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C-H activation for the construction of C-B bonds
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Abstract
A number of studies were conducted to demonstrate C-H activation for the construction of C-B bonds. Investigations revealed that the conversion of C-H bonds to C-B bonds was both thermodynamically and kinetically favorable. The reaction at a primary C-H bond of methane or a higher alkene B ₂(OR) ₄ formed an alkylboronate ester R' -B(OR)₂ and the accompanying borane H-B (OR₂. The ester and the borane were formed on the basis of calculated bond energies for methylboronates and dioaborolanes. The rates of key steps along the reaction pathway for the conversion of a C-H bond in an alkane or arene to the C-B bond in an alkyl or arylboronate ester were favorable. These studies also highlighted the accessible barriers for C-H bond cleavage and B-C bond formation during the borylation of alkanes and arenes.