A MOLECULAR STRUCTURE STUDY OF 1,3,5-TRICHLOROBENZENE

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The paper presents the structure and molecular correlations in liquid 1,3,5-trichlorobenzene $C_6H_3Cl_3$ determined for the first time by the X-ray diffraction method [1]. Trichlorobenzene characterized by the melting point of 338 K and boiling point of 481 K ($M = 181.45$ g/mol). This paper reports the first studies of liquid trichlorobenzene performed by the counter method for the range of the angular measurements intensity extended to the value of $\theta = 60°$ (Fig. 1). Trichlorobenzene samples of 99% purity were purchased from Aldrich-Chemie (Germany).

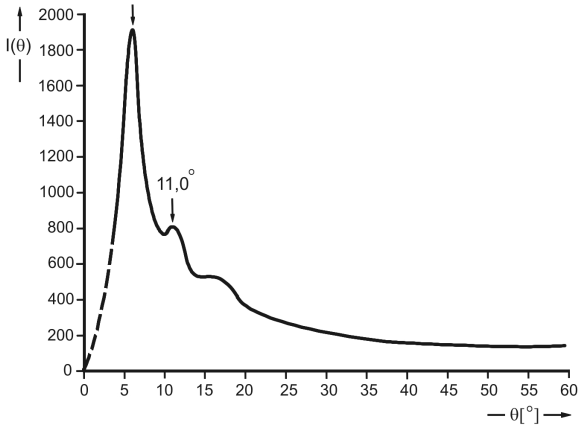

Figure 1: Mean angular distribution of the scattered intensity for pure 1,3,5-trichlorobenzene $C_6H_3Cl_3$.

From the position of the main maximum $I(\theta)$ of the east intermolecular distance, which is also the radius of the first coordination sphere, was determined.

The attractive dipole interaction between neighbouring molecules can favour the plane arrangement of molecules one over another in antiparallel arrangement (Fig. 2 and Fig. 3 — for liquid chlorobenzene). The distance between the centres of two neighbouring molecules is defined by van der Waals atomic radii.

The physical sense of the molecular packing coefficient [2] and its role in solving the near-range ordering in liquids chloronenzene is explained.

On the basis of the differential radial distribution functions (DRDFs) it is possible to conclude about the mutual orientations of the functional groups (-*Cl*) of molecules with respect to the benzene rings of the neighbouring molecules. The antiparallel arrangement of the molecules dipole moments is indicated by the positions of the maxima on the functions and the size of the molecules. Because of the supposed role of the benzene ring and functional group (-*Cl*) attached to it at the *ortho*-, *meta*-, *para*-position, for mutual configurations of molecules in liquids studied, it seems very probable that the proposed models of local arrangements can also hold for other derivatives of benzene in the liquid phase.

The use of short-wave radiation Mo K_α enabled determination of the shortest interatomic distances within the benzene ring.

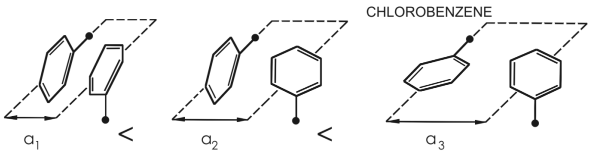

Figure 2: The model of probable configuration of molecules in chlorobenzene C_6H_5Cl.

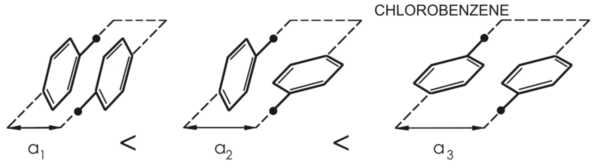

Figure 3: The arrangement of molecules in liquid chlorobenzene.

References

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