

Supporting Information

Vapor-Liquid Equilibria of Water + Alkylimidazolium-based Ionic Liquids: Measurements and Perturbed-Chain Statistical Associating Fluid Theory Modeling

Helena Passos^{a,1}, Imran Khan^{a,1}, Fabrice Mutelet^b, Mariana B. Oliveira^a, Pedro J. Carvalho^a, Luís M. N. B. F. Santos^c, Christoph Held^{d*}, Gabriele Sadowski^d, Mara G. Freire^a and João A. P. Coutinho^{a*}

^a *Departamento de Química, CICECO, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal;*

^b *Université de Lorraine, Ecole Nationale Supérieure des Industries Chimiques, Laboratoire Réactions et Génie des Procédés, CNRS (UMR7274), 1 rue Grandville, BP 20451 54001 Nancy, France;*

^c *Centro de Investigação em Química, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre, 687, 4169-007 Porto, Portugal;*

^d *Laboratory of Thermodynamics, Department of Biochemical and Chemical Engineering, Technische Universität Dortmund, Emil-Figge-Str. 70, 44227 Dortmund, Germany.*

*Corresponding authors

Tel: +351 234370200; Fax: +351 234370084; E-mail address: jcoutinho@ua.pt;

Tel: +49231 7552086; Fax +49231 7552572; E-mail address: christoph.held@bci.tu-dortmund.de.

¹ Equally contributing authors.

Table S 1. Electrical conductivity (κ) data for the water + [C₄C₁im]Cl system at 298.15 K and atmospheric pressure.

[IL] / (mol·kg ⁻¹)	κ / (mS·cm ⁻¹)
0.55	30.3
1.21	47.3
2.03	57.6
3.07	62.4
4.44	62.9

Table S 2. Electrical conductivity (κ) data for the water + [C₄C₁im]Br system at 298.15 K and atmospheric pressure.

[IL] / (mol·kg ⁻¹)	κ / (mS·cm ⁻¹)
0.56	31.6
1.29	47.9
2.24	57.0
3.54	61.3
5.53	61.6

Table S 3. Electrical conductivity (κ) data for the water + [C₄C₁im][SCN] system at 298.15 K and atmospheric pressure.

[IL] / (mol·kg ⁻¹)	κ / (mS·cm ⁻¹)
0.025	2.24
0.051	3.95
0.103	7.16
0.266	14.51
0.434	19.52
0.561	23.00
1.244	33.30
2.155	40.20
3.309	44.70

Table S 4. VLE data for the water + [C₄C₁im][CF₃SO₃] system at 0.1, 0.07 and 0.05 MPa.

x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w
0.1 MPa						0.07 MPa						0.05 MPa					
0.994	373.23	0.993	0.818	375.69	1.103	0.994	363.40	0.995	0.818	367.44	1.040	0.994	355.46	0.970	0.818	358.44	1.045
0.990	373.40	0.990	0.803	375.97	1.113	0.991	363.65	0.989	0.803	368.26	1.028	0.991	355.94	0.955	0.802	359.01	1.042
0.982	373.47	0.995	0.794	376.27	1.114	0.983	364.17	0.976	0.793	368.10	1.046	0.982	355.96	0.962	0.794	359.13	1.049
0.977	373.53	0.998	0.785	376.69	1.110	0.978	364.30	0.977	0.786	368.40	1.045	0.978	356.06	0.963	0.785	359.27	1.054
0.972	373.59	0.999	0.776	377.09	1.107	0.973	364.44	0.977	0.776	369.03	1.034	0.974	356.13	0.965	0.776	359.37	1.063
0.963	373.66	1.006	0.758	377.80	1.106	0.964	364.53	0.984	0.759	369.54	1.038	0.963	356.17	0.975	0.758	359.99	1.062
0.947	373.76	1.021	0.748	377.83	1.121	0.949	364.69	0.992	0.747	369.99	1.037	0.950	356.20	0.986	0.748	360.28	1.065
0.933	373.98	1.028	0.735	378.33	1.120	0.932	365.04	0.997	0.736	370.27	1.042	0.932	356.36	0.996	0.735	360.70	1.065
0.914	374.16	1.042	0.726	379.09	1.105	0.918	365.47	0.997	0.725	370.81	1.037	0.920	356.48	1.002	0.725	360.79	1.076
0.901	374.40	1.050	0.719	379.37	1.105	0.901	365.56	1.013	0.719	371.07	1.036	0.902	356.60	1.022	0.719	361.18	1.070
0.886	374.53	1.063	0.708	379.82	1.104	0.888	365.64	1.025	0.708	371.36	1.040	0.892	356.72	1.028	0.708	361.46	1.074
0.875	374.62	1.071	0.703	379.97	1.107	0.874	366.22	1.018	0.704	371.71	1.034	0.866	357.07	1.046	0.705	361.93	1.060

0.870	374.83	1.069	0.688	380.56	1.108	0.868	366.39	1.019	0.690	371.97	1.046	0.861	357.17	1.047	0.690	362.26	1.070
0.862	374.92	1.076	0.676	381.14	1.107	0.863	366.63	1.016	0.678	372.46	1.046	0.862	357.27	1.039	0.677	362.68	1.073
0.843	375.02	1.097	0.665	381.67	1.105	0.843	366.80	1.033	0.665	373.02	1.045	0.843	357.49	1.053	0.665	363.13	1.075
0.838	375.41	1.088				0.838	367.03	1.030				0.838	357.83	1.046			

^a Standard uncertainties x_w , T^b and γ_w are 0.001, 0.02 K and 0.001, respectively.

Table S 5. VLE data for the water + [C₄C₁im][SCN] system at 0.1, 0.07 and 0.05 MPa.

x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w
0.1 MPa						0.07 MPa						0.05 MPa					
0.996	372.67	1.010	0.795	382.27	0.903	0.995	363.46	0.994	0.773	372.30	0.922	0.996	354.69	1.000	0.783	362.25	0.941
0.989	373.38	0.991	0.711	387.36	0.853	0.989	363.79	0.989	0.717	377.41	0.830	0.989	355.14	0.990	0.719	366.03	0.891
0.981	373.66	0.989	0.669	390.87	0.811	0.981	363.87	0.991	0.658	380.87	0.803	0.981	355.19	0.993	0.661	370.29	0.828
0.971	373.93	0.989	0.609	395.48	0.771	0.968	364.09	0.996	0.605	385.26	0.754	0.969	355.25	1.003	0.609	373.87	0.790
0.955	374.30	0.992				0.951	364.47	0.999				0.951	355.70	1.004			
0.937	375.11	0.984				0.922	365.71	0.982				0.929	356.85	0.984			
0.921	375.67	0.982				0.903	366.16	0.987				0.917	357.11	0.986			
0.896	376.35	0.982				0.891	366.70	0.980				0.896	357.61	0.986			
0.860	378.30	0.961				0.860	368.15	0.963				0.869	358.75	0.972			
0.842	378.89	0.962				0.830	369.30	0.958				0.841	359.68	0.971			
0.804	381.69	0.912				0.793	371.14	0.938				0.811	360.61	0.971			

^a Standard uncertainties x_w , T^b and γ_w are 0.001, 0.02 K and 0.001, respectively.

Table S 6. VLE data for the water + [C₄C₁im][TOS] system at 0.1, 0.07 and 0.05 MPa.

x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w
0.1 MPa						0.07 MPa						0.05 MPa					
0.996	373.33	0.986	0.888	378.03	0.936	0.996	363.53	0.988	0.893	367.76	0.942	0.996	354.88	0.988	0.898	358.14	0.962
0.995	373.41	0.986	0.875	379.50	0.903	0.995	363.65	0.987	0.874	368.90	0.923	0.995	355.01	0.987	0.876	359.11	0.949
0.990	373.56	0.986	0.859	380.51	0.890	0.990	363.78	0.987	0.857	369.84	0.908	0.995	355.01	0.987	0.865	359.93	0.935
0.984	373.75	0.982	0.839	381.53	0.879	0.986	363.88	0.985	0.838	370.88	0.894	0.990	355.13	0.985	0.852	360.75	0.917
0.983	373.94	0.976	0.826	382.89	0.852	0.986	364.04	0.980	0.830	371.90	0.870	0.985	355.46	0.977	0.830	362.40	0.888
0.975	374.12	0.978	0.813	385.38	0.798	0.975	364.04	0.990	0.811	374.40	0.815	0.975	355.58	0.982	0.809	364.69	0.833
0.965	374.34	0.980	0.797	386.14	0.796	0.966	364.22	0.993	0.792	375.50	0.802	0.966	355.67	0.987	0.798	365.39	0.821
0.958	374.45	0.983	0.791	387.13	0.776	0.958	364.50	0.991	0.789	376.12	0.789	0.958	355.94	0.987	0.797	365.92	0.806
0.952	374.98	0.973	0.784	388.67	0.744	0.952	364.89	0.982	0.787	376.81	0.771	0.953	356.10	0.986	0.792	366.64	0.790
0.935	375.55	0.970	0.766	390.82	0.709	0.934	365.66	0.974	0.771	378.16	0.752	0.937	356.60	0.983	0.774	367.27	0.790
0.924	376.10	0.963	0.746	393.73	0.663	0.921	366.65	0.951	0.763	379.53	0.724	0.921	357.30	0.971	0.764	369.01	0.752
0.896	377.28	0.953				0.900	366.95	0.964				0.907	357.52	0.976			

^a Standard uncertainties x_w , T^b and γ_w are 0.001, 0.02 K and 0.001, respectively.

Table S 7. VLE data for the water + [C₄C₁im][CF₃CO₂] system at 0.1, 0.07 and 0.05 MPa.

x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w
0.1 MPa						0.07 MPa						0.05 MPa					
0.994	373.03	0.997	0.911	377.30	0.938	0.993	363.93	0.979	0.911	367.32	0.938	0.993	354.91	0.990	0.908	358.12	0.955
0.990	373.31	0.991	0.896	378.26	0.922	0.989	364.20	0.973	0.895	368.29	0.921	0.991	355.26	0.979	0.895	358.85	0.941
0.985	373.46	0.990	0.878	379.20	0.911	0.985	364.23	0.976	0.875	369.32	0.909	0.985	355.38	0.978	0.884	359.58	0.925
0.980	373.69	0.987	0.866	380.10	0.895	0.979	364.46	0.973	0.862	369.99	0.898	0.980	355.70	0.971	0.870	360.27	0.916
0.974	374.03	0.983	0.852	381.00	0.881	0.974	364.70	0.967	0.849	370.72	0.889	0.974	356.03	0.965	0.852	361.00	0.908
0.966	374.36	0.979	0.834	381.56	0.885	0.967	364.89	0.967	0.832	371.80	0.872	0.968	356.31	0.962	0.835	362.20	0.887
0.958	374.92	0.968	0.812	382.50	0.880	0.960	365.50	0.954	0.812	372.89	0.859	0.960	356.77	0.953	0.815	363.40	0.869
0.948	375.50	0.957	0.794	384.49	0.841	0.951	366.12	0.941	0.794	374.28	0.836	0.950	357.19	0.947	0.799	364.63	0.845
0.939	375.92	0.953	0.773	386.48	0.808	0.942	366.26	0.944	0.775	375.12	0.832	0.941	357.24	0.955	0.780	365.80	0.827
0.928	376.31	0.950	0.739	388.96	0.781	0.932	366.37	0.950	0.741	377.09	0.812	0.930	357.29	0.964	0.741	367.70	0.812
0.920	376.82	0.944	0.693	391.48	0.767	0.922	366.86	0.943	0.697	380.04	0.780	0.922	357.72	0.956	0.704	370.03	0.785

^a Standard uncertainties x_w , T^b and γ_w are 0.001, 0.02 K and 0.001, respectively.

Table S 8. VLE data for the water + [C₄C₁im]Br system at 0.1, 0.07 and 0.05 MPa.

x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w
0.1 MPa						0.07 MPa						0.05 MPa					
0.995	373.23	0.981	0.908	378.09	0.915	0.995	363.86	0.979	0.908	368.13	0.915	0.995	355.24	0.976	0.909	359.20	0.915
0.990	373.25	0.986	0.894	378.90	0.903	0.989	363.91	0.982	0.893	368.93	0.903	0.990	355.28	0.979	0.892	359.91	0.907
0.984	373.28	0.990	0.886	379.69	0.888	0.984	363.97	0.985	0.877	369.94	0.887	0.984	355.34	0.982	0.884	360.49	0.894
0.976	373.76	0.982	0.877	380.21	0.881	0.976	364.40	0.974	0.871	370.25	0.883	0.977	355.79	0.974	0.875	361.04	0.885
0.967	374.25	0.974	0.865	381.57	0.852	0.967	364.84	0.968	0.861	371.03	0.868	0.966	356.19	0.970	0.866	361.30	0.884
0.960	374.66	0.964	0.851	382.36	0.843	0.959	365.11	0.967	0.849	371.76	0.857	0.958	356.57	0.961	0.855	361.60	0.885
0.953	375.05	0.958	0.817	385.67	0.787	0.950	365.38	0.963	0.813	374.64	0.801	0.949	356.92	0.957	0.822	365.38	0.799
0.946	375.46	0.951	0.794	388.81	0.731	0.945	365.76	0.957	0.793	377.51	0.748	0.943	357.26	0.950	0.798	366.81	0.781
0.938	375.82	0.947	0.780	390.74	0.697	0.938	366.12	0.950	0.769	378.97	0.734	0.937	357.56	0.945	0.767	369.59	0.729
0.929	376.77	0.931	0.737	394.73	0.651	0.926	366.72	0.943	0.732	383.62	0.659	0.926	358.02	0.939	0.748	372.82	0.669
0.920	377.25	0.925	0.729	399.88	0.559	0.918	367.28	0.932	0.695	388.24	0.595	0.919	358.45	0.930			

^a Standard uncertainties x_w , T^b and γ_w are 0.001, 0.02 K and 0.001, respectively.

Table S 9. VLE data for the water + [C₄C₁im][C₁SO₃] system at 0.1, 0.07 and 0.05 MPa.

x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w
0.1 MPa						0.07 MPa						0.05 MPa					
0.995	373.28	0.987	0.904	379.68	0.870	0.996	363.39	0.994	0.904	369.80	0.865	0.995	354.60	1.001	0.904	360.54	0.877
0.988	373.38	0.990	0.893	380.90	0.845	0.989	363.79	0.987	0.891	370.86	0.845	0.990	355.03	0.991	0.893	361.32	0.862
0.983	373.76	0.983	0.885	381.50	0.835	0.983	363.97	0.984	0.880	372.20	0.813	0.984	355.36	0.982	0.881	362.60	0.829
0.981	373.92	0.980	0.876	382.47	0.816	0.981	364.21	0.980	0.868	373.50	0.786	0.981	355.51	0.981	0.868	363.87	0.802
0.978	374.11	0.977	0.858	384.71	0.774	0.978	364.47	0.973	0.859	374.57	0.766	0.978	355.65	0.978	0.859	364.83	0.780
0.968	374.86	0.961	0.837	386.91	0.738	0.968	365.16	0.957	0.843	375.69	0.750	0.968	356.31	0.963	0.844	365.59	0.771
0.955	375.59	0.949	0.819	389.27	0.697	0.956	365.84	0.944	0.821	378.44	0.699	0.954	356.94	0.952	0.830	367.47	0.731
0.946	376.19	0.938	0.800	391.54	0.664	0.946	366.45	0.931	0.796	381.08	0.659	0.946	357.59	0.936	0.815	369.43	0.693
0.936	376.82	0.927	0.784	393.56	0.635	0.938	367.08	0.917	0.786	382.26	0.641	0.938	358.25	0.923	0.788	370.80	0.683
0.925	377.61	0.913	0.766	395.75	0.606	0.925	367.92	0.903	0.774	383.28	0.629	0.927	358.98	0.903	0.783	372.26	0.652
0.913	378.40	0.900	0.719	400.30	0.562	0.917	368.76	0.885	0.719	389.10	0.559	0.921	359.75	0.883			

^a Standard uncertainties x_w , T^b and γ_w are 0.001, 0.02 K and 0.001, respectively.

Table S 10. VLE data for the water + [C₄C₁im][C₁CO₂] system at 0.1, 0.07 and 0.05 MPa.

x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w	x_w	T^b / K	γ_w
0.1 MPa						0.07 MPa						0.05 MPa					
0.994	373.33	0.987	0.865	383.38	0.800	0.994	363.56	0.991	0.885	372.02	0.813	0.994	354.66	1.001	0.886	362.59	0.824
0.987	373.51	0.988	0.853	384.81	0.775	0.987	363.76	0.990	0.872	373.48	0.783	0.987	355.09	0.991	0.876	363.76	0.797
0.980	373.83	0.984	0.837	386.24	0.753	0.982	364.14	0.981	0.860	374.74	0.760	0.982	355.26	0.990	0.865	364.86	0.773
0.971	374.21	0.982	0.825	388.23	0.717	0.975	364.50	0.975	0.847	375.97	0.739	0.976	355.38	0.991	0.853	366.00	0.753
0.962	375.05	0.960	0.813	390.09	0.685	0.961	365.23	0.960	0.828	377.78	0.711	0.963	355.69	0.992	0.839	368.01	0.711
0.952	375.73	0.948	0.802	391.75	0.657	0.951	365.93	0.944	0.813	379.71	0.677	0.954	356.60	0.965	0.822	369.76	0.680
0.932	377.26	0.918	0.792	393.45	0.631	0.940	366.70	0.930	0.803	381.13	0.652	0.942	357.83	0.934	0.816	370.66	0.663
0.920	378.09	0.904	0.781	395.73	0.597	0.930	367.77	0.903	0.793	382.60	0.628	0.933	358.48	0.917	0.807	372.27	0.632
0.906	379.46	0.874	0.767	398.08	0.565	0.920	368.20	0.901	0.783	384.38	0.600	0.922	359.21	0.902	0.787	374.36	0.604
0.894	380.76	0.848				0.909	369.27	0.876	0.764	386.86	0.566	0.911	360.27	0.876	0.773	375.59	0.590
0.881	382.07	0.823				0.896	370.56	0.848				0.898	361.52	0.847			

^a Standard uncertainties x_w , T^b and γ_w are 0.001, 0.02 K and 0.001, respectively.