Chalcogens Outerly and Innerly Functionalize Various Boron-Based Cages. Molecular Structures of the Resulting Heteroboranes Determined Using Electron Diffraction and Computational Protocols

Drahomír Hnyk,[a] Josef Holub, Tomáš Baše, [a] Jan Macháček,[a] Yury V. Vishnevskiy, [b] Christian G. Reuter,[b] Norbert W. Mitzel[b] and Derek A. Wann[c]
hnyk@iic.cas.cz

The development of modern computational methods, linked to improved methods for analysis of experimental gas-phase structural data, has allowed the stereochemistry of many boranes and heteroboranes to be determined with great accuracy over the past two decades. Many of these compounds have been prepared in the Institute of Inorganic Chemistry, Czech Academy of Sciences and gas-phase electron diffraction (GED) data have been obtained mainly at the University of Edinburgh and also at the University of Oslo and at the University of Bielefeld. Structural tools based on the concerted use of GED (using Edinburgh-based, Oslo-based, and Bielefeld-based refinement programs) and computations of the geometries and ^{11}B chemical shifts (*MOCED, SARACEN)* have been employed [1,2]. (^{11}B chemical shifts are often employed as an additional refinement condition.) Different *closo*- and *nido*-geometrical shapes containing sulfur and selenium are reported.

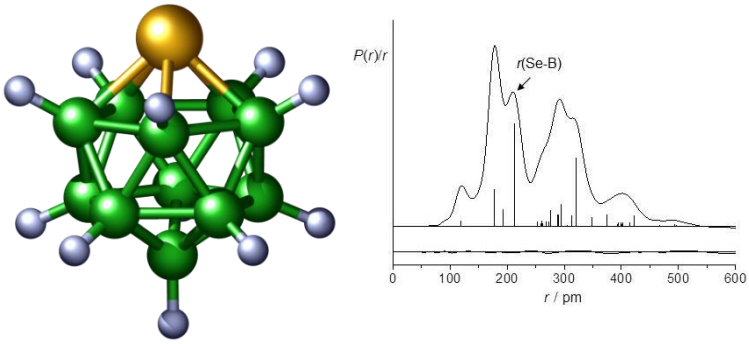

Figure 1: closo-1-$SeB_{11}H_{11}$, its molecular structure with radial distribution curve from GED as an example.

References

1. D. Hnyk, D.W.H. Rankin, *Dalton Trans.* (2009**)**, 585.
2. D. Hnyk, D. A. Wann, Boron – the Fifth Element, Chapter 2, *Challenges and Advances in Computational Chemistry and Physics.* Vol 20, (Eds. D. Hnyk, and M. McKee), Springer, Heidelberg, New York, Dordrecht and London, 2015.