

# On the nucleophilicity of boryllithium compounds. A theoretical study

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Boron compounds are widely used in synthetic chemistry. The synthesis of the compounds is relatively easy, presenting thermodynamic stability and synthetic versatility. Almost all of them show electrophilic reactivity. Recently, some boryllithium species have been reported as a base or a nucleophile in reaction with organic electrophiles in  $S_N2$  reactions. In the present work, the proton affinity (PA) of boryllithium compounds was calculated. These values can be useful as theoretical reference values and to provide valuable complementary information for the interpretation and discussion of the basicity of these compounds. The proton affinity was calculated using a theoretical method based on density functional theory and high-level theoretical methods through MP2 and G2MP2 levels of theory. In addition, some global and local reactivity indexes based on density functional theory (DFT) on boryllithium compounds were studied. In order to compare and discuss the chemical reactivity of these