

**DEVELOPMENT OF WAYS OF IMPROVING EFFECTIVENESS OF IZOPREN
PRODUCTION BY "DIOXANE" METHOD IN PRESENCE OF ZEOLITES
OF GROUP Si_xO_y**

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The possibility of increasing the selectivity of the formation of the 4,4-dimethyl-1,3-dioxane 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 of Si_xO_y composition with pores of different cross 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 6.25–7.01, 7.24–7.59 Å. Obviously, in this case, the TS can most conveniently be placed inside the pore of the zeolite and stabilized by intermolecular interactions with the entire inner surface of the pore.

At a pore diameter of 6.8, 7.47 Å, the TS stabilizes only partly due to interaction with the zeolite surface. In the case of zeolites with a large pore diameter, intermolecular interactions can be performed with a fragment of the inner or outer surface of the pore.

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

Zeolite	d, Å	ethylene	propylene	buthene-1	isobuthylene	trans-2-buthene
MTF	6.25	136.68	158.88	171.88	130.45	174.724
VET	6.39	110.89	130.95	147.67	139.31	151.39
SFE	6.66	127.99	94.67	112.77	87.02	112.19
STO	6.8	78.04	73.73	74.82	66.37	68.8
ISV	7.01	108.13	125.56	144.62	146.63	138.14
IFR	7.24	118.29	131.37	154.45	150.68	152.73
CFI	7.47	93.59	112.9	129.91	132.25	132.92
SFF	7.59	114.78	137.52	158.79	155.95	158.54
STF	7.63	110.39	129.58	152.02	151.94	153.4
ITE	8.3	109.18	129.78	146.35	150.81	149.01

This type of TS stabilization indicates the possibility of increasing the selectivity of the formation of 1,3-dioxanes by the Prince reaction in the presence of zeolites with pore sizes of 6.25–7.01, 7.24–7.59 Å.

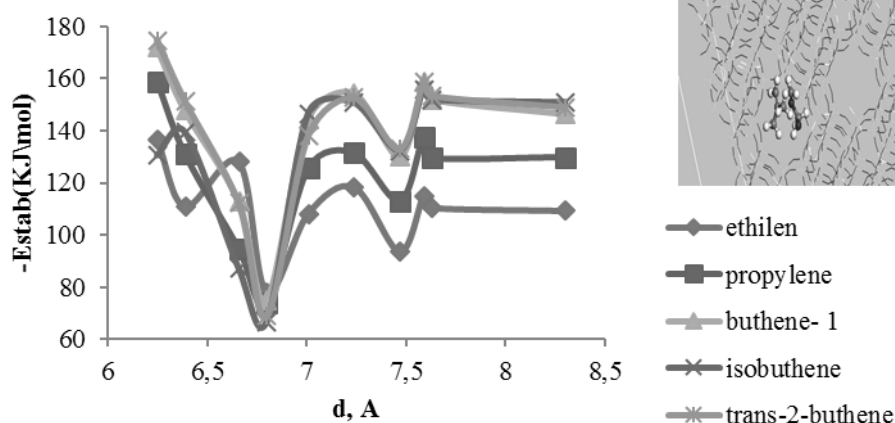


Fig. Stabilization of the transition state of the formation of 1,3-dioxanes in the presence of group zeolites Si_xO_y

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