Supporting Information

The non ideality of solutions of NH_3, SO_2 and H_2S in ionic liquids and the prediction of their solubilities using the Flory Huggins model

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Table S1. Deviations, Δp, between the available VLE[1, 2] and the equilibrium pressure predicted by the Flory-Huggins model, as function of SO_2 mole fractions and temperature, for the IL + SO_2 systems.

x_{SO2}	Δp /MPa	x_{SO2}	Δp /MPa	x_{SO2}	Δp /MPa	x_{SO2}	Δp /MPa	x_{SO2}	Δp /MPa
SO_2 + [C_6mim][NTf_2] [1]						**SO_2 + [C_6mim][NTf_2] [2]**			
298 K		**313 K**		**333 K**		**283 K**		**298 K**	
0.310	-0.005	0.103	-0.005	0.0676	-0.004	0.171	0.005	0.124	0.008
0.478	0.001	0.228	0.004	0.136	0.004	0.512	0.01	0.377	0.02
0.616	0.005	0.367	-0.03	0.248	0.02	0.616	0.01	0.477	0.03
0.711	0.005	0.533	-0.05	0.374	0.04	0.706	0.01	0.553	0.03
0.781	0.003	0.655	-0.07	0.488	0.07	0.767	0.01	0.667	0.03
0.844	-0.2	0.719	-0.1	0.58	0.1	0.825	0.01	0.752	0.03
						0.875	0.005	0.82	0.03
								0.881	0.03
x_{SO2}	Δp /MPa	x_{SO2}	Δp /MPa	x_{SO2}	Δp /MPa				
SO_2 + [C_6mim][NTf_2] [2]				**x_{SO2} + [C_6mpy][NTf_2] [1]**					
323 K		**348 K**		**298 K**					
0.049	0.005	0.037	0.01	0.138	-0.01				
0.192	0.02	0.124	0.03	0.343	-0.001				
0.266	0.03	0.169	0.04	0.522	0.003				
0.329	0.03	0.21	0.05	0.660	0.005				
0.431	0.04	0.28	0.06	0.775	0.003				
0.513	0.05	0.343	0.08	0.854	0.01				
0.581	0.06	0.401	0.1						
0.639	0.07	0.457	0.1						

Table S2. Deviations, Δp, between the available VLE[3, 4] and the equilibrium pressure predicted by the Flory-Huggins model, as function of NH_3 mole fractions and temperature, for the IL + NH_3 systems.

x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa
NH_3 + [C_2mim][EtSO$_4$] [4]				**NH_3 + [C_2mim][Ac] [4]**				***NH_3 + [C_4mim][PF_6] [4]***					
283 K		**298 K**		**283 K**		**298 K**		**283 K**		***298 K***		***325 K***	
0.536	-0.1	0.518	-0.1	0.624	-0.1	0.599	-0.1	0.371	-0.04	0.351	*-0.02*	0.292	-0.02
0.707	-0.1	0.694	-0.2	0.749	-0.1	0.730	-0.1	0.471	-0.05	0.435	*-0.06*	0.389	-0.04
0.805	-0.1	0.798	-0.1	0.802	-0.1	0.788	-0.1	0.584	-0.06	0.557	*-0.05*	0.492	-0.04
0.839	-0.1	0.833	-0.1	0.834	-0.1	0.825	-0.1	0.862	-0.05	0.740	*-0.07*	0.681	-0.1
0.875	-0.1	0.871	-0.1	0.847	-0.1	0.839	-0.1			0.854	*-0.04*	0.828	-0.06
				0.877	-0.1	0.871	-0.1						
x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa
NH_3 + [C_4mim][BF_4] [4]				***NH_3 + [C_4mim][BF_4] [3]***									
282 K		**298 K**		**324 K**		**293 K**		**298 K**		***313 K***		**323 K**	
0.201	-0.04	0.173	-0.06	0.122	-0.1	0.2645	-0.03	0.3175	-0.07	0.0989	-0.02	0.1296	-0.04
0.303	-0.05	0.266	-0.08	0.199	-0.1	0.3818	-0.02	0.4654	-0.08	0.2001	-0.05	0.2798	-0.1
0.404	-0.07	0.367	-0.09	0.292	-0.2	0.5087	-0.05	0.5555	-0.08	0.3368	-0.08	0.3799	-0.2
0.582	-0.08	0.548	-0.1	0.473	-0.2	0.691	-0.06	0.595	-0.1	0.4431	-0.08	0.4697	-0.2
0.709	-0.09	0.683	-0.1	0.622	-0.2	0.7531	-0.05	0.6635	-0.2	0.5615	-0.07	0.5087	-0.2

0.844	-0.04	0.833	-0.08	0.805	-0.07						
x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa
NH_3 + $[C_4mim][BF_4]$ [3]		NH_3 + $[C_2mim][BF_4]$ [3]								NH_3 + $[C_6mim][BF_4]$ [3]	
333 K		293 K		298 K		313 K		323 K		*333 K*	
293 K											
0.0608	-0.01	0.2153	-0.06	0.1474	-0.05	0.1255	-0.06	0.0838	-0.05	0.1185	-0.07
0.1103	-0.05	0.3392	-0.1	0.4169	-0.1	0.2546	-0.1	0.2043	-0.1	0.175	-0.1
0.1689	-0.06	0.4976	-0.1	0.4669	-0.1	0.3238	-0.1	0.2853	-0.2	0.2284	-0.2
0.2519	-0.09	0.578	-0.2	0.5386	-0.2	0.4466	-0.2	0.3304	-0.2	0.2538	-0.2
0.3397	-0.1	0.6921	-0.1	0.6176	-0.2	0.5257	-0.1	0.3896	-0.2	0.2549	-0.3
0.3815	-0.01										
0.4933	-0.07										
0.6032	-0.08										
0.724	-0.06										
0.7543	-0.08										
x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa
NH_3 + $[C_6mim][BF_4]$ [3]								NH_3 + $[C_8mim][BF_4]$ [3]			
298 K		313 K		323 K		*333 K*		293 K		298 K	
313 K											
0.3673	-0.04	0.2722	-0.04	0.1898	-0.01	0.128	-0.001	0.4202	0.05	0.2788	0.004
0.4977	-0.06	0.3861	-0.06	0.3548	-0.03	0.1983	-0.001	0.5409	-0.002	0.438	-0.002
0.5756	-0.08	0.4829	-0.09	0.4106	-0.02	0.2949	0.03	0.6402	0.001	0.7028	0.04
0.6992	-0.06	0.5769	-0.03	0.455	-0.02	0.3703	0.04	0.7596	0.06	0.5868	-0.01
0.6974	-0.1	0.6236	-0.06	0.5779	0.05	0.5106	0.1	0.8081	0.04	0.7476	-0.03
0.2832	0.02										
0.3982	0.02										
0.5051	0.06										
0.5741	0.06										
0.6438	0.09										

x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa	x_{NH3}	Δp /MPa
$NH_3 + [C_8mim][BF_4]$ [3]				$NH_3 + [C_2mim][NTf_2]$ [4]				$NH_3 + [C_6mim][Cl]$ [4]			
323 K		333 K		283 K		299 K		323 K		283 K		298 K	
0.1564	0.03	0.1321	0.02	0.220	-0.1	0.171	-0.1	0.089	-0.1	0.095	-0.02	0.086	-0.03
0.3471	0.07	0.2555	0.05	0.504	-0.1	0.430	-0.1	0.305	-0.1	0.254	-0.03	0.231	-0.04
0.4525	0.1	0.3798	0.1	0.634	-0.1	0.568	-0.2	0.444	-0.2	0.363	-0.05	0.337	-0.07
0.5485	0.2	0.4447	0.1	0.811	-0.1	0.768	-0.2	0.673	-0.2	0.562	-0.06	0.537	-0.08
0.6002	0.2	0.5022	0.2	0.931	-0.1	0.921	-0.1	0.888	-0.003	0.745	-0.09	0.728	-0.1
				0.948	-0.04	0.943	-0.05	0.926	0.10	0.837	-0.08	0.828	-0.1

x_{NH3}	Δp /MPa
$NH_3 + [C_6mim][Cl]$ [4]	
324 K	
0.060	-0.06
0.194	-0.04
0.294	-0.06
0.479	-0.1
0.681	-0.2
0.799	-0.2

Table S3. Deviations, Δp, between the available VLE[5, 6] and the equilibrium pressure predicted by the Flory-Huggins model, as function of H_2S mole fractions and temperature, for the IL + H_2S systems.

x_{H2S}	Δp /MPa	x_{H2S}	Δp /MPa	x_{H2S}	Δp /MPa	x_{H2S}	Δp /MPa	x_{H2S}	Δp /MPa
H_2S + [C_4mim][BF_4] [6]						***H_2S + [C_6mim][BF_4]*** [5]			
303 K		**313 K**		**323 K**		**303 K**		**313 K**	
0.039	-0.01	0.038	-0.01	0.035	-0.01	0.072	-0.03	0.07	-0.03
0.081	-0.02	0.076	-0.03	0.074	-0.02	0.144	-0.03	0.139	-0.03
0.120	-0.04	0.111	-0.04	0.11	-0.03	0.233	-0.05	0.226	-0.04
0.163	-0.08	0.166	-0.07	0.168	-0.04	0.303	-0.05	0.295	-0.03
0.183	-0.09	0.180	-0.08	0.187	-0.05	0.38	-0.09	0.371	-0.07
0.228	-0.1	0.220	-0.1	0.225	-0.1	0.441	-0.1	0.433	-0.09
0.270	-0.1	0.250	-0.1	0.24	-0.1	0.469	-0.1	0.46	-0.09
0.310	-0.2	0.280	-0.1	0.28	-0.1	0.499	-0.1	0.491	-0.1
0.354	-0.2	0.32	-0.2	0.303	-0.1				
x_{H2S}	Δp /MPa	x_{H2S}	Δp /MPa	x_{H2S}	Δp /MPa	x_{H2S}	Δp /MPa		
H_2S + [C_4mim][NTf_2] [6]				***H_2S + [C_6mim][PF_6]*** [5]					
303 K		**313 K**		**303 K**		**313 K**			
0.07	-0.03	0.065	-0.03	0.067	-0.07	0.063	-0.07		
0.128	-0.06	0.120	-0.06	0.113	-0.1	0.108	-0.1		
0.174	-0.08	0.163	-0.08	0.166	-0.1	0.159	-0.1		
0.209	-0.1	0.196	-0.1	0.244	-0.2	0.233	-0.2		
0.241	-0.1	0.227	-0.1	0.296	-0.2	0.284	-0.2		
0.273	-0.1	0.258	-0.1	0.345	-0.3	0.333	-0.3		
0.307	-0.2	0.291	-0.2	0.396	-0.3	0.383	-0.3		
0.364	-0.2	0.347	-0.2	0.441	-0.3	0.428	-0.3		
0.444	-0.2	0.434	-0.2						
0.51	-0.2	0.065	-0.03						

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