

Electronic Supplementary Information to “Modelling the Effects of Salt Solutions on the Hydration of Calcium Ions”

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Table SI.1. The average simulation cell lengths and concentrations for each MX (M = Na, K and Cs; X = F, Cl, Br and I) NPT simulation.

	Number of MX units	Number of H ₂ O	Cell length (Å)	Concentration of MX (m)
Aqueous NaF solution	1	998	31.08	0.06
	2	996	31.05	0.11
	4	992	30.98	0.22
	8	984	30.86	0.45
	16	968	30.63	0.92
Aqueous NaCl solution	1	998	31.10	0.06
	2	996	31.09	0.11
	4	992	31.07	0.22
	8	984	31.04	0.45
	16	968	30.98	0.92
	32	936	30.87	1.90
Aqueous NaBr solution	1	998	31.11	0.06
	2	996	31.10	0.11
	4	992	31.09	0.22
	8	984	31.08	0.45
	16	968	31.06	0.92
	32	936	31.03	1.90
Aqueous NaI solution	1	998	31.12	0.06
	2	996	31.13	0.11
	4	992	31.15	0.22
	8	984	31.19	0.45
	16	968	31.27	0.92
	32	936	31.43	1.90
Aqueous KCl solution	1	998	31.11	0.06
	2	996	31.10	0.11
	4	992	31.10	0.22
	8	984	31.10	0.45
	16	968	31.09	0.92
	32	936	31.10	1.90
Aqueous CsCl solution	1	998	31.11	0.06
	2	996	31.12	0.11
	4	992	31.13	0.22
	8	984	31.15	0.45
	16	968	31.20	0.92
	32	936	31.31	1.90
Ca ²⁺ in aqueous solution		999	31.05	
CaCl ₂ in aqueous solution		997	31.10	
CaCl ₂ in aqueous NaF solution	2	993	31.01	0.11
	4	989	30.98	0.22
	8	981	30.83	0.45
CaCl ₂ in aqueous NaCl solution	2	993	31.08	0.11

	4	989	31.07	0.22
	8	981	31.04	0.45
	16	965	30.97	0.92
	32	933	30.87	1.90
CaCl ₂ in aqueous KCl solution	2	993	31.10	0.11
	4	989	31.10	0.22
	8	981	31.09	0.45
	16	965	31.09	0.92
	32	933	31.09	1.90
CaCl ₂ in aqueous CsCl solution	2	993	31.12	0.11
	4	989	31.13	0.22
	8	981	31.15	0.45
	16	965	31.20	0.92
	32	933	31.32	1.90

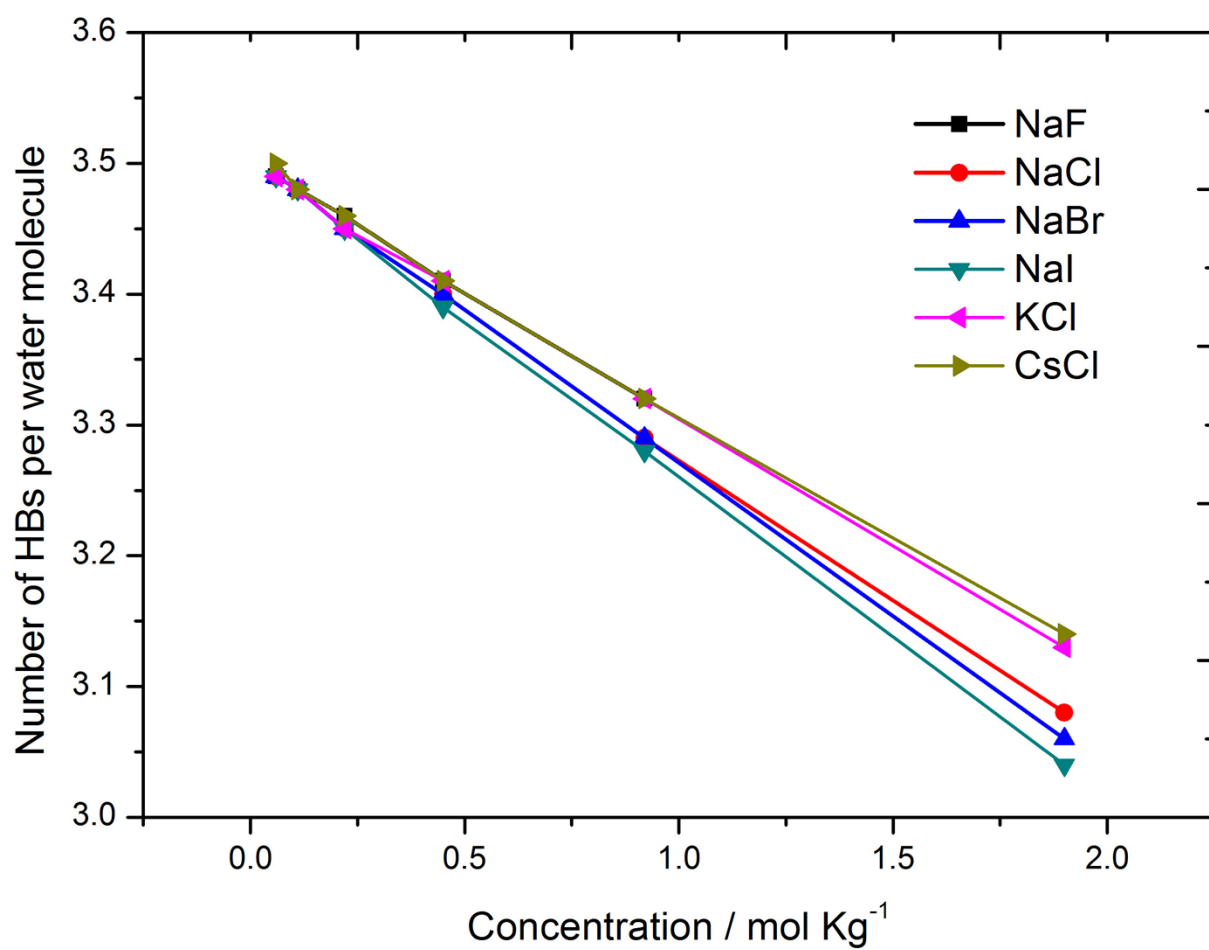


Figure SI.1. The average number of hydrogen bonds per water molecule in aqueous alkali halide solutions as a function of salt concentration.

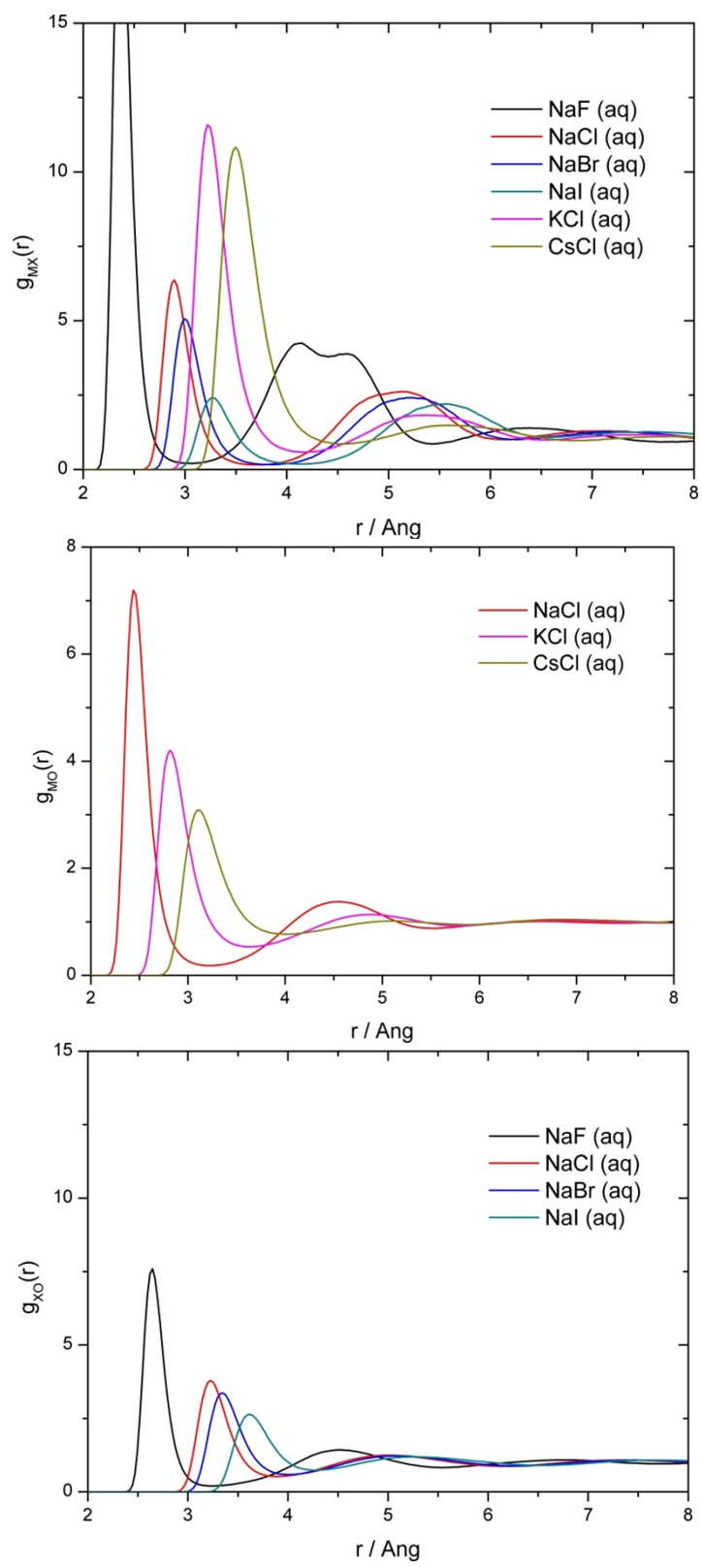


Figure SI.2. Alkali-halide, alkali-oxygen and halide-oxygen radial distribution function obtained from the aqueous solutions with a salt concentration of 0.92 mol kg^{-1} .