Alkali Halide Solutions under Thermal Gradients: Soret Coefficients and Heat Transfer Mechanisms

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Table 1: Thermal conductivity data from simulations of aqueous KCl and NaCl solutions: Salt concentration, density with respect to water, temperature gradient, heat flux and thermal conductivity.

c/mol kg^{-1}	$\rho_{\mathrm{ave,H_2O}}$/g cm^{-3}	∇T/K nm^{-1}	J_U / 10^{10} W m^{-2}	λ / W m^{-1} K^{-1}
KCl, DGS ions, T_{ave}/K = 350, p/bar = 500				
1	0.9562	-37.60±0.02	3.12±0.07	0.83±0.02
2	0.9346	-37.00±0.02	2.96±0.07	0.80±0.02
3	0.9115	-36.54±0.02	2.82±0.07	0.77±0.02
4	0.8930	-36.38±0.03	2.72±0.07	0.75±0.02
KCl, DGS ions, T_{ave}/K = 300, p/bar= 1				
1	0.9562	-18.91±0.02	1.51±0.06	0.80±0.03
2	0.9346	-18.65±0.02	1.44±0.06	0.77±0.03
3	0.9115	-18.40±0.02	1.36±0.06	0.74±0.03
4	0.8930	-18.31±0.02	1.32±0.06	0.72±0.03
KCl, DHV ions, T_{ave}/K = 350, p/bar = 500				
1	0.9562	-37.86±0.02	3.14±0.07	0.83±0.02
2	0.9346	-37.37±0.03	3.01±0.07	0.80±0.02
3	0.9115	-36.71±0.02	2.85±0.07	0.78±0.02
4	0.8930	-36.57±0.03	2.77±0.07	0.76±0.02
NaCl, DGS ions, T_{ave}/K = 350, p/bar = 500				
1	0.9692	-37.68±0.02	3.20±0.07	0.85±0.02
2	0.9582	-37.09±0.02	3.11±0.07	0.84±0.02
3	0.9481	-36.73±0.02	3.04±0.07	0.83±0.02
4	0.9394	-36.58±0.02	3.01±0.07	0.82±0.02
NaCl, DGS ions, T_{ave}/K = 350, p/bar = 100				
1	0.9621	-37.91±0.03	3.17±0.09	0.84±0.02
2	0.9531	-37.34±0.03	3.11±0.09	0.83±0.03
3	0.9457	-36.99±0.02	3.02±0.09	0.82±0.03
4	0.9335	-36.73±0.03	2.99±0.09	0.81±0.03

Table 2: The Soret coefficient for NaCl solutions at different concentrations, temperature and pressures from simulations: Average temperature and salt concentration in observed region and Soret coefficient.

$\frac{T}{\mathrm{K}}$	$\frac{m}{\mathrm{mol\ kg^{-1}}}$	$\frac{s_T}{10^{-3}\mathrm{K}^{-1}}$	$\frac{T}{\mathrm{K}}$	$\frac{m}{\mathrm{mol\ kg^{-1}}}$	$\frac{s_T}{10^{-3}\mathrm{K}^{-1}}$
p/bar = 500			p/bar = 100		
318	1.22±0.02	1.71±0.26	299	1.22±0.02	-1.80±0.59
318	2.31±0.03	1.34±0.34	299	2.43±0.03	-0.08±0.62
318	3.50±0.04	1.61±0.24	299	3.64±0.03	0.68±0.35
318	4.59±0.04	1.27±0.22	299	4.64±0.03	0.67±0.21
328	1.18±0.03	2.54±0.09	309	1.20±0.02	1.08±0.30
328	2.28±0.05	2.38±0.08	309	2.39±0.03	1.40±0.19
328	3.41±0.06	1.70±0.07	309	3.57±0.05	1.55±0.10
328	4.51±0.06	1.45±0.04	309	4.61±0.03	0.79±0.06
339	1.13±0.04	3.06±0.12	318	1.17±0.03	2.23±0.14
339	2.22±0.07	2.68±0.08	318	2.34±0.04	1.65±0.07
339	3.33±0.07	1.61±0.04	318	3.51±0.06	1.56±0.05
339	4.43±0.08	1.44±0.03	318	4.55±0.04	0.83±0.05
348	1.10±0.04	3.46±0.14	328	1.16±0.03	3.44±0.20
348	2.16±0.07	2.68±0.08	328	2.30±0.04	2.05±0.14
348	3.30±0.07	1.93±0.04	328	3.47±0.05	1.81±0.08
348	4.38±0.08	1.61±0.03	328	4.52±0.04	1.00±0.07
358	1.07±0.05	4.00±0.17	338	1.11±0.04	4.34±0.36
358	2.10±0.07	2.87±0.09	338	2.25±0.04	2.14±0.13
358	3.24±0.07	2.02±0.04	338	3.39±0.05	1.95±0.13
358	4.30±0.08	1.77±0.03	338	4.46±0.06	1.56±0.15

Table 3: The Soret coefficient for KCl solutions at different concentrations, temperature, pressures and potential models from simulations: Average temperature and salt concentration in observed region and Soret coefficient.

$\frac{T}{\mathrm{K}}$	$\frac{m}{\mathrm{mol\ kg^{-1}}}$	$\frac{s_T}{10^{-3}\mathrm{K}^{-1}}$	$\frac{T}{\mathrm{K}}$	$\frac{m}{\mathrm{mol\ kg^{-1}}}$	$\frac{s_T}{10^{-3}\mathrm{K}^{-1}}$	$\frac{T}{\mathrm{K}}$	$\frac{m}{\mathrm{mol\ kg^{-1}}}$	$\frac{s_T}{10^{-3}\mathrm{K}^{-1}}$
DGS ions, p/bar = 500			DGS ions, p/bar = 1			DHV ions, p/bar = 500		
334	1.22±0.05	3.23±0.13	288	1.19±0.02	-2.98±0.11	299	1.35±0.01	-0.80±0.20
334	2.48±0.09	3.15±0.12	288	2.39±0.03	-0.41±0.20	299	1.35±0.01	-0.80±0.20
334	3.71±0.10	2.31±0.07	288	3.67±0.07	1.69±0.26	299	2.69±0.03	-0.36±0.27
334	4.97±0.15	2.25±0.10	288	4.96±0.07	2.16±0.09	299	3.93±0.04	-0.25±0.25
341	1.20±0.05	3.44±0.14	297	1.20±0.02	-1.77±0.17	299	5.16±0.06	0.77±0.30
341	2.43±0.10	3.60±0.15	297	2.39±0.03	1.82±0.16	308	1.34±0.02	0.82±0.22
341	3.64±0.11	2.59±0.08	297	3.62±0.08	3.94±0.14	308	2.63±0.05	1.51±0.22
341	4.89±0.17	2.70±0.11	297	4.84±0.09	3.13±0.11	308	3.86±0.06	1.34±0.19
348	1.17±0.05	3.58±0.15	306	1.20±0.02	0.89±0.24	308	5.07±0.08	1.52±0.14
348	2.37±0.11	3.92±0.17	306	2.33±0.05	3.85±0.13	317	1.31±0.03	1.99±0.16
348	3.57±0.12	2.85±0.10	306	3.54±0.08	3.65±0.15	317	2.57±0.06	2.12±0.13
348	4.81±0.18	3.15±0.12	306	4.68±0.10	3.60±0.12	317	3.78±0.09	2.05±0.12
355	1.15±0.05	3.67±0.16	315	1.18±0.03	4.05±0.20	317	4.99±0.09	1.74±0.07
355	2.31±0.11	4.16±0.19	315	2.25±0.06	4.87±0.14	325	1.31±0.05	6.17±0.71
355	3.49±0.13	3.10±0.12	315	3.40±0.06	3.18±0.12	325	2.54±0.09	5.12±0.89
355	4.71±0.20	3.53±0.14	315	4.52±0.13	5.08±0.15	325	3.73±0.10	3.87±0.24
362	1.12±0.05	3.77±0.17				325	4.91±0.07	1.93±0.25
362	2.24±0.11	4.37±0.21				334	1.26±0.05	4.92±0.27
362	3.41±0.14	3.45±0.14				334	2.47±0.07	3.48±0.25
362	4.60±0.21	3.86±0.16				334	3.63±0.10	3.44±0.14
369	1.08±0.05	3.94±0.18				334	4.82±0.07	1.98±0.07
369	2.17±0.12	4.70±0.24						
369	3.33±0.15	3.85±0.16						
369	4.49±0.22	4.20±0.18						

Table 4: Results from TDFRS experiments of aqueous NaCl and KCl solutions: Soret Coefficient s_T, Diffusion Coefficient D, Thermal Diffusivity D_{th} and Thermal Diffusion Coefficient D_T.

T/K	$s_T/10^{-3}\mathrm{K}^{-1}$	$D/10^{-5}\mathrm{cm}^2\mathrm{s}^{-1}$	$D_{\mathrm{th}}/10^{-3}\mathrm{cm}^2\mathrm{s}^{-1}$	$D_T/10^{-8}\mathrm{cm}^2\mathrm{s}^{-1}\mathrm{K}^{-1}$
NaCl, c/mol kg^{-1} = 4				
298	1.879±0.007	2.184±0.023	2.101±0.158	4.11±0.06
308	2.097±0.080	2.823±0.136	2.056±0.031	5.93±0.51
318	2.103±0.010	3.322±0.022	2.061±0.060	6.99±0.01
328	2.315±0.127	4.118±0.144	2.204±0.108	9.55±0.87
338	2.358±0.001	4.708±0.110	2.206±0.084	11.11±0.27
NaCl, c/mol kg^{-1} = 2				
298	1.623±0.010	2.104±0.036	2.022±0.027	3.42±0.04
308	1.980±0.045	2.635±0.015	2.053±0.052	5.21±0.09
318	2.219±0.004	3.215±0.010	2.111±0.014	7.13±0.01
328	2.468±0.012	3.862±0.036	2.151±0.007	9.53±0.04
338	2.522±0.027	4.593±0.006	2.208±0.001	11.58±0.14
NaCl, c/mol kg^{-1} = 0.5				
298	1.209±0.107	2.043±0.030	1.987±0.056	2.47±0.25
308	1.828±0.034	2.508±0.088	2.063±0.017	4.59±0.18
318	2.330±0.011	3.027±0.064	2.087±0.005	7.05±0.12
328	2.780±0.051	3.729±0.125	2.156±0.030	10.36±0.16
338	3.155±0.064	4.228±0.142	2.171±0.020	13.35±0.72
KCl, c/mol kg^{-1} = 2				
298	0.947±0.001	2.026±0.004	1.541±0.002	1.92±0.01
308	1.477±0.018	2.414±0.034	1.528±0.010	3.57±0.09
318	1.931±0.018	2.982±0.012	1.609±0.034	5.76±0.08
328	2.199±0.012	3.500±0.016	1.613±0.000	7.70±0.07
338	2.654±0.010	4.004±0.005	1.621±0.009	10.63±0.02
KCl, c/mol kg^{-1} = 0.5				
288	-0.567±0.011	1.648±0.012	1.436±0.023	-0.93±0.02
298	0.494±0.029	1.520±0.120	1.465±0.004	0.78±0.14
308	1.361±0.031	2.073±0.136	1.511±0.036	2.82±0.25
318	2.058±0.053	2.537±0.039	1.549±0.003	5.22±0.21