

Supporting Information to: Water and Hexane in an Ionic Liquid: Computational Evidence of Association under High Pressure

by
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System	# Ionic Pairs	# Water	# Hexane
PTN	1000	0	0
PWA	1000	87	0
PHE	1000	0	87
PWH	1000	87	87

Table S1: Simulation boxes details

Atoms in the cluster	Cluster	Probability		
		1 bar	5 kbar	10 kbar
3	Water ₁	3.97e-1	3.04e-1	1.15e-1
6	Water ₂	4.58e-2	5.22e-2	8.57e-2
9	Water ₃	1.81e-2	1.15e-2	1.02e-2
12	Water ₄	4.78e-3	1.34e-5	6.79e-6
20	Hexane ₁	4.48e-1	3.58e-1	2.36e-1
23	Water ₁ -Hexane ₁	2.18e-2	2.61e-2	3.18e-2
26	Water ₂ -Hexane ₁	4.90e-4	1.24e-3	5.27e-3
29	Water ₃ -Hexane ₁	1.29e-3	2.10e-3	3.40e-3
32	Water ₄ -Hexane ₁	5.45e-5	6.20e-5	4.20e-3
40	Hexane ₂	4.42e-2	3.70e-2	5.42e-2
43	Water ₁ -Hexane ₂	1.82e-3	2.85e-3	1.10e-2
46	Water ₂ -Hexane ₂	0.00	3.63e-3	5.70e-2
60	Hexane ₃	7.58e-3	3.95e-3	9.25e-4
63	Water ₁ -Hexane ₃	1.09e-3	2.89e-3	6.61e-2
66	Water ₂ -Hexane ₃	0.00	8.33e-4	1.36e-3
80	Hexane ₄	3.13e-4	2.69e-5	0.00
83	Water ₁ -Hexane ₄	1.63e-4	9.78e-2	2.41e-1
86	Water ₂ -Hexane ₄	6.81e-3	9.57e-2	7.60e-2

Table S2: Clusters' probability

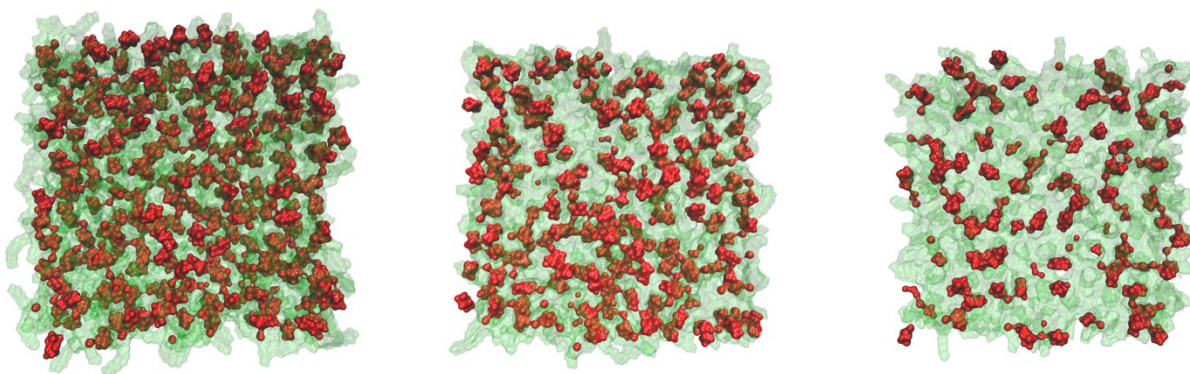


Figure S1: Snapshots of the simulation boxes for neat trihexyl, tetradecylphosphonium bis(trifluoromethyl-sulfonyl) amide at three different pressures, only a slice of 15 Å thickness is shown for clarity. 1 bar (left); 5 kbar (centre); 10 kbar (right). The domains are reported in different colours. Apolar (green, transparent); polar (red, opaque).

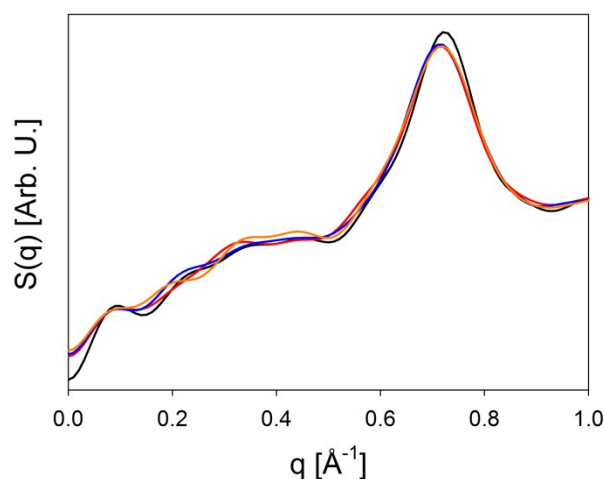


Figure S2: Partial $S(q)$ considering just the CF_3 on the anion for the systems studied. PTF (black); PWA (red); PHE (blue); PWH (orange)

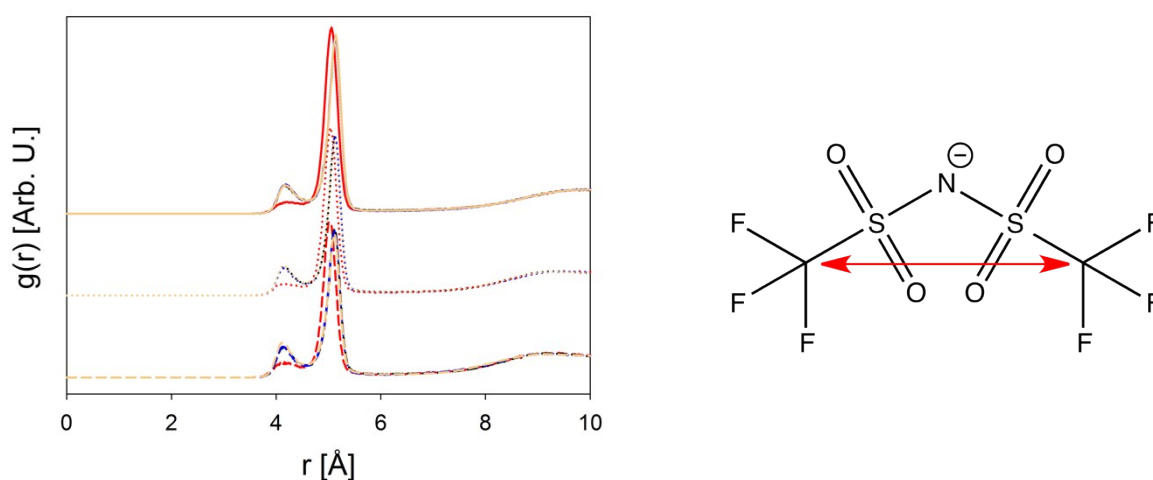


Figure S3: (left) Pair distribution functions for the correlation indicated by the red arrow in the right panel. PTF (black); PWA (red); PHE (blue); PWH (orange). 1 bar (solid line); 5 kbar (dotted line); 10 kbar (dashed line). Curves for different pressures are vertically shifted for clarity.

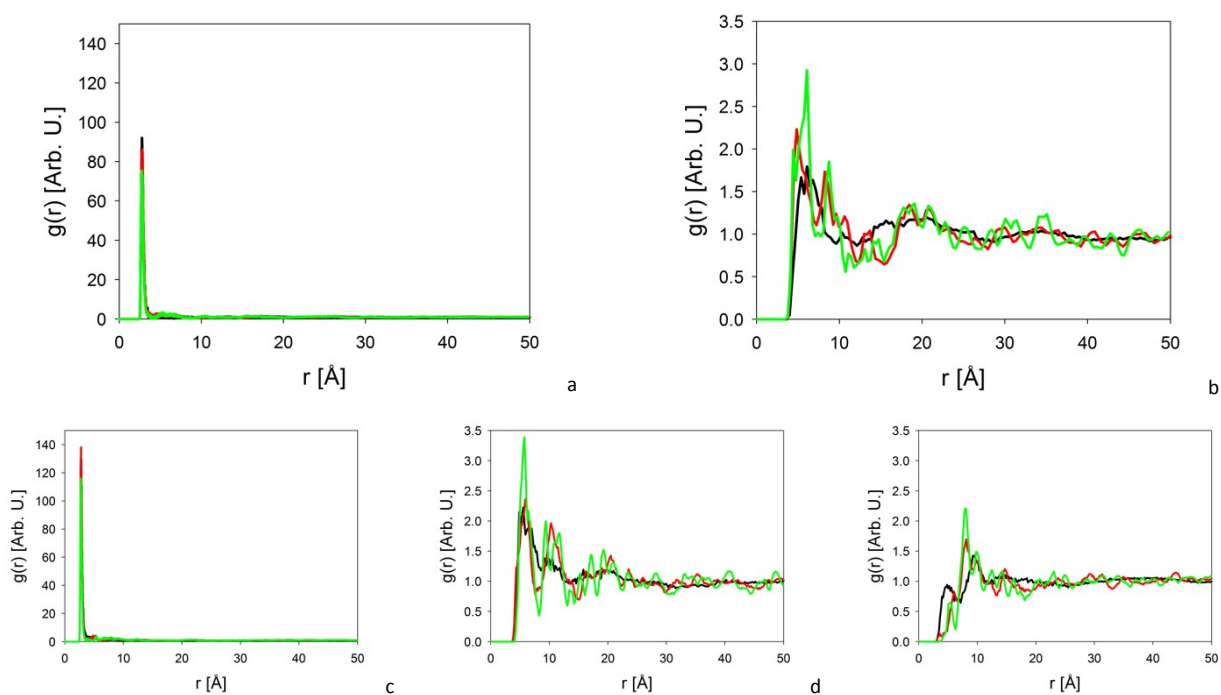


Figure S4: Pair distribution functions for the centers of mass. (a) PWA water-water; (b) PHE hexane-hexane; (c) PWH water-water; (d) PWH hexane-hexane; (e) PWH water-hexane. 1 bar (black); 5 kbar (red); 10 kbar (green).