Effect of Substituents on the Ligating Properties of N-Heterocyclic Carbenes with Inorganic Back Bones: A Theoretical Study

Abstract

Density functional calculations at BP86/TZVP level of theory have been carried out to investigate the effect of substituents on the ligating properties of *N*-heterocyclic carbenes (NHCs) with inorganic (B, Al, Ga) back bones. Both σ and π donor substituents attached to group 13 elements are chosen for this study to investigate their effect on the ligating properties of these carbenes. While π donating substituents increases their σ donation abilities, σ donating substituents increases their π accepting abilities. Comparison of their ligating properties with Arduengo type NHCs reveals that the π accepting abilities of NHCs can be enhanced by introduction of inorganic back bones such as group 13 elements without compromising their σ donation abilities.