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

Effect of Ion Structure on the Physicochemical Properties and Gas Absorption of Surface Active Ionic Liquids

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Supplementary Information

Ionic liquids synthesis and characterization

We designed 7 SAILs as shown in Fig. 1a – Fig. 1g. The synthesis follow the method described before.[1] Ions metastasis of chloride or bromine precursor with sodium precursor in dichloromethane and water phases. The chemical structure of the synthesized SAILs was confirmed by ^1H-NMR:

[$P_{6,6,6,14}$][AOT]:^1H-NMR (CD_3Cl, 400 MHz): ($\delta = 4.06 - 3.81$, -OCH_2-, OCH_2-, -CH−S, 5H) ($\delta = 3.25 - 3.03$, CH_2−COO, 2H) ($\delta = 2.31 - 2.22$, -CH_2P, 8H) ($\delta = 1.48, 1.30 - 1.24$, -$CH_2$-, -CH, 66H) ($\delta = 0.9 - 0.8$, -$CH_3$, 24H).

[$P_{6,6,6,14}$][DS]: ^1H-NMR (CD_3Cl, 400 MHz): ($\delta = 3.94$, -CH_2−S, 2H) ($\delta = 2.23 - 2.18$, -CH_2−P, 8H) ($\delta = 1.52 - 1.35, 1.29 - 1.20, 1.17 - 1.20$, -$CH_2$-, 70H) ($\delta = 0.84 - 0.79$, -$CH_3$, 15H).

[$P_{4,4,4,4}$][AOT]: ^1H-NMR (CD_3Cl, 400 MHz): ($\delta = 4.09 - 3.86$, -OCH_2-, -OCH_2-, -CH−S-, 5H) ($\delta = 3.29 - 3.07$, -CH_2−COO, 2H) ($\delta = 2.31 - 2.22$,-CH_2P, 8H) ($\delta = 1.54 - 1.44, 1.38 - 1.16$, -$CH_2$-, -CH-, 34H) ($\delta = 0.96 - 0.8$, -$CH_3$, 24H).

[$P_{4,4,4,4}$][DS]: ^1H-NMR (CD_3Cl, 400 MHz): ($\delta = 3.99$, -CH_2−S, 2H) ($\delta = 2.31 - 2.24$, CH_2−P, 8H) ($\delta = 1.51 - 1.39, 1.24 - 1.09$, -$CH_2$, 36H) ($\delta = 0.93 - 0.88$, -$CH_3$ 12H, $\delta = 0.82 - 0.79$, -CH_3 3H).

[$N_{4,4,4,4}$][AOT]: ^1H-NMR (CD_3Cl, 400 MHz): ($\delta = 4.06 - 3.85$, -OCH_2-, -OCH_2-, -CH−S, 5H) ($\delta = 3.25 - 3.21$,-CH_2N, 8H) ($\delta = 3.10 - 3.05$, -CH_2−COO, 2H) ($\delta = 1.64 - 1.56, 1.38 - 1.33, 1.33 - 1.15$, -$CH_2$, -CH, 34H) ($\delta = 0.99 - 0.95, 0.86 - 0.79$, -$CH_3$, 24H).

[$N_{4,4,4,4}$][DS]: ^1H-NMR (CD_3Cl, 400 MHz): ($\delta = 3.95$, -CH_2−S, 2H) ($\delta = 3.27 - 3.23$, CH_2−N, 8H) ($\delta = 1.57 - 1.65, 1.45 - 1.36, 1.26 - 1.21$, -$CH_2$, 36H) ($\delta = 0.98 - 0.95$, -$CH_3$ 12H, $\delta 0.86 - 0.82$, -CH_3, 3H).

[C_4mim][AOT]: ^1H-NMR (CD_3Cl, 400 MHz): ($\delta = 9.56, 7.41, 7.30$, imidazolium ring, 3H) ($\delta = 4.25 - 3.88$, -CH_2−N, CH_3−N, -OCH_2-, -OCH_2-, -CH−S-, 10H) ($\delta = 3.27 - 3.09$, -CH_2−COO, 2H) ($\delta = 1.39 - 1.24$, -CH_2, 22H) ($\delta = 0.95 - 0.91$, -CH_3, 3H, $\delta = 0.87 - 0.81$, -CH_3, 12H).

Table S1: Molecular weight and water content in the surfactant ionic liquids measured using the Karl Fisher coulometric titration method (Mettler Toledo C20S using Hydranal Coulomat E as reagent).

IL	M_w / g mol^{-1}	Water content / ppm	x_{H_2O}
[C_4mim][AOT]	560.78	32	0.001
[$N_{4,4,4,4}$][AOT]	664.02	65	0.002
[$P_{4,4,4,4}$][AOT]	680.99	58	0.002
[$P_{6,6,6,14}$][AOT]	905.41	42	0.002
[$N_{4,4,4,4}$][DS]	507.84	27	0.0008
[$P_{4,4,4,4}$][DS]	524.81	6	0.0002
[$P_{6,6,6,14}$][DS]	749.23	45	0.002

Surface tension equations

MacLeod[2] proposed the following empirical equation which states a temperature independent relation between surface tension and the liquid density:

$$\gamma^{1/4} = K\rho \tag{S1}$$

where K is a constant characteristic of each substance. The product of K by the molar mass, M, is known as the Parachor the compound $P_{ch} = KM$[3]. One of the best known empirical correlation of γ versus T is the Eötvos rule[4], which takes into account that γ vanishes at the critical point and assumes that γ behaves linear with T:

$$\gamma V^{2/3} = k_{\text{Eotvos}}(T_c - T) \tag{S2}$$

where V is the molar volume of the liquid and k_{Eotvos} is a constant. An improvement of this equation was made by Guggenheim[5], who applied the Principle of Corresponding States to a more accurate modification of the Eötvos rule made previously by Katayama, leading to:

$$\gamma = k_{\text{Guggenheim}}(1 - T/T_c)^{9/11} \tag{S3}$$

where $k_{\text{Guggenheim}}$ is another constant.

Micellization parameters

The minimum molecular area at the air-liquid interface, A_{mim}, gives insights on the packing density of the solute at the interface and it was calculated by assuming ideality from the Gibbs equation:

$$A_{\mathrm{min}} = \frac{10^{20}}{N_A \Gamma_{\mathrm{max}}} \tag{S4}$$

where N_A is the Avogadro's number and Γ_{max} is the maximum surface excess concentration at the air-liquid interface of the SAILs:

$$\Gamma_{max} = -\frac{1}{2.303RT}\left(\frac{\partial\gamma}{\partial(\ln c)}\right)_T \tag{S5}$$

where R is the universal gas constant, T the temperature, c the mole concentration of the SAILs and $\partial\gamma/\partial(\ln c)$ is the variation of the surface tension bellow the cmc, listed in Table S9, in the monomers zone. The standard free energy of micellization, ΔG^0_{mic}, was estimated by the following approximation for the SAILS:

$$\Delta G^0_{\mathrm{mic}} = RT\ln(cmc) \tag{S6}$$

The standard free energy of adsorption, ΔG^0_{ad}, describes the free energy change for the adsorption of amphiphiles to the liquid-air interface:

$$\Delta G^0_{\mathrm{ad}} = \Delta G^0_{\mathrm{mic}} - (\gamma_0 - \gamma_{\mathrm{cmc}})A_{\mathrm{min}} \tag{S7}$$

where γ_0 and γ_{cmc} are the surface tension of the neat solvent (70.45 ± 0.28 mN m^{-1}) and at the cmc, respectively (Table 3).

Density and viscosity data

Table S2: Experimental densities of the ionic liquid-based surfactants, ρ, the molar volumes, V_m, and molar volumes calculated from the group contribution method using literature parameters ${V_m}^{GCM}$. $\Delta V_m/\%$ represents the relative difference between the experimental and calculated molar volume using the GCM. All parameters and groups are listed in Tables S4 and S5.

T/K	ρ/g cm^{-3}	V_m/cm^3 mol^{-1}	${V_m}^{GCM}$/cm^3 mol^{-1}	$\Delta V_m/\%$
		[C_4mim][AOT]		
293.154	1.059712	529.1803	521.9309	1.4
303.154	1.052830	532.6393	522.8199	1.8
313.154	1.046002	536.1163	523.7175	2.3
323.154	1.039224	539.6129	524.6238	2.8
333.154	1.032498	543.1281	525.5386	3.2
343.154	1.025813	546.6676	526.4620	3.7
353.154	1.019163	550.2345	527.3941	4.2
		[$N_{4,4,4,4}$][AOT]		
293.146	1.000319	663.8105	661.1358	0.4
303.154	0.993891	668.1037	661.3207	1.0
313.154	0.987398	672.4970	662.1863	1.5
323.154	0.980991	676.8892	663.7327	1.9
333.154	0.974615	681.3175	665.9596	2.3
343.154	0.968267	685.7842	668.8672	2.5
353.155	0.961948	690.2891	672.4558	2.6
363.154	0.955653	694.8361	676.7242	2.6
373.154	0.949366	699.4375	681.6737	2.5
		[$P_{4,4,4,4}$][AOT]		
293.150	1.001861	679.7243	677.5053	0.3
303.154	0.995279	684.2195	680.6987	0.5
313.154	0.988724	688.7557	683.8937	0.7
323.154	0.982205	693.3270	687.0915	0.9
333.154	0.975727	697.9301	690.2922	1.1
343.154	0.969277	702.5745	693.4958	1.3
353.154	0.962834	707.2759	696.7023	1.5
363.154	0.956426	712.0146	699.9116	1.7
373.154	0.950045	716.7969	703.1238	1.9
		[$P_{6,6,6,14}$][AOT]		
293.149	0.951927	951.1353	946.6786	0.5
303.154	0.945429	957.6725	950.5845	0.7
313.154	0.938956	964.2745	954.5122	1.0
323.154	0.932522	970.92766	958.4636	1.3
333.154	0.926122	977.6372	962.4386	1.6
343.154	0.919740	984.4210	966.4374	1.8
353.155	0.913373	991.2833	970.4602	2.1
363.155	0.907025	998.2210	974.5063	2.4
373.154	0.900710	1005.2196	978.5756	2.7
		[$N_{4,4,4,4}$][DS]		
293.149	0.959667	529.1893	531.5725	-0.5
303.152	0.953708	532.4958	533.1797	-0.1

T/K	ρ/g cm^{-3}	V_m/cm^3 mol^{-1}	$V_m{}^{GCM}$/cm^3 mol^{-1}	ΔV_m/%
313.152	0.947788	535.8219	535.4025	0.1
323.151	0.941898	539.1725	538.2408	0.2
333.152	0.936017	542.5602	541.6955	0.2
343.151	0.930094	546.0153	545.7655	0.0
353.152	0.924127	549.5409	550.4521	-0.2
363.152	0.918189	553.0948	555.7542	-0.5
373.152	0.912318	556.6541	561.6722	-0.9
		[$P_{4,4,4,4}$][DS]		
293.149	0.966762	542.8561	547.9418	-0.9
303.152	0.960651	546.3093	552.5572	-1.1
313.152	0.954561	549.7947	557.1094	-1.3
323.152	0.948500	553.3080	561.5997	-1.5
333.152	0.942462	556.8528	566.0280	-1.6
343.152	0.936442	560.4326	570.3945	-1.8
353.152	0.930420	564.0599	574.6992	-1.9
363.152	0.924416	567.7234	578.9419	-2.0
373.152	0.918431	571.4230	583.1228	-2.0
		[$P_{6,6,6,14}$][DS]		
293.151	0.921538	813.0264	817.1164	-0.5
303.152	0.915338	818.5334	822.4429	-0.5
313.152	0.909162	824.0937	827.7278	-0.4
323.152	0.903022	829.6970	832.9716	-0.4
333.152	0.896912	835.3492	838.1743	-0.3
343.152	0.890805	841.0760	843.3359	-0.3
353.152	0.884698	846.8819	848.4565	-0.2
363.152	0.878612	852.7481	853.5360	-0.1
373.152	0.872545	858.6774	858.5744	0.0

Table S3: Fitting parameters from the second order polynomial used to fit the molar volume as a function of temperature, $V_m = A_0 + A_1 T + A_2 T^2$, and absolute average deviation $AAD = \frac{100}{N} \sum_{i=1}^{N} \left(\frac{|Vm_{\mathrm{exp},i} - Vm_{\mathrm{cal},i}|}{Vm_{\mathrm{cal},i}} \right)$.

Sample	A_0/cm^3 mol^{-1}	A_1/cm^3 mol^{-1} K^{-1}	A_2/cm^3 mol^{-1} K^{-2}	AAD/%
[C_4mim][AOT]	437.30	0.2824	1.0587×10^{-4}	0.0005
[$N_{4,4,4,4}$][AOT]	554.03	0.3188	1.8979×10^{-4}	0.002
[$P_{4,4,4,4}$][AOT]	566.54	0.3255	2.0672×10^{-4}	0.0009
[$P_{6,6,6,14}$][AOT]	789.91	0.4512	3.3711×10^{-4}	0.0008
[$N_{4,4,4,4}$][DS]	452.82	0.1956	2.2151×10^{-4}	0.003
[$P_{4,4,4,4}$][DS]	457.87	0.2373	1.7954×10^{-4}	0.0008
[$P_{6,6,6,14}$][DS]	679.90	0.3629	3.1128×10^{-4}	0.001

The VFT equation is a modified version of the Arrhenius equation with an added T_0 term, which

Table S4: Number of groups (n_j) taken into account for the calculation of the molar volume of the studied ILs using the group contribution method expressed by Eq. 5 (main text).

Group j	n_j	
	$[C_4mim][AOT]$	
$[C_4ImC_1]^+$	1	
$[AOT]^-$	1	
	$[N_{4,4,4,4}][AOT]$	$[N_{4,4,4,4}][DS]$
$[N_{4,4,4,1}]^+$	1	1
$-CH_2-$	3	7
$[AOT]^-$	1	0
$[C_8H_{17}SO_4]^-$	0	1
	$[P_{4,4,4,4}][AOT]$	$[P_{4,4,4,4}][DS]$
$[P_{4,4,4,14}]^+$	1	1
$-CH_2-$	-10	-6
$[AOT]^-$	1	0
$[C_8H_{17}SO_4]^-$	0	1
	$[P_{6,6,6,14}][AOT]$	$[P_{4,4,4,4}][DS]$
$[P_{6,6,6,14}]^+$	1	1
$-CH_2-$	0	4
$[AOT]^-$	1	0
$[C_8H_{17}SO_4]^-$	0	1

Table S5: Group contribution parameters used to calculate the molar volume using Eq. 5 (main text).

Group j	$\frac{C_0}{\mathrm{cm^3\,mol^{-1}}}$	$\frac{C_1}{\mathrm{cm^3\,mol^{-1}\,K^{-1}}}$	$\frac{C_2}{\mathrm{cm^3\,mol^{-1}\,K^{-2}}}$	Ref.
$[C_4ImC_1]^+$	134.260	8.890×10^{-2}	4.304×10^{-5}	6
$[N_{4,4,4,1}]^+$	222.128	1.428×10^{-2}	3.409×10^{-3}	6
$[P_{4,4,4,14}]^+$	460.657	3.332×10^{-1}	-5.102×10^{-6}	6
$[P_{6,6,6,14}]^+$	560.514	3.904×10^{-1}	1.184×10^{-4}	6
$-CH_2^-$	16.967	1.399×10^{-3}	-1.946×10^{-6}	7
$[AOT]^-$	388.114	0.000	0.000	6
$[C_8H_{17}SO_4]^-$	191.402	1.366×10^{-1}	-3.160×10^{-4}	6

Table S6: Experimental viscosities (m Pa s) of the surfactant ionic liquids $[C_4mim][AOT]$, $[N_{4,4,4,4}][AOT]$, $[P_{4,4,4,4}][AOT]$, $[P_{6,6,6,14}][AOT]$, $[N_{4,4,4,4}][DS]$, $[P_{4,4,4,4}][DS]$ and $[P_{6,6,6,14}][DS]$ in the temperature range of 283–323 K.

	η/m Pa s						
T/K	$[P_{6,6,6,14}][AOT]$	$[P_{6,6,6,14}][DS]$	$[P_{4,4,4,4}][AOT]$	$[P_{4,4,4,4}][DS]$	$[N_{4,4,4,4}][AOT]$	$[N_{4,4,4,4}][DS]$	$[C_4mim][AOT]$
284.435	3074.92	2793.01	6557.99	4639.67	26133.1	21614.5	12931
285.8	2824.14	2566.63	5983.4	4239.17	24249.2	20074.4	11980.6
287.173	2577.74	2352.83	5393.85	3829.3	21953.8	18305.3	10860.4
288.52	2349.32	2146.09	4855.12	3457.34	19627.5	16429.8	9750.75
289.871	2138.48	1956.18	4359.76	3117.21	17432.7	14470.7	8688
291.214	1946.63	1786.32	3913.81	2805.47	15406.8	12943.1	7730.38
292.599	1773.13	1627.58	3512.8	2527.58	13606.8	11363.3	6868.03
293.937	1615.9	1486.36	3163.12	2282.43	12029.5	10041	6107.71
295.255	1477.81	1361.75	2846.69	2058.94	10644.1	8860.8	5424.99
296.601	1350.46	1244.01	2566.25	1864.97	9407.99	7869.25	4827.5
297.968	1236.29	1139.29	2315.12	1686.45	8319.4	7028.06	4310.14
299.327	1132.11	1043.42	2094.36	1528.8	7393.88	6237.18	3854.49
300.694	1038.45	956.143	1898.92	1391.58	6562.83	5562.9	3450.4
302.026	954.397	880.419	1723.63	1265.72	5857.16	4994.19	3096.78
303.361	879.199	809.774	1563.31	1154.73	5209.73	4449.49	2778.53
304.737	809.453	747.706	1424.9	1051.87	4645.32	3970.71	2499.64
306.073	746.472	689.032	1294.41	965.73	4160.13	3615.98	2255.84
307.399	690.125	639.892	1184.89	882.471	3732.08	3285.13	2037.51
308.766	639.186	589.475	1080.23	809.748	3346.21	2919.45	1843.55
310.164	590.11	546.599	985.762	742.254	3009.16	2728.03	1666.92
311.459	547.789	507.181	905.194	682.432	2710.79	2424.74	1516.86
312.791	509.033	470.149	828.787	627.009	2445.84	2127.37	1379.12
314.192	472.115	436.398	762.934	578.171	2211.42	1978.38	1257.49
315.527	439.705	406.712	702.472	533.937	2000.87	1795.29	1147.43
316.843	409.713	379.257	648.096	491.671	1814.74	1607.59	1049.16
318.241	381.651	355.887	596.645	458.175	1647.53	1445.96	956.976
319.571	356.188	329.909	551.111	421.869	1501.14	1321.2	874.96
320.9	333.165	306.982	509.855	389.984	1364.42	1213.41	807.047
322.279	310.609	287.366	471.176	359.847	1248.59	1094.26	738.409
323.237	295.521	270.695	443.014	340.418	1159.43	1025.89	697.193

refers to the theoretical glass transition temperature of the sample[8]:

$$\ln(\eta) = \ln(\eta_\infty) + \frac{E_\eta}{R(T - T_0)} \tag{S8}$$

The Arrhenius and VFT fitted parameters are listed in Table S7.

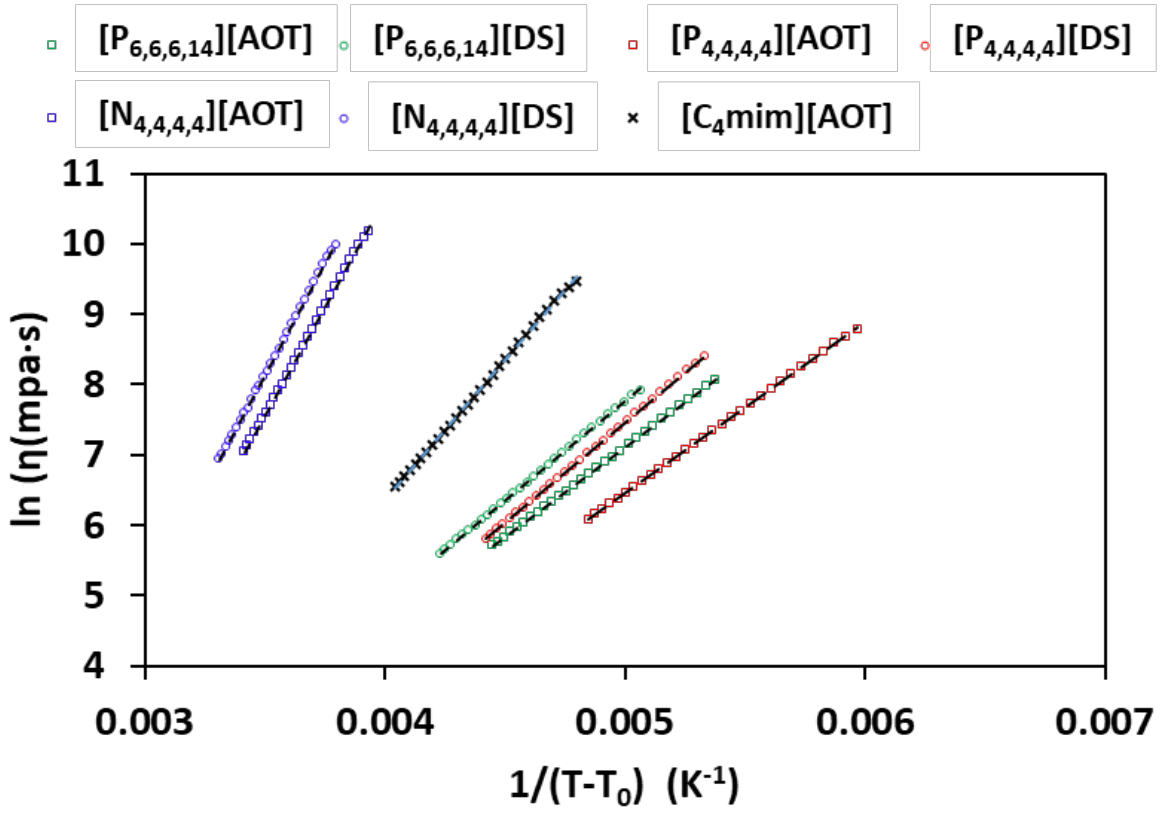

Figure S1: The VFT fits of viscosity vs temperature at a fixed shear rate of $50\,s^{-1}$.

Table S7: Parameters, η_∞ and E_η, from Arrhenius and VFT functions used to fit experimental viscosity as a function of temperature and the corresponding R^2 of each curve.

SAILs	Arrhenius fitting			VFT fitting			
	E_η ($kJ\,mol^{-1}$)	η_∞ ($1 \times 10^{-6} m\,Pa\,s$)	R^2	E_η ($kJ\,mol^{-1}$)	η_∞ ($1 \times 10^{-6} m\,Pa\,s$)	T_0	R^2
$[N_{4,4,4,4}][AOT]$	63.05	0.07	0.9996	51.07	0.92	30.35	0.9996
$[N_{4,4,4,4}][DS]$	61.37	0.13	0.9996	53.08	0.69	21.27	0.9996
$[C_4mim][AOT]$	59.00	0.20	0.9995	33.14	69.75	75.93	0.9996
$[P_{4,4,4,4}][AOT]$	53.61	0.95	0.9995	20.19	3400.00	116.96	0.9999
$[P_{4,4,4,4}][DS]$	51.37	1.68	0.9997	23.73	1114.83	97.04	0.9999
$[P_{6,6,6,14}][AOT]$	46.57	9.03	0.9997	21.19	3594.40	98.59	0.9999
$[P_{6,6,6,14}][DS]$	46.09	9.73	0.9997	23.41	1816.85	87.04	0.9999

Surface tension data

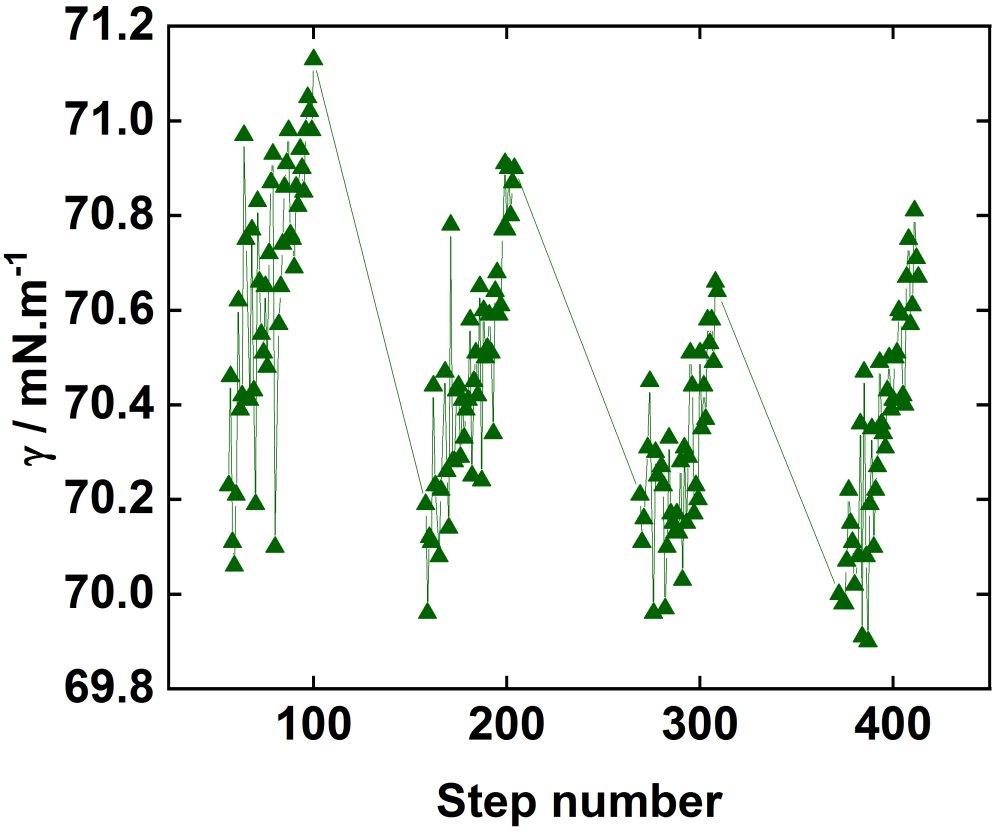

Figure S2: Surface tension fluctuation of the pure water at 298.15 K.

Sample preparation and CMC measurements at 298.15 K.

Table S9: Sample composition and surface tension data of the ILs/water mixtures. The slope of the curves at concentrations lower than the cmc are also depicted in the table.

$\frac{m_{IL}}{\mathrm{g}}$	$\frac{m_{H_2O}}{\mathrm{g}}$	$\frac{IL_{conc}{}^{(H_2O)}}{mM}$	$\frac{\gamma}{mN\mathrm{m}^{-1}}$	$\frac{\partial\gamma/\partial(\ln c)}{mN\mathrm{m}^{-1}}$
		[C_4mim][AOT]		
0.00247	7.47951	0.59	31.95	-14.8
0.00424	7.48036	1.01	28.44	
0.00668	7.47574	1.59	25.55	
0.00941	7.47612	2.23	25.36	
0.01321	7.46796	3.14	25.25	
0.01713	7.45589	4.07	25.39	
0.02199	7.45567	5.23	25.40	

$\frac{m_{IL}}{\mathrm{g}}$	$\frac{m_{H_2O}}{\mathrm{g}}$	$\frac{IL_{conc}{}^{(H_2O)}}{mM}$	$\frac{\gamma}{mN\mathrm{m}^{-1}}$	$\frac{\partial\gamma/\partial(\ln c)}{mN\mathrm{m}^{-1}}$
		$[\mathrm{N}_{4,4,4,4}][\mathrm{AOT}]$		
0.00141	7.47217	0.28	33.45	-11.6
0.00253	7.48230	0.51	30.42	
0.00362	7.47864	0.73	28.01	
0.00420	7.47592	0.84	28.35	
0.00462	7.47194	0.93	38.35	
0.00801	7.47039	1.61	27.36	
0.01019	7.46987	2.05	28.27	
		$[\mathrm{P}_{4,4,4,4}][\mathrm{AOT}]$		
0.00112	7.48066	0.22	31.22	-5.1
0.00292	7.48055	0.57	28.75	
0.00334	7.47982	0.65	29.07	
0.00574	7.47618	1.12	29.06	
0.00874	7.47172	1.71	29.19	
0.00974	7.47060	1.91	29.10	
0.01420	7.46616	2.78	29.07	
0.02146	7.46081	4.20	29.02	
		$[\mathrm{P}_{6,6,6,14}][\mathrm{AOT}]$		
0.00196	7.48493	0.29	47.96	-36.4
0.00309	7.47224	0.46	40.71	
0.00527	7.47392	0.78	40.91	
0.00642	7.46852	0.94	40.79	
0.01094	7.46581	1.61	40.69	
0.01413	7.46136	2.08	40.12	
0.01945	7.45689	2.86	40.29	
0.02491	7.44424	3.67	40.01	
		$[\mathrm{N}_{4,4,4,4}][\mathrm{DS}]$		
0.00213	7.494055	0.56	33.19	-19.5
0.00247	7.48812	0.65	32.63	
0.00321	7.47991	0.84	29.81	
0.00496	7.48291	1.30	28.19	
0.00756	7.47599	1.98	29.89	
0.01119	7.46912	2.94	30.39	
0.01621	7.455645	4.26	31.03	
		$[\mathrm{P}_{4,4,4,4}][\mathrm{DS}]$		
0.00118	7.49441	0.30	36.32	-13.1
0.00224	7.48590	0.57	32.84	
0.00282	7.48040	0.72	31.46	
0.00358	7.48058	0.91	30.41	
0.00513	7.47450	1.30	30.39	
0.00877	7.46993	2.23	30.47	
0.01146	7.46131	2.91	30.40	
0.01358	7.46248	3.45	30.39	
		$[\mathrm{P}_{6,6,6,14}][\mathrm{DS}]$		

$\frac{m_{IL}}{\mathrm{g}}$	$\frac{m_{H_2O}}{\mathrm{g}}$	$\frac{IL_{conc}{}^{(H_2O)}}{mM}$	$\frac{\gamma}{mN\mathrm{m}^{-1}}$	$\frac{\partial\gamma/\partial(\ln c)}{mN\mathrm{m}^{-1}}$
0.001655	7.47879	0.29	38.90	-4.8
0.00252	7.476545	0.45	37.58	
0.00399	7.47489	0.71	36.17	
0.00593	7.474505	1.05	36.44	
0.00813	7.47468	1.45	35.34	
0.01176	7.47167	2.09	34.53	
0.014315	7.461525	2.55	34.91	
0.02367	7.452495	4.21	33.82	

Gas absorption data

Table S10: Average absorption of CO_2 by the ionic liquid-based surfactants as a function of pressure from 0.5–5 bar at 303 K. The uncertainties of temperature, pressure and gas absorption are also depicted in the table.

CO_2 — Average absorption		
T/K	p/bar	x(CO_2)
	[C_4mim][AOT]	
303.239 ± 0.067	0.0000 ± 0.0000	0.0000 ± 0.0000
303.146 ± 0.004	0.4984 ± 0.0006	0.0224 ± 0.0002
303.141 ± 0.010	0.7485 ± 0.0003	0.0331 ± 0.0003
303.158 ± 0.006	0.9992 ± 0.0002	0.0434 ± 0.0005
303.148 ± 0.007	2.5003 ± 0.0004	0.1013 ± 0.0000
303.134 ± 0.000	4.9993 ± 0.0000	0.1834 ± 0.0000
	[$N_{4,4,4,4}$][AOT]	
303.155 ± 0.010	0.0000 ± 0.0000	0.0000 ± 0.0000
303.158 ± 0.021	0.4970 ± 0.0023	0.0275 ± 0.0004
303.151 ± 0.011	0.7487 ± 0.0000	0.0403 ± 0.0006
303.146 ± 0.004	0.9979 ± 0.00024	0.0523 ± 0.0006
303.139 ± 0.006	2.4994 ± 0.0003	0.1202 ± 0.0001
303.138 ± 0.000	4.9977 ± 0.0000	0.2143 ± 0.0000
	[$P_{4,4,4,4}$][AOT]	
303.206 ± 1.013	0.0000 ± 0.0000	0.0000 ± 0.0000
303.177 ± 0.060	0.4985 ± 0.0002	0.0274 ± 0.0006
303.105 ± 0.054	0.7480 ± 0.0018	0.0400 ± 0.0006
303.148 ± 0.007	0.9991 ± 0.0003	0.0525 ± 0.0004
303.087 ± 0.101	2.4992 ± 0.0005	0.1200 ± 0.0003
303.158 ± 0.000	4.9991 ± 0.0000	0.2137 ± 0.0000
	[$P_{6,6,6,14}$][AOT]	
304.587 ± 1.496	0.0000 ± 0.0000	0.0000 ± 0.0000

CO_2 — Average absorption		
T/K	p/bar	x(CO_2)
303.160 ± 0.003	0.4983 ± 0.0001	0.0373 ± 0.0010
303.146 ± 0.004	0.7479 ± 0.0008	0.0541 ± 0.0013
303.151 ± 0.004	0.9994 ± 0.0001	0.0702 ± 0.0013
303.151 ± 0.004	2.4993 ± 0.0003	0.1558 ± 0.0012
303.181 ± 0.000	4.9987 ± 0.0000	0.2686 ± 0.0000
	$[N_{4,4,4,4}][DS]$	
303.186 ± 0.141	0.0000 ± 0.0000	0.0000 ± 0.0000
303.201 ± 0.013	0.4980 ± 0.0009	0.0185 ± 0.0007
302.917 ± 0.212	0.7488 ± 0.0012	0.0277 ± 0.0008
303.148 ± 0.014	0.9993 ± 0.0004	0.0361 ± 0.0001
303.137 ± 0.030	2.4994 ± 0.0007	0.0857 ± 0.0000
303.148 ± 0.000	4.9980 ± 0.0000	0.1585 ± 0.0000
	$[P_{4,4,4,4}][DS]$	
303.134 ± 0.006	0.0000 ± 0.0000	0.0000 ± 0.0000
303.150 ± 0.017	0.4979 ± 0.0008	0.0198 ± 0.0006
303.148 ± 0.014	0.7484 ± 0.0010	0.0289 ± 0.0007
303.141 ± 0.004	0.9990 ± 0.0007	0.0380 ± 0.0006
303.191 ± 0.047	2.4996 ± 0.0004	0.0877 ± 0.0005
303.134 ± 0.000	4.9997 ± 0.0000	0.1603 ± 0.0000
	$[P_{6,6,6,14}][DS]$	
303.320 ± 0.223	0.0000 ± 0.0000	0.0000 ± 0.0000
303.168 ± 0.013	0.4981 ± 0.0003	0.0276 ± 0.0001
303.148 ± 0.020	0.7479 ± 0.0002	0.0403 ± 0.0001
303.146 ± 0.011	0.9995 ± 0.0004	0.0530 ± 0.0004
303.153 ± 0.007	2.4992 ± 0.0005	0.1211 ± 0.0009
303.158 ± 0.000	4.9975 ± 0.0000	0.2159 ± 0.0000

Table S11: Average absorption of N_2 by the ionic liquid-based surfactants as a function of pressure from 0.5–5 bar at 303 K. The uncertainties of temperature, pressure and gas absorption are also depicted in the table.

N_2 — Average absorption		
T/K	p/bar	x(N_2)
	$[C_4mim][AOT]$	
303.155 ± 0.105	0.0000 ± 0.0000	0.0000 ± 0.0000
303.129 ± 0.041	0.4984 ± 0.0007	0.0034 ± 0.0019
303.134 ± 0.027	0.7495 ± 0.0001	0.0055 ± 0.0014
303.151 ± 0.011	0.9995 ± 0.0002	0.0074 ± 0.0010
303.143 ± 0.007	2.4985 ± 0.0004	0.0201 ± 0.0002
303.077 ± 0.000	4.9984 ± 0.0000	0.0407 ± 0.0000
	$[N_{4,4,4,4}][AOT]$	
303.958 ± 1.017	0.0000 ± 0.0000	0.0000 ± 0.0000

N_2 — Average absorption		
T/K	p/bar	x(N_2)
303.187 ± 0.074	0.4975 ± 0.0007	0.0086 ± 0.0005
303.165 ± 0.111	0.7466 ± 0.0004	0.0121 ± 0.0007
303.139 ± 0.021	0.9992 ± 0.0002	0.0161 ± 0.0007
303.150 ± 0.017	2.4994 ± 0.0003	0.0357 ± 0.0007
303.143 ± 0.000	4.9980 ± 0.0000	0.0664 ± 0.0000
	$[P_{4,4,4,4}][AOT]$	
303.239 ± 0.121	0.0000 ± 0.0000	0.0000 ± 0.0000
303.165 ± 0.077	0.4985 ± 0.0002	0.0086 ± 0.0008
303.184 ± 0.050	0.7493 ± 0.0002	0.0124 ± 0.0005
303.187 ± 0.101	0.9989 ± 0.0006	0.0159 ± 0.0005
303.168 ± 0.013	2.4987 ± 0.0001	0.0364 ± 0.0004
303.224 ± 0.000	4.9984 ± 0.0000	0.0674 ± 0.0000
	$[P_{6,6,6,14}][AOT]$	
303.789 ± 0.556	0.0000 ± 0.0000	0.0000 ± 0.0000
303.151 ± 0.118	0.4981 ± 0.0000	$0.0124 pm 0.0001$
303.203 ± 0.051	0.7489 ± 0.0001	0.0178 ± 0.0001
303.220 ± 0.021	0.9997 ± 0.0005	0.0228 ± 0.0008
303.091 ± 0.061	2.4988 ± 0.0002	0.0519 ± 0.0005
303.248 ± 0.000	4.9989 ± 0.0000	0.0969 ± 0.0000
	$[N_{4,4,4,4}][DS]$	
303.225 ± 0.209	0.0000 ± 0.0000	0.0000 ± 0.0000
303.146 ± 0.011	0.4986 ± 0.0001	0.0054 ± 0.0014
303.148 ± 0.007	0.7486 ± 0.0002	0.0080 ± 0.0006
303.141 ± 0.017	0.9989 ± 0.0004	0.0107 ± 0.0001
303.151 ± 0.004	2.4990 ± 0.0007	0.0266 ± 0.0002
303.134 ± 0.000	4.9973 ± 0.0000	0.0517 ± 0.0000
	$[P_{4,4,4,4}][DS]$	
303.255 ± 0.044	0.0000 ± 0.0000	0.0000 ± 0.0000
303.148 ± 0.007	0.4982 ± 0.0006	0.0066 ± 0.0001
303.167 ± 0.000	0.7491 ± 0.0002	0.0096 ± 0.0001
303.136 ± 0.003	0.9988 ± 0.0009	0.0126 ± 0.0004
303.148 ± 0.020	2.4991 ± 0.0004	0.0292 ± 0.0001
303.138 ± 0.000	4.9987 ± 0.0000	0.0553 ± 0.0000
	$[P_{6,6,6,14}][DS]$	
304.215 ± 0.161	0.0000 ± 0.0000	0.0000 ± 0.0000
303.139 ± 0.013	0.4981 ± 0.0007	0.0095 ± 0.0003
303.139 ± 0.013	0.7486 ± 0.0004	0.0135 ± 0.0000
303.141 ± 0.004	0.9989 ± 0.0008	0.0178 ± 0.0004
303.158 ± 0.000	2.4992 ± 0.0012	0.0413 ± 0.0001
303.167 ± 0.000	4.9984 ± 0.0000	0.0771 ± 0.0000

Table S8: Experimental surface tension, γ, for the ionic liquid-based surfactants [C_4mim][AOT], [$N_{4,4,4,4}$][AOT], [$P_{4,4,4,4}$][AOT], [$P_{6,6,6,14}$][AOT], [$N_{4,4,4,4}$][DS], [$P_{4,4,4,4}$][DS] and [$P_{6,6,6,14}$][DS] (about 700 ppm of water) in the temperature range 293.15–353.15 K in air at ambient pressure.

T/K	γ / mN m^{-1}	T/K	γ / mN m^{-1}
[C_4mim][AOT]		[$N_{4,4,4,4}$][AOT]	
293.2	27.65	293.2	30.51
303.2	27.21	303.2	29.80
313.3	26.90	313.2	29.23
323.2	26.41	323.1	28.45
333.1	26.06	333.1	27.81
343.1	25.54	343.1	26.88
353.2	24.89	353.3	26.17
[$P_{4,4,4,4}$][AOT]		[$P_{6,6,6,14}$][AOT]	
293.2	30.00	293.2	28.83
303.2	29.58	303.3	28.17
313.1	28.97	313.3	27.58
323.2	28.26	323.3	26.91
333.2	27.58	333.1	26.28
343.2	26.91	343.0	25.77
353.2	26.14	353.2	25.19
[$N_{4,4,4,4}$][DS]		[$P_{4,4,4,4}$][DS]	
293.2	32.32	293.1	31.89
303.3	31.43	303.3	31.07
313.2	30.83	313.2	30.48
323.2	30.08	323.1	29.71
333.1	29.31	333.0	29.11
343.1	28.61	343.2	28.47
353.0	28.06	353.2	27.71
[$P_{6,6,6,14}$][DS]			
293.1	29.88		
303.2	29.24		
313.1	28.54		
323.1	27.91		
333.1	27.23		
343.1	26.56		
353.2	25.86		

Table S12: Absorption and desorption of CO_2 by the ionic liquid-based surfactants as a function of pressure from 0.5–5 bar at 303.15 K.

T / K	p / bar	b / mmol g^{-1}	T / K	p / bar	b / mmol g^{-1}
CO_2 — Absorption					
[C_4C_1im][AOT]					
303.29	0.0000	0.0000			
303.14	0.4988	0.0226			
303.13	0.7483	0.0329			
303.16	0.9993	0.0430			
303.14	2.5001	0.1014			
303.13	4.9993	0.1834			
[$N_{4,4,4,4}$][AOT]			[$N_{4,4,4,4}$][DS]		
303.15	0.0000	0.0000	303.09	0.0000	0.0000
303.17	0.4953	0.0272	303.19	0.4986	0.0190
303.14	0.7487	0.0398	302.77	0.7497	0.0283
303.15	0.9961	0.0518	303.14	0.9996	0.0362
303.13	2.4992	0.1202	303.12	2.4989	0.0857
303.14	4.9977	0.2143	303.15	4.9980	0.1585
[$P_{4,4,4,4}$][AOT]			[$P_{4,4,4,4}$][DS]		
303.20	0.0000	0.0000	303.14	0.0000	0.0000
303.13	0.4984	0.0270	303.14	0.4974	0.0194
303.07	0.7493	0.0396	303.14	0.7477	0.0285
303.14	0.9989	0.0522	303.14	0.9995	0.0376
303.02	2.4988	0.1198	303.16	2.4994	0.0873
303.16	4.9991	0.2137	303.13	4.9997	0.1603
[$P_{6,6,6,14}$][AOT]			[$P_{6,6,6,14}$][DS]		
305.64	0.0000	0.0000	303.16	0.0000	0.0000
303.16	0.4984	0.0366	303.16	0.4984	0.0276
303.14	0.7484	0.0531	303.13	0.7477	0.0402
303.15	0.9993	0.0692	303.14	0.9997	0.0527
303.15	2.4995	0.1550	303.16	2.4988	0.1205
303.18	4.9987	0.2686	303.16	4.9975	0.2159
CO_2 — Desorption					
[C_4C_1im][AOT]					
303.13	4.9993	0.1834			
303.15	2.5006	0.1013			
303.15	0.9991	0.0438			
303.15	0.7487	0.0333			
303.15	0.4979	0.0223			
303.19	0.0000	0.0000			
[$N_{4,4,4,4}$][AOT]			[$N_{4,4,4,4}$][DS]		
303.14	4.9977	0.2143	303.15	4.9980	0.1585
303.14	2.4996	0.1202	303.16	2.4999	0.0857
303.14	0.9996	0.0527	303.16	0.9991	0.0360
303.16	0.7487	0.0407	303.07	0.7480	0.0272

$\frac{T}{\mathrm{K}}$	$\frac{p}{\mathrm{bar}}$	$\frac{b}{\mathrm{mmol\,g^{-1}}}$	$\frac{T}{\mathrm{K}}$	$\frac{p}{\mathrm{bar}}$	$\frac{b}{\mathrm{mmol\,g^{-1}}}$
303.14	0.4986	0.0278	303.21	0.4974	0.0180
303.16	0.0000	0.0000	303.29	0.0000	0.0000
$[P_{4,4,4,4}][AOT]$			$[P_{4,4,4,4}][DS]$		
303.16	4.9991	0.2137	303.13	4.9997	0.1603
303.16	2.4995	0.1201	303.22	2.4999	0.0881
303.15	0.9993	0.0528	303.14	0.9985	0.0384
303.14	0.7468	0.0404	303.16	0.7491	0.0294
303.22	0.4986	0.0278	303.16	0.4985	0.0202
303.22	0.0000	0.0000	303.13	0.0000	0.0000
$[P_{6,6,6,14}][AOT]$			$[P_{6,6,6,14}][DS]$		
303.18	4.9987	0.2686	303.16	4.9975	0.2159
303.15	2.4991	0.1566	303.15	2.4995	0.1217
303.15	0.9995	0.0711	303.15	0.9992	0.0533
303.15	0.7473	0.0550	303.16	0.7480	0.0404
303.16	0.4982	0.0380	303.18	0.4979	0.0275
303.53	0.0000	0.0000	303.48	0.0000	0.0000

Table S13: Absorption and desorption of N_2 by ionic liquid-based surfactants as a function of pressure from 0.5–5 bar at 303.15 K.

$\frac{T}{\mathrm{K}}$	$\frac{p}{\mathrm{bar}}$	$\frac{b}{\mathrm{mmol\,g^{-1}}}$	$\frac{T}{\mathrm{K}}$	$\frac{p}{\mathrm{bar}}$	$\frac{b}{\mathrm{mmol\,g^{-1}}}$
N_2 — Absorption					
$[C_4C_1im][AOT]$					
303.23	0.0000	0.0000			
303.10	0.4989	0.0048			
303.11	0.7494	0.0065			
303.14	0.9996	0.0081			
303.15	2.4983	0.0202			
303.08	4.9984	0.0407			
$[N_{4,4,4,4}][AOT]$			$[N_{4,4,4,4}][DS]$		
303.24	0.0000	0.0000	303.08	0.0000	0.0000
303.24	0.4979	0.0083	303.14	0.4985	0.0064
303.24	0.7469	0.0116	303.15	0.7487	0.0084
303.15	0.9993	0.0156	303.13	0.9992	0.0108
303.14	2.4992	0.0352	303.15	2.4995	0.0265
303.14	4.9980	0.0664	303.13	4.9973	0.0517
$[P_{4,4,4,4}][AOT]$			$[P_{4,4,4,4}][DS]$		
303.15	0.0000	0.0000	303.22	0.0000	0.0000
303.22	0.4986	0.00807	303.14	0.4978	0.00668
303.22	0.7491	0.01204	303.17	0.7490	0.00957
303.12	0.9985	0.01558	303.13	0.9995	0.01232
303.16	2.4987	0.03613	303.13	2.4988	0.02916
303.22	4.9984	0.06743	303.14	4.9987	0.05534

T / K	p / bar	b / mmol g^{-1}	T / K	p / bar	b / mmol g^{-1}
[$P_{6,6,6,14}$][AOT]			[$P_{6,6,6,14}$][DS]		
303.40	0.0000	0.0000	304.10	0.0000	0.0000
303.23	0.4981	0.01249	303.15	0.4986	0.00970
303.17	0.7490	0.01790	303.15	0.7483	0.01346
303.21	1.0000	0.02228	303.14	0.9995	0.01747
303.05	2.4987	0.05153	303.16	2.5001	0.04137
303.25	4.9989	0.09686	303.17	4.9984	0.07707
N_2 — Desorption					
[C_4C_1im][AOT]					
303.08	4.9984	0.0407			
303.14	2.4988	0.0200			
303.16	0.9993	0.0067			
303.15	0.7495	0.0045			
303.16	0.4979	0.0021			
303.08	0.0000	0.0000			
[$N_{4,4,4,4}$][AOT]			[$N_{4,4,4,4}$][DS]		
303.14	4.9980	0.0664	303.13	4.9973	0.0517
303.16	2.4996	0.0362	303.15	2.4985	0.0267
303.12	0.9991	0.0167	303.15	0.9986	0.0107
303.09	0.7463	0.0126	303.14	0.7484	0.0075
303.13	0.4970	0.0090	303.15	0.4986	0.0044
304.68	0.0000	0.0000	303.37	0.0000	0.0000
[$P_{4,4,4,4}$][AOT]			[$P_{4,4,4,4}$][DS]		
303.22	4.9984	0.0674	303.14	4.9987	0.0553
303.18	2.4988	0.0366	303.16	2.4994	0.0293
303.26	0.9993	0.0162	303.14	0.9982	0.0128
303.15	0.7494	0.0128	303.17	0.7493	0.0097
303.11	0.4984	0.0092	303.15	0.4986	0.0065
303.32	0.0000	0.0000	303.29	0.0000	0.0000
[$P_{6,6,6,14}$][AOT]			[$P_{6,6,6,14}$][DS]		
303.25	4.9989	0.0969	303.17	4.9984	0.0771
303.13	2.4989	0.0523	303.16	2.4984	0.0413
303.23	0.9993	0.0234	303.14	0.9984	0.0180
303.24	0.7488	0.0177	303.13	0.7488	0.0135
303.07	0.4981	0.0123	303.13	0.4977	0.0093
304.18	0.0000	0.0000	304.33	0.0000	0.0000

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