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**LOGNORMAL DISTRIBUTION AS UNIVERSAL
FUNCTION OF TEMPERATURE DEPENDENCE OF
HEAT CAPACITY**

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Heat capacity is a fundamental value of thermodynamics that allows us to calculate all other thermodynamic parameters required for behavior prediction of complex physical and chemical systems.

Theoretically the temperature dependence of the isochoric heat capacity of most solids must obey the well-known theoretical dependences of Debye, Einstein, and Tarasov [1]. It would allow quite accurately approximate the experimental data that are necessary for scientific and engineering calculations [2], but in practice many substances have anomalous behavior of heat capacity (deviation from the theoretical value) and as a result, purely empirical or semi-empirical dependencies are more widespread for practical thermodynamic calculations [3].

Such empirical dependencies are simpler for calculations and have greater accuracy compared with theoretical dependencies in useful for practice temperature range. But at the same time they can result a significant deviation from the “reasonable” behavior just beyond of interval of experimental data and so any theoretical conclusions based on them may contradict the theoretical foundations. In addition such empirical dependencies is characterized by complexity of calculations of thermodynamic quantities (S , H , G), deficiency of techniques for obtaining required empirical parameters and absence of physical meaning of such parameters.

Thus, for now, even if a large amount of experimental data has been collected, the contribution of various factors to the heat capacity has been established and many methods for its determination and calculations have been developed. Modern chemical thermodynamics does not have a unified, theoretically justified, convenient for use, adequate to experimental data, and understandable for scientists approach for calculating of heat capacity.

So the aim of this work is the determination of the dependence, which could be used for the maximum range of parameters and maximum number of substances and meet the requirements of theory and computational practice. And for this, three basic concepts of modern thermodynamics were considered.

First, the physical nature of the heat capacity is associated to the statistical state of matter, which is determined by its internal structure. Second, such a state is the sum of different statistical states that can be independent of each other. Third concepts based on the fact that the proposed functions of Debye, Einstein and Tarasov are only particular cases of more general energy state distribution.

Analysis of experimental data of temperature dependences of heat capacity for solids and gases showed that as such

universal distribution function with logarithm of temperature as argument (Log-normal distribution) can be Laplace function (probability function). It is important that this function is the limiting distribution function according to the theory of mathematical statistics (Central Limit Theorem) [4] and have only 2 parameters with some physical meaning

$$Q(x) = \frac{1 + \operatorname{Erf}\left(\frac{\sqrt{2}}{2}x\right)}{2}$$

$$x = \frac{\ln(T) - \ln(\zeta)}{\nu} = \frac{1}{\nu} \ln\left(\frac{T}{\zeta}\right)$$

where

T – temperature, K

ζ – scale factor (characteristic temperature), K

ν – rate of state changes

$C_\nu(T)$ – Laplace dependence of heat capacity from temperature

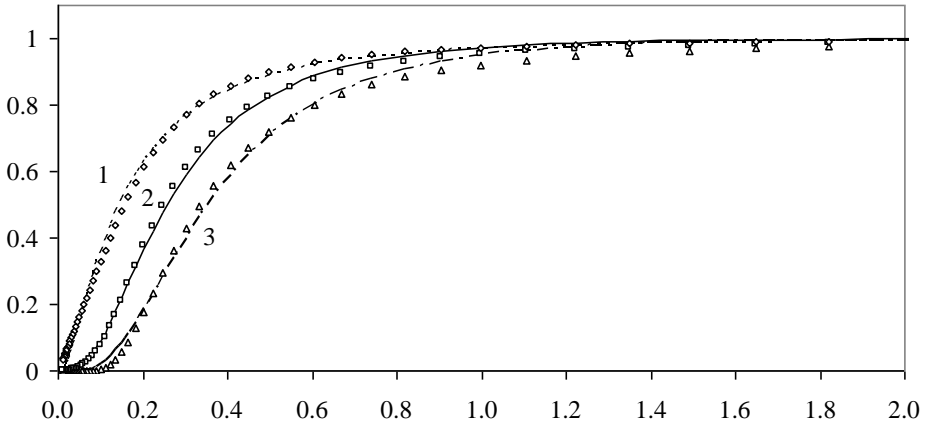


Fig.1. Tarasov (1), Debye (2) and Einstein (3) functions and fitted Laplace function for $x=T/\zeta$

As can be seen from Figure 1, functions of Einstein, Debye or Tarasov can be well approximated by the normal distribution function. Values of parameters for fitted Laplace function to Einstein, Debye and Tarasov functions and accuracy of approximation (\square) for x from 0 to 10 are given in the Table 1.

Table1. Coefficients values of the equation $C_v(T)$ and the difference between the Laplace function and the Einstein, Debye, and Tarasov functions

Function	ζ	\square	\square
Enshstein	0.352	1.589	0.031
Debye	0.257	1.421	0.021
Tatasov	0.143	0.987	0.040

The scale factor (ζ) numerically corresponds to value of argument at which the function value is 50% of its maximum. So, one of the benefits of using Laplace function is possibility to evaluate fast the characteristic temperature ζ . Its value can be defined as the temperature at which the heat capacity is 50% of the maximum $(3 \cdot n \cdot R)/2$.

This parameter is closely related to parameters of Einstein, Debye and Tarasov functions. Therefore, with an error not exceeding 4% its possible take ζ if Einstein, Debye and Tarasov temperature is known

$$\zeta = \frac{\theta_D}{3.90}, \zeta = \frac{\theta_E}{2.85}, \zeta = \frac{\theta_T}{6.83}$$

The value of distribution of logarithm of temperature ($\square\square\square$ determines the width of the transition zone to the sum

of most probable state and can be determined from already known structural data. It can be accepted with an average value of 1.5 (distribution close to the Debye and Einstein functions) for the most crystalline materials with three-dimensional structure (metals, diamond-like and vitreous structure), to layered structures (graphite-like substance) with an average value of 1.2, and for linear (polymers) with an average value of 0.9 (close to Tarasov function).

However, in the absence of the substance structure data, and in the presence of experimental data on the heat capacity for a range $C_V \approx (1 \div 2R)$ ν can be calculated with precision about 2% according to the given bellow equation

$$\nu = \frac{2\sqrt{2}}{3 \cdot R \cdot n} \cdot \frac{C_1 - C_2}{\ln(T_1) - \ln(T_2)}$$

Therefore, to estimate temperature dependences of specific heat it is sufficient to know experimental data of heat capacity for two temperatures, preferably from a range close to ζ . Values that are more precise can be obtained by any of the statistical methods of evaluation.

It should be noted that the use of the Laplace function gives also some advantages in terms of computation of other thermodynamic quantities. The determination of entropy and enthalpy values requires an additional calculation only of the

error function, its derivative and integral, which is quite easy to do due to a sufficient number of works in this area [5,6].

$$S(T) = \int \frac{C_v(T)}{T} dT = 3R \cdot \int \frac{Q(x)}{T} dT = 3R \cdot \left[\nu \cdot Q(x) \cdot x + \frac{dQ(x)}{dx} \cdot \nu^2 \cdot T + \ln(\zeta) \right]$$

$$S(T) = 3R \cdot \left[Q\left(\frac{1}{\nu} \ln\left(\frac{T}{\zeta}\right)\right) \cdot \ln\left(\frac{T}{\zeta}\right) + \nu^2 \cdot T \cdot \frac{\sqrt{2}}{2 \cdot \sqrt{\pi}} e^{-\frac{\left[\frac{1}{\nu} \ln\left(\frac{T}{\zeta}\right)\right]^2}{2}} + \ln(\zeta) \right]$$

$$H(T) = \int C_v(T) dT = 3R \cdot \left[\int Q(x) dT = \frac{\int \operatorname{Erf}\left(\frac{\sqrt{2}}{2} \frac{1}{\nu} \ln\left(\frac{T}{\zeta}\right)\right) dT}{2} + \frac{T}{2} \right]$$

where,

H(T) – temperature dependence of enthalpy

S(T) – temperature dependence of entropy

Many literature data, internet resource and software product have been used for the testing dependence which confirms its reliability [7-11]. The most typical experimental literature data of temperature dependence of heat capacity were been approximated by all theoretical relationships. But only using Laplace function allows to describe heat capacity of both

crystalline and linear macromolecular substances with almost the same accuracy.

Thus, the proposed dependence is universal and describes the isochoric specific heat of solids, which does not contradict existing theoretical dependence but complements them. It has greater accuracy in comparison with theoretical dependencies for all structures of solids.

Parameters of proposed dependence have a clear physical meaning which relates to structural features of substances. So in case of absence of accurate thermochemical data from experimental data such structural features can be used for preliminary evaluation of parameters of dependence.

Proposed dependence is simpler in calculation in comparison with other theoretical, empirical and semi-empirical dependences both at the stage of evaluating its parameters and for calculation of all thermodynamic quantities.

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