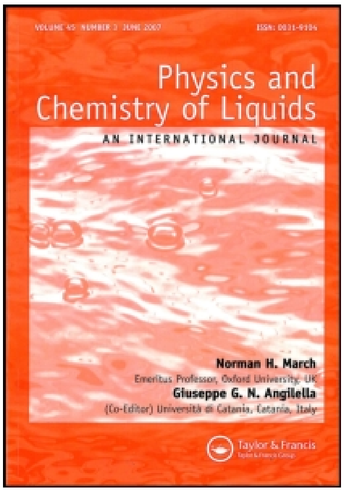

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THE PACKING COEFFICIENT OF LIQUID 2-PHENYLNAPHTHALENE MOLECULES AT 396 K

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A method of measuring the angular intensity distribution of monochromatic MoK$_\alpha$ radiation, $\lambda = 0.71069\,\text{Å}$ scattered by a thin layer of liquid 2-phenylnaphthalene $C_{10}H_7$–C_6H_5 is proposed and results of such an experiment are presented. Fourier analysis of this distribution by the procedure of Warren–Krutter–Morningstar yielded electron-density radial-distribution function (EDRDF). The curve of radiation intensity was analysed by the pair functions method. The determined mean, mutual distances between molecules of liquid studied are: $\bar{r}_1 = 5.30\,\text{Å}$, $\bar{r}_2 = 7.43\,\text{Å}$, $\bar{r}_3 = 12.35\,\text{Å}$. X-ray structural analysis was applied to determine the packing coefficient of 2-phenylnaphthalene molecules at 396 K. From the known volume of the first coordination sphere $\bar{V}$ as well as the specific volume of the molecule V_0 and taking into regard the structural model of intermolecular interactions, the most probable value of the packing coefficient of the molecules was found to be $\bar{k} = 0.64$. This value falls in the range of $\bar{k}$ values permissible for liquid phase. The results concern a wide class of molecular liquids, in particular polar compounds being naphthalene derivatives.

Keywords: X-ray scattering in liquids; Angular-distribution function; Liquid 2-phenylnaphthalene; Packing coefficient

1. INTRODUCTION

The packing coefficient of molecules in liquid due to its physical sense plays an important role in determining the structure of short-range molecular arrangement. The short-range arrangement is characterized

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by the values of the distances between the nearest molecules determined by the so-called radii of coordination spheres and a number of molecules in subsequent coordination spheres around one molecule chosen as central. In liquids we cannot talk about a three-dimensional periodicity of structure in such a sense as in solids, so we cannot define an elementary unit such as in solids. However, we can introduce a concept of a spherical pseudo-elementary cell [1]. From the course of EDRDF we can find the mean radii of the coordination spheres, corresponding to the points enhanced electron density [2]. The distances assigned to the subsequent maxima of the function in the range $\bar{r} \geq 4.5\,\text{Å}$ EDRDF, are the most probable distances between the atoms of the neighbouring molecules. The thickness of the coordination sphere is the distance between the two neighbouring minima of this function in the range $4.5 < \bar{r} \leq 20\,\text{Å}$ [1]. The ranges of particular spheres correspond to subsequent minima in EDRDF. In this way, the spheres have been determined by Radnai and Ohtaki [3] for water studied in high temperatures and under high pressures, by Cargill [4] for non-crystalline nickel–phosphorus alloy and by Kasai [1] for amorphous polymers (polystyrene glass). The data proving the existence of spheres of intermolecular ordering in amorphous polyethylene in the range from 4.50 Å to 20 Å are presented in the work by Skryshevskii [2].

The temperature study of the packing coefficient behaviour in benzene [5] and cyclohexane [6] proved that in the liquid phase the molecules can occupy almost twice as much space as in the crystal. A comparison of mean values of the molecule packing coefficient in liquids and crystals leads to the inequality:

$$\bar{k}_l < k_c, \qquad (1)$$

where $\bar{k}_l$ is the mean packing coefficient in liquids and k_c, the packing coefficient in the crystal. This inequality confirms the assumption that in liquids the packing and intermolecular interactions are lesser than in the crystals.

The structures of 1,2,3,4-tetraphenylnaphthalene [7] and octaphenylnaphthalene [8] have been studied in the crystal phase. The density of crystalline 2-phenylnaphthalene is $d = 1.218\,\text{g/cm}^3$ [9]. On the basis of the known liquid structures of 1-methylnaphthalene [10,11],

TABLE I Physical and structural parameters of liquid 2-Phenylnaphthalene ($\sum_j Z_j$ denotes the sum of the atom numbers in one molecule)

Mean effective number of electrons per		$\sum_j \bar{K}_j$	$\sum_j Z_j$	*Macroscopic density* [g/cm^3]	*Molecular mass* [g/mol]	*Mean electron density* [el/Å^3]
hydrogen atom $\bar{K}_H$	*carbon atom* $\bar{K}_C$					
0.670	6.365	108.000	108	1.009	204.27	0.3213

1-chloronaphthalene [12] and 1-phenylnaphthalene [13] we can predict the structures of their weakly polar derivatives. However, 2-phenylnapthalene has not been studied in the liquid phase by diffraction methods [14].

The values of the structural and physical parameters of the liquid studied are collected in Table I. The compounds to be studied (of 99% purity) were purchased from Aldrich-Chemie (Germany).

The most probable model of the short-range order structure was obtained using the method of exact analysis of the distribution curve in terms of EDRDF and of pair functions *P*(*r*).

2. EXPERIMENTAL

X-ray scattering in liquid 2-phenylnaphthalene $C_{10}H_7$–C_6H_5 (melting point 376 K, boiling point 630 K), at a temperature of (396 ± 0.1) K was measured by applying MoK_α radiation generated by a 1375 W tube ($U = 55$ kV, $I_A = 25$ mA). The intensity of the scattered radiation was recorded by a proportional counter coupled with a pulse counter at the counting rate up to 3.10^5 per second. The diffracted X-ray pulses are counted in the time of 40 s. The angular range of the measurements was from $\vartheta_{\min} = 3^\circ$ to $\vartheta_{\max} = 60^\circ$ with a scanning step equal to 0.2°. The radiation was monochromatized by reflection from the (002) planes of flat graphite with the angle of monochromatization of $\Theta_m = 6^\circ 00'$ ($\Delta\Theta_m = 2.2'$). The X-ray diffraction patterns were recorded on a typical X-ray diffractometer equipped with a special cell for measurements of liquids, described by North *et al.* [15] and Drozdowski [10].

Intensity of radiation scattered by a layer of the studied liquid was determined by the transmission method, Fig. 1.

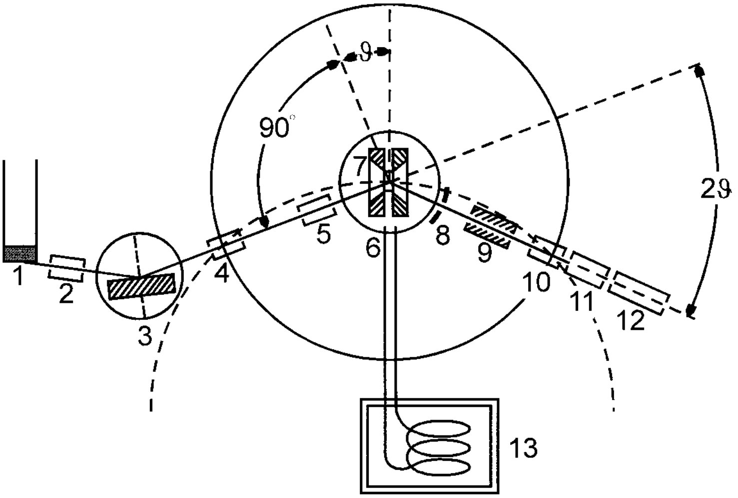

FIGURE 1 A scheme of a measuring system of a goniometer in the transmission method; 1 – X-ray lamp anode, 2 – a system of output slits of the lamp, 3 – monochromator, 4 – a system of input slits of the goniometer, 5 – slits controlling the width and divergence of the beam, 6 – the goniometer table, 7 – cell with the liquid studied, 8 – a shield against the scattered parasite radiation, 9 – Soller slits, 10 – a system of output slits, 11 – radiation counter, 12 – electronic amplifier, 13 – ultrathermostat.

The liquid studied was placed in an electrically heated cell closed on both sides with windows made of Bengal mica of 0.025 ± 0.001 mm in thickness. The distance between the mica windows was 1.00 ± 0.01 mm. The brass blocks were heated with four electric heaters of the power $P = 800\,\mathrm{W}$ and inner resistance $r = 58.3$ ohms each. The temperature in the cell was measured by a platinum sensor connected to a temperature control unit and power supply unit. Absorption in the cuvette windows was neglected. The construction of the cell facilitated its filling, adjustment in the goniometric holder and thermostating.

The measured intensity was corrected for: the background (air scattering) and noise counter [16], polarization [17], absorption by a sample [18], multiple scattering [19] and anomalous dispersion [20]. In processing the data, I used the computer procedure prepared by Renninger and Kaplow [21]. The scattered X-radiation was normalized to electron units [e.u] according to the Krogh-Moe [22] and Norman [23] method.

3. CALCULATIONS

On the basis of the mean value of volume of the first coordination sphere $\bar{V}$ and specific volume of the molecules V_0, the packing coefficient $\bar{k}$ of molecules in the liquid is calculated from the formula [24]:

$$\bar{k} = \bar{N}\frac{V_0}{\bar{V}}, \tag{2}$$

where $\bar{N}$ is the mean number of molecules in the volume of the first coordination sphere $\bar{V}$. The specific volume of the molecules V_0 was determined on the basis of the volume increments corresponding to the contributions of particular atoms in the total volume. The mean volume per one molecule of the liquid is calculated from the known macroscopic density, molecular mass and the Avogadro number according to the formula [24]:

$$V^{\max} = \frac{M}{N_A d}, \tag{3}$$

where M is the *molecular mass* of the liquid (g /mol), d the liquid density at a certain temperature and N_A the *Avogadro constant* [mol^{-1}]. The volume $V^{\max}$ is the maximum because the liquid density d in formula (3) concerns the whole volume of the liquid, including microvoids characteristic of the liquid phase [25]. A molecule of 2-phenylnaphthalene takes on the average a volume $V^{\max} = 322.8$ Å^3, whereas an increment of the molecule volume is $V_0 = 209.8$ Å^3.

The experimental results were interpreted by the electron-density radial-distribution function which is described in detail in earlier works [12,26]. The information on close-range ordering was obtained after verification of the two-molecular model by comparing the experimental and model functions of atomic pair distribution $P(r)$. This comparison was also an additional criterion of correctness of the assumed model of interactions. From the measured intensities, the pair function, $P(r)$, was evaluated. The $P(r)$ function is given by the equation:

$$P(r) = 4\pi r^2\langle\rho_0\rangle + 2\bar{r}\pi^{-1}\int_{S_0}^{S_{\max}} \mathrm{SF}(S)\exp(-\beta^2 S^2)\sin(S\bar{r})\,dS, \tag{4}$$

where $\langle\rho_0\rangle$ is the average atomic density, $S = 4\pi\sin\vartheta/\lambda$, $\exp(-\beta^2 S^2)$ denotes the temperature factor, and $F(S)$ is the interference function given by:

$$F(S) = \bar{I}(S) - \langle f^2(S)\rangle / \langle f(S)\rangle^2, \tag{5}$$

where $\bar{I}(S)$ is the coherent scattered intensity in electron units, $\langle f(S)\rangle = \sum_{i=1}^{n} c_i f_j(S)$ – atomic scattering factor, $\langle f^2(S)\rangle = \sum_{i=1}^{n} \times c_i f_j^2(S)$ – mean of the squares of atomic factors, $\langle f(S)\rangle^2$ – square of the mean value of atomic factors; c_i – concentration of atoms in the molecule (molar fraction): $\sum_{i=1}^{n} c_i = 1$.

The model $P(r)$ function was calculated according to Warren [27] as follows:

$$P(r) = \sum_{uc} \sum_{i} |N_{ij}/r_{ij}| P_{ij}(r), \tag{6}$$

where$\sum_{uc}$ – summation over a structural unit, N_{ij} – mean value of the nearest neighbours in the ith sphere about the atom j at a distance of r_{ij} from that atom, P_{ij} is the partial atom pair distribution function.

For a given type of interatomic interactions, on the basis of Eqs. (4)–(6), the pair function $P_{ij}(r)$ is calculated as follows:

$$P_{ij}(r) = \int_{S_0}^{S_{\max}} f_i f_j / g^2(S) \exp(-\beta^2 S^2) \sin(S r_{ij}) \sin(S r)\, dS, \tag{7}$$

where $g(S)$ is the sharpening factor. The model pair function was calculated by using the same values of β and $S_{\max}$ as in the experimental $P(r)$ function. The numerical calculation of the integral from Eq. (4) was performed by the Simpson method at a step 0.20° and for $\bar{r}$ changed every 0.05 Å.

The random error of the radial distribution function has been estimated according to the Konnert and Karle method [28] and does not exceed 3%.

4. RESULTS

The normalized angular-distribution function $\bar{I}(S)$, in electron units [e.u], of 2-phenylnaphthalene (Fig. 2) is characterized by four general maxima which correspond to intermolecular interactions. The first maximum, at $S_1 = 0.61 \pm 0.01\,\text{Å}^{-1}$, less intense, corresponds to the

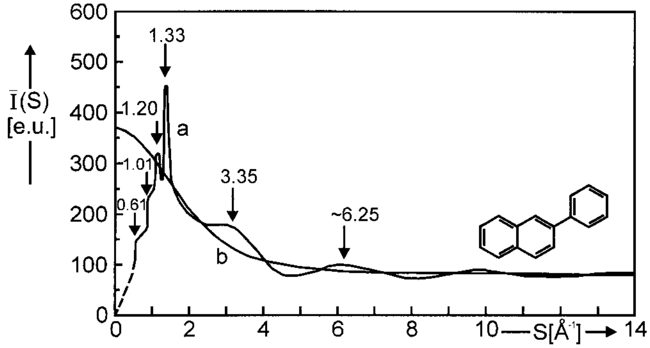

FIGURE 2 Normalized, experimental curve of angular distribution of X-ray scattered intensity (a), and total independent scattering curve (b) in liquid 2-phenylnaphthalene $C_{10}H_7$–C_6H_5.

distance $\bar{r}_1 = 12.37 \pm 0.15$ Å, between molecules and the next one $S_2 = 1.01 \pm 0.01$ Å^{-1} to the distance of $\bar{r}_2 = 7.35 \pm 0.15$ Å. The third peak at $S_3 = 1.20 \pm 0.01$ Å^{-1} corresponds to the distance $\bar{r}_3 = 6.14 \pm 0.12$ Å and the fourth maximum $S_4 = 1.33$ Å^{-1} to $\bar{r}_4 = 5.51 \pm 0.12$ Å.

The mean intermolecular distances were found on the basis of the experimental distribution function of scattered radiation intensity [29]. Small-angle scattering result was extrapolated to the origin of the coordination system using a second-order function [21].

The EDRDF of liquid 2-phenylnaphthalene (Fig. 3) has ten maxima in the range of the distance $\bar{r}$ below 20 Å. Their positions correspond to the most probable interatomic and intermolecular distances in the studied liquid, they are considered in detail below.

The total functions of atom pair distribution, with EDRDF for gas scattering taken into account were calculated for $\beta = 0.03$ and $S_{max} = 14$ Å^{-1}. The best agreement between the model and experimental pair function is shown in Fig. 4. The model and experimental forms of $P(r)$ were calculated with the use of the same S_{max} and β.

From the chemical structure of the molecule, the bond length within it and van der Waals radii of its atoms and functional group, a model of the molecule can be constructed. The 2-phenylnaphthalene molecule can be described by three values (length x width x height) which are obtained in orthogonal projections of the model onto three mutually perpendicular planes (Fig. 5).

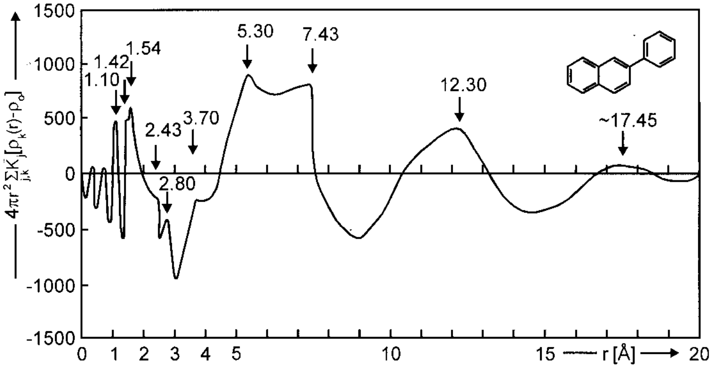

FIGURE 3 The electron-density radial-distribution function $4\pi r^2\sum_{j,k}^{n}\bar{K}_j[\rho_k(r)-\rho_0]$ for liquid 2-phenylnaphthalene.

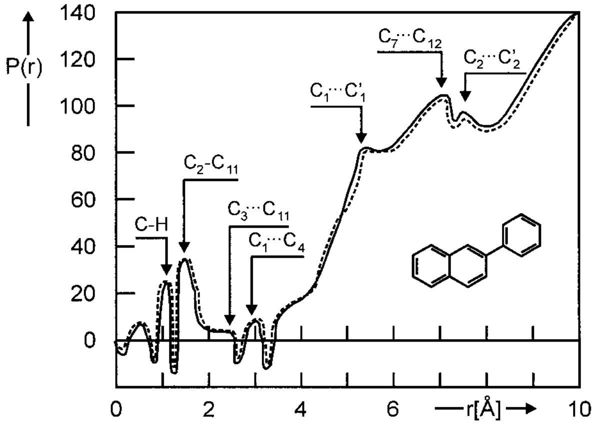

FIGURE 4 Solid line – the experimental pair function; dashed line – the best-fit model pair function.

For the calculation of mean amplitudes of vibrations ($\bar{u}_{ij}$) of different pairs of atoms of the liquid studied, the empirical formula of Mastryukov and Cyvin was applied [30]: $\bar{u}_{ij} = a + br + cr^2$, where r is the internuclear distance in the molecule, and a, b, c are constants equal to 0.0013837, 0.023398 and −0.000147 respectively. The formula was proposed by Mastryukov and Cyvin on the basis of a large body of data from electron diffraction studies.

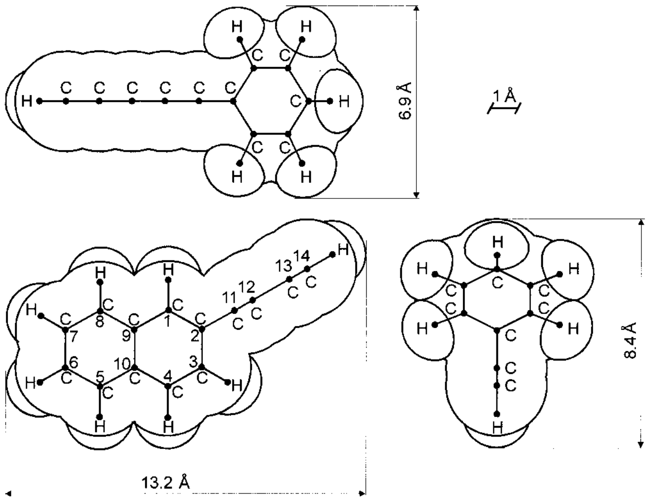

FIGURE 5 A model of 2-phenylnaphthalene molecule structure $C_{10}H_7$–C_6H_5 ($\mu = 1.81$ D; $d = 1.009$ g/cm^3; $\rho_0 = 0.3213$ el/Å^3).

A simple model of short-range arrangement of the molecules in liquid 2-phenylnaphthalene was proposed (Fig. 6). This model is judged to be correct if the whole experimental curve shows a good arrangement with the model curve with respect both to the position and to the surface area of the maxima obtained.

The mean distances between pairs of different atoms belonging to neighbouring molecules of 2-phenylnaphthalene are given in Table II. The numbering of the atoms is consistent with the notation assumed in Fig. 6.

5. DISCUSSION

It is interesting to note that already from the positions of the peaks in the angular distribution (Fig. 2) in the range of $0.43\,\text{Å}^{-1} \leq S \leq 2.20\,\text{Å}^{-1}$ we can conclude about not only mean intermolecular distances but also the distances between phenyl groups in two neighbouring molecules of liquid 2-phenylnaphthalene. This result is possible thanks to the use of the short-wave radiation from the anode of a molybdenum lamp.

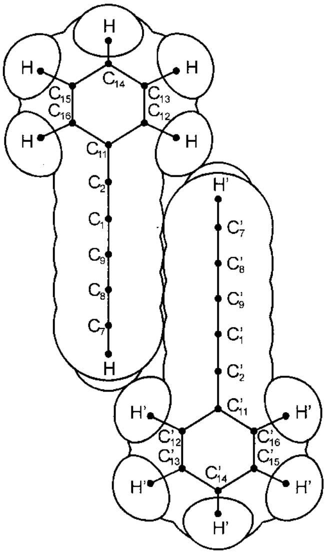

FIGURE 6 The model of probable conformation of molecules in liquid 2-phenylnaphthalene $C_{10}H_7–C_6H_5$. The arrangement of molecules corresponding to the maxima in the EDRDF and $P(r)$.

TABLE II The mean distances $\bar{r}_{ij}$ and root-mean-square variation ($\bar{u}_{ij}$) between pairs of atoms in liquid 2-Phenylnaphthalene

Distances between pairs of atoms	*Distances*		
	calculated from the model [Å]	*determined from the EDRDF* [Å]	*Mean amplitude* $\bar{u}_{ij}$ [Å]
$C_1 \ldots C'_1$	5.34	5.30	0.12_6
$C_2 \ldots C'_2$	7.40	7.43	0.16_7
$C_6H_5 \ldots C_6H'_5$	12.35	12.30	0.26_7

A common feature of the radial distribution functions (Figs. 3 and 4) is that in the range of distances $1 < \bar{r} \leq 4$ Å the effects of intramolecular diffraction appear. They are manifested as three maxima at distances 1.42 Å, 2.43 Å, 2.80 Å. They correspond to the distances between the carbon atoms in the positions *ortho*, *meta* and *para* in the naphthalene ring. The maximum assigned to the C–H bond corresponds to the distance 1.10 Å within the ring. In the range of the argument below 1 Å, the values of the EDRDF (Fig. 3) making the interpretation difficult or even impossible are not uncommon. They seem to be due to some approximations assumed in the method, e.g., to the extrapolation of small angle scattering results [21]. The maxima on the EDRDF in the range $1 < \bar{r} \leq 4\,\text{Å}$ have been ascribed to the following pairs of atoms: $C_1\text{–}H = (1.10 \pm 0.01)\,\text{Å}$, $C_1 \cdots C_9 = (1.42 \pm 0.01)\,\text{Å}$, $C_2\text{–}C_{11} = (1.54 \pm 0.01)\,\text{Å}$, $C_1 \cdots C_3 = (2.43 \pm 0.02)\,\text{Å}$, $C_1 \cdots C_4 = (2.80 \pm 0.02)\,\text{Å}$, $C_1 \cdots C_5 = (3.70 \pm 0.05)\,\text{Å}$.

The maxima in the range $4 \leq \bar{r} < 6\,\text{Å}$, are interpreted as due to intra- and intermolecular diffraction, whereas those for $\bar{r} > 6\,\text{Å}$ are due to intermolecular diffraction. In the range of distances $\bar{r} \in \langle 4\,\text{Å}\text{–}20\,\text{Å}\rangle$ we can talk about the spheres of intermolecular ordering in the liquid studied. The mean number of molecules in the volume of the first coordination sphere is $\bar{N} = 8.6$.

Because of the permanent dipole moment of the molecule, 2-phenylnaphthalene $\mu = 1.81D$ [31], the neighbouring molecules are arranged so that their dipolar moments are antiparallel (Fig. 6). This orientation is confirmed by the peaks on the EDRDF appearing at: $C_1 \cdots C_1' = 5.30\,\text{Å}$, $C_2 \cdots C_2' = 7.43\,\text{Å}$ and $C_6H_5 \cdots C_6H_5' = 12.30\,\text{Å}$.

A comparison of the mean values of the packing coefficients of the α- [13] and β-phenylnaphthalene molecules leads to the relation:

$$\bar{k}_a > \bar{k}_\beta, \tag{8}$$

where $\bar{k}_\alpha$ and $\bar{k}_\beta$ are the mean packing coefficients of α- and β-phenylnaphthalene. The inequality (8) holds because the following relations are valid

$$\bar{r}_\alpha < \bar{r}_\beta \quad \text{and} \quad d_\alpha > d_\beta, \tag{9}$$

where $\bar{r}_\alpha$ and $\bar{r}_\beta$ are the mean least intermolecular distances, d_α and d_β are the macroscopic densities of α- and β-phenylnaphthalene.

6. CONCLUSIONS

As the molecules of 2-phenylnaphthalene have permanent electric moment in liquid they should assume such an orientation that their dipolar moments would be antiparallel. Such an orientation is confirmed by the occurrence of intermolecular interactions suggested in the model of the molecule.

The results of the X-ray diffraction study have proved that the function of angular distribution of scattered radiation intensity $\bar{I}(S)$ and the radial functions /EDRDF, $P(r)$/ are sensitive to the shape of the molecule of the liquid studied, which enables a construction of a model of the molecule. It is possible to construct and verify local binary models of intermolecular interactions and identify steric restrictions of spatial models. The applied methods of measurements and calculations permitted a determination of the mean structural parameters and local ordering of the molecules in the liquid 2-phenylnaphthalene.

The structure of liquid 2-phenylnaphthalene is determined by the presence of the naphthalene ring, which is not deformed within the measuring uncertainties. The presence of clear maxima in the range $1 < \bar{r} \leq 4\,\text{Å}$ in the course of the EDRDF (Fig. 5) and $P(r)$ (Fig. 6) functions confirms that the phenyl ring does not have a deforming influence on the structure of the naphthalene ring. A realistic estimation of the uncertainties of the interatomic distances $\Delta\bar{r} = (\pm 0.01\text{–}0.02)\,\text{Å}$ determined in the range $1 < \bar{r} \leq 3\,\text{Å}$ justifies putting forward a hypothesis that the method of X-ray diffraction in liquids does not allow determinations of possible deformations in the naphthalene ring (0.0003 Å – 0.01 Å). The maxima on the EDRDF in the range $1 < \bar{r} \leq 4\,\text{Å}$ are attributed to intramolecular interactions. The three maxima corresponding to the C–C distances appear at 1.42 Å, 2.43 Å and 2.80 Å for the molecule studied. These distances correspond to those between the carbon atoms in the *ortho*, *meta* and *para* positions in the naphthalene ring.

The proposed model of interactions is related to mutual orientations of phenyl groups of neighbouring molecules. The values of $\bar{r} = 5.30\,\text{Å}$ and $\bar{r} = 7.43\,\text{Å}$ determined provide the information about intermolecular spatial configurations in the liquid studied. The proposed approximate binary model of interactions is related to the mutual antiparallel orientation of phenyl groups from the neighbouring molecules. The analysis of the angular and radial functions has confirmed the antiparallel orientation of the dipole moments and the fact that the naphthalene rings are stacked one over the other. The results can be interpreted on the basis of simple models of local ordering of molecules.

The packing coefficient of molecules in liquid 2-phenylnaphthalene is equal 0.64. This value falls within the range of $\bar{k}$ values acceptable for the liquid phase substances. These results are also consistent with the values presumed in the conformational structure investigation of 2-phenylnaphthalene performed by empirical and semi-empirical MO-LCAO calculations [32].

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