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

ESI for:

X-Ray and Molecular Dynamics Studies of Butylammonium Butanoate-Water Binary Mixtures

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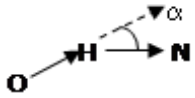
Online Supplementary Information

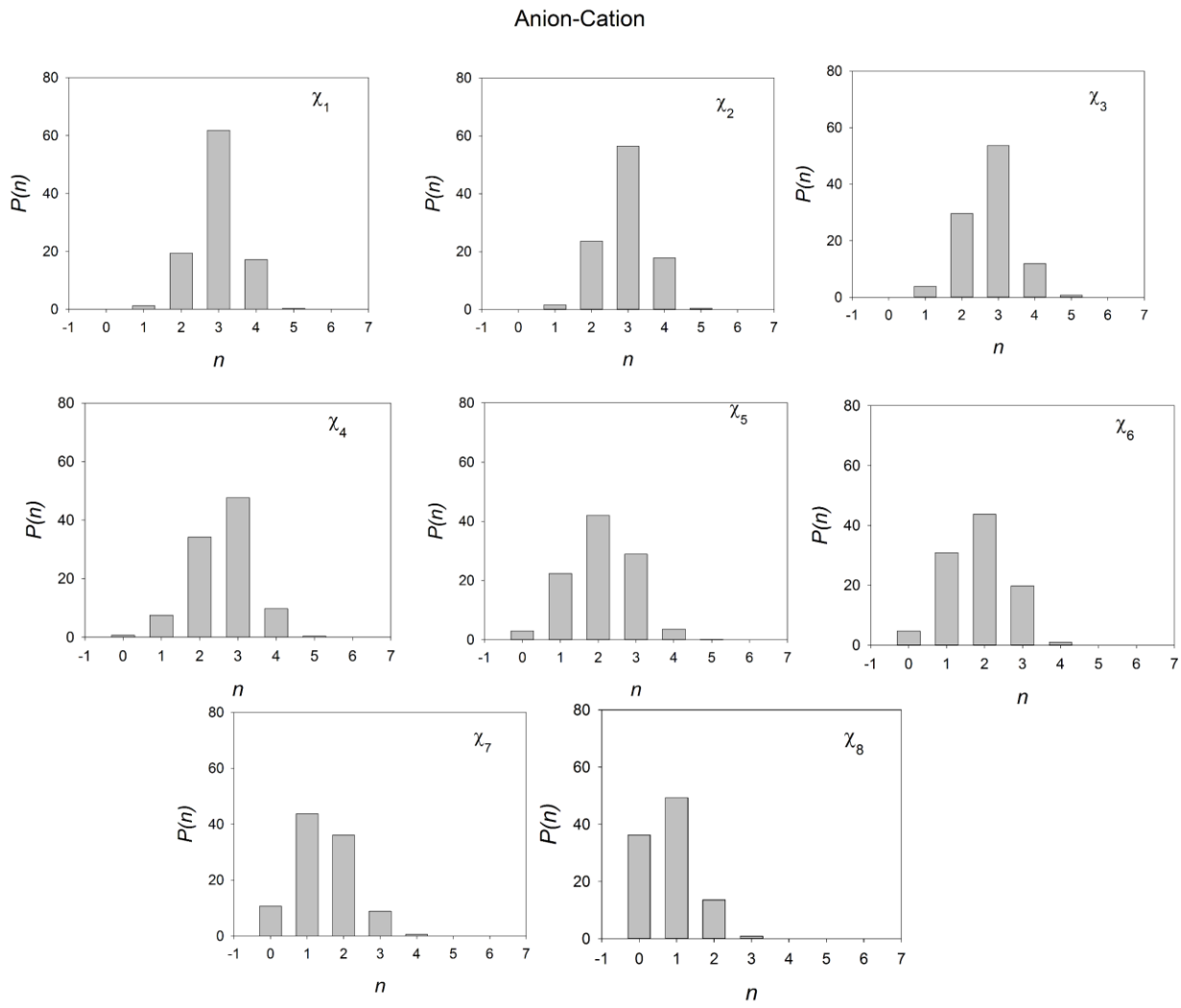
Details on H-bonds analysis

The MD trajectories were scanned with Travis software to look for hydrogen bonds. For the three possible triplets (N-H----O water, O---H-O water and N-H---O anion), a given contact was considered as

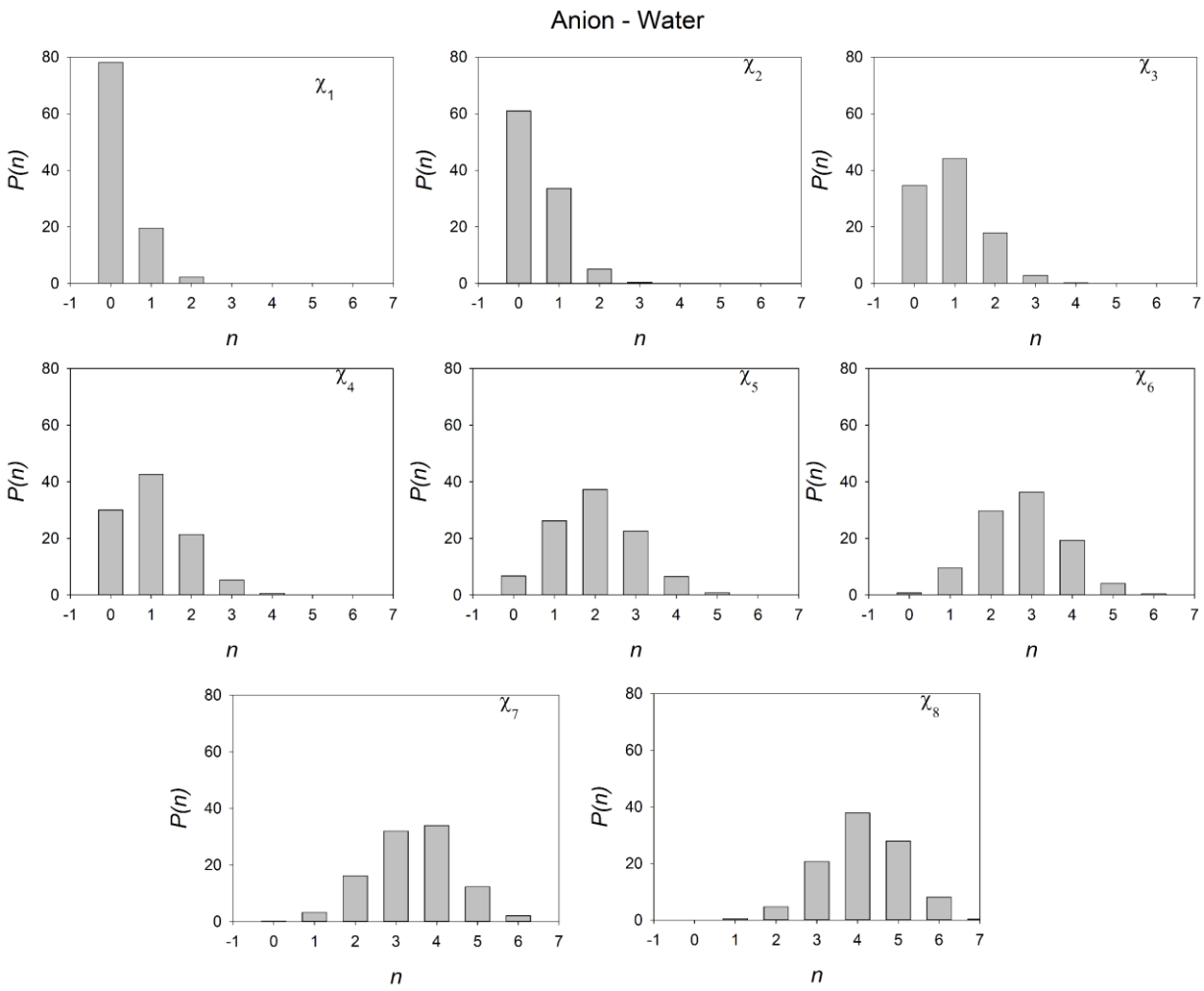


H-bond if the distance and angle cutoffs (3.5 Å and 30 degrees, respectively) were satisfied for the donor-acceptor distance and the hydrogen bond angle α.

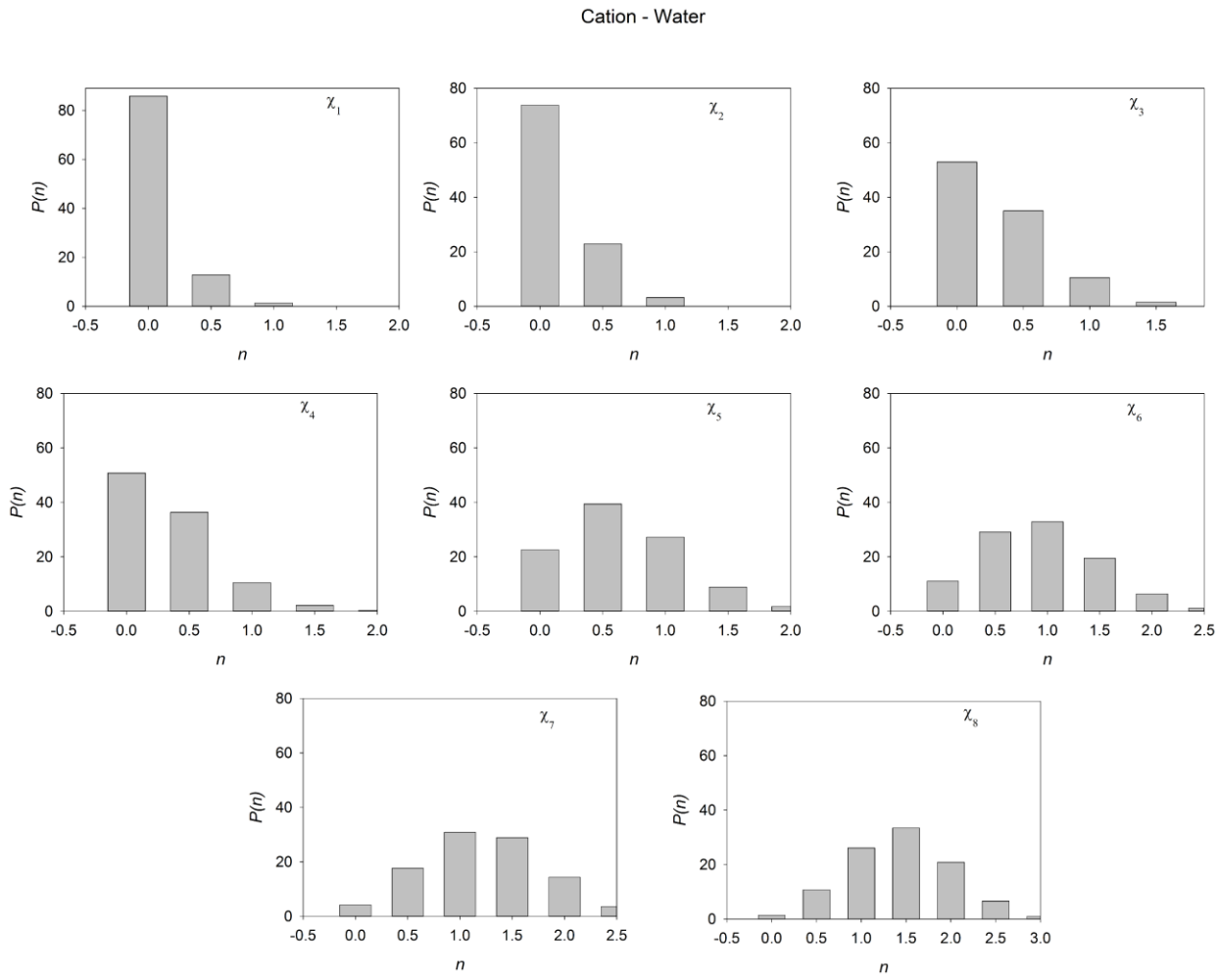
In the following pictures, the percent frequencies of occurrence *(P(n))* of a given number *(n)* of HB contacts relative to the total number of interactions are grouped into histograms. The data are reported for anion-cation (a), anion-water (b) and cation-water (c) at increasing water concentration from χ_1 to χ_8. The histogram bin size is 1 for a-b and 0.5 for c (according to the lesser solvation of cations).



(a)



(b)



(c)

Figure S1. Anion-cation (a), anion-water (b) and cation-water (c) coordination number (n) distribution calculated from the MD simulation of $[N_{0004}][C_3CO_2]$-water mixtures at different concentrations.

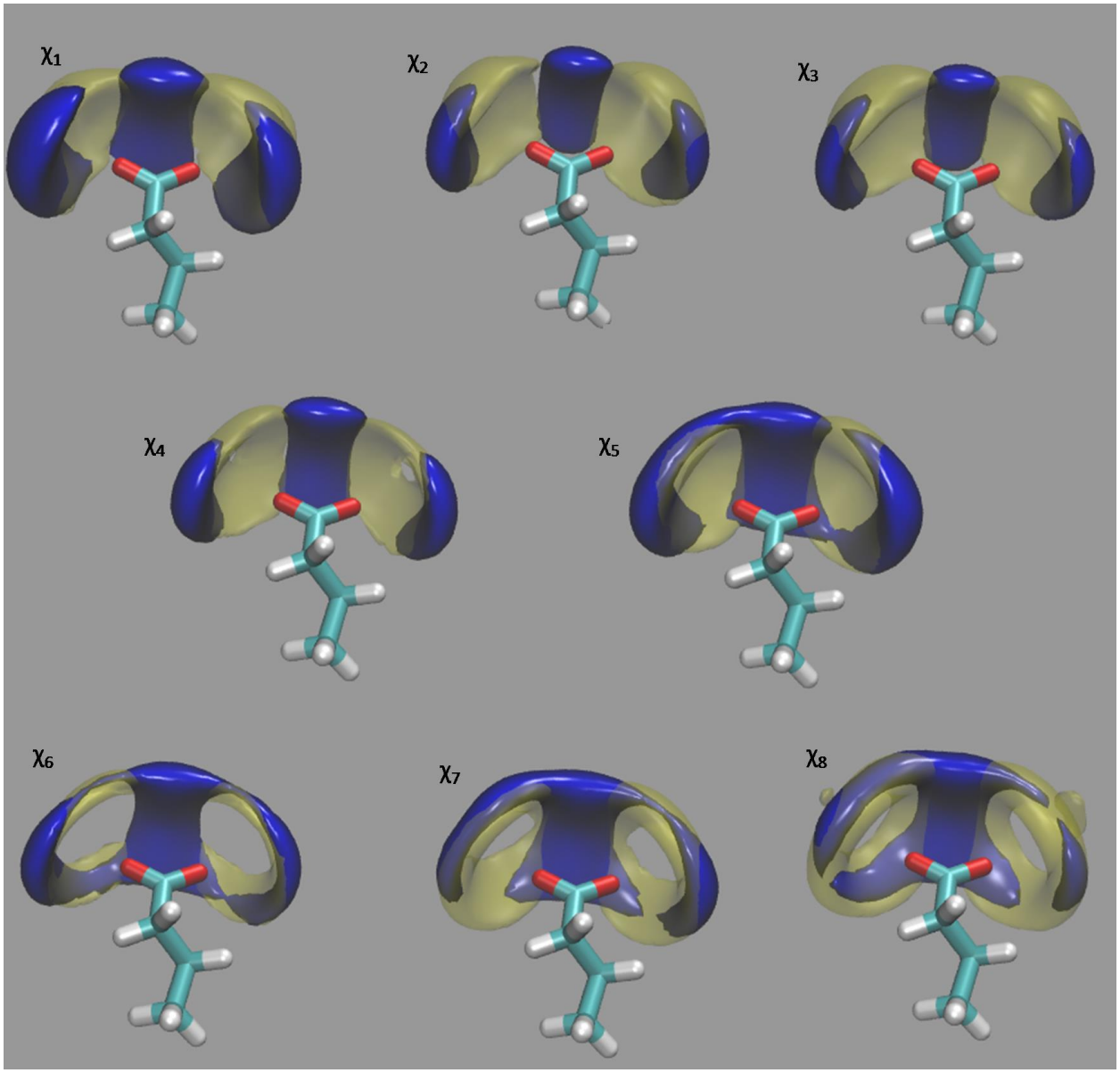


Figure S2. Spatial distribution functions of atoms of cation and water around a butanoate anion. Clouds are plotted for an isosurface of nitrogen of cation (blue) and oxygen of water (yellow) at all concentrations of water in $[N_{0\ 0\ 0\ 4}][C_3CO_2]$. The Isosurface values of cation and water around the anion are between 6-2.012 nm^{-3} from χ_1 to χ_8 mixtures. The TRAVIS and VMD software are used to generate the figures.

Table S1. AMBER PARAMETERS (GAFF) of ALKYLAMMONIUM ALKANOATES + TIP4P WATER

(Amber format)

Atom names, types and charges (AMBER format)

Atom	Charge	Mass	Residue	Type
N1	-0.37720	14.0	CAT	n4
H1	0.32992	1.0	CAT	hn
H2	0.32992	1.0	CAT	hn
H3	0.32992	1.0	CAT	hn
C1	0.10560	12.0	CAT	c3
H4	0.08112	1.0	CAT	hx
H5	0.08112	1.0	CAT	hx
C2	-0.17462	12.0	CAT	c3
H6	0.07326	1.0	CAT	hc
H7	0.07326	1.0	CAT	hc
C3	0.08743	12.0	CAT	c3
H8	0.02277	1.0	CAT	hc
H9	0.02277	1.0	CAT	hc
C4	-0.20996	12.0	CAT	c3
H10	0.07490	1.0	CAT	hc
H11	0.07490	1.0	CAT	hc
H12	0.07490	1.0	CAT	hc
C1	-0.28657	12.0	ANI	c3
H1	0.03501	1.0	ANI	hc
H2	0.03501	1.0	ANI	hc
H3	0.03501	1.0	ANI	hc
C2	0.25305	12.0	ANI	c3
H4	-0.05319	1.0	ANI	hc
H5	-0.05319	1.0	ANI	hc
C3	-0.14424	12.0	ANI	c3
H6	-0.01283	1.0	ANI	hc
H7	-0.01283	1.0	ANI	hc
C4	0.67439	12.0	ANI	c
O2	-0.73482	16.0	ANI	o
O1	-0.73482	16.0	ANI	o
O	0.00000	16.0	WAT	OW
H1	0.52422	1.0	WAT	HW
H2	0.52422	1.0	WAT	HW
EPW	-1.04844	0.0	WAT	EP

MASS

n4	14.010	0.000
hn	1.008	0.000
c3	12.010	0.000
hx	1.008	0.000
hc	1.008	0.000
c	12.010	0.000
o	16.000	0.000
OW	16.000	0.000
HW	1.008	0.000
EP	0.000	0.000

BOND

c3-hc	337.300	1.092
c3-c3	303.100	1.535
c3-hx	338.700	1.091
hn-n4	369.000	1.033
c3-n4	293.600	1.499
c -o	648.000	1.260
c -c3	328.300	1.508
HW-HW	553.000	1.514
EP-OW	553.000	0.125
HW-OW	553.000	0.957

ANGLE

hc-c3-hc	39.430	108.350
c3-c3-hc	46.370	110.050
c3-c3-c3	63.210	110.630
c3-c3-hx	46.020	111.740
hx-c3-hx	39.040	110.740
c3-n4-hn	46.190	110.110
hn-n4-hn	40.520	108.110
hx-c3-n4	49.020	107.910
c3-c3-n4	64.450	114.320
o -c -o	78.170	130.380
c -c3-hc	47.200	109.680
c3-c -o	68.030	123.110
c -c3-c3	63.790	110.530

DIHEDRAL

hc-c3-c3-hc	1	0.150	0.000	3.000
c3-c3-c3-hc	1	0.160	0.000	3.000
hc-c3-c3-hx	1	0.156	0.000	3.000
c3-c3-c3-c3	1	0.200	180.000	-1.000
c3-c3-c3-c3	1	0.250	180.000	-2.000
c3-c3-c3-c3	1	0.180	0.000	3.000
hc-c3-c –o	1	0.800	0.000	-1.000
hc-c3-c –o	1	0.080	180.000	3.000
c3-c3-c –o	1	0.000	180.000	2.000
IMPROPER				
c3-o -c -o	1	1.100	180.000	2.000