

Supporting Information
Evaluating the Importance of Long-Range Interactions in the Thermodynamic Description of Choline Chloride/Water System

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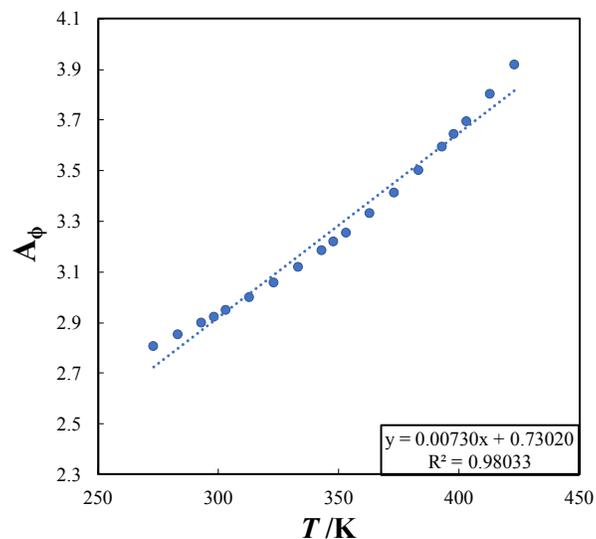


Figure S1. Debye-Hückel Parameter of water as a function of temperature. Data were taken from Clarke and Glew¹

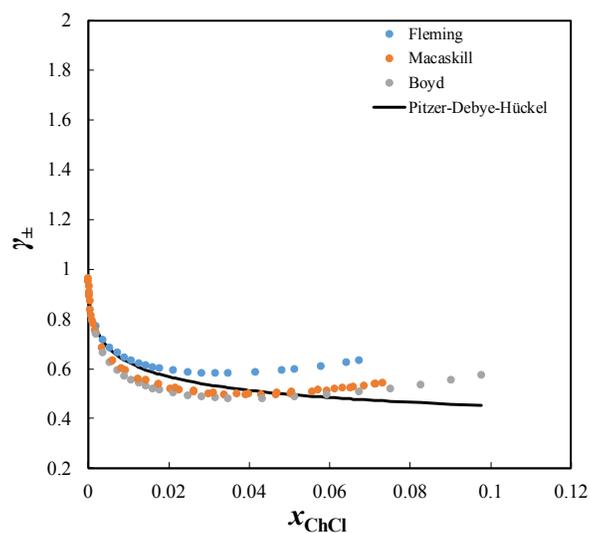


Figure S2. Mean activity coefficients of choline chloride (ChCl) in water at 298.15 K. The line shows the mean activity coefficients calculated by Pitzer-Debye-Hückel term using the closest approach parameter of 14.9. Experimental data were taken from²⁻⁴

Saturation Pressure of Water

The saturation pressure of water was calculated as follows ⁵

$$P_{sat} = P_c \exp \left(\frac{T_c}{T} \times (B_1\tau + B_2\tau^{1.5} + B_3\tau^3 + B_4\tau^{3.5} + B_5\tau^4 + B_6\tau^{7.5}) \right) \quad (1)$$

$$\tau = 1 - \frac{T}{T_c} \quad (2)$$

The parameters are available in **Table S1**.

Table S1. Parameters used to calculate the saturation pressure of water.

P_c	22064 kPa
T_c	647.14 K
B_1	-7.85823
B_2	1.83991
B_3	-11.7811
B_4	22.6705
B_5	-15.9393
B_6	1.77516

Table S2. Binary interaction parameters obtained in this work.

Approach	Component 1	Component 2	A_{12}/R	A_{21}/R
Melting Properties Set 1				
Associated ions	ChCl	Water	-648.6168	-448.2319
Associated ions no long-range	ChCl	Water	-648.5446	-448.2199
Dissociated ions	Ch ⁺	Cl ⁻	0	-1261.7513
	Ch ⁺	Water	2195.0926	-1590.5220
	Cl ⁻	Water	-889.7643	601.3952
Melting Properties Set 2				
Associated ions	ChCl	Water	2342.3743	-573.4183
Associated ions no long-range	ChCl	Water	2372.9372	-559.8990
Dissociated ions	Ch ⁺	Cl ⁻	626.3170	240.5581
	Ch ⁺	Water	1954.5345	-962.2324
	Cl ⁻	Water	1924.4647	240.5581

Table S3. The weights of error in each type of data when summing up the objective function.

Approach	SLE	VLE	Isopiestic data	Water activity	Sum of OF
Melting Properties Set 1					
Associated ions	11.4%	2.43%	86.02%	0.15%	9878.01
Associated ions no long-range	1.41%	0.14%	98.44%	0.01%	69587.48
Dissociated ions	70.0%	3.48%	26.48%	0.04%	7741.22
Melting Properties Set 2					
Associated ions	82.0%	15.90%	0.66%	1.46%	12020.30
Associated ions no long-range	48.43%	6.85%	44.02%	0.7%	17634.44
Dissociated ions	66.57%	29.90%	1.23%	2.3%	5832.61

References

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