Report: The aim of experiment SC-4035 was to study changes in the local structure of monohydroxy alcohols and their mixtures using high energy x-ray diffraction with the ultimate goal to do a pair distribution analysis to determine the local structural changes causing dynamic anomalies referred to as Debye process and to compare these results with molecular dynamic simulations. The huge difference of the dielectric absorption due to the Debye process is often assigned to different topologies of supramolecular arrangements in the liquids which has not been probed directly so far [1]. The hydrogen bonded oxygen atoms build the skeleton of such a cluster and the carbon chains are radiating outwards and so chain or ring like structures are prevailed depending on the shape of the carbon chain and the position of the OH-group. Moreover the Debye process is strongly dependent on temperature and can also be influenced by mixing of two monohydroxy alcohols [2, 3]. We used beamline ID22 to measure high energy x-ray diffraction pattern of different alcohols and specific mixtures. The samples were contained in glass capillaries of 2 mm in diameter and fixed in a spinning mount on the diffractometer where its temperature was controlled by a liquid nitrogen jet. Diffraction pattern were measured employing the image plate detector of ID22 at a distance of 59 cm and a incident energy of 72 keV. For each temperature 25 pattern with an exposure time of five seconds were averaged. First we measured 1-octanol as a reference at room temperature and did a pair distribution analysis employing pdfgetx3 [4]. As presented in figure 1 we were able to reproduce the PDF measured by Vahvaselkä et al. (1995) with improved resolution [5]. The first peak of the PDF is due to O-H and C-H distances, the second one arises from C-C and C-H distances. There is also a clear resolved peak which is representing the typical distance between two hydrogen bonded oxygen atoms. Figure 2 shows the PDFs of the monohydroxy alcohols 2-ethyl-1-hexanol (2E1H) and 4-methyl-3-heptanol (4M3H), 2E1H displays a strong Debye process compared to 4M3H. The correlation number calculated from the area below this O-O peak is higher for 4M3H then for 2E1H which indicates that there are more dimers in 4M3H then in 2E1H. The peak at twice the O-O distance (5.3 Å) gives rise to a higher correlation number in 2E1H than in 4M3H and lead to the assumption that there are more oxygen atoms in the second coordination shell so the number of trimers is higher in 2E1H. These results correspond to the increased Debye process in 2E1H. The next step is to study the temperature induced changes in both alcohols to investigate the origin of the nonlinear temperature evolution of the Debye process. In addition we will compare the experimental

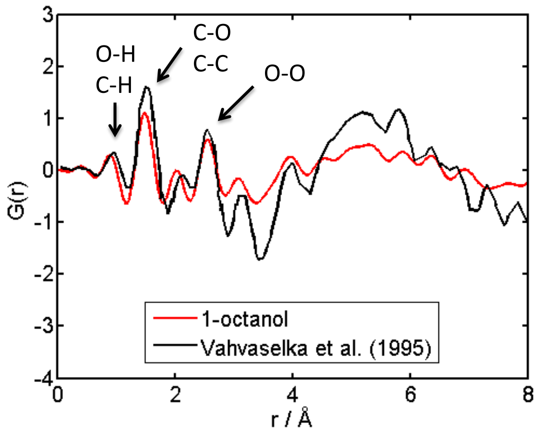

Figure 1: Pair distribution function of 1-octanol measured at ID22 in red and by Vahvaselka et al. in black. Theoretical values for several distances are shown as vertical lines: O-H 0.956 Å, C-H 1.096 Å, C-O 1.427 Å, C-C 1.540 Å, O-O hydrogen bond 2.7 Å

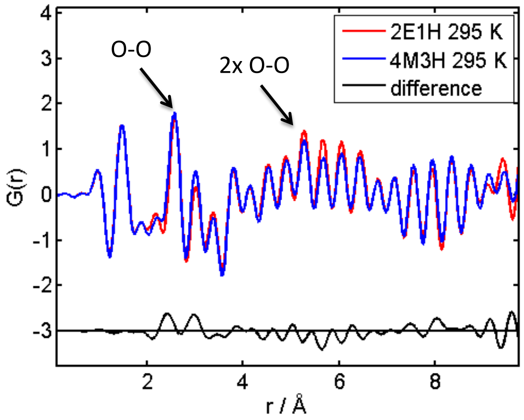

Figure 2: Pair distribution function of 2-ethyl-1-hexanol and 4-methyl-3-heptanol.

results with molecular dynamic simulations that we are carrying out at the moment. Furthermore we measured the mixtures of two ring building alcohols for which a structural rearrangement to more chain like structures is known.

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