Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field

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Supporting Information

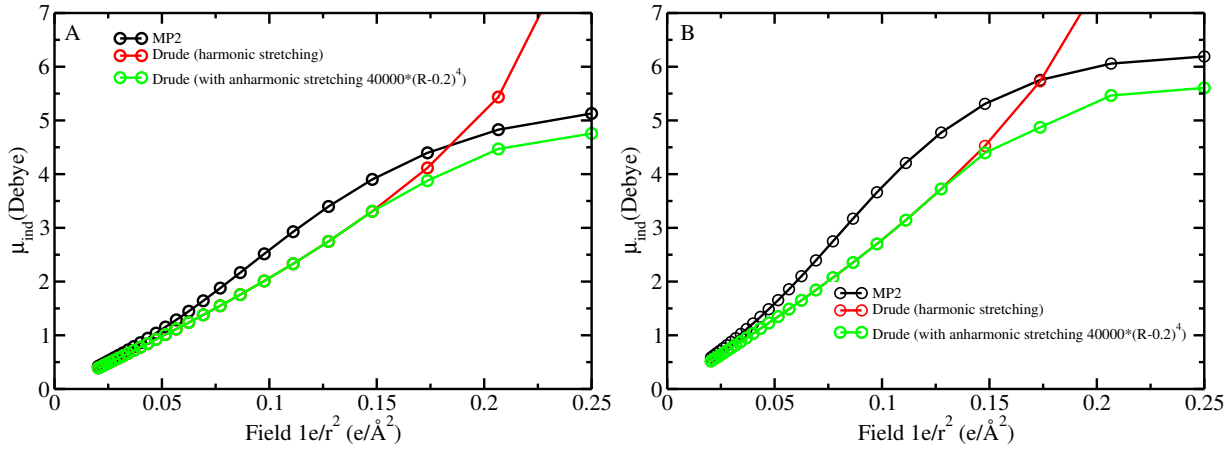

Figure 1: The induced dipole moments of Cl^- (A) or Br^- (B) as a function of the field strength produced by a point charge. The MP2 results were obtained with the 6-311++G(2df,2pd) basis set.

Table 1: Hydration Free Energy Differences for Monovalent Cations and Anions (kcal/mol)

	Cluster		Extra Thermo. Hypothesis			Electrochem.		Drude	
	Tissandier[a]	Klots[b]	Marcus[c]	Noyes[d]	Schmid[e]	Randles[f]	Gomer[g]	relative[h]	absolute[i]
Li^+									
	-25.2	-23.9	-26.2	-23.8	-25.1	-23.9	-27.4	-24.2	-24.2
Na^+									
	-17.2	-17.6	-16.7	-17.7	-17.4	-17.6	-17.5	-17.3	-17.7
K^+									
	-5.4	-5.1	-4.9	-5.1	-5.3	-5.1		-5.2	-4.9
Rb^+									
		-7.7	-6.0	-7.7	-5.5	-7.7		-7.1	-7.2
Cs^+									
F^-									
	-29.7	-28.0	-29.9	-13.4	-30.6	-28.4	-29.3	-30.0	-29.6
Cl^-									
	-6.4	-3.3	-6.0	-6.9	-6.5	-5.8	-5.3	-6.5	-6.8
Br^-									
	-8.9	-11.1	-9.6	-8.9	-8.4	-7.7		-8.5	-8.5
I^-									

a: Taken from Ref.;[1] *b*: Taken from Ref.;[2] *c*: Taken from Ref.;[3] *d*: Taken from Ref.;[4] *e*: Taken from Ref.;[5] *f*: Taken from Ref.;[6] *g*: Taken from Ref.;[7] *h*: Calculated from free energy perturbation $\Delta\Delta G$ (Ion A$\rightarrow$Ion B); *i*: Calculated from the absolute hydration free energies of Ions A and B: ΔG (Ion B) - ΔG (Ion A).

Table 2: Hydration Free Energy Differences for Divalent Cations (kcal/mol)

	Extra Thermo. Hypothesis Marcus[a]	Schmid[c]	Electrochem. Gomer[d]	Drude
Zn^{2+}	-107.6	-	-	-90.3
Mg^{2+}	-77.7	-77.9	-80.3	-77.3
Ca^{2+}	-29.8	-30.6	-32.9	-32.9
Sr^{2+}	-31.1	-30.6	-27.9	-27.0
Ba^{2+}				

a: Taken from Ref.;[3] *b*: Taken from Ref.;[4] *c*: Taken from Ref.;[5] *d*: Taken from Ref.[7] The entry for Zn^{2+} is defined as $\Delta G^{\text{real}}_{\text{hydr}}(Zn^{2+}) - \Delta G^{\text{real}}_{\text{hydr}}(Ca^{2+})$.

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