STABILIZATION OF THE TRANSITION STATE OF THE FORMATION OF 1,3-DIOXANES ON THE PRINCE REACTION IN THE PRESENCE OF CARBON NANOTUBES

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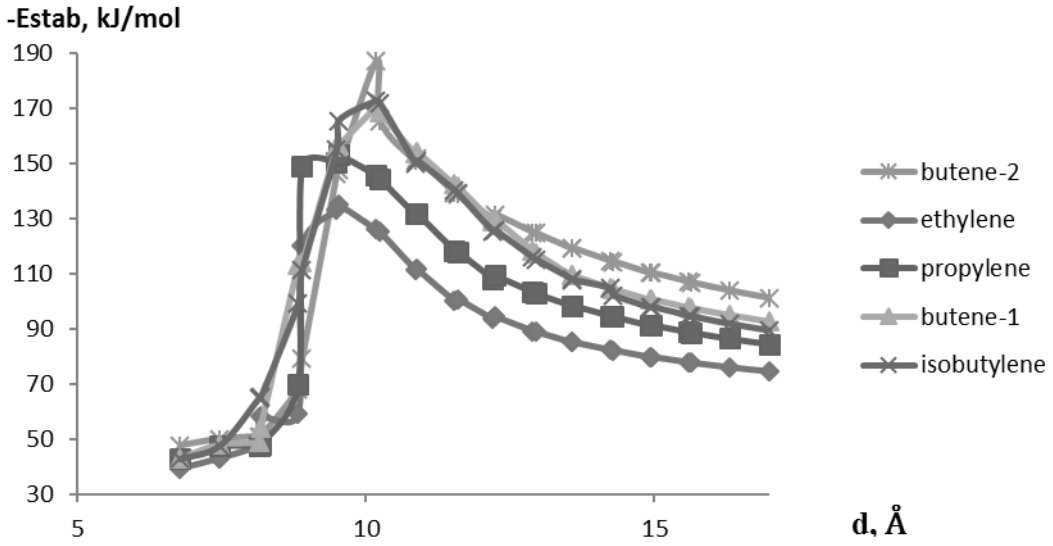
The possibility of increasing the selectivity of the formation of 4,4-dimethyl-1,3-dioxane by the Prins reaction, which is a key intermediate in the synthesis of isoprene by the "dioxane" method, has been studied using quantum chemistry and molecular dynamics. We considered the stabilization of the TS in carbon nanotubes.

Influences of the CNT diameter on the energy of TS stabilization were determined. As model compounds, ethylene, propylene, butene-1, isobutylene and trans-2-butene were considered. In modeling TS adsorption on CNT, we considered nanotubes with diameters from 6 to 17 Å. Below we present the dependence of the stabilization energy TS 1,3-D on the diameter of carbon nanotubes.



The stabilization of the TS of the reaction for the formation of 1,3-dioxane becomes greatest with nanotube diameters from 9.49–12.23 Å. The maximum stabilizing effect is observed when the diameter is 10.18 A.

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