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Abstract and conclusions

This monograph should be treated as an introduction in the attempts to apply Wide Angle X-ray Scattering (WAXS) method in the analysis of structure of selected soft materials.

In the first, second and third chapter the scope of the work is determined. This range comprises: a draft of theory bases, measuring methods and analytical developments description. The radial distributions were obtained by numerical analysis, applying digital computer methods to experimental angular functions of intensity distribution, $\bar{I}(\Theta)$ with all corrections included, and afterwards normalization of the curves [4–8, 80–82] with the help of the Fourier transform of the function, $\bar{I}_{e,u}(S)$ [33, 44]. Methodical instructions for solving the short-range liquid structure as well as estimation of the conditions that should be fulfilled in interpretation of experimental data are given.

X-ray diffractometer applied in the structural studies of soft materials by Freiberger Präzisionsmechanik (Germany) is composed of a generator TuR M-62, X-ray lamp with a linear focal point, flat graphite monochromator and a goniometer HZG-3 with a radiation counter and an electronic device for measurements, registration and control. The focusing system in a HZG-3 goniometer were applied according to the Bragg and Brentano method [66, 67].

Molecular geometry is a sensitive indicator of intra- and intermolecular interactions [151]. The method of reduction proposed by Mozzi and Warren with modifications introduced by the author [123] has been applied to verify the assumed models of the molecules studied and to separate the intra- from intermolecular interactions. Analysis of intramolecular interactions between pairs of atoms and intermolecular interactions has been made taking into account the values of the temperature factors.

Atomic and molecular structures were determined for liquid benzene tri-derivatives (chapter 5 and 6) and *ortho*-nitroanisole solution in *p*-Xylene (chapter 7). The most probable structural models for series of studied liquids and solution are presented. For the first time the theoretically predicted models of their structure were experimentally confirmed. The presence of short-range ordering reaching to about 20 Å has been proved.

In the sixth chapter the description of conformational analysis of molecules of the liquid benzene tri-derivatives by the minimisation of the potential energy is presented.

In this work in the eighth chapter we report the results of the investigations of the blood serum samples which were collected from the patients who suffered from neoplasmic diseases by the X-ray diffraction method. The diffraction patterns were referred to that of pure water.

X-ray diffraction seems to be a promising in diagnostics and therapy of patients with cancer.

The most important results of this work are listed below.

- Preparation of experimental procedure to obtain the optimum results for selected soft materials.
- Obtaining new information about the structure of selected liquid benzene tri–derivatives on the basis of the diffraction experiments.
- Determining the influence of functional groups on the geometry of the benzene ring.
- New experimental data on the structure of the 10% solution of *ortho*-nitroanisole in *p*-Xylene.
- The Lennard-Jones 12–6 potentials in the parametrization of the Kitaigorodsky for benzene tri-derivatives were determined.
- It has been established that changes in the blood serum caused by development of neoplasmic condition can be detected early by the X-ray method.

The approach proposed in this work gives a good description of intra- and intermolecular interactions in selected of soft materials and is a useful X-ray method for their analysis. The WAXS method enables the study of various materials in the soft phase, from molecular liquids to solutions and biological systems (human blood serum).