Steric Versus Electronic Control During the Carbonylation of Substituted Thexylboranes. A Semi-Empirical Investigation

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Abstract

AM1 and PM3 calculations have been carried out to study the reaction of substituted thexylboranes with carbon monoxide. Exhaustive investigation of the complete potential energy surfaces of thexylborane and several substituted derivatives was carried out in order to determine the relative importance of steric and electronic factors in determining the ability of thexylboranes to form stable adducts with carbon monoxide. It is concluded that the primary reason that methyl-isopropy-thexylborane forms a less stable adduct with CO than does dimethyl-thexylborane is because of the increased steric demands around the boron atom when one of the alkyl substituents on the thexylborane is branched. These results help to explain recent experimental observations regarding the reactivity of branched versus straight chain thexylboranes.