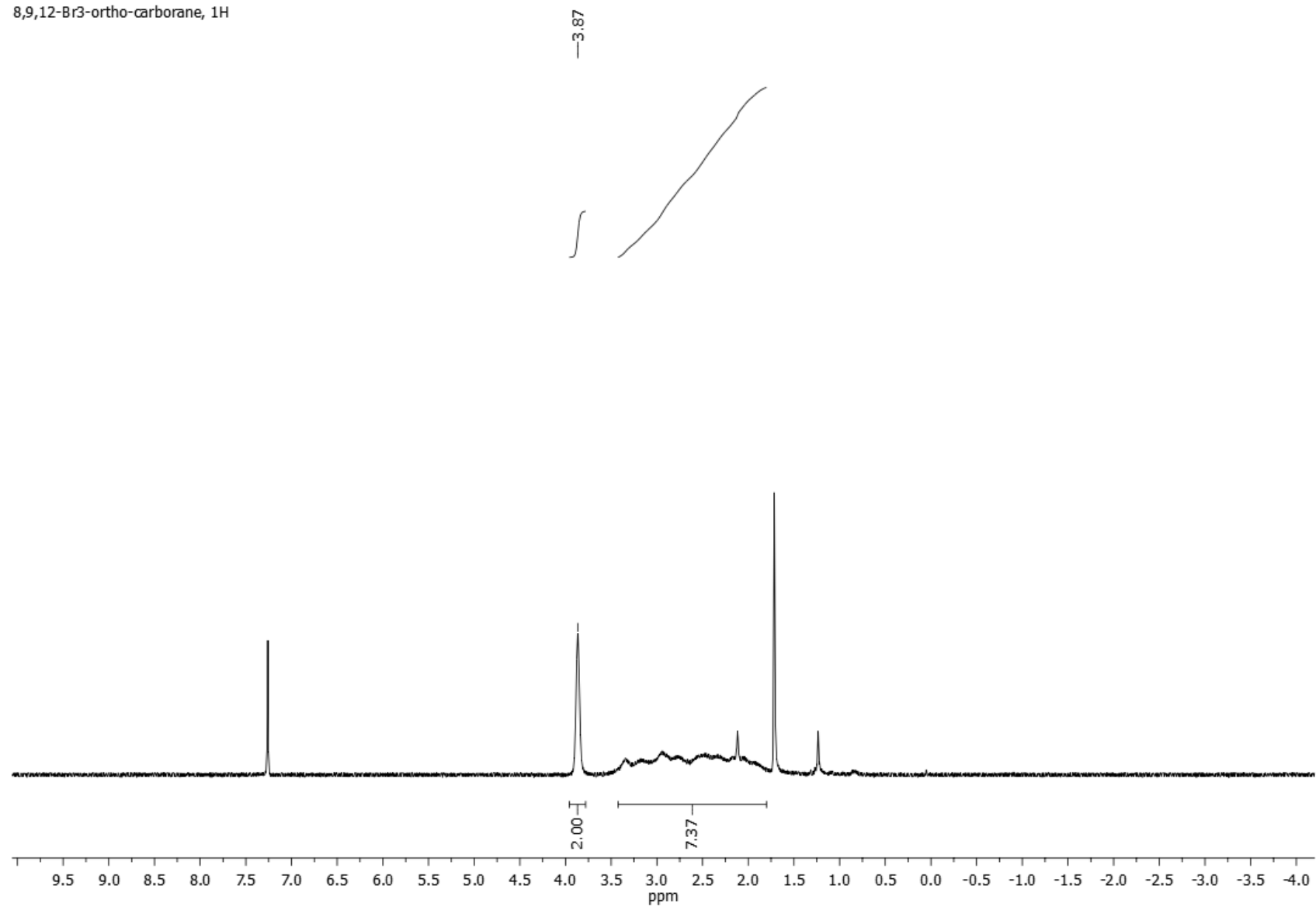
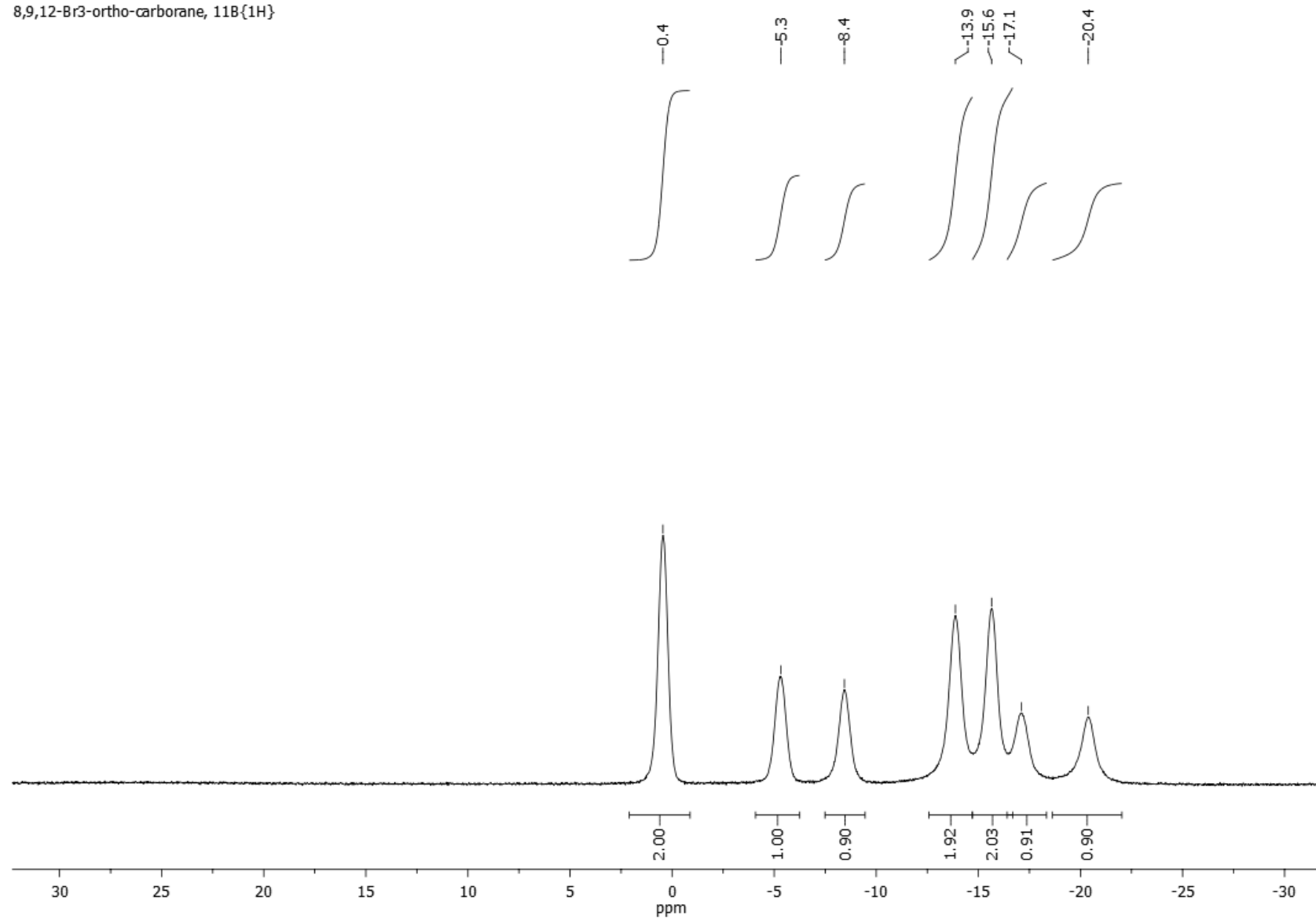


8,9,12-Br<sub>3</sub>-ortho-carborane, 1H



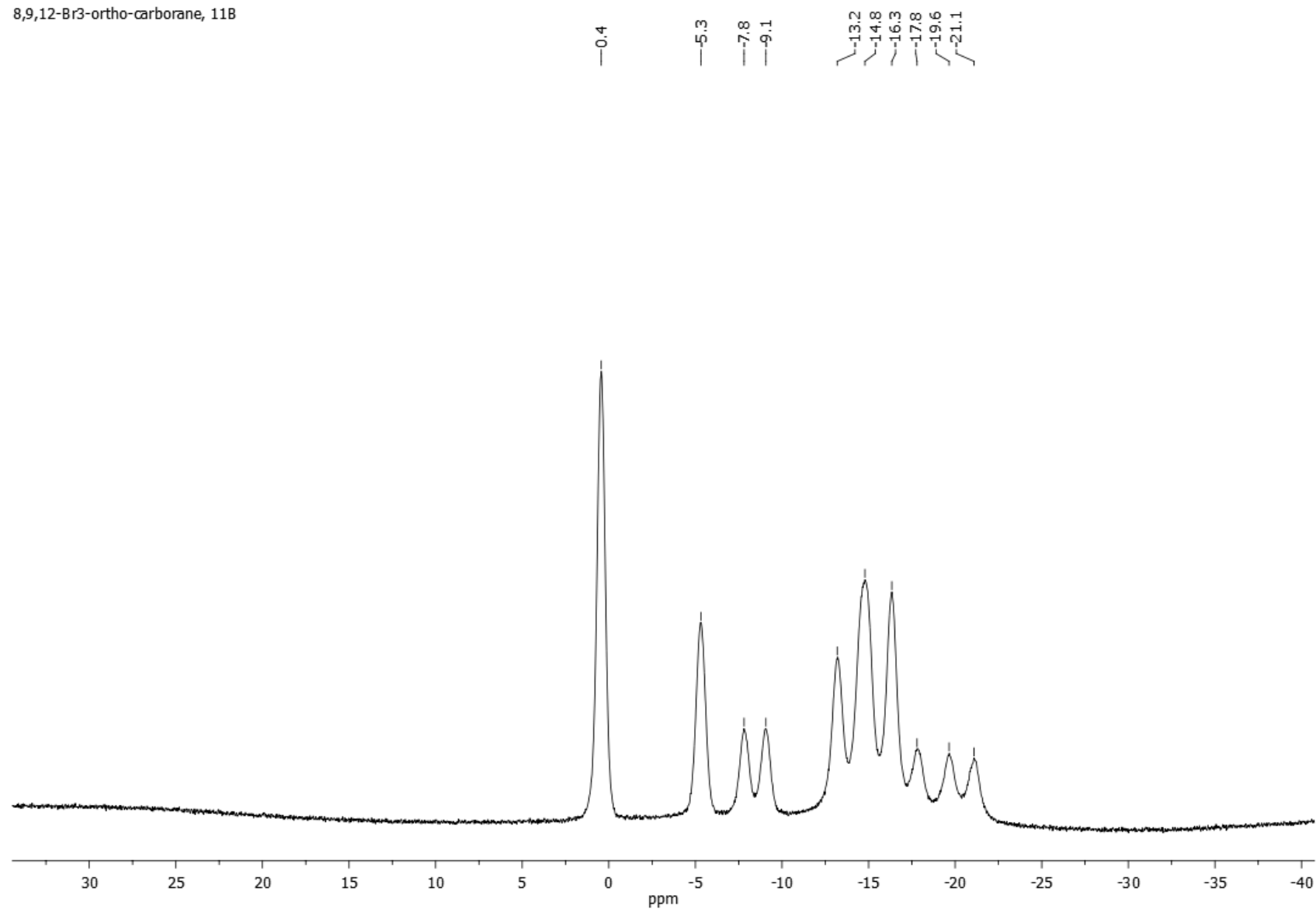
**Figure S1.** <sup>1</sup>H NMR spectrum of 8,9,12-Br<sub>3</sub>-*ortho*-carborane.

8,9,12-Br<sub>3</sub>-ortho-carborane, <sup>11</sup>B{<sup>1</sup>H}



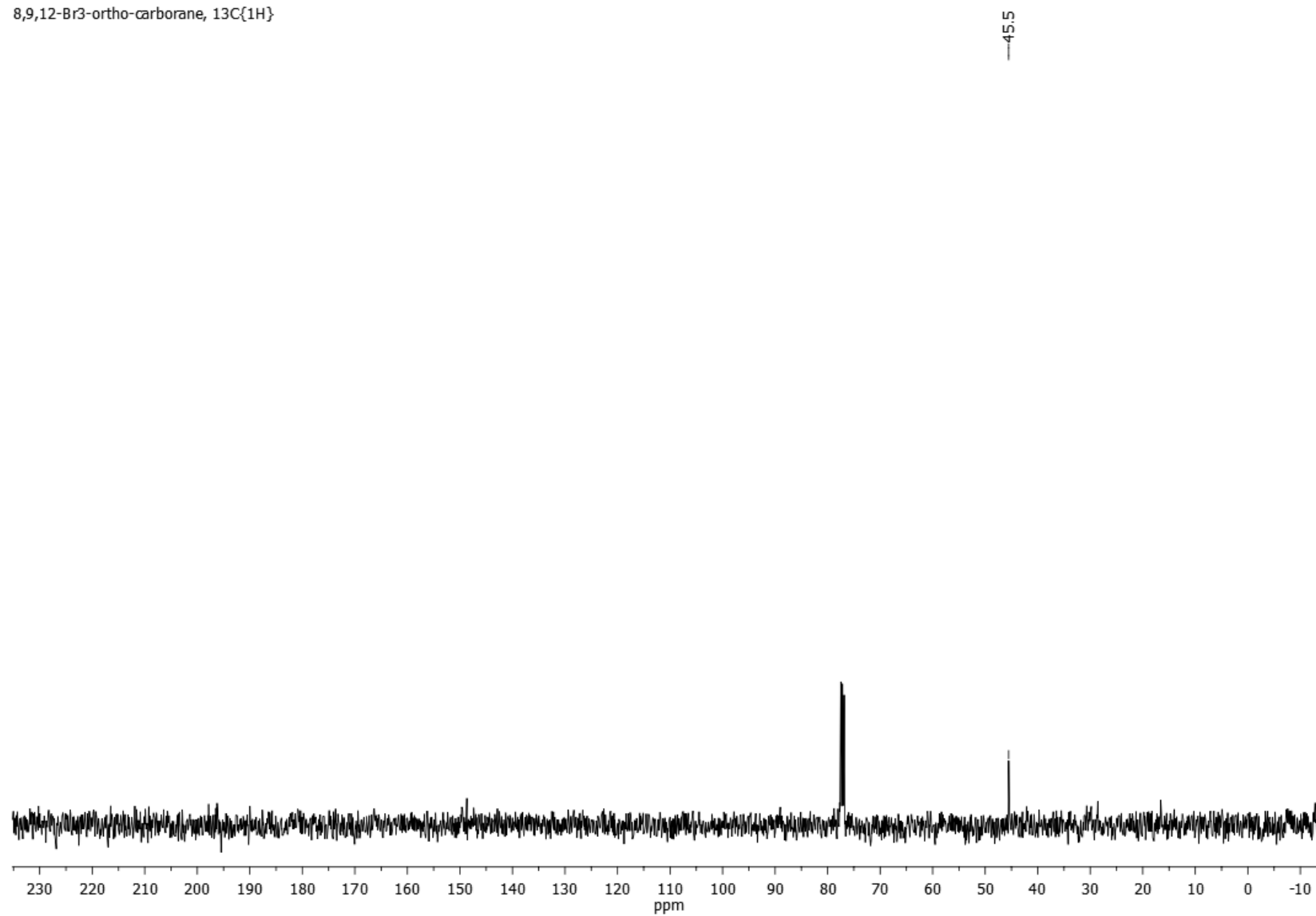
**Figure S2.** <sup>11</sup>B{<sup>1</sup>H} NMR spectrum of 8,9,12-Br<sub>3</sub>-ortho-carborane.

8,9,12-Br<sub>3</sub>-ortho-carborane, 11B

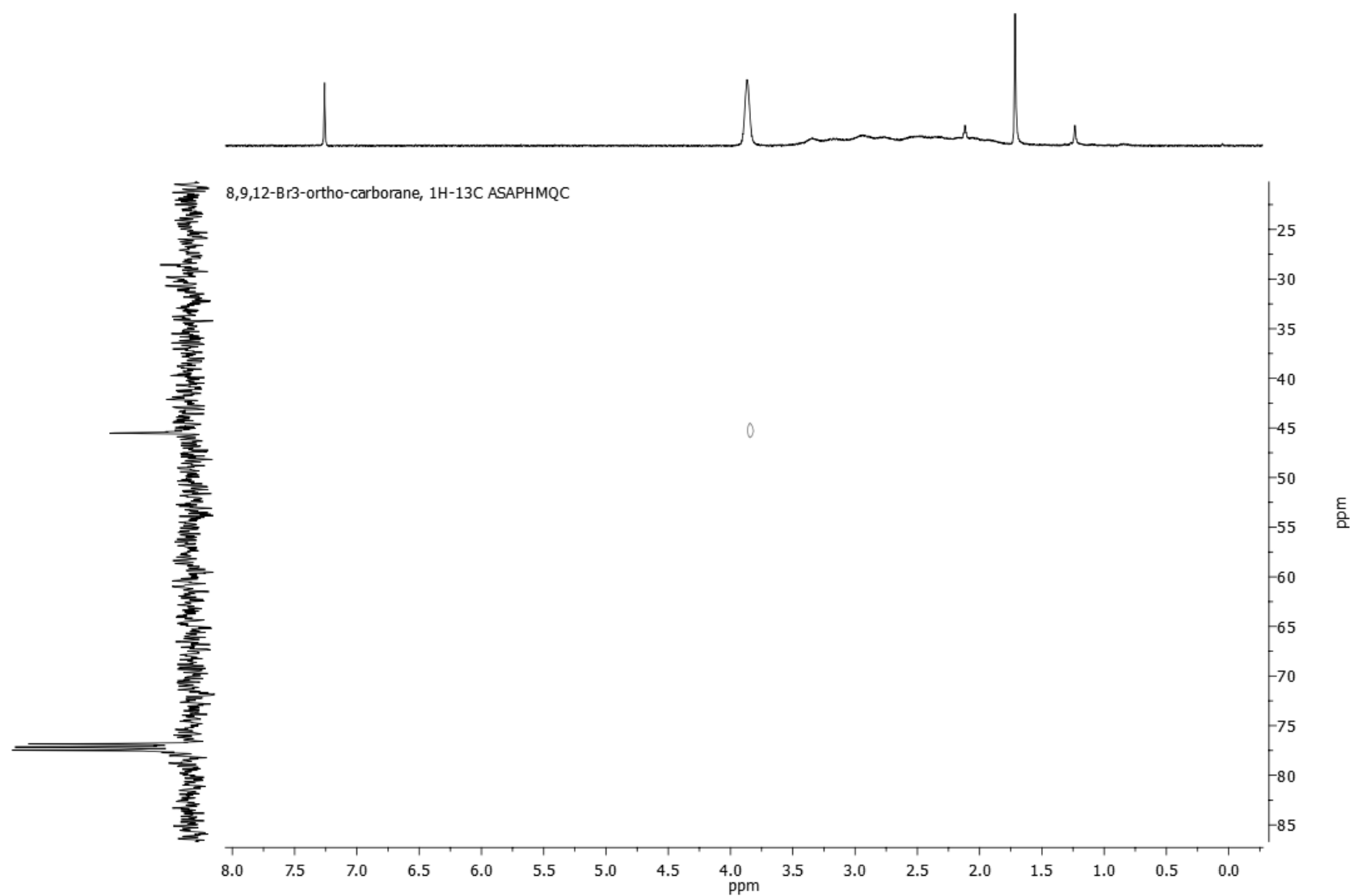


**Figure S3.** <sup>11</sup>B NMR spectrum of 8,9,12-Br<sub>3</sub>-*ortho*-carborane.

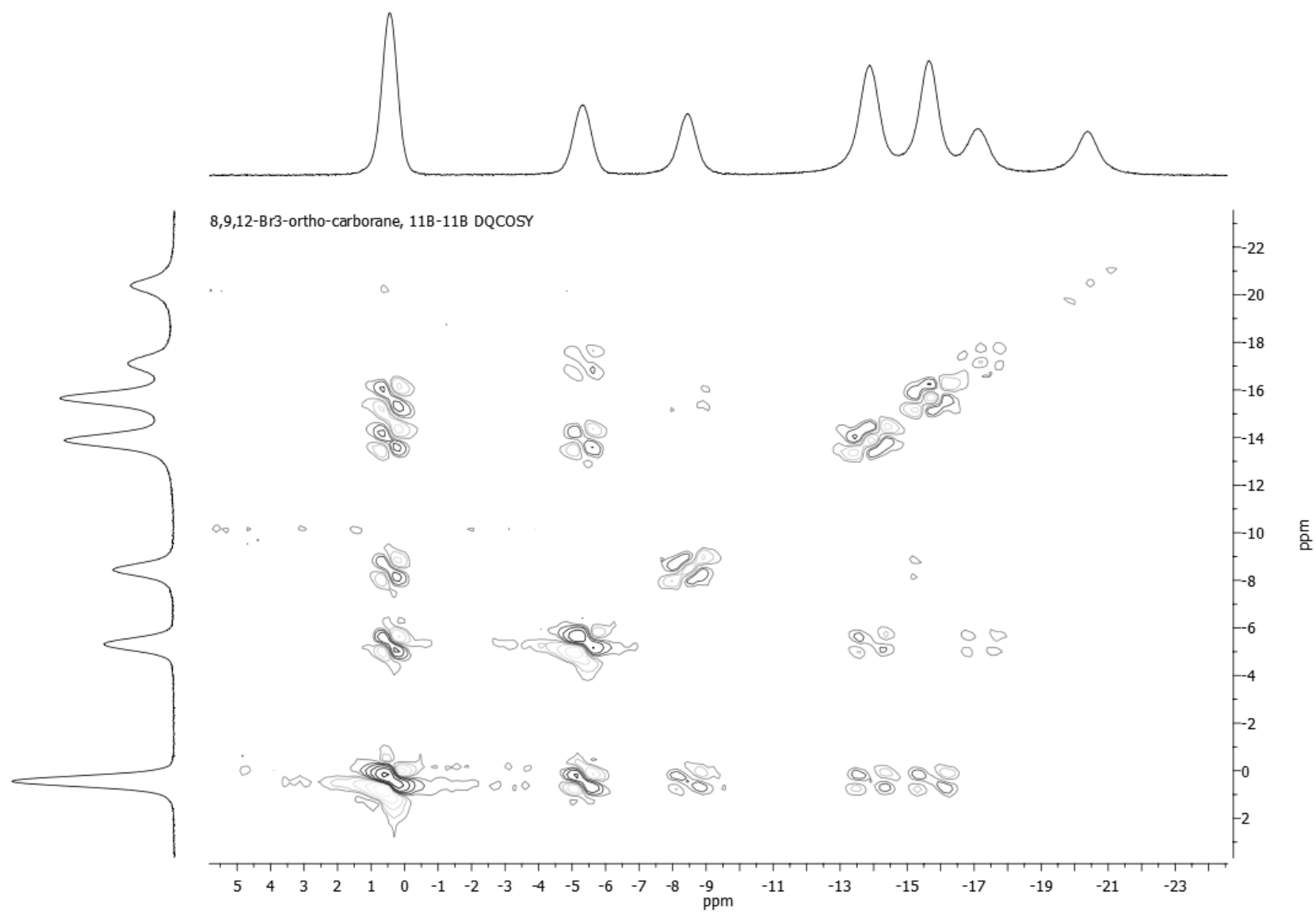
8,9,12-Br<sub>3</sub>-ortho-carborane, <sup>13</sup>C{<sup>1</sup>H}



**Figure S4.** <sup>13</sup>C NMR spectrum of 8,9,12-Br<sub>3</sub>-*ortho*-carborane.

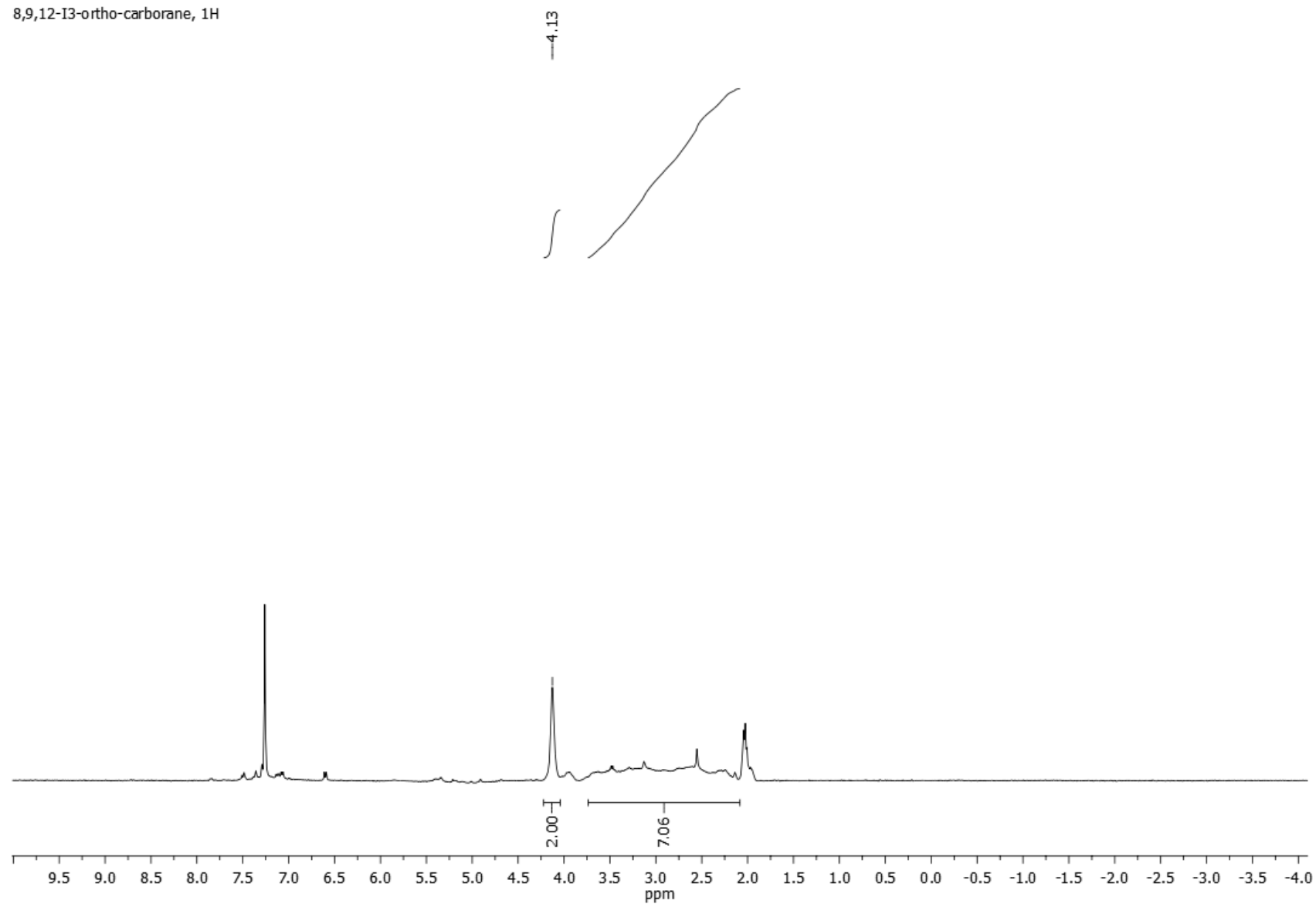


**Figure S5.** <sup>1</sup>H-<sup>13</sup>C ASAPHMQC NMR spectrum of 8,9,12-Br<sub>3</sub>-*ortho*-carborane.

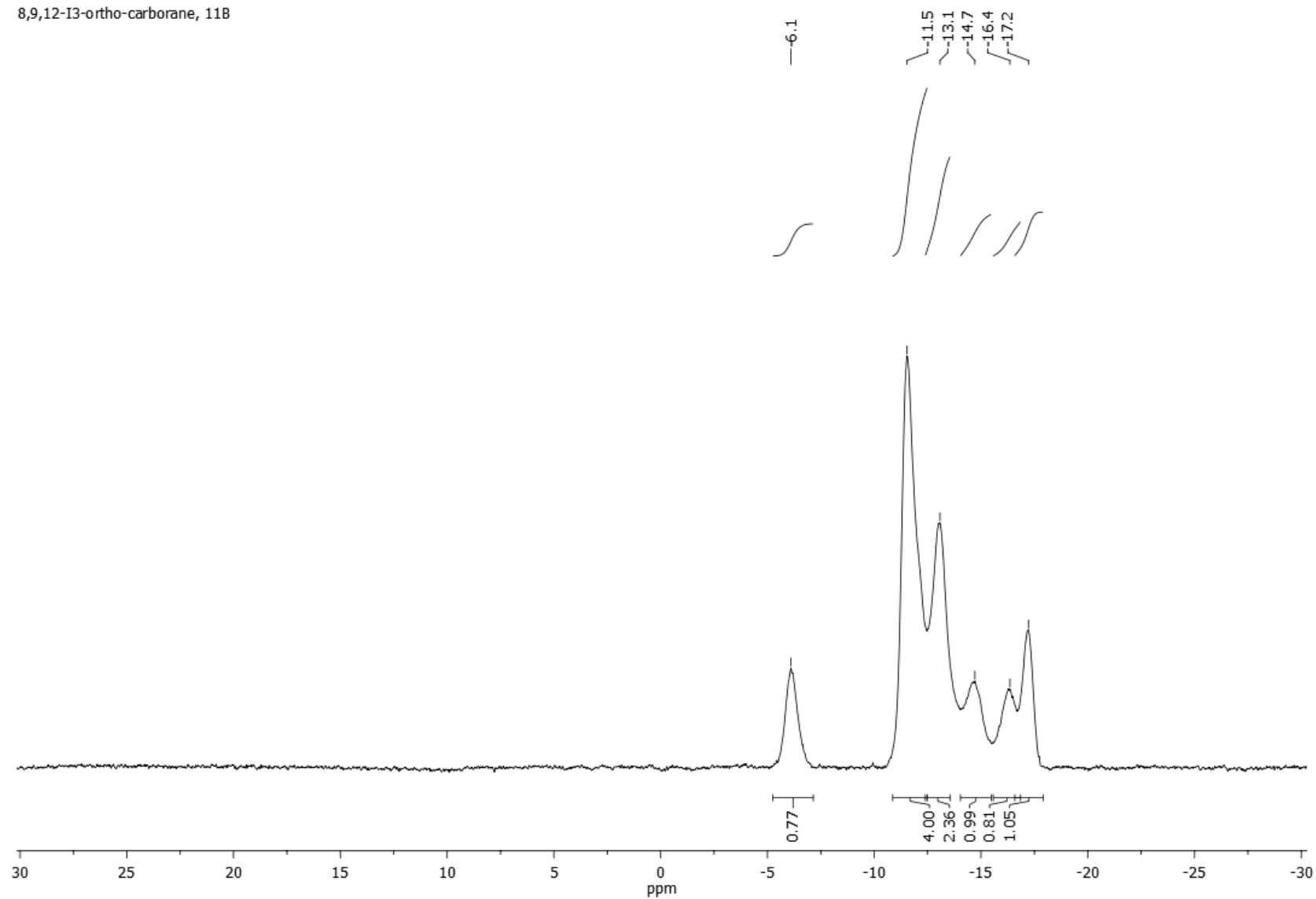


**Figure S6.**  $^{11}\text{B}$ - $^{11}\text{B}$  DQCOSY NMR spectrum of 8,9,12-Br<sub>3</sub>-*ortho*-carborane.

8,9,12-I<sub>3</sub>-ortho-carborane, 1H



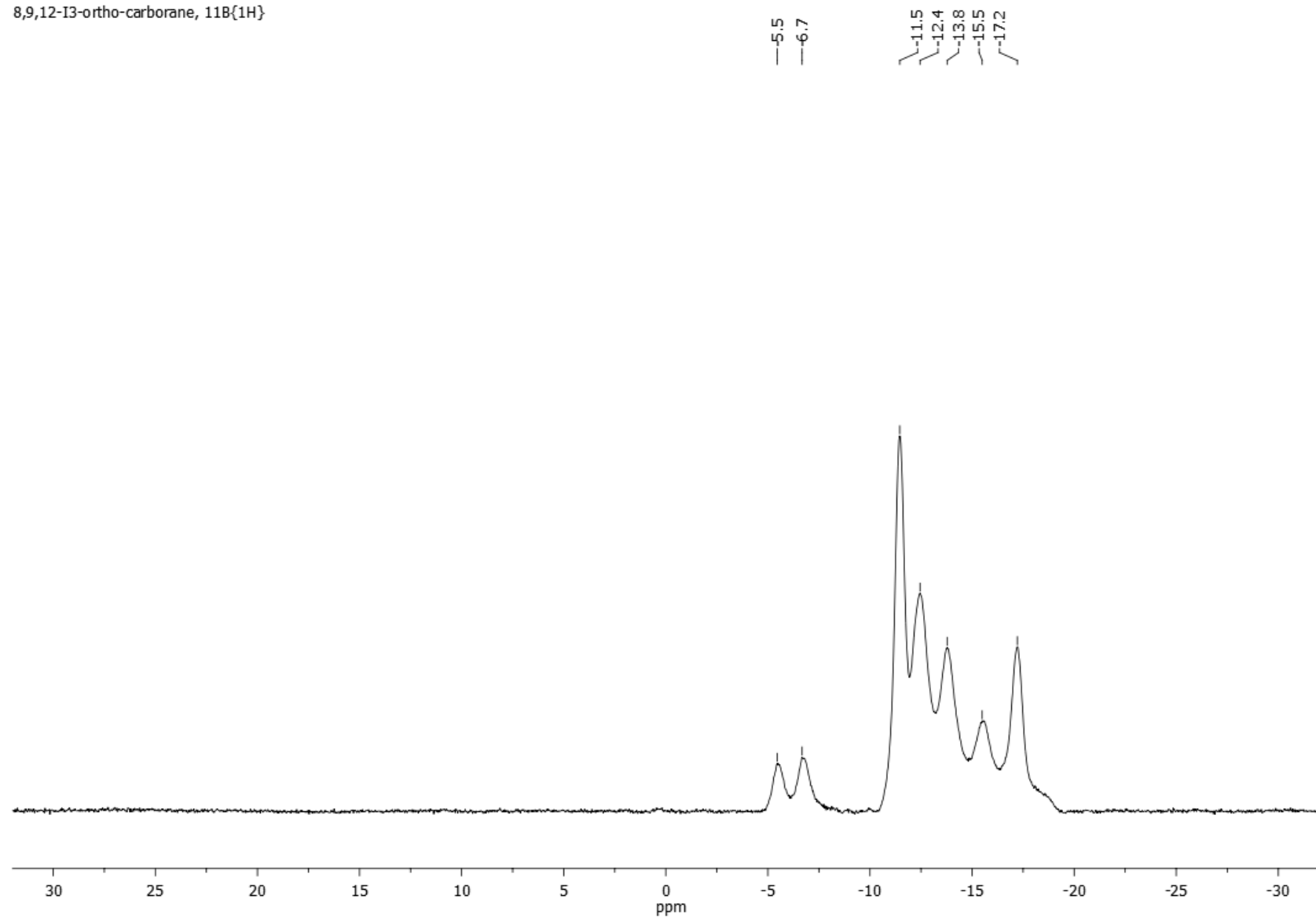
**Figure S7.** <sup>1</sup>H NMR spectrum of 8,9,12-I<sub>3</sub>-*ortho*-carborane.



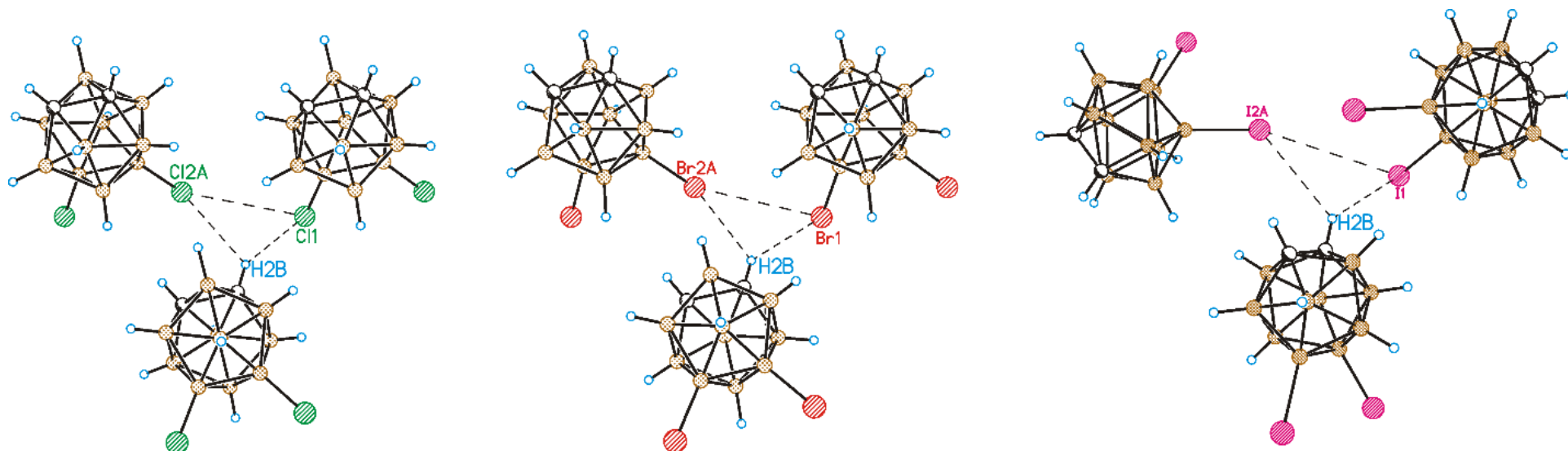
**Figure S8.** <sup>1</sup>H NMR spectrum of 8,9,12-I<sub>3</sub>-ortho-carborane.



8,9,12-I<sub>3</sub>-ortho-carborane, 11B{<sup>1</sup>H}



**Figure S9.** <sup>11</sup>B{<sup>1</sup>H} NMR spectrum of 8,9,12-I<sub>3</sub>-ortho-carborane.



**Figure S10.** View of trimeric associates in 9,12-dichloro-, 9,12-dibromo- and 9,12-diiodo- (from left to right) derivatives of *ortho*-carborane. Chloro- and bromo-derivatives are isostructural while crystal packing of iodo-derivative is different. Trimeric associate of iodo-derivative can be considered only from the formal point of view: only I1...H2B contact is shorter than sum of van-der-Waals radii while I1...I2A and I2A...H2B contacts are significantly longer.