

CALCULATION OF HEAT CONDUCTIVITY OF ORGANIC LIQUIDS AS FUNCTION OF TEMPERATURE

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UDC 531.756

Results of generalization of experimental data on heat conductivity of a series of organic liquids as a function of temperature at atmospheric pressure are presented. The approximation dependence for calculation of heat conductivity of liquid organic compounds as a function of temperature, normal boiling temperature, and molar mass is obtained.

Previously, experimental studies of heat conductivity within the temperature range of 153–573 K at atmospheric pressure were carried out for the following compounds [1, 4, 8, 9]: saturated hydrocarbons (hexane, heptane, octane, nonane, decane, undecane, tetradecane, pentadecane, hexadecane, heptadecane, and nonadecane), unsaturated hydrocarbons and cycloparaffins (hexane-1, heptane-1, octane-1, decene-1, dodecene-1, tetradecene-1, pentyne-1, hexyne-1, heptyne-1, undecyne-5, and dodecyne-6), esters and ethers (domethyl, diethyl, dipropyl, dibutyl, diamyl, dihexyl, diheptyl, dioctyl, diallyl, methylpropyl, ethylbutyl, methylamyl, ethylamyl, propylbutyl, ethylhexyl, methylheptyl, ethylheptyl, and ethyloctyl), ketones (dimethyl, diethyl, dipropyl, dibutyl, diamyl, dihexyl, diheptyl, methylethyl, methylpropyl, methylbutyl, methylamyl, methylhexyl, methylheptyl, methyloctyl, ethylpropyl, ethylbutyl, ethylamyl, ethylhexyl, ethylheptyl, ethyloctyl and others), aldehydes (butyraldehyde, valeraldehyde, caproaldehyde, enanthal, octanal, nonanal, decanal, hendecanal, and dodecanal), saturated monohydric alcohols (methanol, pentanol, hexanol, heptanol, octanol, nonyl alcohol, 1-decanol, undecylic alcohol, dodecyl alcohol, tridecyl alcohol, pentadecyl alcohol, hexadecyl alcohol, heptadecyl alcohol, octadecyl alcohol, and ethanol), and acetates (methyl acetate, ethyl acetate, butyl acetate, isobutyl acetate, amyl acetate, and isoamyl acetate).

The heat conductivity of the above organic liquids was measured on specially designed experimental installations using the method of the heated thread and the cylindrical bicalorimeter of the regular thermal regime [5, 6].

To obtain an equation for calculations of heat conductivity of organic liquids as a function of temperature at atmospheric pressure we processed experimental data from [1-4] using the following functional dependence:

$$\frac{\lambda}{\lambda_1} = f\left(\frac{T}{T_1}\right), \quad (1)$$

where λ is the heat conductivity at temperature T ; λ_1 is the heat conductivity at temperature $T_1 = 383$ K.

A generalization for the dependence (1) for organic liquids is shown in Fig. 1, from which one can see that the experimental data fit the common curve rather well. We write the equation for this curve:

$$\lambda = \left[0.393 \left(\frac{T}{T_1}\right)^2 - 1.432 \frac{T}{T_1} + 2.039 \right] \lambda_1. \quad (2)$$

The analysis of the value of λ_1 for organic liquids has shown that this quantity is a function of the molar weight (Fig. 2). Then the experimental data presented in Fig. 2 were processed in the form of the functional dependence

$$\frac{\lambda_1}{\lambda_1^*} = f\left(\frac{\mu}{\mu_1}\right), \quad (3)$$

K. Dzhravaev State Pedagogical University, Dushanbe, Tadzhikistan. Translated from *Inzhenerno-Fizicheskii Zhurnal*, Vol. 68, No. 3, pp. 451-455, May-June, 1995. Original article submitted December 3, 1991; revision submitted October 13, 1993.

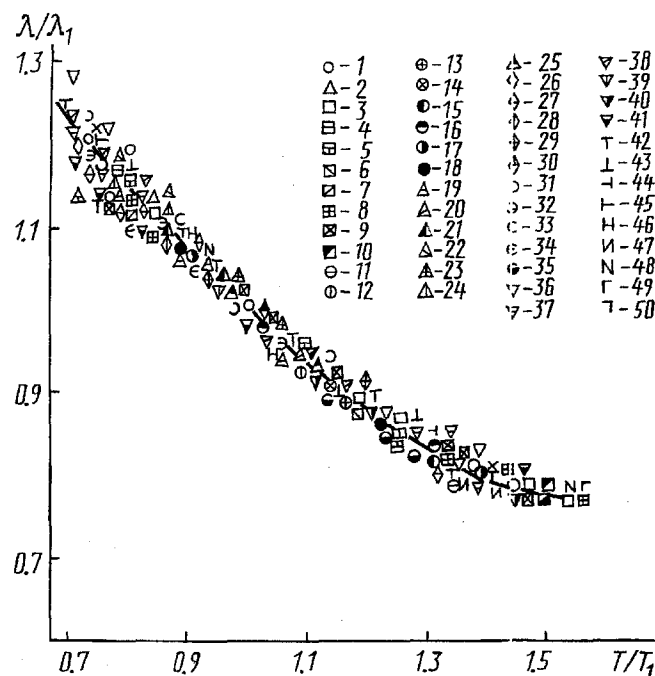


Fig. 1. Dependence of the relative heat conductivity λ/λ_1 on the relative temperature T/T_1 of organic liquids: 1-10) saturated hydrocarbons; 11-18) cycloparaffins; 19-25) olefin hydrocarbons; 26-30) alcohols; 31-35) ketones; 36-41) ethers; 42-45) aldehydes; 46-50) acetates.

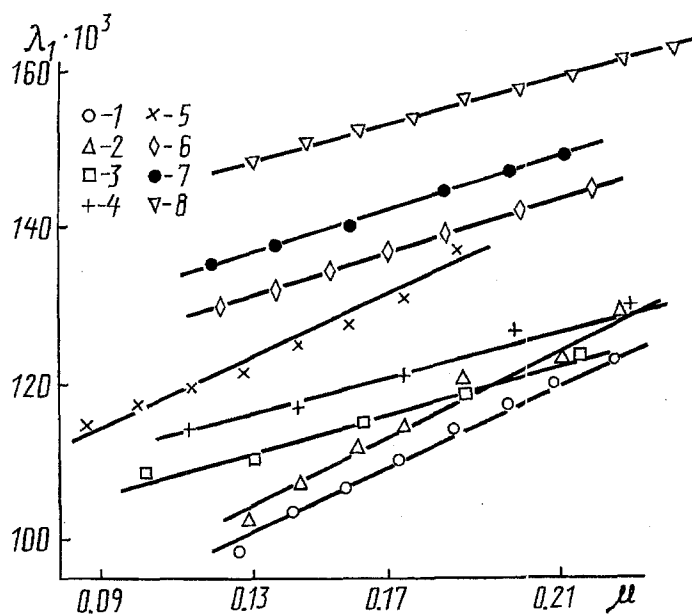


Fig. 2. Dependence of λ_1 on μ : 1) olefin hydrocarbons; 2) paraffin hydrocarbons; 3) ethers; 4) ketones; 5) aldehydes; 6) alcohols; 7) butyrates; 8) acetates. λ_1 , W/(cm·K); μ , kg/mole.

TABLE 1. Values of μ_1 and T_{boil} of Organic Liquids

Organic liquid	Amine acetate	Ethyl ether	Dodecene-1	<i>n</i> -Dodecane	Diamyl ketone	Dodecanal	Dodecyl alcohol
μ_1 , kg/mole	0.136	0.158	0.168	0.170	0.170	0.184	0.186
T_{boil} , K	405	464	486	489	499.4	535.2	546.6

TABLE 2. Comparison of Experimental Data with Calculated Values of Heat Conductivity $\lambda \cdot 10^{-3}$, W/(cm · K) for Several Organic Liquids

T, K	Dibutyl ester			Diheptyl ketone			Enanthal			Pentadecyl alcohol				
	λ_{exp}	λ_{calc}	$\Delta, \%$	λ_{exp}	λ_{calc}	$\Delta, \%$	λ_{exp}	λ_{calc}	$\Delta, \%$	T, K	λ_{exp}	λ_{calc}	$\Delta, \%$	
273	135	134	0,8	162	155	3,9	155	152	2	273	200	195	2,6	
293	128	128	0	154	148	4,5	148	146	1,4	333	179	174	2,8	
313	124	124	0	148	143	5	143	139	2,9	373	166	164	1,2	
333	119	119	0	141	138	2,2	140	136	2,9	413	155	152	1,9	
353	117	116	0,8	134	134	0	136	130	3,2	493	140	134	4,9	
373	114	112	1,8	130	129	0,8	130	126	3,2	533	134	129	3,8	
393	110	108	2,9	125	125	0,8	127	124	2,4	573	127	124	2,4	
413	107	104	2,9	120	120	0	125	118	5,1					
n-Tridecane														
T, K	λ_{exp}	λ_{calc}	$\Delta, \%$	Pentadecene -1			n-Octadecane			n-Heptane				
T, K	λ_{exp}	λ_{calc}	$\Delta, \%$	λ_{exp}	λ_{calc}	$\Delta, \%$	T, K	λ_{exp}	λ_{calc}	$\Delta, \%$	T, K	λ_{exp}	λ_{calc}	$\Delta, \%$
273	143	139	2,2	139	139	4,3	313	149	153	2,7	273	132	127	4
413	116	116	0	122	122	1,6	333	145	145	0	293	129	124	3,9
473	108	106	1,9	116	116	2,6	353	142	140	1,4	313	123	121	1,6
				106	106	3,8	373	138	136	1,4	333	118	117	0,8
							393	134	130	2,9	363	113	113	0
							413	131	126	3,8				
							433	127	124	3,2				

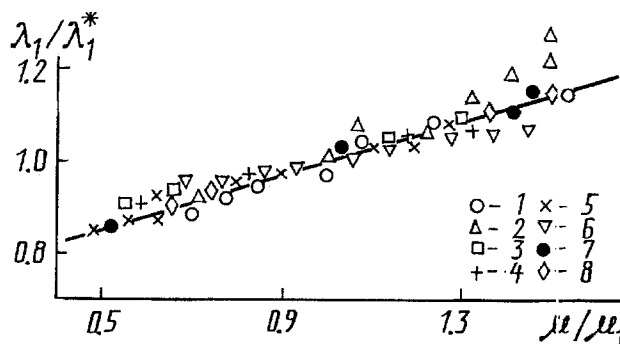


Fig. 3. Dependence of relative heat conductivity λ_1/λ_1^* on the relative molar weight μ/μ_1 of organic liquids: 1) olefin hydrocarbons; 2) paraffin hydrocarbons; 3) ethers; 4) ketones; 5) aldehydes; 6) alcohols; 7) butyrates; 8) acetates.

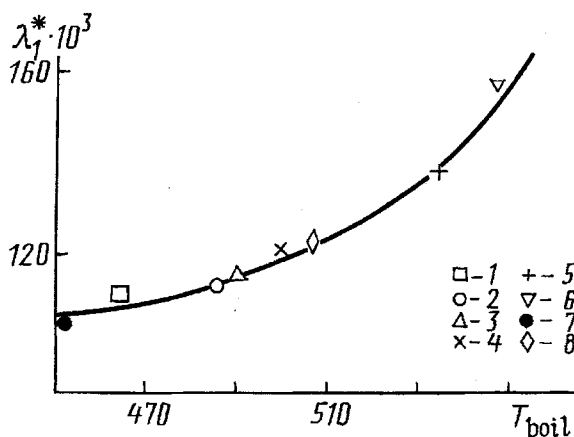


Fig. 4. Dependence of λ_1^* on the normal boiling temperature T_{boil} of organic liquids: 1) 1-ethyloctyl ester; 2) dodecene-1; 3) *n*-dodecane; 4) dimethyl ketone; 5) lauryl alcohol; 6) dodecyl alcohol; 7) amyl acetate; 8) octyl butyrate.

where λ_1^* is the heat conductivity corresponding to the value of μ_1 . The quantity μ_1 possesses different values for each of the homologous series (Table 1).

An approximation of the dependence (3) for all liquids is shown in Fig. 3, from which is clearly seen that the experimental points fit for the common curve well. The curve is described by the equation

$$\lambda_1 = \left(0.3 \frac{\mu}{\mu_1} + 0.7 \right) \lambda_1^*, \quad (4)$$

with the help of which the values of λ_1 can be calculated as a function of the molar weight, provided the values of λ_1^* are known.

Analysis of the values of λ_1^* for the above organic liquids has shown that λ_1^* is a function of the normal boiling temperature (Fig. 4). We describe the curve in the figure by the expression

$$\lambda_1^* = 5.45 \cdot 10^{-6} T_{\text{boil}}^2 - 4.972 T_{\text{boil}} + 1.24, \quad \text{W}/(\text{m} \cdot \text{K}). \quad (5)$$

Analysis of μ_1 for the liquids under investigation has shown that this quantity is also a function of the normal boiling temperature and is described by the equation:

$$\mu_1 = 3 \cdot 10^{-4} T_{\text{boil}} + 0.022, \quad \text{kg}/\text{mole}. \quad (6)$$

From relationship (2) in view of Eqs. (4)-(6) we obtain a relationship for calculation of the heat conductivity of liquid organic substances as a function of temperature

TABLE 3. Calculated Values of Heat Conductivity ($\lambda_{\text{calc}} \cdot 10^3$, W/(m·K)) of Several Organic Liquids Previously not Studied Experimentally

T, K	Dichloromethane	Pentyl acetate	Methylchloroacetate	Dimethyl ester ethyleneglycol (1,2-methoxyethane)	Benzyl alcohol	Benzoaldehyde
273	127	120	115	112	149	130
293	121	115	109	107	143	125
313	117	111	106	103	138	121
333	113	107	103	100	134	117
353	109	104	99	97	129	113
373	106	101	96	93	126	109
393	102	97	92	90	121	105
413	99	94	89	87	117	102

$$\lambda = \left[0.393 \left(\frac{T}{T_1} \right)^2 - 1.432 \frac{T}{T_1} + 2.039 \right] \left(\frac{0.3\mu}{3 \cdot 10^{-4} T_{\text{boil}} + 0.022} + 0.7 \right) \times \left(5.45 \cdot 10^{-6} T_{\text{boil}}^2 - 4.972 \cdot 10^{-3} T_{\text{boil}} + 1.24 \right), \quad \text{W/(m}\cdot\text{K)}, \quad (7)$$

where T_{boil} is the normal boiling temperature (see Table 1).

Using Eq. (7) one can calculate the heat conductivity as a function of temperature at atmospheric pressure for liquid organic compounds previously not studied experimentally, provided the values of the molar weight and normal boiling temperature are known. Verification of this equation has shown that it describes heat conductivity of liquid organic compounds within the temperature range from the room temperature to the boiling temperature with an error of 2–5%.

Table 2 presents a comparison of the results of calculation by Eq. (7) with the experimental data on heat conductivity of several organic liquids.

Using Eq. (7) we calculated the heat conductivity of liquid organic compounds previously not studied experimentally (Table 3).

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