

Name of the research group: Liquid Structure

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Aqueous solutions of simple sugars. — Aqueous solutions of four simple sugars, α -D-glucose, β -D-glucose, α -D-mannose and α -D-galactose were investigated by ab initio molecular dynamics (AIMD) simulations. Hydrogen bonding (HB) properties were analyzed, including the number of hydrogen bond donors and acceptors, as well as the lengths and strengths of the hydrogen bonds between sugar and water molecules. Related electronic properties, such as the dipole moments of water molecules and partial charges of the sugar O-atoms, were calculated. The spatial distribution functions were used to characterize the hydrophilic and hydrophobic shells. It was observed that β -D-glucose forms the highest number of hydrophilic and the smallest number of hydrophobic connections to neighboring water molecules. The average hydrogen bond length in sugar-water was shortest for β -D-glucose, indicating that these hydrogen bonds are the strongest. Additionally, β -D-glucose stands out due to the symmetry properties of both its hydrophilic and hydrophobic hydration shells. In summary, in all aspects considered here, there seems to be a correlation between the distinct characteristics of β -D-glucose, which is one important factor associated with its outstanding solubility in water. [1]

Network structure of alcohols vs. T, p. —The cluster formation ability of two pure monohydroxy alcohols, namely the 2-ethyl-1-hexanol (2E1H) and 2-methyl-3-hexanols (2M3H) are studied via synchrotron x-ray diffraction and classical molecular dynamics simulations on wide temperature (between 163K and 413K) and pressure (between 0.1GPa and 3GPa) range (Figure 1). The simulation results are validated by the satisfactory agreement between the experimental and calculated structure factors. Based on the analysis of the configurations, the hydrogen-bonded network elements are categorized into monomer, ring, linear- and branched chain motifs. At room temperature, linear and branched chains dominate in 2E1H, while linear chains and rings in 2M3H. Generally, increasing temperature promotes linear chains and monomer structures, which are supported by the breaking of branched chains in 2E1H and rings in 2M3H. Interestingly, raising the pressure does not affect the probabilities of the different motifs in the 2M3H network, but linear chains start to form branched chains in 2E1H. [2]

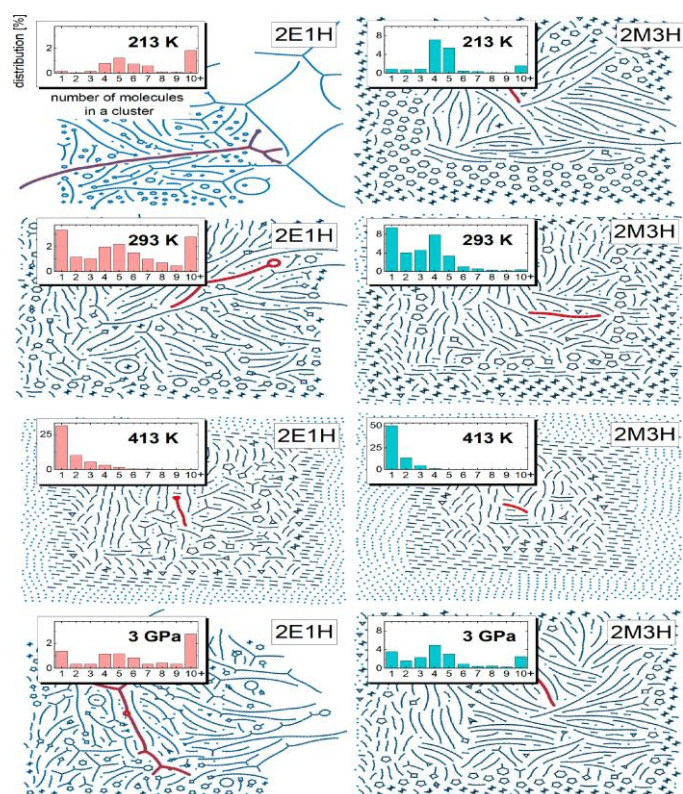


Figure 1. Visualization of lone and bonded hydroxyl groups derived from one configuration of simulation trajectory for 2E1H and 2M3H. The cluster colored in red is the largest one in the configuration. The insets show the histograms of the number of molecules in a cluster.[2]

Atomic structure and devitrification of vitreous $\text{Mg}_{82}\text{Ca}_8\text{Au}_{10}$. —Short range order of a ternary $\text{Mg}_{82}\text{Ca}_8\text{Au}_{10}$ biodegradable amorphous alloy was studied by combining diffraction datasets and Au L3 edge EXAFS data by the Reverse Monte Carlo simulation technique. It was found that while the Mg–Mg bond length agrees well with the empirical atomic diameter of Mg, both the Mg–Ca and Mg–Au mean interatomic distances are $\sim 9\%$ shorter than the sum of the corresponding atomic radii. The Ca–Au bond length exhibits $\sim 14\%$ shortening. The linear expansion coefficients of the glass determined from the temperature induced shift of the first peak of the structure factor and the reduced pair distribution function are $\sim 3.7 \times 10^{-5} \text{K}^{-1}$ and $\sim 3.1 \times 10^{-5} \text{K}^{-1}$, respectively. During devitrification, two crystalline phases emerge from the amorphous alloy: hexagonal AuMg_3 and the solid solution of Ca in hexagonal close packed Mg. The thermal expansion behaviour of the AuMg_3 unit cell was also determined using diffraction data. [3]

References (choose maximum 5 articles, each must begin with <https://>):

[1] <https://doi.org/10.3390/molecules29102205>

[2] <https://doi.org/10.1021/acs.jpcllett.4c000857>

[3] <https://doi.org/10.1016/j.jnoncrysol.2024.123157>