STUDY OF THE STRUCTURE AND OF THE INTERNAL ORDERING DEGREE IN LIQUID CYCLOHEXYLAMINE C_6H_{11}–NH_2

H. Drozdowski * and K. Nowakowski

Faculty of Physics, Adam Mickiewicz University,
ul. Umultowska 85, PL 61-614 Poznań, Poland

Keywords: angular-distribution function, intermolecular ordering

**) e-mail: riemann@amu.edu.pl*

The study of the structure and molecular correlations of cyclohexylamine is a continuation of earlier works on methylcyclohexane in the liquid phase [1].

The structure of cyclohexylamine (Fig. 1) at 293 K was investigated using the X-ray diffraction method. The scattered intensity distribution was measured for the angles $6° \leq 2\theta \leq 120°$ at every 0.2°, where 2θ is the scattering angle. An angular distribution of X-ray radiation scattered in liquid cyclohexylamine was measured (Fig. 2).

The use of short-wave radiation MoK_α enabled determination of the shortest interatomic distances within cyclohexane ring. The bond distances and bond angles used were: C–C = 1.53 Å; C–NH_2 = 1.36 Å; C–H = 1.09 Å; <CCC = <CCH = regular tetrahedral.

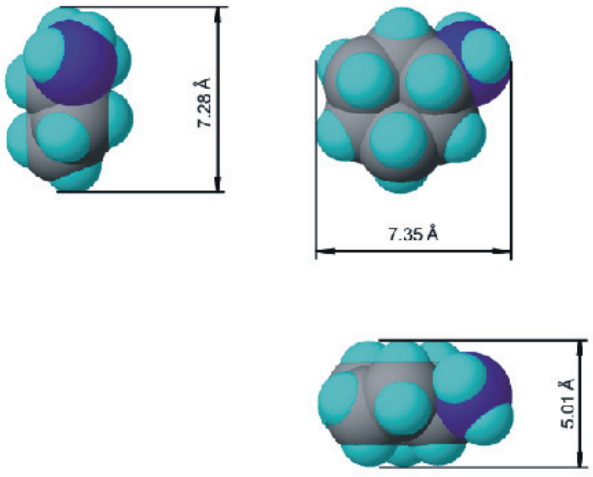

Figure 1. A model of liquid cyclohexylamine structure projected onto three orthogonal planes (d = 0.867 g/cm^3; M = 99.18 g/mol; V_0 = 190 Å^3).

A simple model of short-range arrangement of the molecules was proposed [2]. In liquid cyclohexylamine only in the aniparallel conformation the distance between the centres of the amine groups is $NH_2(1)\ldots NH_2(2)$ = 6.70 Å [2].

The interpretation of the results was carried out using the reduction method of Blum and Narten [3].

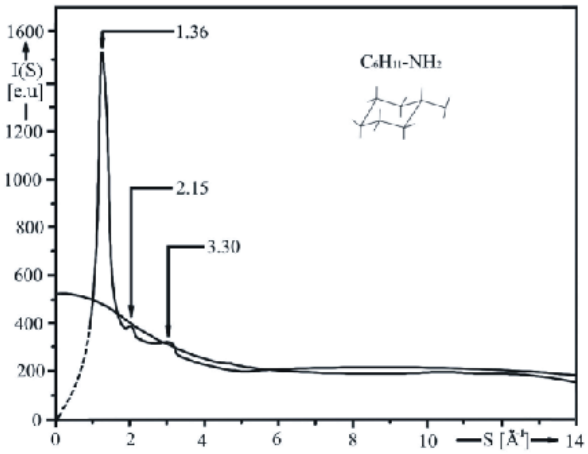

Figure 2. Normalized, experimental curve of angular distribution of X-ray scattered intensity, and total independent scattering curve in liquid cyclohexylamine.

These results are also consistent with the values presumed in the conformational structure investigation of the liquids studied performed by empirical and semi-empirical MOLCAO calculations [4].

References

[1] 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** (2) (2008) 383–389.

[2] H. Drozdowski, K. Nowakowski, Z. Błaszczak, "A relation between X-ray diffraction based liquid cyclohexylamine C_6H_{11}–NH_2 structure and packing coefficient", *Pol. Crystallogr. Meet*. **51** (2009) 268–269.

[3] H. Drozdowski, K. Nowakowski, "X-ray scattering in liquid cyclohexane derivatives at 293 K", *J. Mol. Struct*. (2009) in press.

[4] J.M. Haile, *Molecular Dynamics. Elementary Methods* (John Wiley & Sons, New York, 1992).