

SUPPLEMENTARY MATERIAL

PHASE EQUILIBRIA AND CORRELATION OF SYSTEMS INVOLVING 1-HEXYL-3-METHYLPYRIDINIUM TRIFLUOROMETHANESULFONATE

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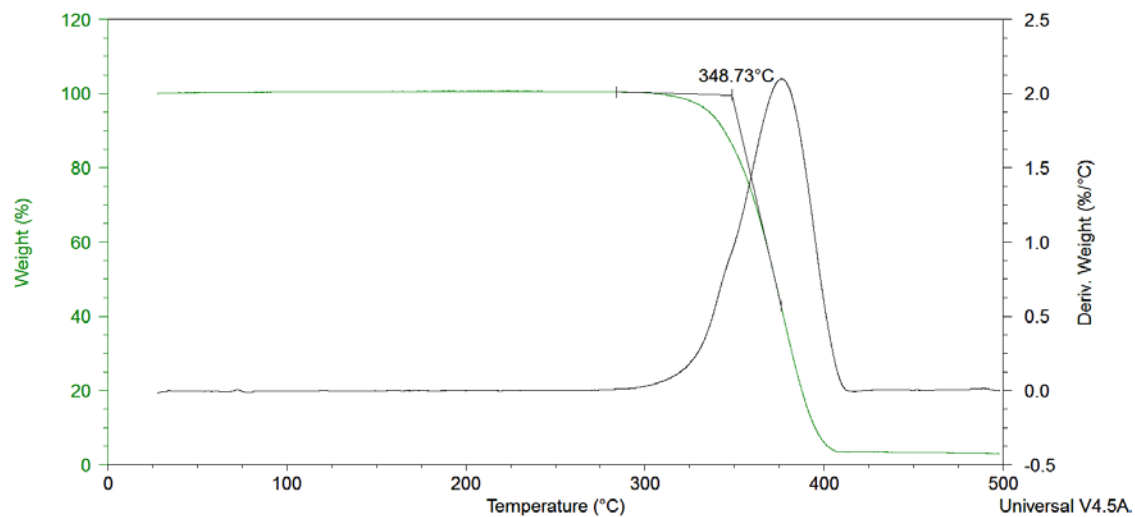


Figure S1. T_d calculation from TGA thermogram of [C₆C₁py][OTf].

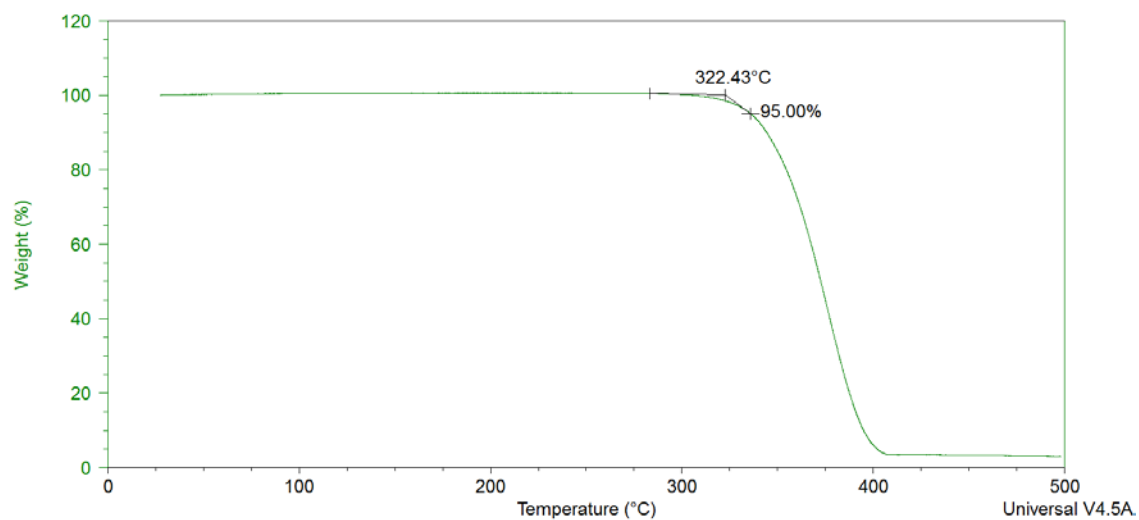


Figure S2. $T_{d,5\%}$ calculation from TGA thermogram of [C₆C₁py][OTf].

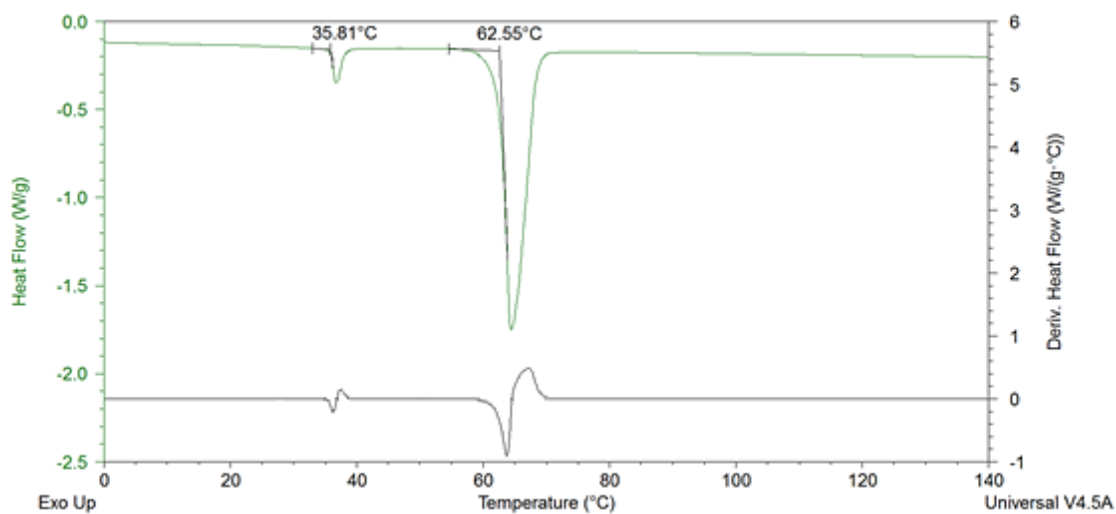


Figure S3. Thermal events calculation (onset) from DSC thermogram of [C₆C₁py][OTf].

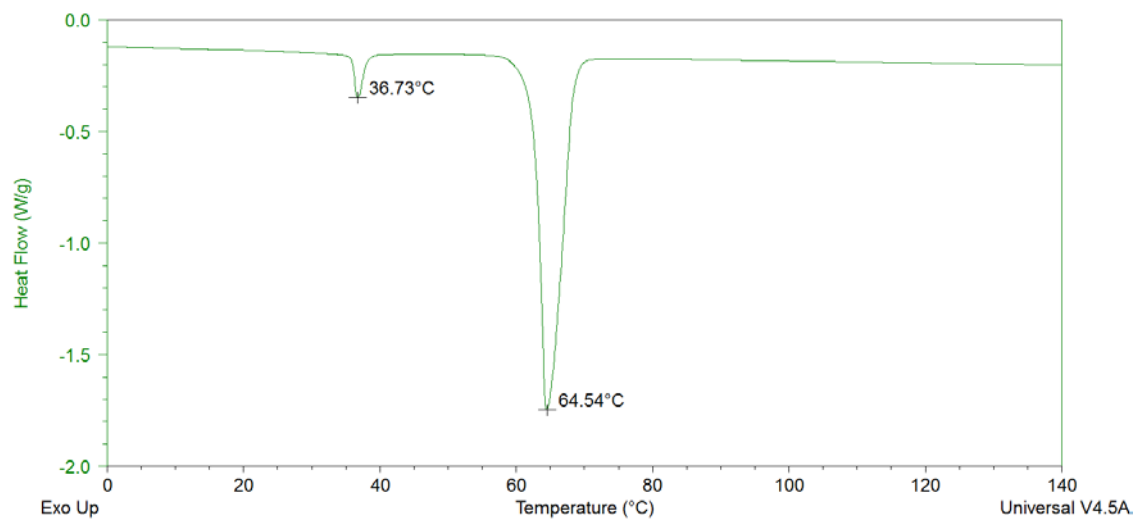


Figure S4. Thermal events calculation (midpoint) from DSC thermogram of [C₆C₁py][OTf].

Table S1. Liquid-liquid equilibrium of the ternary system water (1) + [C₆C₁py][OTf] (2) + *n*-octane (3) at 298.15 K and 0.1 MPa.

Biphasic region 1								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	1.000	0.000	0.000			
0.000	0.000	1.000	0.986	0.014	0.000			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 2								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.972	0.028	0.000	0.179	0.821	0.000			
0.972	0.028	0.000	0.179	0.821	0.000			
$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 3								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	0.110	0.879	0.011			
0.000	0.000	1.000	0.092	0.896	0.012			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$			
Triphasic region								
Upper Phase			Medium Phase			Lower phase		
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.000	0.000	1.000	0.972	0.028	0.000	0.174	0.817	0.009
0.000	0.000	1.000	0.972	0.028	0.000	0.174	0.817	0.009
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$

$u(P) = 5$ kPa, $u(T) = 0.05$ K. All the uncertainties are standard.

Table S2. Liquid-liquid equilibrium of the ternary system water (1) + [C₆C₁py][OTf] (2) + *n*-octane (3) at 323.15 K and 0.1 MPa.

Biphasic region 1								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	1.000	0.000	0.000			
0.000	0.000	1.000	0.975	0.025	0.000			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 2								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.965	0.035	0.000	0.210	0.790	0.000			
0.965	0.035	0.000	0.210	0.790	0.000			
$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 3								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	0.177	0.814	0.009			
0.000	0.000	1.000	0.127	0.862	0.011			
0.000	0.000	1.000	0.060	0.922	0.019			
0.000	0.000	1.000	0.021	0.958	0.020			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$			
Triphasic region								
Upper Phase			Medium Phase			Lower phase		
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.000	0.000	1.000	0.965	0.035	0.000	0.203	0.788	0.009
0.000	0.000	1.000	0.965	0.035	0.000	0.203	0.788	0.009
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$

$u(P) = 5$ kPa, $u(T) = 0.05$ K. All the uncertainties are standard.

Table S3. Liquid-liquid equilibrium of the ternary system water (1) + [C₆C₁py][OTf] (2) + toluene (3) at 298.15 K and 0.1 MPa.

Biphasic region 1								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	1.000	0.000	0.000			
0.000	0.000	1.000	0.985	0.015	0.000			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 2								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.972	0.028	0.000	0.179	0.821	0.000			
0.972	0.028	0.000	0.107	0.787	0.106			
0.972	0.028	0.000	0.078	0.741	0.182			
0.972	0.028	0.000	0.055	0.676	0.270			
$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 3								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	0.000	0.550	0.450			
0.000	0.000	1.000	0.022	0.603	0.376			
0.000	0.000	1.000	0.032	0.617	0.351			
0.000	0.000	1.000	0.042	0.627	0.331			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$			
Triphasic region								
Upper Phase			Medium Phase			Lower phase		
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.000	0.000	1.000	0.972	0.028	0.000	0.056	0.639	0.305
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$

$u(P) = 5$ kPa, $u(T) = 0.05$ K. All the uncertainties are standard.

Table S4. Liquid-liquid equilibrium of the ternary system water (1) + [C₆C₁py][OTf] (2) + toluene (3) at 323.15 K and 0.1 MPa

Biphasic region 1								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	1.000	0.000	0.000			
0.000	0.000	1.000	0.983	0.017	0.000			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 2								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.965	0.035	0.000	0.210	0.790	0.000			
0.965	0.035	0.000	0.140	0.787	0.073			
0.965	0.035	0.000	0.113	0.767	0.119			
0.965	0.035	0.000	0.097	0.749	0.154			
0.965	0.035	0.000	0.072	0.687	0.241			
$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 3								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	0.000	0.559	0.441			
0.000	0.000	1.000	0.012	0.584	0.404			
0.000	0.000	1.000	0.024	0.612	0.364			
0.000	0.000	1.000	0.031	0.623	0.346			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$			
Triphasic region								
Upper Phase			Medium Phase			Lower phase		
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.000	0.000	1.000	0.965	0.035	0.000	0.072	0.649	0.279
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$

$u(P) = 5$ kPa, $u(T) = 0.05$ K. All the uncertainties are standard.

Table S5. Solid-liquid equilibrium of the ternary system water (1) + [C₆C₁py][OTf] (2) + toluene (3) at several temperatures and 0.1 MPa.

Liquid Phase (298.15 K)			Liquid phase (323.15K)		
w_1	w_2	w_3	w_1	w_2	w_3
0.112	0.888	0.000	0.033	0.967	0.000
0.055	0.878	0.067	0.023	0.967	0.010
0.022	0.809	0.169	0.010	0.932	0.058
0.000	0.641	0.359	0.000	0.896	0.104
$u(w_1)=0.002$	$u(w_2)=0.002$	$u(w_3)=0.001$	$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$

$u(P) = 5$ kPa, $u(T) = 0.05$ K. All the uncertainties are standard.

Table S6. Liquid-liquid equilibrium of the ternary system water (1) + [C₆C₁py][OTf] (2) + cyclohexane (3) at 298.15 K and 0.1 MPa.

Biphasic region 1								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	1.000	0.000	0.000			
0.000	0.000	1.000	0.981	0.019	0.000			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 2								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.972	0.028	0.000	0.179	0.821	0.000			
$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 3								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	0.159	0.818	0.024			
0.000	0.000	1.000	0.124	0.846	0.030			
0.000	0.000	1.000	0.088	0.879	0.033			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.002$	$u(w_2)=0.002$	$u(w_3)=0.001$			
Triphasic region								
Upper Phase			Medium Phase			Lower phase		
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.000	0.000	1.000	0.972	0.028	0.000	0.170	0.803	0.027
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.002$	$u(w_2)=0.002$	$u(w_3)=0.001$

$u(P) = 5$ kPa, $u(T) = 0.05$ K. All the uncertainties are standard.

Table S7. Liquid-liquid equilibrium of the ternary system water (1) + [C₆C₁py][OTf] (2) + cyclohexane (3) at 323.15 K and 0.1 MPa.

Biphasic region 1								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	1.000	0.000	0.000			
0.000	0.000	1.000	0.979	0.021	0.000			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 2								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.965	0.035	0.000	0.210	0.790	0.000			
$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$			
Biphasic region 3								
Upper Phase			Lower phase					
w_1	w_2	w_3	w_1	w_2	w_3			
0.000	0.000	1.000	0.151	0.820	0.029			
0.000	0.000	1.000	0.116	0.853	0.032			
0.000	0.000	1.000	0.090	0.874	0.036			
0.000	0.000	1.000	0.071	0.890	0.039			
0.000	0.000	1.000	0.042	0.915	0.043			
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.002$	$u(w_2)=0.002$	$u(w_3)=0.001$			
Triphasic region								
Upper Phase			Medium Phase			Lower phase		
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.000	0.000	1.000	0.965	0.035	0.000	0.164	0.809	0.027
$u(w_1)=0.001$	$u(w_2)=0.001$	$u(w_3)=0.001$	$u(w_1)=0.003$	$u(w_2)=0.003$	$u(w_3)=0.001$	$u(w_1)=0.002$	$u(w_2)=0.002$	$u(w_3)=0.001$

$u(P) = 5$ kPa, $u(T) = 0.05$ K. All the uncertainties are standard.