Properties of Imidazolium Ionic Liquids Bearing both Benzylic and *n*-Alkyl Substituents

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Reports of imidazolium ionic liquids (ILs) with at least one benzylic substituent bound to the imidazolium cation are far less common than the ubiquitous 1-alkyl-3-methylimidazolium ILs ([$C_n$mim][X]). Yet, considerable motivation exists to study structure−property relationships for imidazolium-based ILs with at least one benzylic substituent.[1] Not only are these ILs just as straightforward to synthesize as [$C_n$mim][X] ILs, but ILs with benzylic substituents are also representative segments of poly(ILs) and ionenes where imidazolium cations with benzylic groups are commonly found. For the studied series, we found published data in the IUPAC database *ILThermo*[2] for just one of six ILs. This presentation focuses on the influence of benzyl and methylbenzyl substituents on measured specific density and dynamic viscosity of a series of imidazolium cations paired with bis[(trifluoromethyl)sulfonyl]imide (commonly known as bistriflimide) ([Tf_2N]−) anions. Furthermore, the solubility of CO_2 in 1-benzyl-3-methylimidazolium bistriflimide [Bnmim][Tf_2N] (CASRN: 433337-24-7) was measured along isotherms at (303.15, 318.15, 333.15, and 348.15) K and at pressures in the range of (1 to 9) bar.

References

[1] Bara, J. E. Finotello, A., Magee, J. W., Qian, S., O'Harra, K. E., Dennis, G. P. and Noble, R. D., "110th Anniversary: Properties of Imidazolium-based Ionic Liquids Bearing both Benzylic and n-Alkyl Substituents," Ind. Eng. Chem. Res. 58, 17956-17964 (2019) [DOI: 10.1021/acs.iecr.9b03159].

[2] Kazakov, A. F., Magee, J. W., Chirico, R. D., Diky, V., Kroenlein, K. G., Muzny, C. D. and Frenkel, M., "Ionic Liquids Database – ILThermo (v2.0)" NIST Standard Reference Database 147, National Institute of Standards and Technology, Gaithersburg, MD (2013).