

The influence of charge ordering in the microscopic structure of monohydroxy alcohols

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Monohydroxy alcohols are well known to form hydrogen bonded clusters of various linear shapes [1, 2, 3]. The signature of this clustering is faithfully reproduced through the pre-peak feature of the calculated X-ray scattering intensities, as obtained from computer simulations with various force fields, and more importantly in excellent agreement with experiments [4, 5]. Since classical force fields simulate the H-bonding through the Coulomb association, it is naturally tempting to interpret the related clustering from a pure electrostatic point of view. Since charge order, *i.e.* the alternated positioning of positively and negatively charged atoms, dominates the microscopic distribution of molecular entities, it is interesting to examine how the constraints of oppositely charged oxygen and hydrogen atoms of the hydroxyl groups, as well as the constraints posed by the neutral atomic groups of the hydrophobic tails, act on the charge ordering and the molecular clustering. The influence of the branching of the tails is equally examined. The atom-atom pair correlation functions, which appear in calculation of the X-ray scattered intensities (through the atom-atom structure factors) are the focus of this study. The role of the cancellation of the positive like-charge correlations and negative cross correlations contributions to the pre-peak feature are analyzed. The analysis reveals several non-intuitive details about how charge ordering and neutral tail correlations adjust to each other to produce the actual structure of these monohydroxy alcohols.

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