DETERMINATION OF ELECTRON RADIAL DISTRIBUTION FUNCTION FOR LIQUID CYCLOHEXYLAMINE BY X-RAY DIFFRACTION

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An angular distribution of X-ray radiation scattered in liquid cyclohexylamine C_6H_{11}–NH_2 was measured. The electron-density radial-distribution function was calculated. Structural parameters, the mean distances between the neighbouring molecules as well as the coordination numbers were found.

X-ray scattering in liquid cyclohexylamine (melting point 256 K, boiling point 406 K), at a temperature of 293 K, was measured by applying MoK_α radiation, λ = 0.71069 Å, monochromatized by a graphite crystal. The scattered intensity distribution was measured by a goniometer HZG-3 for the angles $3° < \theta < 60°$, where 2θ is the scattering angle. Small-angle scattering ($0 < \theta < 3°$) results were extrapolated to the origin of the coordinate system using a second-order function.

Shapes of the scattered intensity were analyzed subsequent to correction for polarization of the monochromatic radiation and absorption in plane samples and after normalization to electron units (Fig. 1).

The method of Warren *et al*. [1] was applied to obtain the electron density radial distribution function. The most probable intermolecular distances were found from the positions of the maxima of the radial distribution function (Fig. 2), whereas the corresponding coordination numbers were obtained from the area delimited by these maxima.

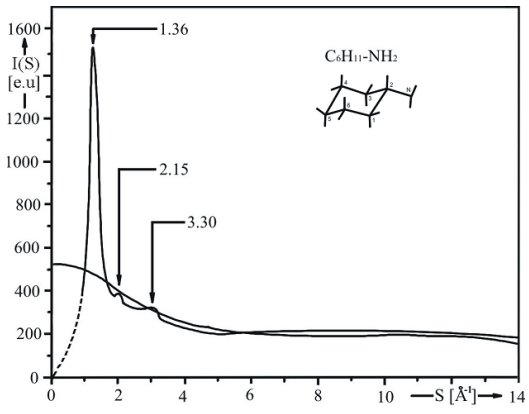

Figure 1. Normalized, experimental curve of angular distribution of X-ray scattered intensity of liquid cyclohexylamine.

The mean distance calculated for two molecules of cyclohexylamine in the antiparallel arrangement between the nitrogen atoms of the functional groups (NH_2) is 7.30 Å (Fig. 3).

References

[1] H. Drozdowski, "Local structure and molecular correlations in liquid 1-methylnaphthalene at 293 K", *Chem. Phys. Lett.* **351** (2002) 53–60.

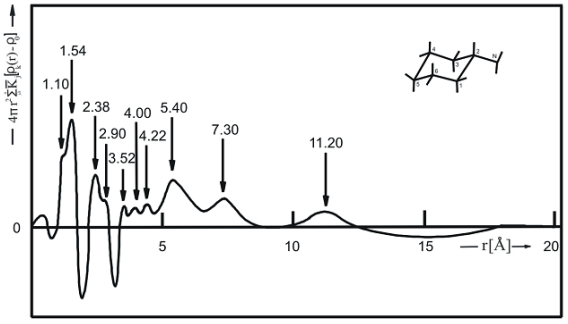

Figure 2. Electron density radial distribution function of liquid cyclohexylamine.

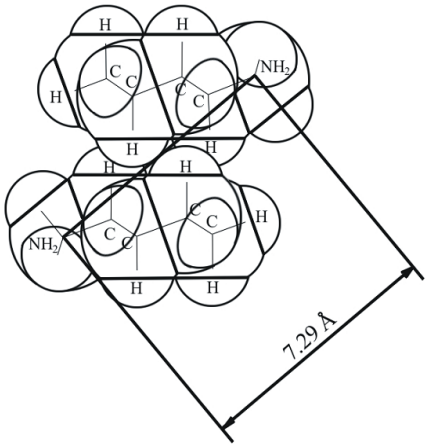

Figure 3. Model of probable conformation of molecules in liquid cyclohexylamine. The antiparallel arrangement of molecules.