Supporting information for:
Hydration of alkali and halide ions. I. Structure and energetics based on simulations with a polarizable force field

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Table 1: Hydration free energy data and computations from the literature

a) Alkali ions

Source[b]	Standard state[a] Gas	Solution	Li^+	Na^+	K^+	Rb^+	Cs^+	Comments
Extrathermodynamic hypothesis								
Noyes62	1 atm	1 M	−120.8	−97.0	−79.3	−74.2	−66.5	$\Delta F^\circ_{\mathrm{el}}$ from Table I, plus $\Delta F^\circ_{\mathrm{neut}} = 1.325$ kcal/mol
Marcus86-87	1 MPa	1 M	−116.8	−91.5	−74.5	−68.9	−67.6	
Electrochemistry								
Randles56	1 atm	1 M	−122.1	−98.2	−80.6	−75.5	−67.8	Table 1
Gomer77	1 atm	1 M	−118.1	−90.6	−73.1			$\Delta G^\circ_{\mathrm{solv}}$ from Table IV
Cluster measurements								
Klots81	1 atm	1 M	−124.0	−100.1	−82.5	−77.4	−69.7	ΔG° from Table I
Tissandier98	1 atm	1 M	−126.5	−101.3	−84.1	−78.7		$\Delta G^\circ_{\mathrm{aq}}$ from Table 3, with $X = -264.0$ kcal/mol
Theory								
Zhan2001	1 atm	1 M	−124.9	−99.7	−82.5	−77.1	−69.7	Derived from the hydration free energy of H^+
Asthagiri2003	1 M	1 M	−112.7	−88.7				Column SPC/E from Table II
	1 atm	1 M	−110.8	−86.8				Column SPC/E from Table II, plus 1.9 kcal/mol
Grossfield2003	1 atm	1 M		−89.9	−72.6			Table 4
This work	1 M	1 M	−125.0	−98.5	−81.3	−75.7	−68.4	ΔG from TI with SSBP
	1 atm	1 M	−123.1	−96.6	−79.4	−73.8	−66.5	ΔG from TI with SSBP +1.9 kcal/mol = $\Delta G^{\mathrm{real}}_{\mathrm{hydr}}$

b) Halide ions

Source[b]	Standard state[a] Gas	Solution	F^-	Cl^-	Br^-	I^-	Comments
Extrathermodynamic hypothesis							
Noyes62	1 atm	1 M	−88.2	−74.8	−67.9	−59.0	$\Delta F^\circ_{\mathrm{el}}$ from Table I, plus $\Delta F^\circ_{\mathrm{neut}} = 1.325$ kcal/mol
Marcus86-87	1 MPa	1 M	−112.1	−82.4	−76.1	−67.0	
Electrochemistry							
Randles56	1 atm	1 M	−99.1	−70.7	−64.9	−57.2	Table 2
Gomer77	1 atm	1 M	−110.7	−81.4	−76.1		$\Delta G^\circ_{\mathrm{solv}}$ from Table IV
Cluster measurements							
Klots81	1 atm	1 M	−101.9	−73.9	−70.6	−59.5	ΔG° from Table I
Tissandier98	1 atm	1 M	−102.5	−72.7	−66.3	−57.4	$\Delta G^\circ_{\mathrm{aq}}$ from Table 3, with $X = -264.0$ kcal/mol
Theory							
Zhan2001	1 atm	1 M	−104.1	−74.3	−67.9	−59.0	Derived from the hydration free energy of H^+
Zhan2004	1 atm	1 M	−104.3				
Grossfield2003	1 atm	1 M		−84.6			Table 4
This work	1 M	1 M	−108.7	−79.1	−72.6	−64.0	ΔG from TI with SSBP
	1 atm	1 M	−106.8	−77.2	−70.7	−62.1	ΔG from TI with SSBP +1.9 kcal/mol = $\Delta G^{\mathrm{real}}_{\mathrm{hydr}}$

[a] Free energies in the (1 M, 1 M) standard state are converted to the (1 atm, 1 M) standard state by adding 1.9 kcal/mol, the entropic contribution associated with confining 1 mol of ions from a volume of 24.465 ℓ to a volume of 1 ℓ.

[b] Source for all values: Noyes62,[1] Marcus86-87,[2, 3, 4] Randles56,[5] Gomer77,[6] Klots81,[7] Tissandier98,[8] Zhan2001,[9] Zhan2004,[10] Asthagiri2003,[11] Grossfield2003.[12]

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