P-15

The application of X-Ray diffraction and computer experiments in the studies of structure of liquids and amorphous solids

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The application of the X-ray diffraction method for study the structure of liquids and amorphous solids is described. The main sources of errors are discussed. A numerical analysis is performed of the influence of X-ray data termination on the normalization constants, radial distribution functions (RDF), and on interatomic distances and coordination numbers determined from these functions. Computations are carried out for liquid dichloroalkanes [1,2], carbon tetrachloride [3,5] and naphthalene [4]. The strong dependence of coordination number on the termination angle, observed by other authors, is confirmed. An approximately linear dependence of coordination numbers on wave vector S is found.

Use of RDF, to compute a coordination number, N_1, for liquids is discussed for four methods: 1/ symmetrizing the first peak in RDF; 2/ symmetrizing the first peak in r^2 $RDF(r)$; 3/ decomposition of r^2 $RDF(r)$ into shells; 4/ computation of area to the first minimum in r^2 $RDF(r)$.

Figure 1 shows the calculated RDF of 1,12-dichloroalkanes decomposed into the various atomic peaks. These composite peaks are resolved into atomic peaks on the assumptions that the shape of an atomic peak can be represented by an equation of the form: $e^{-x^2/c}$ where c is a constant, i. e. that the curve is Gaussian, and also that the area under an atomic peak formed by two atoms multiplied by the distance between the two atoms is proportional to the product of the scattering powers of the two atoms.

The coordination numbers and interatomic and intermolecular distances in a liquid are mean values and undergo fluctuations. Therefore, it seems that the best method to estimate the total experimental uncertainty of

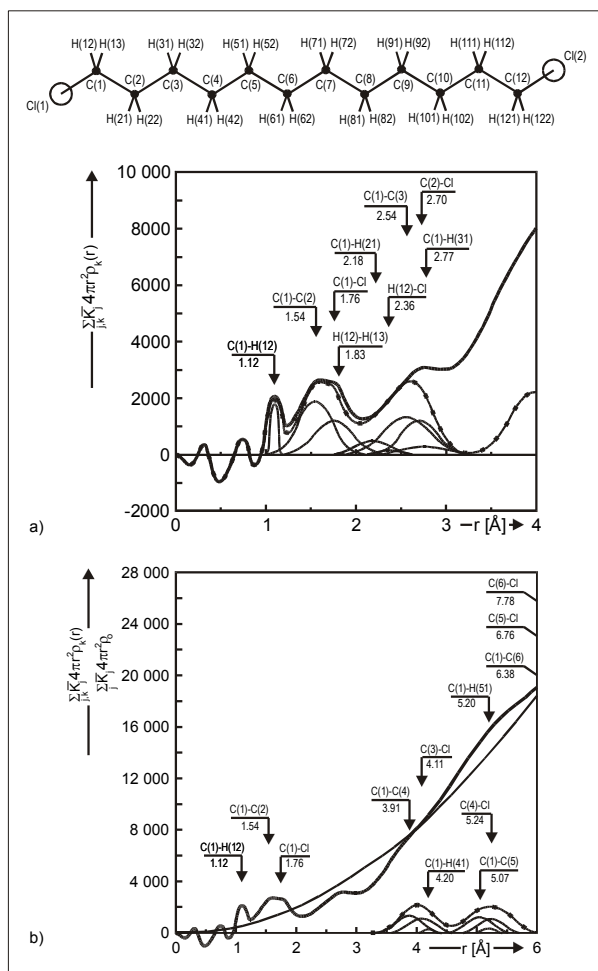RDF determination is a comparison of results obtained independently by X-ray diffraction [4].

Figure 1. The experimental RDF of 1,12-dichlorododecane decomposed into its atomic peaks.

[1] H. Drozdowski, *J. Mol. Liquids* **122** (1–3) (2005) 32.
[2] H. Drozdowski, *Phys. Chem. Liquids* **42** (6) (2004) 577.
[3] M. Śliwińska-Bartkowiak, H. Drozdowski, M. Kempiński, M. Jażdżewska, Y. Long, J. C. Palmer, K. E. Gubbins, *Phys. Chem. Chem. Physics* **14** (19) (2012) 7145.
[4] H. Drozdowski, *Acta Phys. Slovaca* **54** (5) (2004) 447.
[5] Y. Long, M. Śliwińska-Bartkowiak, H. Drozdowski, M. Kempiński, K.A. Phillips, J.C. Palmer, K. Gubbins, *Coll. Surf. A: Physicochem. Engineer. Aspects* **437** (2013) 33.