

**Supporting Information for: Extending Timescale of Molecular Simulations by Using
Time-Temperature Superposition: Rheology of Ionic Liquids**

Adegbola Balogun¹, Daria Lazarenko², Fardin Khabaz^{2, 3*}, and Rajesh Khare^{1*}

¹Department of Chemical Engineering, Texas Tech University,
Lubbock, TX 79409

²School of Polymer Science and Polymer Engineering, The University of Akron,
Akron, OH 44325

³Department of Chemical, Biomolecular, and Corrosion Engineering, University of Akron,
Akron, OH 44325

*Corresponding authors email: fardin.khabaz@uakron.edu and rajesh.khare@ttu.edu

Table of Contents

Table S1: Simulation run information of the steady shear for viscosity calculation

Table S2: Simulation run information of the oscillatory shear for moduli calculation

Table S3: Zero shear viscosity at different temperatures

Figure S1: Master curve of the phase angle values

Figure S2: Master curve of the moduli data using the same shift factors obtained from the MSD master curves

Table S1: Simulation run information of the steady shear for viscosity calculation.

Shear rate, $\dot{\gamma}$ (s^{-1})	Simulation run time (ns)
5×10^6	40
7×10^6	40
1×10^7	40
1.5×10^7	40
2.5×10^7	10
5×10^7	10
1×10^8	10
2.5×10^8	10
1×10^9	10
1×10^{10}	10
5×10^{10}	10
1×10^{11}	10

Table S2: Simulation run information of the oscillatory shear for moduli calculation.

Frequency, ω (rad s^{-1})	Number of oscillations	simulation run time (ns)
2×10^9	24	72
5×10^9	70	84
1×10^{10}	120	72
2×10^{10}	120	36
5×10^{10}	120	14.4
1×10^{11}	120	7.2

Table S3: Zero shear viscosity at different temperatures

Temperature (K)	Zero shear viscosity, η_o (Pa s)
300	0.7729 ± 0.0428
340	0.0720 ± 0.0014
380	0.0171 ± 0.0004
420	0.0070 ± 0.0008
460	0.0038 ± 0.0004

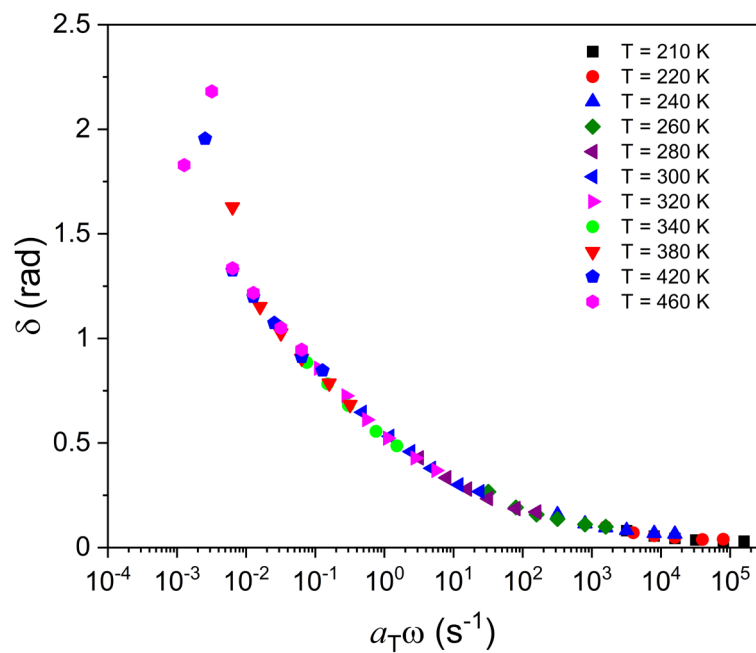


Fig. S1 Master curve of phase angle as a function of the rescaled frequency constructed at a reference temperature of 300 K.

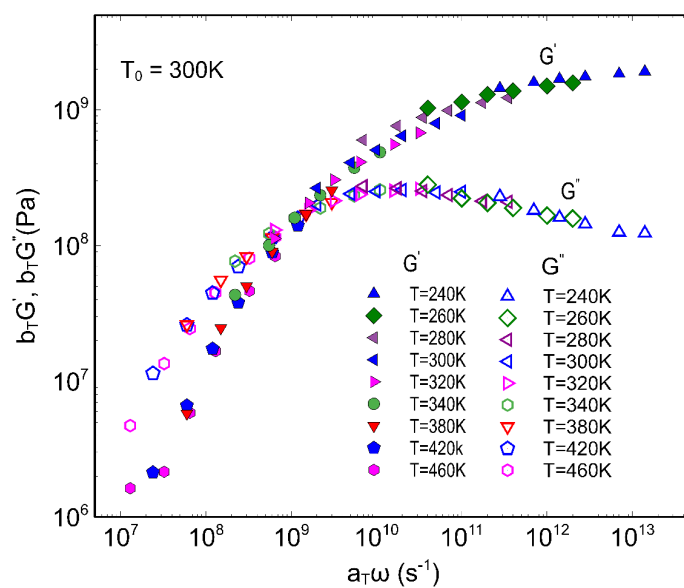


Fig. S2 Master curve of the moduli data using the same shift factors obtained from the MSD master curves at a reference temperature of 300 K.