Supplementary Material (ESI) for PCCP

Supplementary Information

Solubility of Alkanes, Alkanols and Their Fluorinated Counterparts in Tetraalkyl-Phosphonium Ionic Liquids

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Table S1. Cloud point temperatures for the system $[P_{6\,6\,6\,14}]Cl + H_2O$ and interfacial surface tension (IFT) of $[P_{4\,4\,4\,14}]Cl + H_2O$. The data are presented graphically in Figure 2 (and its inset) of the main text (x_{IL} and $x_{V,IL}$ hold, respectively, for the IL mole fraction and the IL volume fraction).

$[P_{6\,6\,6\,14}]Cl + H_2O$		
x_{IL}	$x_{V,IL}$	T / K
0.188	0.861	356.0
0.194	0.865	323.7
0.197	0.868	293.2
$[P_{4\,4\,4\,14}]Cl + H_2O$		
[IL], mM	$x_{V,IL}$	IFT, $mN.m^{-1}$
0.0137	0.00001	71.65
0.1369	0.00006	57.72
0.2738	0.00013	50.94
0.4108	0.00020	48.01
0.6846	0.00033	44.93
0.9584	0.00046	42.92
1.3692	0.00066	42.3
2.7384	0.00131	41.52
4.1076	0.00197	40.93
6.8460	0.00328	39.91
9.5844	0.00458	39.77
13.692	0.00654	39.15
41.076	0.01937	37.47
68.46	0.0319	36.96
136.92	0.0619	35.8

Table S2. Cloud point temperatures in the systems containing phosphonium-based ionic liquids, except those already presented in Table S1 (chloride-based). The data are presented graphically in figures 3, 4, 7, and 8 of the main text (x_{IL} and $x_{V,IL}$ hold, respectively, for the IL mole fraction and the IL volume fraction).

$[P_{6\,6\,6\,14}][Ac]$								
C_6H_{14}			$C_{10}H_{14}$			$C_{14}H_{30}$		
x_{IL}	$x_{V,IL}$	T/K	x_{IL}	$x_{V,IL}$	T/K	x_{IL}	$x_{V,IL}$	T/K
0.005	0.023	283.5	0.002	0.006	277.9	0.008	0.019	320.7
0.011	0.049	295.5	0.004	0.012	286.3	0.015	0.035	333.2
0.013	0.058	296.7	0.007	0.022	297.2	0.024	0.055	336.9
0.016	0.070	296.7	0.009	0.028	304.7	0.003	0.007	293.1
0.019	0.083	296.7	0.011	0.034	307.7	0.004	0.009	302.6
0.023	0.099	296.1	0.014	0.043	310.2	0.006	0.014	313.6
0.026	0.111	295.1	0.017	0.051	310.7	0.009	0.021	323.5
0.030	0.126	294.7	0.019	0.057	311.0	0.011	0.026	329.4
0.036	0.148	292.3	0.024	0.071	310.9	0.014	0.032	332.4
0.048	0.190	288.9	0.030	0.088	310.7	0.02	0.046	335.6
0.061	0.233	282.8	0.037	0.107	310.5	0.022	0.050	336.7
0.004	0.018	272.2	0.045	0.129	309.6	0.026	0.059	336.9
0.006	0.027	286.9	0.061	0.169	307.3	0.031	0.070	337.1
0.009	0.041	292.4	0.084	0.223	303.0	0.041	0.091	336.7
0.049	0.194	288.2	0.113	0.285	295.8	0.053	0.116	336.3
0.076	0.277	273.9	0.146	0.349	287.0	0.072	0.154	335.3
0.093	0.324	263.9				0.098	0.204	332.4
0.105	0.354	256.4				0.128	0.257	327.6
0.002	0.009	257.3				0.173	0.330	319.0
0.003	0.014	264.1						
0.005	0.023	277.8						
0.039	0.159	290.7						
0.061	0.233	281.4						
0.007	0.032	288						
0.009	0.041	291.8						
0.053	0.207	285.4						
0.083	0.297	270.1						
0.121	0.391	247.8						

Table S2. (cont.)

$[P_{6\,6\,6\,14}][Otf]$			$[P_{6\,6\,6\,14}]$ [DCA]		
C_6H_{14}			C_6H_{14}		
x_{IL}	$x_{V,IL}$	T /K	x_{IL}	$x_{V,IL}$	T /K
0.002	0.010	287.4	0.273	0.639	289.2
0.003	0.015	301.5	0.281	0.648	245.9
0.005	0.024	312.4	0.255	0.618	315
0.007	0.034	320.9	0.246	0.606	331.2
0.008	0.038	325.9	0.273	0.639	291.4
0.01	0.047	331.1	0.255	0.618	316.2
0.012	0.056	333.1	0.269	0.635	296.3
0.014	0.065	334	0.286	0.654	220.2
0.017	0.079	335.4	0.276	0.643	280.5
0.02	0.091	335.9	0.269	0.635	298.6
0.022	0.100	335.7	0.264	0.629	306.5
0.025	0.112	335.5	0.259	0.623	311.6
0.028	0.124	335.4	0.255	0.618	315.4
0.034	0.148	335	0.248	0.609	329
0.041	0.174	334.3	0.25	0.611	324
0.051	0.209	332.4	0.239	0.597	341.4
0.063	0.249	328.6	0.244	0.604	334.6
0.078	0.294	323.3	0.224	0.577	350.8
0.095	0.341	318.2			
0.116	0.393	310.5			
0.141	0.447	303.4			

Table S2. (cont.)

$[P_{6\,6\,6\,14}][Ntf_2]$					
C_6H_{14}			C_8H_{18}		
x_{IL}	$x_{V,IL}$	T /K	x_{IL}	$x_{V,IL}$	T /K
0.002	0.011	296.6	0.008	0.034	350.6
0.003	0.016	318.7	0.008	0.034	350.5
0.002	0.011	308.6	0.013	0.055	354.6
0.001	0.005	296.1	0.022	0.090	357
0.003	0.016	318.4	0.031	0.123	356.1
0.004	0.022	323.7	0.041	0.158	353.5
0.005	0.027	328.1	0.05	0.188	351
0.007	0.037	332	0.059	0.216	347.7
0.008	0.042	334.1	0.07	0.249	342.5
0.011	0.057	335	0.085	0.290	333.9
0.016	0.082	335.7	0.101	0.331	325
0.019	0.096	334.8	0.118	0.370	314.4
0.025	0.123	333.3	0.135	0.407	305
0.032	0.153	330.6	0.159	0.454	291
0.014	0.072	335.3	0.188	0.504	272
0.02	0.100	334.6	0.223	0.558	250.6
0.028	0.136	332.6			
0.042	0.194	325.7			
0.055	0.242	316.9			
0.075	0.307	303.1			
0.095	0.365	289.8			
0.113	0.411	272.7			
0.13	0.450	261.1			

Table S2. (cont.)

$[P_{6\,6\,6\,14}][Ntf_2]$								
C_6F_{14}			C_7F_{16}			C_8F_{18}		
x_{IL}	$x_{V,IL}$	T /K	x_{IL}	$x_{V,IL}$	T /K	x_{IL}	$x_{V,IL}$	T /K
0.896	0.968	301.6	0.962	0.988	291.7	0.96	0.986	321.8
0.871	0.960	312.6	0.95	0.984	301.4	0.955	0.984	326.2
0.852	0.953	320	0.936	0.979	311.6	0.939	0.978	340.7
0.913	0.974	288	0.925	0.975	315.5	0.923	0.972	346.7
0.879	0.963	310.7	0.91	0.970	325.1	0.912	0.968	353.4
0.864	0.958	316.6	0.893	0.964	331.3			
0.840	0.949	322.2	0.864	0.953	338.9			

Table S2. (cont.)

$[P_{6\,6\,6\,14}][Ntf_2]$					
$C_8F_5H_{12}OH$		$C_8F_{13}H_4OH$		$C_8F_{13}H_5$	
x_{IL}	T/K	x_{IL}	T/K	x_{IL}	T/K
0.041	247.1	0.015	283.8	0.842	283.6
0.07	252.9	0.021	290.3	0.785	310.3
0.094	253.8	0.035	295.9	0.822	292.8
0.123	255	0.048	300	0.779	312.6
0.035	241.5	0.063	302.4	0.749	325.6
0.06	249.6	0.084	303.6	0.735	328.9
0.09	253.1	0.134	305.5	0.886	246.1
0.109	254.1	0.18	306.1	0.856	272.1
0.126	253.7	0.234	306.1	0.824	294.1
0.145	253.8	0.381	303.2	0.79	309.8
0.166	253.5	0.445	300.7	0.776	312.6
0.186	253	0.518	295.8	0.755	323.7
0.223	253	0.634	284.3	0.701	342.1
0.257	252.5	0.686	278.2	0.683	347.1
0.298	251.6	0.013	280.9	0.661	354.1
0.544	231.6	0.028	293.6		
0.487	236.7	0.058	301.7		
0.443	240.1	0.085	303.9		
0.406	243.6	0.114	305.3		
0.37	248.7	0.163	306		
0.331	250.9	0.215	306		
		0.268	305.8		
		0.315	304.8		
		0.77	263.3		
		0.568	292		

Table S3. Cloud point temperatures (both LLE and LSE) for the systems containing imidazolium-based ionic liquids. The data are presented graphically in Figure 5 of the main text (x_{IL} and $x_{V,IL}$ hold, respectively, for the IL mole fraction and the IL volume fraction).

[C_{14}mim][Ntf_2]								
C_7H_{16}			$C_{10}H_{14}$			$C_{14}H_{30}$		
x_{IL}	$x_{V,IL}$	T/K	x_{IL}	$x_{V,IL}$	T/K	x_{IL}	$x_{V,IL}$	T/K
0.956	2.086	308.0	1.000	2.100	308.1	1.000	2.100	308.1
0.924	2.075	307.3	0.963	2.084	307.8	0.949	2.073	307.3
0.889	2.062	306.8	0.941	2.074	307.2	0.619	1.856	304.6
0.860	2.051	306.2	0.910	2.060	306.4	0.405	1.666	304.6
0.840	2.043	305.9	0.862	2.037	305.6	0.284	1.531	304.5
0.827	2.038	305.5	0.817	2.014	304.7	0.177	1.391	304.5
0.762	2.010	304.5	0.744	1.974	303.9	0.076	1.236	304.6
0.790	2.022	305.1	0.695	1.944	303.1	0.030	1.157	304.5
0.772	2.014	304.7	0.621	1.896	302.5	0.017	1.132	304.3
0.737	1.999	304.1	0.060	1.231	301.2	0.972	2.085	307.7
0.717	1.989	303.8	0.143	1.384	301.4	0.929	2.061	306.9
0.685	1.973	303.1	0.086	1.284	301.3	0.879	2.033	306.2
0.656	1.958	302.8	0.055	1.222	301.3	0.851	2.016	305.8
0.631	1.944	302.2	0.028	1.163	301.2	0.828	2.002	305.4
0.564	1.903	300.8	0.645	1.913	302.6	0.807	1.989	305.2
0.509	1.866	299.9	0.533	1.831	301.6	0.774	1.968	304.8
0.604	1.928	301.4	0.445	1.757	301.6	0.738	1.944	304.6
0.572	1.908	300.9	0.300	1.606	301.5	0.708	1.923	304.6
0.525	1.877	300.2	0.168	1.425	301.4	0.647	1.878	304.6
0.432	1.806	298.7	0.746	1.975	304.0	0.527	1.781	304.6
0.388	1.767	298.0	0.629	1.902	302.4	0.439	1.700	304.6
0.352	1.731	298.0	0.593	1.876	302.0	0.375	1.634	304.6
0.301	1.676	297.9	0.557	1.850	301.6	0.212	1.440	304.6
0.234	1.591	297.8	0.489	1.795	301.6	0.012	1.122	304.1
0.189	1.524	297.8	0.377	1.690	301.5	0.005	1.110	303.7
0.139	1.437	297.8	0.217	1.498	301.5			
0.485	1.848	299.5	0.157	1.408	301.5			
0.456	1.826	298.9	0.097	1.304	301.4			
0.433	1.807	298.6	0.022	1.152	301.0			
0.399	1.777	298.2	0.011	1.126	300.8			
0.363	1.743	297.9	0.007	1.117	300.6			
0.330	1.709	297.8						
0.291	1.665	297.8						
0.236	1.593	297.8						
0.033	1.196	297.2						
0.012	1.136	296.2						
0.173	1.498	297.9						
0.089	1.335	297.5						
0.052	1.247	297.3						
0.146	1.450	297.8						
0.013	1.139	295.9						