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Theoretical Study of Oxidative Addition to Platinum Metal Complexes: V. Kinetic Substrate Selectivity of Dichlorobis(phosphine)platinum(II) in Reactions with Alkanes

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Abstract

Complete geometry optimization has been performed for products of oxidative addition of alkanes to trans-PtCl2(PH3)2, transition states for concerted insertion of the metal into hydrocarbon C-H bond have been localized, and the energies of stationary points on the potential energy surface have been calculated. The kinetic and thermodynamic selectivities of the complex have been estimated.