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THE MOLECULAR STRUCTURE OF LIQUID 1-PHENYLNAPHTHALENE BY X-RAY DIFFRACTION

H. Drozdowski [1]
Non-Crystalline Materials Division, Institute of Physics, A. Mickiewicz University,
Grunwaldzka 6, 60-780 Poznań 2, Poland

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The paper reports results of the X-ray diffraction structural studies of liquid 1-phenylnaphthalene, $\mathrm{C_{10}H_7}$ — $\mathrm{C_6H_5}$ at 338 K, with the use of $\mathrm{MoK_\alpha}$ radiation of the wavelength $\lambda = 0.071069$ nm. The curves of reduced radiation intensity were analysed by the reduction method of Blum and Narten. Experimental distributions of X-ray scattered intensity were compared with theoretical results predicted by the proposed model of 1-phenylnaphthalene molecule. The electron-density radial-distribution function $4\pi r^2 \sum\limits_{j,k}^{n} \bar{K}_j[\rho_k(r) - \rho_0]$ was calculated and some intra- and intermolecular distances in liquid 1-phenylnaphthalene were determined.

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1 Introduction

X-ray diffraction is a very efficient method of studying the structure of matter in both solid and liquid phase [1]. Recently [2,3] it has been shown that the X-ray diffraction method on liquid media allows not only determination of interatomic distances in a molecule but also brings information on the kind of interaction among the molecules and degree of their ordering. In view of the above, an attempt was made at structural analysis of liquid 1-phenylnaphthalene. The aim of the study was to acquire experimental data for structural analysis of intermolecular interactions in dilute binary solutions of naphthalene nitroderivative-nitrophenyl in phenylnaphthalene and naphthalene. Results of the study concerning molecular correlations in liquid phase may be important for explanation of mechanisms of certain physical and chemical processes taking place in such systems, e.g. diffusion or thermal conductivity [4].

Naphthalene has been studied in three phases: gas [5], liquid [6] and solid [7,8]. The structures of 1,2,3,4-Tetraphenylnaphthalene [9] and Octaphenylnaphthalene [10] have been studied in the crystal phase. However, 1-phenylnaphthalene $\mathrm{C_{10}H_7}$ — $\mathrm{C_6H_5}$ (melting point 318 K, boiling point 598 K) has not been studied in the liquid phase by diffraction methods [11].

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[1] E-mail address: riemann@main.amu.edu.pl

This work reports the first studies of liquid 1-phenylnaphthalene performed by the counter method for the range of the angular measurements intensity extended to the value of ϑ=60°. Monochromatic radiation MoK$_\alpha$ enabled a determination of the scattered radiation intensity between $S_0 = 9.25$ nm^{-1} and $S_{\max} = 153.13$ nm^{-1}.

The interpretation of the results was carried out using the reduction method [12,13]. The X-ray diffraction method permitted determination of the mean structural parameters of liquid 1-phenylnaphthalene (the intra- and intermolecular distances, the radii of coordination spheres) at 338 K. X-ray structural analysis was applied to determine the packing coefficient of 1-phenylnaphthalene molecules. The values of the structural and physical parameters of liquid 1-phenylnaphthalene are collected in Table I. Phenylnaphthalene samples of 99% purity were purchased from Aldrich-Chemie (Germany).

Table I. Physical and structural parameters of liquid 1-phenylnaphthalene ($\sum_j Z_j$ denotes the sum of the atom numbers in one molecule).

Mean effective number of electrons per hydrogen atom $\bar{K}_H$	Mean effective number of electrons per carbon atom $\bar{K}_C$	$\sum_j \bar{K}_j$	$\sum_j Z_j$	Macroscopic density [g/cm^3]	Molecular mass [g/mol]	Mean electron density [el/nm^3]
0.650	6.335	108.000	108	1.085	204.27	345.5

2 Experimental

The intensity of radiation scattered by a layer of the studied liquid was determined by the transmission method using a typical X-ray diffractometer adapted for measurements of liquids [14]. The angular distribution of the X-ray scattered intensity was measured by applying MoK$_\alpha$ (λ=0.071069 nm) radiation for the angles $6° \leq 2\vartheta \leq 120°$ at every 0.2°, where 2ϑ is the scattering angle. The radiation was monochromatised by reflection from the (002) planes of flat graphite with the angle of monochromatisation of α=6°00′ [15]. The scattered X-ray intensities were measured by a VA-G-120 proportional counter (made by Otto Schön, Germany) and the results were recorded by a computer. Deviations in intensity due to instability the diffractometer work were of about 1% in the whole range considered.

The studies were carried out with a special cuvette with exchangeable plates and closed with 0.01 mm thick foil windows, constructed in our laboratory [16]. Absorption in the cuvette windows was neglected [17].

The cuvette was connected with a flow-through ultrathermostate U-10. X-ray diffraction investigation of liquid 1-phenylnaphthalene was performed at 338 K. Temperature inside the cuvette was measured by a probe made by Testoterm GmbH&Lenzkirch, Germany.

3 Calculations

The scattered X-radiation was normalized to electron units [e.u.] according to the Krogh-Moe [18] and Norman [19] method. This normalization was performed by approximating the experimental curve $I(S)$ for large values of S to the theoretical curve given by the expression $\sum_{i=1}^{n} x_i f_i$, where x_i is the concentration of atoms of species i and f_i is the respective atomic factor, recurring to the circumstance that for large angles ϑ interatomic and intermolecular interference can be neglected. Oscillations of the experimental curve $I(S)$ need not be taken into account then, and the experimental intensity distribution curve coincides with the theoretical one. Normalization of the experimental curve of intensity distribution is performed by taking into account the corrections for uncoherent radiation [20].

Normalization was also performed on the basis of a comparison between the area under the experimental curve given as a function of $I(S)S^2$ with the area under the theoretical curve given by: $\left(\sum_{i=1}^{n} x_i f_i\right) S^2$, where $S = 4\pi \sin\vartheta/\lambda$. For the liquid studied the following normalization relationship was obtained:

$$C_n \int_0^\infty I(S)S^2 \mathrm{d}S = \sum_{i=1}^{n} \int_0^\infty f_i^2(S) S^2 \mathrm{d}S, \tag{1}$$

in which C_n is a normalization coefficient and $f_i(S)$ stands for atomic scattering factors expressed in electron units [21].

Before normalization of the intensity curve, corrections for the background (air scattering and noise counter) [22], polarisation of the X-ray beam reflected by the sample and monochromator [23], absorption by a sample [24], multiple scattering [25] and anomalous dispersion [26] were applied.

For a given atomic composition of a scattering structural unit, the curve of intensity of independent scattering can be obtained from tabulated atomic scattering factors [27]. The shape of this curve depends on a given scattering structural unit. In the case of liquid 1-phenylnaphthalene, the definition of a structural unit can be much simplified [28].

The experimental values of scattered radiation intensity were corrected by the computer program [29] according to the scheme:

$$I = \left(I^{\mathrm{exp}} - I^{\mathrm{INC}} - I^{\mathrm{MULT}} - T\right) PA \tag{2}$$

where I^{exp} is the experimentally obtained intensity of scattered radiation, I^{INC} - intensity of incoherent radiation, I^{MULT} - intensity of multiple scattering, T - apparatus background and noise of the analysing system, P - polarising factor, and A - absorption factor.

The interpretation of the experimental results was performed by the method of the electron-density radial-distribution function (EDRDF) calculated from the equation [30]:

$$\sum_{j=1}^{n}\sum_{k=1}^{n} \bar{K}_j 4\pi r^2 \rho_k(r) = \sum_{j=1}^{n} \bar{K}_j 4\pi r^2 \rho_0 + \frac{2r}{\pi} \int_0^\infty S\, i(S) \exp(-\alpha^2 S^2) \sin(Sr) \mathrm{d}S. \tag{3}$$

In Eq.(3) the function $i(S)$ is defined as:

$$i(S)=\frac{I_{\rm eu}(S)/N-\sum\limits_{\rm uc} f_j^2(S)}{g^2(S)}, \tag{4}$$

where $I_{\rm eu}(S)/N$ is the experimentally observed total coherent intensity of scattered radiation per one structural unit, $\sum\limits_{\rm uc} f_j^2(S)$ denotes the theoretical independent scattering on atoms of one structural unit, $g(S)$ is a sharpening factor, often written in the form: $\sum\limits_{\rm uc} f_j$ or $\sum\limits_{\rm uc} f_j/\sum\limits_{\rm uc} Z_j$ and $\exp(-\alpha^2 S^2)$ is a convergence factor, with coefficient $\alpha=0.06$. The mean number of electrons in a unit volume (1 nm^3) is given by the formula [31]:

$$\rho_0={\rm d}N_A 10^{-21}\sum_j Z_j/M, \tag{5}$$

where ${\rm d}$ is the macroscopic density of the liquid, N_A - the *Avogadro constant*, Z_j is the number of electrons in the j-th atom and M *- molar mass* (see Table I). The summation in Eq. (3) runs over all atoms of the molecule: $\sum\limits_j \bar{K}_j = n_{\rm C}\bar{K}_{\rm C}+n_{\rm H}\bar{K}_{\rm H}$ where $n_{\rm C}$ and $n_{\rm H}$ are the numbers of carbon and hydrogen atoms, respectively, in one molecule, $\bar{K}_{\rm C}$ and $\bar{K}_{\rm H}$ are the average effective numbers of electrons in the atoms of carbon and hydrogen. The mean effective number of diffracting electrons as found from the integral average:

$$\bar{K}_j=\frac{1}{S_{\max}-S_0}\int\limits_{S_0}^{S_{\max}} K_j {\rm d}S, \tag{6}$$

where $S=4\pi\sin\vartheta/\lambda$, 2ϑ the angle of scattering and λ the X-ray scattering wavelength. The calculations have been performed for a finite range of S values from $S_0=9.25$ nm^{-1} to $S_{\max}=153.13\,{\rm nm}^{-1}$.

The least mean intermolecular distances were found from the Voigtlaender-Tetzner formula [32]:

$$\bar{R}=7.73/S_{\max}-0.03\ \ [{\rm nm}]. \tag{7}$$

The correcting factor ”0.03 [nm]” for molecular liquids has been found empirically [32]. The maximum experimental error in determination of EDRDF was estimated to be ± 3%. The mean least inter- and intramolecular distances were determined with the following accuracy: for $0.1<\bar{r}\leq 0.2$ nm: $\Delta\bar{r}=\pm 0.001$ nm, for $0.2\leq\bar{r}\leq 0.3$ nm: $\Delta\bar{r}=\pm 0.005$ nm, for $\bar{r}>0.3$ nm: $\Delta\bar{r}=\pm 0.010$ nm [33]. Computer techniques were used to minimise the effects of experimental errors, uncertainties in the scattering factors, and termination errors. X-ray diffraction data of the studied liquid was analyzed by Renninger-Kaplow program package [29].

4 Results

The normalized angular-distribution function $I(S)$ (where $S=4\pi\sin\vartheta/\lambda$) of 1-phenylnaphthalene (Fig. 1) is characterized by two general maxima which are corresponding to intermolecular interaction. The first maximum, at $S_1 = 12.00 \pm 0.10\ \mathrm{nm}^{-1}$, less intense, is related to the distance of $\bar{R}_1 = 0.62 \pm 0.01$ nm, between molecules and the next one $S_2 = 13.30 \pm 0.10\ \mathrm{nm}^{-1}$ is related to the distance of $\bar{R}_2 = 0.551 \pm 0.01$ nm. The positions of the S_1 and S_2 maxima were found using the Lagrange polynomials method. Small-angle scattering result ($0^\circ < \vartheta < 3^\circ$) was extrapolated to the origin of the coordinate system using a second-order function [29].

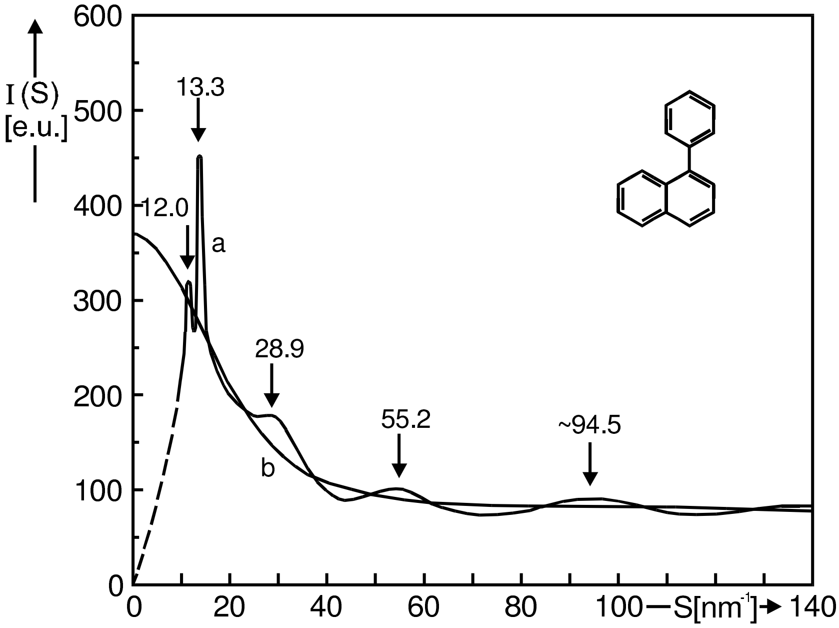

Fig. 1. (a) normalized, experimental curve of angular distribution of X-ray scattered intensity. (b) total independent scattering curve in liquid 1-phenylnaphthalene.

Using the experimental values of $I(S)$, presented in Fig. 1 and Eq. (2), the values of $i(S)$, so the total function of the structure, were calculated. By the reduction method [12,13], the function $i(S)$ which is an important component of the Fourier integral in Eq. (3) can be separated from the total value of intensity $I_{\mathrm{eu}}(S)/N$. In order to employ the reduction method, the function $i(S)$ which is now referred to as the total structure function must be redefined and expressed as the sum:

$$i(S) = i_{\mathrm{m}}(S) + i_{\mathrm{d}}(S), \tag{8}$$

where $i_{\mathrm{m}}(S)$ is the molecular structure function describing the scattering by a single molecule and $i_{\mathrm{d}}(S)$ is the distinct structure function providing the information about intermolecular correlations from the experimental data. The molecular structure function $i_{\mathrm{m}}(S)$ calculated from the equation [34]:

$$i_{\mathrm{m}}(S) = \frac{1}{\left[\sum_i f_i(S)\right]^2} \left[\sum_{\mathrm{uc}} \sum_{i \neq j} f_i f_j \exp\left(-A_{ij} S^2\right) \frac{\sin(S r_{ij})}{S r_{ij}} \right]. \tag{9}$$

In Eq. (9) the symbols i and j denote summation over stoichiometric unit; $A_{ij} = \frac{1}{2}u_{ij}$, $u_{ij} = \left\langle (\Delta r_{ij})^2 \right\rangle^{0.5}$ denoting the root-mean-square variation in the distance r_{ij} between pairs of atoms [35]. The calculated mean amplitudes of vibration (u_{ij}) for 1-phenylnaphthalene are shown in Table II. The numbering of atoms follows common usage in organic chemistry.

Atomic scattering factors f_{C}, f_{H}, f_{CH} were calculated according to the formula [27]:

$$f\left(\frac{\sin\vartheta}{\lambda}\right) = \sum_{i=1}^{4} a_i \exp\left(-\frac{b_i \sin^2\vartheta}{\lambda^2}\right) + C \tag{10}$$

using the a_i, b_i and C values determined by Narten [28].

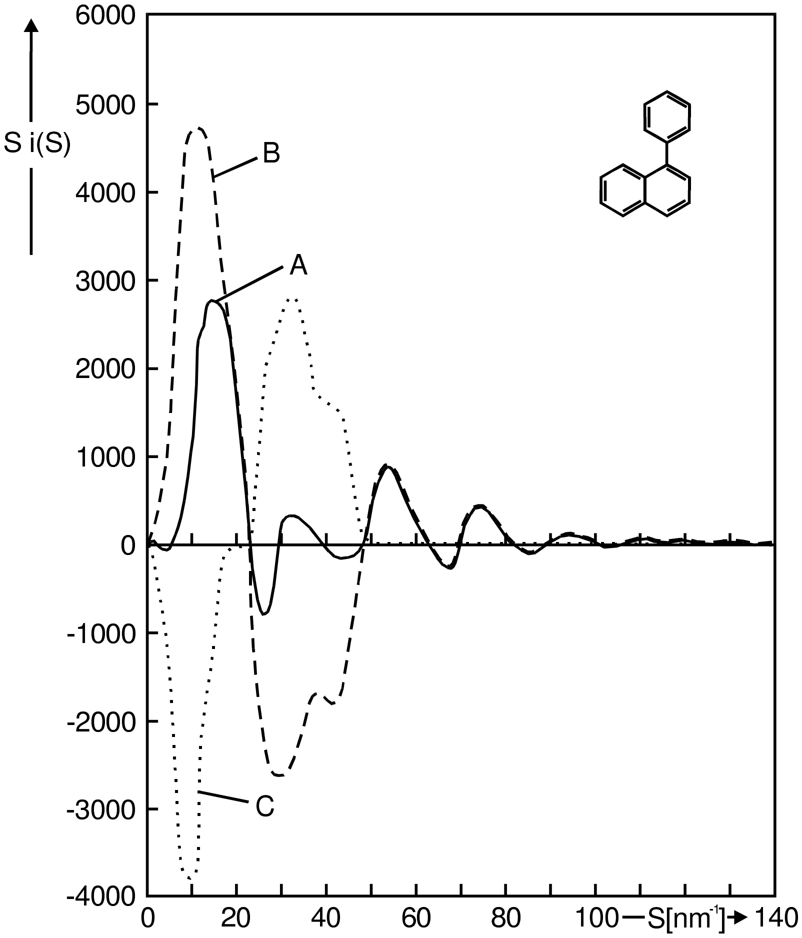

Fig. 2. Curve A (continuous line), the experimental structure function $S\ i(S)$. Curve B (broken line), the molecular structure function $S\ i_{\mathrm{m}}(S)$ calculated according to Debye. Curve C (dotted line), subtraction of the calculated curve B from the curve A, $S\ [i(S) - i_{\mathrm{m}}(S)]$.

The values of $i_{\mathrm{m}}(S)$ from Fig. 1 have been calculated from the Debye formula (9) for the proposed model of 1-phenylnaphthalene, which is shown in Fig. 3. Molecular parameters r_{ij} (Table II) have been fitted by the Narten's method [28], assuming that $i(S) \approx i_{\mathrm{m}}(S)$ for $S \geq 50$ nm^{-1}.

Table II. The values of parameters of 1-phenylnaphthalene molecule model applied in Debye formula Eq. (9). Atoms notation the same as in Fig. 3 (u_{ij} denotes the root-mean-square variation in the distance r_{ij} between pairs atoms [35]).

Type of intramolecular interactions C — C and C $\cdots$ C	Intramolecular distances $r_{ij} \times 10^{-3}$ [nm]	Mean amplitude $u_{ij} \times 10^{-3}$ [nm]
C_2 — H	110	7.7
C_1 — C_2	136	4.6
C_2 — C_3	141	6.1
C_1 — C_9	142	4.7
C_1 — C_{11}	154	4.8
$C_2 \cdots C_{11}$	230	6.7
$C_1 \cdots C_3$	243	6.2
$C_1 \cdots C_{12}$	254	7.3
$C_1 \cdots C_4$	280	5.6
$C_8 \cdots C_{11}$	290	8.0
$C_2 \cdots C_{12}$	325	8.8
$C_8 \cdots C_{12}$	340	9.2
$C_1 \cdots C_5$	370	5.8
$C_3 \cdots C_{11}$	375	10.0
$C_1 \cdots C_{13}$	384	10.6
$C_1 \cdots C_6$	422	6.3
$C_1 \cdots C_{14}$	434	11.3
$C_7 \cdots C_{11}$	435	11.3
$C_8 \cdots C_{13}$	446	11.6
$C_4 \cdots C_{11}$	450	11.7
$C_2 \cdots C_{13}$	451	11.7
$C_3 \cdots C_{12}$	465	12.3
$C_7 \cdots C_{12}$	480	12.5
$C_2 \cdots C_7$	483	5.7
$C_2 \cdots C_6$	503	6.1
$C_5 \cdots C_{11}$	506	12.8
$C_8 \cdots C_{14}$	510	12.9
$C_2 \cdots C_{14}$	516	13.1
$C_6 \cdots C_{11}$	525	13.3
$C_4 \cdots C_{12}$	535	13.5
$C_5 \cdots C_{12}$	574	14.3
$C_7 \cdots C_{13}$	576	14.4

(continued)

Type of intramolecular interactions C — C and C $\cdots$ C	Intramolecular distances $r_{ij} \times 10^{-3}$ [nm]	Mean amplitude $u_{ij} \times 10^{-3}$ [nm]
$C_6 \cdots C_{12}$	585	14.6
$C_3 \cdots C_{13}$	594	14.8
$C_7 \cdots C_{14}$	635	15.6
$C_3 \cdots C_{14}$	656	16.2
$C_4 \cdots C_{13}$	670	16.4
$C_6 \cdots C_{13}$	690	16.8
$C_5 \cdots C_{13}$	698	17.1
$C_4 \cdots C_{14}$	730	17.6
$C_6 \cdots C_{14}$	755	18.2
$C_5 \cdots C_{14}$	776	18.7

The molecular function of structure $i_{\mathrm{m}}(S)$ was calculated by the Debye formula (9) for the Bragg angle ϑ varying from 0° to 60°. The courses of the dependencies $i(S)$, $i_{\mathrm{m}}(S)$ and $i_{\mathrm{d}}(S)$ are shown in Fig. 2.

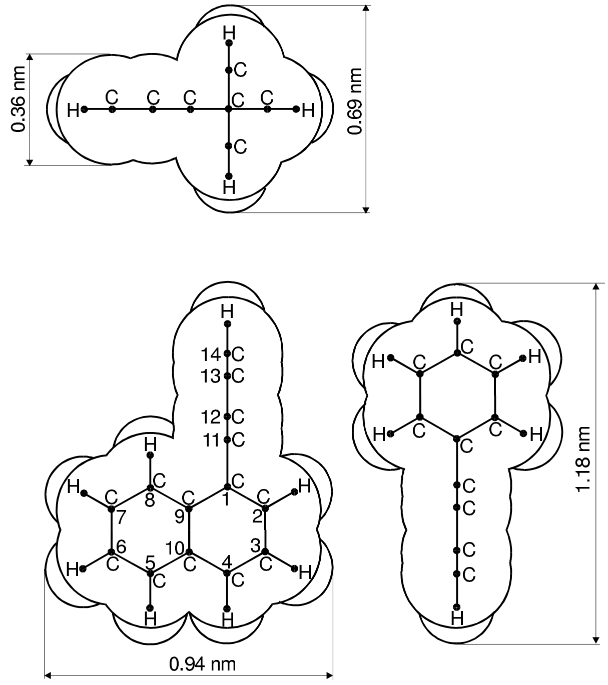

Fig. 3. A model of 1-phenylnaphthalene $C_{10}H_7 - C_6H_5$ molecule structure.

Fourier analysis of the function $S\ i(S)$ yielded the function of radial distribution of electron density shown in Fig. 4. Their positions correspond to the most probable interatomic and intermolecular distances in the liquid studied. These function bring the information about the difference between the observed and the average distribution of electron density [1].

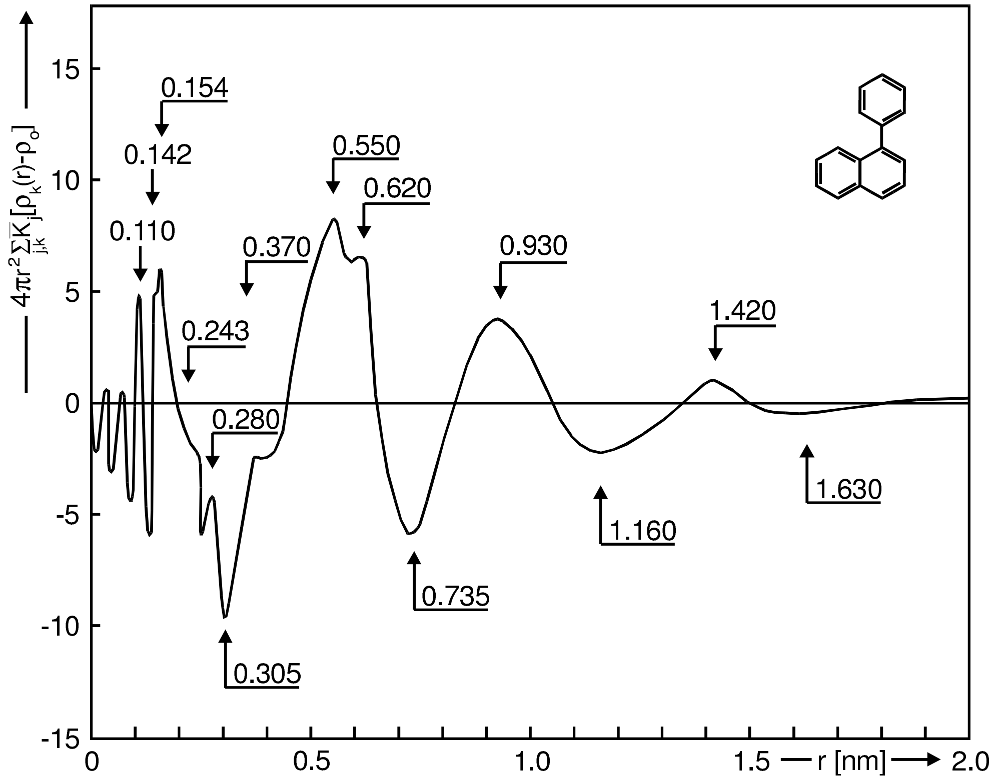

Fig. 4. The electron-density radial-distribution function $4\pi r^2 \sum_{j,k}^{n} \bar{K}_j[\rho_k(r) - \rho_0]$ for liquid 1-phenylnaphthalene.

In liquid 1-phenylnaphthalene the presence of the coordination spheres of intermolecular ordering [36] was established. Subsequently, the ranges of the spheres and coordination numbers (Table III) were determined. Coordination shells are delimited by minima of EDRDF [37].

Table III. The range of coordination spheres and the mean number of molecules in each sphere for the studied 1-phenylnaphthalene.

Sphere	Range [nm]	Number of molecules
1 st	0.305 — 0.735	8.1
2 nd	0.735 — 1.160	27.2
3 rd	1.160 — 1.630	54.7

5 Discussion

In this work the experimental data $S\ i(S)$ (Fig. 2, curve A) were complemented with theoretical data of the curve $i_{\mathrm{m}}(S)$ (Fig. 2, curve B) to the $S_{\max}$ value equal to 140 nm^{-1}. The obtained coincidence of these two curves proves that the proposed model of 1-phenylnaphthalene molecule, and in particular the interatomic distances in the molecule, is correct. In this situation the EDRDF (Fig. 4) was calculated. The function of the radial distribution of electron density $4\pi r^2 \sum\limits_{j,k}^{n} \bar{K}_j [\rho_k(r) - \rho_0]$ is, according to Eq. (3), determined by the integral,

$$\frac{2r}{\pi} \int\limits_0^\infty S\ i(S) \exp(-\alpha^2 S^2) \sin(Sr) \mathrm{d}S$$

calculated by the numerical Simpson method for $0 \le \bar{r} \le 2$ nm at a step of 0.005 nm.

The EDRDF is charged with a certain error following from the application of the integral Fourier formula derived for infinite limits of integration to an experimental situation in which measurements are conducted in a finite range of argument values. Replacement of the Fourier transform from Eq. (3) by the proper integral in Eq. (6) implies the appearance of additional oscillations for $0 < \bar{r} \le 0.1$ nm. These maxima have no physical meaning and are only a mathematical effect, a consequence of the approximations applied.

The size of a 1-phenylnaphthalene molecule is 0.94 nm (length) × 0.36 nm (width) × 1.18 nm (height). On the average, it takes a volume of V=0.3126 nm^3, whereas an increment of the molecule volume [38] is V=0.2098 nm^3. The packing coefficient of molecules in liquid 1-phenylnaphthalene is k=67%. Due to the size of the 1-phenylnaphthalene molecule, Fig. 3 which can be evaluated from the van der Waals radii of carbon and hydrogen atoms, the first six maxima of the EDRDF, Fig. 4, should be ascribed to the interferences inside a respective single molecule. The maxima fall within the range $0.1 < \bar{r} \le 0.4$ nm and their positions correspond to the distances between the following atomic pairs: C_2 — H = 0.110 nm, C_1 — C_9 = 0.142 nm, C_1 — C_{11} = 0.154 nm, $C_1 \cdots C_3$ = 0.243 nm, $C_1 \cdots C_4$ = 0.280 nm and $C_1 \cdots C_5$ = 0.370 nm.

The subsequent maxima of the EDRDF correspond to the mean intermolecular distances in the liquid studied. The positions of the maxima of this function (Fig. 4) corresponding to the mean least intermolecular distances are directly related to the main maxima at the function of intensity distribution. According to the data from Fig. 1 and Table II, the intensity distribution for liquid 1-phenylnaphthalene shows two maxima corresponding to intermolecular interactions. The first of them, for $S_1 = 12.00$ nm^{-1}, corresponds to the intermolecular distance of $\bar{R}_1 = 0.614 \pm 0.010$ nm, calculated [32] from Eq. (7). The second maximum on the intensity distribution curve at $S_2 = 13.30$ nm^{-1}, corresponds to $\bar{R}_2 = 0.551 \pm 0.010$ nm. This maximum should be attributed to intermolecular interactions considering its high intensity and the fact of the occurrence of EDRDF maximum for $\bar{r}_7 = 0.550$ nm (Fig. 4). In the range $\approx 0.4 \le \bar{r} < 2.0$ nm, the function can be divided into three regions corresponding to three spheres of intermolecular ordering.

The most probable simple configurations of neighbouring molecules in the liquid in question can be examined by fitting the positions of the maxima of the EDRDF to the distances between the centres of the neighbours, resulting from their van der Waals models. Such models can be constructed on the basis of the bond lengths within the molecule and the van der Waals radii of C and H atoms.

6 Conclusions

The applied methods of measurements and calculations permitted a determination of the mean structural parameters (the inter- and intramolecular distances, the radii of coordination spheres, the coordination numbers) and local ordering of the molecules in the liquid 1-phenylnaphthalene. The use of short-wave radiation from an X-ray tube with a molybdenum anode permitted determination of the 3 spheres of intermolecular ordering, that is the supermolecular structure in the liquid studied.

The appearance of distinct maxima in the angular distribution function of X-ray scattered radiation and electron-density radial-distribution function obtained for liquid 1-phenylnaphthalene, indicates the presence of the short-range ordering in liquid 1-phenylnaphthalene up to a distance of about 2.0 nm. In this range three spheres of intermolecular ordering were distinguished. The maxima on the EDRDF in the range $0.1 < \bar{r} \leq 0.4$ nm are attributed to intramolecular interactions. The three maxima corresponding to the C — C distances appear at 0.142 nm, 0.243 nm and 0.280 nm 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 maximum assigned to the C — H bond corresponds to the distance 0.110 nm within the ring. The maxima in the range $0.4 \leq \bar{r} < 0.6$ nm, are interpreted as due to intra- and intermolecular diffraction, whereas those for $\bar{r} > 0.6$ nm are due to intermolecular diffraction. These results can be interpreted in terms of a simple model of local arrangement of molecules, which probably can be valid for a larger class of molecular liquids, i.e.weakly polar monosubstituted derivatives of naphthalene.

The values of $\bar{r}_7$=0.550 nm and $\bar{r}_8$=0.620 nm determined provide the information about intermolecular spatial configurations in the liquid studied. The maxima of EDRDF at $\bar{r}_9$=0.930 nm and $\bar{r}_{10}$=1.420 nm bring the information about the difference between the observed and the average distribution of electron density. The packing coefficient of molecules in liquid 1-phenylnaphthalene is approximately constant in all coordination spheres and equal to 67%. This value falls within the range of k values acceptable for the liquid phase substances. These results are also consistent with the values presumed in the conformational structure investigation of 1-phenylnaphthalene performed by empirical and semi-empirical MO-LCAO calculations [39].

The approach proposed in this paper gives a good description of intermolecular interactions in liquids and is a useful X-ray method for their analysis.

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