Obtaining aromatic carbohydrates by catalytic aromatization of hexane with a linear structure

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Abstract. In this article, the kinetics of the synthesis of benzene-free aromatic hydrocarbons by aromatizing hexane with the modified 2%La/N-YuKTs-40 and 2%La*2%Cu*8%Zn/N-YuKTs-40 catalysts in the presence of catalysts was studied. 2%La*2%Cu*8%Zn/N-YuKTs-30 for a catalyst with higher catalytic activity was selected for aromatization of hexane with a linear structure to obtain aromatic hydrocarbons Ekaj 2%La*2%Cu*8%Zn/N-YuKTs-20 was found to be smaller than the catalyst with higher activity selected for the aromatization of hexane with a linear structure to produce aromatic hydrocarbons. 2%La*2%Cu*8%Zn/N-YuKTs-30 and 2%La*2%Cu*8%Zn/N-YuKTs-20 with higher catalytic activity were selected for aromatization of hexane with a linear structure to obtain aromatic hydrocarbons the process of improvement of low-octane 85-1800C gasoline fractions on catalysts was studied at atmospheric pressure, in the temperature range of 400-5000C, without hydrogen-containing gas circulation. It was found that the 2%La*2%Cu*8%Zn/N-YuKTs-30 catalyst with high catalytic activity, selected for the catalytic aromatization of hexane with a linear structure, produces a high-octane catalyst with aromatic hydrocarbons as its main.

1 Introduction

Modern processes of oil refining and petrochemicals are based on catalytic technologies. One of the primary methods for refining oil that yields the high octane content of motor fuels and individual aromatic compounds like xylene, toluene, and benzene is catalytic reforming. Increasing the share of high-octane, benzene-free components (alkylates, isomers, oxygenates), as well as the use of environmentally non-toxic anti-detonation agents are of interest to world scientists [1-2].

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To meet the strict requirements of oil refining processes, the international market offers the latest catalytic technologies: ultra-deep hydro treating, chain branches and hydrogen release process as well as hydrogen recycling. Development and renewal of the process, abandoning the old technology, oil and gas processing is the most important and manifested itself in connection with the increased requirements for the quality of gasoline as a motor fuel, that is, first of all, their octane number [3-5].

With high-silicon-modified mesoporous aluminosilicates, the selectivity of ArU increases to 60% for n-hexane, and the yield of important substances resulting from the process is significantly reduced. In particular, a catalyst with high activity and selectivity selected for the aromatization of n-hexane to aromatic hydrocarbons contains about 15% propane about 5% each of methane, and about 5% ethane. The mechanism of aromatization is a very complex process [6, 8].

In addition to the above-mentioned point of view, the activation mechanism of lower molecular saturated hydrocarbon molecules through the elimination of hydride ions of carbanions or the release of primary hydrogen has been proposed. The need for automobile gasoline and aromatic hydrocarbons is increasing day by day, and research aimed at increasing the production of hydrocarbons with an increased octane number by improving the production process of liquid fuel by catalytic aromatization of hydrocarbons is urgent [9-11].

2 Methods

Qualitative and quantitative composition of gaseous products formed while obtaining aromatic hydrocarbons by catalytic aromatization of liquid and linear hexane for modified 2%La/N-YuKTs-40 and 2%La*2%Cu*8%Zn/N-YuKTs-40 catalysts analysis was done using gas-liquid chromatography on a "Krystallyuks-4500M" chromatograph with a flame ionization detector. The reaction products were analyzed using a phytochrome-I column (6 m x 3 mm). The stationary phase is 15% triethylene glycol dibutyrate. The temperature of the columns is 500C [12, 13].

The magnitude of the constant coefficient Const depends on the selection of the graph scale in the structure of the curves x=f(no). The magnitude of the observed activation energy was determined based on the following equation at a constant rate of change of the initial substance according to the temperature dependence of the observed rate of the reaction [14-17].

$$W = -Const \cdot n_0^2 \frac{dx}{dn_0} \tag{1}$$

Where Const WT1 and Const WT2 are observed reaction rate constants at temperatures T1 and T2. It is also possible to graphically determine the observed activation energy from the tangent of the tilt angle of the Arrhenius line, which represents the dependence of LgConstW on 1/T.

To calculate the kinetic laws of linear hexane conversion, using the Frost equation, a series of experiments were conducted with increasing feed rates to reduce the depth of conversion of linear hexane. To calculate the kinetic laws of linear hexane conversion, using the Frost equation, a series of experiments were conducted with increasing feed rates to reduce the depth of conversion of linear hexane

3 Results and Discussion

T2%La*2%Cu*8%Zn/N-YuKTs-20 and 2%La*2%Cu*8%Zn/N-YuKTs-30 have high catalytic activity selected for catalytic aromatization of hexane with linear structure to obtain aromatic hydrocarbons Tables 1-2 show the results of changes in hexane with a linear structure in catalysts at temperatures of 400, 450, 5000C.

As the volumetric rate of raw material transfer increases, the linear structure hexane conversion depth and target product yield decrease.

The calculation results presented in Tables 3-6 and illustrated in Figures 1-4 show the kinetic dependence of the total transformation of hexane with a linear structure and its compliance with the Frost equation in the studied temperature range [15, 17-19].

Table 1. Distribution of transformation products of linear hexane in 2%La*2%Cu*8%Zn/N-YuKTs-20 catalyst with higher activity selected for aromatization of linear hexane to obtain aromatic hydrocarbons.

T,^{0}C	V, c^{-1}	A, %	Catalyst content,%				
			Alkanes	Isoalkanes	Aromatic	Cycloparaffins	Olefins
400	1.0	18.35	85.85	6.125	5.410	0.502	0.915
	2.0	13.64	89.90	4.645	4.745	0.401	0.613
	2.5	10.12	94.08	3.112	3.625	0.303	0.401
450	1.0	24.78	77.86	3.014	13.35	0.605	2.02
	2.0	19.98	82.70	2.714	10.84	0.503	0.901
	2.5	14.45	88.12	2.202	8.012	0.504	0.703
500	1.0	39.80	63.24	2.705	24.25	0.402	2.102
	2.0	31.25	71.65	2.615	19.85	0.325	0.804
	2.5	28.70	74.24	2.501	18.85	0.326	0.705

Here, A is the depth of change in hexane with a linear structure.

2%La*2%Cu*8%Zn/N-YuKTs-20 catalysts with high activity were selected for the aromatization of linear hexane to obtain aromatic hydrocarbons. The amount of aromatic hydrocarbons in the catalyst was 24.25%.

Table 2. Distribution of transformation products of linear hexane in 2%La*2%Cu*8%Zn/N-YuKTs-30 catalyst with high activity selected for aromatization of linear hexane to obtain aromatic hydrocarbons.

T,^{0}C	V, c^{-1}	A, %	Catalyst content,%				
			Alkanes	Isoalkanes	Aromatic	Cycloparaffins	Olefins
400	1.0	47.21	56.95	12.74	26.45	-	0.501
	2.0	40.48	66.44	9.450	21.54	3.112	0.503
	2.5	27.35	79.15	5.112	14.25	2.265	0.440
450	1.0	60.84	43.35	4.065	43.50	1.012	1.012
	2.0	54.95	49.34	3.332	39.68	2.330	1.025
	2.5	42.25	62.03	2.612	29.40	2.303	0.804
500	1.0	71.51	2.75	3.385	51.25	3.450	2.235
	2.0	64.98	39.40	3.412	46.50	2.894	2.221
	2.5	47.42	56.95	0.704	33.64	1.015	1.016

Here, A is the depth of hexane conversion with a linear structure

2%La*2%Cu*8%Zn/N-YuKTs-30 catalysts with high activity were selected for the aromatization of linear hexane to obtain aromatic hydrocarbons at a temperature of 500^{0}C. the amount of aromatic hydrocarbons in the catalyst was 51.25%.

Table 3. Calculation of the value of the Frost equation for the total transformation of hexane with a linear structure in 2%La*2%Cu*8%Zn/N-YuKTs-20.

T,^{0}C	Size speed s^{-1}	$v_0.10^4$ mol/g·h	y	$v_0.y.10^4$	v_0•ln(1/l-y).10^3	α .10^4 mol/g·h	β
300	1.0	60	0.1752	2.044	2.148	2.5	0.87
	2.0	120	0.1284	2.524	2.615		
	2.5	240	0.0983	3.208	3.225		
400	1.0	60	0.2452	1.425	2.520	5.0	
	2.0	120	0.1980	3.267	3.610		
	2.5	240	0.1425	4.245	4.420		
500	1.0	60	0.4954	3.335	3.910	7.5	
	2.0	120	0.4046	4.640	5.335		
	2.5	240	0.3782	7.645	8.710		

The calculation results given in Table 3, i.e. V0•y =7,665 x10^3 when the temperature is 500 0C, v_0•ln(1/l-y) =8,775 x10^3, show the kinetic dependence of the general change of hexane with a linear structure and its compliance with the Frost equation in the studied temperature range.

Table 4. Calculation of the value of the Frost equation for the dehydrocyclization of hexane with a linear structure in 2%La*2%Cu*8%Zn/N-YuKTs-20.

T,^{0}C	Size speed s^{-1}	$v_0.10^4$ mol/g·h	y	$v_0.y.10^4$	v_0•ln(1/l-y).10^3	$\alpha \cdot 10^4$ mol/g·h	β
300	1.0	60	0.046	3.651	3.710	2.0	0.84
	2.0	120	0.040	5.445	5.525		
	2.5	240	0.028	7.225	7.331		
400	1.0	60	0.125	8.330	8.774	2.5	
	2.0	120	0.010	12.75	13.520		
	2.5	240	0.073	18.05	18.660		
500	1.0	60	0.235	14.90	16.820	3.5	
	2.0	120	0.190	23.54	25.975		
	2.5	240	0.180	43.71	48.030		

The calculation results given in Table 4, i.e. V0·ln(1/l-y) =48.05.10^3 when the temperature is 500 ^{0}C, V0·y =43.74.10^3, show the kinetic dependence of the general change of hexane with a linear structure and its compliance with the Frost equation in the studied temperature range shows

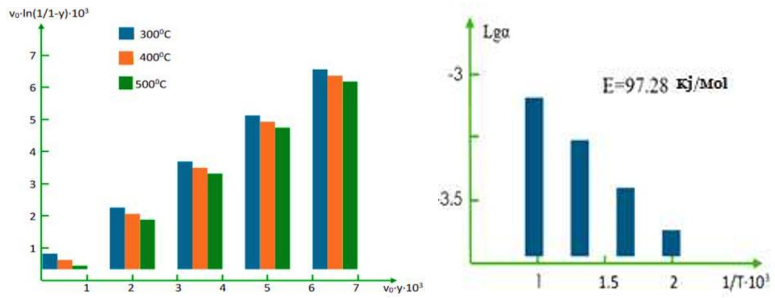

Fig. 1. Kinetics of the general transformation of linear hexane in the catalyst with high activity selected for the aromatization of linear hexane to aromatic hydrocarbons in the coordinates of the Frost equation 2%La*2%Cu*8%Zn/N-YuKTs-20.

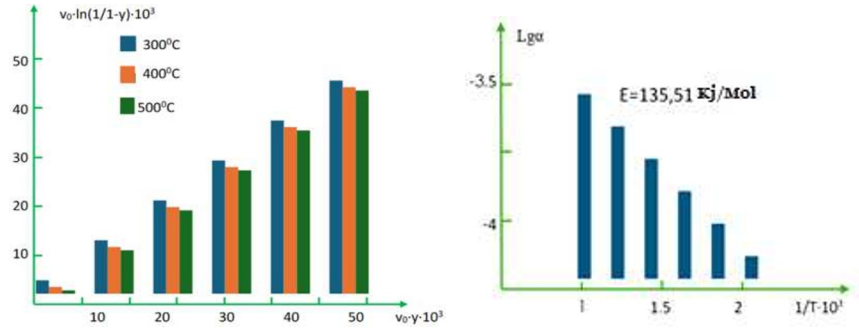

Fig. 2. Dehydrocyclization kinetics of linear hexane in the catalyst with high activity elected for the aromatization of linear hexane to aromatic hydrocarbons in the coordinates of the Frost equation 2%La*2%Cu*8%Zn/N-YuKTs-20.

Table 5. Calculation of the value of the Frost equation for the total transformation of hexane with a linear structure in 2%La*2%Cu*8%Zn/N-YuKTs-30.

T,^{0}C	Size speed s^{-1}	$v_0.10^4$ mol/g·h	y	$v_0.y.10^4$	v_0•ln(1/l-y).10^3	α .10^4mol/g·h	β
300	1.0	84.15	0.520	4.841	6.152	4.0	0.78
	2.0	111.0	0.430	5.330	6.523		
	2.5	222.5	0.321	6.820	7.654		
400	1.0	84.15	0.615	5.885	8.445	4.5	
	2.0	111.0	0.622	6.920	9.523		
	2.5	222.5	0.513	10.12	12.650		
500	1.0	84.15	0.804	6.770	11.120	6.5	
	2.0	111.0	0.730	8.080	12.330		
	2.5	222.5	0.560	11.290	17.815		

The calculation results presented in Table 5, i.e. V0·y =11,292.103 when the temperature is 500˚C, V0·ln(1/l-y) =12,323.103, show the kinetic dependence of the total transformation of hexane with a linear structure and its compliance with the Frost equation in the studied temperature range.

Table 6. Calculation of the value of the Frost equation for dehydrocyclization of hexane with a linear structure in 2%La*2%Cu*8%Zn/N-YuKTs-30.

T,^{0}C	Size speed s^{-1}	$v_0.10^4$ mol/g·h	y	$v_0.y.10^4$	v_0•ln(1/ly).10^3	α.10^4 mol/g·h	β
300	1.0	84.15	0.350	3.121	3.440	0.8	0.84
	2.0	111.0	0.302	3.225	3.552		
	2.5	222.5	0.213	3.985	4.145		
400	1.0	84.15	0.520	4.526	5.601	1.7	
	2.0	111.0	0.480	5.280	5.425		
	2.5	222.5	0.382	7.230	8.401		
500	1.0	84.15	0.602	5.120	6.880	2.5	
	2.0	111.0	0.525	6.045	7.775		
	2.5	222.5	0.420	8.327	8.883		

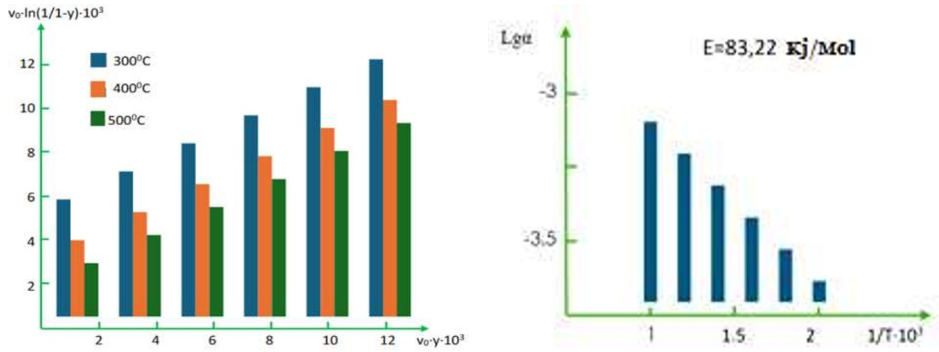

Fig. 3. Kinetics of the overall conversion of linear hexane in the 2%La*2%Cu*8%Zn/N-YuKTs-30 catalyst with high activity selected for the aromatization of linear hexane in the coordinates of the Frost equation.

The calculation results shown in Figure 3 show the kinetic dependence of the total transformation of hexane with a linear structure and its compliance with the Frost equation in the studied temperature range

Table 7. Kinetic description of the transformation of linear hexane according to x=f(no) curves on the 2%La*2%Cu*8%Zn/N-YuKTs-20 catalyst with high catalytic activity selected for catalytic aromatization of linear hexane to aromatic hydrocarbons.

Reaction	T, ^{0}C	x,%	$n_0 \cdot 10^4$	$dx/dn \cdot 10^{-3}$	ConstW·10^5	Lg(ConstW)	Enable, KJ/mol	
							beat. 4	graph
Total conversion of n-hexane	300	0.2	1.620	11.5260	0.2586	-6.5235		98.125
	400		2.815	5.1753	0.3340	-6.6140	99.10	
	500		11.321	0.4350	0.4329	-6.3842	97.15	
	Average						98.12	
Digidrocyclization	300	0.1	0.625	4.5520	0.0210	-7.9065		135.55
	400		2.515	0.8265	0.0510	-6.3885	134.60	
	500		8.335	0.5105	0.4162	-6.4045	136.50	
	Average						135.55	

Table 8. Kinetic description of the transformation of linear hexane according to x=f(no) curves on 2%La*2%Cu*8%Zn/N-YuKTs-20 catalyst with high catalytic activity selected for catalytic aromatization of linear hexane to aromatic hydrocarbons.

Reaction	T,^{0}C	x,%	no.10^4mol/g·h	$dx/dn \cdot 10^{-3}$	ConstW·10^5 mol/sec	Lg(ConstW)	Enable, KJ/mol	
							beat.4	graph
Total conversion of n-hexane	300	0.5	3.520	2.632	0.1520	-6.9815	-	84.13
	400		6.015	0.826	0.2018	-6.7105	82.71	-
	500		7.775	0.649	0.3045	-6.6032	85.55	
	Average						84.13	
Digidrocyclization	300	0.4	2.515	0.864	0.1622	-6.8275	-	-
	400		6.520	0.805	0.3290	-6.6084	111.25	
	500		8.010	0.601	0.4095	-6.4560	115.30	113.27
	average						113.27	

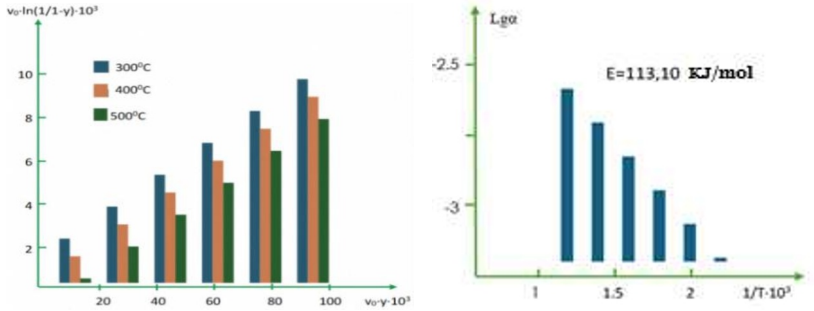

Fig. 4. Kinetics of linear structure hexane dihydrocyclization on 2%La*2%Cu*8%Zn/N-YuKTs-20 catalyst in Frosto equation coordinates.

The calculation results shown in Fig. 4 show the kinetic dependence of the total transformation of hexane with a linear structure and its compliance with the Frost equation in the studied temperature range

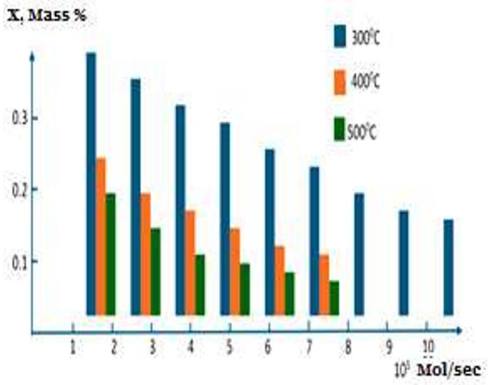

Fig. 5. Dependence of linear structure hexane conversion depth on 2%La*2%Cu*8%Zn/N-YuKTs-20 catalyst consumption rate.

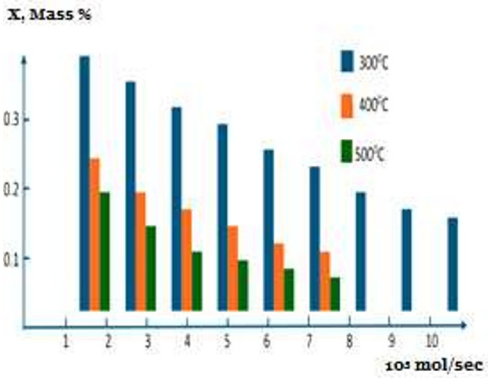

Fig. 6. Dependence of the imaginary constant on the total conversion rate of linear hexane on the 2%La*2%Cu*8%Zn/N-YuKTs-20 catalyst with high catalytic activity selected for catalytic aromatization of linear hexane to obtain aromatic hydrocarbons.

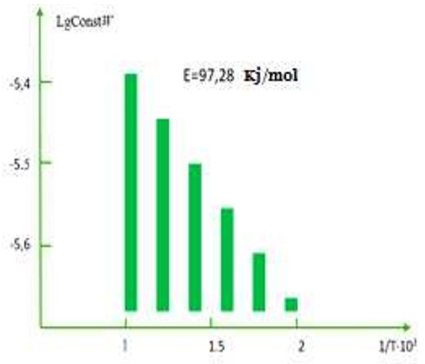

Fig. 7. Dependence of linear hexane dehydrocyclization on raw material transfer rate on 2%La*2%Cu*8%Zn/N-YuKTs-20 catalyst with high catalytic activity selected for catalytic aromatization of linear hexane to obtain aromatic hydrocarbons.

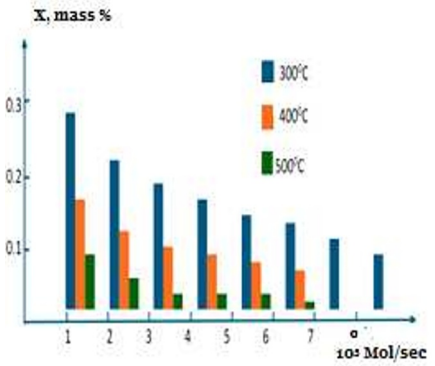

Fig. 8. The dependence of the imaginary constant on the rate of linear hexane dehydrocyclization on the 2%La*2%Cu*8%Zn/N-YuKTs-20 catalyst with high catalytic activity selected for the catalytic aromatization of linear hexane to obtain aromatic hydrocarbons.

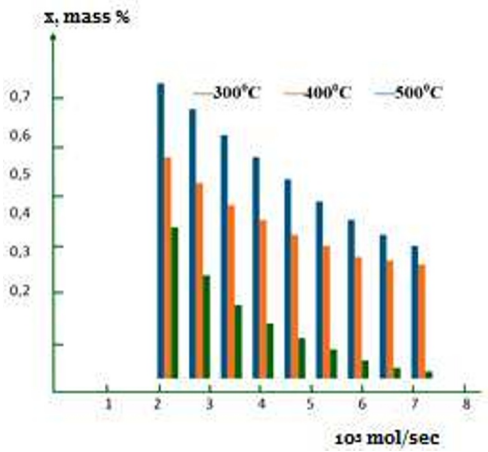

Fig. 9. Dependence of the conversion depth of linear hexane on the rate of raw material transfer in the 2%La*2%Cu*8%Zn/N-YuKTs-30 catalyst with high catalytic activity selected for catalytic aromatization of linear hexane to obtain aromatic hydrocarbons.

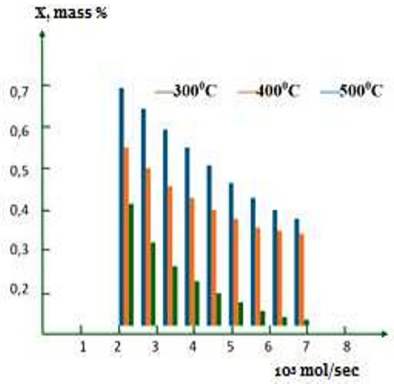

Fig. 10. Dependence of the imaginary constant on the total conversion rate of linear hexane in the 2%La*2%Cu*8%Zn/N-YuKTs-30 catalyst with high catalytic activity selected for the catalytic aromatization of linear hexane to obtain aromatic hydrocarbons.

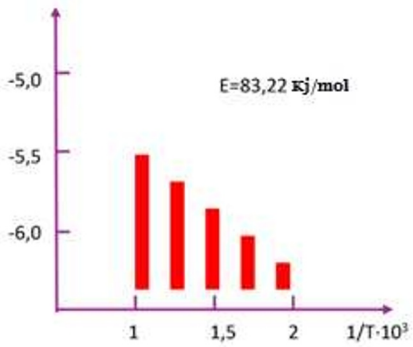

Fig. 11. Dependence of raw material transfer rate on the dehydrocyclization of linear hexane on the 2%La*2%Cu*8%Zn/N-YuKTs-30 catalyst with high catalytic activity selected for the catalytic aromatization of linear hexane to obtain aromatic hydrocarbons.

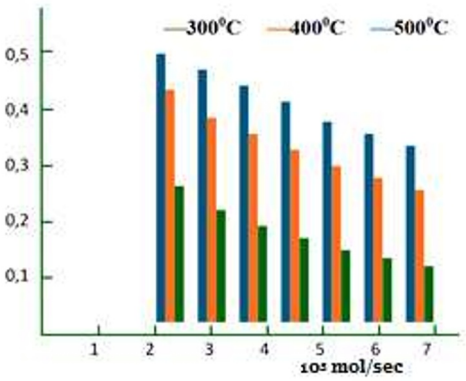

Fig. 12. Dependence of the imaginary constant on the rate of linear hexane dehydrocyclization on the 2%La*2%Cu*8%Zn/N-YuKTs-30 catalyst with high catalytic activity selected for the catalytic aromatization of linear hexane to obtain aromatic hydrocarbon.

4 Conclusion

Using two independent kinetic methods (Frost equation and graphical differentiation equation of experimental data), a total transformation of hexane with a linear structure and activation energies for the dehydrocyclization reaction were calculated. It was found that 2%La*2%Cu*8%Zn/N-YuKTs-30 linear structure catalyst with high catalytic activity selected for catalytic aromatization of hexane to obtain aromatic hydrocarbons is Ekaj 2%La*2%Cu*8%Zn/N -YuKTs-20 is smaller than the catalyst with high catalytic activity selected for the catalytic aromatization of linear hexane to obtain aromatic hydrocarbons: 83 and 97 kDj/mol for the total conversion of linear hexane, and 113 and 135 kDj/mol for the dehydrocyclization reaction.

In addition, 2%La*2%Cu*8%Zn/N-YuKTs-30 and 2%La*2%Cu*8%Zn/N-YuKTs with high catalytic activity selected for obtaining aromatic hydrocarbons by catalytic aromatization of hexane with a linear structure The process of improvement of low-octane 85-1800C gasoline fractions on -20 catalysts was studied at atmospheric pressure, in the temperature range of 400-5000C without hydrogen-containing gas circulation. 2%La*2%Cu*8%Zn/N-YuKTs-30 catalyst with high catalytic activity selected for catalytic aromatization of linear hexane to obtain aromatic hydrocarbons. It was shown that the 2%La*2%Cu*8%Zn/N-YuKTs-20 catalyst with high catalytic activity selected for obtaining aromatic hydrocarbons from catalytic aromatics produces a large number of compounds of isostructures, which are the main high-octane and environmentally friendly components of automotive fuels.

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