

X-ray Raman scattering study of hydrothermal fluids: The case of aqueous sodium chloride solutions

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Aqueous solutions play a key role in many natural and industrial processes. Particularly, hydrothermal fluids (i.e. hot aqueous fluids with dissolved electrolytes, silica, CO₂, or other solutes) are essential in mass and energy transfer in the Earth's crust and upper mantle, which happens predominantly in subduction zones [1]. These fluids cause the formation of most ore deposits. The system H₂O + NaCl is of special interest in geosciences as NaCl is long known to be the major solute in aqueous fluids in Earth's crust [2].

Interestingly, the effect of electrolytes on the water structure at sub- and supercritical conditions has only been investigated for a handful of chemical compounds. The role of additional protons and hydroxide ions in aqueous solution is still debated [3,4] and the spatial extend of the ion's influence on the local water structure is controversially discussed [5]. In order to reveal the microscopic structure of this fascinating liquid and to investigate the influence of the alkali halide on the hydrogen bond network up to the supercritical regime, we present an in situ x-ray Raman scattering study of aqueous sodium chloride solutions at high pressure and high temperature. Probing the oxygen K-edge of the salt solution yields unique information about the oxygen's local coordination around the ions, e.g. solvation-shell structure and ion pairing. Using x-ray Raman scattering in combination with yet to perform ab initio modelling of the liquid's molecular structure we aim to constrain the structural effects of sodium chloride on the hydrogen-bond network providing unique understanding of NaCl solvation in hot aqueous fluids.

References

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