Supporting Information

Corrections in the CHARMM36 parameterization of chloride interactions with proteins, lipids and alkali cations, and extension to other halide anions

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Table S1. Properties of the radial distribution functions for each of the halide ions in liquid water.

$g_{\text{ion-O}}$ (r)					$g_{\text{ion-H}}$ (r)				
Property	F^-	Cl^-	Br^-	I^-	Property	F^-	Cl^-	Br^-	I^-
r_{max1}	2.67	3.13	3.30	3.58	r_{max1}	1.73	2.22	2.38	2.67
g_{max1}	7.6	4.4	3.7	2.9	g_{max1}	8.6	3.9	3.1	2.2
r_{min1}	3.30	3.80	3.90	4.19	r_{min1}	2.40	2.92	3.05	3.33
g_{min1}	0.2	0.5	0.6	0.8	g_{min1}	0.1	0.3	0.4	0.5
CN1	6.7	7.7	8.0	8.7	CN1	6.7	7.3	7.3	7.6
r_{max2}	4.6	5.0	5.3	–	r_{max2}	3.02	3.48	3.65	3.92
g_{max2}	1.3	1.1	1.1	–	g_{max2}	2.3	1.5	1.4	1.3
r_{min2}	5.7	6.3	6.5	–	r_{min2}	3.5	4.0	4.2	4.5
g_{min2}	0.9	0.9	0.9	–	g_{min2}	0.7	0.8	0.9	1.0
CN2	27	35	38	–	CN2	15	19	21	23

Table S2. Calculated and experimental osmotic pressures of aqueous solutions of lithium halides.[a,b]

Salt	molality (m)	Calculated Π (bar)		Expt. Π (bar)
		Generic	NBFIX[c]	
LiCl	0.5	18 ± 3	27 ± 3 (23 ± 3)	24
	1.0	30 ± 4	50 ± 3 (47 ± 2)	50
	3.0	71 ± 5	177 ± 10 (135 ± 7)	182
	5.0	110 ± 13	346 ±11 (223 ± 17)	366
LiBr	0.5	23 ± 3	24 ± 3	24
	1.0	44 ± 4	52 ± 5	50
	3.0	116 ± 6	188 ± 5	190
	5.0	190 ± 13	372 ± 17	387
LiI	0.5	24 ± 2	24 ±2	25
	1.0	53 ± 4	53 ± 4	51
	3.0	195 ± 10	195 ± 10	194
	5.0	372 ± 12	372 ± 12	–

[a] Calculated values used the CHARMM36m forcefield and either generic LJ parameters or NBFIX pair-specific corrections. [b] No data are shown for LiF as it is sparingly soluble in water (0.133 wt% at 25.4 °C). The dashes indicate that no experimental data are available. [c] Data in brackets are calculated using the NBFIX parameters reported in Ref. 107 (ϵ_{LiCl} = -0.0187 kcal/mol and $R_{\text{min,LiCl}}$ = 3.6875 Å).

Table S3. Calculated and experimental osmotic pressures of aqueous solutions of sodium halides.[a]

Salt	molality (m)	Calculated Π (bar)		Expt. Π (bar)
		Generic	NBFIX	
NaF	0.5	17 ± 3	23 ± 2	23
	1.0	10 ± 3	47 ± 6	44
NaCl	0.5	25 ± 3	26 ± 4	23
	1.0	52 ± 4	52 ± 4	46
	3.0	166 ± 10	161 ± 12	150
	5.0	138 ± 9	285 ± 7	273
NaBr	0.5	26 ± 2	26 ± 2	23
	1.0	48 ± 3	48 ± 3	47
	3.0	165 ± 12	165 ± 12	155
	5.0	275 ± 19	275 ± 19	286
NaI	0.5	27 ± 2	25 ± 5	23
	1.0	52 ± 3	49 ± 5	47
	3.0	204 ± 12	165 ± 4	159
	5.0	394 ± 9	283 ± 10	292

[a] No data are shown for NaF at 3 and 5 m as its solubility limit in water is 0.987 m at 25 °C.

Table S4. Calculated and experimental osmotic pressures of aqueous solutions of potassium halides.

Salt	molality (m)	Calculated Π (bar)		Expt. Π (bar)
		Generic	NBFIX	
KF	0.5	22 ± 4	22 ± 3	23
	1.0	43 ± 1	44 ± 4	46
	3.0	95 ± 4	133 ± 8	157
	5.0	160 ± 8	235 ± 9	297
KCl	0.5	24 ± 2	22 ± 2	22
	1.0	45 ± 5	45 ± 3	44
	3.0	111 ± 4	149 ± 6	130
	5.0	150 ± 7	238 ± 10	219
KBr	0.5	24 ± 1	24 ± 3	22
	1.0	46 ± 1	48 ± 3	44
	3.0	129 ± 8	143 ± 5	129
	5.0	178 ± 1	214 ± 8	214
KI	0.5	24 ± 1	23 ± 3	23
	1.0	52 ± 3	45 ± 3	44
	3.0	155 ± 7	136 ± 7	128
	5.0	257 ± 10	204 ± 7	208

Table S5. Calculated and experimental osmotic pressures of aqueous solutions of rubidium halides.

Salt	molality (m)	Calculated Π (bar)		Expt. Π (bar)
		Generic	NBFIX	
RbF	0.5	19 ± 2	23 ± 4	24
	1.0	43 ± 5	45 ± 4	48
	3.0	121 ± 4	140 ± 4	155
	5.0	206 ± 15	243 ± 8	N/A
RbCl	0.5	24 ± 1	24 ± 1	22
	1.0	44 ± 2	44 ± 2	43
	3.0	130 ± 6	130 ± 6	125
	5.0	202 ± 13	202 ± 13	206
RbBr	0.5	25 ± 3	23 ± 2	22
	1.0	48 ± 3	46 ± 4	42
	3.0	139 ± 6	128 ± 6	120
	5.0	207 ± 9	201 ± 6	193
RbI	0.5	23 ± 1	24 ± 3	22
	1.0	49 ± 2	46 ± 3	41
	3.0	151 ± 11	124 ± 7	116
	5.0	248 ± 13	182 ± 5	183

Table S6. Calculated and experimental osmotic pressures of aqueous solutions of cesium halides.

Salt	molality (m)	Calculated Π (bar)		Expt. Π (bar)
		Generic	NBFIX	
CsF	0.5	23 ± 3	24 ± 3	24
	1.0	46 ± 2	45 ± 3	48
	3.0	140 ± 6	157 ± 5	167
	5.0	257 ± 10	281 ± 15	N/A
CsCl	0.5	21 ± 3	22 ± 4	22
	1.0	48 ± 3	45 ± 3	41
	3.0	146 ± 6	122 ± 7	117
	5.0	240 ± 10	190 ± 4	191
CsBr	0.5	22 ± 1	24 ± 4	21
	1.0	45 ± 4	43 ± 3	41
	3.0	150 ± 10	115 ± 4	113
	5.0	238 ± 5	180 ± 11	180
CsI	0.5	25 ± 2	23 ± 3	21
	1.0	50 ± 2	42 ± 2	40
	3.0	150 ± 5	107 ± 9	103
	5.0	251 ± 4	130 ± 9	N/A

Table S7. Gas-phase interaction energies and contact distances for energy-minimized complexes of alkali and halide ions.[a]

Alkali ion	Halide ion	Generic FF		Optimized FF[b]	
		E^{MM}	r^{MM}	$E^{MM,opt}$	$r^{MM,opt}$
Li^+	F^-	-176.2	1.73	-158.6	1.92
	Cl^-	-148.3	2.06	-137.2	2.23
	Br^-	-140.7	2.17	-131.9	2.32
	I^-	-129.1	2.36	–	–
Na^+	F^-	-148.8	2.05	-143.1	2.14
	Cl^-	-126.1	2.43	-124.3	2.46
	Br^-	-119.9	2.55	–	–
	I^-	-110.4	2.78	-113.9	2.69
K^+	F^-	-129.9	2.35	-125.5	2.44
	Cl^-	-111.4	2.75	-110.0	2.79
	Br^-	-106.3	2.89	-105.7	2.91
	I^-	-98.5	3.12	-99.4	3.09
Rb^+	F^-	-122.1	2.51	-119.6	2.56
	Cl^-	-105.1	2.92	–	–
	Br^-	-100.5	3.06	-100.7	3.05
	I^-	-93.3	3.30	-94.6	3.25
Cs^+	F^-	-114.4	2.68	-111.5	2.75
	Cl^-	-99.0	3.10	-100.5	3.06
	Br^-	-94.8	3.25	-96.2	3.20
	I^-	-88.3	3.50	-90.7	3.39

[a] E^{MM} and $E^{MM,opt}$ are interaction energies (in kcal/mol) calculated with the CHARMM36m forcefield, either with generic LJ parameters or pair-specific NBFIX corrections, respectively; and *r* refers to the distance (in Å) between the two ions. [b] The NBFIX parameters used for NaCl and KCl are reproduced from reference 35. Note that no NBFIX parameters were required for LiI, NaBr or RbCl.

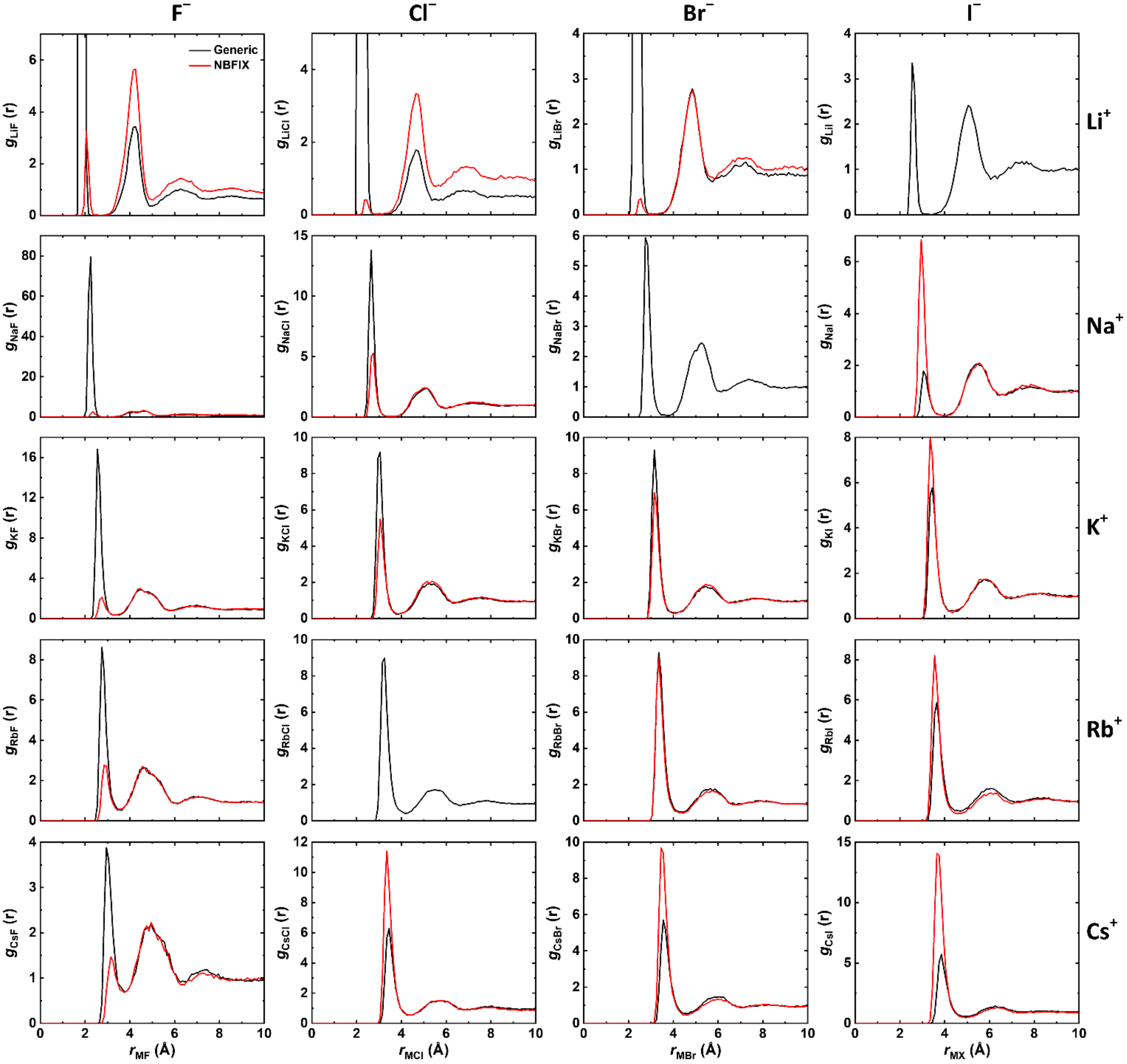

Figure S1. Association of alkali halides in water. $g_{MX}(r)$ radial distribution functions calculated from 100-ns MD simulations of a single M^+X^- pair in 250 H_2O molecules (at 298.15 K and 1.0 atm) show the structure of contact-ion and solvent-shared ion-pairs. Data are shown for calculations using the CHARMM36m forcefield, and either generic LJ parameters (black) or with NBFIX pair-specific parameters (red). The NBFIX parameters for NaCl and KCl are reproduced from reference 35 Note that no NBFIX parameters were required for LiI, NaBr, or RbCl.

Table S8. Calculated and experimental osmotic pressures of aqueous solutions of guanidinium halides.[a]

Anion	molality (m)	Calculated		Expt.
		Generic FF	NBFIX	
Fluoride	0.5	11 ± 1	19 ± 2	21
	1	19 ± 2	40 ± 3	39
	3	25 ± 5	90 ± 8	106
	5	52 ± 5	160 ± 10	165
Chloride	0.5	22 ± 2	20 ± 3	21
	1	41 ± 4	33 ± 3	38
	3	110 ± 9	81 ± 6	89
	5	173 ± 14	131 ± 5	126
Bromide	0.5	24 ± 2	20 ± 3	21
	1	43 ± 5	36 ± 3	38
	3	131 ± 7	82 ± 5	88
	5	218 ± 15	129 ± 11	122
Iodide	0.5	25 ± 2	21 ± 3	21
	1	50 ± 3	32 ± 2	38
	3	156 ± 5	81 ± 3	86
	5	275 ± 7	115 ±7	119

[a] Calculated values used the CHARMM36m forcefield and either generic LJ parameters or NBFIX pair-specific corrections.

Table S9. Calculated and experimental osmotic pressures of aqueous solutions of tetramethylammonium halides.

Anion	molality (m)	Calculated		Expt.
		Generic FF	NBFIX	
Fluoride	0.5	31 ± 1	27 ± 2	25
	1	60 ± 2	54 ± 3	52
	3	283 ± 7	208 ± 7	204
	5	651 ± 17	408 ± 17	405
Chloride	0.5	27 ± 3	20 ± 1	21
	1	57 ± 4	38 ± 3	39
	3	220 ± 7	114 ± 7	114
	5	447 ± 12	180 ± 3	189
Bromide	0.5	24 ± 1	23 ± 2	20
	1	53 ± 4	39 ± 5	36
	3	198 ± 5	89 ± 8	94
	5	379 ± 10	142 ± 9	143
Iodide	0.5	24 ± 2	19 ± 3	–
	1	49 ± 3	36 ± 4	–
	3	164 ± 4	88 ± 6	–
	5	292 ± 12	120 ± 4	–

Table S10. Calculated and experimental osmotic pressures of aqueous solutions of methylammonium halides.

Anion	molality (m)	Calculated		Expt.
		Generic FF	NBFIX	
Fluoride	0.5	17 ± 2	25 ± 1	–
	1	30 ± 2	53 ± 7	–
	3	78 ± 5	183 ± 5	–
	5	145 ± 13	345 ± 14	–
Chloride	0.5	24 ± 1	20 ± 3	22
	1	49 ± 2	41 ± 2	42
	3	148 ± 2	117 ± 5	119
	5	253 ± 5	185 ± 6	188
Bromide	0.5	25 ± 5	22 ± 2	–
	1	49 ± 3	38 ± 2	–
	3	166 ± 4	101 ± 5	–
	5	290 ± 9	150 ± 6	–
Iodide	0.5	25 ± 2	22 ± 2	–
	1	54 ± 6	37 ± 3	–
	3	183 ± 5	93 ± 8	–
	5	314 ± 5	136 ± 7	–

Table S11. Calculated osmotic pressures of aqueous solutions of imidazolium halides.

Anion	molality (m)	Calculated		Expt.
		Generic FF	NBFIX	
Fluoride	0.5	16 ± 3	25 ± 2	–
	1	36 ± 3	50 ± 5	–
	3	101 ± 3	186 ± 10	–
	5	208 ± 16	340 ± 20	–
Chloride	0.5	24 ± 3	22 ± 2	–
	1	51 ± 2	46 ± 3	–
	3	165 ± 6	134 ± 5	–
	5	295 ± 14	258 ± 10	–
Bromide	0.5	25 ± 3	22 ± 3	–
	1	54 ± 1	42 ± 2	–
	3	169 ± 9	119 ± 6	–
	5	305 ± 16	202 ± 9	–
Iodide	0.5	24 ± 3	21 ± 2	–
	1	50 ± 3	35 ± 4	–
	3	161 ± 5	104 ± 5	–
	5	287 ± 14	170 ± 7	–

Table S12. Ion-ligand distance (r_1 and r_2 in Å) at the minimum potential of mean force (PMF1 and PMF2, in kcal/mol) for the halide ion complexes with the cationic analogs in bulk water[a]

Ion	Ligand	Generic				NBFIX			
		r_1	PMF1	r_2	PMF2	r_1	PMF1	r_2	PMF2
Fluoride	Guanidinum	3.3	-3.0	5.5	-0.6	3.7	-1.0	5.4	-0.6
	Tetramethylammonium	-	-	5.8	-0.2	3.8	-1.2	6.4	-0.1
	Methyl ammonium	2.7	-3.1	4.8	-0.6	2.8	-0.5	4.8	-0.6
	Imidazolium	3.8	-2.7	5.7	-0.4	4.1	-0.2	5.8	-0.5
Chloride	Guanidinum	3.7	-1.2	6.1	-0.3	3.7	-1.9	6.1	-0.3
	Tetramethylammonium	4.6	-0.5	7.2	-0.2	4.3	-1.7	7.2	-0.2
	Methyl ammonium	3.2	-1.6	5.4	-0.4	3.1	-2.1	5.2	-0.4
	Imidazolium	4.3	-0.9	6.6	-0.2	4.2	-1.6	6.7	-0.2
Bromide	Guanidinum	3.9	-0.7	6.3	-0.2	3.8	-2.0	6.7	-0.2
	Tetramethylammonium	4.7	-0.8	7.2	-0.2	4.4	-1.9	7.2	-0.2
	Methyl ammonium	3.3	-1.3	5.4	-0.4	3.2	-2.4	5.6	-0.3
	Imidazolium	4.4	-1.0	6.8	-0.2	4.3	-1.8	6.7	-0.2
Iodide	Guanidinum	4.6	-0.4	6.7	-0.3	3.9	-1.9	6.8	-0.1
	Tetramethylammonium	4.8	-0.9	7.7	-0.1	4.7	-1.7	7.9	-0.1
	Methyl ammonium	3.6	-0.6	5.4	-0.4	3.4	-2.1	5.7	-0.3
	Imidazolium	4.7	-1.0	7.1	-0.2	4.4	-2.4	7.2	-0.2

[a]Dashes indicate absence of a metastable free-energy minimum.

Table S13. Gas-phase interaction energies and contact distances for energy-minimized binary complexes of the halide anions and cationic protein/lipid analogs.[a]

Ion	Ligand (structure)	Generic FF		Optimized FF	
		r^{MM}	E^{MM}	$r^{MM,opt}$	$E^{MM,opt}$
Fluoride	Guanidinum	3.05	-123.2	3.18	-116.6
	Tetramethylammonium	3.22	-97.0	2.92	-106.8
	Methylammonium	2.54	-125.4	2.65	-118.9
	Imidazolium	2.54	-106.5	2.69	-100.1
Chloride	Guanidinum	3.55	-101.8	3.51	-103.3
	Tetramethylammonium	3.68	-85.7	3.49	-90.1
	Methylammonium	2.96	-106.2	2.92	-107.6
	Imidazolium	3.02	-90.9	2.95	-92.3
Bromide	Guanidinum	3.71	-96.5	3.62	-99.2
	Tetramethylammonium	3.83	-82.6	3.64	-86.6
	Methylammonium	3.10	-101.2	3.02	-103.9
	Imidazolium	3.18	-87.2	3.02	-89.8
Iodide	Guanidinum	3.98	-88.8	3.81	-93.3
	Tetramethylammonium	4.10	-77.8	3.92	-80.8
	Methylammonium	3.34	-93.6	3.15	-98.0
	Imidazolium	3.44	-81.4	3.18	-85.7

[a]E^{MM} and $E^{MM,opt}$ are interaction energies (in kcal/mol) calculated with the CHARMM36m forcefield and either generic LJ parameters or pair-specific NBFIX corrections, respectively; and r refers to the distance (in Å) between the anion and the C atom of guanidinium, or the nearest N atom of the other ligands.

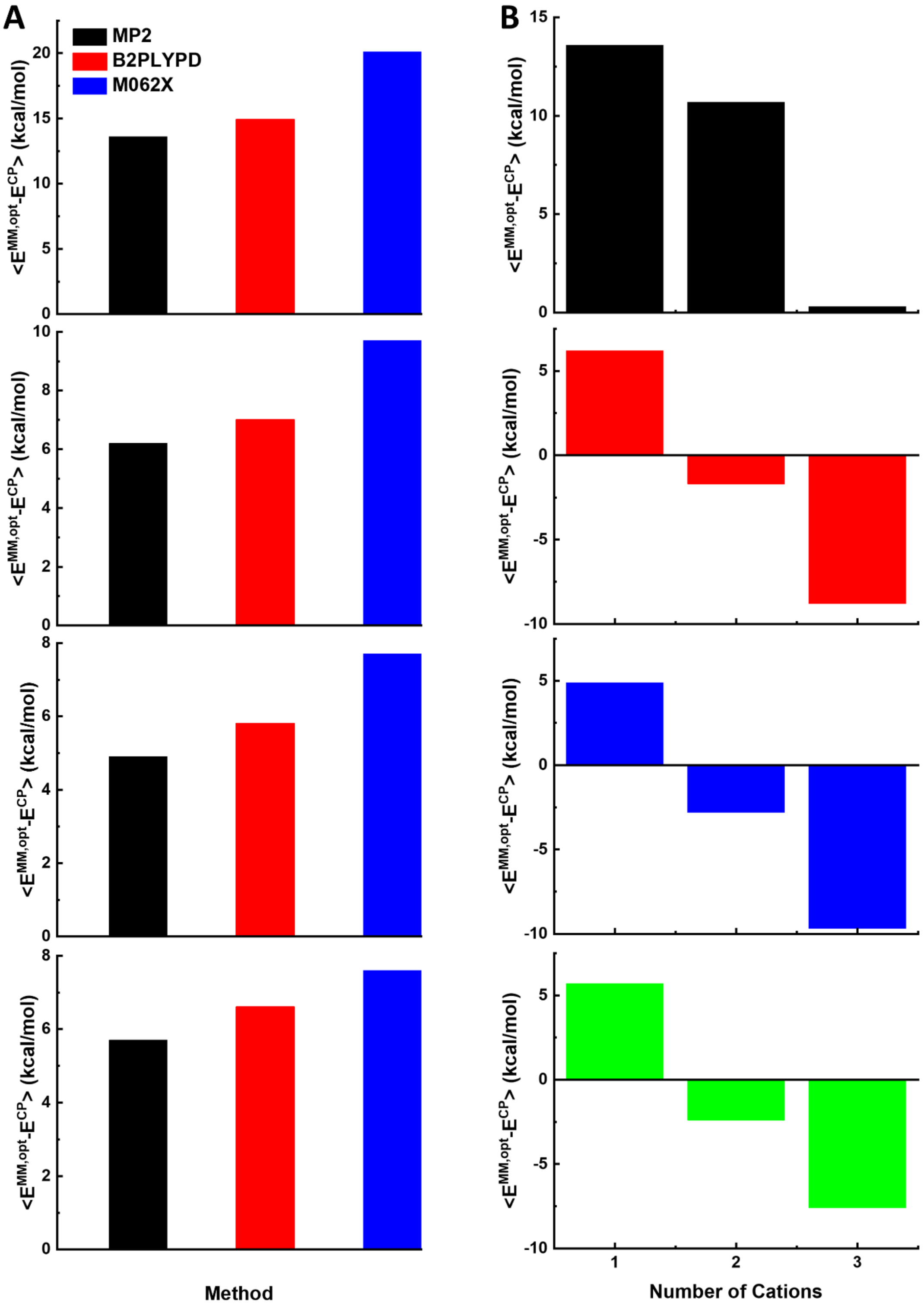

Figure S2. Average error of the optimized model for F^-, Cl^-, Br^-, and I^- (top to bottom) over (**A**) the ab-initio E^{CP} interaction energies with a single cationic analog calculated with the MP2 (*black*), B2PLYPD (red) and M062X (*blue*) and (*B*) the ab-initio E^{CP} interaction energies with one to three cationic analogs calculated with the MP2 energy function.

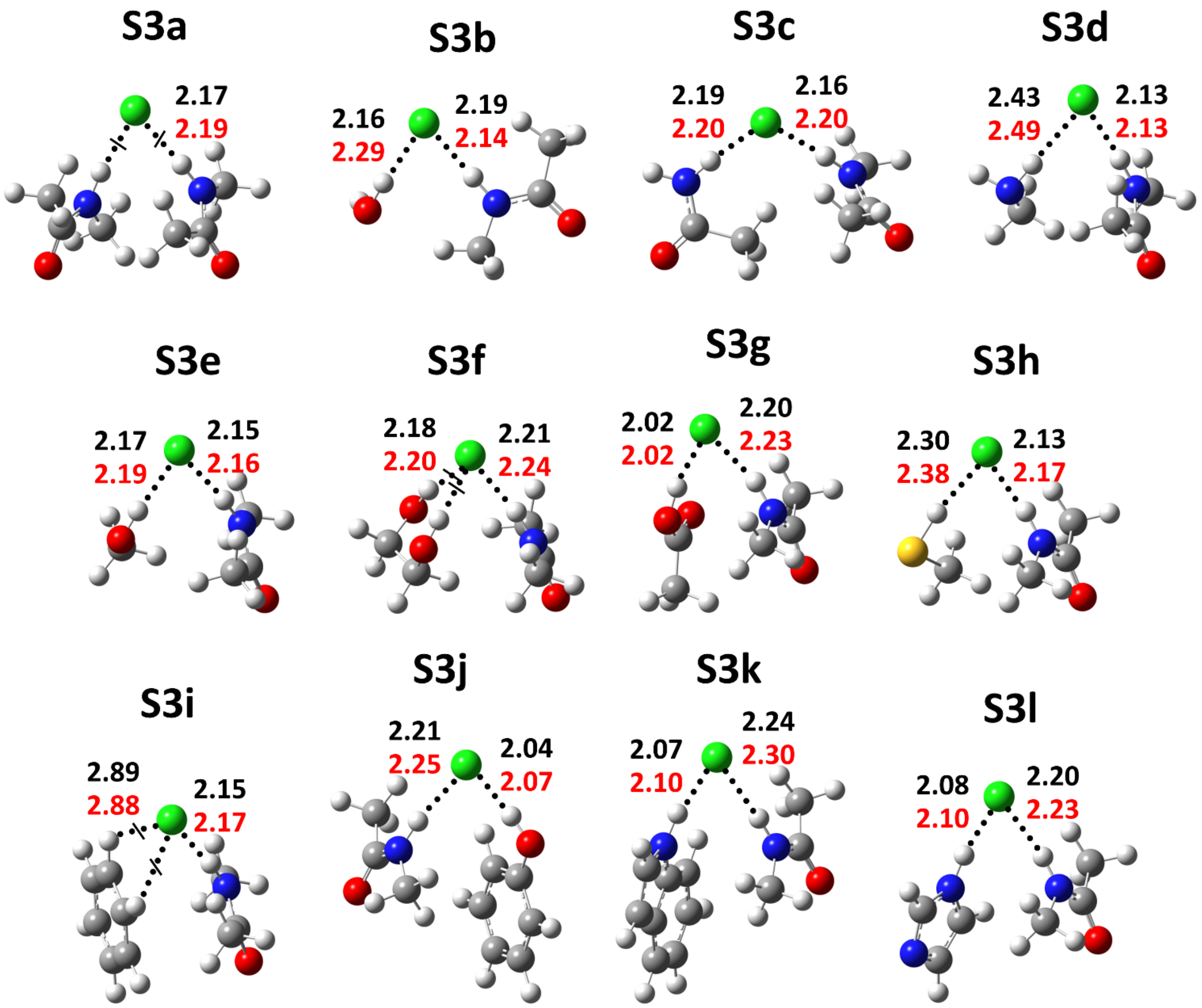

Figure S3. Ab-initio optimized, global energy-minimum structures of Cl^-, one molecule of NMA and an additional ligand L, for L = NMA (**S3a**), water (**S3b**), acetamide (**S3c**), methylamine (**S3d**), methanol (**S3e**), ethylene glycol (**S3f**), acetic acid (**S3g**), methanethiol (**S3h**), benzene (**S3i**), phenol (**S3j**), indole (**S3k**), and imidazole (**S3l**). For all complexes, the distance between the atoms connected with dotted lines is indicated, in Å; in *black* from B2LYPD/6-311++G(d,p) calculations; in *red* from M062X/6-311++G(d,p) calculations. Atom color code: H (white), C (gray), N (blue), O (red), S (yellow), Cl^- (green).

Table S14. Interaction energies (in kcal/mol) for the Cl^- complexes shown in **Figure S3**.[a]

Ligand (structure)	B2PLYPD/6-311++G(d,p)		M062X/6-311++G(d,p)	
	E	E^{CP}	*E*	E^{CP}
NMA (**S3a**)	-45.7	-41.3	-46.1	-44.7
Water (**S3b**)	-38.4	-35.3	-38.8	-37.6
Acetamide (**S3c**)	-44.4	-40.6	-45.2	-43.9
Methylamine (**S3d**)	-34.0	-30.5	-34.7	-33.6
Methanol (**S3e**)	-39.6	-35.7	-41.0	-39.7
Ethylene glycol (**S3f**)	-50.5	-45.7	-51.0	-49.4
Acetic acid (**S3g**)	-44.2	-39.9	-44.9	-43.4
Methanethiol (**S3h**)	-36.7	-32.4	-38.4	-36.9
Benzene (**S3i**)	-33.3	-29.0	-33.7	-32.4
Phenol (**S3j**)	-47.3	-42.5	-47.4	-45.7
Indole (**S3k**)	-46.8	-41.9	-45.8	-44.3
Imidazole (**S3l**)	-47.2	-43.0	-46.4	-45.1

Table S15. Ion-ligand distance (r_1 and r_2 in Å) and potential of mean force (PMF1 and PMF2, in kcal/mol) in metastable states of F^- complexes in bulk water.[a]

Ligand	Generic				NBFIX			
	r_1	PMF1	r_2	PMF2	r_1	PMF1	r_2	PMF2
NMA	-	-	-	-	2.7	-0.3	-	-
Acetamide	-	-	-	-	2.7	-0.9	-	-
Methylamine	-	-	-	-	-	-	-	-
Methanol	2.7	-0.9	-	-	2.7	-0.5	6.8	-0.1
Ethylene glycol	2.2	-1.4	4.1	-0.1	2.4	-0.4	-	-
Acetic acid	2.1	-1.6	-	-	2.7	-1.1	-	-
Methanethiol	-	-	-	-	3.3	-0.6	-	-
Benzene	-	-	-	-	4.6	-0.5	7.3	-0.1
Phenol	2.7	-0.9	-	-	2.7	-2.4	4.3	-0.3
Indole	-	-	-	-	2.7	-0.8	4.1	-0.9
Imidazole	2.8	-0.3	-	-	2.7	-1.3	6.4	-0.1

[a] Dashes indicate absence of a metastable free-energy minimum.

Table S16. Ion-ligand distance (r_1 and r_2 in Å) and potential of mean force (PMF1 and PMF2, in kcal/mol) in metastable states of Cl^- complexes in bulk water.[a]

Ligand	Generic				NBFIX			
	r_1	PMF1	r_2	PMF2	r_1	PMF1	r_2	PMF2
NMA	-	-	-	-	3.2	-0.7	-	-
Acetamide	3.3	-0.2	-	-	3.2	-1.0	-	-
Methylamine	-	-	-	-	3.2	-0.3	-	-
Methanol	3.2	-0.6	5.1	-0.1	3.1	-1.9	5.2	-0.1
Ethylene glycol	-	-	4.4	-0.4	2.6	-1.4	3.8	-1.2
Acetic acid	3.1	-0.7	-	-	3.0	-2.2	-	-
Methanethiol	-	-	-	-	3.7	-1.1	-	-
Benzene	-	-	-	-	5.1	-1.2	7.7	-0.2
Phenol	3.2	-0.8	7.6	-0.1	3.0	-3.3	5.0	-0.3
Indole	3.3	-0.3	-	-	3.1	-2.3	4.9	-0.5
Imidazole	3.3	-0.2	-	-	3.1	-2.3	6.7	-0.1

[a] Dashes indicate absence of a metastable free-energy minimum.

Table S17. Ion-ligand distance (r_1 and r_2 in Å) and potential of mean force (PMF1 and PMF2, in kcal/mol) in metastable states of Br^- complexes in bulk water.[a]

Ligand	Generic				NBFIX			
	r_1	PMF1	r_2	PMF2	r_1	PMF1	r_2	PMF2
NMA	3.6	-0.2	5.4	-0.1	3.3	-0.7	-	-
Acetamide	3.6	-0.4	6.3	-0.1	3.3	-1.1	6.3	-0.2
Methylamine	-	-	5.2	-0.1	3.4	-0.4	5.2	-0.1
Methanol	3.3	-0.5	5.1	-0.2	3.1	-1.8	5.1	-0.2
Ethylene glycol	-	-	4.7	-0.2	2.7	-1.6	3.9	-1.6
Acetic acid	3.3	-0.5	-	-	3.1	-2.2	-	-
Methanethiol	-	-	-	-	3.7	-0.9	-	-
Benzene	5.4	-0.2	-	-	5.2	-1.2	7.9	-0.1
Phenol	3.3	-0.6	7.4	-0.1	3.1	-3.1	5.4	-0.4
Indole	3.4	-0.3	-	-	3.3	-1.5	5.1	-0.5
Imidazole	3.4	-0.4	6.2	-0.1	3.2	-1.8	6.7	-0.1

[a] Dashes indicate absence of a metastable free-energy minimum.

Table S18. Ion-ligand distance (r_1 and r_2 in Å) and potential of mean force (PMF1 and PMF2, in kcal/mol) in metastable states of I^- complexes in bulk water.[a]

Ligand	Generic				NBFIX			
	r_1	PMF1	r_2	PMF2	r_1	PMF1	r_2	PMF2
NMA	3.8	-0.3	5.4	-0.2	3.6	-1.0	-	-
Acetamide	3.8	-0.6	6.4	-0.2	3.6	-1.4	6.6	-0.2
Methylamine	3.9	-0.3	5.4	-0.3	3.6	-0.6	5.3	-0.1
Methanol	3.6	-0.3	5.3	-0.3	3.3	-2.1	5.3	-0.3
Ethylene glycol	-	-	4.9	-0.3	2.9	-1.8	4.2	-1.6
Acetic acid	-	-	6.2	-0.2	3.3	-2.2	6.6	-0.1
Methanethiol	4.6	-0.2	-	-	3.9	-1.3	-	-
Benzene	5.4	-0.4	-	-	5.3	-1.6	8.1	-0.1
Phenol	3.6	-0.3	7.7	-0.3	3.3	-3.3	5.6	-0.6
Indole	3.7	-0.4	-	-	3.4	-1.6	5.2	-0.6
Imidazole	3.8	-0.5	-	-	3.4	-1.8	6.3	-0.1

[a] Dashes indicate absence of a metastable free-energy minimum.