

**STUDY OF THE FEATURES OF STABILIZATION OF TRANSITION STATES
OF THE PRINCE REACTION ON CLUSTERS FROM CARBON AND BORNITRIDE
NANOTUBES**

*Zaytunova G. G.*¹, Pasko P. A.¹, Vakulin I. V.¹, Talipova G. R.¹, Vakulina A. I.²

¹Bashkir state University, Ufa, Russia

²Ural State University of Economics, Yekaterinburg, Russia

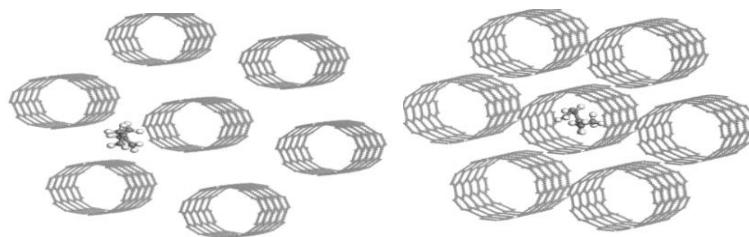
zajtunovag010@gmail.com

An increase in 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 section. We considered the stabilization of the TS in clusters of nanotubes, which are characterized by an additional TS stabilization site. To build clusters, we used nanotubes with the optimum diameter found earlier. The table shows the sections of the cavity that arises between the tubes in the cluster at different distances between the walls of the tubes.

Table

d nnt (Å)	L (distance between nanotube walls, Å)							
	0,847	1,5	2,5	3,347	5,847	8,347	10,847	13,347
D (cavities in a cluster, Å)								
8,89	5,62	5,98	6,56	7,06	8,50	9,94	11,38	12,82
9,49	5,96	6,34	6,92	7,40	8,84	10,29	11,73	13,17
9,52	5,98	6,36	6,94	7,42	8,86	10,31	11,74	13,20
10,18	6,36	6,74	7,32	7,80	9,24	10,70	12,13	13,58
10,24	6,38	6,78	7,34	7,84	9,28	10,73	12,16	13,61
10,85	6,74	7,12	7,70	8,19	9,63	11,08	12,51	13,96
11,53	7,14	7,52	8,10	8,58	10,02	11,46	12,90	14,35
12,20	7,52	7,90	8,48	8,97	10,41	11,85	13,29	14,73
13,58	8,32	8,70	9,28	9,76	11,20	12,64	14,08	15,52

In all cases, stabilization of the transition state inside the tube proves to be more advantageous than stabilization in the cavity between the walls.



It is interesting to note, that the profitability of the stabilization of the transition state between the walls is also of extreme nature, but the maximum of stabilization is achieved at large values of the cavity cross section as compared to the diameter of the nanotube.

This research is supported by the grant № 17-43-020754 of Russian Fund of Basic Researches.