

**DEVELOPMENT OF WAYS OF IMPROVING EFFECTIVENESS OF IZOPREN
PRODUCTION BY "DIOXANE" METHOD IN PRESENCE OF ZEOLITES
OF GROUP $\text{Na}^+_x (\text{H}_2\text{O})_y [\text{Al}_a\text{Si}_b\text{O}_c]$**

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The possibility of increasing the selectivity of the formation of the 4,4-dimethyl-1,3-dioxane reaction of 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 have considered the stabilization of the transition state (TS) of this reaction on zeolites $\text{Na}^+_x (\text{H}_2\text{O})_y [\text{Al}_a\text{Si}_b\text{O}_c]$ with pores of different sections (Table, Fig.). It is shown that the TS stabilization of the formation of 1,3-dioxane becomes most advantageous on zeolites with pore sizes of 6.08–7.72 Å. Obviously, in this case the TS can be placed inside the pore of the zeolite and stabilized due to intermolecular interactions with the entire inner surface of the pore.

With a pore diameter of less than 6.08 Å, the TS is no longer able to fit inside and only partially stabilizes due to interaction with the zeolite surface. In the case of zeolites with a large pore diameter, intermolecular interactions can be carried out with a fragment of the inner or outer surface of the pore.

Table. The dependence of the adsorption energy of transition states on the pore diameter of zeolites, kJ/mol

Zeolite	d, Å	ethylene	propylene	buthene-1	isobutylene	trance-2-buthene
ANA	4.21	-11.8	-12.4	-13.3	-12.9	-16.5
NAT	4.52	-13.2	-13.9	-15.5	-15.2	-15
TON	5.71	-30.8	-21.1	-23	-21.1	-25.7
MTW	6.08	-29.2	-33.6	-38.6	-31.7	-37.1
LOS	6.36	-34	-40.8	-44.1	-45.5	-43.7
EUO	7.00	-32.1	-36.8	-41	-42.7	-40.9
MEL	7.72	-27.7	-32.6	-36.6	-36.3	-36.5
MEI	8.06	-24.9	-27.3	-30.4	-31	-30.4
KFI	10.67	-27	-28.9	-28.3	-29.3	-29.7

This type of TS stabilization indicates the possibility of increasing the selectivity of the formation of 1,3-dioxanes by the Prins reaction in the presence of zeolites with pore sizes from 6.08 to 7.72 Å.

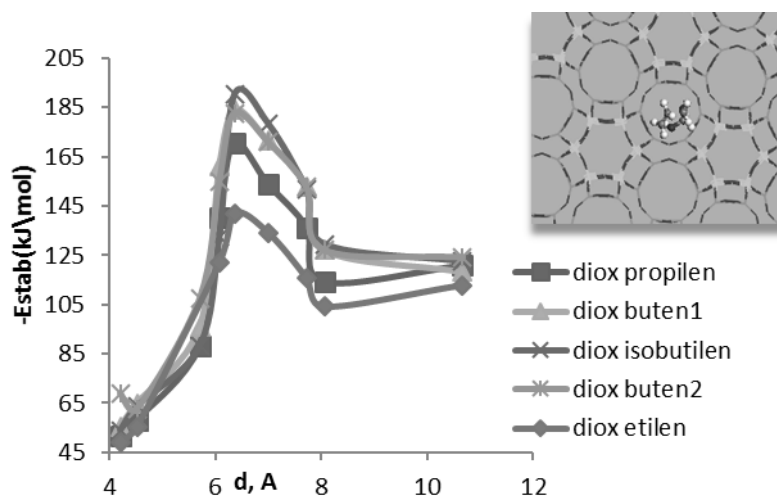


Fig. Stabilization of the transition state of the formation reaction of 1,3-dioxanes in the presence of group zeolites $\text{Na}^+_x (\text{H}_2\text{O})_y [\text{Al}_a\text{Si}_b\text{O}_c]$

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