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# Speed of sound and thermodynamic properties of ternary liquid mixture octane + dodecane + hexadecane

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ABSTRACT

The speed of sound in octane + dodecane + hexadecane liquid mixture was measured within the temperatures from 298 to 433 K and at pressures from 0.1 to 100.1 MPa with an uncertainty 0.1%. Deviations of speed of sound from a mole fraction average have been calculated using known symmetric and asymmetric models. Density, isobaric expansion coefficient, isobaric and isochoric heat capacity, isothermal compressibility for the liquid mixture octane + dodecane + hexadecane of six compositions were evaluated from speed of sound data in the temperature range from 298 to 393 K at pressures up to 100 MPa. The calculated densities were fitted with a Tait equation.



## 1. Introduction

By now, properties of binary liquid mixtures are most widely studied ones of all liquid mixtures. As to experimental data on the properties of ternary liquid mixtures there is scarce information about their properties. At the same time, they may be easily used as samples to demonstrate thermodynamic regularities, which are characteristic for multicomponent mixtures, verify property prediction methods for multicomponent mixtures.

In the recent investigation experimental determination of the thermodynamic properties of ternary liquid mixtures have been mostly done at pressures and temperatures close to ambient. There were a few papers reported density data of compressed ternary liquid mixtures of n-alkanes, and no any data available on the thermodynamic properties of the compressed liquid mixture octane + dodecane + hexadecane. Moreover, there are no available data on heat capacity and compressibility of the ternary liquid mixture of n-alkanes (or at least it is unknown to us). The results of measurements of speed of sound for ternary liquid mixtures of n-alkanes ($C_nH_{2n+2}$) have been reported in papers [1,2]. Speeds of sound for ternary liquid mixtures of n-alkanes $C_7$, $C_{12}$, and $C_{16}$ of four compositions have been reported [1] within the temperatures from 313 to 413 K and at pressures up to 245.2 MPa. The results of measurements of speed of sound for ternary liquid mixtures of n-alkanes $C_6$, $C_7$, and $C_{10}$ have also been reported [2] at atmospheric pressure and temperature 298.15 K. The uncertainty of the speed of sound measurements was estimated by the authors [1] to be 0.1–0.4%. However, most reliable measurements of speed of sound in pure alkanes and their binary mixtures of other authors reveal deviations from the data reported in paper [1] significantly exceeding the above-mentioned uncertainty. It is evident that data [1] are of low accuracy.

The present paper deals with measurement of the speed of sound within the temperatures from 298 to 433 K and at pressures from 0.1 to 100.1 MPa, and calculation of the thermodynamic properties at temperatures from 298 to 393 K and pressures up to 100 MPa for ternary liquid mixture octane(1) + dodecane(2) + hexadecane(3) at mole fraction of component in mixture 0.125, 0.250, 0.500, and 0.750 (at $x_1 + x_2 + x_3 = 1$).

## 2. Experimental

The ultrasonic apparatus, used for the measurement of speed of sound, is based on direct chronometry of the transfer times of pulses within the cell containing the sample. The apparatus and procedure of measurement have been described in detail in [3,4]. The precision of the speed of sound measurements was estimated to be 0.1%. Correctness of the uncertainty is confirmed by some test measurements carried out in water and dodecane and binary mixture octane + dodecane.

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**Table 1**
Material description.

| Chemical name | Source | Mass fraction purity | Purification method |
|---|---|---|---|
| Octane | Aldrich | >0.99 | None |
| Dodecane | Aldrich | >0.99 | None |
| Hexadecane | Aldrich | >0.99 | None |

The samples of the octane, dodecane, and hexadecane, provided by Aldrich, are shown in Table 1. The mixtures were prepared by mass to obtain mole fraction for components of 0.125, 0.250, 0.500, and 0.750 (at $x_1 + x_2 + x_3 = 1$). There are corresponding 6 points on ternary diagram (Fig. 1). Masses were determined using an electronic balance with precision of ±0.02 g. The mass of each sample of the mixture is more than 250 g.

The speed of sound in octane, dodecane, hexadecane, as well as in binary octane + dodecane, octane + hexadecane, and dodecane + hexadecane mixtures were studied by us previously [4–9].

The speeds of sound in octane + dodecane + hexadecane liquid mixture were measured at five temperatures: 298.15, 333.15, 373.15, 393.15 and 433.15 K in the pressure range from 0.1 to 100.1 MPa for the mole fraction of component in the mixture 0.125, 0.250, 0.500 and 0.750. The experimental values associated with the uncertainty are listed in Table 2.

The measurements were performed along isotherms with increasing and then decreasing pressure, whereas the difference between repetitive measurements was less than 0.01%. After having carried out a measurement at five temperatures, a repeated measurement was done at first temperature. The agreement between the results of repeated measurements, in this case, was within 0.03%. Repeated measurements results showed that the mixture composition change during experimental work did not take place.

## 2. Calculation

To calculate the thermodynamic properties of liquid mixture octane + dodecane + hexadecane at high pressures from the speed of sound data, well-known thermodynamic relations for density $\rho$ and isobaric heat capacity $c_p$ were used

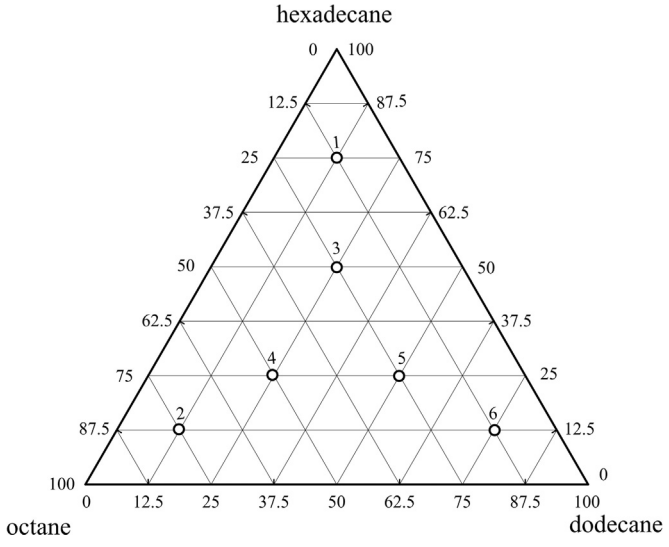


**Fig. 1.** Compositions of the mixtures: the ternary mixtures studied in this paper correspond to points 1–6 on the triple diagram.

$$\rho = \rho_0 + \int_{p0}^{p} \frac{1}{u^2} dp + T \int_{p0}^{p} \frac{\alpha_p^2}{c_p} dp, \tag{1}$$

$$c_p = c_{p0} - \int_{p0}^{p} \frac{T}{\rho} \left[ \alpha_p^2 + \left( \frac{\partial \alpha_p}{\partial T} \right)_p \right] dp, \tag{2}$$

where $p$ is the pressure, $T$ is the temperature; $\rho_0$ and $c_{p0}$ are, respectively, the density and isobaric heat capacity at atmospheric pressure $p_0 = 0.1$ MPa; $\alpha_p$ is the isobaric expansion coefficient defined by $\alpha_p = -1/\rho(\partial\rho/\partial T)_p$. For calculation, we have used the method of step computation of thermodynamic properties from the data on the speed of sound under pressure similar to the algorithm described in [10].

In the calculations, the experimental sound velocities reported in this study have been used. To calculate the thermodynamic properties, the experimental speed of sound data were fitted by the equation

$$\left( \frac{1000}{u} \right)^2 = E_0 + \frac{E_1}{E_2 + \frac{p}{100}} + \frac{E_3}{E_4 + \frac{p}{100}} \tag{3}$$

in which $p$ is the pressure in MPa, $T$ is the temperature in K. $E_0$ and $E_1$ are constants for each composition of mixture, and $E_2$, $E_3$, and $E_4$ are the temperature dependent functions

$$E_2 = e_{21} \left( \frac{T}{100} \right)^n, \tag{4}$$

$$E_3 = e_{31} \left( \frac{T}{100} \right), \tag{5}$$

$$E_4 = e_{41} + e_{42} \left( \frac{T_C - T}{100} \right)^k. \tag{6}$$

The critical temperature was calculated using the equation presented in [11]:

$$T_C = 1426.4 - 4086.3N^{-1/2} + 5992.7N^{-1} - 3665N^{-3/2}. \tag{7}$$

where $N$ is the number of carbon atoms in an alkane molecule.

The average number of carbon atoms $N$ is given by:

$$N = x_1 N_1 + x_2 N_2 + x_3 N_3. \tag{8}$$

where $x_1$, $x_2$, $x_3$ are the mole fraction and $N_1$, $N_2$, $N_3$ a number of carbon atoms of octane, dodecane, hexadecane, respectively.

The coefficients of Eq. (7) were determined by us through the critical temperature values [12] for pure alkanes when changing $N = (5–18)$.

Parameters of Eqs. (3)–(6) are given in Table 3. Eq. (3) describes speeds of sound data with standard and maximum deviations 0.05 and 0.1%, respectively.

There are no literature values for experimental data on density and isobaric heat capacity for the liquid mixture octane + dodecane + hexadecane. On the basis of experimental data, almost-linear dependence of the molar volume and the molar isobaric heat capacity on the molar mass of the n-alkanes and their mixtures [7] from $C_6H_{12}$ to $C_{16}H_{34}$ was found. The standard deviation for the entire array of literature data on the density of alkanes and their binary and ternary mixtures from this dependence is 0.06%. The standard deviation of the literature data on the isobaric heat capacity of alkanes and their mixtures is 0.5%. This correlation was used to calculate missing $\rho_0$ and $c_{p0}$ between 298 and 433 K.