Assessing Potential Energy Surfaces for M-CH₃ Functionalization

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Multiple pathways for the functionalization of metal-bound methyl groups are available to aspirant methane partial oxidation catalysts. Using quantum mechanical simulations, we examine potential energy surfaces underlying reductive elimination and nucleophilic attack, as well as Baeyer-Villager analogues and electrophilic attack by oxidants. Metal complexes known to operate catalytically and other complexes are used to illustrate the feasibility of the elementary steps and the dependence of their thermodynamics on the metal, ligands and oxidant.