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

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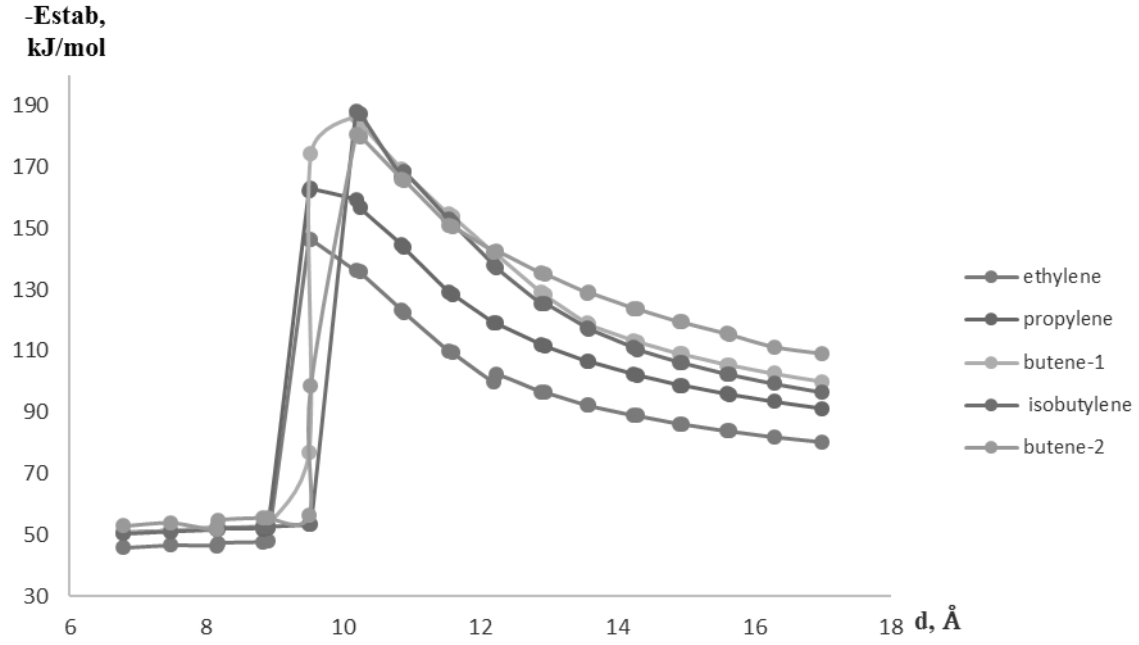
An increasing of the selectivity of the formation of 1,3-dioxanes can be achieved in the presence of substances with a developed surface containing cavities of a certain cross section.

To this end, we studied the interactions of the transition state of formation of oxygen-containing heterocycles according to the Prince reaction with BNNT. The influence of diameter on the energy of stabilization of the transition state was determined. Energy parameters and the nature of the interaction of transition states with BNNT were determined using the Adsorption Locator module included in the program package Accelrys Material Studio.

When modeling TS adsorption on BNNT, we considered nanotubes with diameters from 6 to 17 Å. Below, the dependence of the stabilization energy TS 1,3D on the diameter of boronitride nanotubes.



Stabilization becomes greatest with nanotube diameters from 9.52–12.23 Å. The maximum stabilizing effect is observed at 10.18 Å.

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