

The Influence of Organic Substituents on the Stability of Dative Bonding

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The stability of bonding interactions between MFH_3 molecules and borylene species (R--B), where $\text{M} = \text{Ge}, \text{Si}, \text{and C}$, is investigated. Borylene is by no means a particularly stable species, although under some conditions depending on the identity of the R substituent, the strength of the sigma hole, and the C-H bond activation, the proton transfer does not occur and a dative bond (or weak sigma hole interaction) between the monovalent B--R and the M center forms. The energy barrier going from the monovalent to the trivalent B substituent is examined and discussed for a range of electron withdrawing and donating R substituents. Additionally, due to the strength of a C-H bond, no proton transfer occurs for any of the carbon centers. For M group elements such as Silicon, proton transfer occurred more often, which may be explained by the low electronegativity of Silicon and the weakness of the Si---H bond.