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Title: High Temperature Aqueous Solvent Effect on Stretching Vibrations of the Hydroxyl Radical – MD Simulation Study of Spectral Shifts and Hydrogen Bond Statistics

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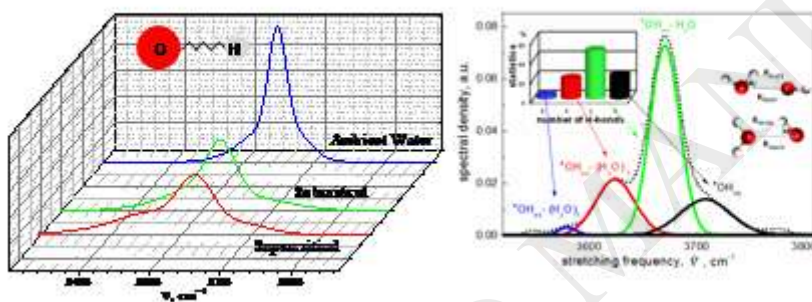
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High Temperature Aqueous Solvent Effect on Stretching Vibrations of the Hydroxyl Radical – MD Simulation Study of Spectral Shifts and Hydrogen Bond Statistics

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Graphical abstract



Highlights

- Power spectrum of $^{\bullet}\text{OH}_{\text{aq}}$ stretching vibrations computed vs temperature and density.
- Decomposition to components assigned to H-bonded complexes $^{\bullet}\text{OH}_{\text{aq}} - (\text{H}_2\text{O})_{\text{nHB}=0,1,2,3}$.
- Hydrogen-bond network effect on fundamental frequencies of band-components shown.
- Statistics of $^{\bullet}\text{OH}$ -water H-bonds assessed from partial area of band-components.

Abstract

The effect of water temperature and density on stretching vibrations power spectrum of $^{\bullet}\text{OH}_{\text{aq}}$ was studied from ambient to supercritical conditions by molecular dynamics

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