

Polyhedral Heteroboranes; from 3D aromatics to cations or superbases

Aleš Růžička^a, Jan Vrana^b, Vlastimil Nemeč^b

^a University of Pardubice

^b Uni Pardubice

* Presenting author: 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. Polyhedral boranes and hereroboranes appear almost exclusively as neutral or anionic species, while the cationic ones are protonated at exoskeletal heteroatoms or they are instable. Taking these considerations into account, one could expect that the addition of a strong σ -donor such as NHCs would increase the electron density on those traditionally taken electron-deficient skeletons and stabilize them like in the many cases of low-valent or cationic main-group elements.

Surprisingly enough, the addition of strong sigma-donors to various (hetero)boranes dramatically exchange its structure and reactivity.

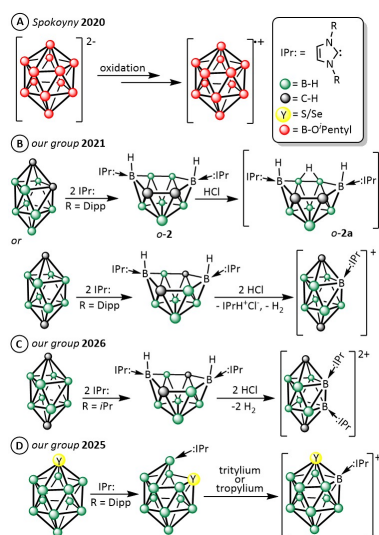


Figure 1 | Uploaded scheme / graphic

References

- Stauber, J. M. et al. A super-oxidized radical cationic icosahedral boroncluster. *J. Am. Chem. Soc.* **142**, 12948–12953 (2020).
 Vrána, J. et al. Access to cationic polyhedral carboranes via dynamic cage surgery with N-heterocyclic carbenes. *Nat. Commun.* **12**, 4971 (2021).
 Nemeč, V. et al. The far side of carboranes: anticancer active monocations and ambiently stable dications. *Angew. Chem., Int. Ed.* **65**, e202621595 (2026).
 Holub, J. et al. Cationic Polyhedral Chalcogenaboranes: Activation without breaking Wade's Rules. *Angew. Chem., Int. Ed.* **64**, e202419677 (2025).