

Title: Coordination vs. Insertion: Competitive Channels for the Bonding of Monovalent Boron

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Abstract: Only isolated or case specific pieces of experimental information are available to date for free monovalent boron and borylene compounds. A systematic theoretical investigation is missing from the literature so there are substantial gaps in our understanding of borylenes and their possible utility in organic and inorganic chemistry – either as ligands or intermediates in complex chemical reactions. We show that the relative stability of borylene complexes varies widely, depending on the electron donating ability of the R groups (considering a diverse range of R substituents). Moreover, an investigation of attractive interactions between several BH_3F Lewis acids (where $\text{M} = \text{C}, \text{Si}, \text{and Ge}$) shows that the $\text{R}'\text{H}_3\text{M} \cdots \text{BR} \rightarrow \text{R}'\text{H}_2\text{M}-\text{BHR}$ reaction is barrierless in some cases. For Si, in fact, a barrier appears only in the case where R is a very strong electron withdrawing group. The barriers are very high for C, and vary significantly for Ge.

