**Supporting information for:**

# Absolute hydration free energy scale for alkali and halide ions established from simulations with a polarizable force field

Guillaume Lamoureux[a)†] and Benoît Roux[b)*]

[a)]Département de physique, Université de Montréal,
C.P. 6128, succ. centre-ville, Montréal, Québec H3C 3J7, Canada

[b)]Department of Biochemistry, Weill Medical College of Cornell University,
1300 York Avenue, New York, NY 10021

[†]Current address: Center for Molecular Modeling, Department of Chemistry, University of Pennsylvania

[*]Corresponding author: Benoit.Roux@med.cornell.edu

Table S1: 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 | $\Delta G^\circ$ 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 | $\Delta G$ from TI with SSBP |
| | 1 atm | 1 M | −123.1 | −96.6 | −79.4 | −73.8 | −66.5 | $\Delta G$ 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 | $\Delta G^\circ$ 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 | $\Delta G$ from TI with SSBP |
| | 1 atm | 1 M | −106.8 | −77.2 | −70.7 | −62.1 | $\Delta G$ 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 $\ell$ to a volume of 1 $\ell$.
[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]

# Complete list of authors for Refs. 93 and 133

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