

Structure of Nanoions in Water-Alcohol Mixtures: Partial Structure Factors and SAXS Predictions

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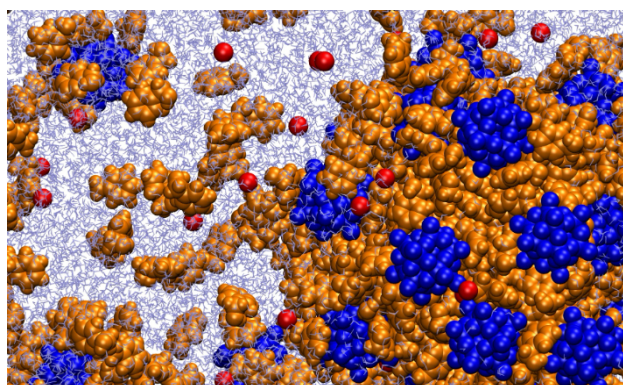
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Understanding the structural organization of ionic polyoxometallates (POMs) in water-alcohol mixtures remains challenging. Experimentally it is difficult to access and resolve the molecular-level correlations that give rise to complex solution structures. This difficulty is compounded by the intrinsic structural complexity of a water-alcohol mixtures themselves, within which the nanoscale organization of POMs occurs. Moreover, the thermodynamic origin of the superchaotropic[1] behavior exhibited by these nanoions is still not fully understood at the molecular level.

To address these issues, we perform all-atom molecular dynamics simulations of keggion ions ($\text{Na}_3[\text{PW}_{12}\text{O}_{40}]$) in water and benzyl alcohol. We analyze the resulting colloidal structures in real space, as illustrated in the figure below. In addition, we compute partial structure factors from the simulations to probe the molecular-level organization of these ionic solutions. These structure factors enable the prediction of small angle X-ray scattering (SAXS) spectra, thereby providing a direct link to experimental observables. This approach not only yields quantitative scattering predictions but also offers detailed insight into the underlying molecular structures governing these complex systems.

Keywords:

Polyoxometalates, Keggin ions, Superchaotropy, Water-Alcohol Mixtures, Molecular Dynamics Simulation, Scattering, Colloids



Solution of keggion ions and sodium ions in water and benzyl alcohol. Blue: $[\text{PW}_{12}\text{O}_{40}]^{3-}$, Red: Na^+ , Orange: Benzyl Alcohol, Purple lines: Water.

References:

[1] Dullinger, P., & Horinek, D. (2023). Solvation of nanoions in aqueous solutions. *Journal of the American Chemical Society*, 145(45), 24922-24930.