

Hydrogen-Bond Acidity of Ionic Liquids: an Extended Scale†

Kiki A. Kurnia^{1,2}, Filipa Lima¹, Ana Filipa M. Cláudio¹, João A. P. Coutinho¹ and Mara G. Freire^{1,*}

¹CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.

²Center of Research in Ionic Liquids, Department of Chemical Engineering, Universiti Teknologi PETRONAS, Tronoh 31750, Malaysia.

Electronic Supplementary Information

*Corresponding author: Tel: +351-234-370200; Fax: +351-234-370084; E-mail: maragfreire@ua.pt (M. G. Freire).

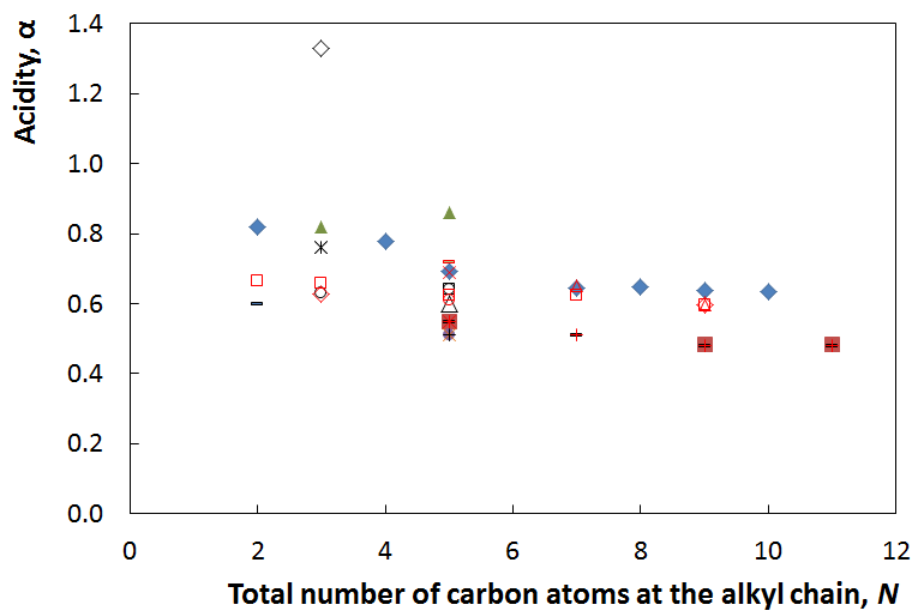


Figure S1. Comparison between experimental hydrogen-bond donating (α) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as a function of the total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [1]; (\blacktriangle), [2]; (\bullet), [3]; (\times), [4]; (+), [5]; (-), [6]; (\ast), [7]; (\diamond), [8]; (\square), [9]; (Δ), [10]; (\circ), [11]; (\times), [12]; (+), [13]; (-), [14]; (\ast), [15]; (\diamond), [16]; (\square), [17]; (Δ), [18]; (\circ), [19]; (\times), [20].

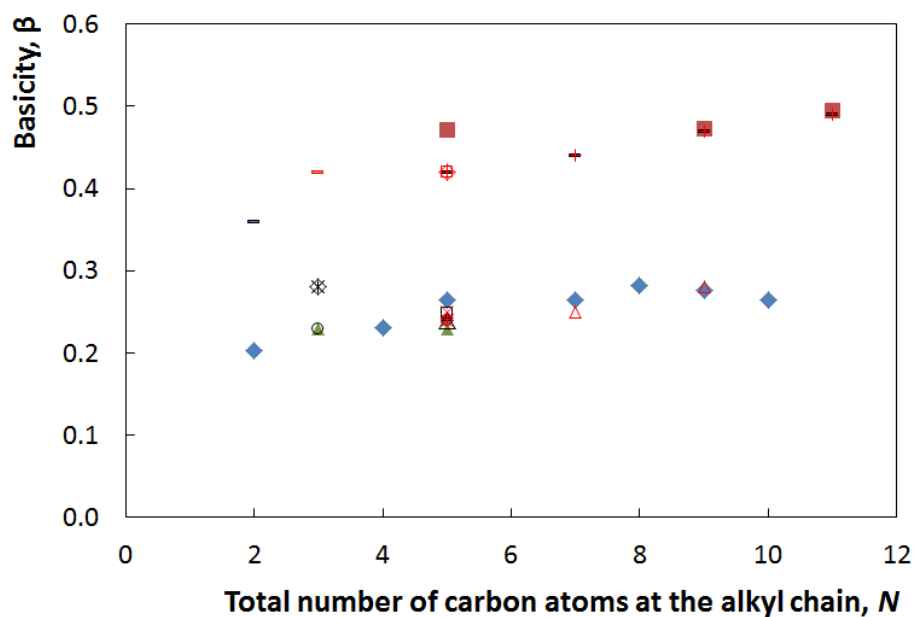


Figure S2. Comparison between experimental hydrogen-bond accepting (β) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [1]; (\blacktriangle), [2]; (\bullet), [3]; (\times), [4]; (+), [5]; (-), [6]; (\ast), [7]; (\diamond), [8]; (\square), [9]; (Δ), [10]; (\circ), [11]; (\times), [12]; (+), [13]; (-), [21]; (\ast), [14]; (\diamond), [22]; (\square), [15]; (Δ), [18]; (\circ), [19]; (\times), [20].

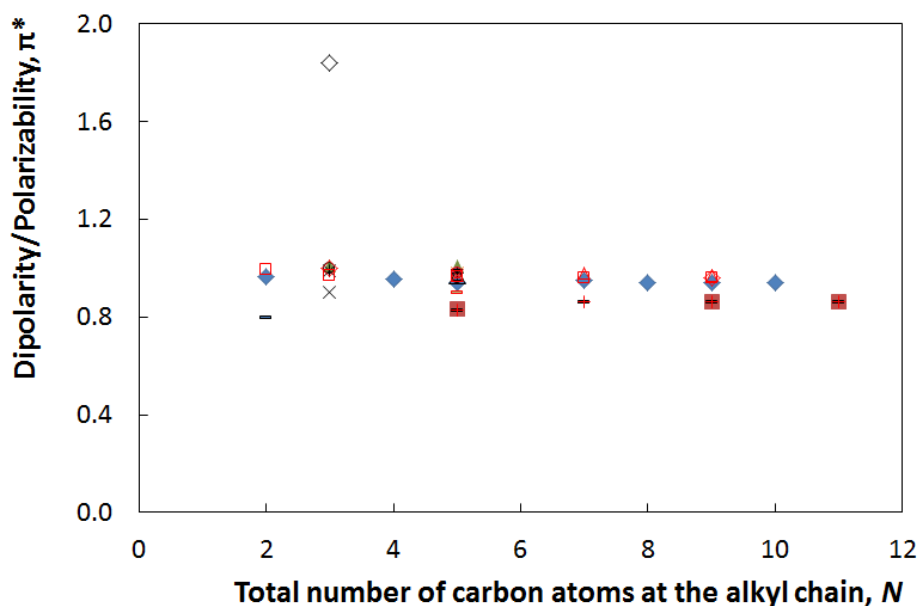


Figure S3. Comparison between experimental dipolarity/polarizability (π^*) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [1]; (\blacktriangle), [2]; (\bullet), [3]; (\times), [4]; (+), [5]; (-), [6]; (\ast), [7]; (\diamond), [8]; (\square), [9]; (Δ), [10]; (\circ), [11]; (\times), [12]; (+), [13]; (-), [14]; (\ast), [15]; (\diamond), [16]; (\square), [17]; (Δ), [18]; (\circ), [19]; (\times), [20].

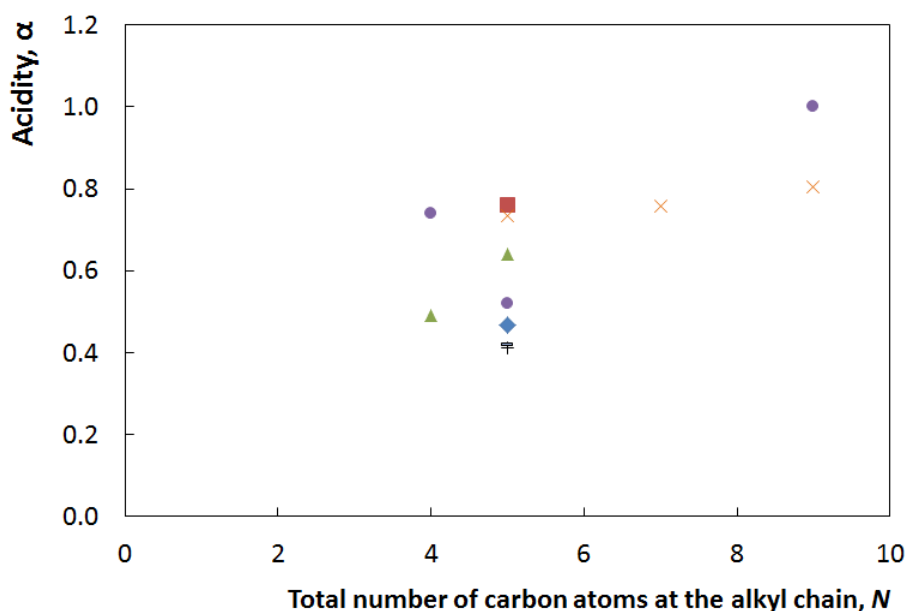


Figure S4. Comparison between experimental hydrogen-bond donating (α) values of 1-alkyl-1-methylpyrrolidinium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [2]; (\blacktriangle), [11]; (\bullet), [23]; (\times), [24]; (+), [17]; (-), [19].

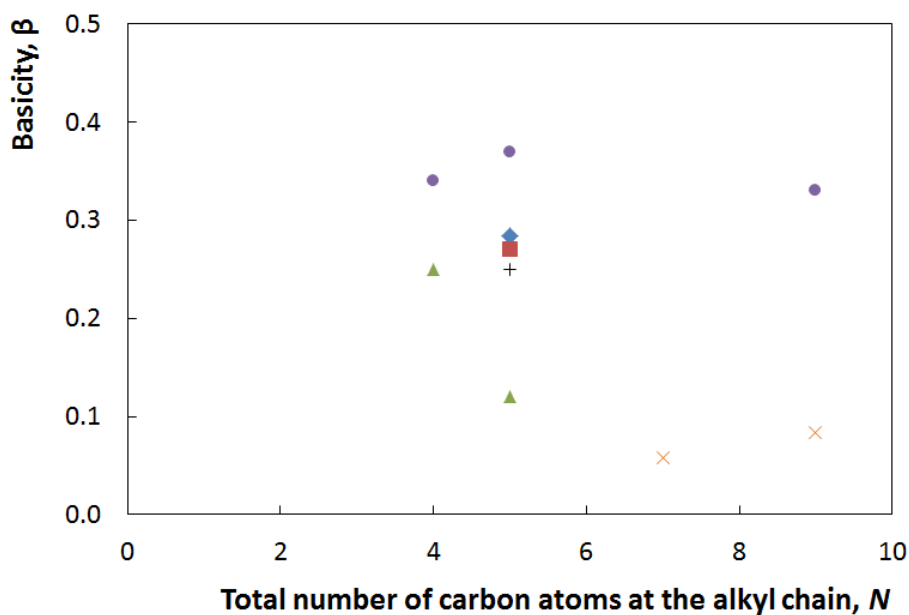


Figure S5. Comparison between experimental hydrogen-bond accepting (β) values of 1-alkyl-1-methylpyrrolidinium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [2]; (\blacktriangle), [11]; (\bullet), [23]; (\times), [24]; (+), [19].

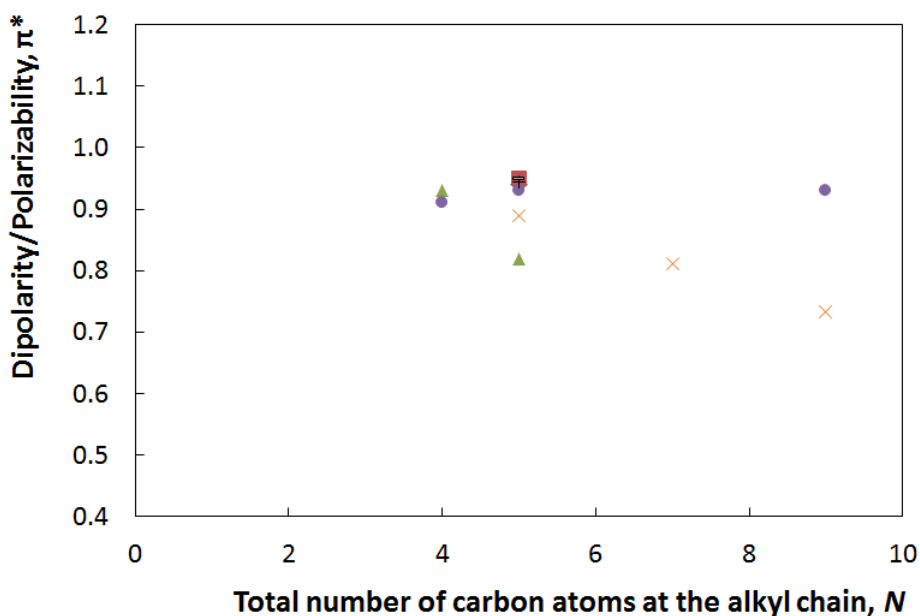


Figure S6. Comparison between experimental hydrogen-bond dipolarity/polarizability (π^*) values of 1-alkyl-1-methylpyrrolidinium-based ILs obtained in this work and in the literature as function of total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [2]; (\blacktriangle), [11]; (\bullet), [23]; (\times), [24]; (+), [17]; (-), [19].

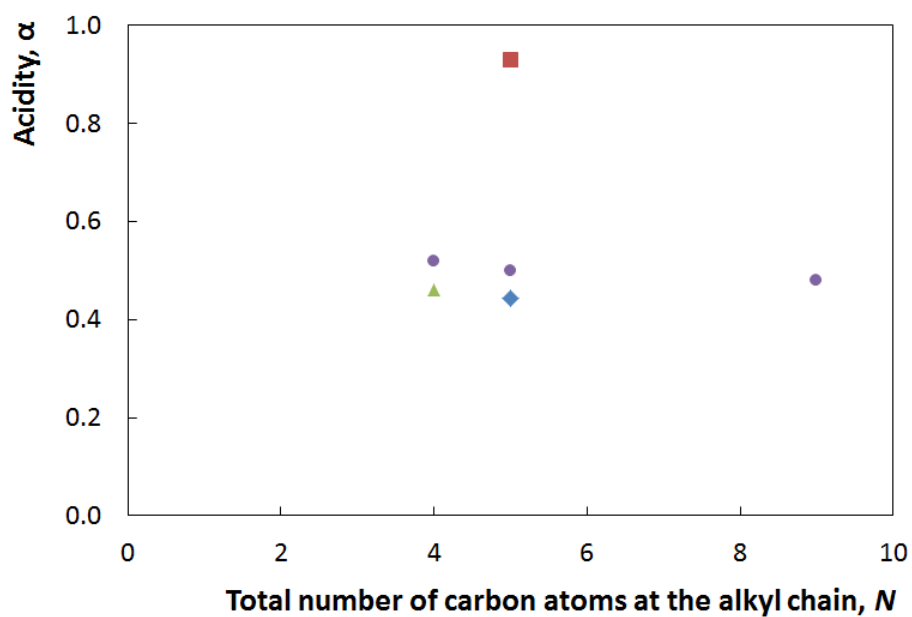


Figure S7. Comparison between experimental hydrogen-bond donating (α) values of 1-alkyl-1-methylpiperidinium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [2]; (\blacktriangle), [11]; (\bullet), [25].

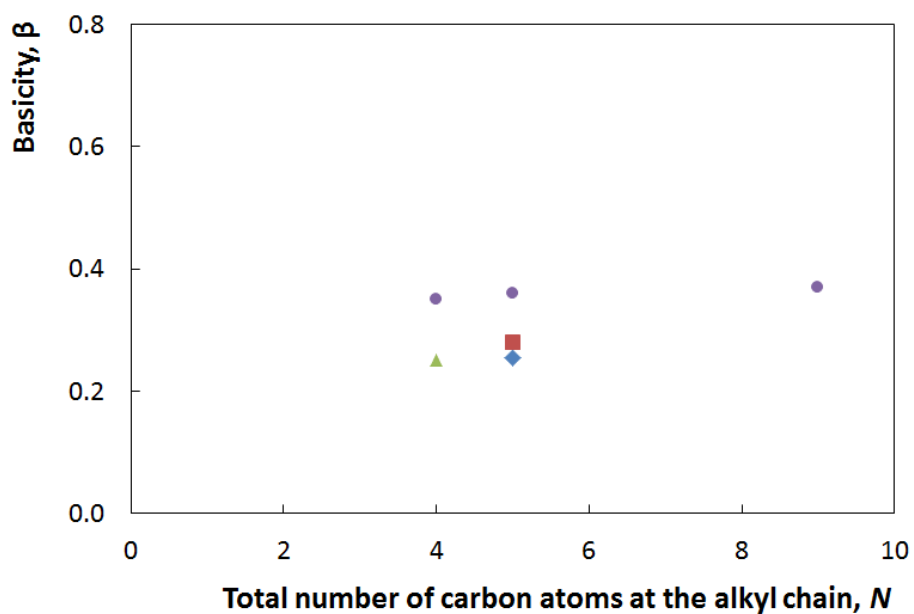


Figure S8. Comparison between experimental hydrogen-bond accepting (β) values of 1-alkyl-1-methylpiperidinium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [2]; (\blacktriangle), [11]; (\bullet), [25].

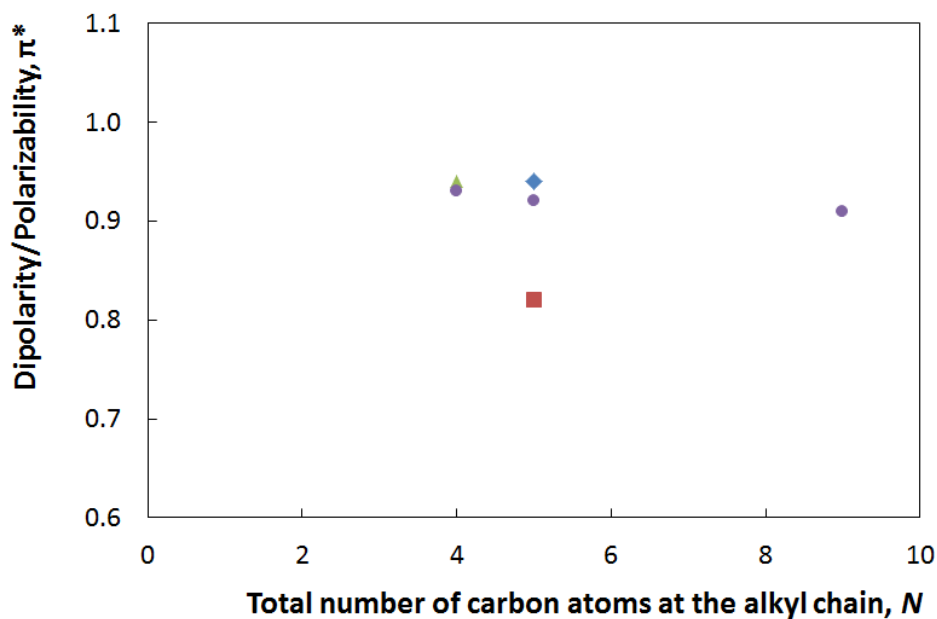


Figure S9. Comparison between experimental dipolarity/polarizability (π^*) values of 1-alkyl-1-methylpiperidinium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (◆), This work; (■), [2]; (▲), [11]; (●), [25].

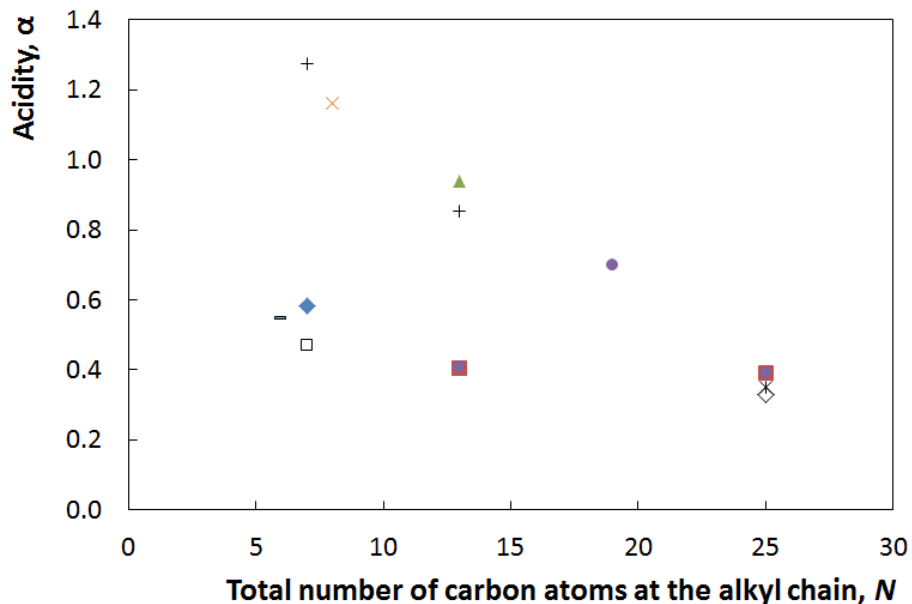


Figure S10. Comparison between experimental hydrogen-bond donating (α) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (◆), This work; (■), [1]; (▲), [2]; (●), [6]; (×), [10]; (+), [26]; (-), [11]; (*), [27]; (◇), [14]; (□), [17].

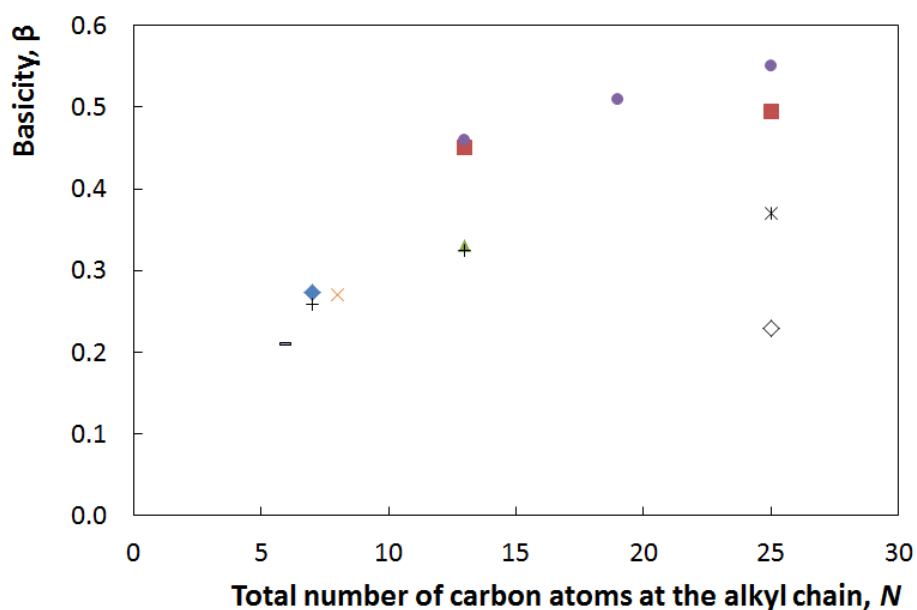


Figure S11. Comparison between experimental hydrogen-bond accepting (β) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [1]; (▲), [2]; (●), [6]; (×), [10]; (+), [26]; (-), [11]; (*), [27]; (◇), [14].

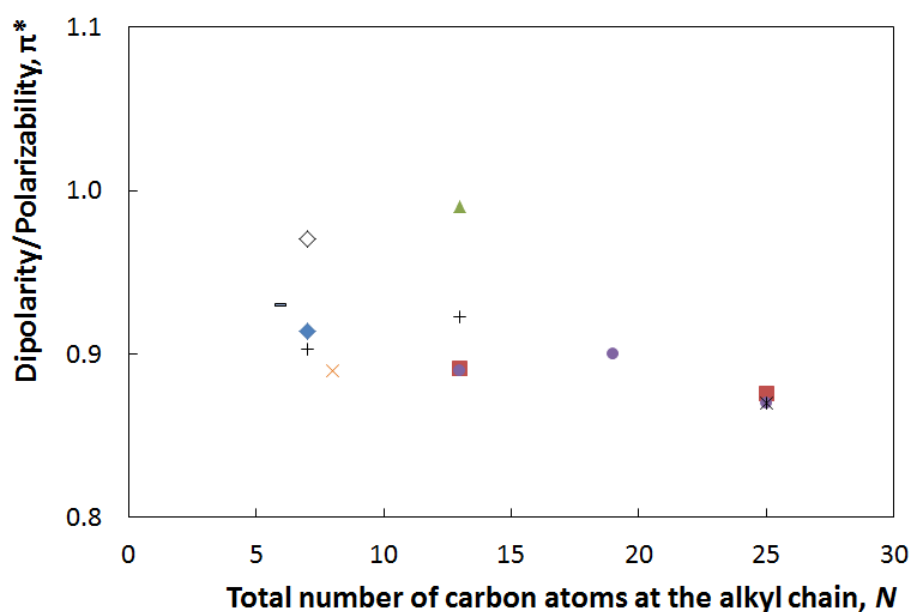


Figure S12. Comparison between experimental dipolarity/polarizability (π^*) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [1]; (▲), [2]; (●), [6]; (×), [10]; (+), [26]; (-), [11]; (*), [14]; (◇), [17].

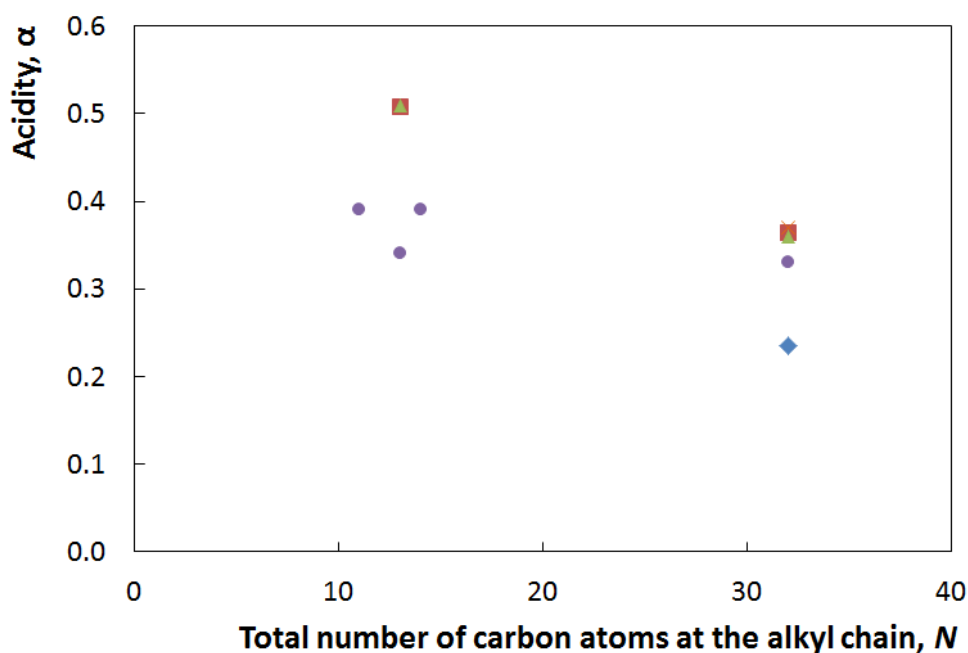


Figure S13. Comparison between experimental hydrogen-bond donating (α) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [1]; (\blacktriangle), [6]; (\bullet), [11]; (\times), [14].

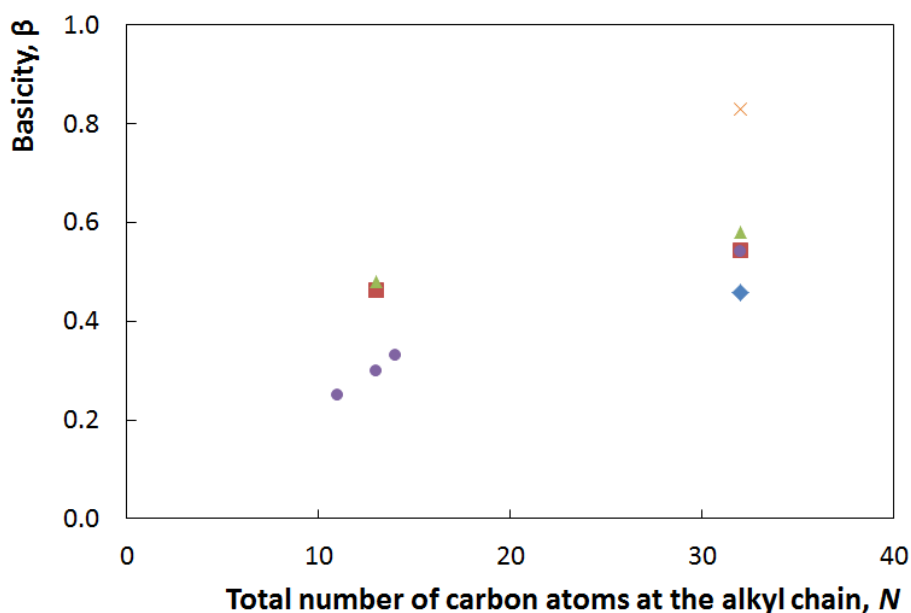


Figure S14. Comparison between experimental hydrogen-bond accepting (β) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [1]; (\blacktriangle), [6]; (\bullet), [11]; (\times), [14].

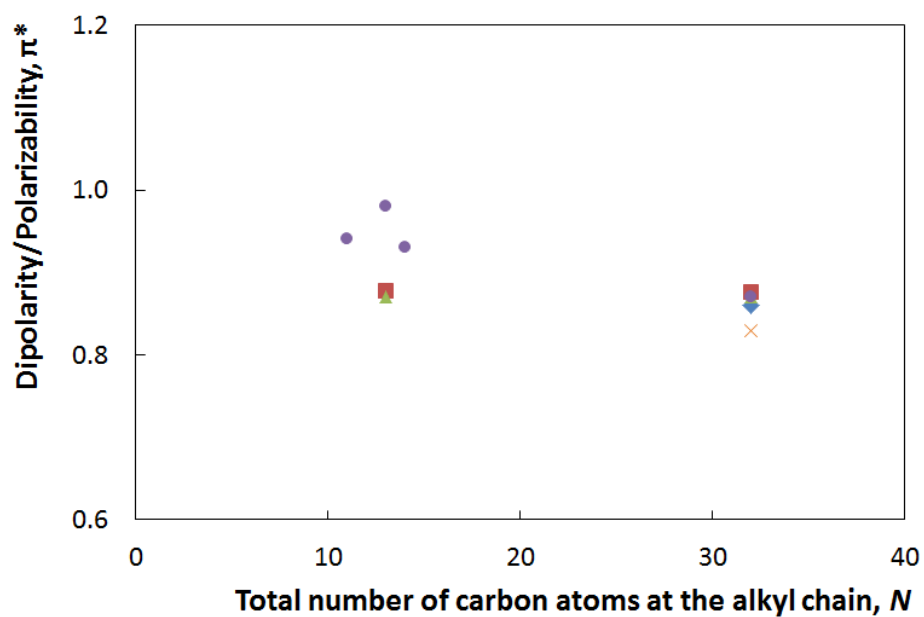


Figure S15. Comparison between experimental dipolarity/polarizability (π^*) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (\blacklozenge), This work; (\blacksquare), [1]; (\blacktriangle), [6]; (\bullet), [11]; (\times), [14].

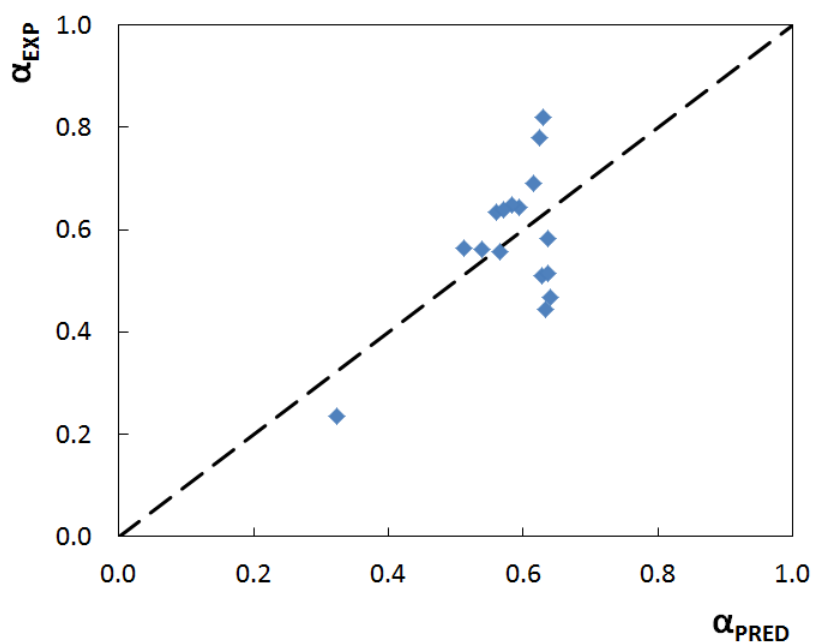


Figure S16. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 3.

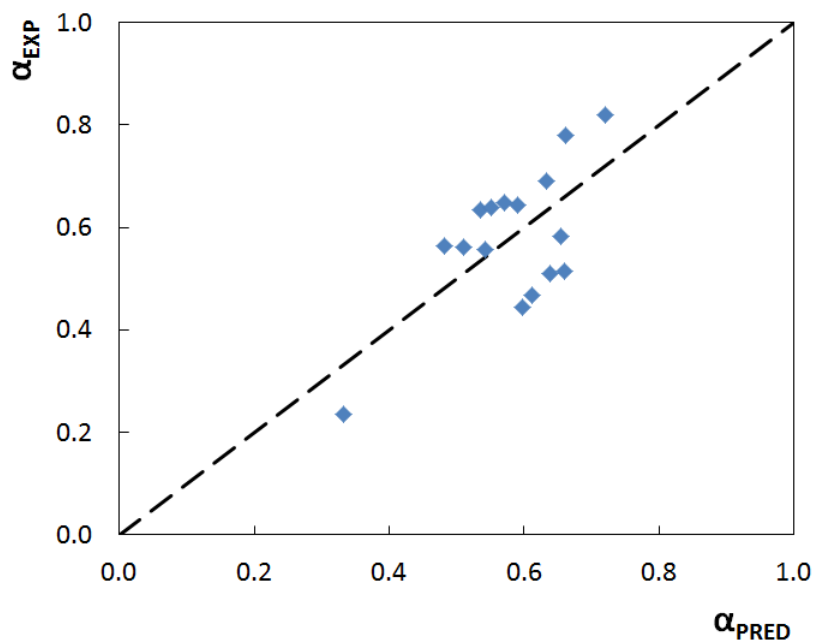


Figure S17. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 4.

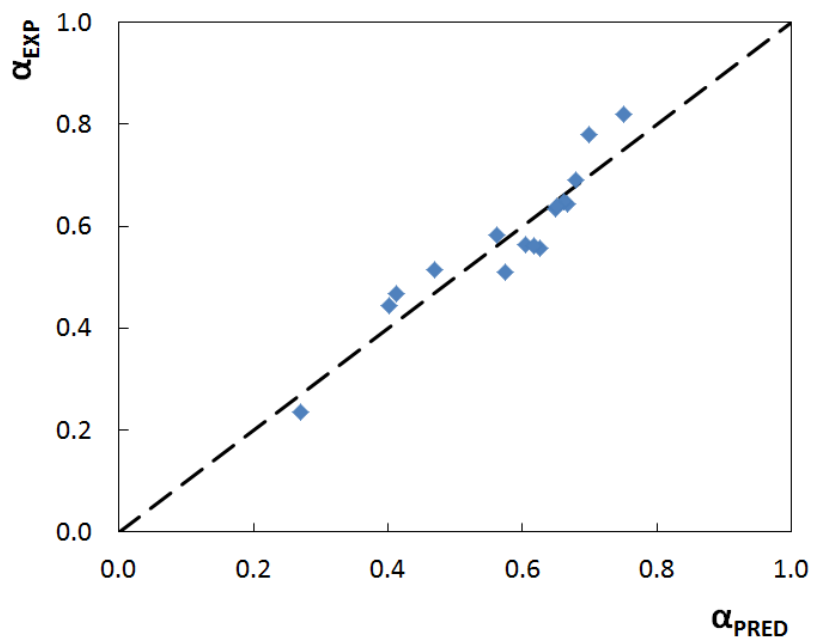


Figure S18. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 5.

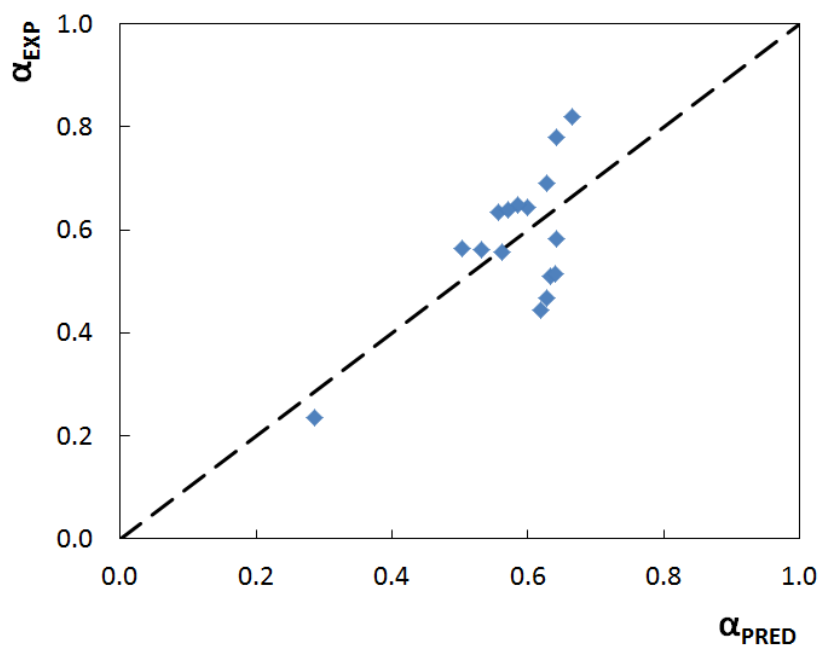


Figure S19. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 6.

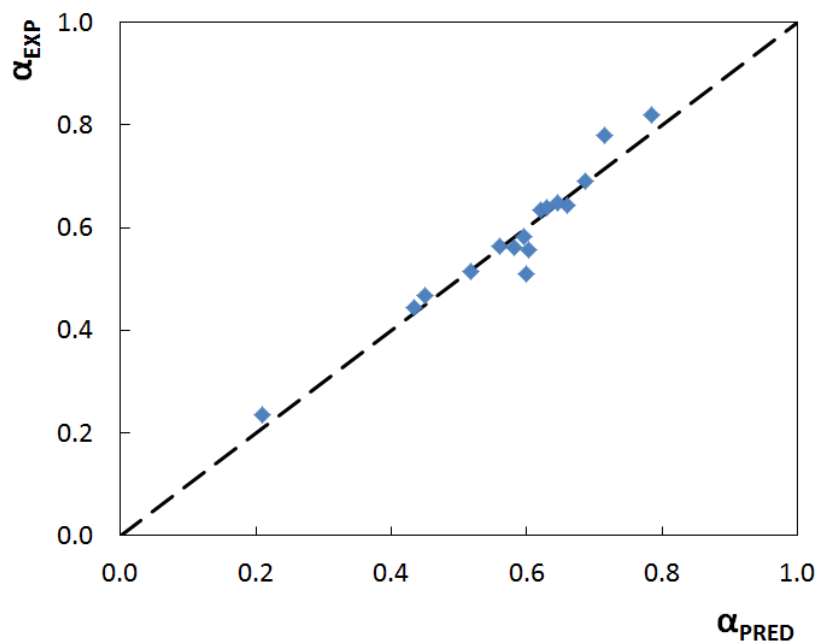


Figure S20. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 7.

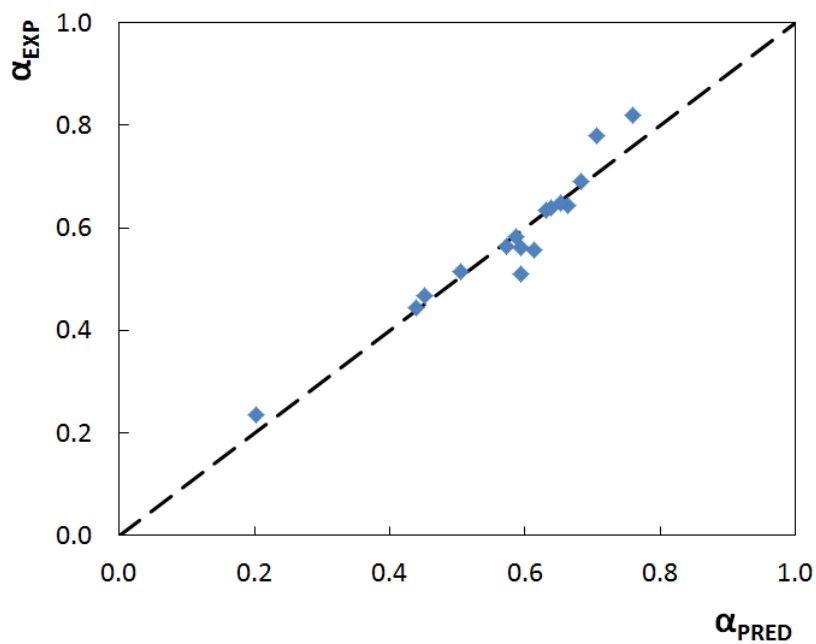


Figure S21. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 8.

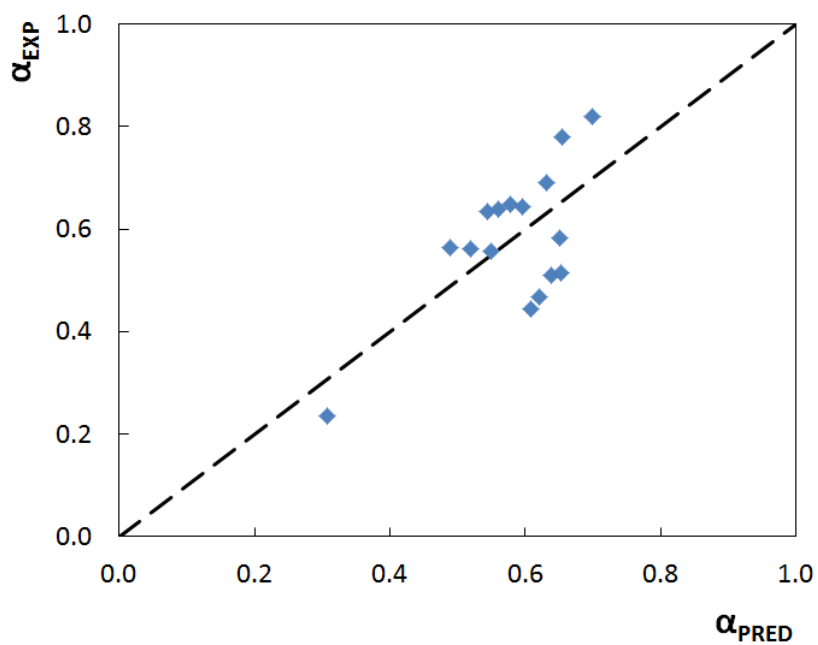


Figure S22. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 9.

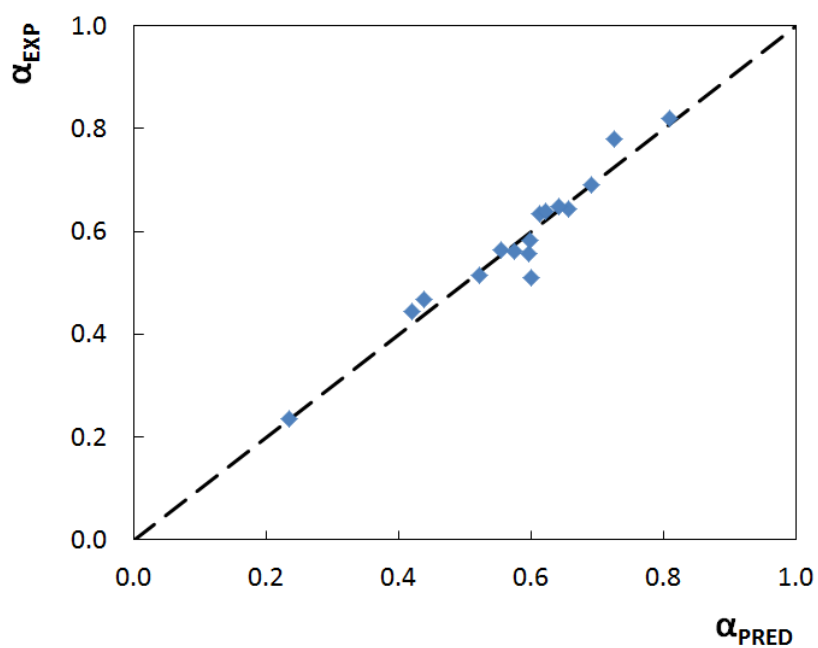


Figure S23. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 10.

The absolute average relative deviation, AARD, was calculated using Equation S1

$$AARD/\% = \frac{1}{N} \sum \frac{|\alpha_{EXP} - \alpha_{PRED}|}{\alpha_{EXP}} \times 100\% \quad (S1)$$

where, N is the number of data, α_{EXP} is the reported experimental data, α_{PRED} is the predicted value.

References

- [1] A. Schade, N. Behme, and S. Spange, *Chemistry - A European Journal* 20 (2014) 2232-2243.
- [2] R. Rai and S. Pandey, *J. Phys. Chem. B* 118 (2014) 11259-11270.
- [3] A. Ali, M. Ali, N. A. Malik, S. Uzair, and A. B. Khan, *Journal of Chemical and Engineering Data* 59 (2014) 1755-1765.
- [4] A. Ali, M. Ali, N. A. Malik, S. Uzair, and U. Farooq, *Fluid Phase Equilib.* 382 (2014) 31-41.
- [5] A. Ali, M. Ali, N. A. Malik, and S. Uzair, *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy* 121 (2014) 363-371.
- [6] S. Spange, R. Lungwitz, and A. Schade, *J. Mol. Liq.* 192 (2014) 137-143.
- [7] L. Kyllönen, A. Parviainen, S. Deb, M. Lawoko, M. Gorlov, I. Kilpeläinen, and A. W. T. King, *Green Chem.* 15 (2013) 2374-2378.
- [8] K. Fujita, D. Kobayashi, N. Nakamura, and H. Ohno, *Enzyme Microb. Technol* 52 (2013) 199-202.
- [9] C. Chiappe, A. Sanzone, D. Mendola, F. Castiglione, A. Famulari, G. Raos, and A. Mele, *J. Phys. Chem. B* 117 (2013) 668-676.
- [10] S. Zhang, Z. Chen, X. Qi, and Y. Deng, *New Journal of Chemistry* 36 (2012) 1043-1050.
- [11] A. Kobayashi, K. Osawa, M. Terazima, and Y. Kimura, *Phys. Chem. Chem. Phys.* 14 (2012) 13676-13683.
- [12] S. Zhang, X. Qi, X. Ma, L. Lu, and Y. Deng, *J. Phys. Chem. B* 114 (2010) 3912-3920.
- [13] V. Strehmel, R. Lungwitz, H. Rexhausen, and S. Spange, *New Journal of Chemistry* 34 (2010) 2125-2131.
- [14] S. Coleman, R. Byrne, S. Minkovska, and D. Diamond, *Phys. Chem. Chem. Phys.* 11 (2009) 5608-5614.
- [15] R. Lungwitz, M. Friedrich, W. Linert, and S. Spange, *New Journal of Chemistry* 32 (2008) 1493-1499.
- [16] R. Bini, C. Chiappe, V. L. Mestre, C. S. Pomelli, and T. Welton, *Organic and Biomolecular Chemistry* 6 (2008) 2522-2529.
- [17] H. Tokuda, S. Tsuzuki, M. A. B. H. Susan, K. Hayamizu, and M. Watanabe, *J. Phys. Chem. B* 110 (2006) 19593-19600.
- [18] B. R. Mellein, S. N. V. K. Aki, R. L. Ladewski, and J. F. Brennecke, *J. Phys. Chem. B* 111 (2006) 131-138.

- [19] L. Crowhurst, R. Falcone, N. L. Lancaster, V. Llopis-Mestre, and T. Welton, *Journal of Organic Chemistry* 71 (2006) 8847-8853.
- [20] C. P. Fredlake, M. J. Muldoon, S. N. V. K. Aki, T. Welton, and J. F. Brennecke, *Phys. Chem. Chem. Phys.* 6 (2004) 3280-3285.
- [21] P. Iiiner, S. Begel, S. Kern, R. Puchta, and R. Van Eldik, *Inorganic Chemistry* 48 (2009) 588-597.
- [22] R. Lungwitz and S. Spange, *New Journal of Chemistry* 32 (2008) 392-394.
- [23] J. M. Lee and J. M. Prausnitz, *Chem. Phys. Lett* 492 (2010) 55-59.
- [24] N. D. Khupse and A. Kumar, *J. Phys. Chem. B* 114 (2009) 376-381.
- [25] J.-M. Lee, *Chem. Eng. J.* 172 (2011) 1066-1071.
- [26] M. L. C. J. Moita, A. F. S. Santos, J. F. C. C. Silva, and I. M. S. Lampreia, *J. Chem. Eng. Data* 57 (2012) 2702-2709.
- [27] A. Jeličić, N. García, H.-G. Löhmansröben, and S. Beuermann, *Macromolecules* 42 (2009) 8801-8808.