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Quantum-chemical methods for studying geometrical structure of hydride complexes of palladium(II) with styrene

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Abstract

In the work the composition of palladium(II) complexes have been discussed, through the formation of which the reaction of styrene carbonylation proceeds. Geometrical structure of the complex of palladium with styrene, chloride-anion and carbon(II) monoxide, as well as hydride complex of palladium with styrene, chloride-anion and acetate-anion have been studied. Calculations were performed by B3LYP method with the use of the combined basic sets in which for the atom of palladium there have been used bases TZVP and DZVP, and for the remaining atoms there have been used different valence-disintegrated bases. After considering the results of calculations there have been made the conclusions concerning the effect of geometric structure of complexes on the ultimate yield of product of carbonylation of styrene.