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

Supporting Information

A neutron scattering and modelling study of aqueous solutions of tetramethylammonium and tetrapropylammonium bromide

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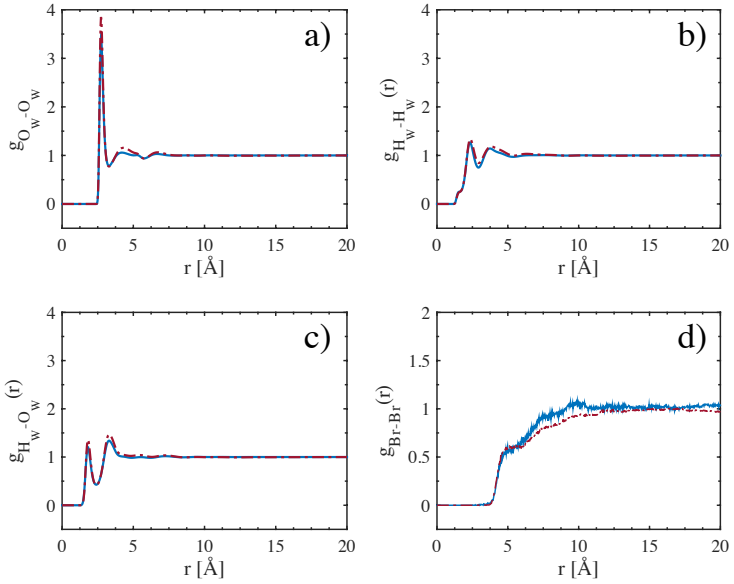

***Figure S1**: Radial distributions of the bromide and water for both the TMABr (solid blue line) and TPABr (dot-dashed red line) in water.*

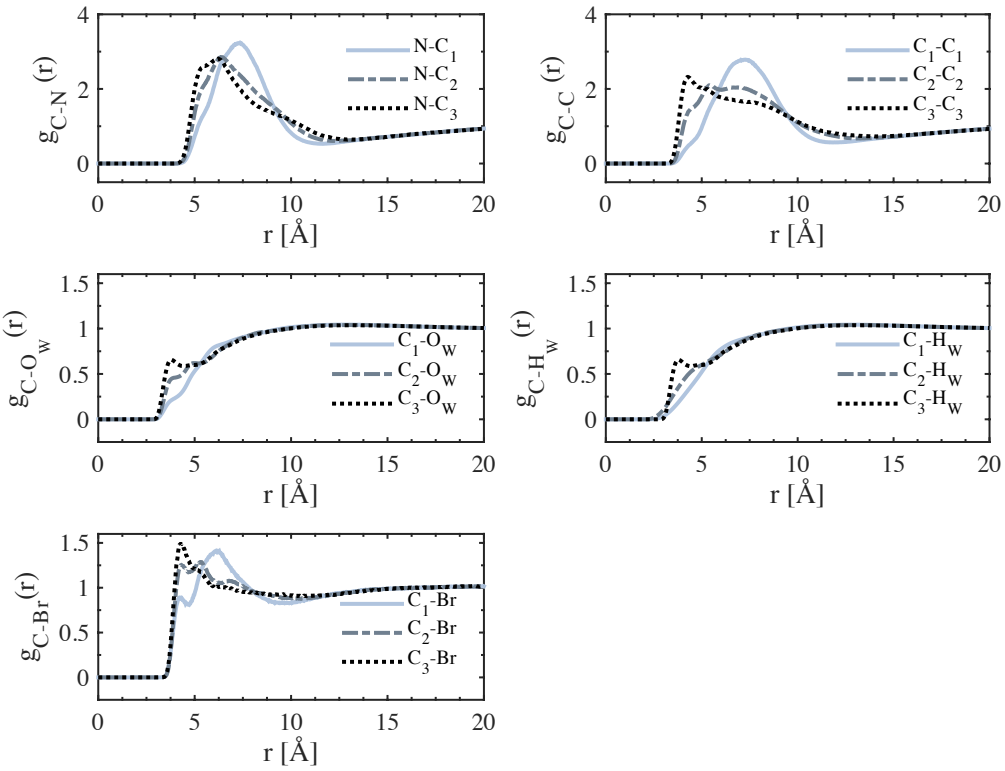

Figure S2: *Radial distributions of the three different carbons in TPABr in water.*

Table S1: Coordination number for 0.4 M TMABr in water, between R_{min} and R_{max}.

pair-correlation	R_{min}	R_{max}	Number of atoms	Standard error
N – N	4.5	7.5	0.94	±1.2
	4.5	10.5	1.9	±1.8
N – C_1	3.6	6.0	1.4	±2.0
	3.6	8.5	4.8	±5.3
N – Br	3.4	6.5	0.48	±0.65
N – O_W	3.0	6.0	23	±3.8
N – H_W	3.0	6.4	7.3	±16
C_1 – C_1	3.0	4.7	0.36	±0.80
	3.0	9.1	5.5	±5.8
	3.0	12.5	11	±9.0
C_1 – Br	3.0	5.0	0.19	±0.41
Br – O_W	2.7	3.3	1.8	±1.0
Br – O_W	2.7	4.6	11	±2.2
Br – H_W	1.5	3.0	4.6	±1.3
Br – Br	3.5	5.9	0.079	±0.28
Br – Br	3.5	10.5	1.0	±0.99
O_W – O_W	2.3	3.3	4.3	±1.2
H_W – H_W	1.2	3.0	6.3	±1.6
O_W – H_W	1.3	2.4	2.0	±0.87

Table S2: Coordination numbers for 0.4 M TPABr in water, between R_{min} and R_{max}.

pair-correlation	R_{min}	R_{max}	Number of atoms	Standard error
N – N	5.0	10.6	2.0	±1.3
N – C_3	3.9	8.3	4.1	±2.8
	3.9	12.6	9.6	±5.7
N – C_1	3.9	11.3	8.3	±5.4
N – C_2	3.9	12.0	8.9	±5.5
N – Br	3.9	5.8	0.15	±0.38
	3.9	8.6	0.66	±0.76
N – O_W	3.5	7.4	31	±6.1
	3.5	10.4	0.00	±0.00
N – H_W	3.2	7.9	0.52	±4.8
	3.2	9.5	0.00	±0.00
C_3 – C_3	3.1	5.9	3.1	±1.6
	3.1	13.8	13.9	±6.1
C_1 – C_1	3.1	11.7	8.7	±5.5
C_2 – C_2	3.1	6.0	3.6	±1.4
	3.1	13.3	13	±6.0
C_3 – Br	3.2	4.9	0.085	±0.29
	3.2	6.0	0.20	±0.43
C_1 – Br	3.2	4.7	0.040	±0.20
	3.2	9.5	0.85	±0.86
C_2 – Br	3.2	4.8	0.066	±0.25
	3.2	6.2	0.22	±0.45
Br – H_W	1.5	3.0	4.3	±1.3
Br – Br	5.7	2.0	0.0	±0.00
	3.5	8.5	0.39	±0.60
	3.5	10.8	0.98	±0.92
O_W – O_W	2.3	3.3	4.4	±1.2
H_W – H_W	1.2	3.0	6.44	±1.7
O_W – H_W	1.3	2.4	1.98	±0.88
Br - O_W	2.7	3.3	1.76	±1.0
Br – O_W	2.7	4.6	10	±2.4

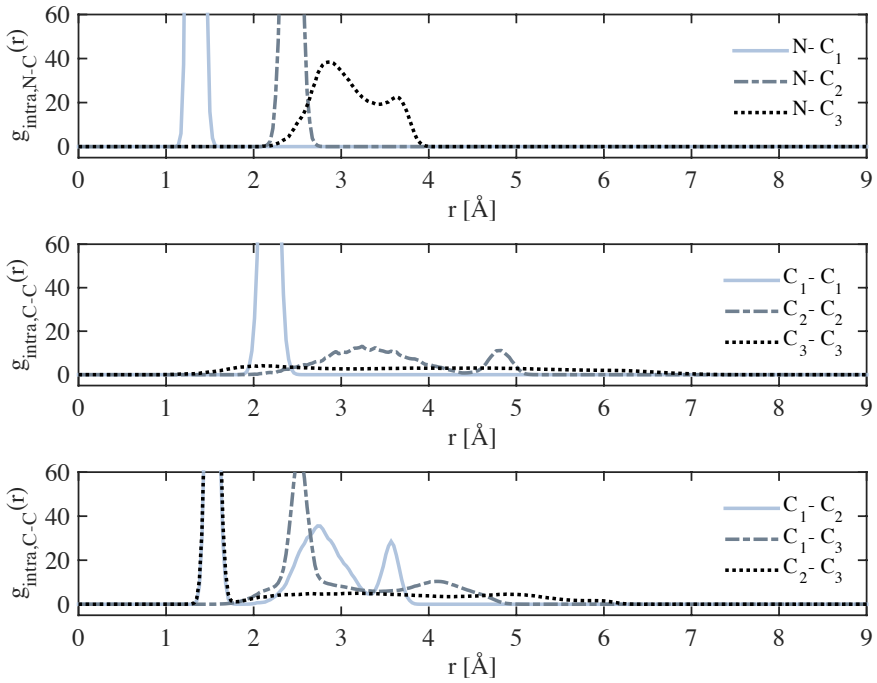

***Figure S3**: Internal partial radial distribution functions for nitrogen and carbons within the same TPA^+ molecule.*

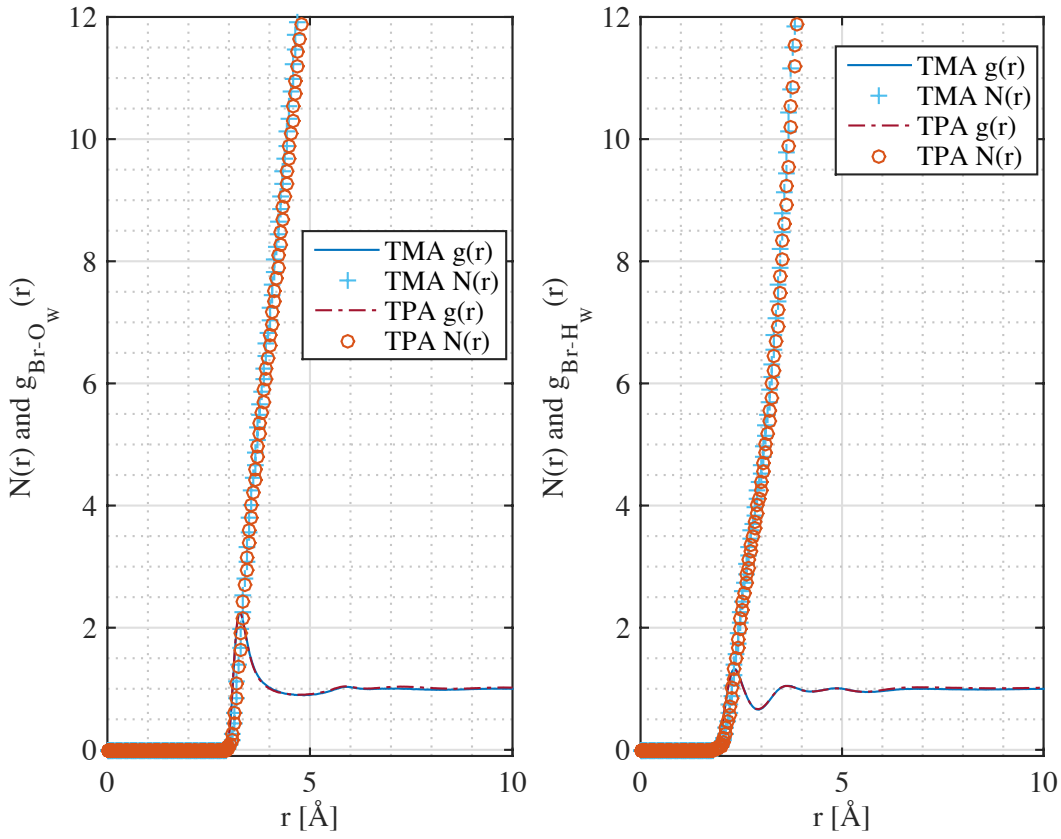

***Figure S4**: RDFs for bromide-water and the corresponding coordination number. N(r).*