

X-RAY DIFFRACTION INVESTIGATION OF CYCLOHEXANE DERIVATIVES AT 293 K

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This paper reports results of X-ray diffraction study of three the cyclohexane derivatives: methylcyclohexane $C_6H_{11}-CH_3$ (Fig. 1a), cyclohexylamine $C_6H_{11}-NH_2$ (Fig. 1b) and cyclohexanol $C_6H_{11}-OH$ (Fig. 1c). The aim of the study was to establish the role of the cyclohexane ring and the functional groups ($-CH_3$, $-NH_2$, $-OH$) attached to it at the equatorial position in configurations of the molecules of the liquids studied.

The measurements of scattered radiation intensity were performed with molybdenum radiation (MoK_{α} , $\lambda = 0.71069 \text{ \AA}$) and graphite monochromator on the diffracted beam in a range 2θ of $6^\circ - 120^\circ$ by the step-scanning method [1] with a step of 0.2° and counting time of 15 s.

The most important results of the paper are listed below:

- 1) New experimental data on the structure of cyclohexane derivatives (Fig. 1) at 293 K.
- 2) New information on mutual arrangement, orientation and packing coefficient of the molecules studied.
- 3) Proposition of models if intermolecular binary radial correlations in the antiparallel orientation of dipole moments in the liquids studied.
- 4) The presence of short-range ordering reaching about 20 \AA has been proved [2].

References

- [1] H. Drozdowski, "Structural analysis of liquid 1,4-dimethylbenzene at 293 K", *J. Mol. Struct.* **783** (2006) 204–209.
- [2] H. Drozdowski, K. Nowakowski, "X-ray diffraction studies of liquid methylcyclohexane $C_6H_{11}-CH_3$ structure at 293 K", *Acta Phys. Polon. A* **114** (2008) 383–389.

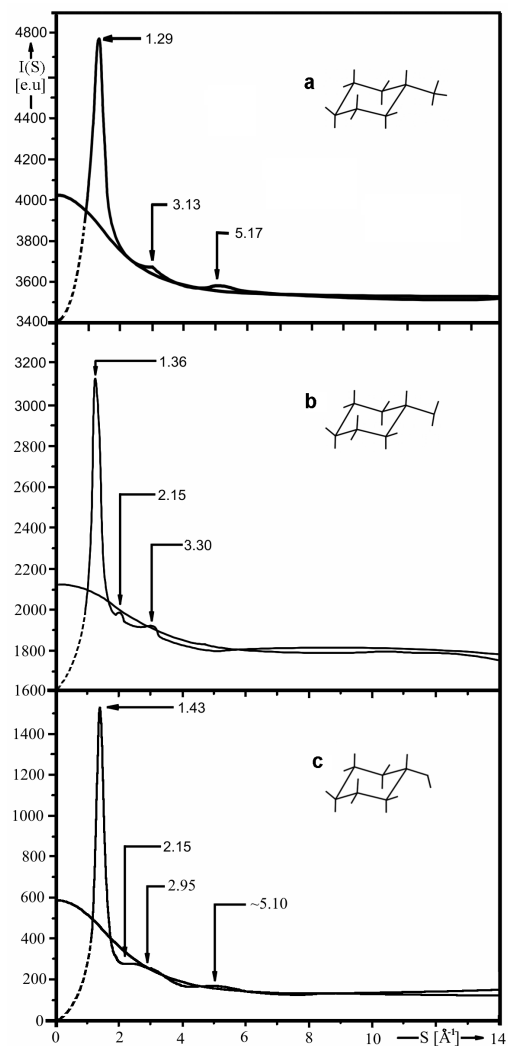


Figure 1. The experimental curves of angular distribution of X-ray scattered intensity in cyclohexane derivatives ($S = 4\pi \sin\theta / \lambda$).