THERMAL PROPERTIES OF SOLID BENZENE

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The results of the numerical analysis of the thermodynamic parameters of solid benzene are presented. The calculations of the temperature dependence of the isochoric heat conductivity of solid benzene have been carried out with the help of various methods. The influence of thermal pressure on elastic properties and the isochoric heat conductivity has been studied. Possible reasons of the exceeding of the isochoric heat conductivity of benzene over the classical law $1/T$ are described within the framework of the phonon concept.

The results of the researches of the thermal properties of molecular crystals point out some their features which go beyond the framework of traditional ideas about thermal processes taking place in dielectric crystals [1–6]. The available theoretical models [7–9] were created mainly on the basis of researches of the simplest crystal structures, atomic crystals. Therefore, the features typical of molecular crystals were not taken into account in them. In particular, the question is about the orientational motion of molecules. In this connection, the necessity to carry out researches of the thermal properties of molecular crystals more systematically has arisen, with the obtained results being applied in future to check and develop the existing theoretical models of thermal processes in dielectric crystals.

Solid benzene was selected as an object of researches. One can note that the situation concerning the temperature dependence of the heat conductivity of the particular substance in the region of submelting temperatures remains rather controversial now. For example, an insignificant increase of the recalculated isochoric heat conductivity λ_V, as the temperature rises in the indicated region, was observed in [10], while the value of λ_V, experimentally determined in [11], is almost constant here. To elucidate this issue and to obtain additional data about thermal properties, we carried out the calculations of thermodynamic parameters of solid benzene and made the analysis of the high-temperature behavior of the heat conductivity in the framework of the Callaway model and taking into account the thermal pressure which arises in specimens during isochoric researches.

It has been established earlier that solid benzene under the pressure of its own saturated vapors exists only in a single crystal modification and has the orthorhombic structure [12] (Fig. 1) with the space symmetry $P_{bca} - D_{2h}^{15}Q$ [13]. The researches of the solid benzene structure [12] testify that there is a significant reduction of the second moment of the nuclear magnetic resonance signal in the temperature interval of 80 – 120 K, which results from molecular reorientations in the ring plane around the axis of the sixth order (the c-axis). The reorientation frequency at 85 K equals 10^4 s^{-1} and considerably increases, as the temperature grows further, reaching the values of about 10^{11} s^{-1} near the melting temperature ($T_\mathrm{m} = 278.5$ K [14]).

The results of the neutron scattering experiments [15] testify that the oscillation frequency of the benzene molecule increases to some extent, as the temperature decreases, while the oscillation amplitudes substantially diminish at the same time. This brings us to a conclusion that solid benzene is a crystal where, provided that the temperature grows, the transition from librations of molecules to their practically free rotations takes place only in a single plane perpendicular to the c-axis.

In the general case of anisotropic solids, the coefficient of volume thermal expansion β can be calculated according to the formula

$$\beta = \alpha(a) + \alpha(b) + \alpha(c), \tag{1}$$

where $\alpha(a), \alpha(b)$, and $\alpha(c)$ are the coefficients of linear thermal expansion along the relevant axes. Their values were obtained making use of the data of [13]. The absence of phase transformations in solid benzene over the whole interval of temperatures under investigation allowed us to carry out their reliable extrapolation to the melting temperature. The obtained results are presented in Table 1 and in Fig. 2.

The temperature dependence of the Grüneisen constant was obtained with the help of the dependence

$$\gamma = \beta V_\mathrm{mol}/C_P \mathrm{X}_S, \tag{2}$$

where X_S is the adiabatic compressibility, V_mol is a molar volume of the studied specimens, C_P is the isobaric heat capacity. The temperature dependence of

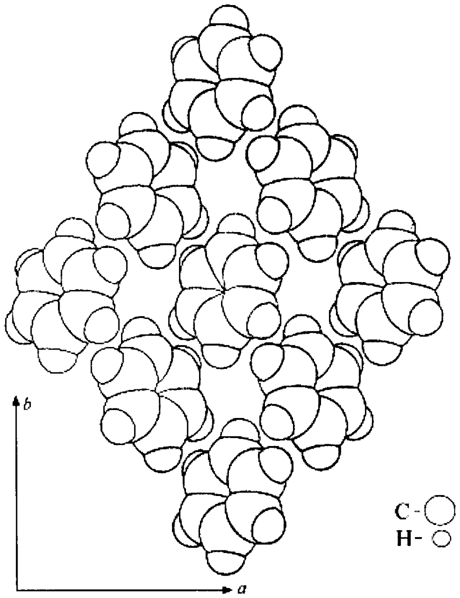

Fig. 1. Crystalline structure of solid benzene

the molar volume $V_{\rm mol}$ (table 1) was obtained from literary data [11,12]. The adiabatic, X_S, and isothermal, X_T, compressibilities were calculated according to the following formulae [16]:

$$X_S = \left[\rho\left(v_\ell^2 - 4/3v_t^2\right)\right]^{-1}, \tag{3}$$

$$X_T = \beta V_{\rm mol}/\gamma C_V, \tag{4}$$

where the corresponding values of the heat capacities at constant pressure, C_P, and constant volume, C_V, were evaluated (table 2) making use of the data of [14] and the well-known relation

$$C_V = C_P/(1+\gamma\beta T), \tag{5}$$

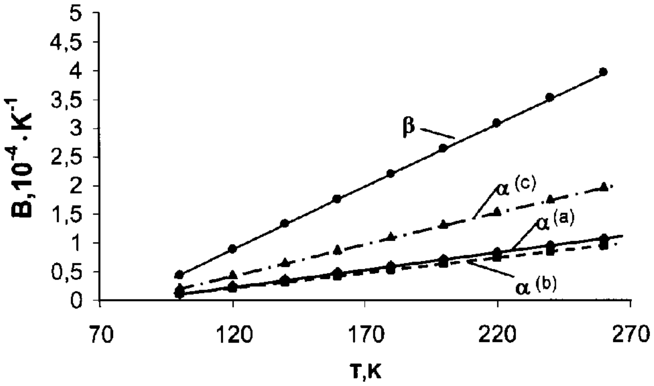

Fig. 2. Temperature dependences of the thermal expansion coefficients β, $\alpha(a)$, $\alpha(b)$, and $\alpha(c)$ of solid benzene

the temperature dependence of the crystal density $\rho(T)$ (Table 1) was obtained on the basis of the data for $V_{\rm mol}$, and v_ℓ^P and v_t^P are the isobaric longitudinal and transverse sound velocities, respectively, in the crystal.

The necessary initial data for the calculations of isobaric sound velocities were taken from [17]. The linear dependence of elastic constants on the temperature allowed us, in the isobaric case, to carry out their reliable extrapolations and calculations in the whole investigated range of temperatures (Fig. 3). In so doing, the following relations [18] were used:

$$v_\ell^P = \left(C_{11}/\rho\right)^{1/2},$$

$$v_t^P = \left(C_{44}/\rho\right)^{1/2}. \tag{6}$$

The Grüneisen constant characterizes the change of the frequency spectrum with the change of the crystal volume. The obtained values for the Grüneisen constant (Table 2) decrease at first with the temperature approximately up to 120 K, with such a behavior agrees

T a b l e 1. Temperature dependences of the thermal expansion coefficients $\beta, \alpha(a), \alpha(b), \alpha(c)$, the density ρ, the molar volume $V_{\rm mol}$, the longitudinal and transverse sound velocities in the benzene crystal for isobaric and isochoric cases

T, K	$\alpha(a)\cdot10^{-4}$, K^{-1}	$\alpha(b)\cdot10^{-4}$, K^{-1}	$\alpha(c)\cdot10^{-4}$, K^{-1}	$\beta\cdot10^{-4}$, K^{-1}	$\rho\cdot10^{3}$, kg/m^3	$V_{\rm mol}\cdot10^{6}$, m^3/mole	v_l^P, m/s	v_t^P, m/s	v_l^V, m/s	v_l^V, m/s
80	—	—	—	—	1.110	70.5	9591	6381	9591	6381
100	0.116	0.104	0.218	0.439	1.103	71.0	9402	6193	9592	6383
120	0.233	0.208	0.437	0.879	1.094	71.6	9205	6016	9593	6385
140	0.350	0.312	0.656	1.318	1.088	72.1	8983	5839	9594	6387
160	0.466	0.416	0.875	1.758	1.078	72.6	8806	5524	9597	6390
180	0.583	0.520	1.094	2.198	1.071	73.2	8539	5328	9599	6394
200	0.700	0.624	1.313	2.673	1.061	73.6	8323	5119	9603	6399
220	0.816	0.728	1.532	3.077	1.048	74.4	8114	4874	9607	6405
240	0.933	0.832	1.751	3.516	1.037	75.2	7850	4543	9611	6412
260	1.050	0.936	1.970	3.956	1.024	76.1	7629	4227	9617	6421
278	1.17	1.040	2.189	4.396	1.013	77.0	7488	4072	9622	6429

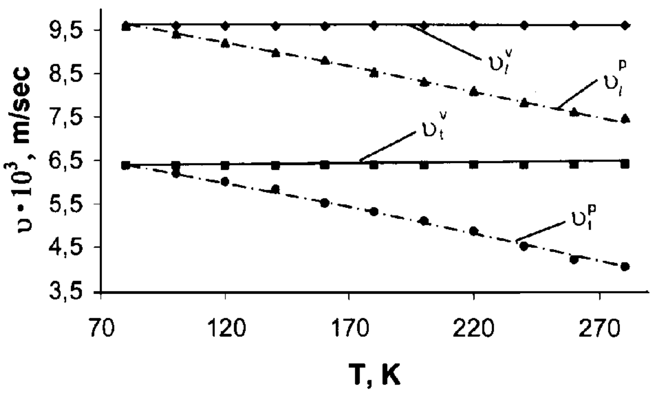

Fig. 3. Theoretical dependences of longitudinal and transverse sound velocities in solid benzene for the isobaric, v^P, and isochoric, v^V, cases

well with the data of [12]. The latter correspond to an untwisting of the benzene molecules in the ring plane at temperatures of 80 – 120 K. Then the curve of the Grüneisen constant (Fig. 4) passes through a minimum and starts to grow, similarly to what takes place for the majority of atomic crystals. The average value of the Grüneisen constant is 1.84, being close to those values which are observed in disordered phases of simple molecular crystals [19] and crystals of inert gases [20].

The temperature dependence of the thermal pressure $P(T)$ in the isochoric case (Fig. 5) was obtained making use of the formula [21]

$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{\gamma C_V}{V_{\mathrm{mol}}}. \tag{7}$$

One can see from Fig. 5 that the thermal pressure in the isochoric specimen changes by more than a factor of 100 over the whole investigated interval of temperatures.

The value of the molar volume depends on the temperature of the crystal growing. The obtained results of calculations are in a good agreement with the data of direct researches of the thermal pressure of solid benzene [11] carried out for specimens with the molar volume $V_{\mathrm{mol}} = 75.05$ cm^3/mole and presented in Fig. 1 by a solid curve *1*. The high-temperature values of the Debye characteristic temperature $\Theta_{\mathrm{D}\infty}$ (table 2) were evaluated according to the formula [22]

$$\Theta_{\mathrm{D}\infty} = \frac{h}{k_{\mathrm{B}}}\left[\frac{4\pi V_{\mathrm{mol}}}{9N}\left(\frac{1}{v_\ell^{P3}} + \frac{2}{v_t^{P3}}\right)\right]^{-\frac{1}{3}}, \tag{8}$$

where k_{B} is the Boltzmann constant and N is a number of atoms in a volume unit.

The results of researches of the heat conductivity of equilibrium spesimens of solid benzene, which have been carried out in [10], are shown in Fig. 6. The isobaric heat conductivity λ_P, which corresponds to a solid curve, falls down as the temperature increases according to the dependence $\lambda_P \sim T^{-1.1}$.The values of the isochoric heat conductivity λ_V at the given temperatures were obtained by recalculating the experimental data for the isobaric heat conductivity λ_P to the constant volume $V_{\mathrm{mol}} = 70.5$ cm^3/mole, occupied by the sample at the temperature of growing. The calculation was carried out with the help of the formula [23]:

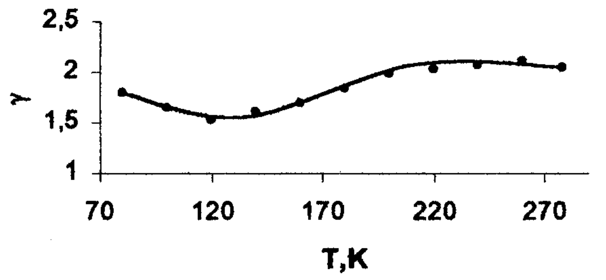

Fig. 4. Temperature dependence of the Grüneisen constant in solid benzene

$$\lambda_V = \lambda_P \left(\frac{V_m\,(T)}{V_{m0}}\right)^g, \tag{9}$$

where $V_m(T)$ is a temperature dependence of the molar volume of a free sample, V_{m0} is the molar volume of the recalculated sample. The Bridgeman factor $g = \partial \ln\lambda/\partial \ln V$ was accepted to equal 7.5 [11].

The temperature dependence of the benzene isobaric heat conductivity is satisfactorily described by the classical dependence $\lambda = B/T$ in the whole investigated interval of temperatures. In the isochoric case, the satisfactory agreement with the law $1/T$ is observed only below 180 K.

Table 2. Temperature dependences of the Grüneisen constant γ, the high-temperature characteristic Debye temperature $\Theta_{\mathrm{D}\infty}$, the theoretical and experimental values of the heat conductivity, and the isobaric C_P and isochoric C_V heat capacities

T, K	γ	$\Theta_{\mathrm{D}\infty}$	λ_{theor}, mW/(cm·K)	λ, mW/(cm·K)	C_P, J/(mole·K)	C_V, J/(mole·K)
80	1.79	190	8.31	8.19	40.7	38.7
100	1.65	185	7.18	6.43	47.6	45.5
120	1.53	179	6.32	5.80	54.2	51.5
140	1.59	174	5.42	5.35	61.8	57.5
160	1.69	166	4.51	5.04	68.9	61.9
180	1.83	160	4.16	4.62	74.8	64.6
200	1.97	154	3.73	4.38	83.6	68.1
220	2.03	147	3.52	4.26	93.5	72.8
240	2.07	138	3.39	4.18	104.2	75.6
260	2.09	130	3.24	4.15	114.5	76.7
278	2.04	125	3.12	4.16	125.5	80.8

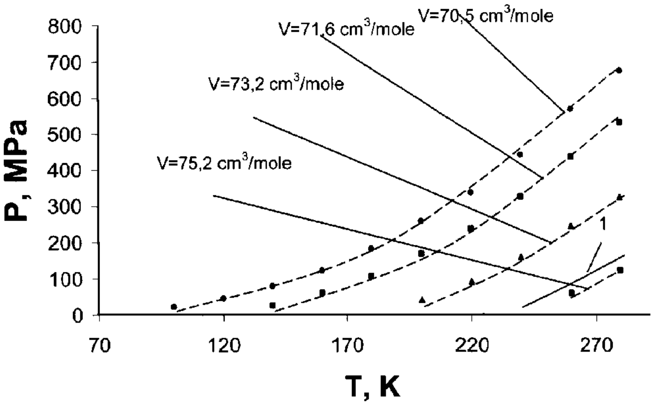

Fig. 5. Temperature dependence of the thermal pressure for the solid benzene specimens with various molar volumes. Curve *1* corresponds to the experimental data [11]

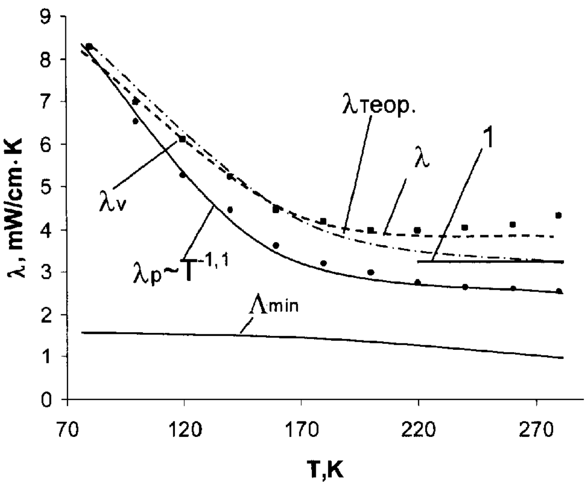

Fig. 6. Temperature dependences of the isobaric, λ_P, and isochoric, λ_V, heat conductivities of solid benzene. The circles present the experimental values of λ_P [10] and the squares the values of λ_V obtained according to Eq. (9). The solid curve corresponds to the smoothed experimental data. The dash-dotted curve shows the results of calculations on the basis of the Callaway method ($\lambda_{\text{theor}} \sim 1/T$). The dashed line shows the values of the heat conductivity obtained according to Eq. (10). It is also shown the limiting heat conductivity $\Lambda_{\min}$ calculated for the isobaric case in the framework of the Einstein model of the diffusion heat transfer directly from atom to atom. Line *1* corresponds to the data of [11] for a specimen with the molar volume $V_{\text{mol}} = 75.05$ cm^3/mole

The results of our calculations and those of the direct researches [11] show (Fig. 6) that the value of λ_V of benzene depends on T more weakly than it is required by the law $1/T$, and at $T > 200$ K practically ceases to depend on it and even starts to grow slightly. It is important to note that this effect cannot be explained for benzene by the influence of the rotational motion of the molecules only because the transition of its molecules to a practically free rotation comes to an end at 120 K, and all this occurs only in a single plane perpendicular to the c-axis. The experiments show [12] that the further temperature growth does not augment the rotation frequency of benzene molecules substantially.

It is interesting to note that the weaker than $1/T$ dependence of the high-temperature isochoric heat conductivity is observed also for crystals of inert elements [23], where the rotational degrees of freedom are absent altogether. The deviations upwards from the law $1/T$ are also typical of other molecular crystals, which consist of asymmetric molecules [6]. Due to this circumstance, the total orientational ordering preserves in those systems up to the melting temperature. Therefore, besides the influence of the orientational disordering on the heat conductivity, one must pay attention to other possible effects in order to explain the exceeding above the law $1/T$.

According to theoretical representations, the speed of phonons in dielectric crystals is practically independent of the temperature in the isochoric case and is equal to an average sound velocity in the crystal.

At carrying out the isochoric experiment with the temperature growth, the measuring ampoule of the practically constant volume prevents from the thermal expansion of the investigated speciment, which leads to an increase of the thermal pressure [11]. It does not exclude an opportunity to affect the thermal properties through the growth of the sound velocity. However, now there are no experimental data of structural researches and measurements of the sound velocity in solid benzene in the isochoric case.

Taking into account that the isochoric heat conductivity exceeds the diffusion minimum of the heat transfer in benzene by a factor of three (Fig. 6), we shall consider the concept of phonons suitable, despite of the exceeding of the Debye temperature in the experiment. We use the well-known relation of the kinetic theory of gases

$$\lambda = {}^1\!/_3 \, (C_V v \, \ell) \, , \tag{10}$$

where ℓ is a mean free path, for the calculation of the isochoric heat conductivity. The average speed of phonons v at the given temperature was defined with the help of the formula

$$\frac{3}{v^3} = \frac{1}{3v_\ell^{V^3}} + \frac{2}{v_t^{V^3}} \, , \tag{11}$$

where v_ℓ^V and v_t^V are the isochoric longitudinal and transverse sound velocities in the crystal, respectively.

At isochoric researches, the crystal sample undergoes the permanently growing pressure of the measuring ampoule walls, because the ampoule has a practically constant volume. This process is analogous to a uniform squeezing with a negative sign, since the thermal pressure, in this case, arises owing to a confinement imposed on the thermal expansion of a polycrystalline specimen. At such a squeezing, each unit of the crystal surface undergoes the pressure, identical by value and directed always normally to the surface. This is just what corresponds to the conditions of isochoric experiment. We use the data obtained for thermal expansions (Table 1) and thermal pressure (Fig. 5) to analyze the influence of thermal pressure upon the isochoric heat conductivity.

It is known [24] that the stress tensor is connected to the strain tensor at a uniform squeezing by the relation $C_{ii} = 3Ku_{ii}$, where $K = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T$ is the volume compressibility of the substance, and is defined exclusively by its diagonal elements. The values of the diagonal elements of the strain tensor were calculated using the thermal expansion data (Table 1). The temperature dependence of $\left(\frac{\partial V}{\partial P}\right)_T$ was obtained with the help of the data for the thermal pressure (Fig. 5) and the molar volume of the research specimens (Table 1). Evaluating the diagonal elements of the stress tensor according to Eqs. (6), the temperature dependences of the values of v_ℓ^V and v_t^V were calculated (Fig. 3). The results of calculations show (see table 1) that the isochoric sound velocity, despite the substantial growth of the thermal pressure, increases only a little, remaining practically constant over the whole interval of studied temperatures. The temperature dependence of the mean free path was calculated using the experimental heat conductivity data and making an assumption that it has a reciprocal temperature dependence at high temperatures. The obtained values of the isochoric sound velocity (Table 1) and the isochoric heat capacity (Table 2) were used to calculate, in accordance with Eq. (10), the heat conductivity λ_V taking into account the of influence of the thermal pressure (see Fig. 6). The curve qualitatively correctly describes the behavior of the temperature dependence of the isochoric heat conductivity and agrees well with the results of its direct researches [11] without any use of fitting parameters. The quantity C_V in Eq. (10) is the isochoric heat capacity of the system per unit volume. Its components may be as follows:

$$C_V = C_{\mathrm{tr}} + C_{\mathrm{rot}} + C_{\mathrm{in}}, \tag{12}$$

where C_{tr}, C_{rot}, and C_{in} are the translational, orientational, and intramolecular heat capacities, respectively. But it is known that for the high-temperature region the elementary excitation of different nature are interdependent. Therefore, the hypothesis of the additivity of their contributions into the total heat capacity does not work [18].

Thus, the analysis, carried out on the basis of the results obtained for equilibrium specimens of solid benzene and the simple dependence $\lambda = \frac{1}{3}C_V v\ell$, shows that the reason of why the isochoric heat conductivity exceeds the law $1/T$ can be seeked in the behavior of C_V as well. In this case, although the isochoric speed of phonons also slightly increases over the whole temperature interval (table 1), it does not influence substantially. In this model, the mean free path, which decreases reciprocally to the temperature, does not cause the exceeding, though the account of the libron scattering relaxation, which is due to the molecule untwisting, undoubtedly will be also favorable for an excess. However, as it has already been noted, concerning the c-axis, it has already taken place at temperatures about 100 K, and concerning other two main axes, the transition to the decelerated rotation is complicated down to the melting temperature.

To analyze the experimental data on the heat conductivity, the Callaway method [25], which is based on the kinetic equation in a relaxation approximation taking into account the special role of normal processes and the Debye model, is widely used. In Fig. 6, the results of theoretical calculations of the heat conductivity λ_{theor} with the help of this method are presented by the dash-dotted line. In accordance to the Callaway method, the heat conductivity is determined by the following relations:

$$\lambda = \lambda_1 + \lambda_2, \tag{13}$$

$$\lambda_1 = \frac{k_\mathrm{B}}{2\pi^2 v}\left(\frac{k_\mathrm{B}}{\hbar}\right)^3 T^3 \int\limits_0^{\Theta_\mathrm{D}/T} \frac{\tau_C x^4 e^x}{\left(e^x - 1\right)^2} dx, \tag{14}$$

$$\lambda_2 = \frac{k_\mathrm{B}}{2\pi^2 v}\left(\frac{k_\mathrm{B}}{\hbar}\right)^3 \times$$

$$\times T^3 \frac{\int\limits_0^{\Theta_\mathrm{D}/T} \left(\tau_C/\tau_N\right) x^4 e^x \left(e^x - 1\right)^{-2} dx}{\int\limits_0^{\Theta_\mathrm{D}/T} \left(\tau_C/\tau_N \tau_R\right) x^4 e^4 \left(e^x - 1\right)^{-2} dx}, \tag{15}$$

$$\tau_C^{-1} = \tau_R^{-1} + \tau_N^{-1}, \tag{16}$$

$$\tau_N^{-1} = A_N T^5 x \left(1+x\right), \tag{17}$$

$$\tau_R^{-1} = \tau_B^{-1} + \tau_U^{-1}, \tag{18}$$

$$\tau_B^{-1} = \frac{\upsilon}{\ell}, \tag{19}$$

$$\tau_U^{-1} = A_U T^3 x^2 e^{-\frac{E}{T}}, \tag{20}$$

where τ_C^{-1} is a combined relaxation time for resistive (τ_R^{-1}) and normal (τ_N^{-1}) processes, τ_B^{-1} and τ_U^{-1} are relaxation times for the limiting and phonon-phonon (the U-processes) scatterings, respectively, A_N and A_U are numerical constants, E is the activation energy of the U-processes, ℓ is a characteristic size of the crystal. Since the influence of the phonon-rotational interaction was not taken into account in this model, the temperature dependence of the heat conductivity appeared close to $1/T$.

The limiting heat conductivity of solid benzene, calculated for the isobaric case in the framework of the Einstein model of the diffusion heat transfer directly from atom to atom [26]

$$\Lambda_{\min} = \left(\frac{\pi}{6}\right)^{1/3} k_{\mathrm{B}} N^{2/3} \times$$

$$\times \sum_i \upsilon_i \left\{ \left(\frac{T}{\Theta_i}\right)^2 \int\limits_0^{\Theta_i/T} \frac{x^3 e^x}{\left(e^x - 1\right)^2} dx \right\}. \tag{21}$$

is shown in the bottom of Fig. 6. The sum is estimated taking into account three oscillation modes (two transverse and one longitudinal) with the sound velocities υ_i, where $i = 1, 2$, and 3, $\Theta_i = \frac{\hbar}{k_{\mathrm{B}}} \upsilon_i \left(6\pi^2 N\right)^{1/3}$ is the limiting Debye frequency for each polarization, expressed in Kelvins. It can be feen from Fig. 6 that the experimental curve of the heat conductivity of equilibrium specimens of solid benzene approach the absolute minimum at $T > 220$ K. But similarly to the isochoric case, it exceeds the diffusion minimum by more that a factor of 2.

Thus, the consideration of the exceeding effect of the isochoric heat conductivity over the classical dependence $1/T$ in the framework of the expression of the kinetic theory of gases shows that all its three factors make contributions to this effect. However, the determination of the quantitative relations among those contributions appears to be rather involved and requires additional studies, both theoretical and experimental. In the framework of the gas-kinetic model, the main contribution to the excess over the law $1/T$ was revealed to be connected to the heat capacity growth, with the contributions connected to the phonon-libron scattering relaxation and the increasung of the phonon speed being smaller.

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ТЕПЛОФІЗИЧНІ ВЛАСТИВОСТІ ТВЕРДОГО БЕНЗОЛУ

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Резюме

Наведено результати чисельного аналізу термодинамічних параметрів твердого бензолу. Проведено розрахунки температурної залежності ізохорної теплопровідності твердого C_6H_6 різними методами. Досліджено вплив термічного тиску на пружні властивості та ізохорну теплопровідність. У рамках концепції фононів описано можливі причини перевищення ізохорної теплопровідності бензолу над класичним законом $1/T$.