

Correction to On the Effects of Temperature, Pressure and Dissolved Salts on the Hydrogen-bond Network of Water

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A small error was found in the program used to analyze the transient broken H-bonds of liquid water, which influenced the H-bond lifetimes presented in Figure 4 for $t^* = 0.1$ ps and t^{**}

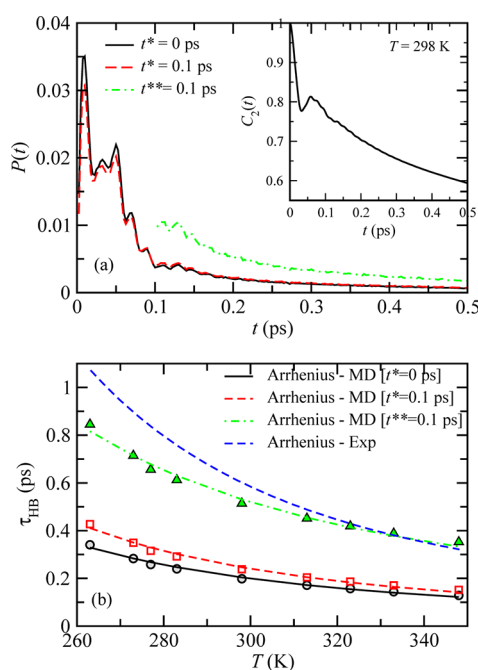


Figure 4. (a) Effect of transient broken H-bonds and transient H-bonds on the H-bond lifetime distribution for neat water at 298 K. The inset shows the first 0.5 ps of the orientational autocorrelation function of AMOEBA water. (b) MD and experimental H-bond lifetimes for neat water at different temperatures. The Arrhenius equation parameters $[A, E_A]$ for the tolerance time, $t^* = 0.1$ ps and $t^{**} = 0.1$ ps are [0.0053 ps, 9.5 kJ/mol] and [0.021 ps, 8.0 kJ/mol], respectively.

$= 0.1$ ps. This error prevented correctly probing every possible H-bond acceptor switching event during a broken H-bond transience period, $t^* = 0.1$ ps. Thus, H-bond lifetimes at the different T 's reported in Figure 4b of the original manuscript are larger by 20–25% than they actually should be when both transient broken H-bonds and transient H-bonds are excluded. Accordingly, a better and worst agreement with experimental depolarized light scattering data is found at high and low temperatures, respectively; the corresponding activation energies are, nevertheless, almost unchanged. This error does not affect any of the other results or conclusions presented in the manuscript. A corrected Figure 4 is given here.

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