STRUCTURE AND INTERMOLECULAR INTERACTIONS IN SELECTED BINARY SOLUTIONS STUDIED BY X-RAY METHODS

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X-ray structural results for liquid orthonitrotoluene and ortho-nitrotoluene $C_7H_7NO_2$ in 1,4-dimethylbenzene are reported. The measurements were performed using the transmission technique (Figure 1).

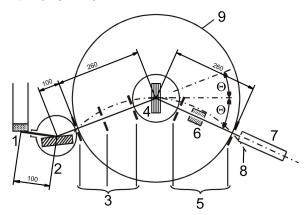


Figure 1: The focusing of the beam passing through the monochromator and goniometer with the preparation studied: 1-X-ray lamp anode, 2- monochromator, 3- a system of input slits of the goniometer, 4- cuvette with the liquid solution studied, 5- a system of output slits, 6- Soller slits, 7- radiation counter, 8- Rowland circle, 9- goniometer circle; distances expressed in mm [1].

Averaged scattered X-ray angular distribution for 10% solution of *ortho*-nitrotoluene in 1,4-dimethylbenzene was determined (Figure 2).

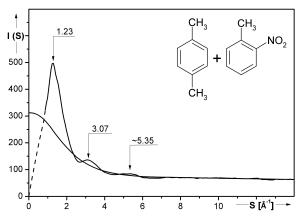


Figure 2: The mean angular distribution of the scattered radiation intensity for binary solution studied.

Radial electron density distribution function was obtained from a modiefied Warren, Krutter and Morningsstar equation [2] (Figure 3).

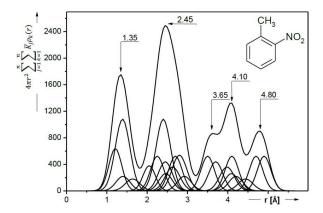


Figure 3: The electron-density radial-distribution function (EDRDF) of the ortho-nitrotoluene is a sum of the curves of the Gauss normal distribution.

To the maxima of I(S), EDRDF, interatomic and intermolecular distances are assigned [3]. The experimental results were used to plot models of the most highly probable mutual disposition of the molecules in liquid *ortho*-nitrotoluene and it solution (Figure 4).

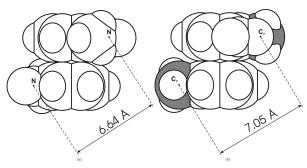


Figure 4: Model of the most highly probable mutual disposition of molecules in 10% solution of orthonitrotoluene in 1,4-dimethylbenzene.

References

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