

1 Proton Jump Rate Determination

Figure 1: Excess proton jump rate. Top: Semilogarithmic plot. Bottom: Linear plot. Small error bars signify a higher number of sampled Oxygen-Hydronium distances and therefore a higher confidence of the jump rate value.



Figure 2: Comparison of excess proton jump rates at 300 K, 350 K and 400 K.

Table 1: Resulting jump rate fit parameters from the $ab\mathchar`initio$ trajectory at 400 K

Parameter	Value	Unit
a	55 ± 6	$\rm ps^{-1}$
d_0	2.415 ± 0.009	Å
c	4.5 ± 0.3	10^{-2}\AA

2 Linear Distance Rescaling in Time



Figure 3: Illustrative example of the distance rescaling within the LMC scheme. Dashed line: Oxygen–Oxygen distance obtained from the MD trajectory. Dash-dotted line: Rescaled Oxygen–Oxygen distance using a conversion function.

Solid line: Relaxing Oxygen–Oxygen distance, which is obtained by interpolating linearly between the beforementioned distances.

For this picture a relaxation time of 0.4 ps was chosen.