

# Supporting Information

## Thermophysical Properties and Water Saturation of [PF<sub>6</sub>]-based Ionic Liquids

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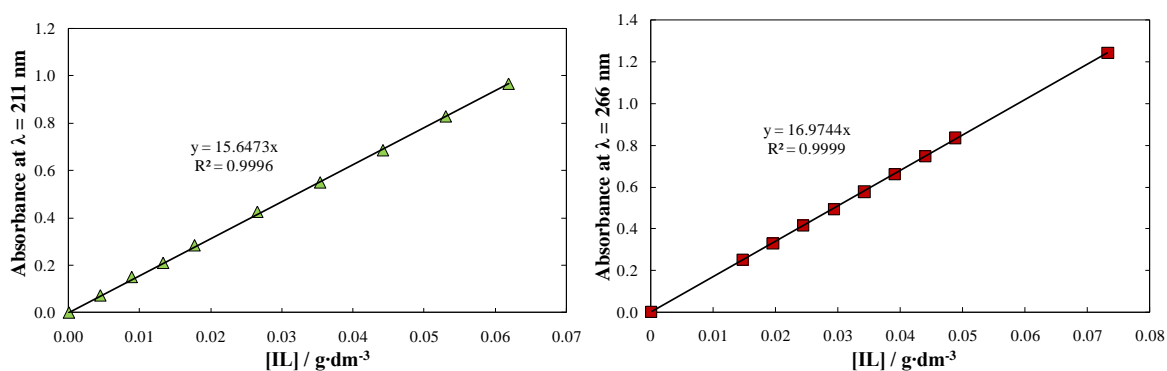
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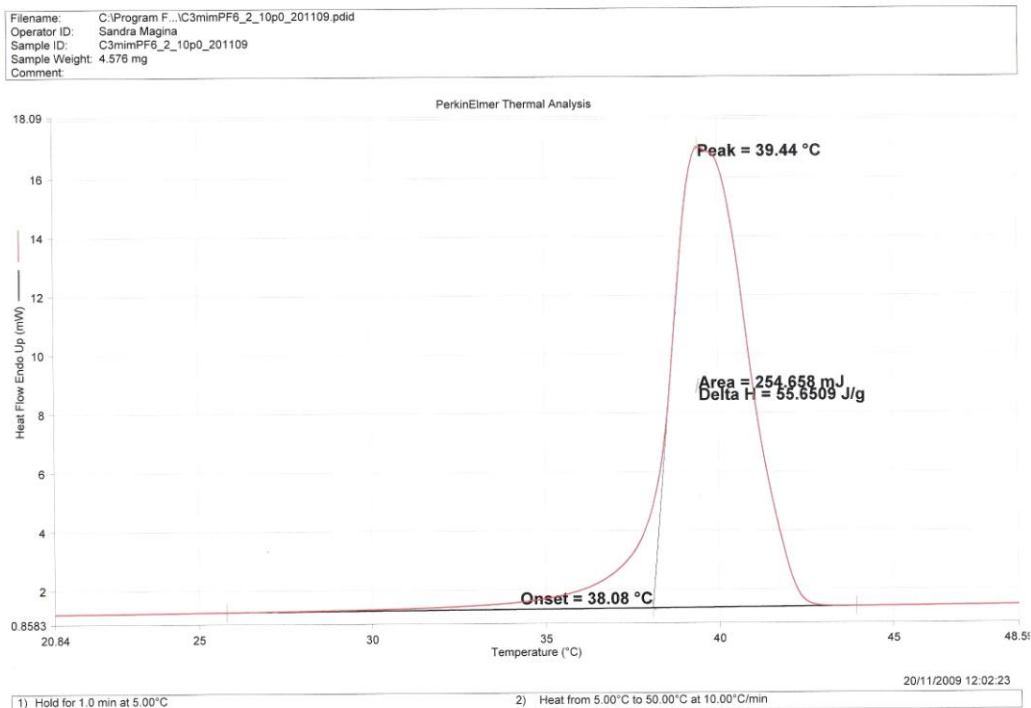
Calibration curves for the ILs solubility in water determination were achieved using a stock solution of each IL in ultra-pure water with a concentration of  $\approx 0.5 \text{ g}\cdot\text{dm}^{-3}$ . Proper dilutions in ultra-pure water of the stock solution guided to nine standard solutions. The concentration of each standard is given in Table S1, and the calibration curves are given in Figure S1. The absorbance of each standard solution is an average of at least 5 independent readings.

**Table S1.** Concentration of the stock solution and respective standard solutions of each IL, as well as respective absorbance at  $\lambda = 211 \text{ nm}$  or  $266 \text{ nm}$ .

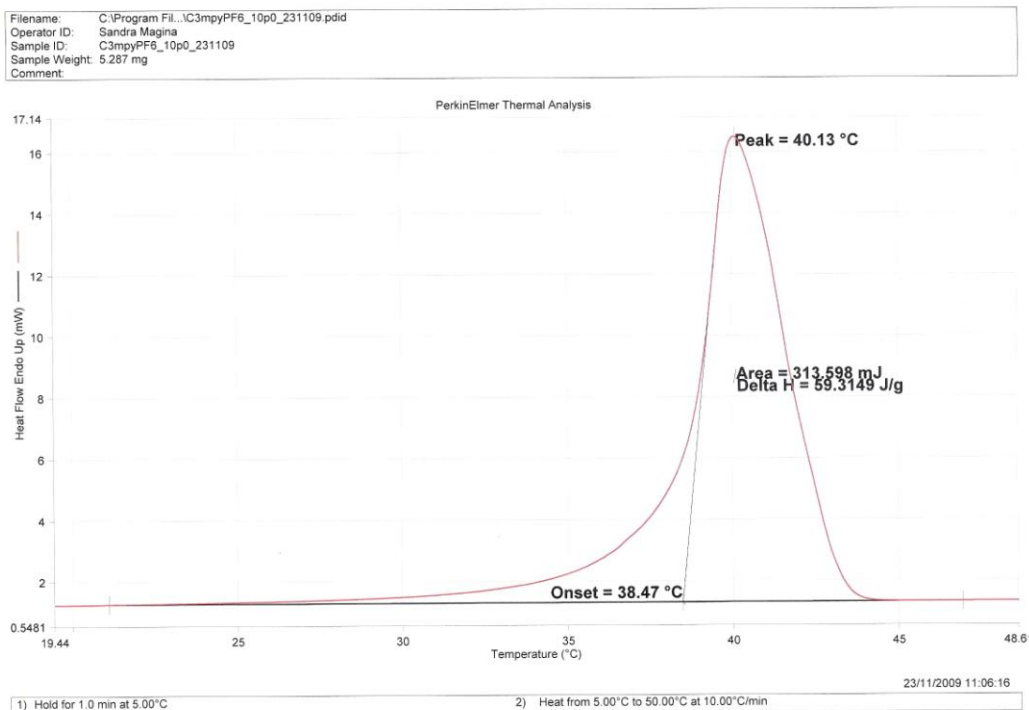
	[C <sub>3</sub> mim][PF <sub>6</sub> ]		[C <sub>3</sub> mpy][PF <sub>6</sub> ]	
Stock Solution / $\text{g}\cdot\text{dm}^{-3}$	0.4424		0.4884	
Standard Solutions	[IL] / $\text{g}\cdot\text{dm}^{-3}$	Absorbance at $\lambda = 211 \text{ nm}$	[IL] / $\text{g}\cdot\text{dm}^{-3}$	Absorbance at $\lambda = 266 \text{ nm}$
1	0.0044	0.072	0.0146	0.251
2	0.0088	0.150	0.0195	0.329
3	0.0133	0.210	0.0244	0.415
4	0.0177	0.284	0.0293	0.494
5	0.0265	0.426	0.0342	0.577
6	0.0354	0.550	0.0391	0.661
7	0.0442	0.686	0.0440	0.747
8	0.0531	0.829	0.0488	0.836
9	0.0619	0.967	0.0733	1.243



**Figure S1.** Calibration Curves (Absorbance at  $\lambda = 211 \text{ nm}$  or  $266 \text{ nm}$  as a function of the IL concentration) for ILs:  $\blacktriangle$ , [C<sub>3</sub>mim][PF<sub>6</sub>];  $\blacksquare$ , [C<sub>3</sub>mpy][PF<sub>6</sub>].



**Figure S2.** Thermogram for  $[C_3mim][PF_6]$  obtained using a Diamond DSC PerkinElmer equipment.



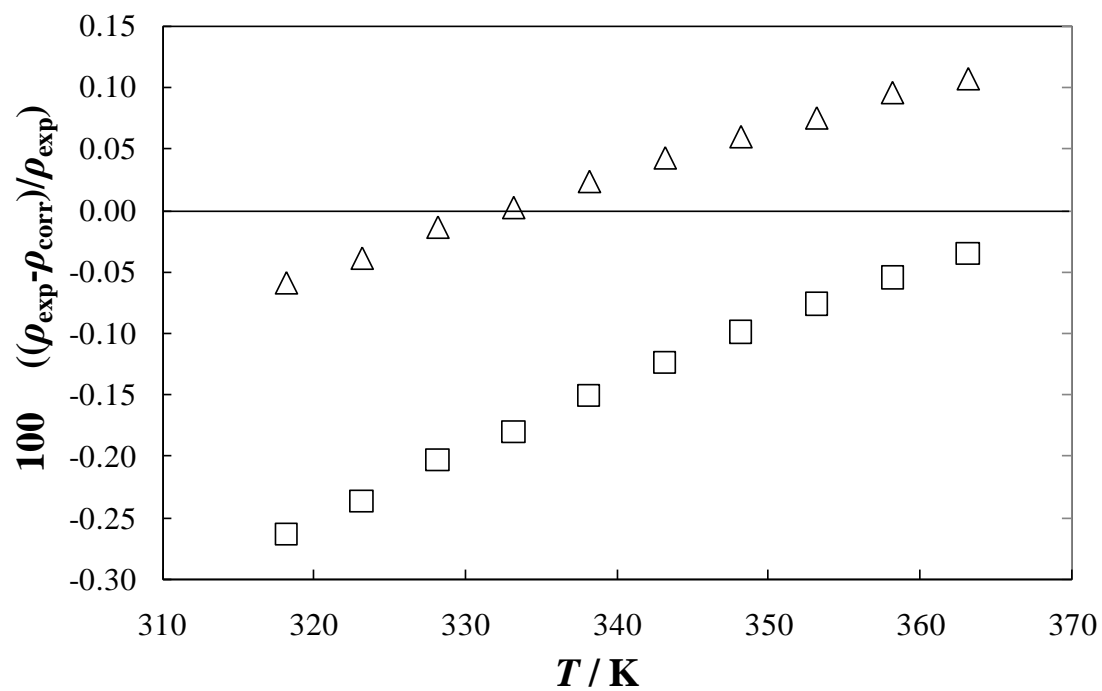
**Figure S3.** Thermogram for  $[C_3mpy][PF_6]$  obtained using a Diamond DSC PerkinElmer equipment.

**Table S2.** Correlation parameters for the mole fraction solubility of water in ILs and ILs in water as a function of temperature using eqs 1 and 2, respectively.

IL	$A$	$B / K$	$R^2$ <sup>(a)</sup>	$C$ <sup>(b)</sup>	$D / K$ <sup>(b)</sup>	$E$ <sup>(b)</sup>	$R^2$ <sup>(a)</sup>
[C <sub>3</sub> mim][PF <sub>6</sub> ]	3.94 ± 0.15	-1541 ± 44	0.9990	-315 ± 405	12816 ± 18676	47 ± 60	0.9969
[C <sub>3</sub> mpy][PF <sub>6</sub> ]	3.99 ± 0.44	-1579 ± 180	0.9965	-425 ± 537	17712 ± 24742	63 ± 80	0.9955

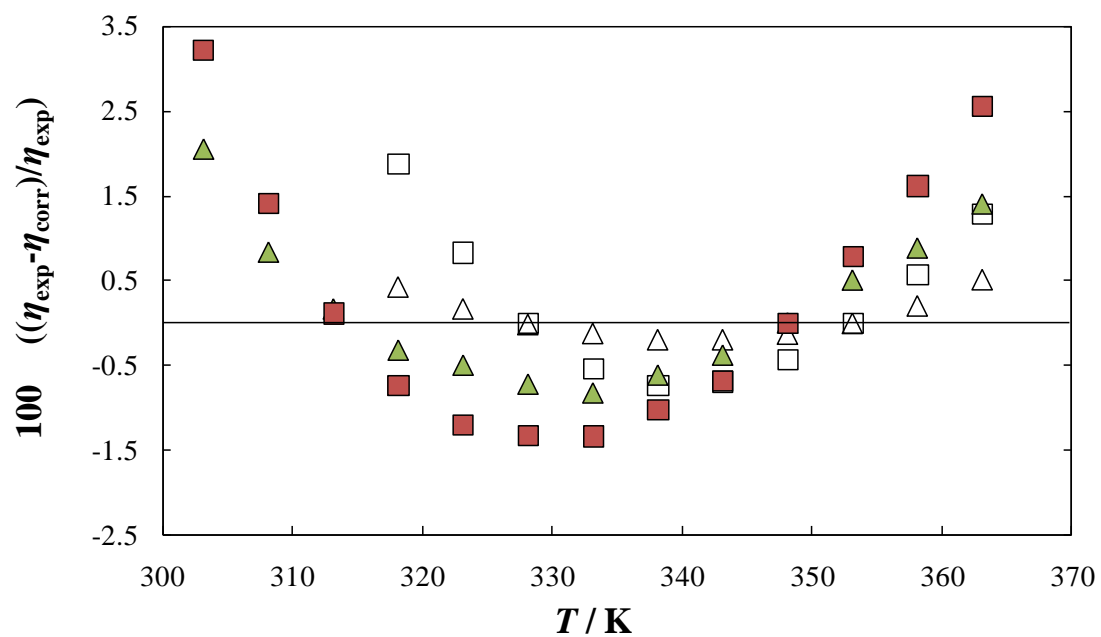
<sup>(a)</sup> Correlation coefficient.

<sup>(b)</sup> Note that three correlation constants were calculated from four experimental data points [from (303.15 to 318.15) K] to avoid discrepancies between liquid-liquid and solid-liquid equilibria.



**Figure S4.** Density deviation plot between measured data and predicted values using eq

6:  $\Delta$ ,  $[\text{C}_3\text{mim}][\text{PF}_6]$ ;  $\square$ ,  $[\text{C}_3\text{mpy}][\text{PF}_6]$ .



**Figure S5.** Viscosity deviation plot between measured data and predicted values using eqs 8 to 10 for pure (empty symbols) and water-saturated (full symbols) ILs:  $\triangle$ ,  $\blacktriangle$ ,  $[\text{C}_3\text{mim}][\text{PF}_6]$ ;  $\square$ ,  $\blacksquare$ ,  $[\text{C}_3\text{mpy}][\text{PF}_6]$ .