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 ($\alpha$) 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 ($\beta$) 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]; (□), [18]; (○), [19]; (×), [20].
Figure S3. Comparison between experimental dipolarity/polarizability ($\pi^*$) 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 ($\alpha$) 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 ($\beta$) 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 ($\pi^*$) 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 ($\alpha$) 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 ($\beta$) 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 ($\pi^*$) 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: ($\bigstar$), This work; ($\blacksquare$), [2]; ($\bigtriangleup$), [11]; ($\bullet$), [25].

Figure S10. Comparison between experimental hydrogen-bond donating ($\alpha$) 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: ($\bigstar$), This work; ($\blacksquare$), [1]; ($\bigtriangleup$), [2]; ($\bullet$), [6]; ($\times$), [10]; ($+$), [26]; ($-$), [11]; ($\ast$), [27]; ($\bigcirc$), [14]; ($\square$), [17].
Figure S11. Comparison between experimental hydrogen-bond accepting ($\beta$) 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 ($\pi^*$) 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 ($\alpha$) 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: ($\circ$), This work; (■), [1]; (▲), [6]; (★), [11]; (×), [14].

Figure S14. Comparison between experimental hydrogen-bond accepting ($\beta$) 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: ($\circ$), This work; (■), [1]; (▲), [6]; (★), [11]; (×), [14].
Figure S15. Comparison between experimental dipolarity/polarizability ($\pi^*$) 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 ($\alpha_{\text{EXP}}$) and predicted ($\alpha_{\text{PRED}}$) values of hydrogen-bond acidity using Equation 3.

Figure S17. Correlation between experimental ($\alpha_{\text{EXP}}$) and predicted ($\alpha_{\text{PRED}}$) values of hydrogen-bond acidity using Equation 4.
Figure S18. Correlation between experimental ($\alpha_{\text{EXP}}$) and predicted ($\alpha_{\text{PRED}}$) values of hydrogen-bond acidity using Equation 5.

Figure S19. Correlation between experimental ($\alpha_{\text{EXP}}$) and predicted ($\alpha_{\text{PRED}}$) values of hydrogen-bond acidity using Equation 6.
Figure S20. Correlation between experimental ($\alpha_{\text{EXP}}$) and predicted ($\alpha_{\text{PRED}}$) values of hydrogen-bond acidity using Equation 7.

Figure S21. Correlation between experimental ($\alpha_{\text{EXP}}$) and predicted ($\alpha_{\text{PRED}}$) values of hydrogen-bond acidity using Equation 8.
Figure S22. Correlation between experimental ($\alpha_{\text{EXP}}$) and predicted ($\alpha_{\text{PRED}}$) values of hydrogen-bond acidity using Equation 9.

Figure S23. Correlation between experimental ($\alpha_{\text{EXP}}$) and predicted ($\alpha_{\text{PRED}}$) values of hydrogen-bond acidity using Equation 10.
The absolute average relative deviation, AARD, was calculated using Equation S1

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AARD / \% = \frac{1}{N} \sum_{\alpha} \left| \frac{\alpha_{\text{EXP}} - \alpha_{\text{PRED}}}{\alpha_{\text{EXP}}} \right| \times 100\%
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where, \( N \) is the number of data, \( \alpha_{\text{EXP}} \) is the reported experimental data, \( \alpha_{\text{PRED}} \) is the predicted value.
References


