ISSN 0036-0244, Russian Journal of Physical Chemistry A, 2016, Vol. 90, No. 4, pp. 754–760. © Pleiades Publishing, Ltd., 2016. Original Russian Text © B. Ya. Stul', 2016, published in Zhurnal Fizicheskoi Khimii, 2016, Vol. 90, No. 4, pp. 532–538.

## CHEMICAL KINETICS AND CATALYSIS

# Kinetics of the *n*-Decanol Oxyethylation Reaction with Allowance for Association

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Abstract—The kinetics of *n*-decanol oxyethylation in the temperature range of  $60-150^{\circ}$ C at a pressure of 1.4 MPa is investigated under conditions of base catalysis and an excess of alcohol in the initial step of the reaction (initial concentration of ethylene oxide in the reaction mixture, approximately 1 mol/L; that of the catalyst,  $10^{-1}$  to  $10^{-3}$  mol/L). The experimental results are satisfactorily described by a kinetic equation that allows for the association of alcohol molecules and is first order with respect to the concentration of alcohol associates. Based on kinetic studies and thermogravimetry, it is concluded that the structural rearrangement of liquid decanol occurs at a temperature of around 87.5°C.

*Keywords:* oxyethylation reaction, *n*-decanol, ethylene oxide, kinetic studies, thermogravimetry. **DOI:** 10.1134/S0036024416040282

#### INTRODUCTION

The kinetics of alcohol oxyethylation are generally described by the scheme

$$\begin{array}{c} \text{ROH} \xrightarrow{C_2H_4O} \text{ROC}_2H_4\text{OH} \\ \xrightarrow{c_2H_4O} \text{RO}(C_2H_4O)_2\text{H} \xrightarrow{C_2H_4O} \text{etc} \end{array}$$

The kinetics of this irreversible sequential reaction for alcohol has been investigated in a number of studies [1]. It is shown in this work that under conditions of base catalysis, the reaction rate in the initial stage with an excess of alcohol follows first order kinetics with respect to the concentrations of ethylene oxide (EO) and catalyst, and exhibits a complex dependence with respect to alcohol concentration. It has been suggested [1] that deviations from first order kinetics with respect to alcohol concentration are due to the association of alcohol molecules as a result of the formation of hydrogen bonds. Both the reaction rate and degree of association depend on the alcohol concentration and the overlapping of these phenomena complicates the general picture.

In [2], we proposed a kinetic model and corresponding equation that satisfactorily described the kinetics of this reaction. This model considered the association of alcohol molecules via the formation of hydrogen bonds and suggested that a monomeric form of the alcohol molecule participated in this reaction not as a kinetically independent unit but rather as a linear chain associate (neither closed nor branched) that consisted of n molecules of alcohol on average. It was shown that in the investigated range of concentrations and conversions, the experimental results in a flow reactor when the impact of the second step of the reaction on the rate of EO consumption was negligible were satisfactorily described by the equation

$$W = (c_{\rm o}^0 - c_{\rm o})/\tau = k_{\rm o,obs.} c_{\rm c} c_{\rm o} (c_{\rm a}^0 - nc_{\rm l}), \qquad (1)$$

where W is the reaction rate determined from EO con-

sumption;  $c_o^0$  and  $c_o$  are the concentrations of EO in the initial mixture and in the reactor, respectively;  $\tau$  is the length of time the reaction mixture is in the reactor;  $k_{o, obs.}$  is the observed reaction rate constant of the first reaction stage;  $c_c$  and  $c_1$  are the concentrations of the catalyst and the first product in the reactor, respectively;  $c_a^0$  is the concentration of alcohol in initial mixture; and *n* is the average number of alcohol molecules in the alcohol associate.

Since n > 1, the calculated concentration of alcohol in this equation, which reflects the reaction rate (the expression in parentheses of the right part of the equation), falls much faster than follows from the stoichiometry. From the viewpoint of chemical kinetics, parameter *n* is a quantitative measure of the deviation of the observed first order kinetics with respect to alcohol concentration. The higher *n*, the greater the deviation. When n = 1 (no association), Eq. (1) is transformed into a general first order equation with respect to alcohol concentration, since  $c_a^0 - c_1 \approx c_a$ . Use of Eq. (1) is limited to the range of concentrations and conversions for which condition  $c_a^0 > c_1 n$  is valid. To substantiate the proposed kinetic model, the following conditions must be met [2]:

1. Alcohol molecules are bound via hydrogen bonds forming linear chain associates with *n* average number of molecules.

2. Only one of two terminal alcohol molecules in a chain associate participates in the reaction with its hydrogen atom of the hydroxyl group not participating in hydrogen bond formation.

3. The corresponding molecule of ethylene glycol monoester formed in the reaction remains in the composition of the associate and, being less reactive, it closes this associate.

It should be noted that point 3 is required in order to fix the associate as a kinetically independent unit. If this point is not met and the molecule of the formed ethylene glycol monoester does not form a complex with the terminal molecule of the alcohol associate, the above model is not valid, and association parameter *n* cannot be determined from it. Fulfillment of condition 3 is indirectly confirmed by IR spectroscopy data [3] showing that, unlike alcohol molecules, the molecules of ethylene glycol monoesters are prone to forming intramolecular hydrogen bonds when the hydrogen atoms of hydroxyl groups bond to the ester oxygen atoms of the same molecules. This causes the hydroxyl groups of the ethylene glycol monoester molecules to become monofunctional with regard to the formation of intermolecular hydrogen bonds, while the hydroxyl groups of alcohol are from this point of view bifunctional. It follows that a monoester molecule in an alcohol solution cannot be located inside the alcohol chain but can only be at its terminus.

If points 1-3 are fulfilled, Eq. (1) can be interpreted as a first order equation with respect to alcohol associate concentration. By factoring out term n in the right part of Eq. (1), an equation identical to it is produced:

$$W = (c_{\rm o}^0 - c_{\rm o})/\tau = k_{\rm o,obs.} n c_{\rm a} c_{\rm o} (c_{\rm a}^0/n - c_{\rm l}), \qquad (2)$$

where the expression in parentheses in the right part of the equation represents the concentration of unreacted alcohol associates in a reactor, since according to the accepted model,  $c_a^0/n$  is the concentration of alcohol associates in the initial mixture;  $c_1$  is the concentration of reacted alcohol associates, which is equal to the concentration of the first reaction product; and product ( $k_{o,obs}$ ,n) is the reaction rate constant in the new scale of alcohol concentration. It follows that the widely accepted physicochemical concept of first order kinetics is preserved in this case, but it applies to the concentration of alcohol associates, rather than the total alcohol concentration.

Since the lifetime of a single hydrogen bond is very short (on the order of  $10^{-13}$  s [4]), the lifetime of an alcohol associate becomes a key parameter for interpreting this mechanism. It was shown experimentally

in [5] with mass spectrometry that methanol associates of  $(CH_3OH)_n$  composition with n = 5-20 have lifetimes in gaseous phase on an order of  $10^{-4}$  to  $10^{-5}$  s. The lifetime of an associate should increase by 1-2 orders of magnitude and be no shorter than  $10^{-3}$  s upon transitioning to the liquid phase, which is sufficient for participation in an elementary chemical act. Considering the results obtained in [6], we may assume that the lifetime of such associates can be much longer.

The results from experiments on the oxyethylation of the normal primary alcohols of  $C_4-C_7$  composition inclusive in the temperature range of  $80-180^{\circ}$ C are presented in [2], along with the results from processing these data with Eq. (1). The reaction rate constants, activation energies, and the values of parameter *n* and its dependence on temperature were determined. It should be noted that the obtained kinetic parameters and parameters of association are in reasonable agreement with the literature data.

In this work, the kinetics of the oxyethylation of  $C_{10}$  alcohol were investigated in a similar manner. This was done with the aim of extending the series of the considered alcohols and comparing the obtained results to those for  $C_4$ – $C_7$  alcohols obtained earlier.

#### **EXPERIMENTAL**

The method employed for  $C_4-C_7$  alcohols in [2] was used to investigate the kinetics of C<sub>10</sub> alcohol oxyethylation. Our experiments were conducted in a flow system made of titanium in a mixing reactor at temperatures in the range of 60–150°C and a pressure of 1.4 MPa. The preset temperature in the reactor was maintained with an accuracy of  $\pm 0.5^{\circ}$ C. The reactor was a hollow cylinder with a volume of  $15 \text{ cm}^3$ . equipped with a magnetic stirrer and all of the necessary connectors. A reaction mixture at a given temperature, pressure, and volume rate was pumped through the reactor and then passed through a condenser, reaching a collector from which cooled samples could be taken for analysis. The reaction mixtures were analyzed by means of GLC. The reactor reached the steady state mode after no fewer than 6 reactor volumes of the reaction mixture were passed through it. Both the preliminary calculations and our experiments showed that the pressure we used was sufficient to prevent the EO state changing from liquid to vapor, the volume of which in our setup was minimal. Errors in the mass balance for EO in our experiments was  $\pm 5\%$  or less. In most cases, errors in determining parameters  $k_{0,obs}$  and *n* did not exceed  $\pm 10$  rel. %.

Commercial *n*-decanol was used with a main component content of no less than 99 wt %. It was desiccated prior to use over molecular sieves. The water content in the *n*-decanol after drying was 0.016 wt %. Sodium *n*-decycloxide was used as a catalyst.

Concentration, mol/L								$k_{0, obs} \times 10^3$ ,	
$c_{\rm c} \times 10^2$	$c_{\rm o}^0$	c <sub>o</sub>	$c_{\mathrm{a}}^{0}$	c <sub>a</sub>	$c_1$	<i>c</i> <sub>2</sub>	$L^2/(mol^2 s)$ at		
	<i>n</i> = 1	<i>n</i> = 49.5							
7.0	0.913	0.839	4.836	4.764	0.070	0.0023	0.52	1.80	
3.50	0.948	0.890	4.802	4.747	0.054	0.0014	0.77	1.71	
2.53	0.956	0.907	4.722	4.674	0.047	0.0011	0.90	1.75	
1.75	0.933	0.892	4.817	4.777	0.039	0.0008	1.08	1.78	
	n = 1	<i>n</i> = 21.1							
4.96	0.932	0.794	4.754	4.619	0.124	0.007	1.49	3.12	
2.48	0.995	0.897	4.690	4.595	0.090	0.0035	1.88	3.09	
1.24	0.968	0.910	4.717	4.659	0.056	0.0015	2.16	2.85	
0.62	0.909	0.872	4.776	4.740	0.035	0.0005	2.83	3.32	
	<i>n</i> = 1	<i>n</i> = 12							
4.57	0.955	0.779	4.676	4.512	0.151	0.011	2.14	3.38	
2.28	0.955	0.841	4.676	4.566	0.104	0.005	2.55	3.40	
1.14	0.886	0.822	4.745	4.683	0.060	0.0017	2.86	3.33	
0.57	0.929	0.891	4.702	4.665	0.0366	0.0006	3.14	3.44	
	<i>n</i> = 1	<i>n</i> = 11.2							
4.96	0.864	0.623	4.712	4.484	0.202	0.017	3.39	6.24	
2.48	0.870	0.699	4.706	4.544	0.147	0.011	4.24	6.32	
1.24	0.893	0.776	4.683	4.571	0.107	0.004	5.21	6.84	
0.62	0.891	0.819	4.685	4.615	0.067	0.002	6.02	7.06	
	<i>n</i> = 1	<i>n</i> = 12.2							
1.24	0.857	0.615	4.501	4.274	0.199	0.020	14.5	30.0	
0.62	0.857	0.699	4.501	4.349	0.140	0.009	16.4	25.6	
0.31	0.873	0.760	4.486	4.376	0.103	0.004	19.6	29.1	
0.15	0.885	0.817	4.474	4.409	0.063	0.002	24.7	29.4	

Table 1. Results from experiments on decanol-1 oxyethylation at different temperatures

The time the reaction mixture was in the reactor was 8.5 min for all experiments.

The water content was determined via the Fischer method using an MKC-500 titrator (Kyoto Electronics). Thermogravimetric experiments were conducted with a SDT Q600 V7.0 Build 84 thermo analyzer (Netzsch). Scanning speed was 8 K/min.

### **RESULTS AND DISCUSSION**

The primary experimental data on the oxyethylation of *n*-decanol at different temperatures, along with the results from data processing using Eq. (1) with n =1 (first order with respect to the total alcohol concentration) and at  $n \neq 1$  (first order with respect to the concentration of alcohol associates) are presented for comparison in Table 1 as an example. It should be noted that as in the case of C<sub>4</sub>-C<sub>7</sub> alcohols [2], the yield of the second product in most cases did not exceed 5–6% of that of the first product of the reaction, which allowing us to assume that the total reaction rate determined from EO consumption could be due entirely to the first stage of this reaction, which is characterized by reaction rate constant  $k_{0, obs}$ . For the most part, the catalyst concentration varied in the series of reactions presented in Table 1, with each series consisting of four experiments. When n = 1, each experiment was processed directly using Eq. (1); when  $n \neq 1$ , the reaction series was processed as a whole. Statistical processing of the experimental data when  $n \neq 1$  involved fitting parameter *n*, using the linear least squares method so that the least square deviations of the reaction rate constant from the average value would be minimal. The minimum of function *F* was thus determined:

$$F = \sum_{i=1}^{N} (k_{o,obs,i} - k_{o,obs,av})^{2},$$
 (3)

where  $k_{0,obs,i}$  is the observed rate constant obtained in the *i*th experiment of a given reaction series at a pre-

t, °C	60	67.5	75	87.5	100	125	150
$k_{\rm o, \ obs.} \times 10^3$ , $L^2  {\rm mol}^{-2}  {\rm s}^{-1}$	$1.76\pm0.04$	$2.3\pm0.15$	$3.1\pm0.2$	$3.4\pm0.05$	$6.6\pm0.4$	$15 \pm 1$	$28.5\pm2$
n	49.5	28.5	21.1	12	11.2	12.6	12.2

**Table 2.** Values of constant  $k_{o, obs.}$  and association parameter *n* in the reaction of decanol-1 oxyethylation at different temperatures

scribed *n* value;  $k_{o,obs,av}$  is the arithmetic mean of the rate constants in this reaction series at the same *n* value; *i* is an index that assumes sequential integer values from 1 to *N*; and *N* is the number of experiments in the reaction series (N = 4). The values of *n* at which function *F* has a minimum and the least square deviation of constants is minimal are presented in Table 1.

As can be seen from the above data, the same pattern is observed when n = 1 as in the case of C<sub>4</sub>-C<sub>7</sub> alcohols; i.e., with all other conditions being equal, the higher the yield of the first reaction product in each series of experiments, the lower the rate constant calculated according to Eq. (1). Formal inhibition by the reaction product is thus observed that is not reflected by Eq. (1) when n = 1. The minimum and the maximum rate constants within each series in this case differ by a factor of  $\sim 1.5-2$ . This is appreciably higher than the experimental error and indicates that Eq. (1)when n = 1 cannot be used to describe the kinetics of this reaction for the investigated ranges of concentration and conversion. At the same time, processing the data according to Eq. (1) when  $n \neq 1$  results in consistent rate constants, as in the case of  $C_4$ – $C_7$  alcohols.

Our results from experiments on decanol-1 oxyethylation are presented in Tables 1 and 2. The dependences of  $\ln n$  and  $\ln k_{0,obs}$  on reciprocal temperature are presented in Fig. 1.

It follows from the presented data that the fundamental difference between this alcohol and the C<sub>4</sub>-C<sub>7</sub> alcohols lies in the temperature dependence of parameter *n*. The arbitrary values of enthalpy of association  $\Delta H^*$  calculated by processing the obtained *n* values in coordinates  $\ln n - 1/T$ , where T is the absolute temperature, were used for quantitative assessment of the temperature dependences of parameter n and their comparison in [2]. These dependences for  $C_4-C_7$ alcohols in coordinates  $\ln n - 1/T$  are straight lines over the investigated range of temperatures with a gradual decline in  $-\Delta H^*$  values from 11 kJ/mol for C<sub>4</sub> alcohol to 4 kJ/mol for C<sub>7</sub> alcohol, due likely to the increasing length of the hydrocarbon radical in this series. Based on this, a further drop in  $-\Delta H^*$  could be expected for  $C_{10}$  alcohol. Parameter *n* of  $C_{10}$  alcohol behaves as expected in the temperature range of 87.5–150°C, and is practically independent of the temperature; i.e.,  $\Delta H^* \approx 0$  within the experimental error, testifying to the high thermal stability of the associate when n = 12 with regard to dissociation. A sharp increase in parameter n is observed when the temperature falls below 87.5°C:  $\Delta H^* = 45.5 \pm 6.4 \text{ kJ/mol}$  in the temperature interval 60–87.5°C. In contrast to the  $C_4$ – $C_7$  alcohols, this dependence for C<sub>10</sub> alcohol consists of two parts that form straight lines which intersect at approximately 87.5°C.

All of the points on the activation energy plot lie on virtually the same straight line, except for the one at 87.5°C. The point at 87.5°C, which corresponds to the inflection point on the  $\ln n - 1/T$  dependence, drops out of the graph. The rate constant value at that temperature was found to be approximately 50% lower than expected, which would put it on the dashed line (Fig. 1). The activation energy determined over the investigated range of temperatures without considering the missing point was  $36.5 \pm 3.2$  kJ/mol.



Fig. 1. (1) Dependences of  $k_0$  and (2) association parameter n on reciprocal temperature.

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Fig. 2. (1) Dependence of the mass loss of a sample  $(\Delta m)$  on temperature and (2) the derivative of this dependence;  $\Delta m = 100(m_0 - m)/m_0$ , where  $\Delta m$  is the mass loss (%),  $m_0$  is the initial mass of the sample, and *m* is the current mass of the sample. The rate of temperature scanning was 8 K/min.

It follows from the above data that the trend of the temperature dependence of parameter *n* changes at a temperature of around 87.5°C. Since parameter n, obtained on the basis of kinetic studies, is related in this model to the microscopic inner structure of liquid decanol, and we would expect this relationship to be preserved on the macrolevel, we may assume that a structural transition occurs in liquid decanol at a temperature of about 87.5°C, and is accompanied by a corresponding change in the trend or pattern of changes in some physical, physicochemical, or spectral properties of *n*-decanol, depending on temperature. It should be noted that our assumption of a structural change was made exclusively on the basis of the change in the trend of *n* dependence on temperature. rather than that of the observed 50% drop in the rate constant, relative to the expected value.

Our analysis of the temperature dependences of the number of physical, physicochemical, and spectral properties of *n*-decanol known from the literature did not reveal any striking anomalies in their behavior around the transition temperature; nevertheless, there were certain indications of these. For example, the dependence of vapor pressure on temperature in coordinates  $\ln P - 1/T$  for C<sub>6</sub> alcohol in the considered range of temperatures is a straight line, while for  $C_{10}$ alcohol this dependence shows a slight bend at 85-90°C [7], which is in agreement with our results. Due to the low impact of the expected effects, their discovery likely requires especially precise experiments in narrow temperature intervals around the transition temperature, while the dependences available in the literature were recorded in wide temperature intervals with large steps.

After a long search, it was established that the existence of the expected structural transition could be confirmed by means of thermogravimetric experi-

ments. The initial *n*-decanol with a water content of 0.016 wt % used in experiments on oxyethylation was used in these experiments. The dependence of the mass loss of the alcohol sample on temperature at a scanning speed of 8 K/min is presented in Fig. 2, along with the same dependence in differential form. As can be seen from the figure, the differential dependence displays a maximum around 87.5°C, which coincides with the temperature determined using the kinetic method. As the temperature rises, the derivative of the mass loss decreases and increases again at 100°C. This pattern is likely due to the presence of 0.016 wt % of water in the sample. It is known [8] that large fluctuations in the thermodynamic parameters are observed near the temperatures of structural transitions. Since the energy of hydrogen bonds is close to that of thermal motion at a given temperature, a great many hydrogen bonds rupture when the temperature reaches 87.5°C, including those that held water molecules in a liquid phase. The factors described above are likely responsible for the sharp influx of water molecules into the vapor phase. The next increase in the rate of desorption into the vapor phase is observed at 100°C, the temperature at which water boils. The decanol sample with a higher water content of 0.32 wt % exhibits a peak at 92.5°C, so the maximum is shifted toward higher temperatures and becomes wider as the water content rises. The participation of water molecules in this process was confirmed by the repeated scanning of a sample that had undergone this procedure earlier failing to produce a peak in the indicated range of temperatures. In this case, water acted as a probe that helped reveal the rearrangement of the liquid phase structure. Using the terminology suggested in [9] for the classification of coil-globule structural transitions in polymer solutions, this transition can be classified as a transition accompanied by a sharp loss

of the adsorbed ligand, recorded by means of thermogravimetry.

It should also be noted that the expression in [10] for phase and structural transitions is valid for the described transition:

$$T_{\rm t} \approx \Delta T n,$$
 (4)

where  $T_t$  is the temperature of transition, K;  $\Delta T$  is the width of the transition, K; *n* is the number of particles in the region of transition (in this case, the association number). According to curve 2 in Fig. 2,  $\Delta T \approx 32$  K. Consequently,  $n \approx 360.75/32 = 11.3$ . This is in good agreement with the results from kinetic studies where  $n = 12 \pm 1.2$ .

To a great extent, the results from thermogravimetric experiments thus support the conclusion, drawn on the basis of based kinetic studies, that a structural transition occurs in *n*-decanol at  $87.5^{\circ}$ C. It is of interest to discuss the nature of this transition and offer some suggestions as to the structure of associates in the series of considered alcohols in the investigated range of temperatures.

Since the dependence of parameter *n* on temperature is not observed for the series of  $C_4$ – $C_7$  alcohols in the investigated range of temperatures, we may assumed that the contact (or, according to the terminology in [9], bulk) interactions of hydrocarbon radicals make a significant contribution (along with hydrogen bonds) to the total energy of interaction for  $C_{10}$  alcohol at temperatures below 87.5°C. In this case, these interactions are likely related to Van der Waals forces, with dispersion interactions providing the major impact. Thermal motion below the transition temperature does not interfere with such arrangements of hydrocarbon radicals relative to one another when these forces are maximal and the system reaches its minimum free energy. We would also expect that at temperatures below the transition temperature, the hydrocarbon radicals of chain associates interact with one another in a stretched trans-conformation and are arranged parallel to one another, since such an arrangement favors this interaction. Thermal motion disrupts this arrangement and the respective interaction of hydrocarbon radicals at temperatures of 87.5°C and above.

It is of interest to estimate the energy of the thermal motion disrupting contact interaction, and thus the energy of contact interaction. For this, we can use the equation

$$\varepsilon = k_{\rm B} N_{\rm A} T_{\rm t}, \qquad (5)$$

where  $\varepsilon$  is the energy of thermal motion,  $k_{\rm B}$  is the Boltzmann constant, and  $N_{\rm A}$  is the Avogadro number. Using the reference values  $k_{\rm B} = 1.38 \times 10^{23}$  J/K and  $N_{\rm A} = 6.02 \times 10^{23}$  mol<sup>-1</sup>, we find that  $\varepsilon = 3$  kJ/mol, which is in good agreement with the estimates of the energy of contact interactions (1–4 kJ/mol) presented in the literature [4].

We may also assume that association occurs mainly via the hydrogen bonds of the hydroxyl groups in  $C_4$ -C<sub>7</sub> alcohols over the range of investigated temperatures, and only at temperatures above  $87.5^{\circ}$ C in C<sub>10</sub> alcohol. Hydrocarbon radicals do not participate directly in the association of alcohol molecules, but they probably shield (protect) the chains of the hydrogen bonds of hydroxyl groups from thermal disruption by wrapping around them and creating a peculiar type of frame. The possibility of such framing, and the term itself, were suggested in [11]. This lowers the  $-\Delta H^*$ values in the series of  $C_4-C_7$  alcohols, due to the growing size of the hydrocarbon radical, which was mentioned above. We suggest that complete shielding is observed for  $C_{10}$  alcohol at temperatures above 87.5°C, and that the disrupted hydrogen bond is restored, since the alcohol molecules that form this bond do not have time to separate, being inside cells made of hydrocarbon radicals.

It is of interest to discuss the purely kinetic consequences of such a structural transition. As can be seen in Fig. 1, the graph for activation energy before the temperature interval where the transition occurs is a continuation of this graph after this interval; i.e., the activation energy and pre-exponential factor in the expression for the reaction rate constant do not change. The observed  $\sim 50\%$  reduction in the observed rate constant at the temperature of transition (Fig. 1) is likely related to the structural disordering (structural chaos) of the liquid phase, which takes place at the transition temperature, and which probably causes the drop in the pre-exponential factor. Based on the obtained data, we may also conclude that the contact interaction of hydrocarbon chains, which occurs at temperatures below the transition temperature for  $C_{10}$ alcohol, does not have any great impact on the reactivity of the terminal hydroxyl group of the alcohol associate that participates directly in the reaction. The abovementioned framing made of hydrocarbon radicals protects the associate from decay at temperatures above 87.5°C, but it also does not affect reactivity of the terminal hydroxyl group.

#### **CONCLUSIONS**

The kinetics of the above reaction allows us to investigate the supramolecular micro-irregular structure of liquid *n*-decanol and predicts the occurrence of a structural transition in the liquid alcohol that is not described in the literature, and has been verified to a great extent by thermogravimetric experiments. Investigations of the structure of liquid decanol at temperatures below and above the transition temperature are required to prove this suggestion conclusively.

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Translated by L. Brovko