Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

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Electronic Supplementary Information

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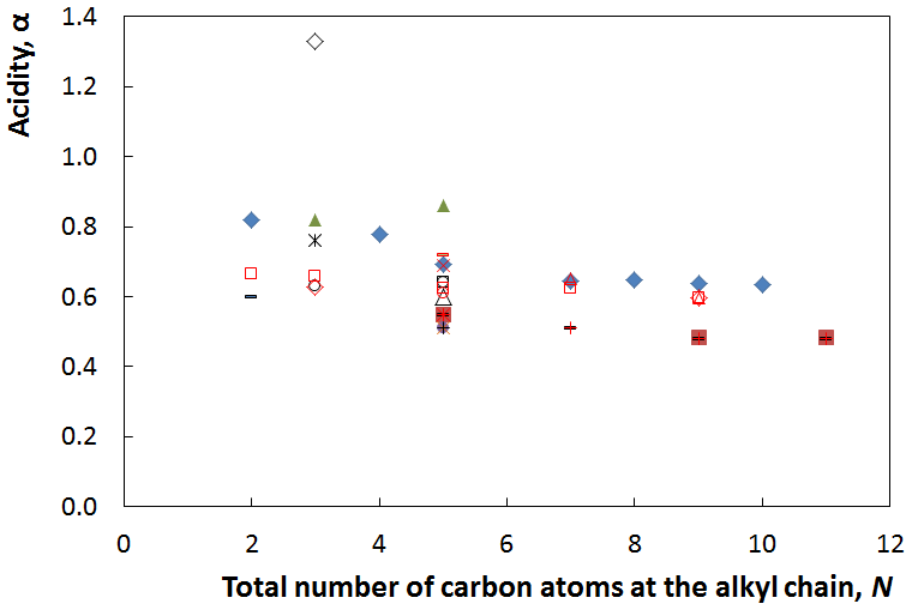

Figure S1. Comparison between experimental hydrogen-bond donating (α) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as a function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [1]; (▲), [2]; (●), [3]; (×), [4]; (+), [5]; (–), [6]; (∗), [7]; (◊), [8]; (□), [9]; (Δ), [10]; (○), [11]; (×), [12]; (+), [13]; (–), [14]; (∗). [15]; (◊), [16]; (□), [17]; (Δ), [18]; (○), [19]; (×), [20].

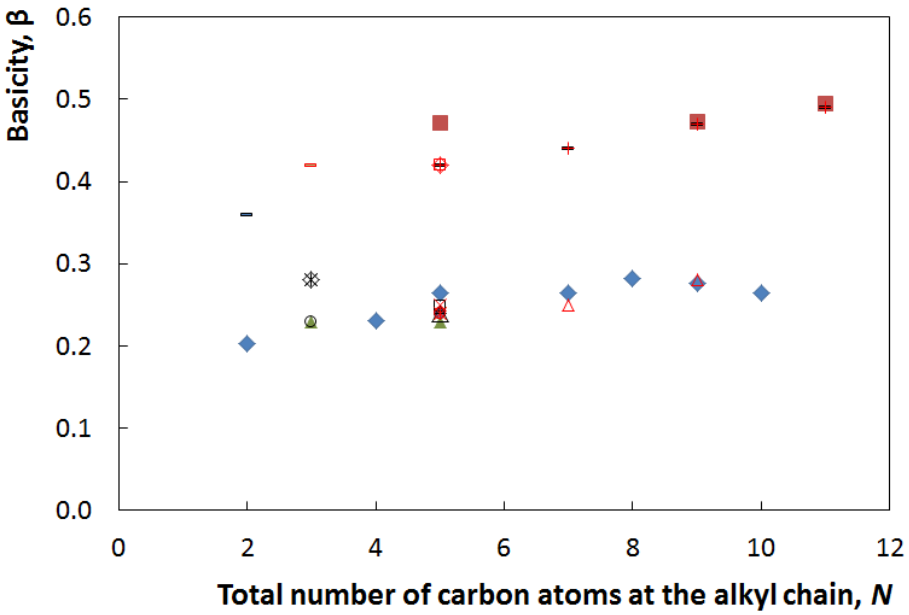

Figure S2. Comparison between experimental hydrogen-bond accepting (β) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [1]; (▲), [2]; (●), [3]; (×), [4]; (+), [5]; (–), [6]; (∗), [7]; (◊), [8]; (□), [9]; (Δ), [10]; (○), [11]; (×), [12]; (+), [13]; (–), [21]; (∗), [14]; (◊), [22]; (□), [15]; (Δ), [18]; (○), [19]; (×), [20].

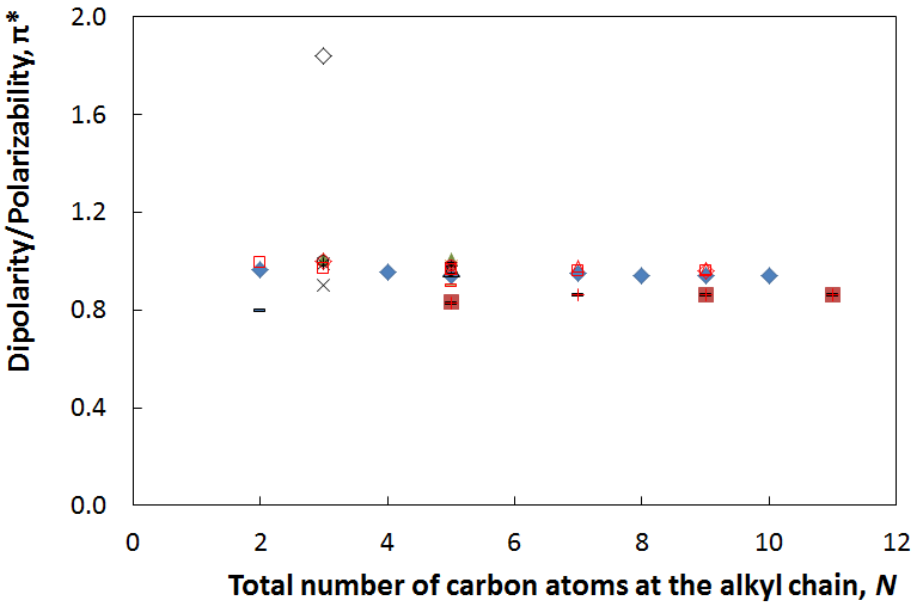

Figure S3. Comparison between experimental dipolarity/polarizability (π^*) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (*N*). Symbols: (♦), This work; (■), [1]; (▲), [2]; (●), [3]; (×), [4]; (+), [5]; (–), [6]; (∗), [7]; (◊), [8]; (□), [9]; (Δ), [10]; (○), [11]; (×), [12]; (+), [13]; (–), [14]; (∗). [15]; (◊), [16]; (□), [17]; (Δ), [18]; (○), [19]; (×), [20].

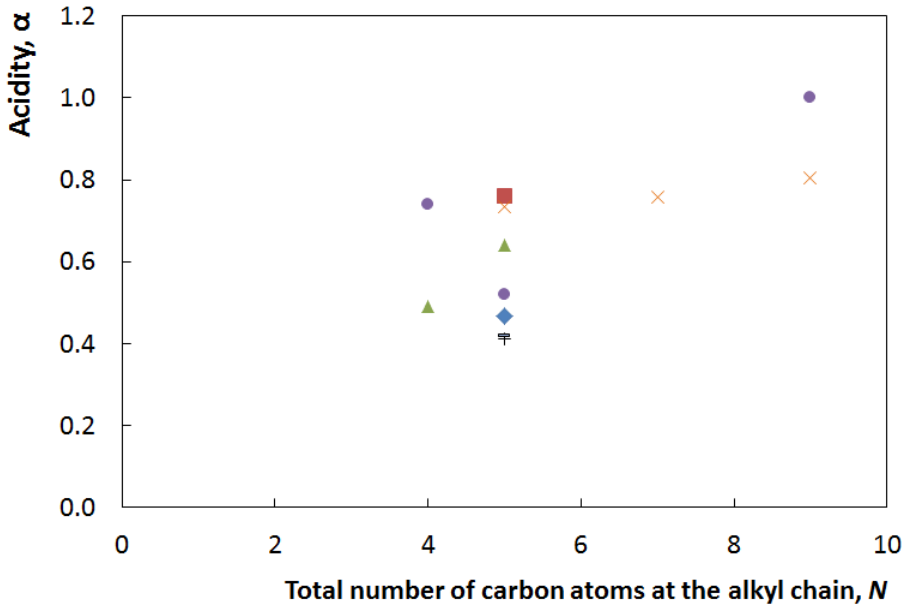

Figure S4. Comparison between experimental hydrogen-bond donating (α) values of 1-alkyl-1-methylpyrrolidinium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (*N*). Symbols: (♦), This work; (■), [2]; (▲), [11]; (●), [23]; (×), [24]; (+), [17]; (–), [19].

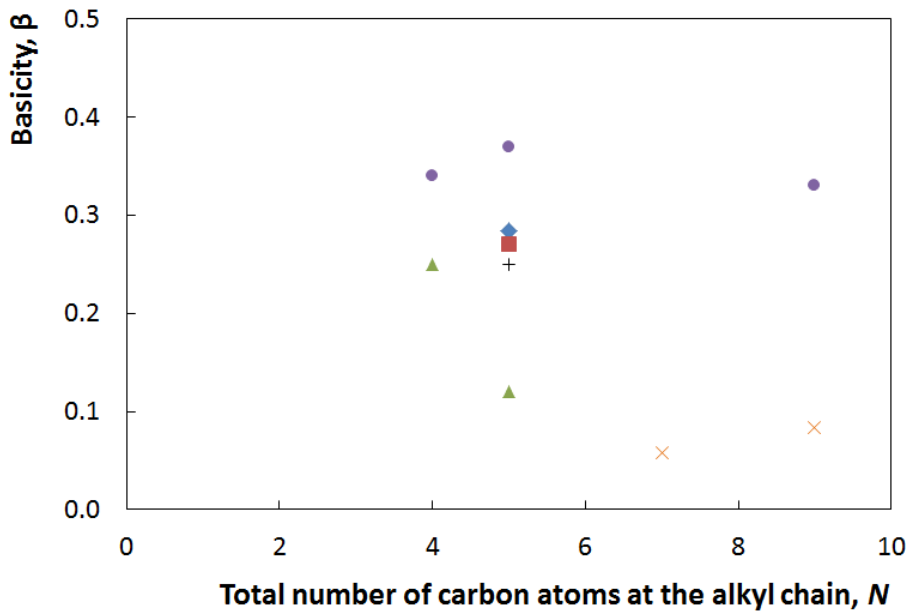

Figure S5. Comparison between experimental hydrogen-bond accepting (β) values of 1-alkyl-1-methylpyrrolidinium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [2]; (▲), [11]; (●), [23]; (×), [24];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

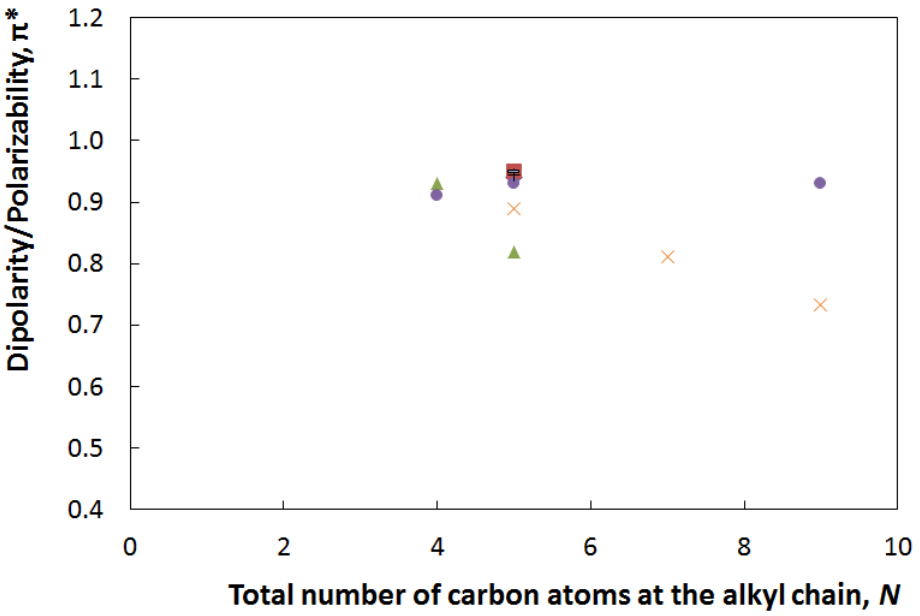

Figure S6. Comparison between experimental hydrogen-bond dipolarity/polarizability (π^*) values of 1-alkyl-1-methylpyrrolidinium-based ILs obtained in this work and in the literature as function of total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [2]; (▲), [11]; (●),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

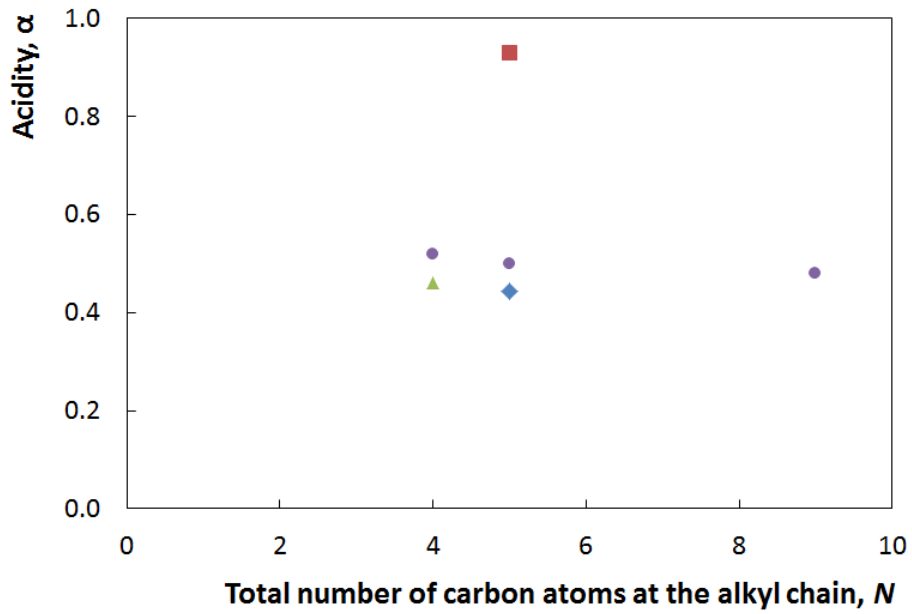

Figure S7. Comparison between experimental hydrogen-bond donating (α) values of 1-alkyl-1-methylpiperidinium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [2]; (▲), [11]; (●), [25].

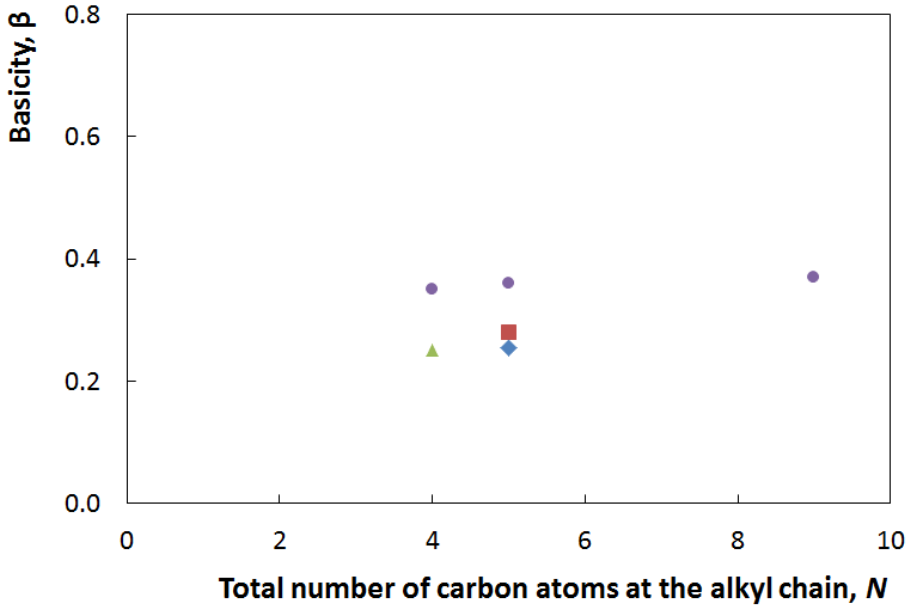

Figure S8. Comparison between experimental hydrogen-bond accepting (β) values of 1-alkyl-1-methylpiperidinium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [2]; (▲), [11]; (●), [25].

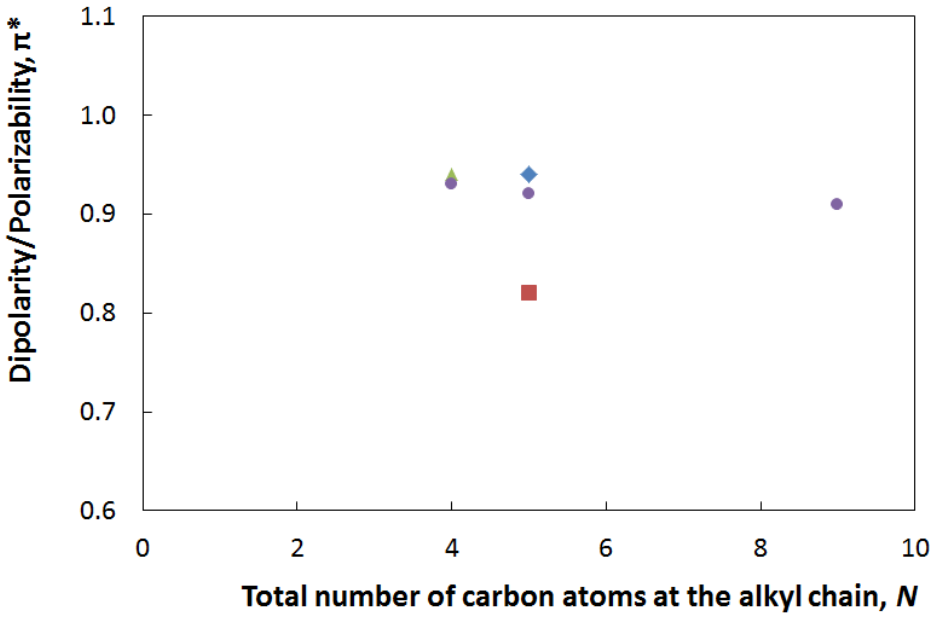

Figure S9. Comparison between experimental dipolarity/polarizability (π^*) values of 1-alkyl-1-methylpiperidinium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (*N*). Symbols: (♦), This work; (■), [2]; (▲), [11]; (●), [25].

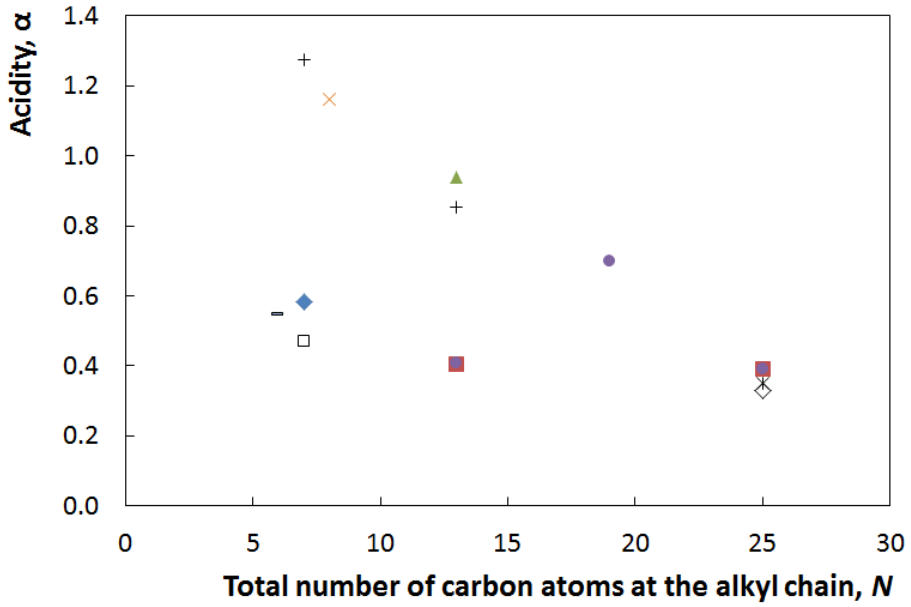

Figure S10. Comparison between experimental hydrogen-bond donating (α) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (*N*). Symbols: (♦), This work; (■), [1]; (▲), [2]; (●), [6]; (×), [10];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

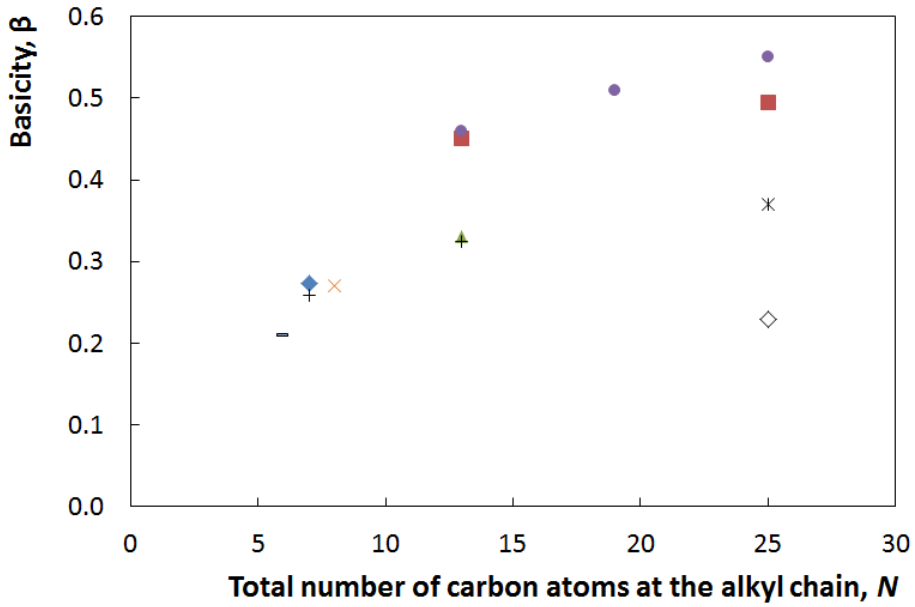

Figure S11. Comparison between experimental hydrogen-bond accepting (β) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [1]; (▲), [2]; (●), [6]; (×), [10];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

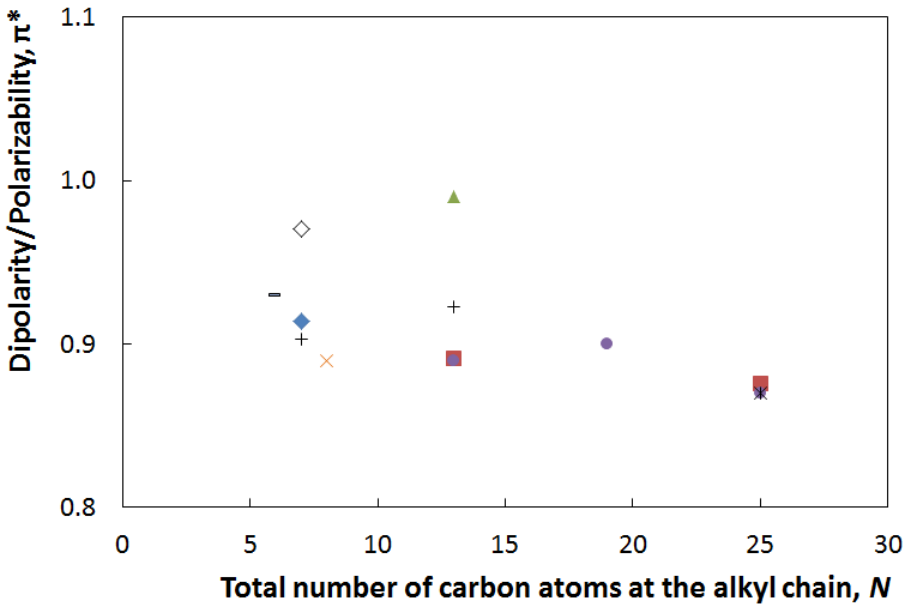

Figure S12. Comparison between experimental dipolarity/polarizability (π*) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [1]; (▲), [2]; (●), [6]; (×), [10];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

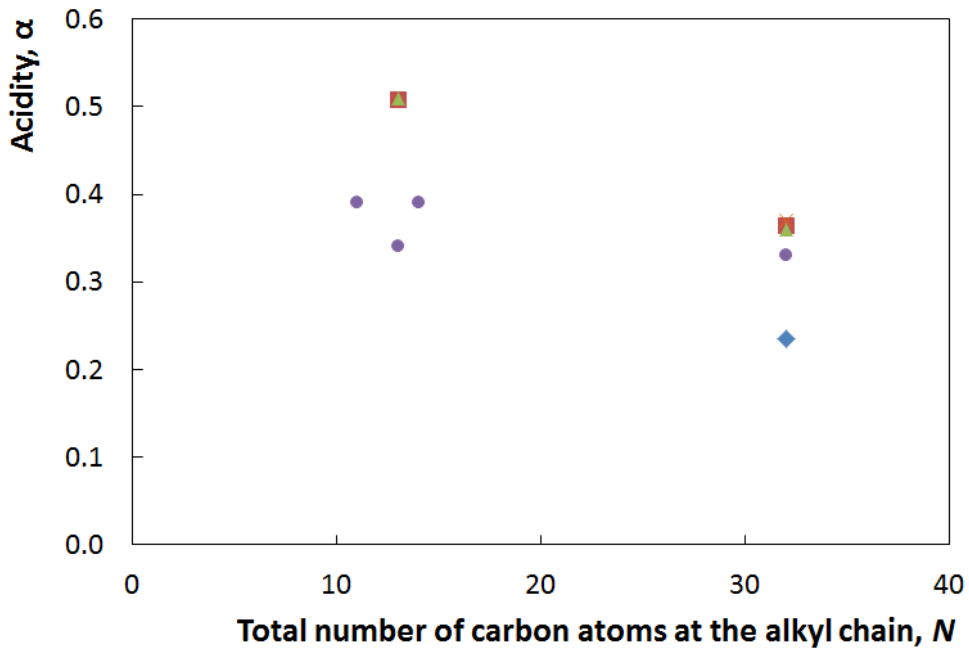

Figure S13. Comparison between experimental hydrogen-bond donating (α) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [1]; (▲), [6]; (●), [11]; (×), [14].

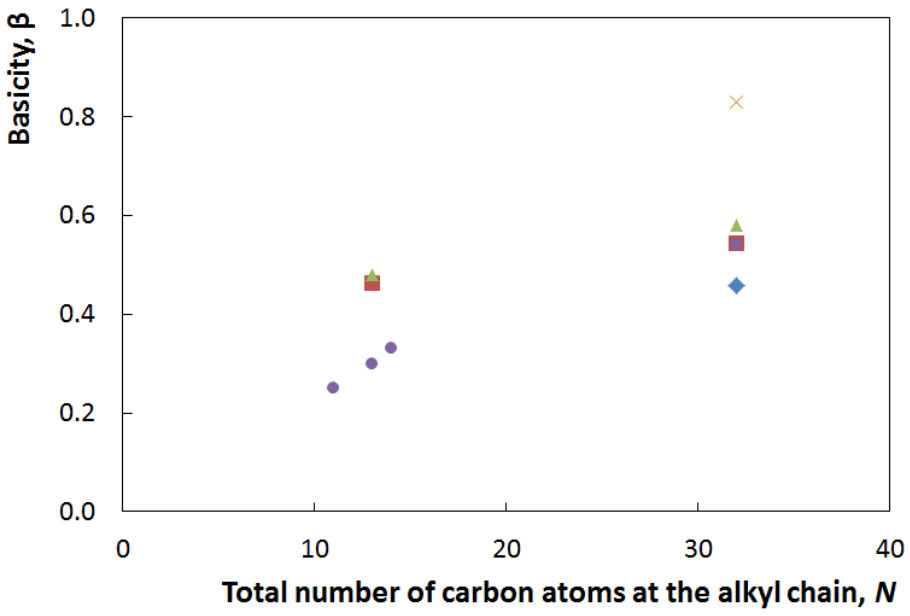

Figure S14. Comparison between experimental hydrogen-bond accepting (β) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (N). Symbols: (♦), This work; (■), [1]; (▲), [6]; (●), [11]; (×), [14].

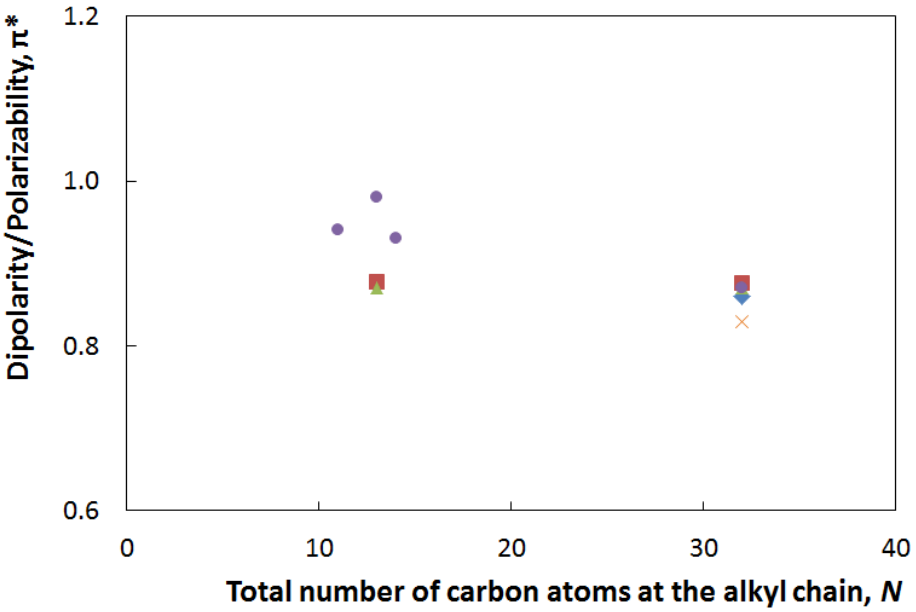

Figure S15. Comparison between experimental dipolarity/polarizability (π^*) values of 1-alkyl-3-methylimidazolium-based ILs obtained in this work and in the literature as function of the total number of carbon atoms at the alkyl chains (*N*). Symbols: (♦), This work; (■), [1]; (▲), [6]; (●), [11]; (×),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

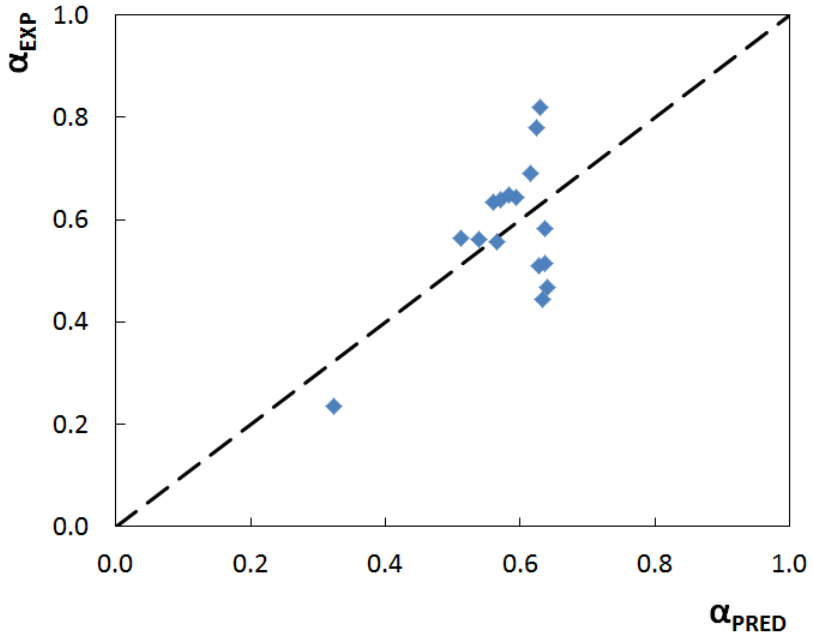

Figure S16. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 3.

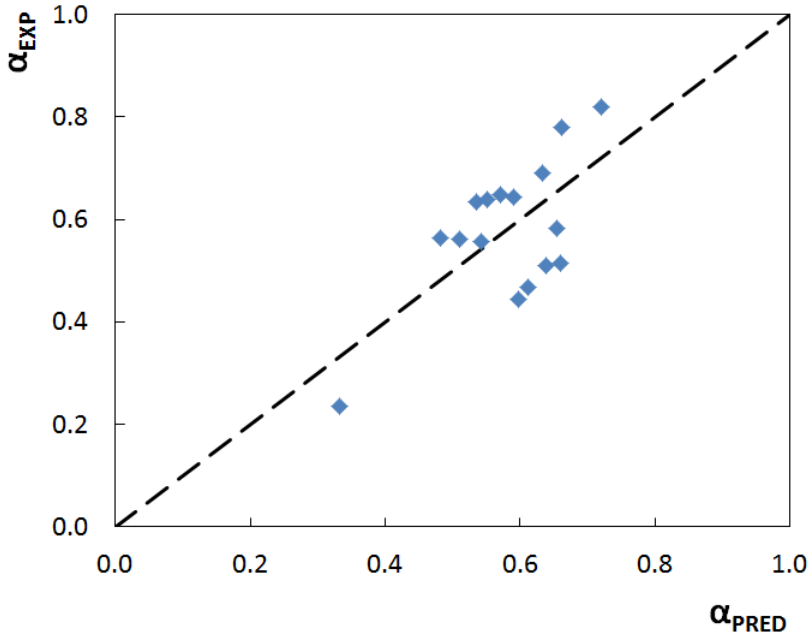

Figure S17. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 4.

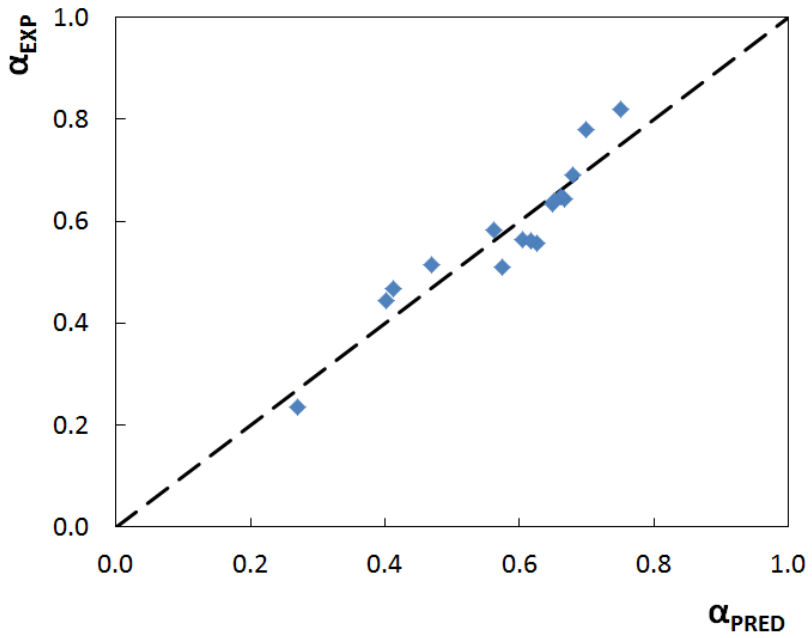

Figure S18. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 5.

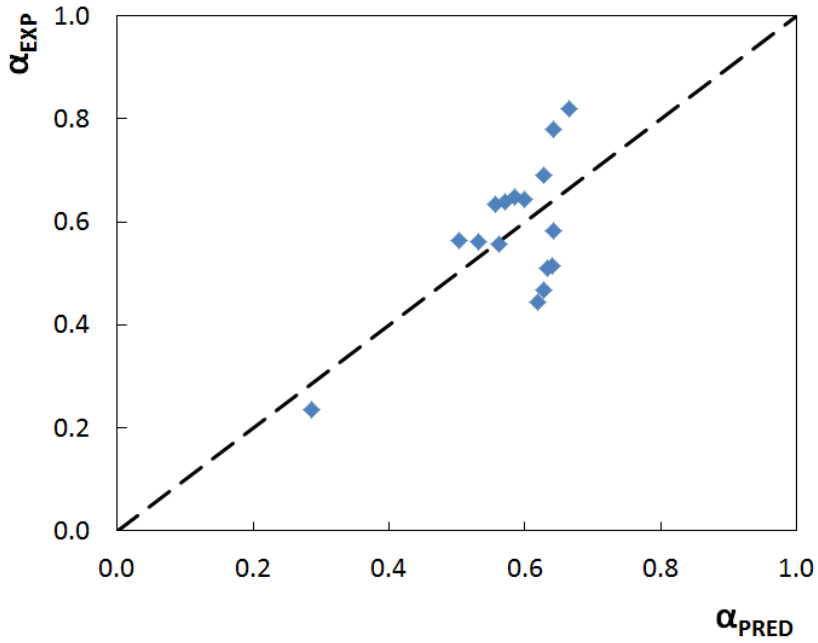

Figure S19. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 6.

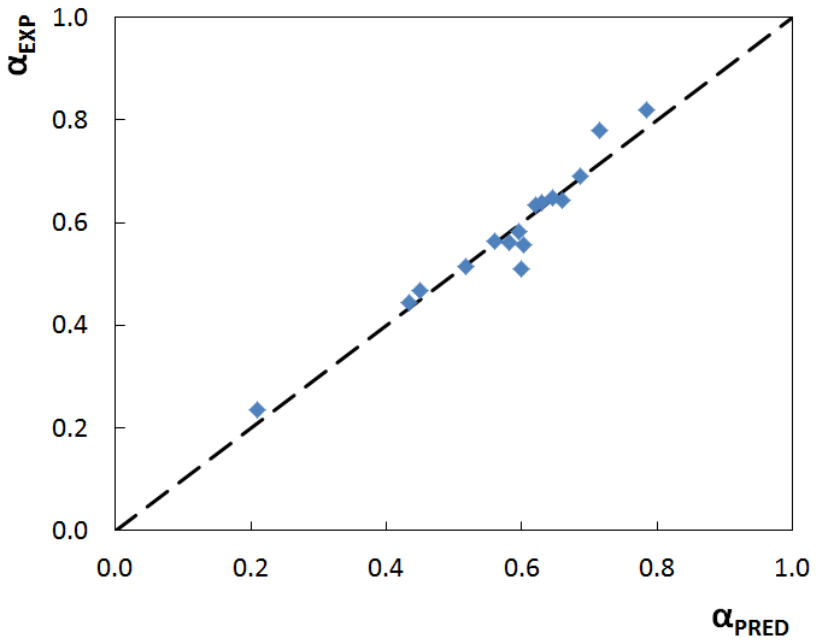

Figure S20. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 7.

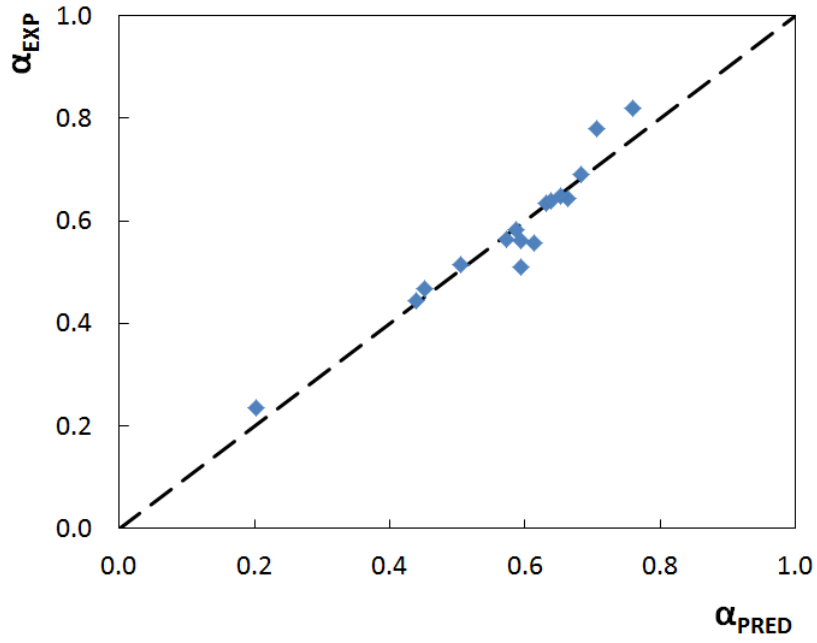

Figure S21. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 8.

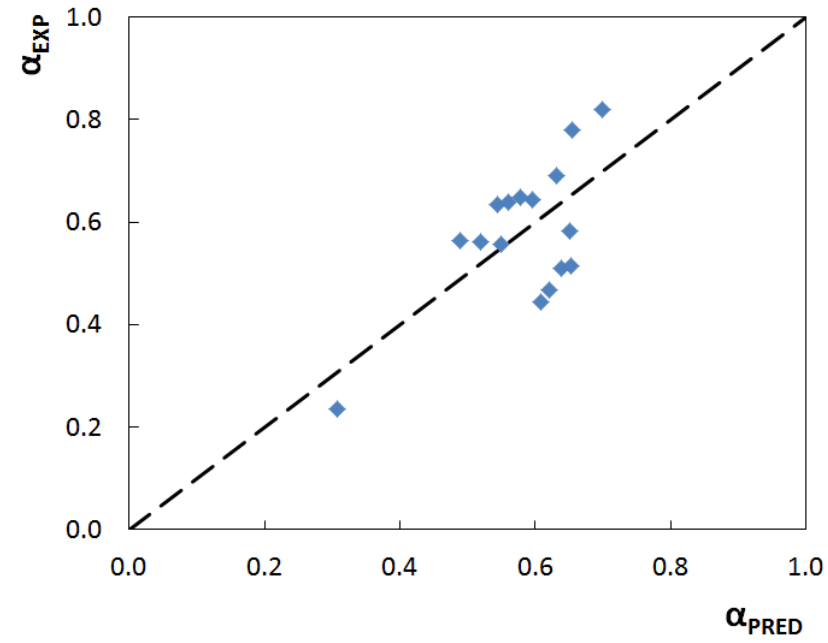

Figure S22. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 9.

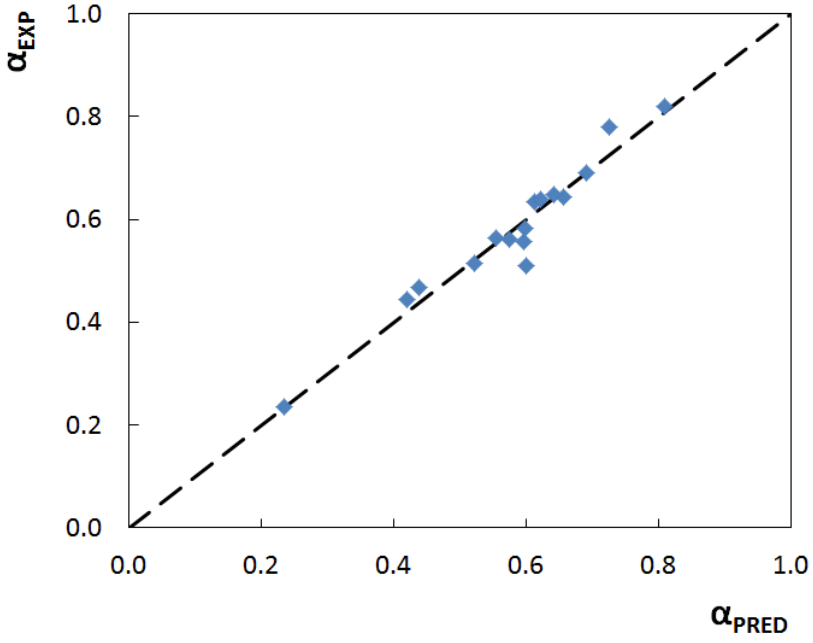

Figure S23. Correlation between experimental (α_{EXP}) and predicted (α_{PRED}) values of hydrogen-bond acidity using Equation 10.

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

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

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

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