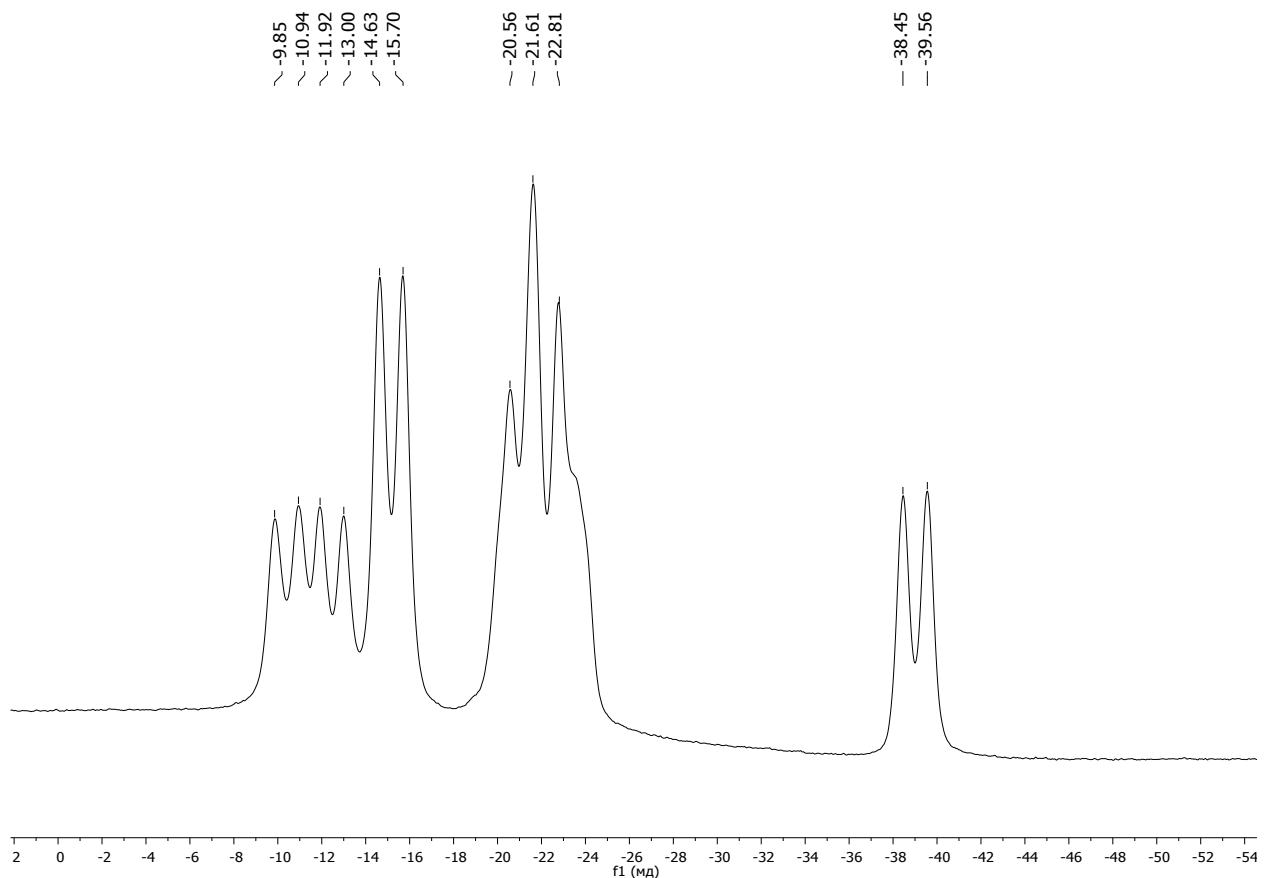


Fig. S12. <sup>11</sup>B NMR spectrum of compounds **2a** and **2b** (acetone-d<sub>6</sub>)

**Spectral data for 10-EtC(NHCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OH)=HN-7,8-C<sub>2</sub>B<sub>9</sub>H<sub>11</sub> (3a, 3b).**

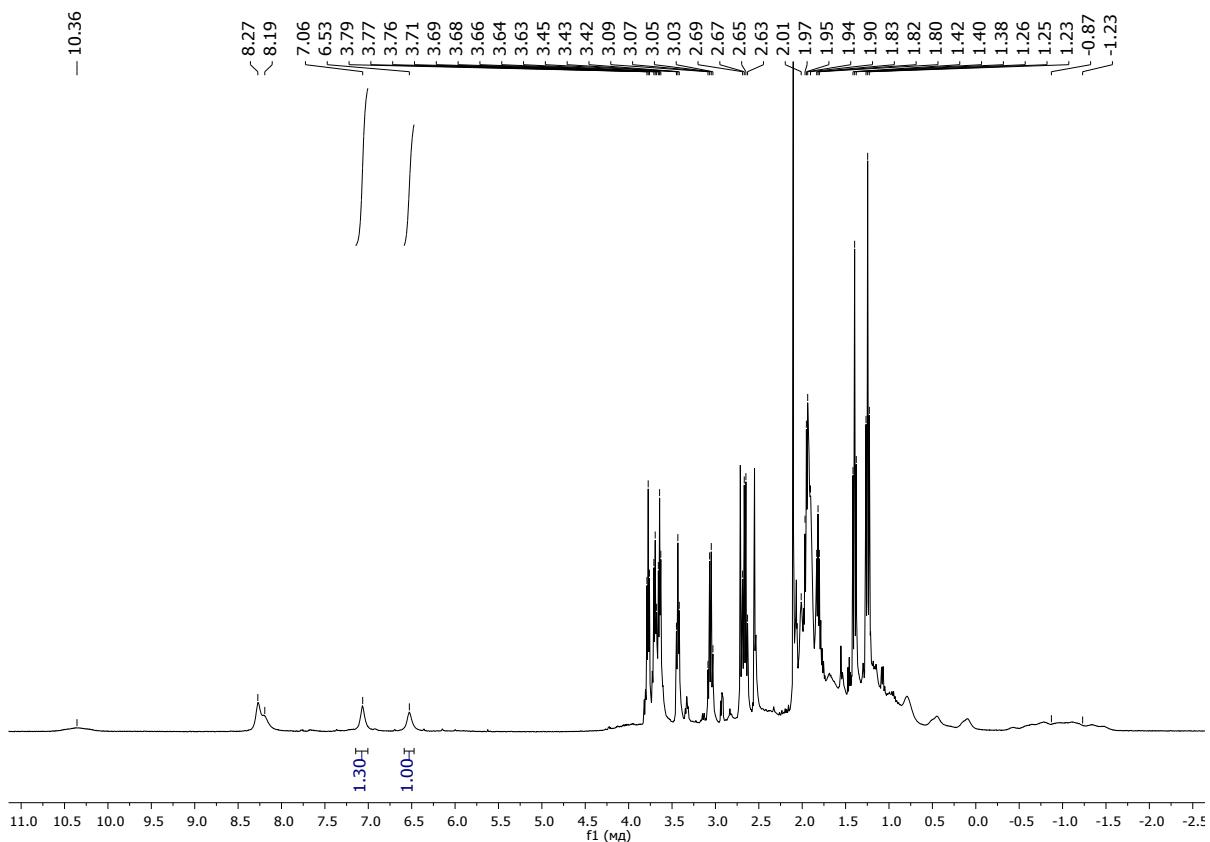


Fig. S13. <sup>1</sup>H NMR spectrum of compounds **3a** and **3b** (acetone-d<sub>6</sub>)

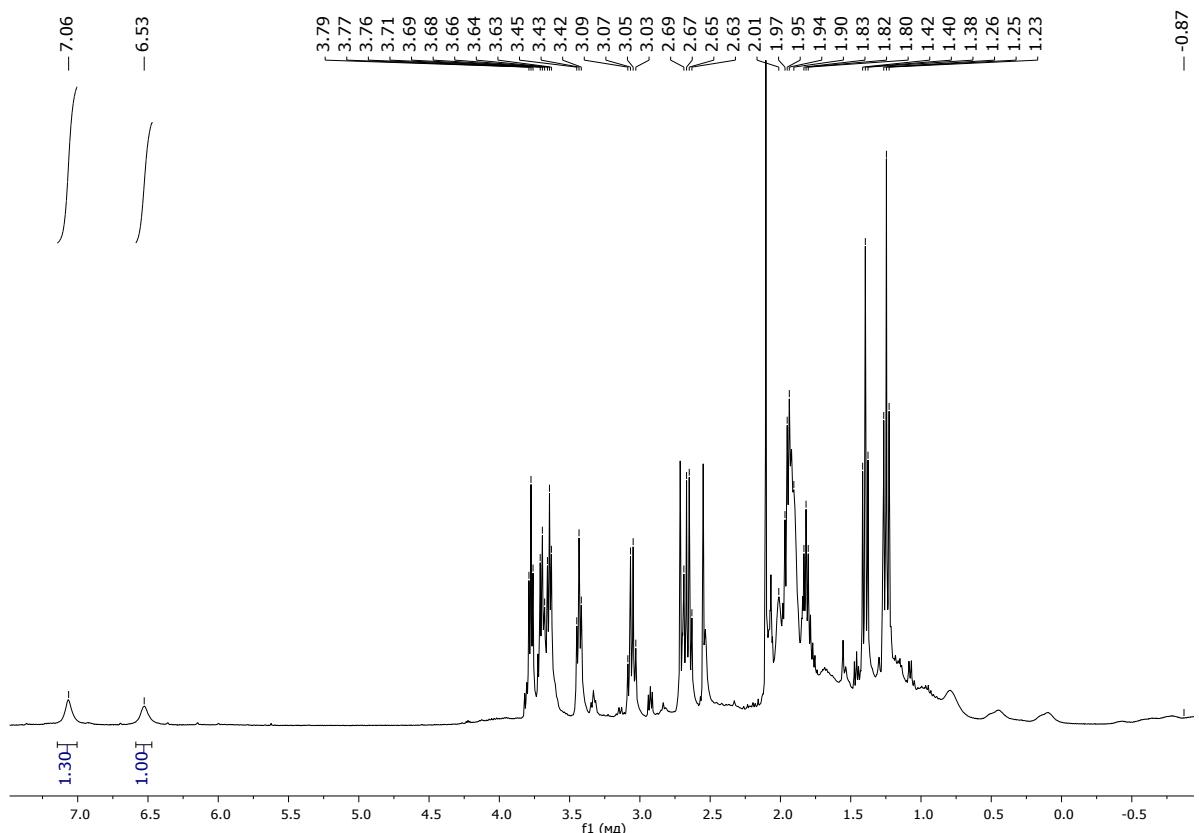


Fig. S14. The fragment of <sup>1</sup>H NMR spectrum of compounds **3a** and **3b** (acetone-d<sub>6</sub>)

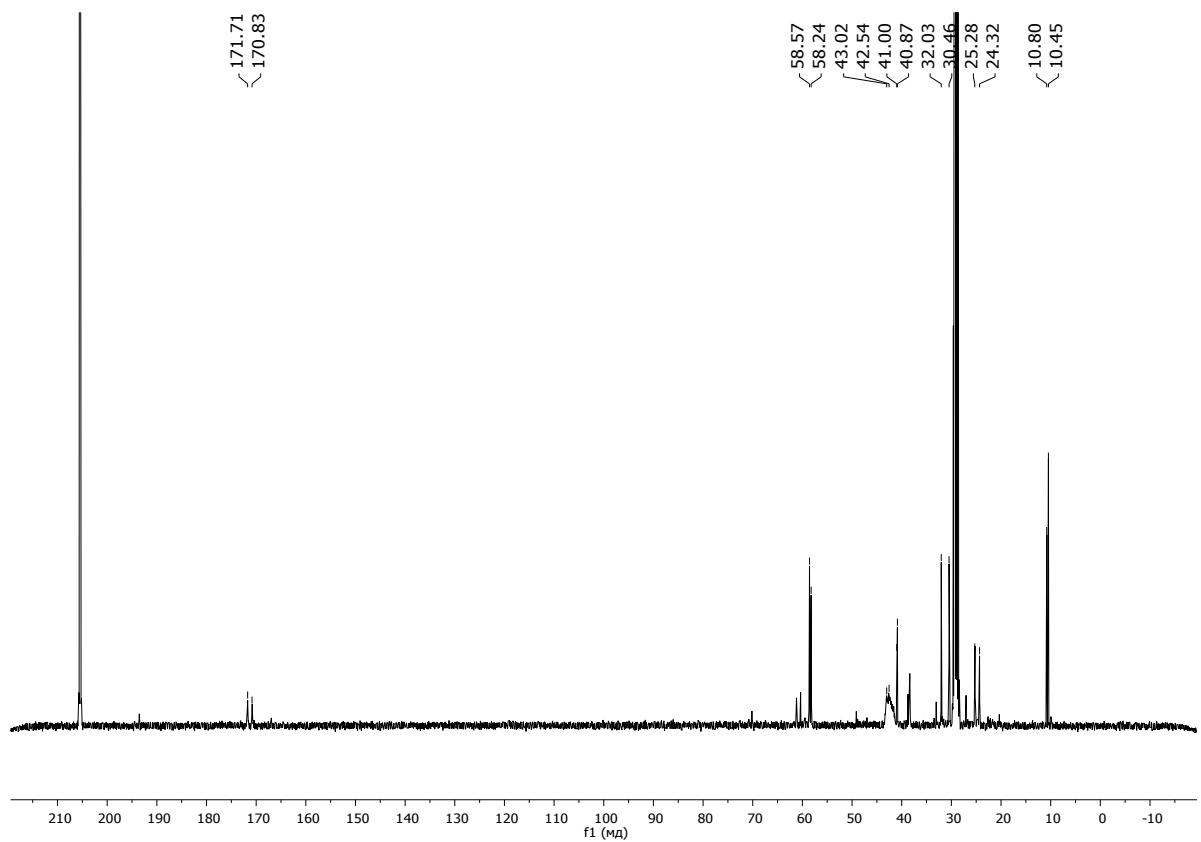


Fig. S15. <sup>13</sup>C NMR spectrum of compounds **3a** and **3b** (acetone-d<sub>6</sub>)

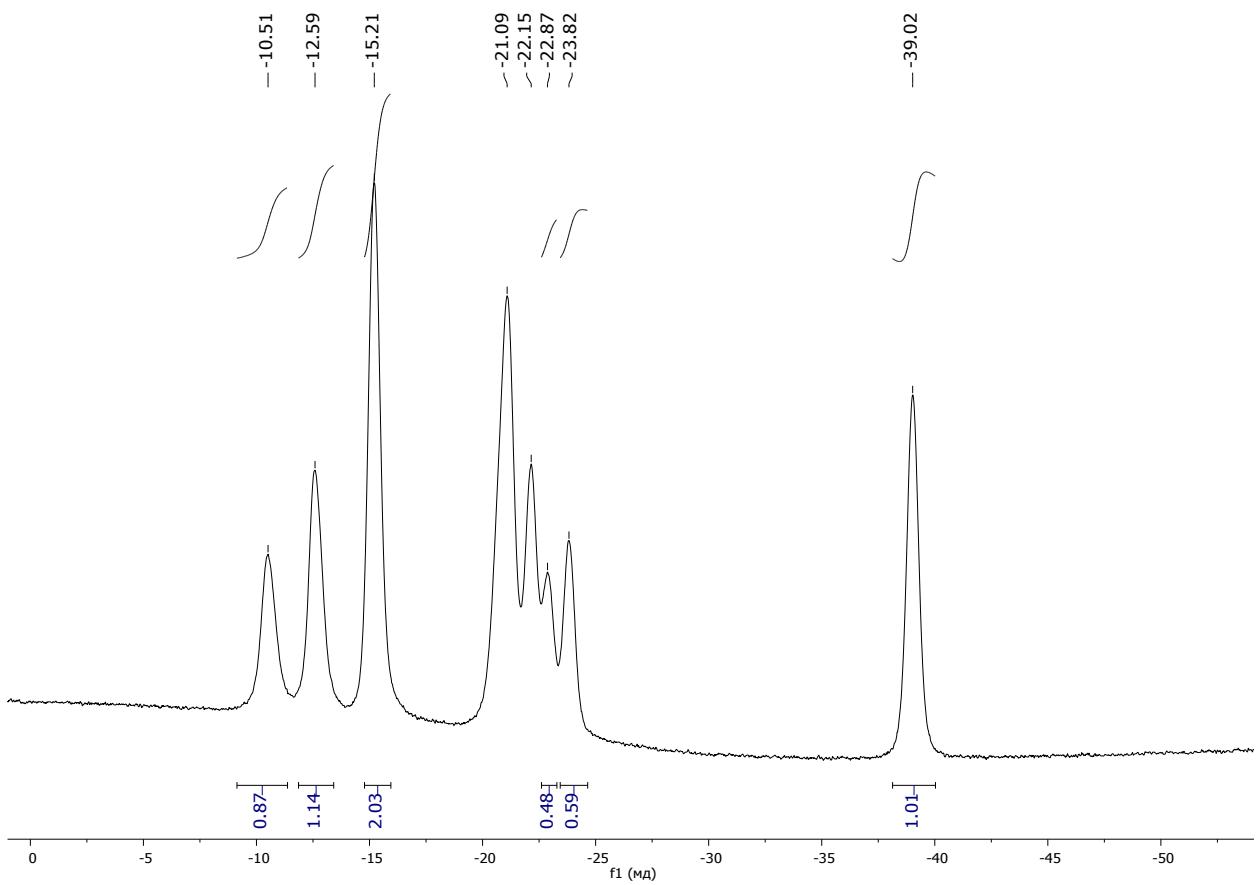


Fig. S16. <sup>11</sup>B{<sup>1</sup>H} NMR spectrum of compounds **3a** and **3b** (acetone-d<sub>6</sub>)

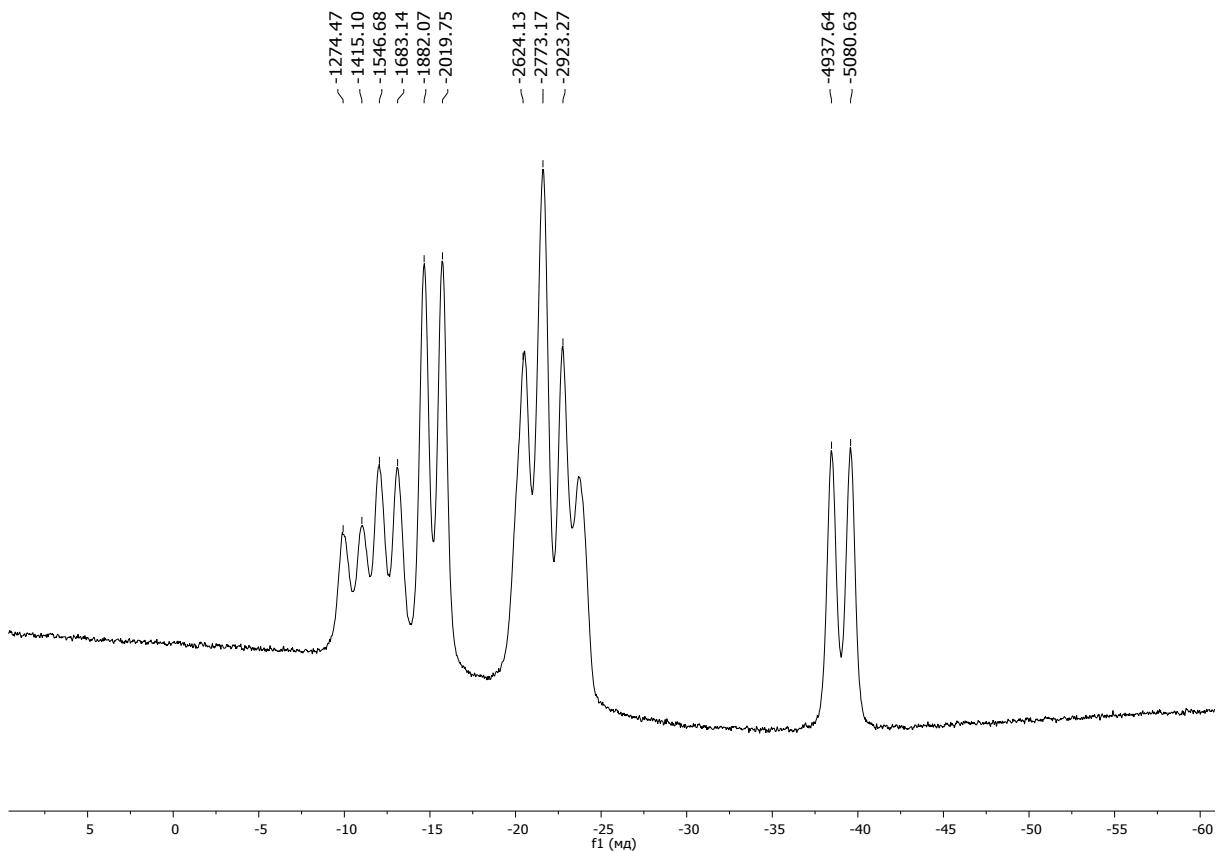


Fig. S17. <sup>11</sup>B NMR spectrum of compounds **3a** and **3b** (acetone-d<sub>6</sub>)

**Spectral data for 10-EtC(NHCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>)=HN-7,8-C<sub>2</sub>B<sub>9</sub>H<sub>11</sub> (4a, 4b).**

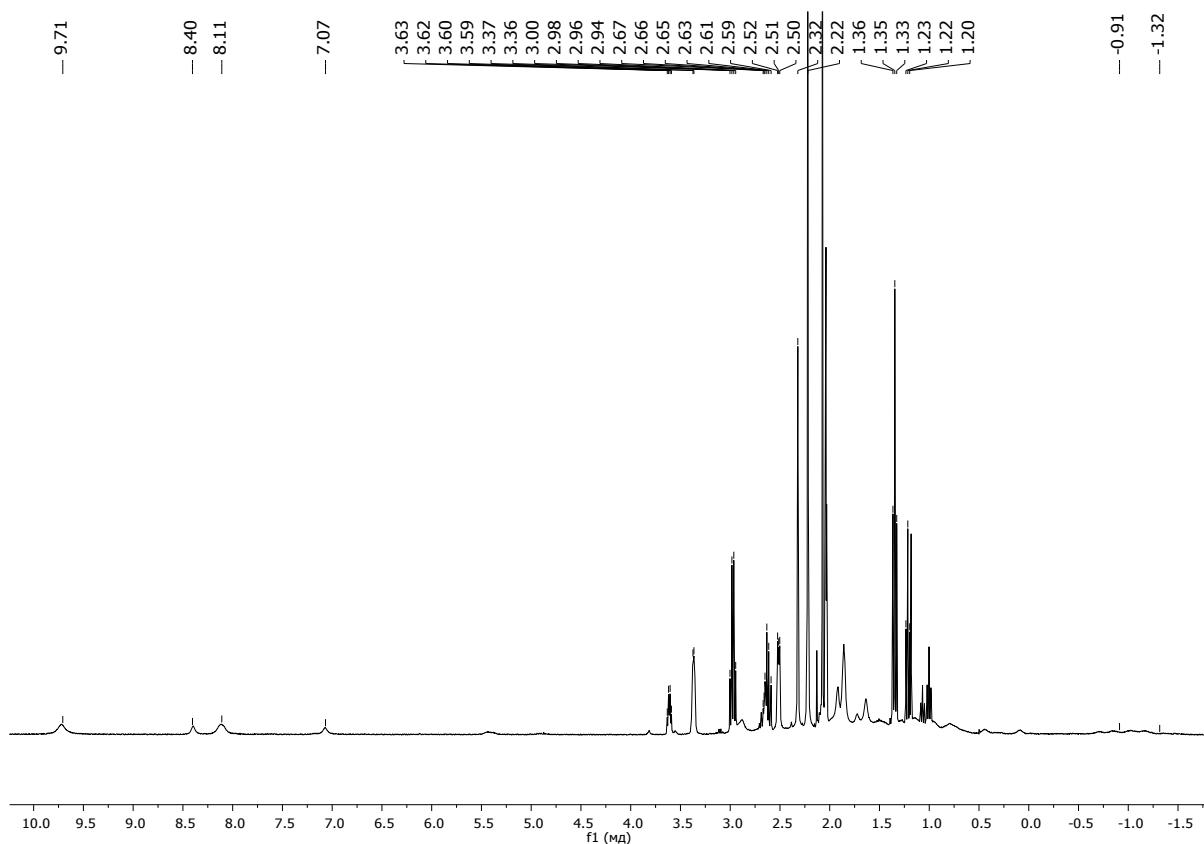


Fig. S18. <sup>1</sup>H NMR spectrum of compounds **4a** and **4b** (acetone-d<sub>6</sub>)

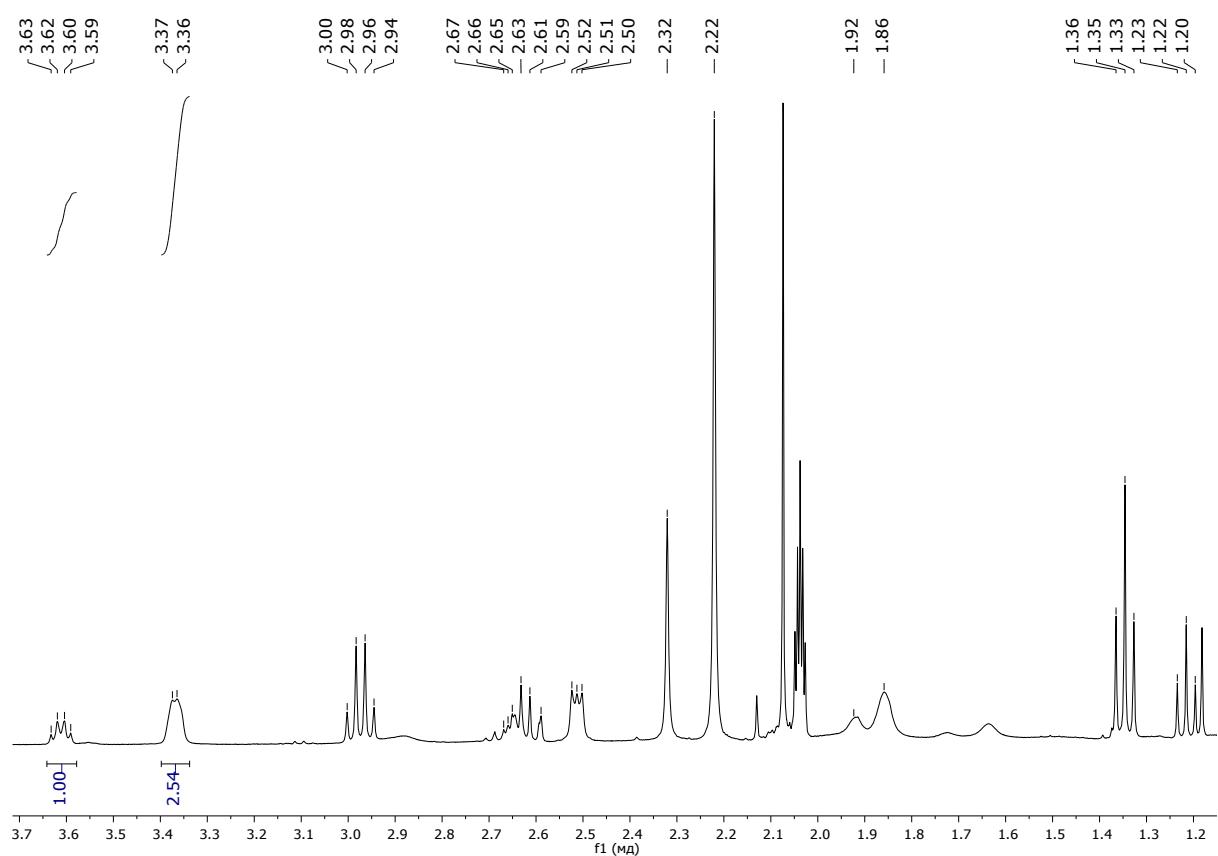


Fig. S19. The fragment of <sup>1</sup>H NMR spectrum of compounds **4a** and **4b** (acetone-d<sub>6</sub>)

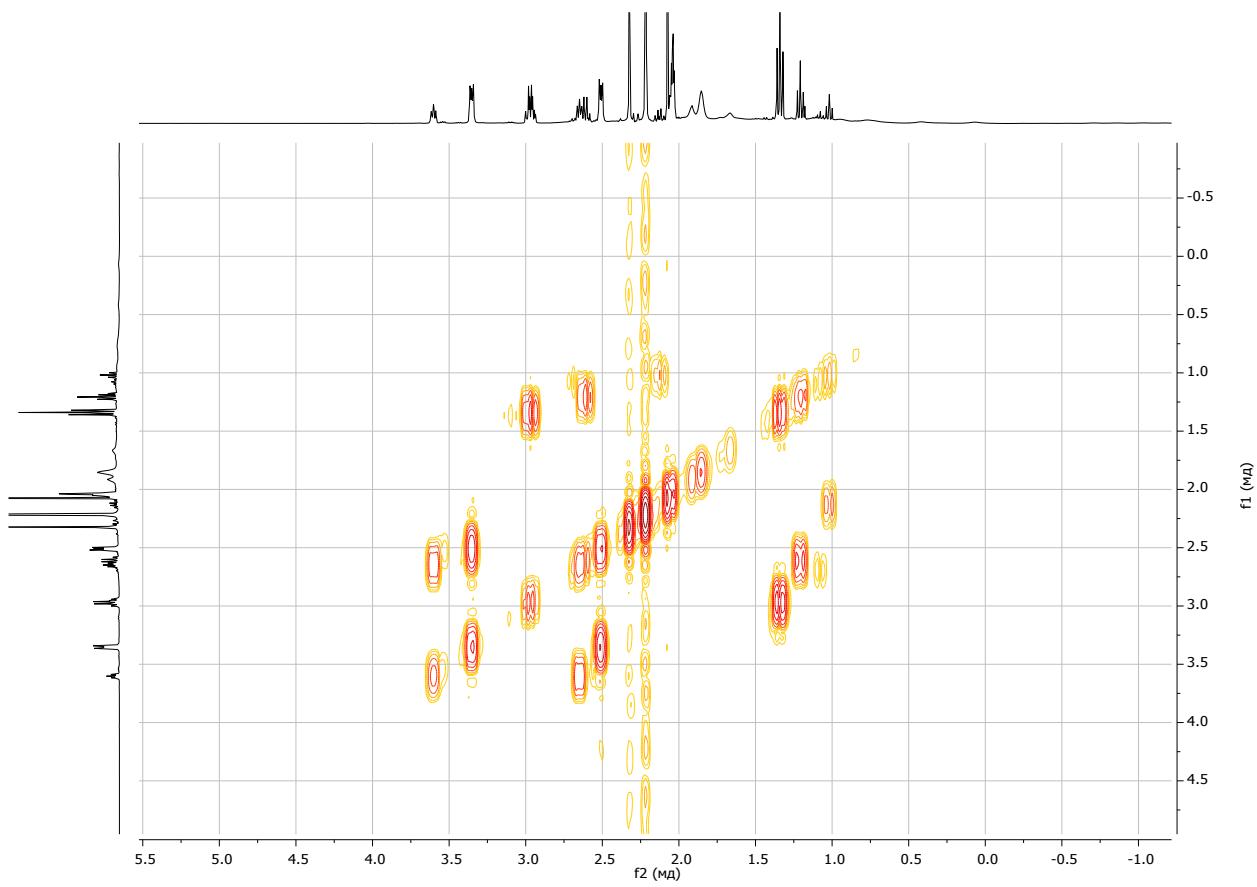


Fig. S20. (HH)gCOSY NMR spectrum of compounds **4a** and **4b** (acetone-d<sub>6</sub>)

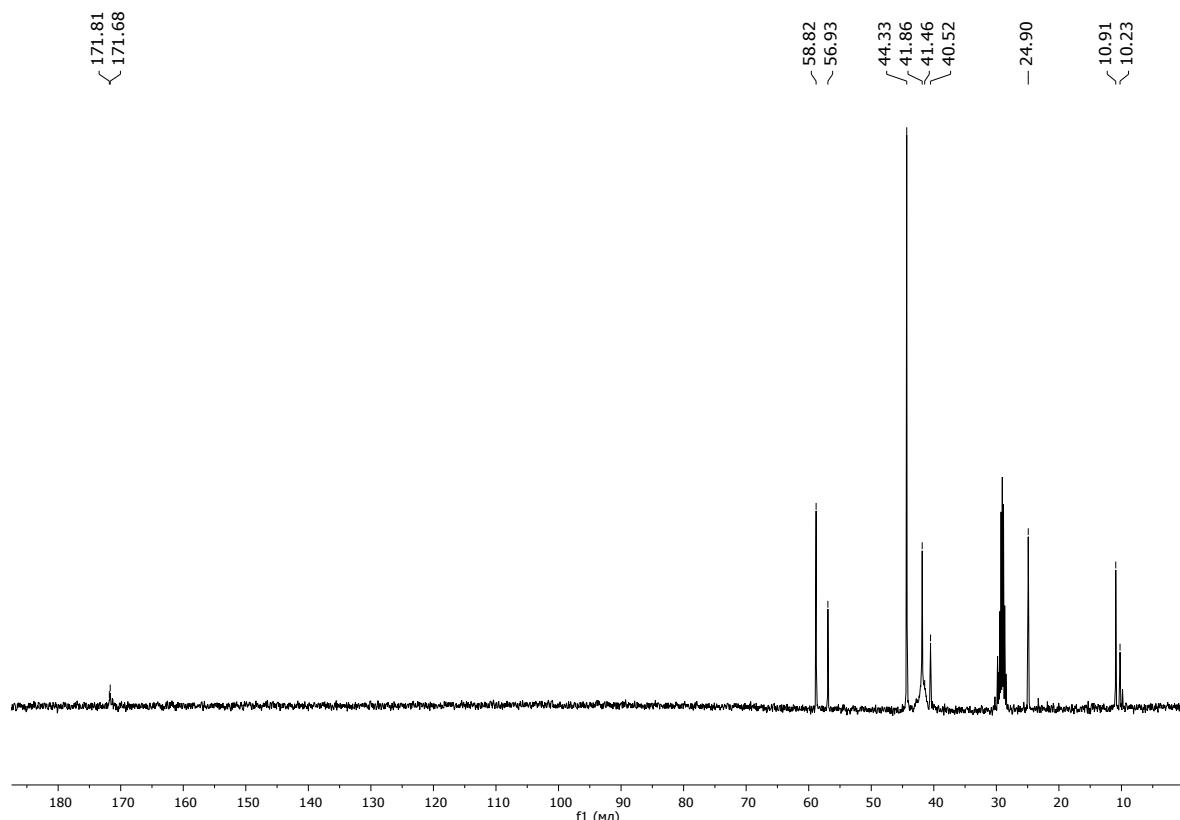


Fig. S21. <sup>13</sup>C NMR spectrum of compounds **4a** and **4b** (acetone-d<sub>6</sub>)

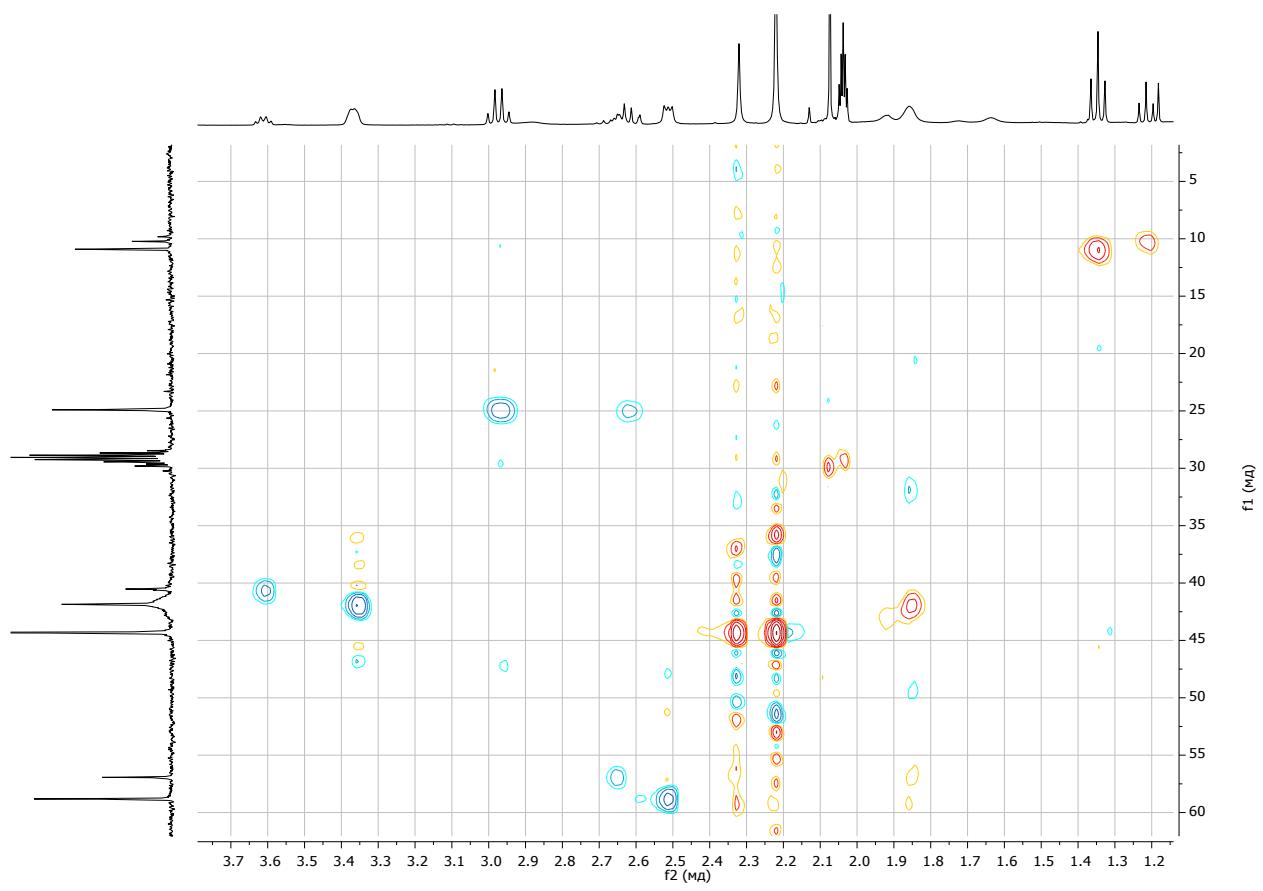


Fig. S22. (HC)HSQC NMR spectrum of compounds **4a** and **4b** (acetone-d<sub>6</sub>)

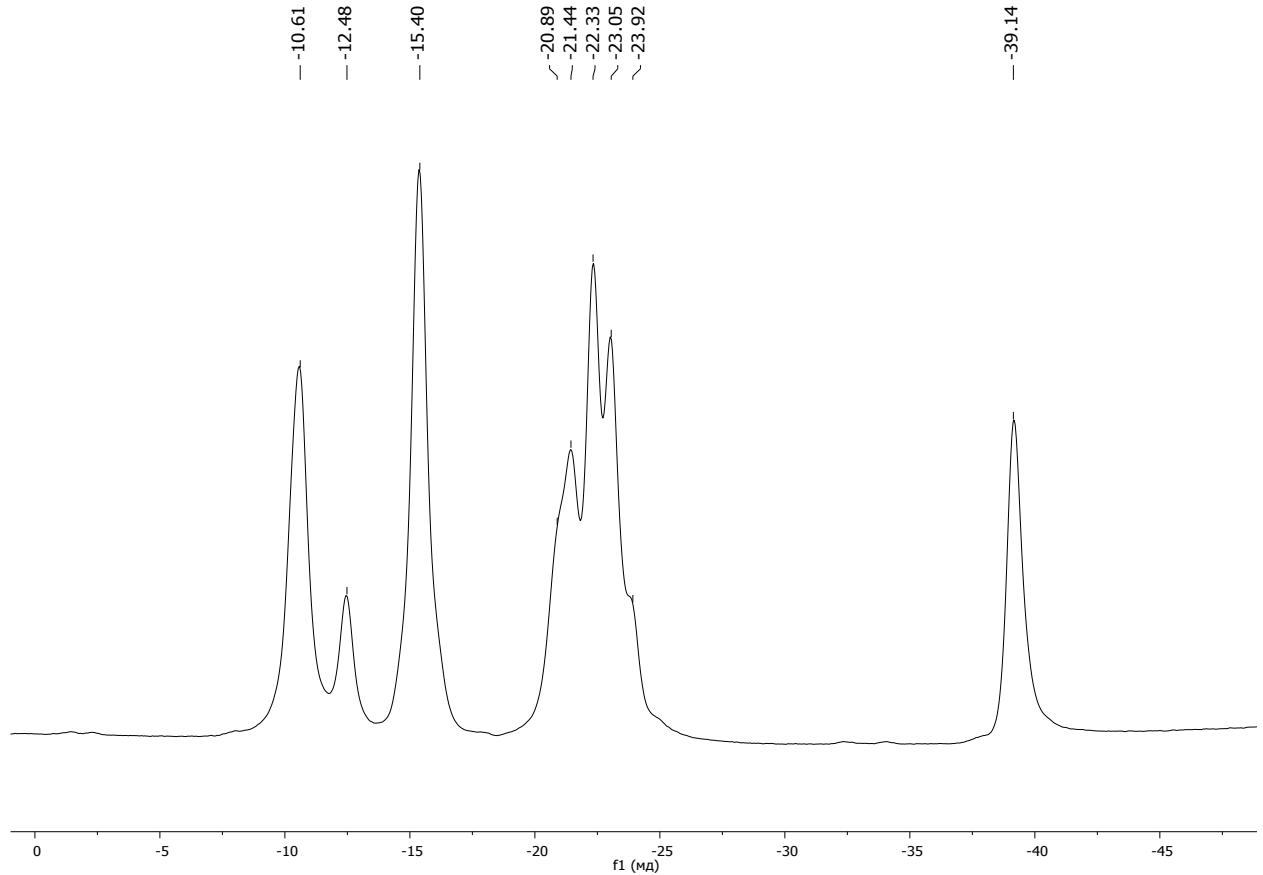


Fig. S23. <sup>11</sup>B{<sup>1</sup>H} NMR spectrum of compounds **4a** and **4b** (acetone-d<sub>6</sub>)

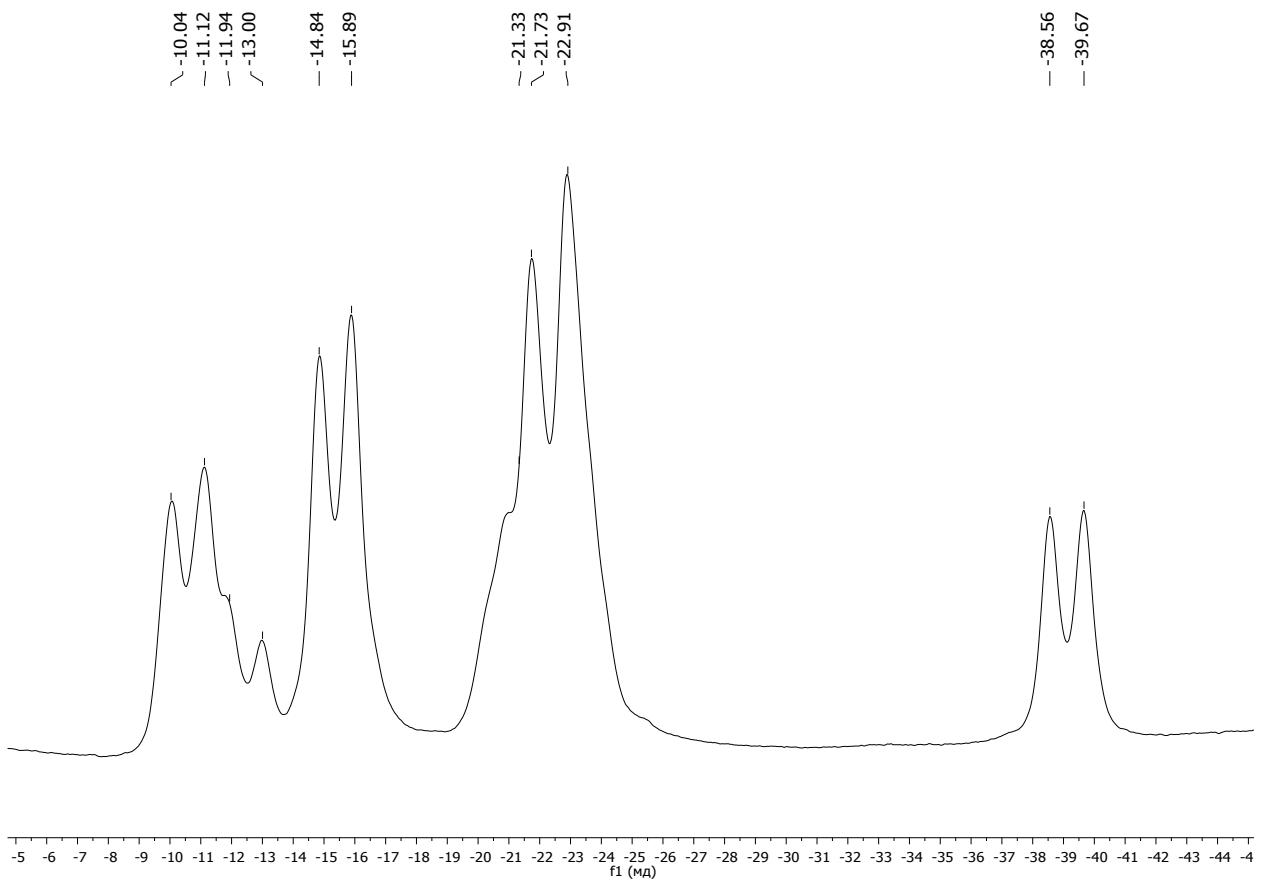


Fig. S24. <sup>11</sup>B NMR spectrum of compounds **4a** and **4b** (acetone-d<sub>6</sub>)

**Spectral data for [3-Ph<sub>3</sub>P-(8-MeOCH<sub>2</sub>CH<sub>2</sub>N=C(Et)NH)-3,1,2-NiC<sub>2</sub>B<sub>9</sub>H<sub>10</sub>] (6)**

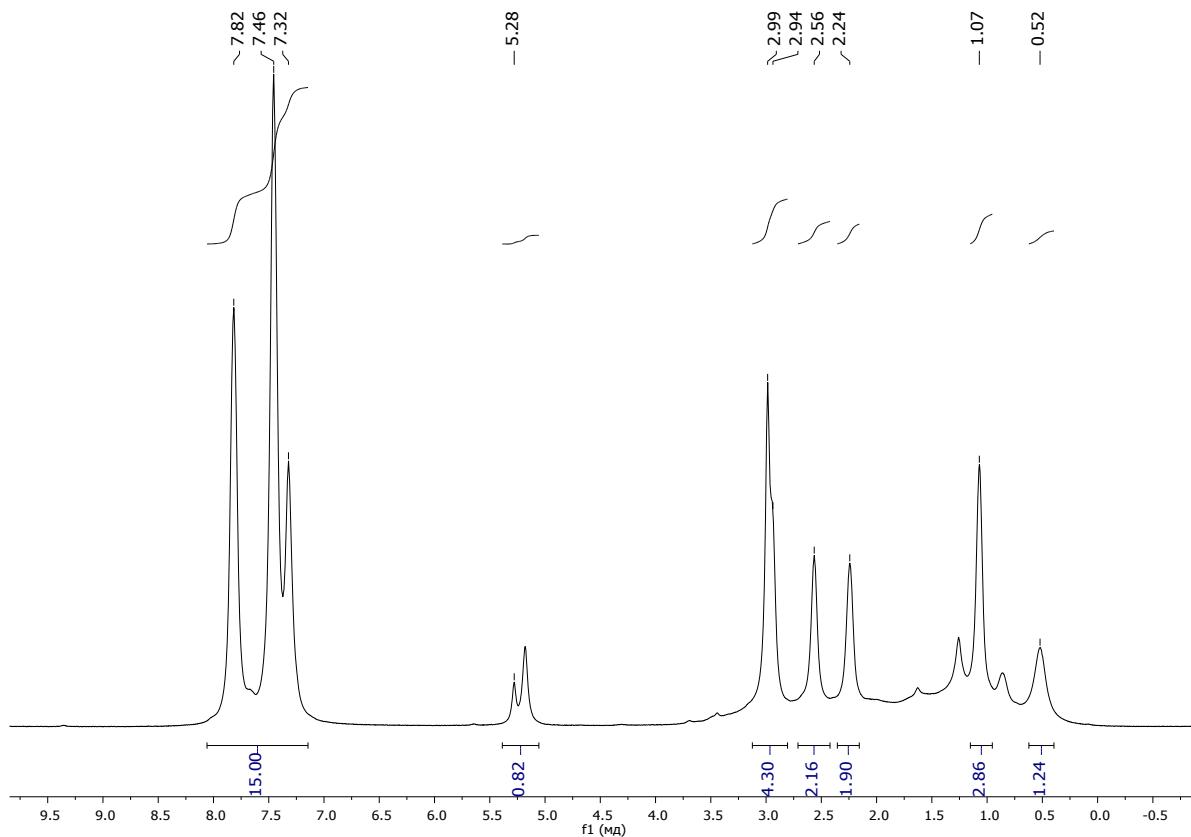


Fig. S25. <sup>1</sup>H NMR spectrum of compound 6 (CDCl<sub>3</sub>)

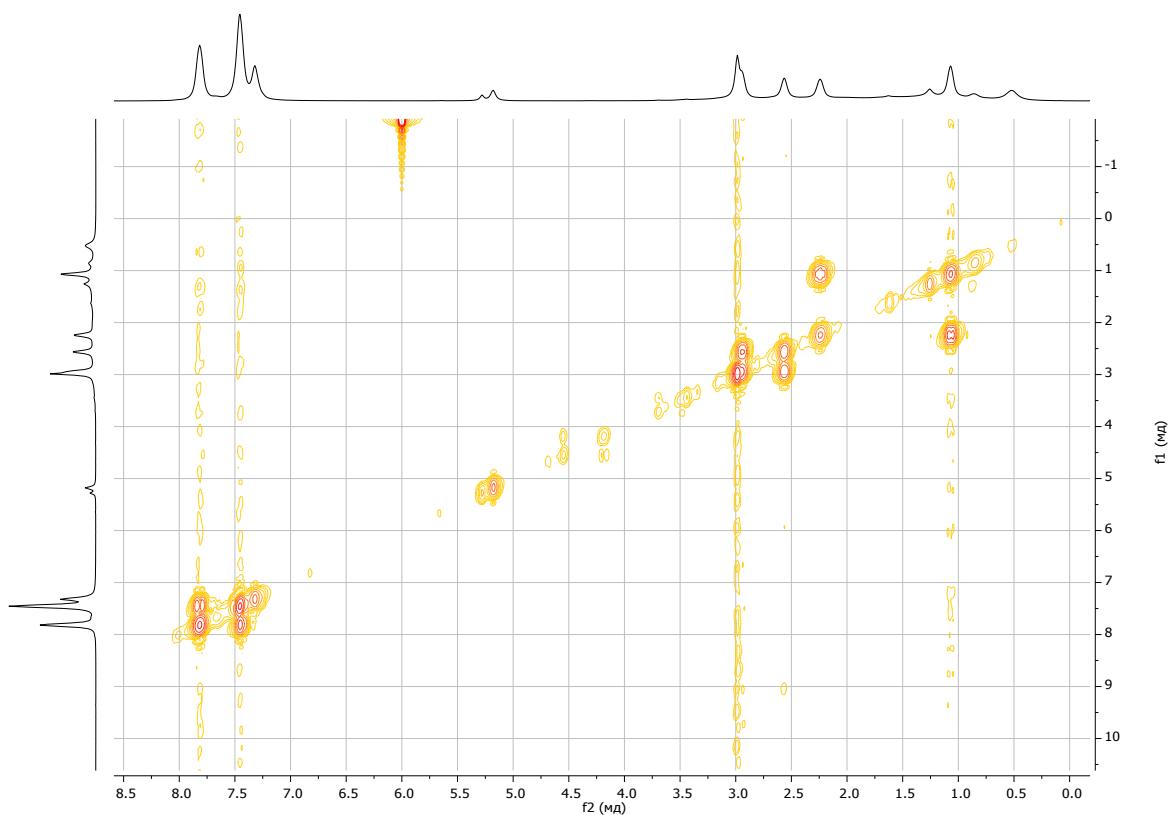


Fig. S26. (HH)gCOSY NMR spectrum of compound 6 (CDCl<sub>3</sub>)

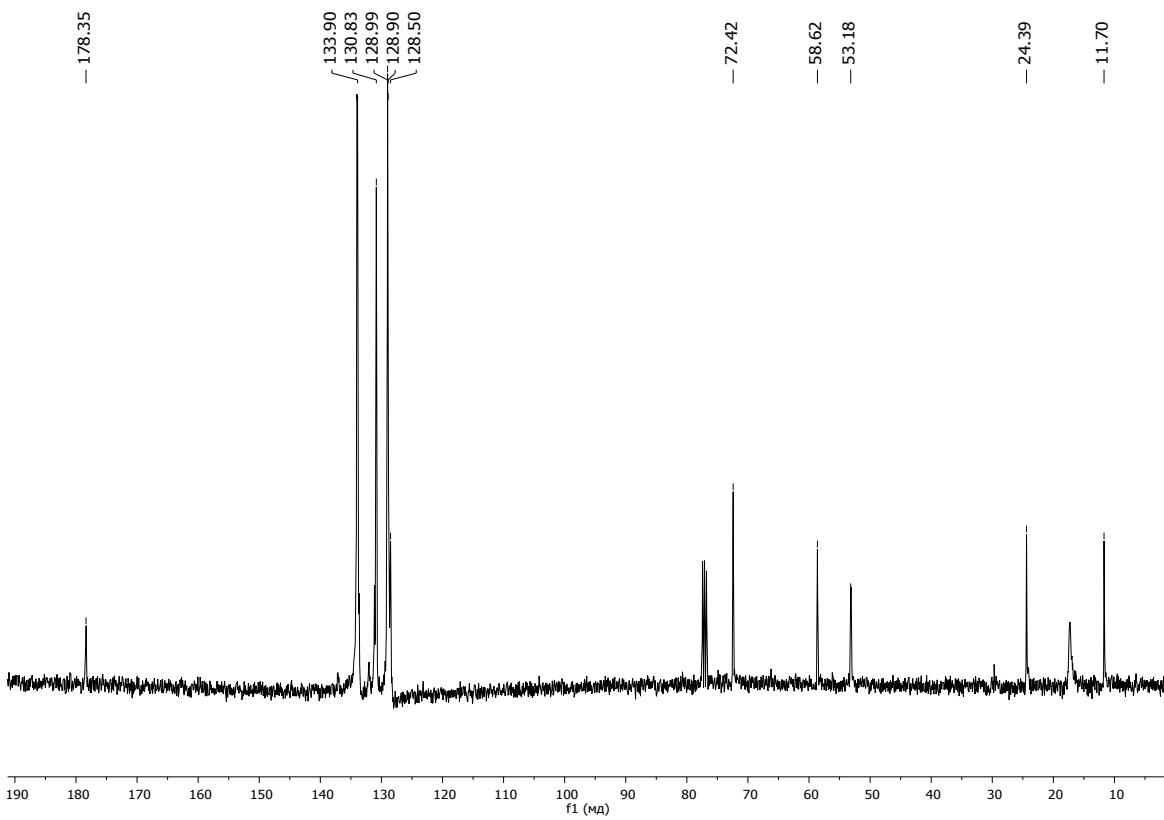


Fig. S27.  $^{13}\text{C}$  NMR spectrum of compound **6** ( $\text{CDCl}_3$ )

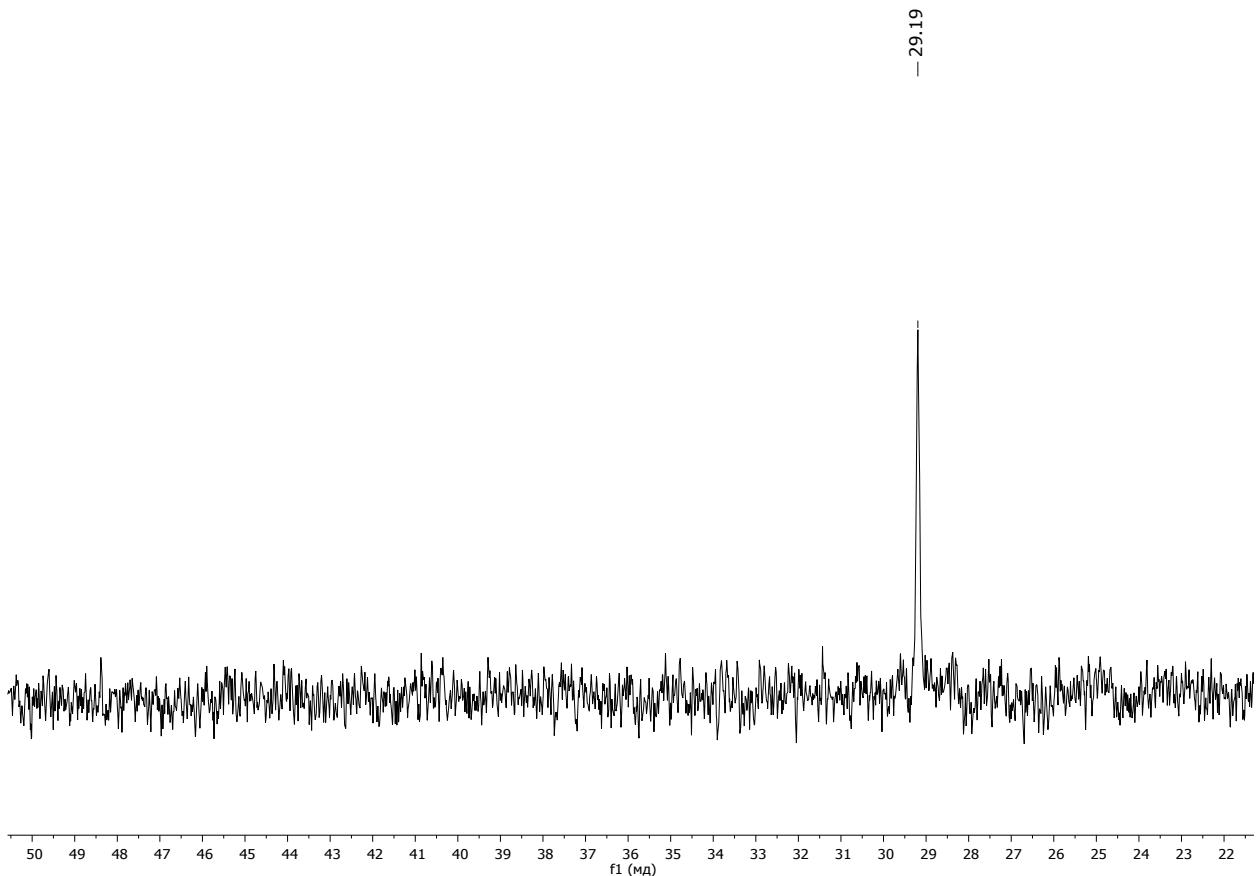


Fig. S28.  $^{31}\text{P}$  NMR spectrum of compound **6** ( $\text{CDCl}_3$ )

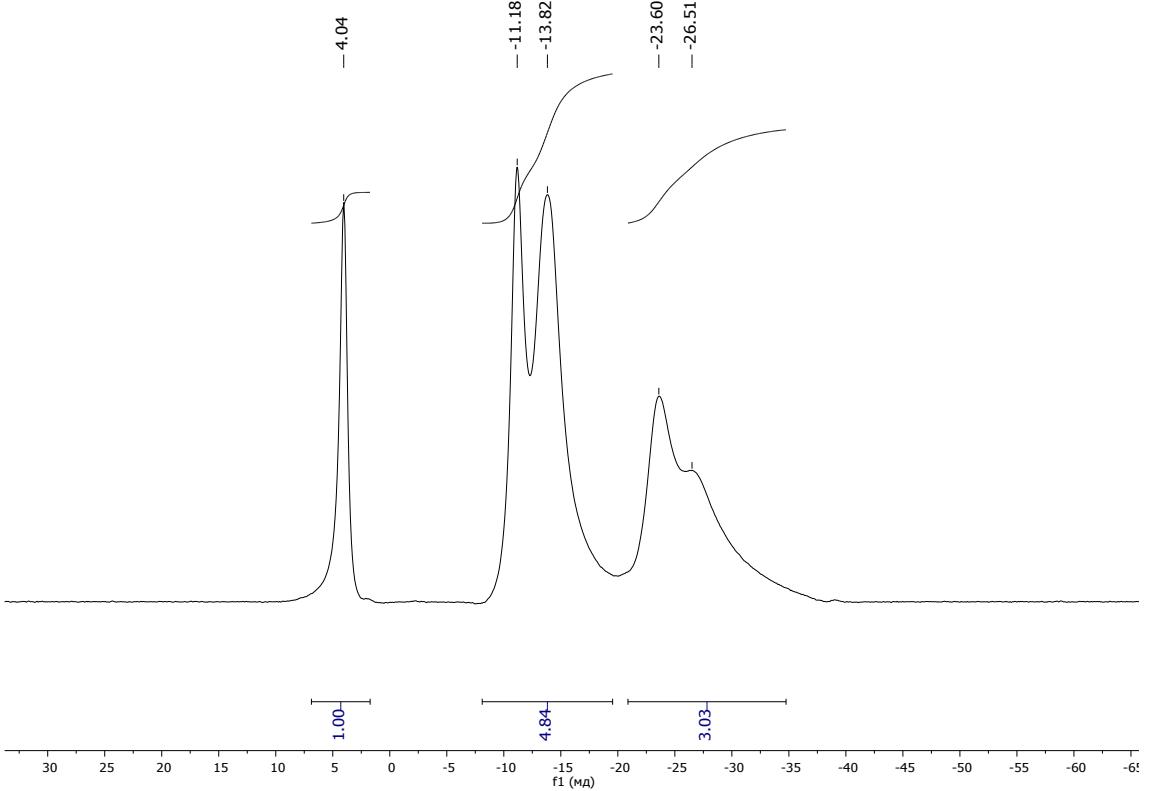


Fig. S29.  $^{11}\text{B}\{\text{H}\}$  NMR spectrum of compound **6** ( $\text{CDCl}_3$ )

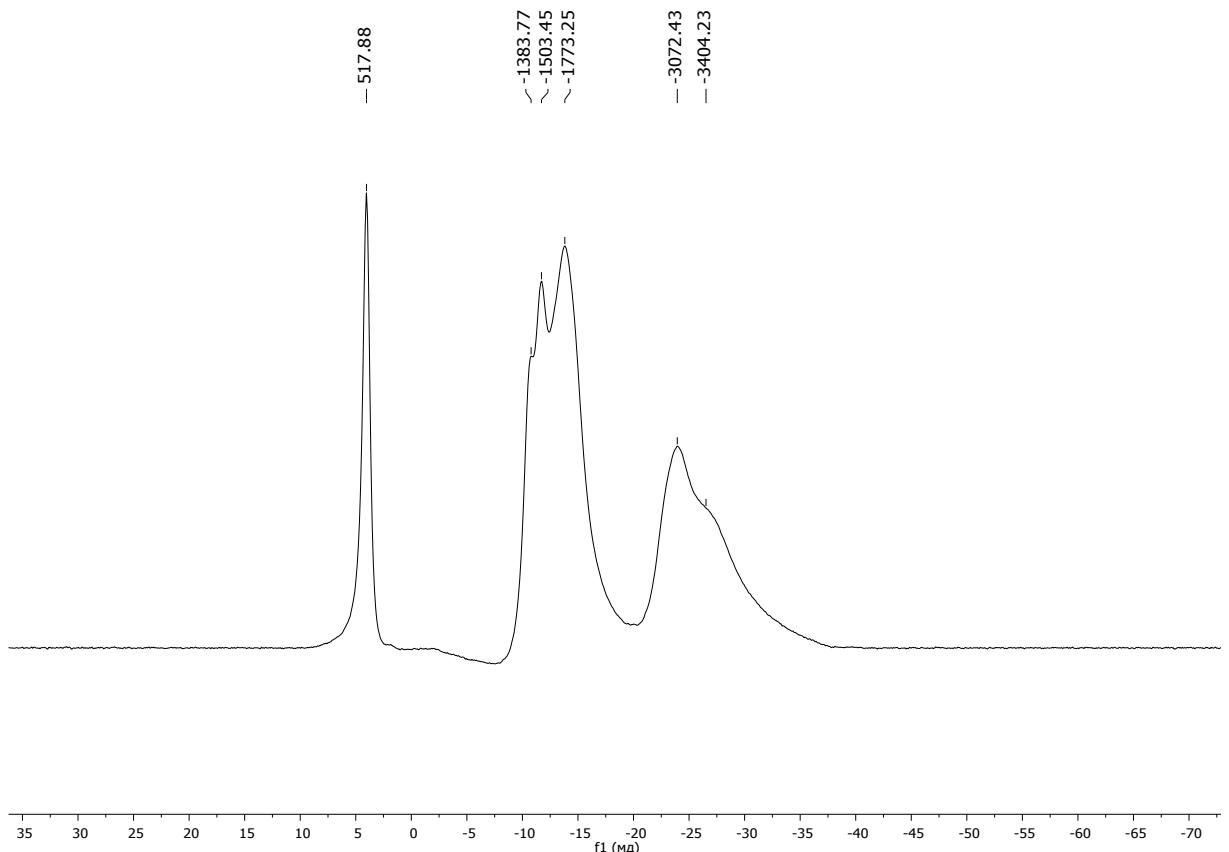


Fig. S30.  $^{11}\text{B}$  NMR spectrum of compound **6** ( $\text{CDCl}_3$ )

**Spectral data for [3-Ph<sub>3</sub>P-(8-MeOCH<sub>2</sub>CH<sub>2</sub>N=C(Et)NH)-3,1,2-PdC<sub>2</sub>B<sub>9</sub>H<sub>10</sub>] (7)**

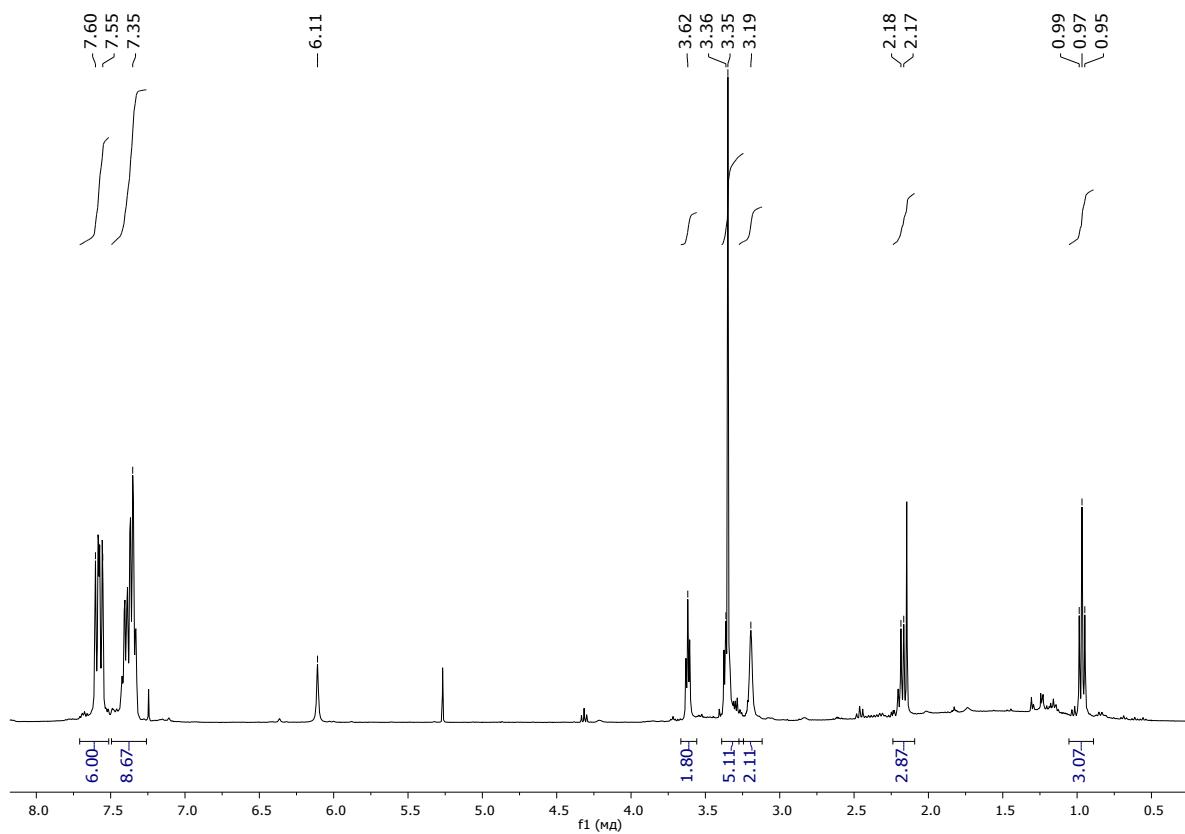


Fig. S31. <sup>1</sup>H NMR spectrum of compound 7 (CDCl<sub>3</sub>)

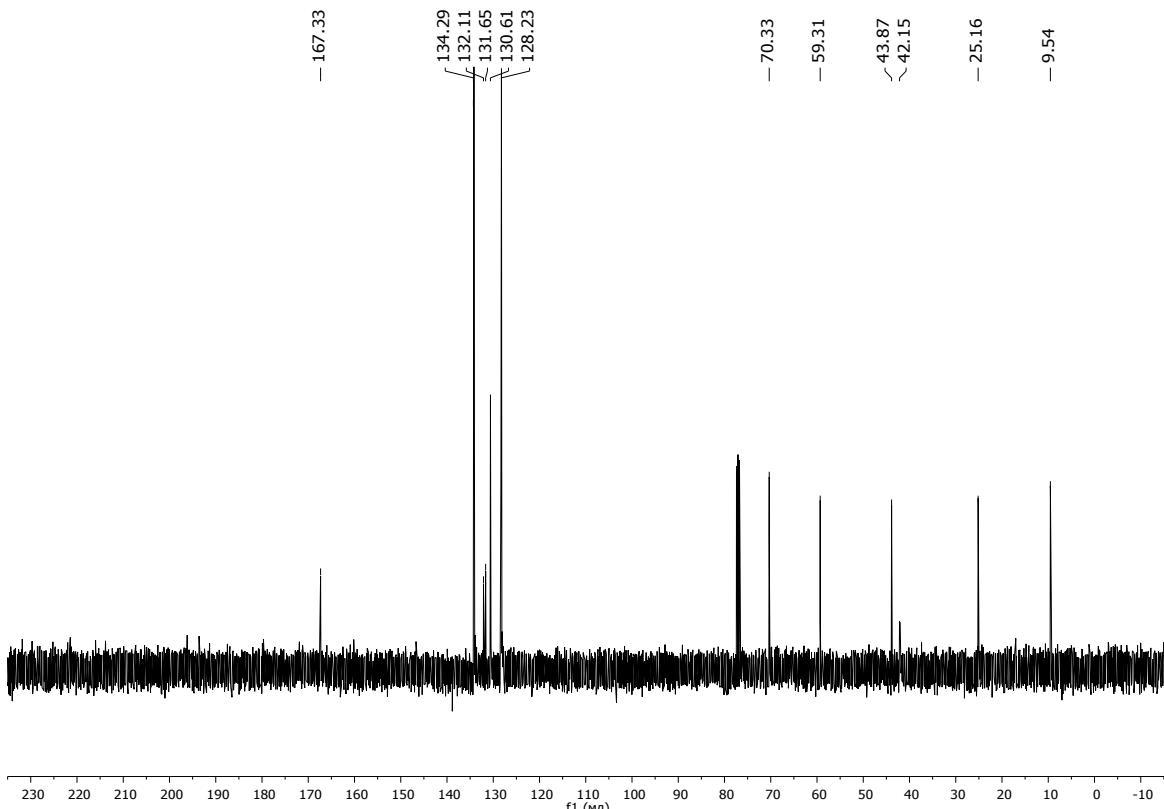


Fig. S32. <sup>13</sup>C NMR spectrum of compound 7 (CDCl<sub>3</sub>)

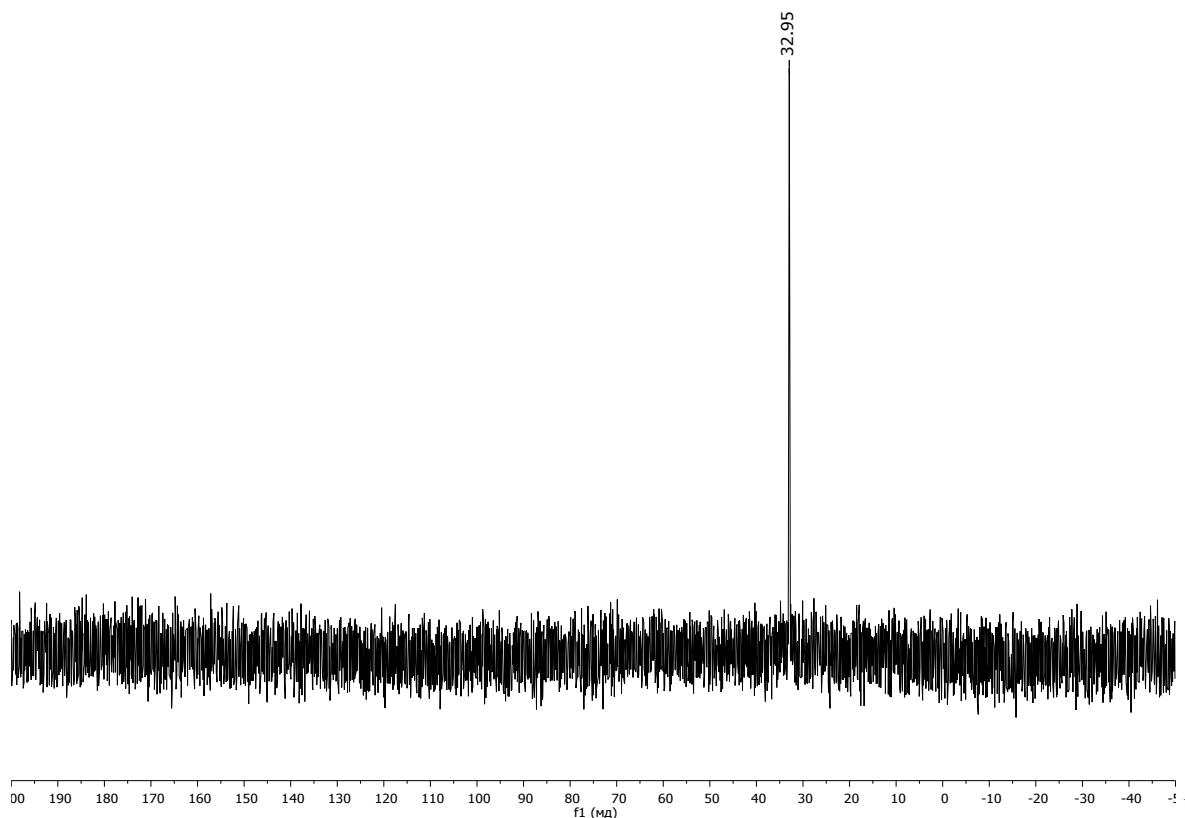


Fig.

Fig. S33.  $^{31}\text{P}$  NMR spectrum of compound 7 ( $\text{CDCl}_3$ )

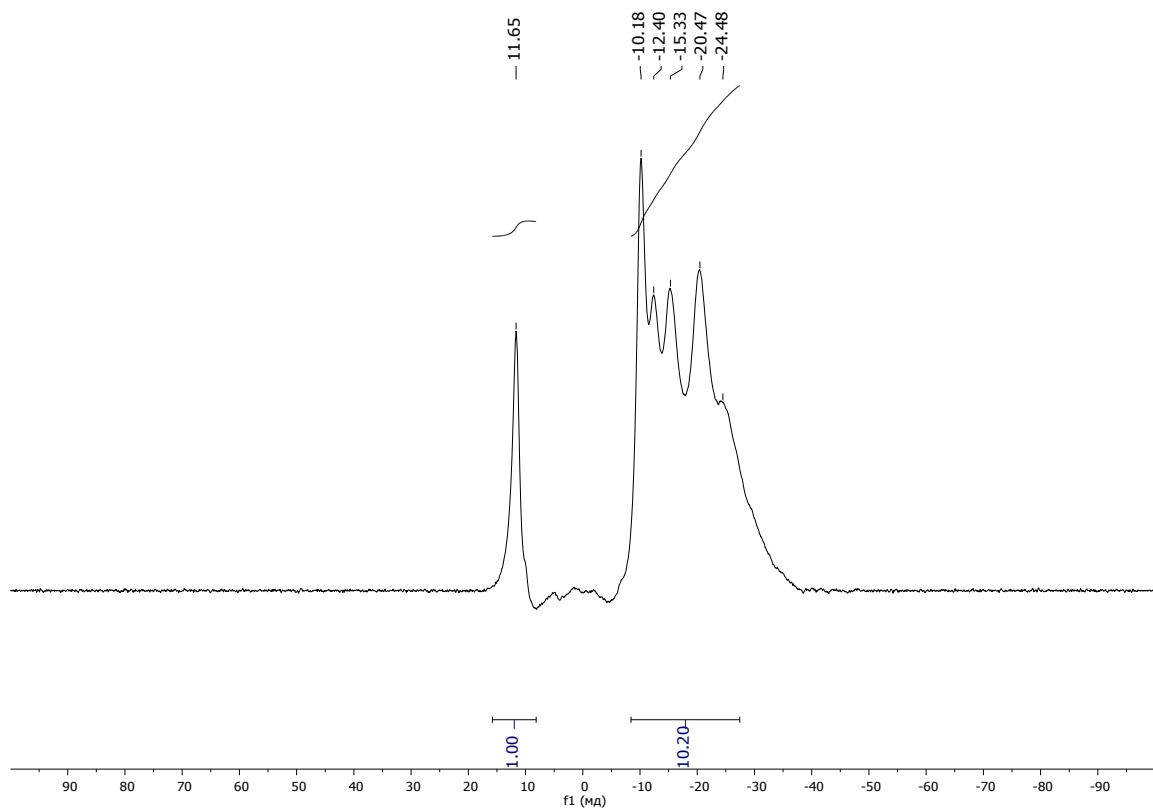


Fig. S34.  $^{11}\text{B}\{\text{H}\}$  NMR spectrum of compound 7 ( $\text{CDCl}_3$ )

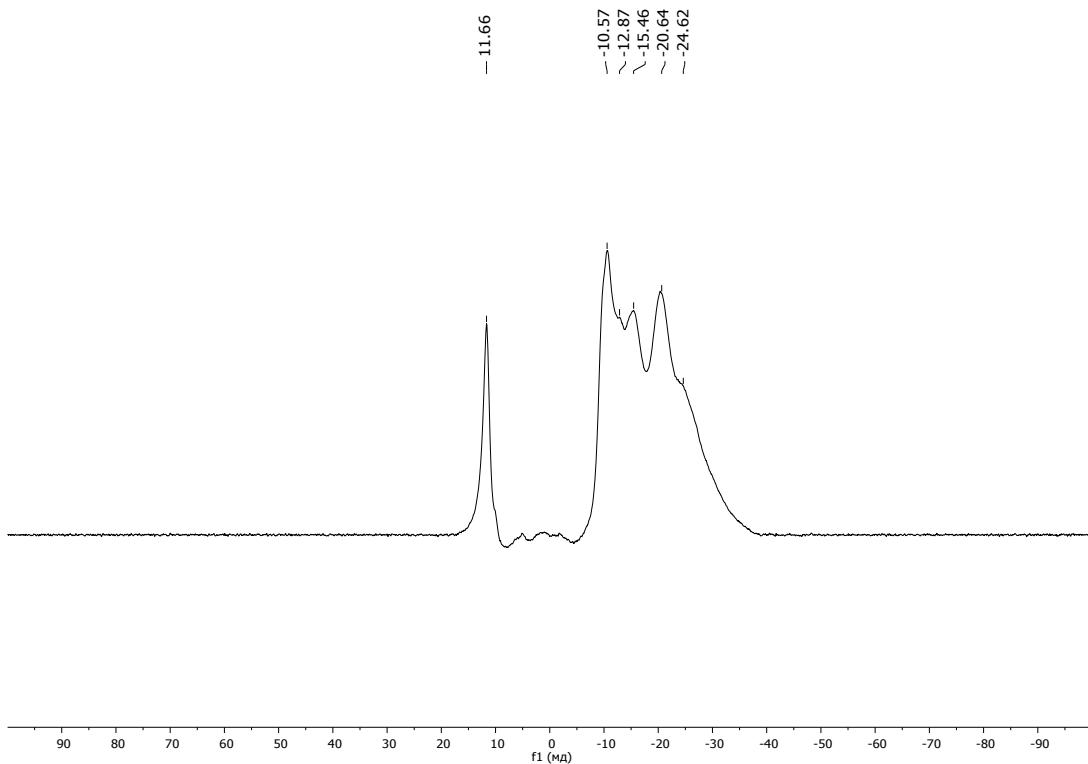


Fig. S35.  $^{11}\text{B}$  NMR spectrum of compound 7 ( $\text{CDCl}_3$ )

**Spectral data for [3,3-(8-Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>N=C(Et)NH)-3,1,2-NiC<sub>2</sub>B<sub>9</sub>H<sub>10</sub>] (8)**

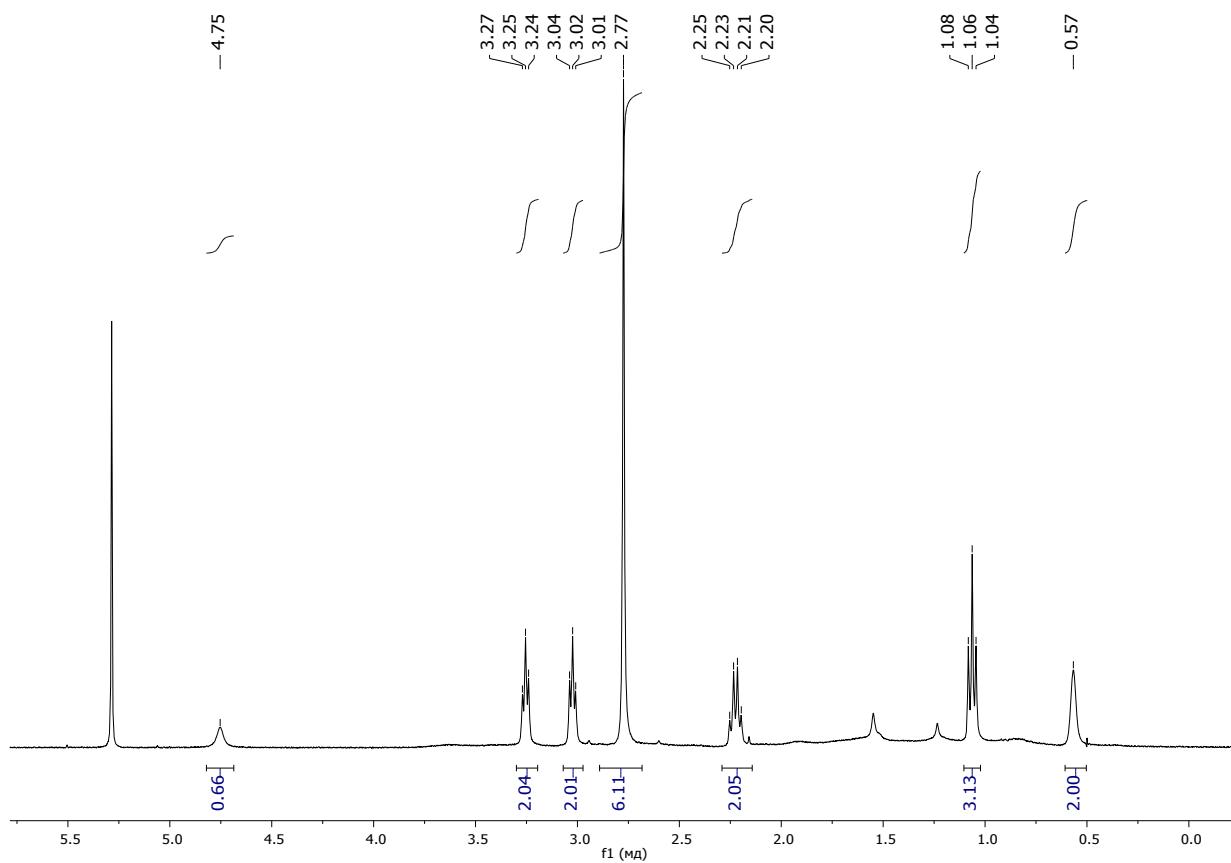


Fig. S36. <sup>1</sup>H NMR spectrum of compound 8 ( $\text{CDCl}_3$ )

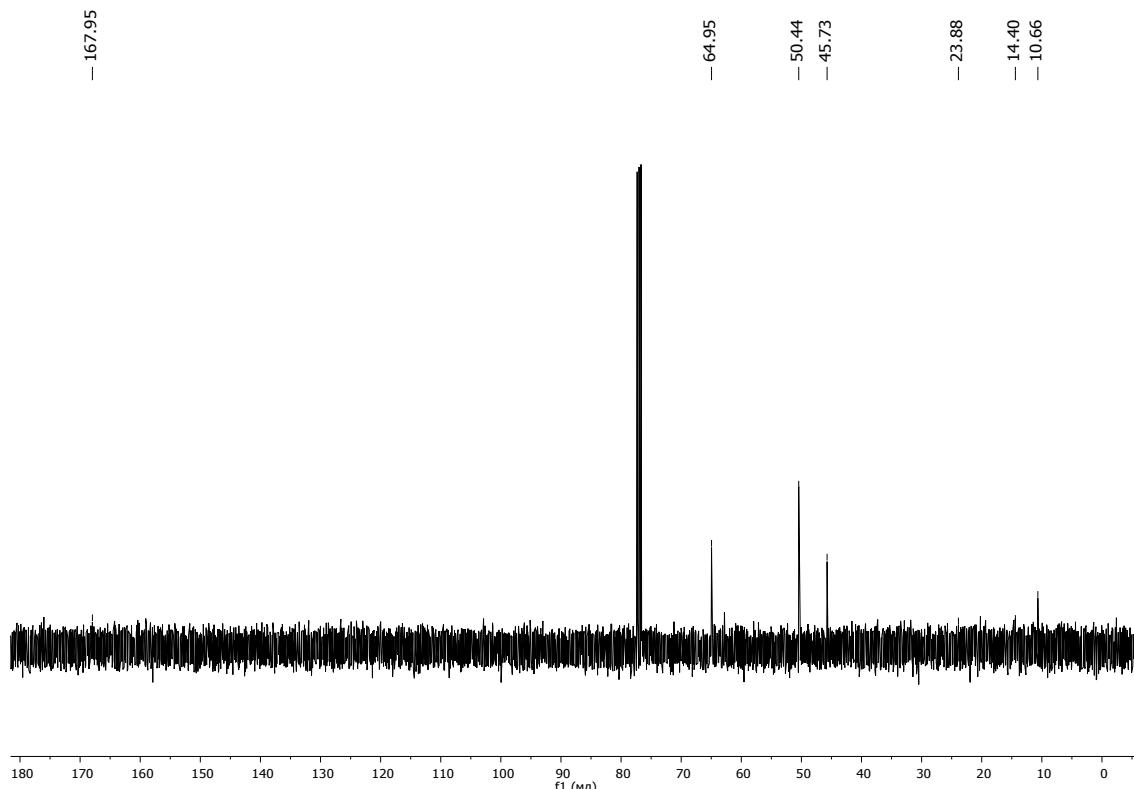


Fig. S37. <sup>13</sup>C NMR spectrum of compound 8 ( $\text{CDCl}_3$ )

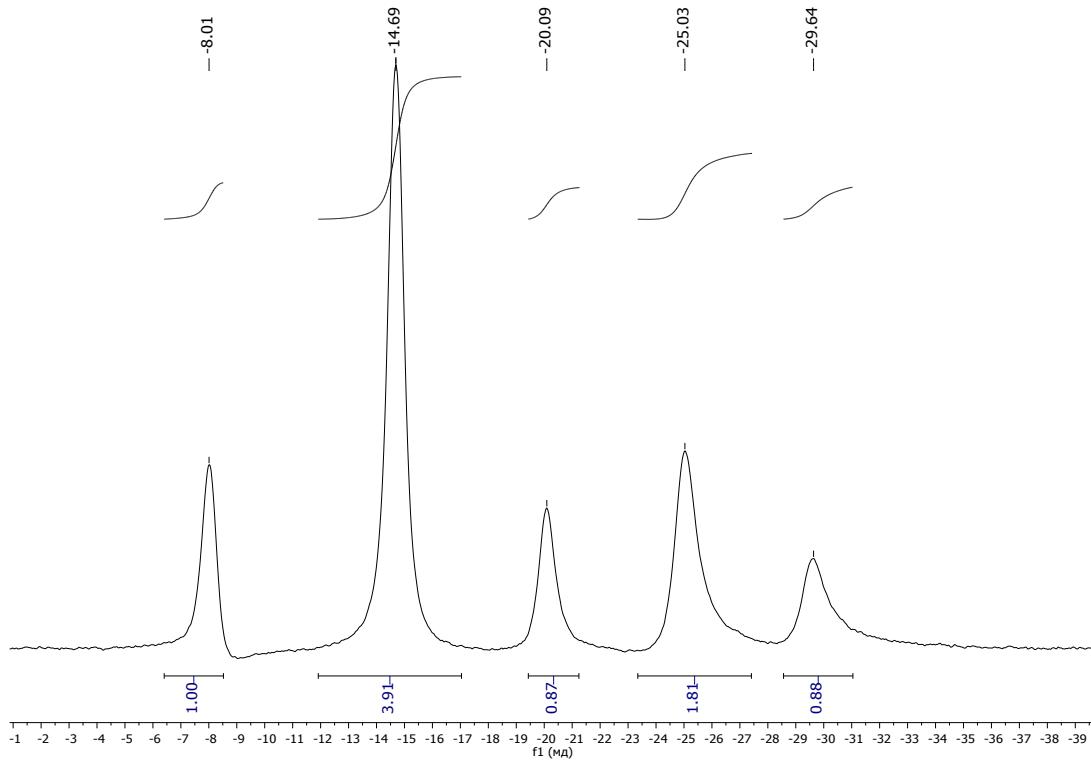


Fig. S38.  $^{11}\text{B}\{^1\text{H}\}$  NMR spectrum of compound **8** ( $\text{CDCl}_3$ )

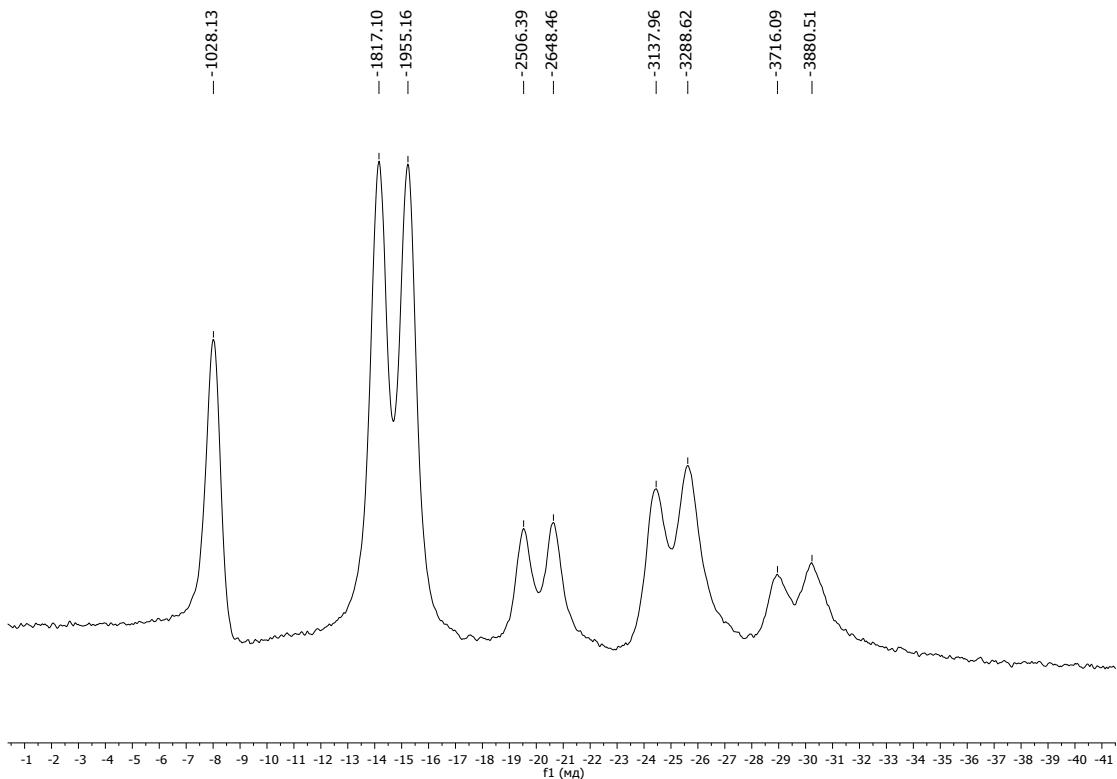


Fig. S39.  $^{11}\text{B}$  NMR spectrum of compound **8** ( $\text{CDCl}_3$ )

**Spectral data for [3,3-(8-Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>N=C(Et)NH)-3,1,2-PdC<sub>2</sub>B<sub>9</sub>H<sub>10</sub>] (9)**

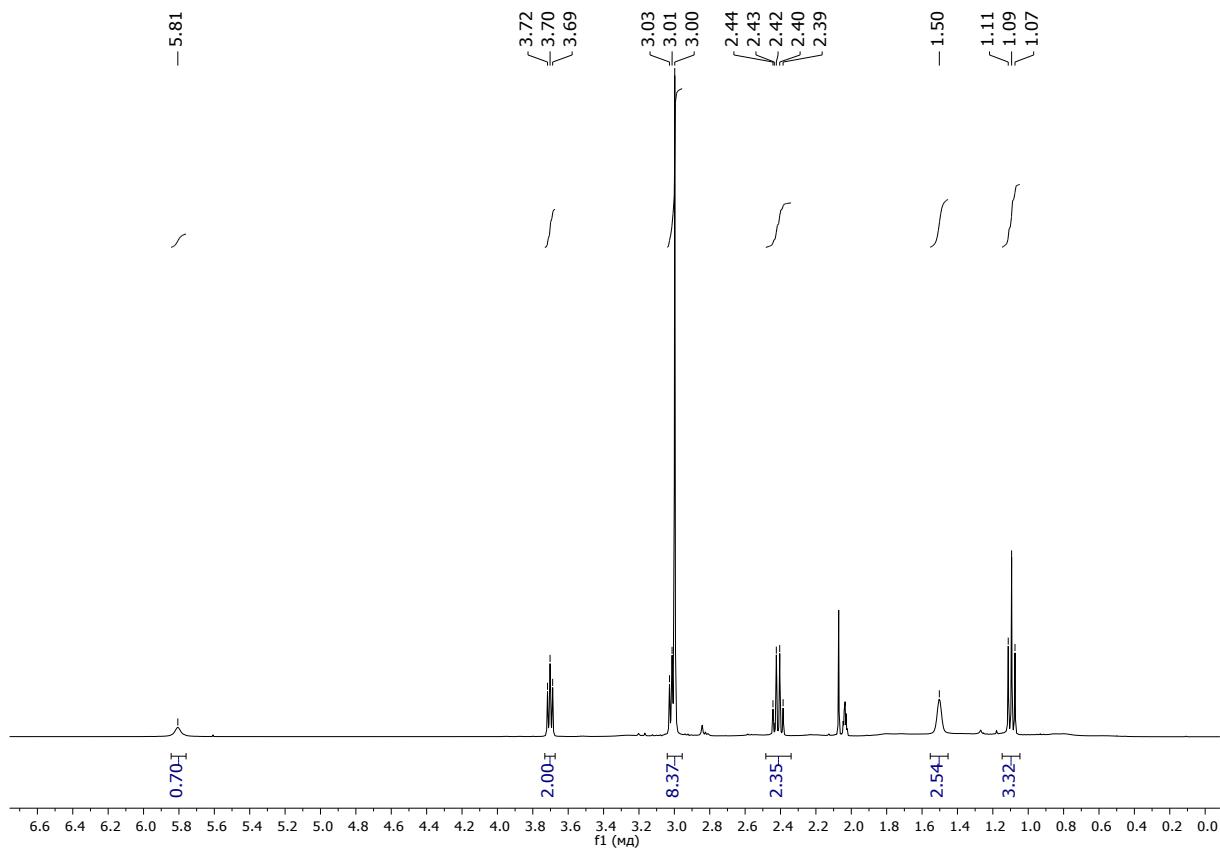


Fig. S40. <sup>1</sup>H NMR spectrum of compound 9 (acetone-d<sub>6</sub>)

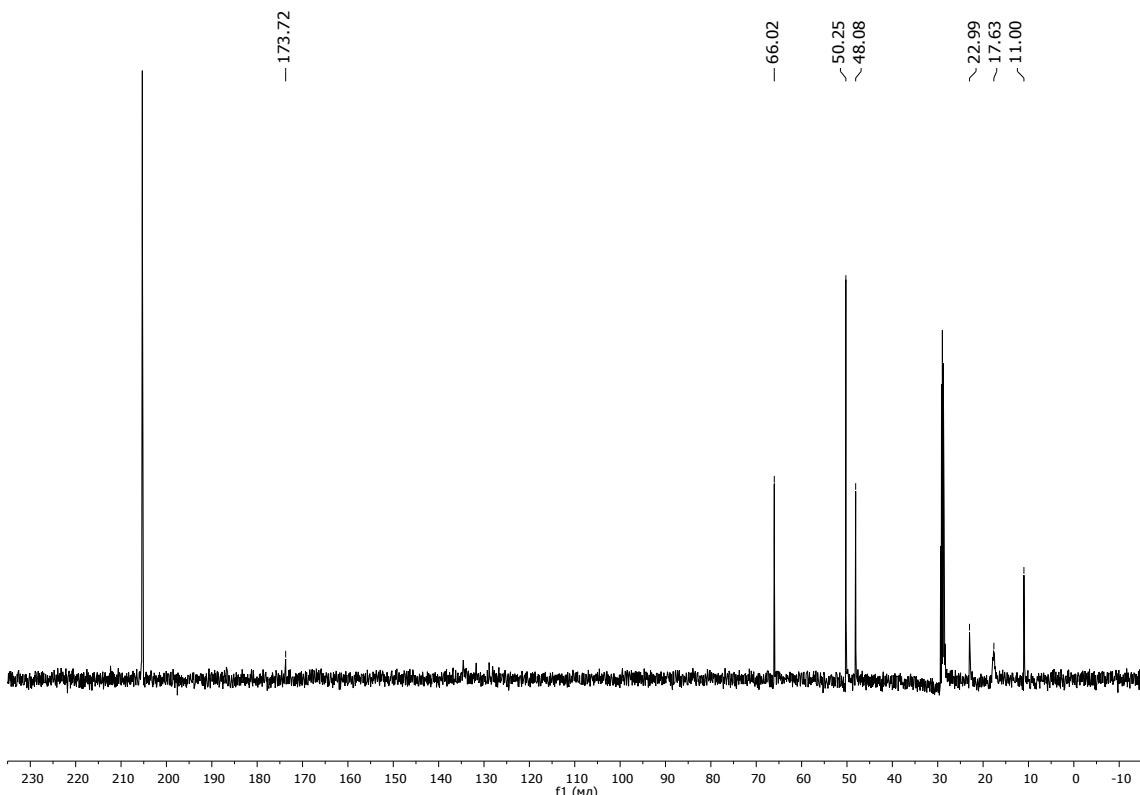


Fig. S41. <sup>13</sup>C NMR spectrum of compound 9 (acetone-d<sub>6</sub>)

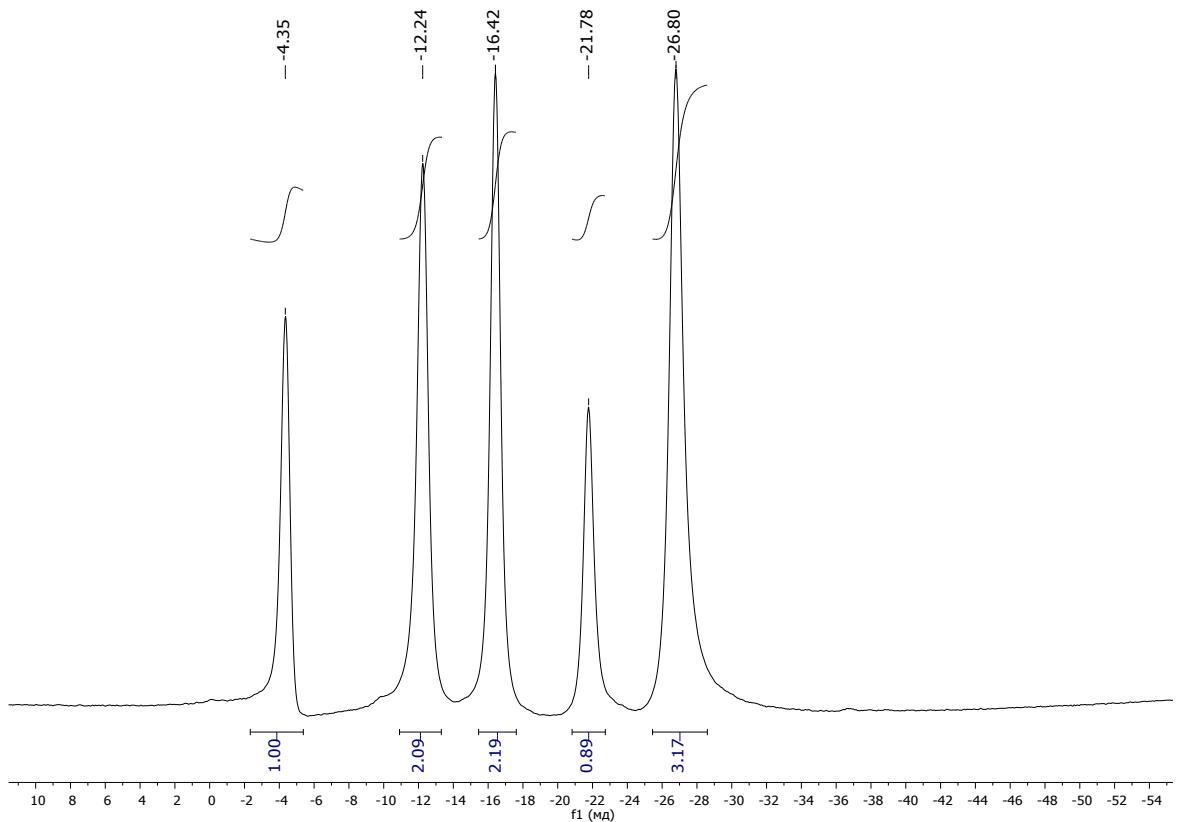


Fig. S42.  $^{11}\text{B}\{^1\text{H}\}$  NMR spectrum of compound **9** (acetone-d<sub>6</sub>)

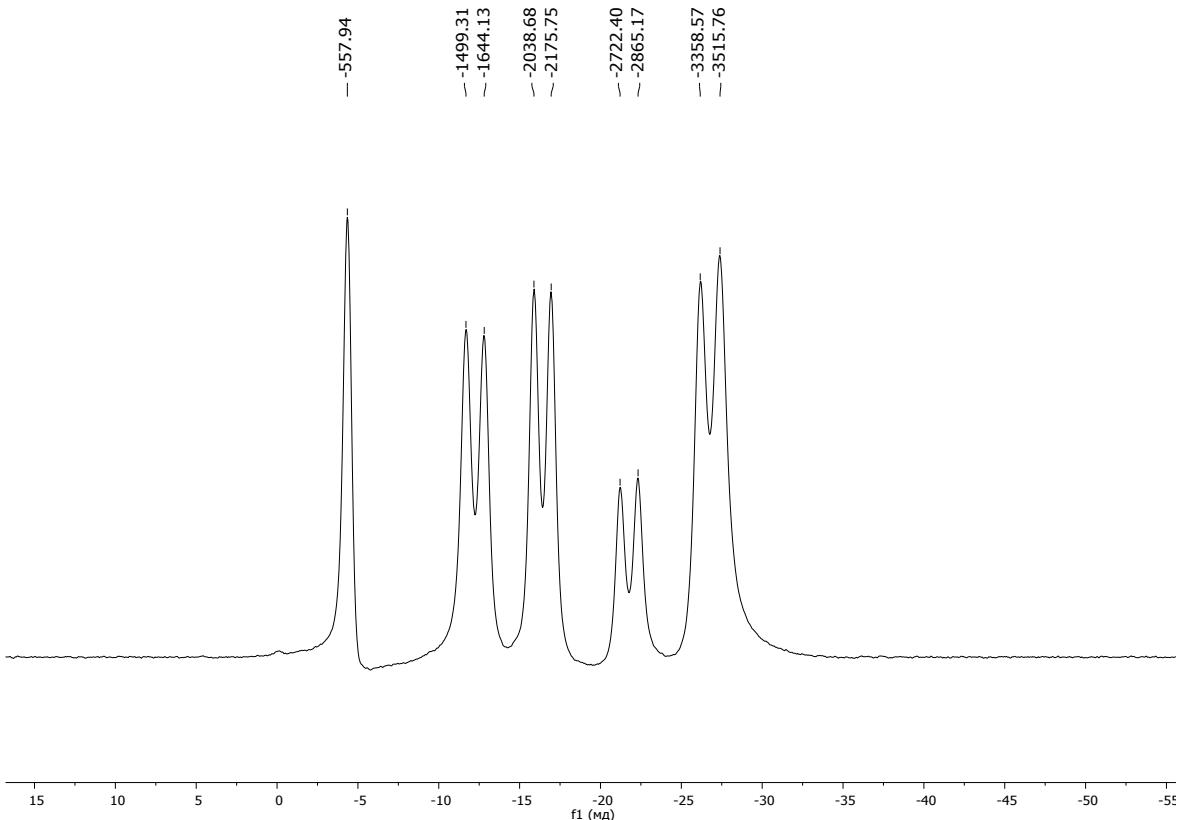


Fig. S43.  $^{11}\text{B}$  NMR spectrum of compound **9** (acetone-d<sub>6</sub>)

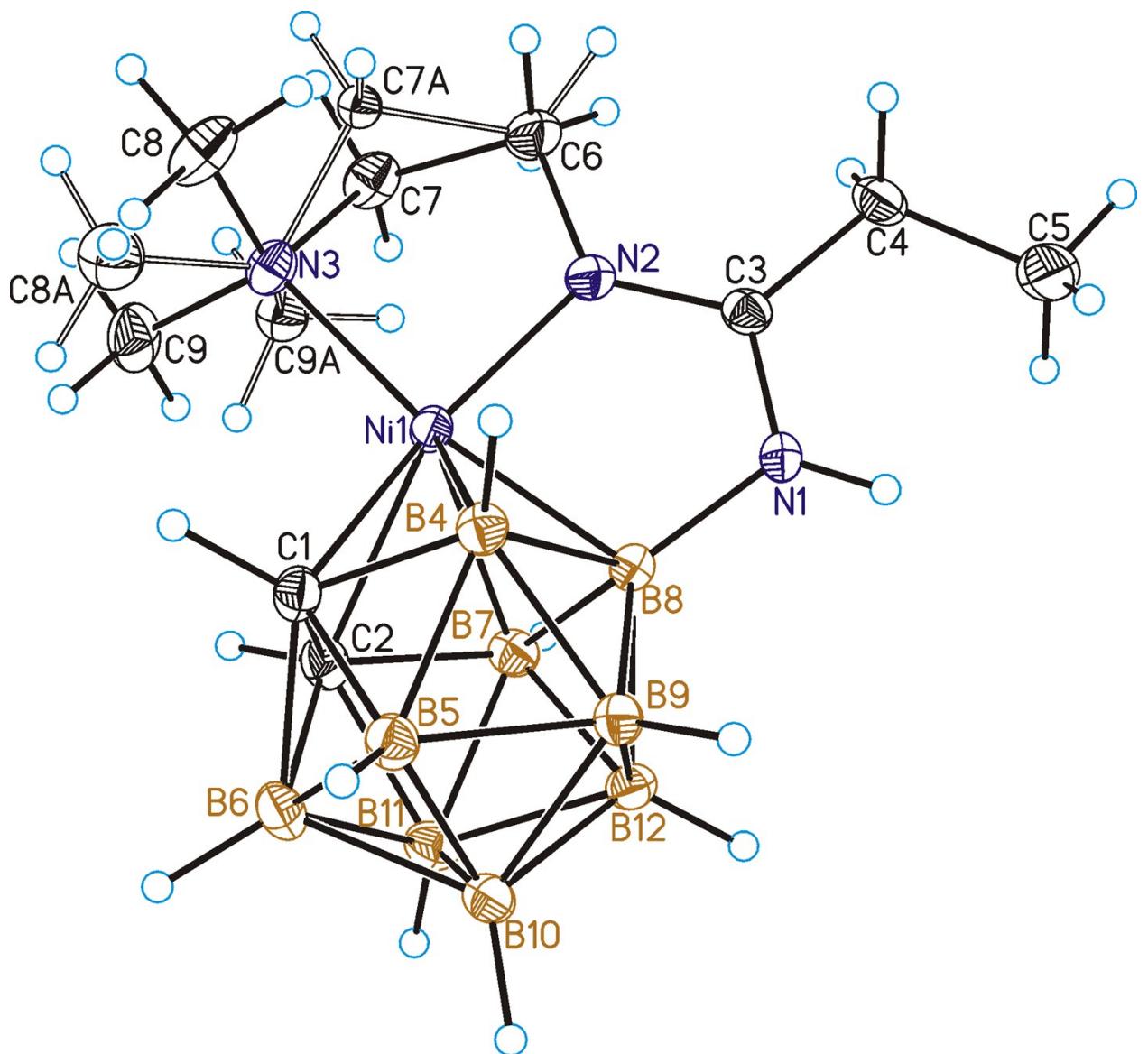


Figure S44. Disorder of complex **8**. Minor part is shown by open lines