

POWER OF ^{11}B NMR SPECTROSCOPY IN STUDIES OF HETEROBORANES

Jan Vrána,^a Josef Holub,^b and Aleš Růžička^a

^a Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentská 573, 532 10 Pardubice, Czech Republic

^b Institute of Inorganic Chemistry, Czech Academy of Sciences, 250 68 Řež, Czech Republic

✉ ales.ruzicka@upce.cz

In the hundred-year-history of boron hydrides and their successors (polyhedral boranes, carboranes and other heteroboranes) and derivatives, the number, molecular shape, reactivity and applications of these species have become enormous, thus establishing a self-consistent field of chemistry. Areas of possible applications of these species ranging from energy/hydrogen storage, synthetic organic chemistry, catalysis and medicine to preparation of new materials.

In contrast to organic chemistry, the reaction mechanisms involving boranes and boron clusters can be very complex since there are very small energy differences between many intermediates and transition states, thus reactions of boron hydrides can involve many competing pathways.

In this work, we would like to illustrate the power of 1D and 2D ^{11}B NMR spectroscopy for understanding numerous boron cluster transformations and structural properties.^[1](Figure 1).

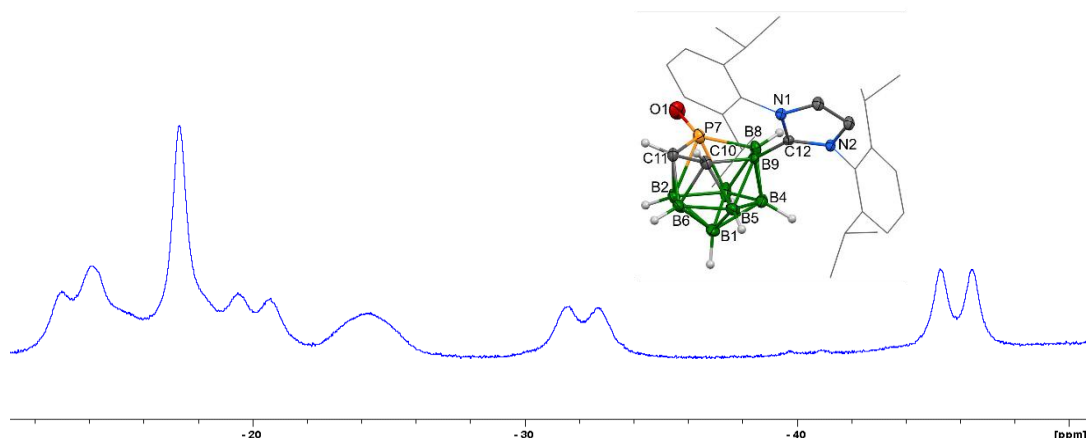


Figure 1. An example of ^{11}B NMR spectrum and structure of shown compound.

Acknowledgements. Authors wish to thank the Czech Science Foundation grant nr. 22-03945S.

REFERENCES

- [1] J. Vrána, J. Holub, M. A. Samsonov, Z. Růžičková, J. Cvačka, M. L. McKee, J. Fanfrlík, D. Hnyk, A. Růžička, *Nat. Commun.* **2021**, *12*, 4971–4977.