

Electronic Supplementary Information for:
Assessing the Reliability of Computing Ion Pair Lifetimes and
Diffusivity to Predict Experimental Viscosity Trends of Ionic
Liquids

Michael T. Humbert, Yong Zhang, Edward J. Maginn

Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre
Dame, Indiana 46556, United States

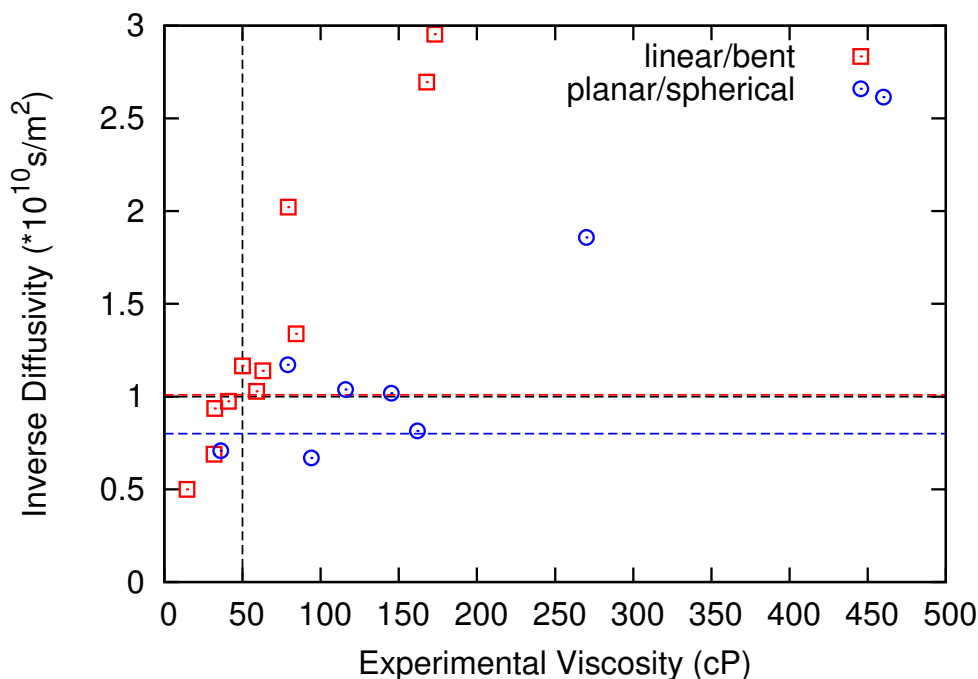


Figure S1: Inverse self-diffusivity vs experimental viscosities for selected ILs. Dashed lines represent various cutoffs used in predictions. The uncertainty estimates were smaller than the symbol size and thus excluded for clarity. Diffusivities were corrected for system size effects using viscosities obtained from a Vogel-Fulcher-Tammann fitting of experimental viscosities

Table S1: All experimental(298 K) and computed (400 K) data used in the analysis. Viscosities have units of cP, ion pair lifetimes have units of ps and diffusivities have units of $\text{*}10^{-11} \text{ m}^2/\text{s}$. Empty Cells represent ionic liquids without Vogel-Fulcher-Tammann parameters so system size corrections were not possible

Ion Pair	Experimental Viscosity	Ion Pair Lifetime	Diffusivity (uncorrected)	Diffusivity (Corrected)	Group
[C4C1IM] [NTF2]	50 ¹	699 \pm 8	4.7 \pm 0.9	8.5 \pm 0.9	Linear/Branched
[C2C1IM] [NTF2]	32.2 ²	488 \pm 7	6.3 \pm 2.0	10.7 \pm 2.0	Linear/Branched
[C4C1PYR] [NTF2]	79.3 ³	1597 \pm 72	2.0 \pm 0.4	4.9 \pm 0.4	Linear/Branched
[C4C1PY] [NTF2]	63 ⁴	678 \pm 35	5.4 \pm 1.1	8.8 \pm 1.1	Linear/Branched
[C4PY] [NTF2]	59.0 ⁵	604 \pm 6	5.9 \pm 1.5	9.7 \pm 4.5	Linear/Branched
[C4C1PIP] [NTF2]	173 ⁶	3146 \pm 335	0.9 \pm 0.2	3.4 \pm 0.2	Linear/Branched
[P2228] [NTF2]	129 ⁷	1793 \pm 197	2.3 \pm 0.2		Linear/Branched
[C4C1IM] [OTF]	84.3 ¹	706 \pm 29	4.3 \pm 1.1	7.5 \pm 1.1	Linear/Branched
[C2C1IM] [OTF]	41 ⁸	433 \pm 12	6.0 \pm 1.4	10.3 \pm 1.4	Linear/Branched
[C4C1PYR] [OTF]	167.8 ⁹	1636 \pm 31	1.3 \pm 0.2	3.7 \pm 0.2	Linear/Branched
[C4C1IM] [DCA]	31.8 ¹⁰	365 \pm 34	8.8 \pm 0.9	14.5 \pm 0.9	Linear/Branched
[C2C1IM] [DCA]	14.5 ¹¹	249 \pm 29	12.3 \pm 1.3	20.0 \pm 1.3	Linear/Branched
[P2224] [DCA]	60 ¹²	294 \pm 15	11.9 \pm 3.7		Linear/Branched
[P2228] [DCA]	104 ¹²	708 \pm 51	6.6 \pm 1.8		Linear/Branched
[C4C1IM] [PF6]	261 ¹³	852 \pm 109	3.1 \pm 0.8		Planar/Spherical
[C4C1IM] [BF4]	116 ¹³	496 \pm 48	6.0 \pm 1.0	9.6 \pm 1.0	Planar/Spherical
[C2C1IM] [BF4]	36.1 ¹¹	270 \pm 8	9.2 \pm 2.1	14.1 \pm 2.1	Planar/Spherical
[C4C1PY] [BF4]	166.7 ¹⁴	455 \pm 13	6.7 \pm 0.9		Planar/Spherical
[C4PY] [BF4]	145.2 ¹⁴	458 \pm 112	6.8 \pm 1.3	9.8 \pm 1.3	Planar/Spherical
[C4C1IM] [CNPYR]	162 ¹⁵	514 \pm 165	8.1 \pm 0.8	12.2 \pm 0.8	Planar/Spherical
[C2C1IM] [CNPYR]	94 ¹⁵	283 \pm 52	11.2 \pm 1.3	14.9 \pm 1.3	Planar/Spherical
[C4C1IM] [4TRIZ]	270 ¹⁵	980 \pm 47	2.7 \pm 0.3	5.4 \pm 0.3	Planar/Spherical
[C2C1IM] [4TRIZ]	79 ¹⁵	447 \pm 5	5.2 \pm 0.5	8.5 \pm 0.5	Planar/Spherical
[C4C1PYR] [4TRIZ]	460 ¹⁵	2099 \pm 163	1.1 \pm 0.1	3.8 \pm 0.1	Planar/Spherical

References

- [1] H. Tokuda, K. Hayamizu, K. Ishii, M. A. B. H. Susan and M. Watanabe, *Journal of Physical Chemistry B*, 2004, **108**, 16593–16600.
- [2] H. Tokuda, K. Hayamizu, K. Ishii, A. Bin, H. Susan and M. Watanabe, *The Journal of Physical Chemistry B*, 2005, **109**, 6103–6110.
- [3] G. McHale, C. Hardacre, R. Ge, N. Doy, R. W. K. Allen, J. M. MacInnes, M. R. Bown and M. I. Newton, *Analytical Chemistry*, 2008, **80**, 5806–5811.
- [4] J. M. Crosthwaite, M. J. Muldoon, J. K. Dixon, J. L. Anderson and J. F. Brennecke, *Journal of Chemical Thermodynamics*, 2005, **37**, 559–568.
- [5] H. Tokuda, K. Ishii, M. A. B. H. Susan, S. Tsuzuki, K. Hayamizu and M. Watanabe, *Journal of Physical Chemistry B*, 2006, **110**, 2833–2839.
- [6] M. L. P. Le, F. Alloin, P. Strobel, J. C. Leprêtre, L. Cointeaux and C. P. del Valle, *Ionics*, 2012, **18**, 817–827.
- [7] K. Tsunashima and M. Sugiya, *Electrochemistry Communications*, 2007, **9**, 2353–2358.
- [8] H. Rodríguez and J. Brennecke, *Journal of Chemical and Engineering Data*, 2006, **51**, 2145–2155.
- [9] F. M. Gaciño, T. Regueira, L. Lugo, M. J. P. Comuñas and J. Fernández, *Journal of Chemical and Engineering Data*, 2011, **56**, 4984–4999.
- [10] P. J. Carvalho, T. Regueira, L. M. N. B. F. Santos, J. Fernandez and J. A. P. Coutinho, *Journal of Chemical and Engineering Data*, 2010, **55**, 645–652.
- [11] C. Schreiner, S. Zugmann, R. Hartl and H. J. Gores, *Journal of Chemical and Engineering Data*, 2010, **55**, 1784–1788.
- [12] K. Tsunashima, S. Kodama, M. Sugiya and Y. Kunugi, *Electrochimica Acta*, 2010, **56**, 762–766.
- [13] W. Li, Z. Zhang, B. Han, S. Hu, Y. Xie and G. Yang, *The Journal of Physical Chemistry B*, 2007, **111**, 6452–6456.
- [14] N. D. Khupse and A. Kumar, *Journal of Solution Chemistry*, 2009, **38**, 589–600.
- [15] C. Shi, A. DeSilva, M. Guzman and J. F. Brennecke, *ECS Transactions*, 2012, **50**, 309.