Electronic Supplementary Material (ESI) for Environmental Science: Atmospheres.

Supporting Information: Lifetimes of pre-reactive complexes of peroxy radicals revisited: Thermostat effects, temperature dependence and highly oxygenated molecules

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Comparison between old and new fits of τ_L versus k_{expt}

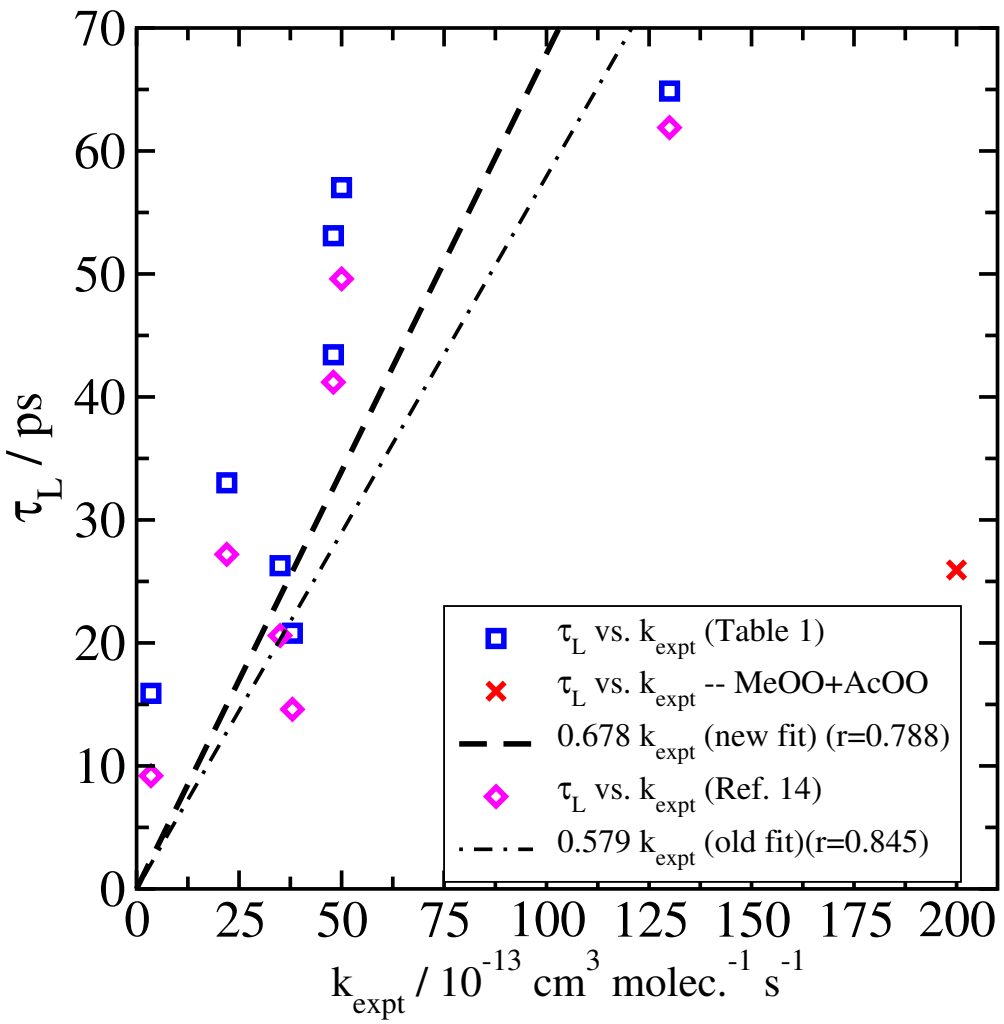

Figure S1: Comparison of the correlation between τ_L and k_{expt} determined in our previous work (Ref. 14 in the main paper, magenta diamonds and dash-dotted line) where the equilibration was done with the Nosé-Hoover thermostat, and the current work (blue squares and dashed line) using the Langevin thermostat.

Association time histograms at varying temperatures

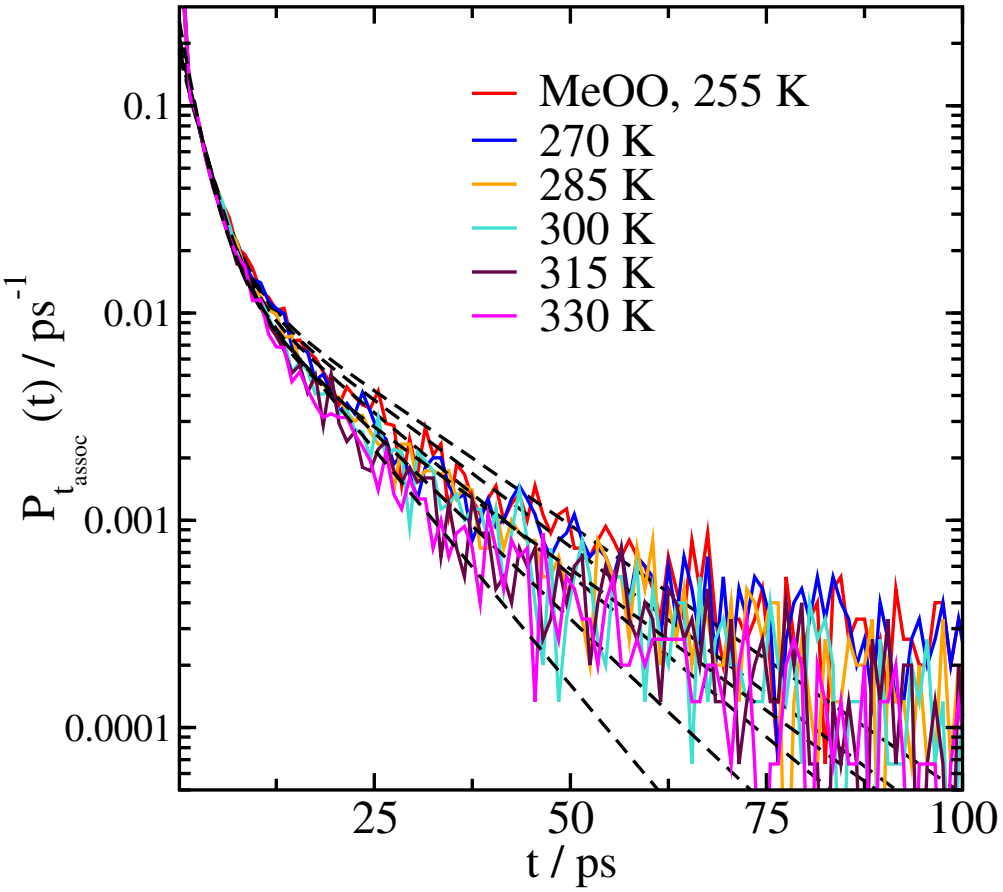

Figure S2: Association time histograms for complexes of two MeOO at different temperatures, and fits to Equation 2 (dashed lines).

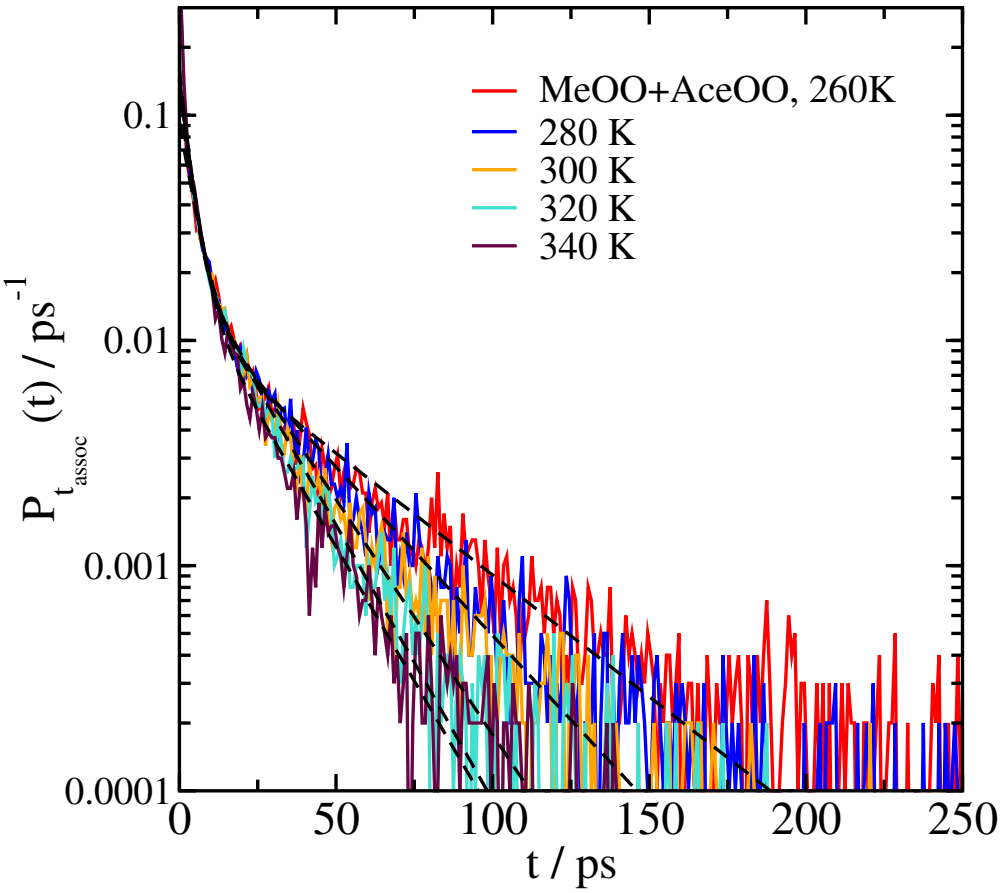

Figure S3: Association time histograms for AceOO + MeOO complexes at different temperatures, and fits to Equation 2 (dashed lines).

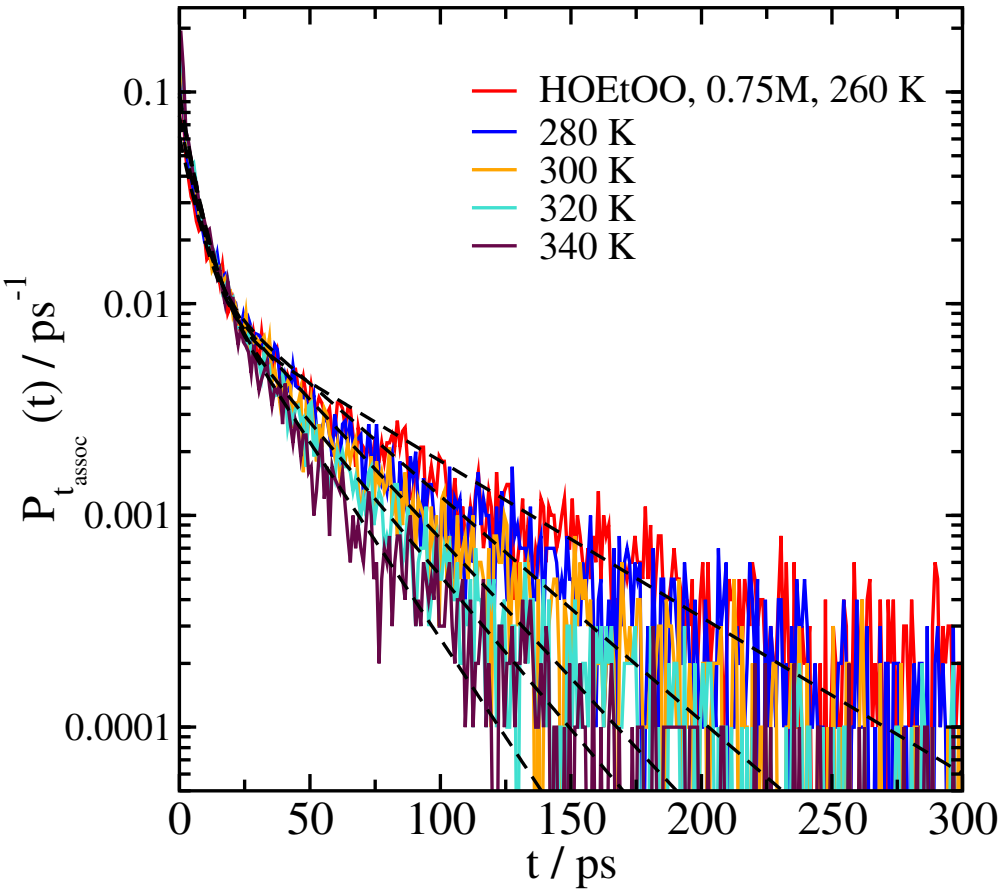

Figure S4: Association time histograms for complexes of two HOEtOO at different temperatures, and fits to Equation 2 (dashed lines).

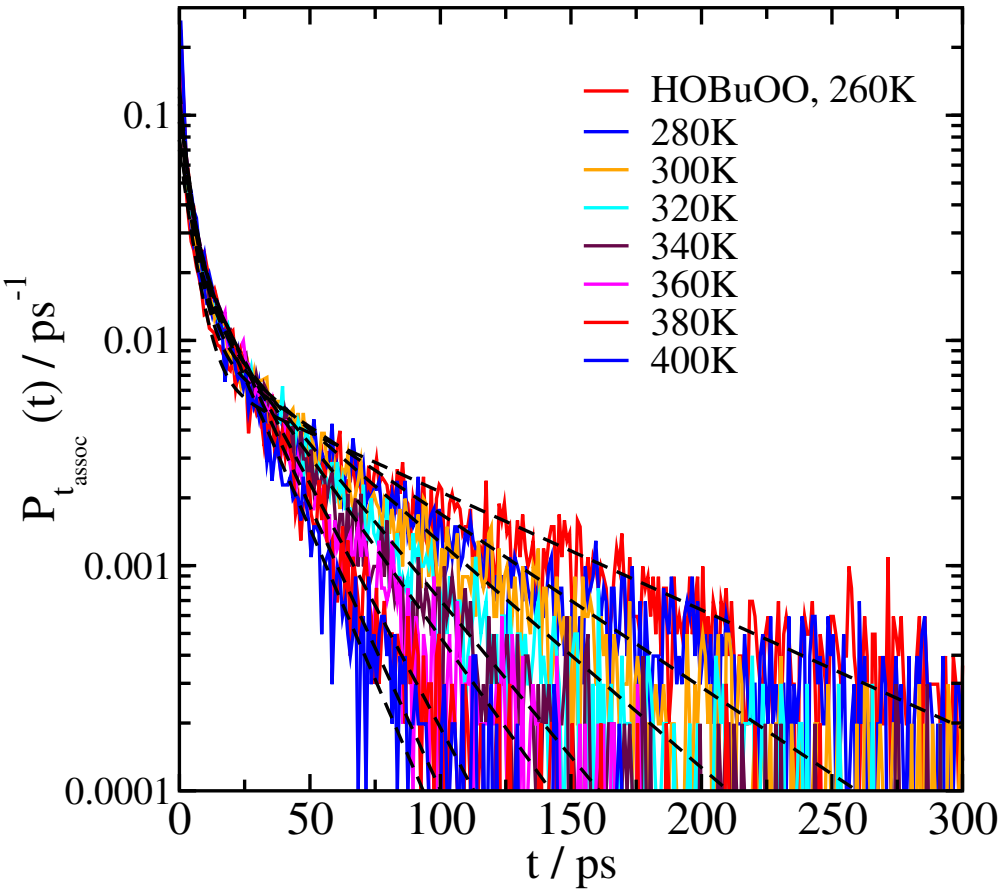

Figure S5: Association time histograms for complexes of two HOBuOO at different temperatures, and fits to Equation 2 (dashed lines).

Input files for LAMMPS

We have attached two examples of LAMMPS 'input' and 'data' files which can be used to initiate a single collision trajectory. Different collision trajectories can be generated by randomly changing the relative orientations of the molecules as well as changing the random number seeds for the initial velocity generation and the random friction force in the Langevin thermostat used during the equilibration phase.