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EXPERIMENTAL INVESTIGATION OF THE DENSITY OF CAPROATES AT HIGH TEMPERATURES AND PRESSURES

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Results of experiments on investigating the density of caproates as a function of temperature and pressure are given. The equation of state of caproates in the liquid phase is composed on the basis of the P–ρ–T data obtained.

Esters of caproic acid, i.e., caproates ($C_5H_{11}COOC_nH_{2n+1}$), are weakly polar liquids, and they differ from normal liquids (alkanes, alkenes, and others) in many properties.

Caproates are widely used in many industries, since they serve as high-temperature solvents of cellulose acetate and nitrate, oils, fats, waxes, rubbers, polyamides, etc. Despite the wide practical use, their thermophysical properties are not understood, in practice.

The thermal conductivity of caproates in the liquid phase as a function of temperature and pressure has been investigated experimentally in [1–7]. However there are no data on their density. The present work seeks to experimentally study the density of caproates (ethyl caproate, propyl caproate, butyl caproate, amyl caproate) in the interval of temperatures 295–600 K and pressures 0.1–58.8 MPa. The results of investigation of the density of other homologs (methyl caproate, nonyl caproate) have been published in [8, 9].

The density was measured by the method of hydrostatic weighing with a maximum error of 0.1% throughout the studied range of the parameters of state. For the investigation we designed and manufactured an experimental setup with the use of the elements of pilot-scale plants [10, 11]. It differs from the existing setups in that the sensor coil is removed from the medium studied; this enabled us to simplify its operation and to improve performance reliability.

We calibrated elements of the suspended system by the method of hydrostatic weighing in water (bidistillate) with the use of a VLA-200 G-M-type analytical balance according to the existing procedure [12, 13]. The density was measured along the isotherms.

We carried out check measurements at the initial temperature and atmospheric pressure to check the chemical stability of the products investigated after the experiments for high parameters. Satisfactory reproducibility of measurement results (0.05%) is a reliable guide for stating that the products are stable in the investigated range of temperatures and pressures.

Figure 1 gives the isobars and isotherms of the density of ethyl caproate and amyl caproate. There are also analogous dependences for the other liquids investigated.

Of the four substances studied, only the the density of ethyl caproate and amyl caproate has been investigated as a function of the temperature and the pressure [14, 15]. The error of these data amounts to 0.2%. The presence of the experimental *P*–ρ–*T* data for caproates enables us to compose an experimentally substantiated equation for them in the form [16]

$$P = A(T)\,\rho^n + B(T)\,\rho^m . \tag{1}$$

It is easy to check the possibility of using the equation of state in such a form and to determine the indices *n* and *m* on the basis of the available experimental data. For this purpose Eq. (1) is reduced to the form

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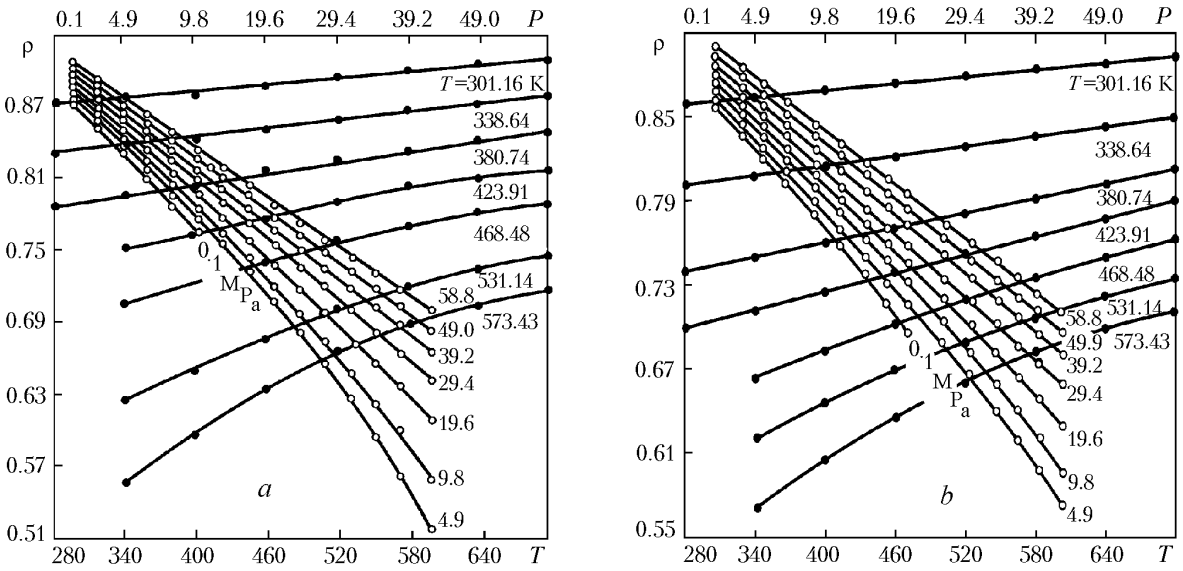

Fig. 1. Isobars and isotherms of the density of ethyl caproate (a) and amyl caproate (b).

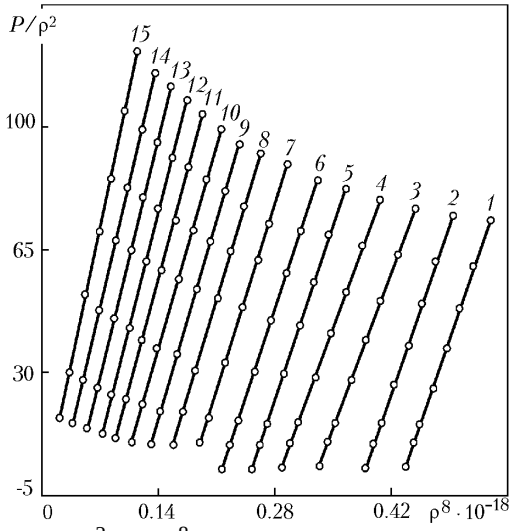

Fig. 2. Dependence $P/\rho^2 = f(\rho^8)$ for ethyl caproate at different temperatures: 1) T = 295.13, 2) 316.21, 3) 338.64, 4) 358.29, 5) 380.74; 6) 402.53, 7) 423.91, 8) 445.32, 9) 466.48, 10) 488.81, 11) 509.00, 12) 531.14, 13) 552.76, 14) 573.43, and 15) 600.98 K.

$$\frac{P}{\rho^n} = A(T) + B(T)\,\rho^{m-n}. \qquad (2)$$

On the basis of the experimental data, we constructed individual isotherms in the coordinate system P/ρ^n–ρ^{m-n} for different values of n and m. Analyzing the resulting plots, we took the values of n and m for which all the isotherms of this liquid are rectilinear in the above coordinates and are characterized by the coefficients $A(T)$ and $B(T)$.

The investigations have shown that for the substances studied the rectilinearity of all the isotherms is satisfied for n = 2 and m = 8. As an example, the above dependence for ethyl caproate is presented in Fig. 2. As is clear from the figure, the T = const lines are straight for all the pressures and the spread in experimental points does not exceed 0.05% and is not systematic.

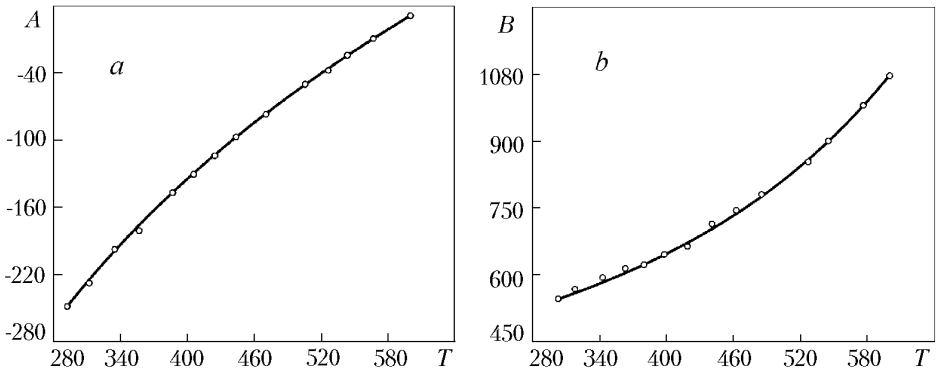

Fig. 3. Dependence of the coefficients $A(T)$ and $B(T)$ for ethyl caproate.

TABLE 1. Values of the Coefficients of Eq. (4)

Substance	Coefficients								
	$a_0 \cdot 10^4$	$a_1 \cdot 10^4$	$a_2 \cdot 10^8$	$a_3 \cdot 10^{10}$	$a_4 \cdot 10^{12}$	$b_0 \cdot 10^4$	$b_1 \cdot 10^4$	$b_2 \cdot 10^8$	$b_3 \cdot 10^{10}$
Ethyl caproate	–8322672	30483	–487181	48326	–2209	–1786602	52057	–1259965	122054
Propyl caproate	–10954000	47791	–792837	49729	0	3067866	21060	–664477	84390
Butyl caproate	–14078060	66114	–1160263	74289	0	1019476	–24002	380895	0
Amyl caproate	–14381370	66600	–1145891	71695	0	15894490	–57728	1049517	–40677

On the basis of the experimental data (Fig. 2) we can represent the equation of state of caproates in the form

$$P = A(T)\,\rho^2 + B(T)\,\rho^8 . \tag{3}$$

The coefficients $A(T)$ and $B(T)$ of Eq. (3) are different for each isotherm. The dependences of $A(T)$ and $B(T)$ for ethyl caproate are shown in Fig. 3. These smooth curves are approximated with a high degree of accuracy using the least-squares method by polynomials of the form

$$A(T) = \sum_{i=0}^{4} a_i T^i , \quad B(T) = \sum_{i=0}^{s} b_i T^i . \tag{4}$$

The values of the coefficients a_i and b_i appearing in (4) for each caproate are given in Table 1.

The equation of state (3) obtained describes the experimental data with account for (4) with a sufficient degree of accuracy. The deviation of the calculated values of the density from the experimental values amounts to no more than 0.2% for all the substances studied throughout the investigated range of temperature and pressure.

Equation (3) can be employed for calculation of the density of caproates in the ranges of the parameters of state for which there are no reliable experimental data and for prediction of the density of the unstudied esters of the class in question.

NOTATION

P, external pressure, MPa; ρ, density, g/cm^3; $A(T)$ and $B(T)$, temperature-dependent coefficients; n and m, positive integers; a_i and b_i, temperature proportionality factors; i, indices of the polynomials a, b, and T.

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