

# Study of the Hydrogen Bond Network in sub- and supercritical Water by Molecular Dynamics Simulations

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For 12 points along the tangent to the saturation curve at the critical point the temperature dependencies of the heights of the first maximum in the O–O RDF, the average number of hydrogen bonds, and the self-diffusion coefficients have been calculated from MD simulations. The curves of these three properties show an inflection near the critical point. To improve the understanding of these changes in going from subcritical to supercritical water the librational spectra and the change in the fractions of water molecules with a given number of hydrogen bonds as a function of temperature have been derived from the simulations, additionally.

*Key words:* Super Critical Water; Molecular Dynamics.