Structure of alcohols under high pressure

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Alcohols are compounds essential in many industrial processes. It is already known that alcohols in the liquid state may form different kinds of supramolecular structures on a length scale larger than ordinary – non-associating liquids[1]. Their simple chemical composition and hydroxyl group make them model substances to study the process of self-association which leads to supramolecular clustering[2]. Currently, the nature of hydrogen bond (HB) interactions and supramolecular clusters formed via HBs is still far from being understood. Especially, little is know about behaviour of H-bonded structures under high pressure up to few gigapascals.

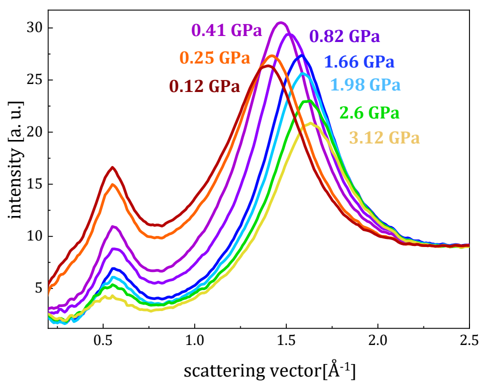

Figure 1. X-ray diffraction data of 2-ethyl-1-hexanol at high pressure measured at ESRF.

The peculiar nanometer size and disordered nature of the supramolecular strcutures make their identification challenging for the current science. One of a few techniques appropriate for their studies is total X-ray scattering, which is sensitive to the local structure and medium range-order of molecules. Importantly, obtaining the experimental diffraction data of a good quality for organic compounds under high pressure is possible by using an intense X-ray synchrotron source and diamond anvil cells. That setup is available only in a few research centers in the world[3]. In addition, characterization of liquids under high pressure is not a well-established field, in contarst to crystalline solid materials[4].

Here, we present the X-ray diffraction data obtained in European Synchrotron Radiation Facility (ESRF) for alcohol compounds under high pressure. Our results showed that the supramolecular structure of these compounds changes significantly with the increase of pressure (Figure 1). Interestingly, the variations in the diffraction peaks intensity and position occur non-monotonically. That finding contributes to the resolving of self-association process at extreme thermodynamic conditions and will be combined with the results of the molecular dynamics simulations. It is also a new pathway of challenging measurements of liquid organic compounds under high pressure.

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