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v Ljubljani

Fakulteta *za kemijo*
in kemijsko tehnologijo

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VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI

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z naslovom:

Neutron and X-ray Scattering for Structural Studies of Molecular Liquids: From Carbon Tetrachloride to Alcohol-Water Mixtures

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Vljudno vabljeni!

Abstract:

Adequate knowledge on the microscopic (i.e., atomic level) structure of liquids is of primary importance: just consider liquid water and aqueous solutions (including the human body…). Unfortunately, standard methods of crystallography cannot be applied in this case, due to the lack of translational symmetry in liquids.

In this lecture, I will try to provide a brief introduction to the experimental methods available for studying disordered structures: neutron and X-ray diffraction. Some elements of the related formalism will also be covered, primarily in order to clearly demonstrate what information is accessible from these measurements. Computational methods that can enhance our understanding of the structure of liquids will also be touched upon.

Next, 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.

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 containing substantial amounts of proton nuclei (like water) has proven to be problematic by neutron diffraction, due to the large 'incoherent cross section' of ^1H. This difficulty has continued to introduce large uncertainties whenever a sample with a ^1H content larger than about 20 % had to be measured by neutron diffraction. 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.

A showcase publication from our group, relevant to the topic of the lecture:
Szilvia Pothoczki, László Temleitner, and László Pusztai:
Structure of Neat Liquids Consisting of (Perfect and Nearly) Tetrahedral Molecules
Chem. Rev. 2015, 115, 13308−13361. DOI:10.1021/acs.chemrev.5b00308