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The DFT study of nickel intermediates in catalytic cycloaddition of ethylacrylate to norbornadiene

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Abstract

The interaction of bis(η^4-norbornadiene)nickel (the catalyst of cycloadditon) with ethylacrylate and norbornadiene was studied by DFT-PBE method using TZ2P basis set. The formation of Ni(0) complexes, containing two, three and four ligands and their isomers were considered. It was shown, that the solvent (toluene) cannot compete with the olefins for coordination site on Ni atom. The formation of cycloadducts with more than three ligands was not favorable kinetically and thermodynamically. The most stable intermediates were found on the basis of thermodynamical analysis (ΔH_0, $\Delta H_0^{\neq}$).