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

Supplementary Information

Factors Affecting Bubble Size in Ionic Liquids

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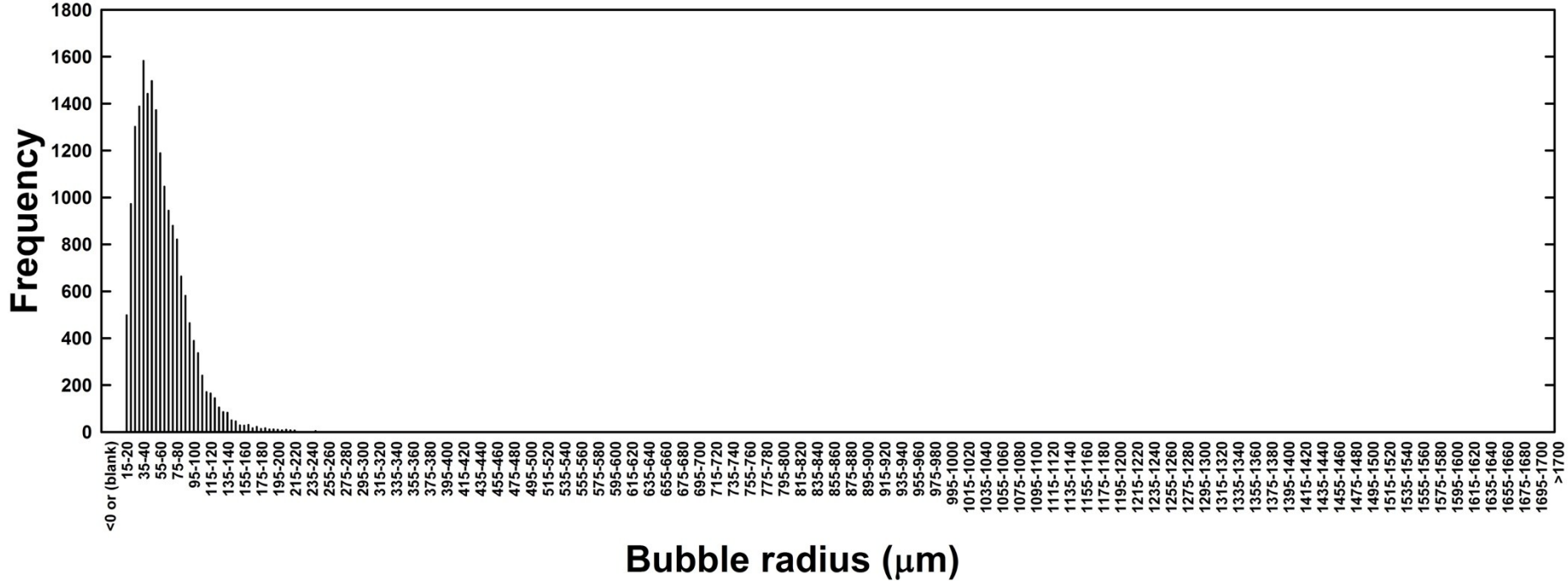

Figure S1. Bubble size distribution for [C_2mim][DCA]

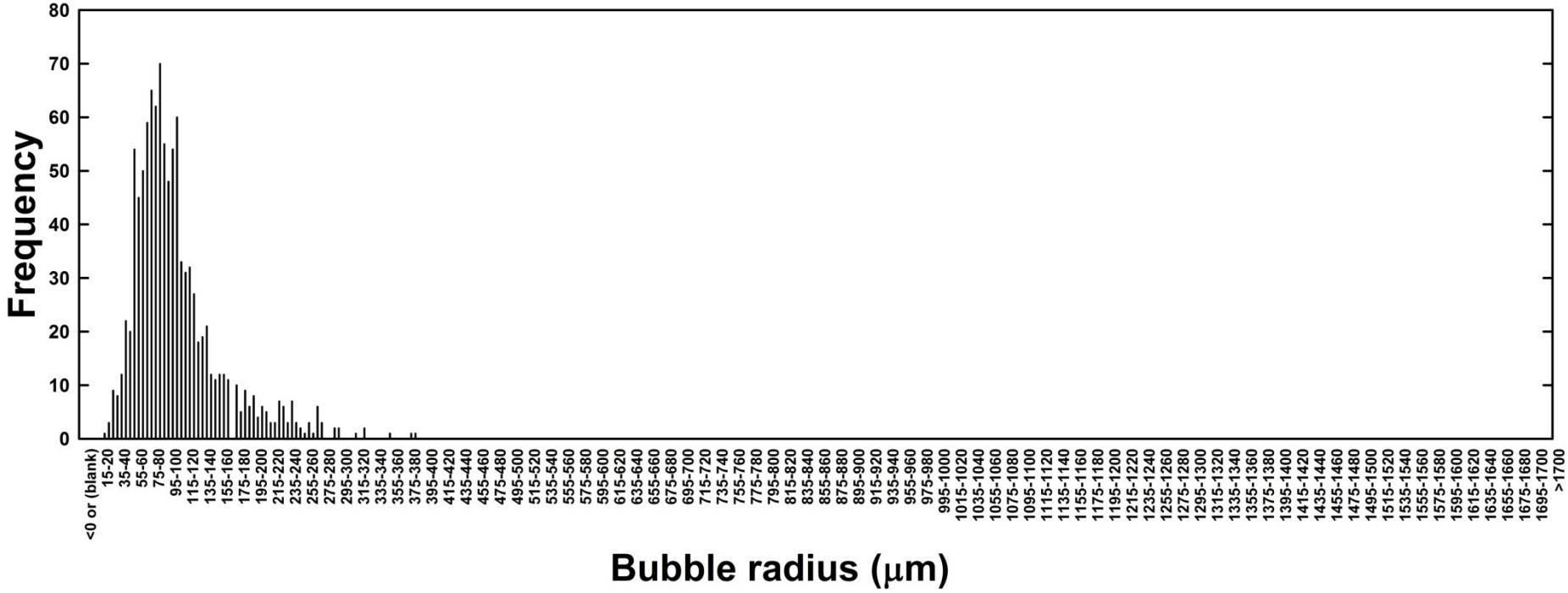

Figure S2. Bubble size distribution for $[C_2mim][EtSO_4]$

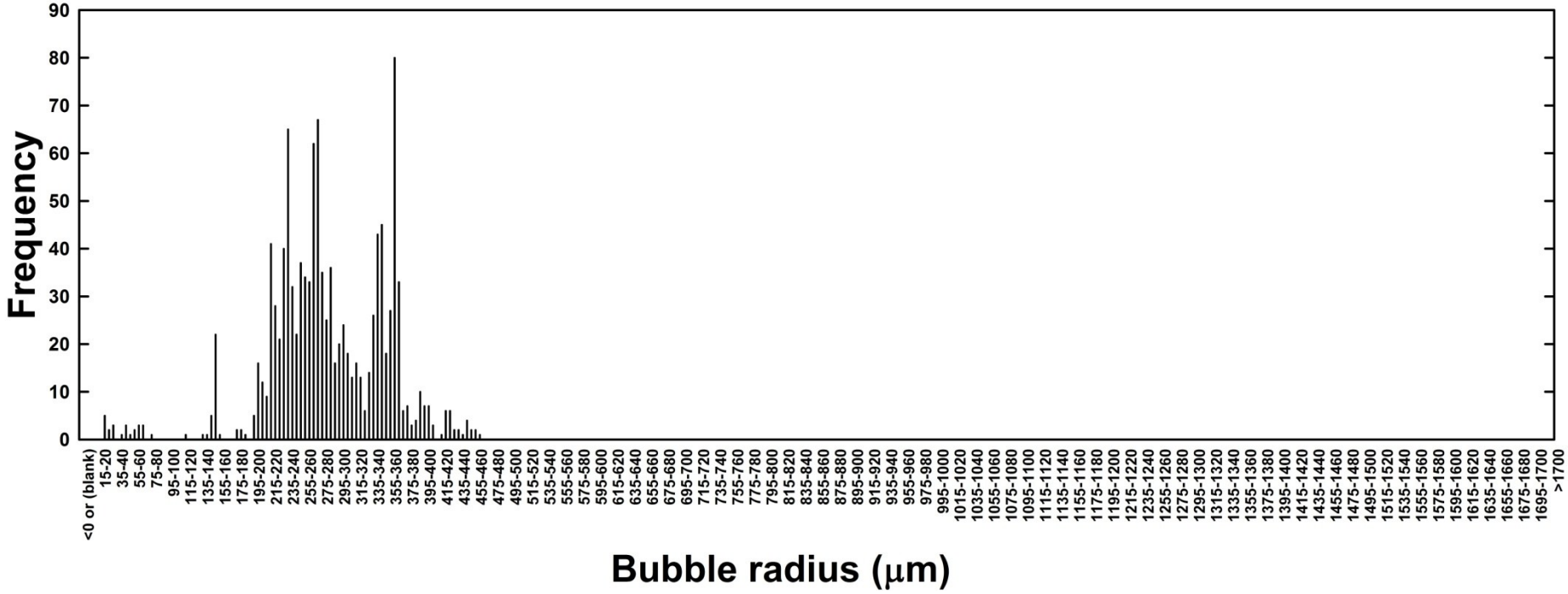

Figure S3. Bubble size distribution for $[C_2mim][NTf_2]$

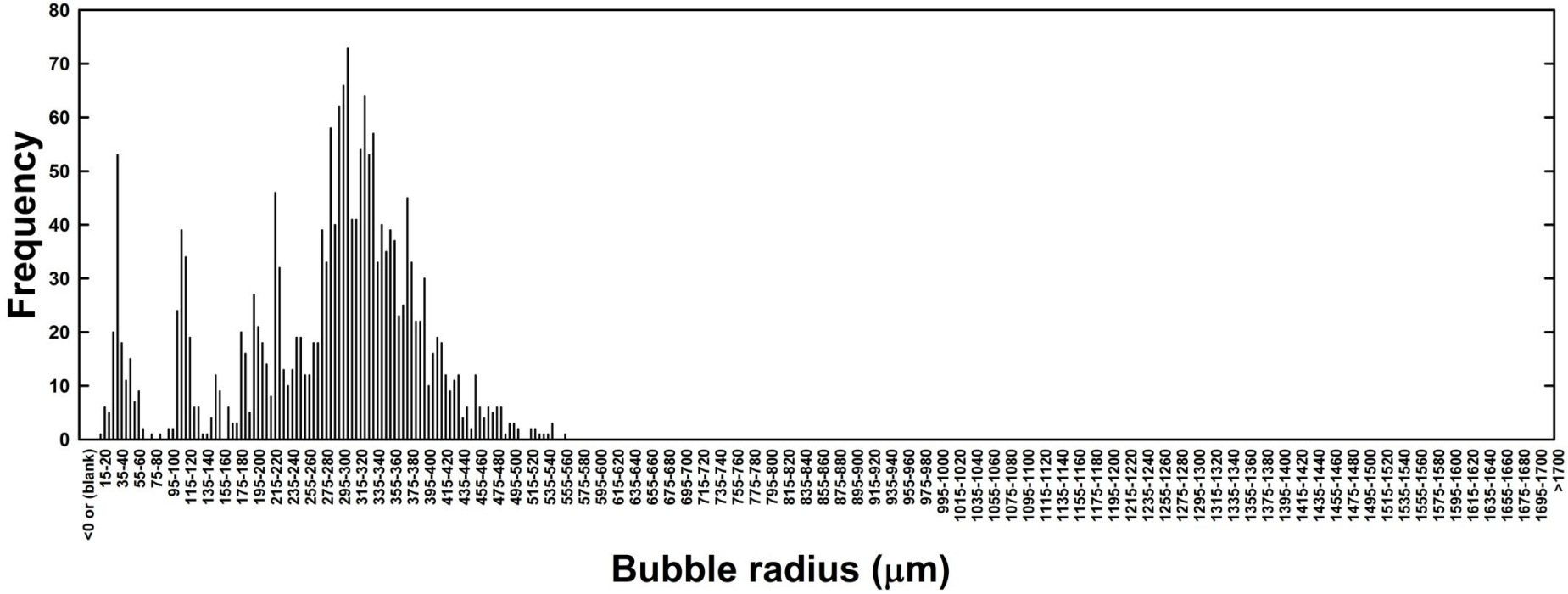

Figure S4. Bubble size distribution for $[C_4mim][NTf_2]$

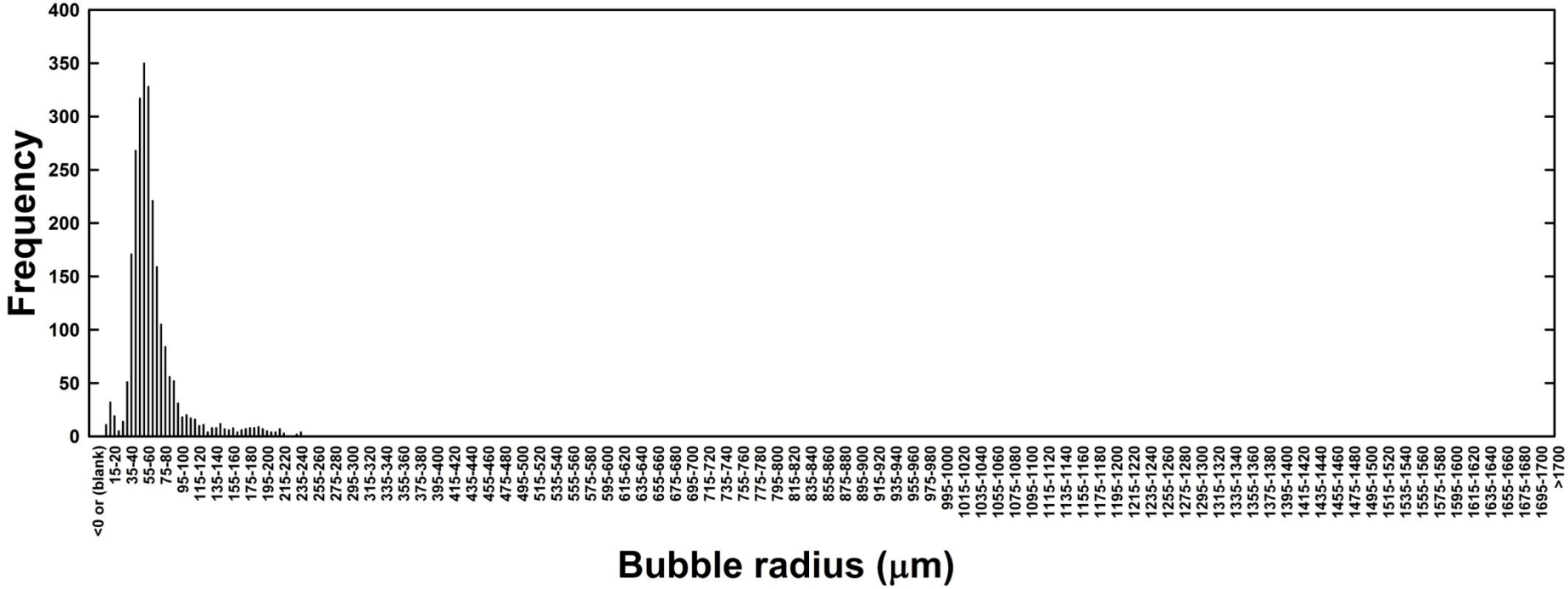

Figure S5. Bubble size distribution for [C_4mim][TFA]

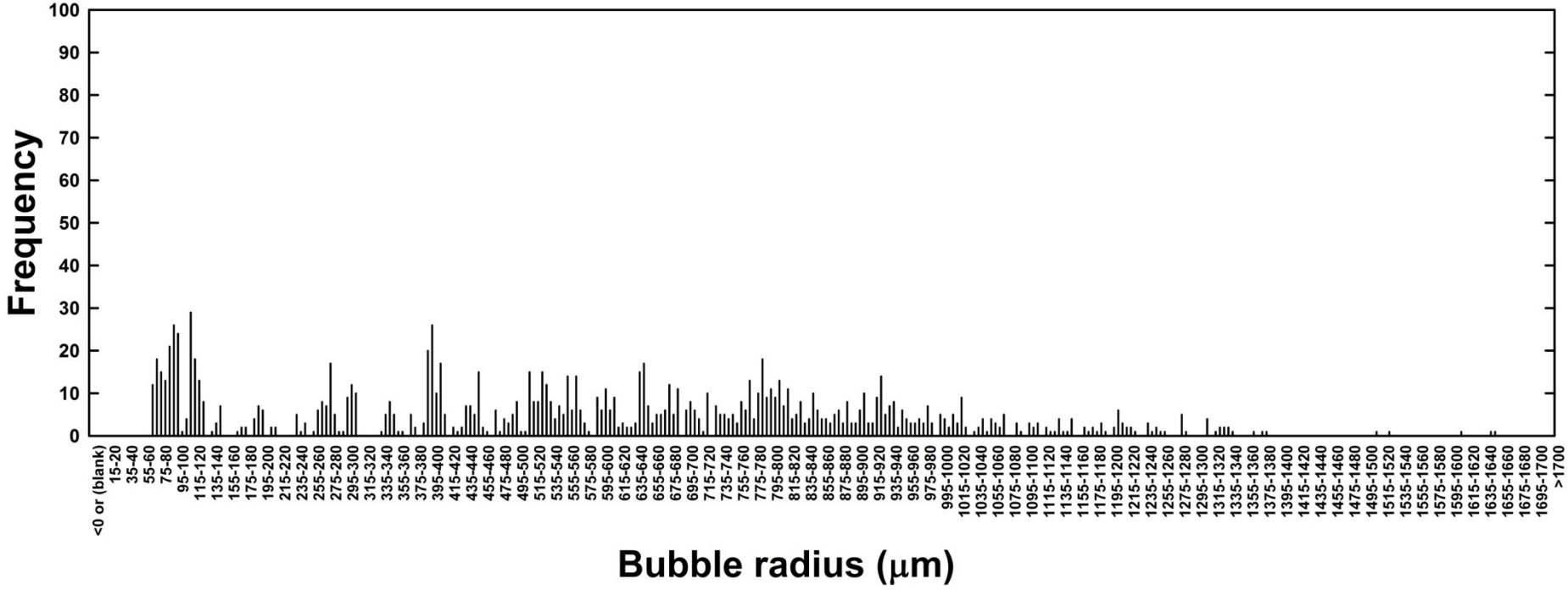

Figure S6. Bubble size distribution for $[P_{66614}]Br$

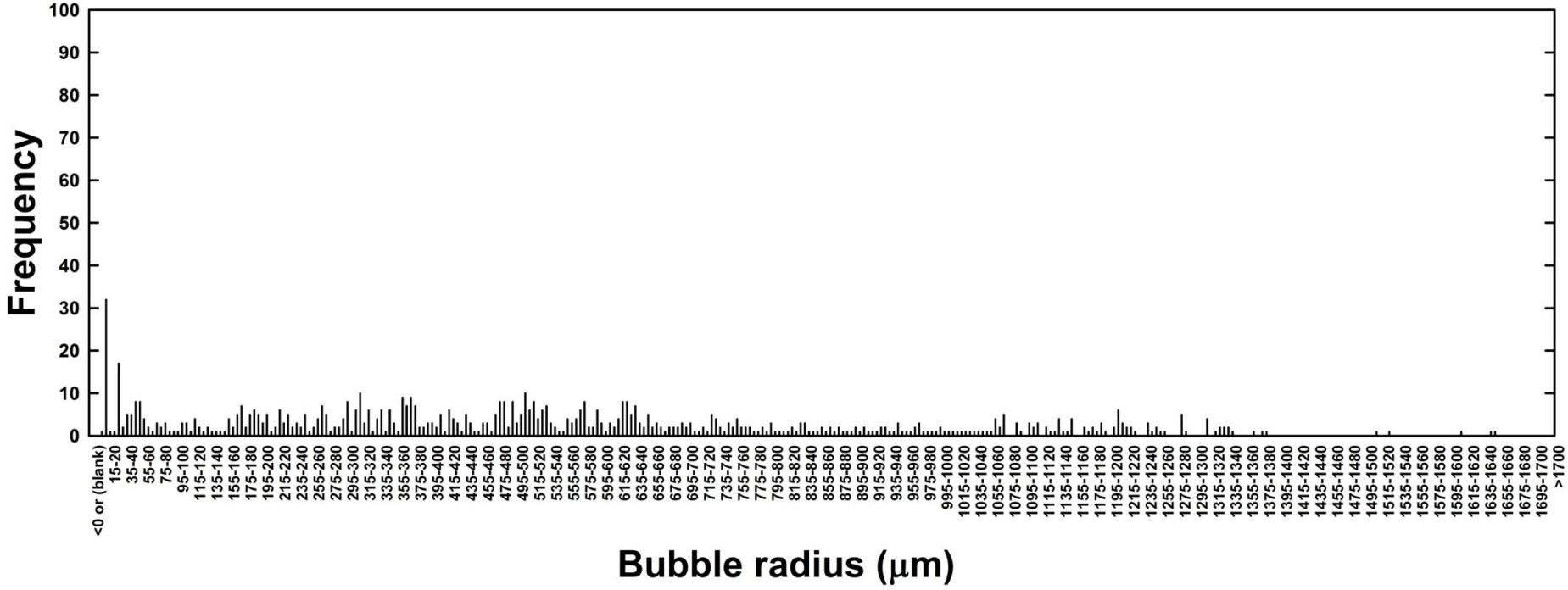

Figure S7. Bubble size distribution for $[P_{66614}]Cl$

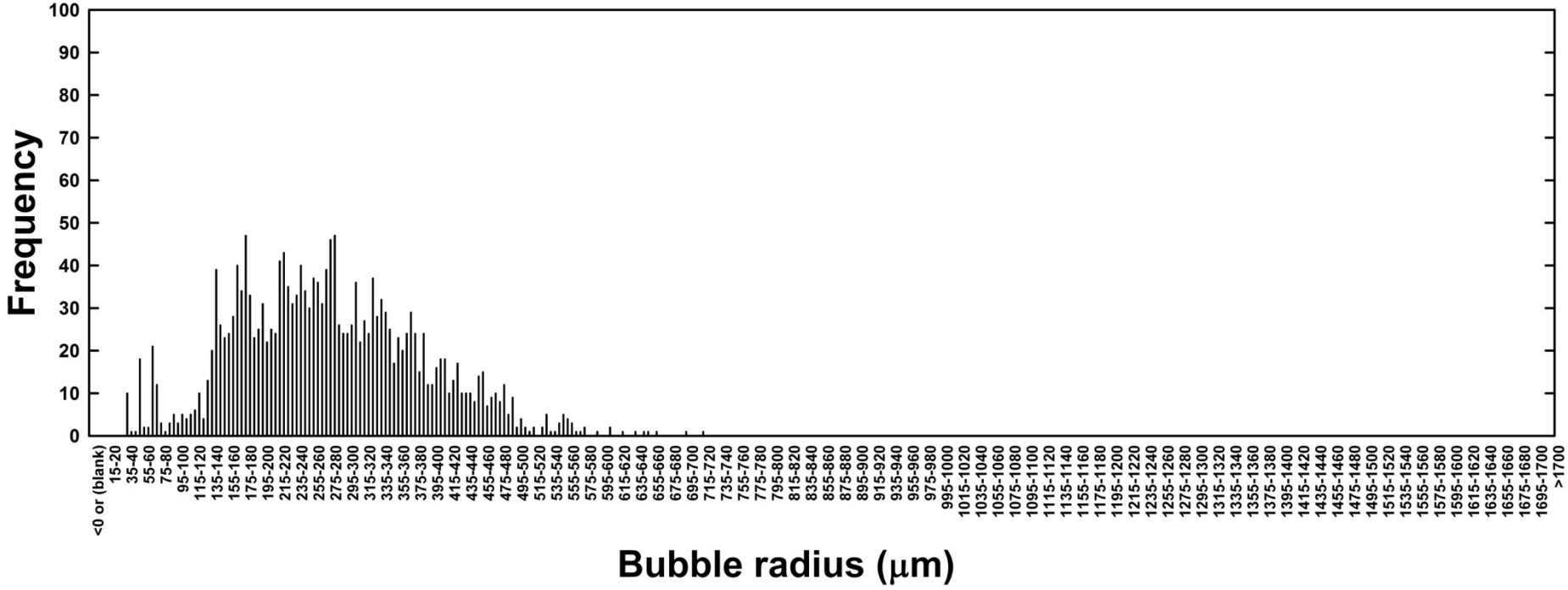

Figure S8. Bubble size distribution for $[P_{66614}][DCA]$

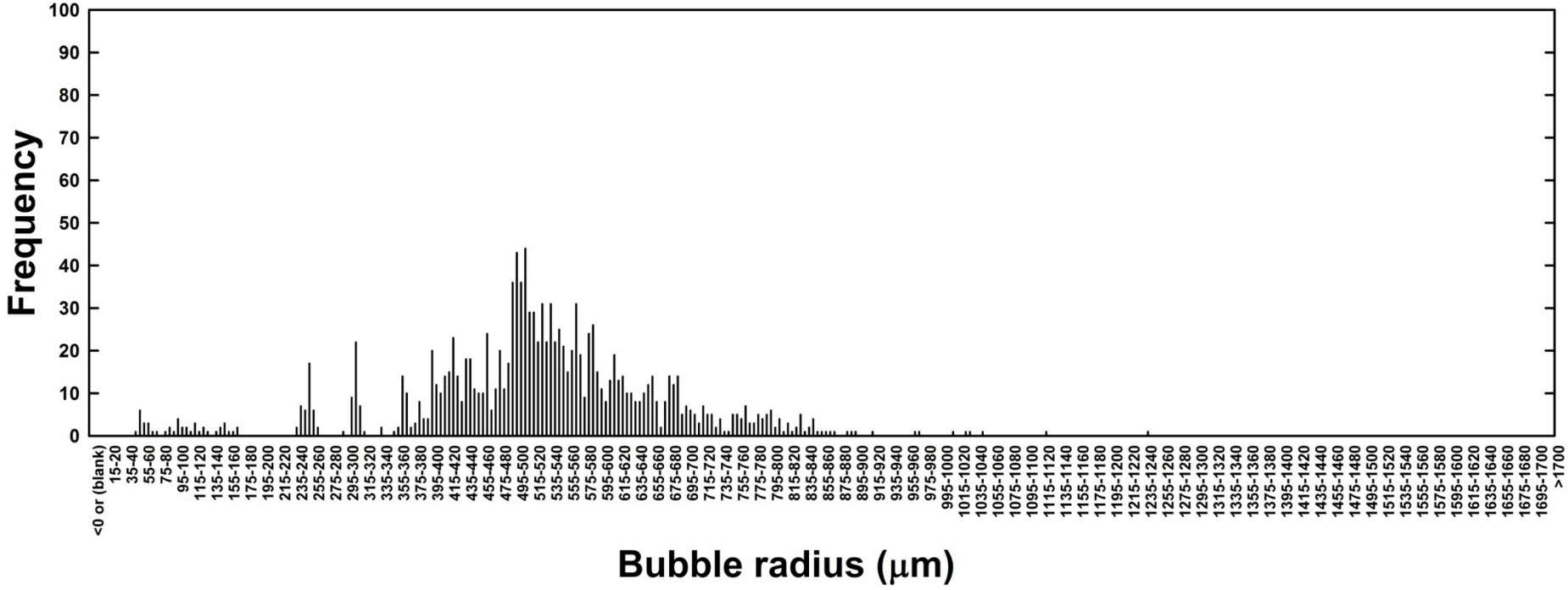

Figure S9. Bubble size distribution for [P_{66614}][Dec]

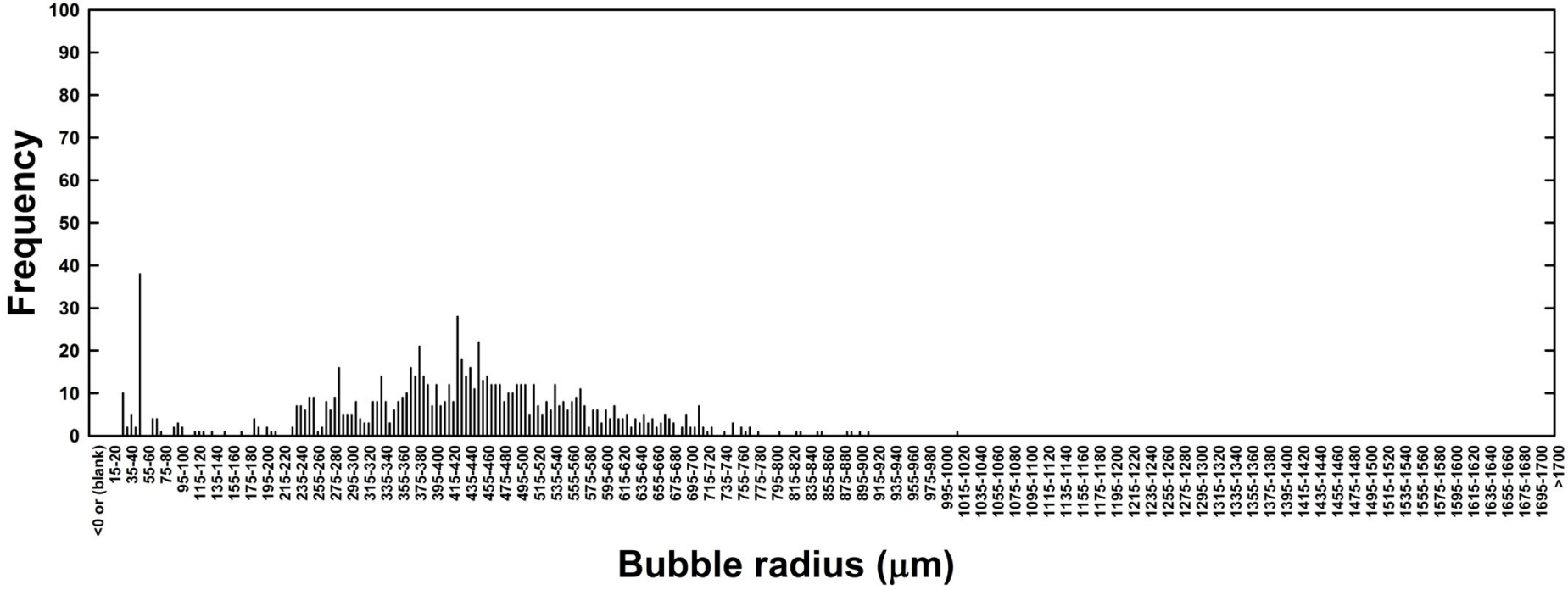

Figure S10. Bubble size distribution for $[P_{66614}][NTf_2]$

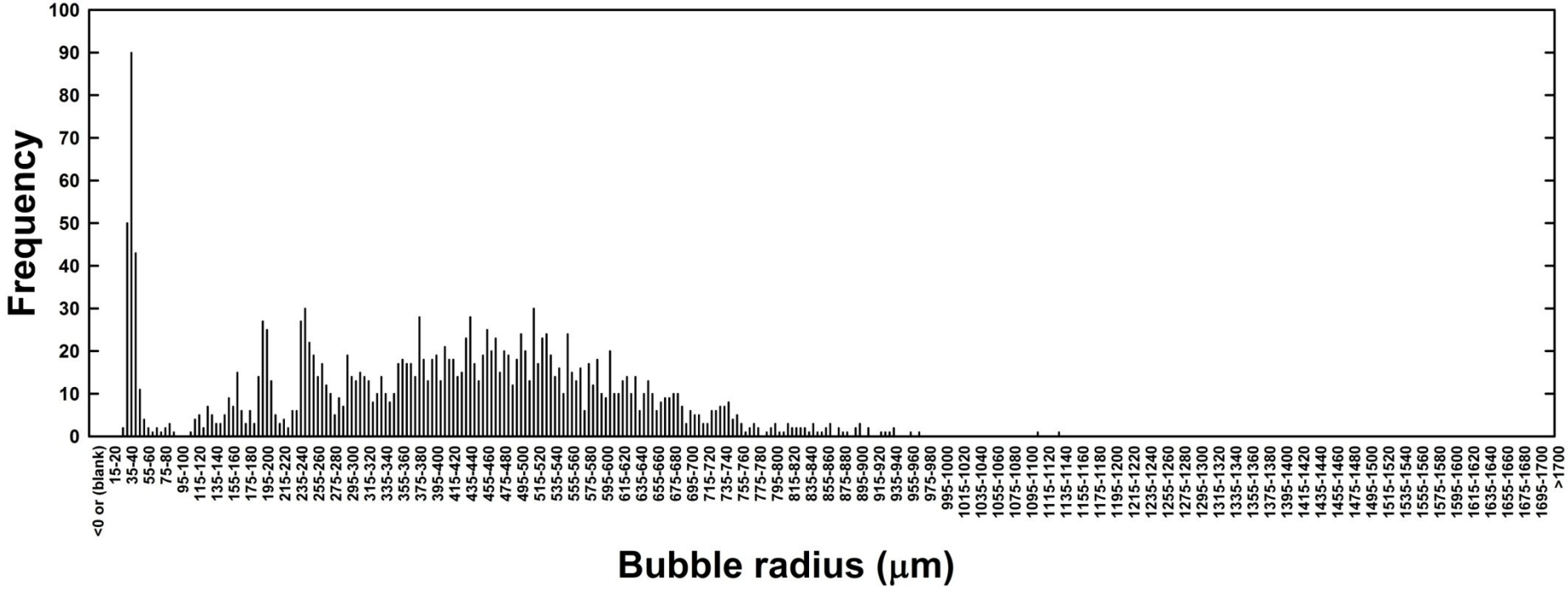

Figure S11. Bubble size distribution for [C_4mpyr][NTf_2]

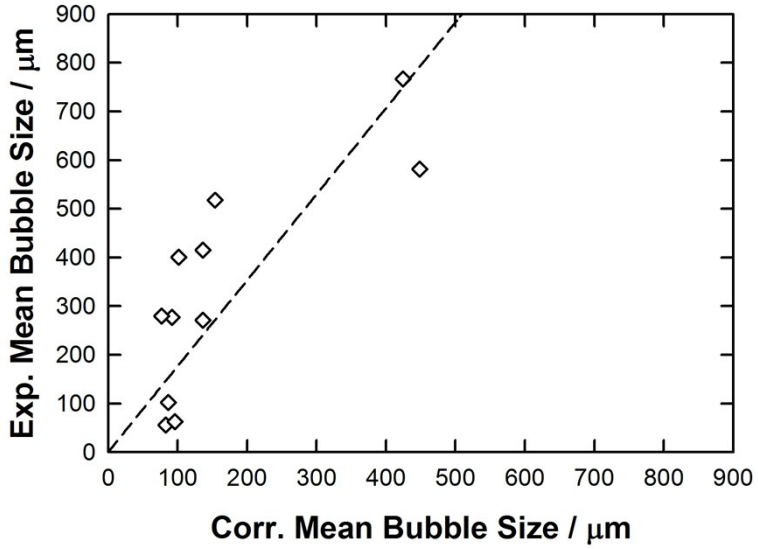

Figure S12. Parity plot between the experimental and correlated mean bubble size using Eq. 8 along with parameters reported in Table S1.

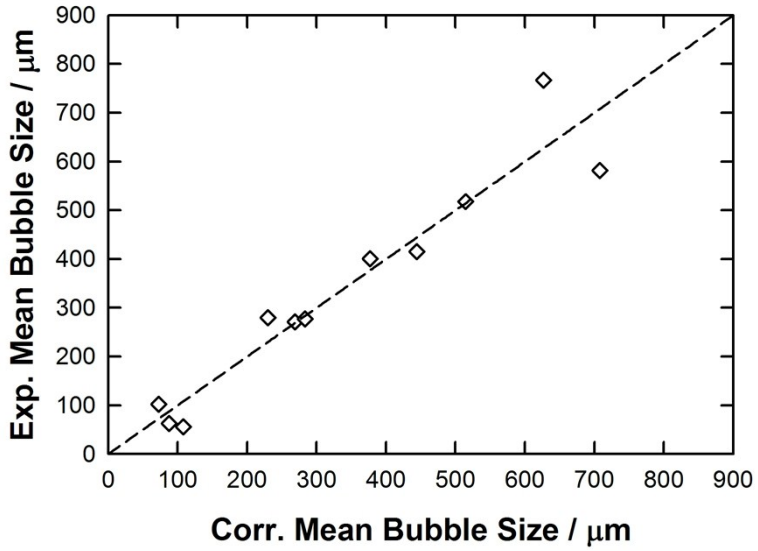

Figure S13. Parity plot between the experimental and correlated mean bubble size using Eqs. 8 and 10 along with parameters reported in Table S3.

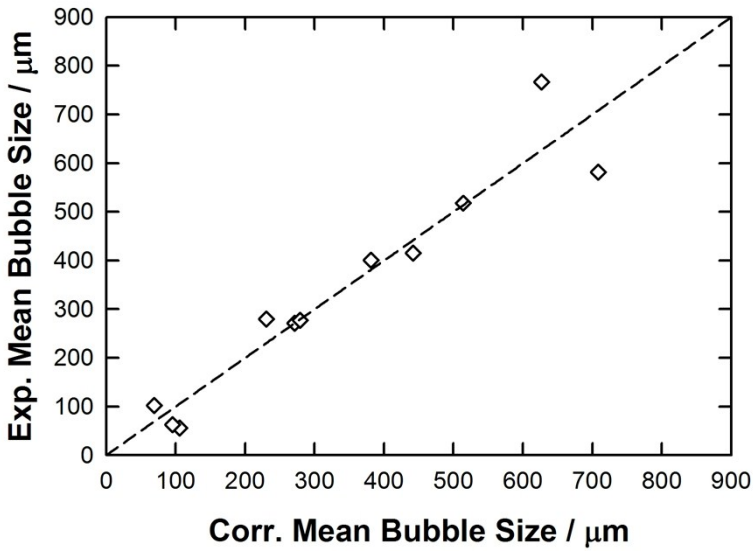

Figure S14. Parity plot between the experimental and correlated mean bubble size using Eqs. 8 and 10 along with parameters reported in Table S4.

Table S1. QSPR-type fitting parameters of the Eq. 8 and comparison between experimental and correlated mean bubble sizes.

a	*b*	*c*	*d*
+ 117.9	– 0.6694	+ 0.6247	0
	Mean bubble radius (μm)		RAD[a]
	Experimental	Correlated	%
[C_2mim][DCA]	56.1	83.3	49
[C_4mim][TFA]	62.9	96.1	53
[C_2mim][$EtSO_4$]	102.0	86.4	15
[P_{66614}][DCA]	270.9	136.6	50
[C_4mim][NTf_2]	276.9	92.1	67
[C_2mim][NTf_2]	279.4	76.8	73
[C_4mpyr][NTf_2]	400.6	101.6	75
[P_{66614}][NTf_2]	415.4	136.4	67
[P_{66614}][Dec]	517.7	153.9	70
[P_{66614}]Br	582.1	448.6	23
[P_{66614}]Cl	766.9	424.7	45

[a] Relative Absolute Deviation (RAD) calculated as follows:

$$RAD\ (\%) = 100 \cdot \frac{|Y_{exp.} - Y_{corr.}|}{Y_{exp.}} \quad (S1)$$

where $Y_{exp.}$ And $Y_{corr.}$ represent the experimental and correlated mean bubble sizes, respectively.

Table S2. Overall population of charge per region for the selected ILs.

	Region 1	Region 2	Region 3	Region 4	Region 5	Region 6
[C_2mim][DCA]	0	20.083	140.119	57.559	53.981	0
[C_4mim][TFA]	0	20.053	162.895	95.427	39.643	2.423
[C_2mim][$EtSO_4$]	0	20.083	178.039	44.175	70.053	0
[P_{66614}][DCA]	0	3.846	494.981	299.388	53.981	0
[C_4mim][NTf_2]	0	20.066	193.090	174.279	42.853	0
[C_2mim][NTf_2]	0	20.096	167.173	157.647	42.853	0
[C_4mpyr][NTf_2]	0	5.817	214.516	169.270	42.853	0
[P_{66614}][NTf_2]	0	3.859	522.035	399.476	42.853	0
[P_{66614}][Dec]	0	3.846	604.569	371.779	23.810	21.367
[P_{66614}]Br	0	3.846	489.030	255.099	58.629	0
[P_{66614}]Cl	0	3.846	489.030	255.099	52.810	0

Table S3. QSPR-type fitting parameters combining the Eqs. 8 and 10, and comparison between experimental and correlated mean bubble sizes.

a	*b*	*c*	*d*	
+ 235.3	– 3.617	– 0.5584	+ 2.048	
e	*f*	*g*	*h*	*i*
– 12.19	– 4.507	+ 5.738	+ 16.05	+ 33.06
		Mean bubble radius (μm)		RAD[a]
		Experimental	Correlated	%
[C_2mim][DCA]		56.1	108.0	93
[C_4mim][TFA]		62.9	87.9	40
[C_2mim][$EtSO_4$]		102.0	72.7	29
[P_{66614}][DCA]		270.9	269.1	0.7
[C_4mim][NTf_2]		276.9	283.4	2.3
[C_2mim][NTf_2]		279.4	230.0	18
[C_4mpyr][NTf_2]		400.6	377.4	5.8
[P_{66614}][NTf_2]		415.4	444.4	7.0
[P_{66614}][Dec]		517.7	514.9	0.5
[P_{66614}]Br		582.1	708.2	22
[P_{66614}]Cl		766.9	627.1	18

[a] Relative Absolute Deviation (RAD) calculated using Eq. S1

Table S4. QSPR-type fitting parameters combining the Eqs. 8 and 10, and comparison between experimental and correlated mean bubble sizes.

a	*b*	*c*	*d*	
+ 230.1	– 3.253	– 0.7441	0	
e	*f*	*g*	*h*	*i*
– 12.38	– 3.721	+ 5.883	+ 14.96	+ 33.09
		Mean bubble radius (μm)		RAD[a]
		Experimental	Correlated	%
[C_2mim][DCA]		56.1	105.9	89
[C_4mim][TFA]		62.9	95.5	52
[C_2mim][$EtSO_4$]		102.0	69.4	32
[P_{66614}][DCA]		270.9	271.7	0.3
[C_4mim][NTf_2]		276.9	279.7	1.0
[C_2mim][NTf_2]		279.4	230.5	17
[C_4mpyr][NTf_2]		400.6	381.4	4.8
[P_{66614}][NTf_2]		415.4	441.8	6.4
[P_{66614}][Dec]		517.7	514.0	0.7
[P_{66614}]Br		582.1	708.4	22
[P_{66614}]Cl		766.9	627.0	18

[a] Relative Absolute Deviation (RAD) calculated using Eq. S1

Table S5. Sigma moments of selected ILs.

	Mean bubble radius (μm)	Area	M_1	M_2	M_3	M_4	M_5	M_6
$[C_2mim][DCA]$	56.1	263.18	0	216.463	114.914	375.141	366.940	835.345
$[C_4mim][TFA]$	62.9	310.38	0	218.720	141.621	452.868	570.656	1294.619
$[C_2mim][EtSO_4]$	102	300.02	0	247.018	151.462	428.912	431.630	905.203
$[P_{66614}][DCA]$	270.9	775.60	0	212.520	151.526	329.209	429.526	753.144
$[C_4mim][NTf_2]$	276.9	406.01	0	179.604	22.152	189.607	32.529	246.383
$[C_2mim][NTf_2]$	279.4	366.24	0	180.216	19.874	191.532	30.807	247.842
$[C_4mpyr][NTf_2]$	400.6	409.00	0	169.425	42.433	156.984	80.802	177.393
$[P_{66614}][NTf_2]$	415.4	878.66	0	176.272	56.486	145.600	93.394	165.641
$[P_{66614}][Dec]$	517.7	922.23	0	286.295	377.472	950.866	2018.458	4704.969
$[P_{66614}]Br$	582.1	732.39	0	250.005	249.085	531.723	817.867	1468.945
$[P_{66614}]Cl$	766.9	726.57	0	268.800	316.733	714.498	1257.229	2459.984
	Hb_acc1	Hb_acc2	Hb_acc3	Hb_acc4	Hb_don1	Hb_don2	Hb_don3	Hb_don4
$[C_2mim][DCA]$	0.258	25.932	15.666	7.559	-0.047	5.093	1.790	0.384
$[C_4mim][TFA]$	0.284	28.448	20.208	12.547	-0.046	5.056	1.776	0.385
$[C_2mim][EtSO_4]$	0.327	32.759	19.179	8.010	-0.047	5.093	1.790	0.384
$[P_{66614}][DCA]$	0.258	25.932	15.666	7.559	-0.002	0.794	0.009	0
$[C_4mim][NTf_2]$	0.074	8.415	1.759	0.080	-0.046	5.056	1.776	0.385
$[C_2mim][NTf_2]$	0.074	8.415	1.759	0.080	-0.047	5.093	1.790	0.384
$[C_4mpyr][NTf_2]$	0.074	8.415	1.759	0.080	-0.003	1.234	0.040	0
$[P_{66614}][NTf_2]$	0.074	8.415	1.759	0.080	-0.002	0.794	0.009	0
$[P_{66614}][Dec]$	0.469	46.992	38.072	29.495	-0.002	0.794	0.009	0
$[P_{66614}]Br$	0.414	41.370	29.644	17.919	-0.002	0.794	0.009	0
$[P_{66614}]Cl$	0.472	47.190	36.628	26.066	-0.002	0.794	0.009	0