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

Supplementary Information

Extended Scale for the Hydrogen-Bond Basicity of Ionic Liquids

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Table S1. Hydrogen-bond basicity (β) data and van der Waals interaction energy in the equimolar cation-anion mixture (E_{vdW} / (kJ·mol^{-1})) taken from COSMO-RS calculations for [C_4mim]-based ILs.

IL	β^{10}	β^{18}	E_{vdW} / (kJ·mol^{-1})
[C_2mim][$N(CF_3SO_2)_2$]	0.23	n.a.	-57.77
[C_4mim][$N(CF_3SO_2)_2$]	0.23	0.42	-65.32
[C_4C_1mim][$N(CF_3SO_2)_2$]	0.24	n.a.	-67.91
[C_5mim][$N(CF_3SO_2)_2$]	0.26	n.a.	-69.16
[C_6mim][$N(CF_3SO_2)_2$]	0.26	0.44	-73.00
[C_8mim][$N(CF_3SO_2)_2$]	0.29	0.47	-80.81
[C_{10}mim][$N(CF_3SO_2)_2$]	n.a.	0.49	-88.72
[C_4mpy][$N(CF_3SO_2)_2$]	0.25	n.a	-67.68
[C_4mpyr][$N(CF_3SO_2)_2$]	0.25	n.a	-67.17
[C_5mpyr][$N(CF_3SO_2)_2$]	0.26	n.a	-70.26
[(C_2OC_2)mpyr][$N(CF_3SO_2)_2$]	0.28	n.a	-66.47
[C_4mim][PF_6]	0.19	0.44	-49.96
[C_6mim][PF_6]	n.a.	0.50	-57.97
[C_8mim][PF_6]	n.a.	0.53	-66.06
[C_{10}mim][PF_6]	n.a.	0.55	-74.20
[C_4mim][BF_4]	0.37	0.55	-48.81
[C_4C_1mim][BF_4]	0.36	n.a.	-51.51
[C_6mim][BF_4]	n.a.	0.60	-56.87
[C_8mim][BF_4]	n.a.	0.63	-64.99
[C_{10}mim][BF_4]	n.a.	0.65	-73.16
[C_4mim][CF_3SO_3]	0.48*	0.57	-55.71
[C_6mim][CF_3SO_3]	n.a.	0.61	-63.67
[C_8mim][CF_3SO_3]	n.a.	0.64	-71.71
[C_{10}mim][CF_3SO_3]	n.a.	0.65	-79.82
[C_4mim][ClO_4]	n.a.	0.55	-52.75
[C_4mim][$C(CN)_3$]	n.a.	0.54	-63.78
[C_4mim][$N(CN)_2$]	0.60	0.64	-56.70
[C_6mim][$N(CN)_2$]	n.a.	0.69	-64.55
[C_8mim][$N(CN)_2$]	n.a.	0.71	-72.50
[C_{10}mim][$N(CN)_2$]	n.a.	0.75	-80.49
[C_4mim][SCN]	n.a.	0.71	-59.37
[C_4mim][NO_3]	n.a.	0.74	-50.83
[C_6mim][NO_3]	n.a.	0.76	-58.83
[C_8mim][NO_3]	n.a.	0.80	-66.91
[C_{10}mim][NO_3]	n.a.	0.81	-75.06
[C_4mim][CF_3CO_2]	0.84*	0.74	-52.72
[C_4mim]I	n.a.	0.75	-61.86
[C_4mim][CH_3SO_4]	0.66	0.75	-59.38
[C_4mim][$C_8H_{17}SO_4$]	0.80*	0.77	-88.15
[C_4mim][CH_3SO_3]	0.77	0.85	-57.95
[C_4mim]Br	n.a.	0.87	-56.46
[C_4mim]Cl	0.84	0.95	-53.53
[C_6mim]Cl	n.a.	0.97	-61.62
[C_8mim]Cl	n.a.	0.98	-69.78
[C_{10}mim]Cl	n.a.	0.98	-77.99
[C_4mim][$(CH_3O)_2PO_2$]	1.12*	1.12	-65.04
[C_4mim][CH_3CO_2]	0.85	1.20	-55.57

*experimental data from this work

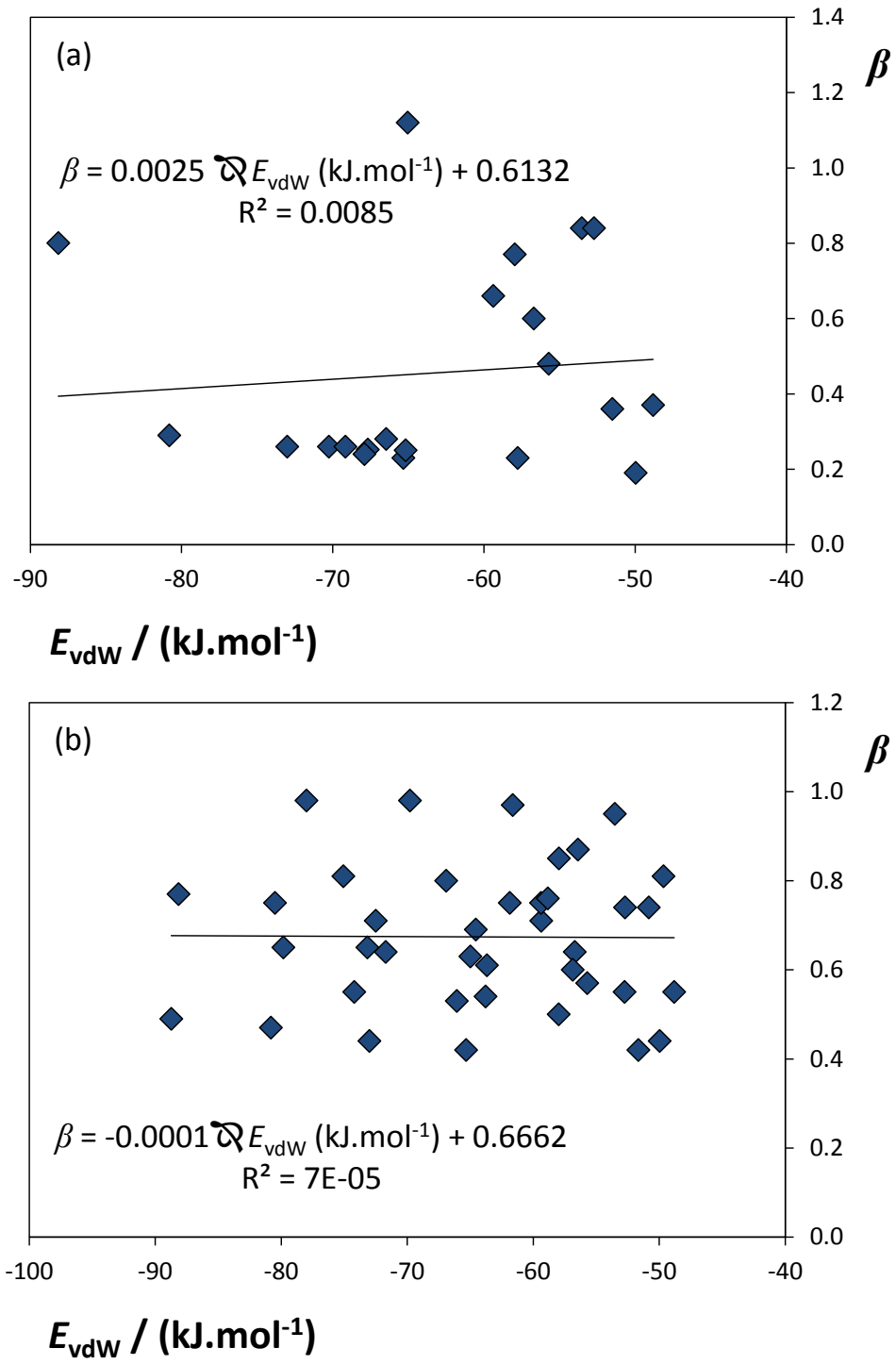

Fig. S1. Correlation between the experimental values of hydrogen-bond basicity (β) and the E_{vdW} predicted by COSMO-RS: (a) experimental data from Welton and co-workers[10]; (b) experimental data from Lungwitz et al.[18].