

SUPPLEMENTARY MATERIAL

Understanding the role of the hydrogen bond donor of the deep eutectic solvents in the formation of the aqueous biphasic systems

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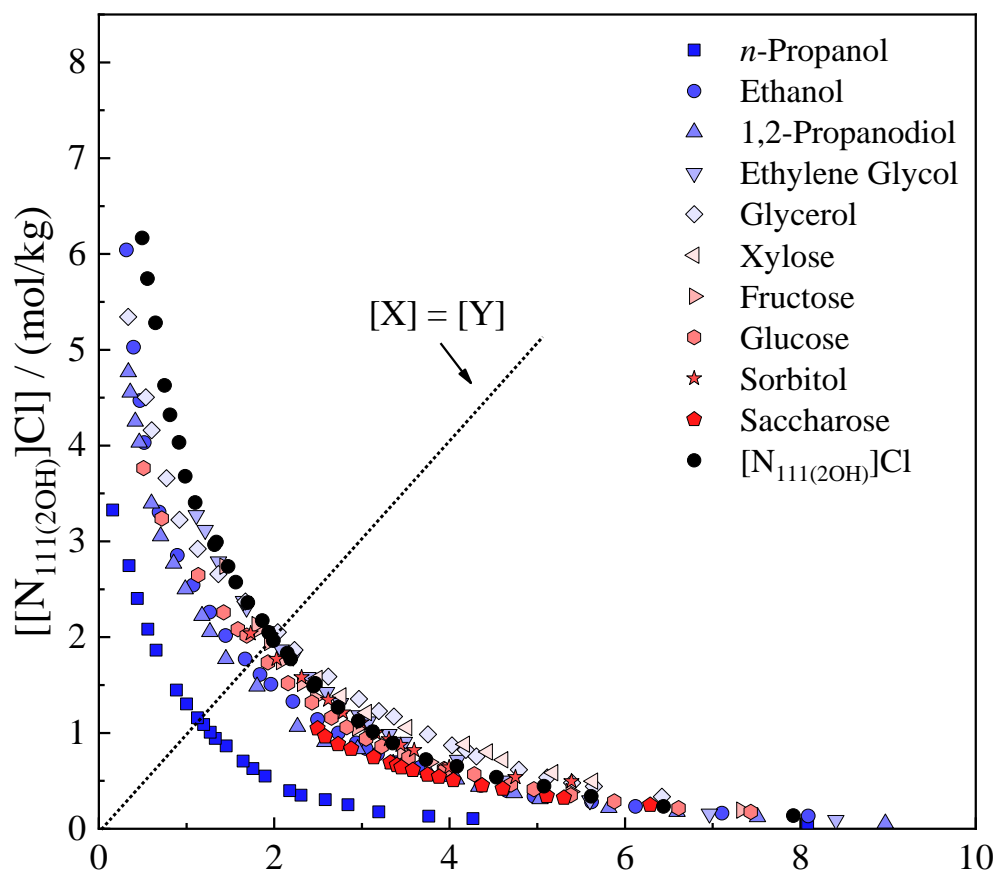


Figure S1 – Phase diagrams at 298 K and atmospheric pressure in function of $[N_{111(2OH)}]Cl$ concentration for ABS composed of $[N_{111(2OH)}]Cl + HBD + K_2HPO_4 + H_2O$, using the follow HBD: *n*-propanol, ethanol, 1,2-propanediol and ethylene glycol [1]; fructose, glucose e saccharose [2] and glycerol, xylose and sorbitol (this work) at 1:1 molar ratio.

Table S1. Experimental binodal data in molality (mol/kg) for the system composed of $[N_{111(2OH)}]Cl + HBD + K_2HPO_4 + H_2O$ at 298.15 K and atmospheric pressure using alcohols as HBD and HBA: HBD molar fraction of 1:1: *n*-propanol, ethanol, 1,2-propanediol and ethylene glycol [1] and glycerol (this work).^a

<i>n</i> -Propanol		Ethanol		1,2-Propanediol		Ethylene glycol		Glycerol	
<i>m</i> Salt	<i>m</i> [N _{111(2OH)}]Cl	<i>m</i> Salt	<i>m</i> [N _{111(2OH)}]Cl	<i>m</i> Salt	<i>m</i> [N _{111(2OH)}]Cl	<i>m</i> Salt	<i>m</i> [N _{111(2OH)}]Cl	<i>m</i> Salt	<i>m</i> [N _{111(2OH)}]Cl
8.08	0.06	8.09	0.12	8.97	0.06	8.41	0.09	0.33	5.34
4.27	0.10	7.11	0.14	7.51	0.12	6.96	0.16	0.54	4.51
3.76	0.13	6.12	0.20	6.59	0.18	5.60	0.29	0.60	4.16
3.19	0.18	5.62	0.24	5.82	0.22	4.60	0.50	0.77	3.66
2.84	0.25	4.96	0.30	5.03	0.31	4.09	0.72	0.92	3.23
2.58	0.30	4.65	0.35	4.74	0.37	3.49	0.90	1.13	2.92
2.31	0.35	4.36	0.39	4.33	0.44	3.31	0.99	1.36	2.66
2.18	0.40	3.95	0.49	4.08	0.52	3.07	1.12	1.67	2.37
1.90	0.55	3.66	0.55	3.76	0.59	2.97	1.18	2.04	2.05
1.76	0.63	3.39	0.60	3.36	0.68	2.76	1.31	2.23	1.87
1.65	0.71	3.18	0.67	2.95	0.83	2.60	1.43	2.62	1.59
1.45	0.86	3.05	0.72	2.58	0.91	2.39	1.58	2.97	1.36
1.33	0.94	2.94	0.77	2.27	1.07	2.22	1.80	3.19	1.23
1.27	1.01	2.73	0.86	1.80	1.49	2.08	1.87	3.36	1.17
1.20	1.09	2.49	0.98	1.45	1.77	1.91	2.06	3.75	0.99
1.12	1.16	2.21	1.14	1.27	2.05	1.68	2.31	4.03	0.87
1.00	1.30	1.96	1.29	1.18	2.22	1.65	2.38	4.18	0.82
0.88	1.45	1.84	1.37	0.99	2.50	1.37	2.79	4.31	0.75
0.65	1.86	1.67	1.51	0.85	2.77	1.21	3.12	4.79	0.62
0.56	2.08	1.45	1.71	0.70	3.05	1.11	3.27	5.11	0.54
0.44	2.40	1.27	1.91	0.60	3.40			5.40	0.48
0.35	2.75	1.08	2.13	0.46	4.03			5.64	0.44
0.16	3.33	0.90	2.38	0.42	4.25			6.42	0.33
		0.69	2.74	0.36	4.55				
		0.52	3.30	0.34	4.77				
		0.47	3.64						
		0.40	4.05						

^a Standard uncertainty u are $u(m) = 0.01$, $u(T) = 0.5$ K, and $u(P) = 10$ kPa.

Table S2. Experimental binodal data in molality (mol/kg) for the system composed of $[N_{111}(2OH)]Cl$ + HBD + K_2HPO_4 + H_2O at 298.15 K and atmospheric pressure using sugars as HBD and HBA: HBD molar fraction of 1:1: **glucose, fructose and saccharose [1]; xylose, sorbitol (this work).**^a

Xylose		Fructose		Glucose		Sorbitol		Saccharose	
<i>m</i> Salt	<i>m</i> [N ₁₁₁ (2OH)]Cl	<i>m</i> Salt	<i>m</i> [N ₁₁₁ (2OH)]Cl	<i>m</i> Salt	<i>m</i> [N ₁₁₁ (2OH)]Cl	<i>m</i> Salt	<i>m</i> [N ₁₁₁ (2OH)]Cl	<i>m</i> Salt	<i>m</i> [N ₁₁₁ (2OH)]Cl
2.49	1.57	7.33	0.19	0.51	3.77	5.39	0.50	2.49	1.06
2.76	1.39	5.38	0.39	0.72	3.24	4.75	0.54	2.58	0.98
3.05	1.21	3.77	0.69	1.13	2.65	3.99	0.64	2.73	0.89
3.51	1.06	3.46	0.80	1.42	2.26	3.60	0.82	2.88	0.84
4.17	0.88	3.08	0.96	1.59	2.08	3.44	0.87	3.14	0.75
4.43	0.80	2.95	1.05	1.69	2.02	3.31	0.93	3.33	0.70
4.61	0.72	2.73	1.21	1.93	1.74	3.16	1.00	3.40	0.67
		2.47	1.37	2.16	1.52	2.99	1.11	3.45	0.65
		2.32	1.52	2.43	1.32	2.78	1.21	3.58	0.62
		2.08	1.74	2.65	1.16	2.62	1.35	3.75	0.57
		1.94	1.94	2.83	1.06	2.31	1.58	3.88	0.55
		1.83	2.08	3.05	0.94	2.03	1.77	4.04	0.51
		1.80	2.13	3.23	0.86	1.73	2.04	4.37	0.46
		1.43	2.74	3.53	0.74	0.66	2.98	4.61	0.42
				3.94	0.62			5.11	0.34
				3.95	0.61			5.30	0.33
				4.28	0.57			6.29	0.25
				4.70	0.46				
				4.96	0.41				
				5.38	0.35				
				5.88	0.29				
				6.61	0.22				
				7.43	0.18				

^a Standard uncertainty u are $u(m) = 0.01$, $u(T) = 0.5$ K, and $u(P) = 10$ kPa.

Table S3. Experimental binodal data in molality (mol/kg) for the system composed of $[\text{N}_{111}(\text{2OH})]\text{Cl} + \text{HBD} + \text{K}_2\text{HPO}_4 + \text{H}_2\text{O}$ at 298.15 K and atmospheric pressure using alcohol as HBD and HBA: HBD molar fraction of 2:1 [1].^a

<i>n</i> -Propanol		Ethanol		1,2-Propanediol		Ethylene glycol	
<i>m</i> Salt	<i>m</i> [N ₁₁₁ (2OH)]Cl	<i>m</i> Salt	<i>m</i> [N ₁₁₁ (2OH)]Cl	<i>m</i> Salt	<i>m</i> [N ₁₁₁ (2OH)]Cl	<i>m</i> Salt	<i>m</i> [N ₁₁₁ (2OH)]Cl
8.30	0.04	8.11	0.15	9.00	0.07	8.82	0.10
5.24	0.06	6.77	0.20	7.68	0.08	6.89	0.22
4.19	0.10	4.82	0.35	6.36	0.22	5.96	0.31
3.90	0.15	4.45	0.40	5.71	0.27	5.27	0.39
3.57	0.20	3.81	0.57	4.99	0.37	4.71	0.48
3.21	0.28	3.47	0.70	4.86	0.44	4.02	0.69
2.62	0.50	3.01	0.89	4.40	0.46	3.60	0.80
2.36	0.70	2.69	1.07	4.11	0.55	3.52	0.85
2.18	0.84	2.40	1.23	3.81	0.62	3.40	0.91
2.08	0.94	2.37	1.25	3.71	0.67	3.27	0.97
1.96	1.04	2.28	1.31	3.44	0.76	3.16	1.04
1.89	1.15	2.05	1.49	3.16	0.88	3.04	1.11
1.85	1.20	1.70	1.83	3.07	0.92	2.92	1.20
1.79	1.29	1.62	1.89	2.71	1.11	2.71	1.33
1.70	1.41	1.26	2.36	2.48	1.25	2.61	1.42
1.60	1.56	1.04	2.66	2.39	1.32	2.41	1.57
1.48	1.72	0.91	2.93	2.21	1.48	2.32	1.67
1.37	1.90	0.79	3.25	2.20	1.52	2.24	1.73
1.30	2.05	0.72	3.46	2.00	1.67	2.05	1.91
1.13	2.39	0.57	4.69	1.79	1.82	1.81	2.16
1.30	2.07	0.48	5.17	1.55	2.11	1.57	2.46
		0.40	6.06	1.46	2.22	1.38	2.75
		0.32	6.88	1.31	2.38	1.20	3.11
				1.19	2.58	1.06	3.47
				1.06	2.85	0.92	3.89
				0.96	3.13	0.69	4.57
				0.85	3.52	0.60	5.49
				0.81	3.55		
				0.76	3.84		
				0.66	4.25		
				0.46	5.34		
				0.30	6.67		

^a Standard uncertainty u are $u(m) = 0.01$, $u(T) = 0.5$ K, and $u(P) = 10$ kPa.

Table S4. Experimental binodal data in molality (mol/kg) for the system composed of $[\text{N}_{111}(\text{2OH})]\text{Cl} + \text{HBD} + \text{K}_2\text{HPO}_4 + \text{H}_2\text{O}$ at 298.15 K and atmospheric pressure using alcohol as HBD and HBA: HBD molar fraction of 1:2 [1].^a

<i>n</i> -Propanol		Ethanol		1,2-Propanediol		Ethylene glycol	
<i>m</i> Salt	<i>m</i> [$\text{N}_{111}(\text{2OH})\text{Cl}$]	<i>m</i> Salt	<i>m</i> [$\text{N}_{111}(\text{2OH})\text{Cl}$]	<i>m</i> Salt	<i>m</i> [$\text{N}_{111}(\text{2OH})\text{Cl}$]	<i>m</i> Salt	<i>m</i> [$\text{N}_{111}(\text{2OH})\text{Cl}$]
8.14	0.15	0.18	17.11	7.79	0.52	7.73	0.42
3.98	0.19	0.24	13.42	6.45	0.73	6.45	0.58
3.42	0.24	0.29	11.87	5.67	0.88	5.84	0.71
3.03	0.35	0.38	9.67	4.49	1.17	5.39	0.90
2.77	0.45	0.47	8.88	3.80	1.35	4.60	1.39
2.34	0.68	0.52	8.07	3.39	1.64	4.17	2.01
1.95	0.96	0.58	7.37	3.05	1.91	3.95	2.29
1.66	1.09	0.67	6.46	2.57	2.50	3.71	2.62
1.35	1.36	0.87	5.48	2.44	2.64	3.29	3.36
1.17	1.55	0.96	4.91	2.20	3.02	2.72	4.69
1.10	1.67	1.11	4.48	2.10	3.24	2.43	5.74
0.93	2.09	1.18	4.22	1.92	3.72	1.91	7.90
0.86	2.33	1.19	4.05	1.63	4.24	1.67	10.09
0.79	2.59	1.31	3.85	1.31	5.34		
0.75	2.75	1.44	3.49	1.18	6.01		
0.69	2.89	1.49	3.38	1.04	6.88		
0.62	3.25	1.64	3.07	0.79	9.33		
0.58	3.58	1.75	2.83	0.66	11.17		
0.54	3.95	1.90	2.58	0.52	15.46		
0.51	4.24	1.99	2.46				
0.45	4.73	2.16	2.13				
0.40	4.98	2.27	1.98				
0.34	5.37	2.40	1.80				
0.31	5.66	2.67	1.48				
0.25	6.16	2.73	1.45				
0.23	6.49	2.84	1.36				
0.18	6.92	3.05	1.16				
0.16	7.27	3.29	0.95				
0.14	7.78	3.46	0.85				
0.12	8.47	3.67	0.73				
0.09	9.10	3.93	0.60				
		4.09	0.54				

^a Standard uncertainty u are $u(m) = 0.01$, $u(T) = 0.5$ K, and $u(P) = 10$ kPa.

Table S5. Experimental binodal data in molality (mol/kg) for the system composed of $[\text{N}_{111}(\text{2OH})]\text{Cl}$ + HBD + K_2HPO_4 + H_2O at 298.15 K and atmospheric pressure using sugars as HBD and HBA: HBD molar fraction of 2:1 and 1:2 [2].^a

Glucose (2:1)		Glucose (1:2)		Fructose (2:1)		Fructose (1:2)	
<i>m</i> Salt	<i>m</i> [$\text{N}_{111}(\text{2OH})\text{Cl}$]	<i>m</i> Salt	<i>m</i> [$\text{N}_{111}(\text{2OH})\text{Cl}$]	<i>m</i> Salt	<i>m</i> [$\text{N}_{111}(\text{2OH})\text{Cl}$]	<i>m</i> Salt	<i>m</i> [$\text{N}_{111}(\text{2OH})\text{Cl}$]
0.35	7.15	2.88	0.89	0.74	5.42	1.58	1.46
0.40	6.48	3.09	0.79	0.89	4.61	1.87	1.27
0.54	5.39	3.23	0.74	1.07	3.94	2.34	1.06
0.73	4.44	3.43	0.68	1.17	3.59	2.51	0.95
0.87	3.97	3.67	0.59	1.27	3.25	2.79	0.86
0.98	3.64	3.83	0.54	1.38	2.97	2.94	0.82
1.03	3.46	4.16	0.47	1.53	2.65	3.06	0.77
1.11	3.28	4.45	0.42	1.71	2.35	3.35	0.69
1.30	2.89	5.23	0.32	1.90	2.10	3.84	0.55
1.34	2.80	5.92	0.25	2.04	1.92	4.28	0.45
1.54	2.52	6.55	0.21	2.21	1.76	4.63	0.38
1.65	2.32			2.37	1.58	5.29	0.30
1.71	2.23			2.59	1.44	6.75	0.20
1.78	2.12			2.82	1.32		
1.95	1.95			2.96	1.22		
2.01	1.88			3.27	1.07		
2.03	1.84			3.78	0.87		
2.10	1.75			3.94	0.81		
2.22	1.65			4.12	0.75		
2.31	1.57			4.36	0.66		
2.36	1.51			4.50	0.59		
2.47	1.44			4.77	0.54		
2.60	1.34			4.91	0.47		
2.93	1.15			5.51	0.38		
3.24	1.00			5.99	0.33		
3.43	0.92			7.10	0.26		
3.75	0.81						
4.20	0.65						
4.44	0.58						
5.01	0.45						
5.31	0.39						
6.00	0.28						
6.66	0.22						
7.17	0.19						
7.82	0.16						

^a Standard uncertainty u are $u(m) = 0.01$, $u(T) = 0.5$ K, and $u(P) = 10$ kPa.

Table S6. Experimental binodal data in molality (mol/kg) for the system composed of [N₁₁₁(2OH)]Cl + K₂HPO₄ + H₂O at 298.15 K and atmospheric pressure [2].^a

[N ₁₁₁ (2OH)]Cl	
<i>m</i> Salt	<i>m</i> [N ₁₁₁ (2OH)]Cl
0.38	7.78
0.50	6.17
0.56	5.74
0.65	5.28
0.75	4.63
0.81	4.32
0.92	4.03
0.99	3.68
1.10	3.40
1.32	2.96
1.34	2.99
1.47	2.74
1.56	2.57
1.70	2.36
1.86	2.17
1.94	2.05
1.99	1.96
2.15	1.83
2.19	1.77
2.45	1.49
2.47	1.52
2.73	1.27
2.96	1.12
3.13	1.01
3.35	0.89
3.73	0.72
4.08	0.65
4.54	0.54
5.08	0.44
5.62	0.34
6.44	0.23
7.92	0.14

^a Standard uncertainty *u* are *u*(*m*) = 0.01, *u*(*T*) = 0.5 K, and *u*(*P*) = 10 kPa.

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