INTERPRETING DIFFRACTION DATA: THE STRUCTURE OF MOLECULAR LIQUIDS

László Pusztai
HUN-REN Wigner Research Centre for Physics, Budapest, Hungary
&
IROAST, Kumamoto University, Japan
(pusztai.laszlo@wigner.hun-ren.hu)

During the first part of the presentation, a general scheme for interpreting diffraction data on liquids and amorphous materials will be introduced in short. The approach makes extensive use of the Reverse Monte Carlo (RMC) method structural modelling [1].

In the main part of the seminar, I will show how the structure of molecular liquids can be determined via neutron and X-ray diffraction experiments, followed by computer modelling. First, a well-known example, the structure of carbon-tetrachloride (CCl_4) will be discussed in some detail, mentioning available diffraction data, as well as the (rather strange) history of interpretations of these data (see [2] for details). Some remarks will be made concerning the structure of the various phases (ordered crystalline, disordered crystalline and liquid) of carbon-tetrabromide (CBr_4).

If time permits, finally a specific but essential class of liquids, of the ones whose basic property is hydrogen-bonding, will be discussed. Neutrons, in contrast to X-rays, *are* sensitive to hydrogen atoms. Still, accurate determination of the so-called 'coherent static structure factor' of liquids that contain substantial amounts of proton nuclei (like water) has proven to be problematic by neutron diffraction, due to the large 'incoherent cross section' of ^1H. In order to expose the case proportionally to its importance, the presentation will end by discussing experimental determination of the structure of pure liquid water [3].

[1] R.L. McGreevy, L. Pusztai, Molec. Simul. 1988, 1, 359.
[2] Sz. Pothoczki, L. Temleitner, L. Pusztai, Chem. Rev. 2015, 115, 13308.
[3] L. Temleitner, A. Stunault, G. Cuello, L. Pusztai, Phys. Rev. B 2015, 92, 014201.