Supporting Information

Ionic Solution: What Goes Right and Wrong with Continuum Solvation Modeling

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Table S-1. Simulated volumes and corresponding molalities after 100ns NPT molecular dynamic simulation for all 10 molalities.

Molality (mol/kg)	Volume ($Å^3$)
0.10	16.10
0.21	16.22
0.31	16.24
0.62	16.33
1.03	16.41
2.06	16.73
3.08	17.04
4.11	17.40
5.14	17.81
6.17	18.22

Table S-2. Excess chemical potential μ^{ex}, volume correction term (Vol term), computed chemical potential μ_{NaCl} (This work), simulation result from Mester and Panagiotopoulos (Mester), and experimental results (Experiment) versus molality. All free energies reported are in the unit of kJ/mol. The chemical potential μ_{NaCl} was computed as the sum of μ^{ex}, μ^0, and volume correction term (eqn (5)).

Molality	μ^{ex}	Vol term	This work	Mester	Experiment
0.05	NA	NA	NA	NA	-409.11
0.06	NA	NA	NA	-407.3	NA
0.10	-743.80	4.58	-405.07	NA	-405.92
0.20	NA	NA	NA	NA	-402.77
0.21	-743.46	7.98	-401.33	NA	NA
0.30	NA	NA	NA	NA	-400.92
0.31	-743.46	9.99	-399.32	NA	NA
0.40	NA	NA	NA	NA	-399.60
0.50	NA	NA	NA	NA	-398.57
0.56	NA	NA	NA	-396.2	NA
0.62	-743.73	13.39	-396.19	NA	NA
1.00	NA	NA	NA	-393.1	-395.29
1.05	-742.55	15.90	-392.50	NA	NA
2.00	NA	NA	NA	-389.3	-391.75
2.06	-741.79	19.24	-388.40	NA	NA
3.00	NA	NA	NA	-386	-389.40
3.08	-742.03	21.16	-386.72	NA	NA
4.00	NA	NA	NA	-383.4	-387.51
4.18	-740.63	22.48	-384.00	NA	NA
5.00	NA	NA	NA	-380.7	-385.85
5.14	-739.11	23.47	-381.49	NA	NA
6.00	NA	NA	N/A	-378.7	-384.34
6.144	NA	NA	N/A	N/A	-384.13
6.17	-737.83	24.26	-379.42	N/A	N/A