Supporting Information: On the Transferability of Ion Parameters to the TIP4P/2005 Water Model using Molecular Dynamics Simulations

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SI. ADAPTATIONS TO MAMATKULOV DATA

The Mamatkulov hydration free energy (ΔG_{solv}) results were presented in the original publication as ion pair ΔG_{solv} with a fictional Cl^-. Consequently, the ΔG_{solv} of the cations is given by

$$\Delta G_{solv}^{X^{2+}} = \Delta G_{solv}^{XCl_2} - 2\Delta G_{solv}^{Cl^-}. \tag{S1}$$

For the $\Delta G_{solv}^{Cl^-}$, the authors assumed 73.1 kcal/mol following the calculations of Horinek[1]. Furthermore, solvation energy was corrected for 3 effects, namely the finite system size, the hypothetical transfer of ions from ideal gas to ideal solution, and the surface potential at the air-water interface

$$\Delta G_{solv}^{X^{2+}} = \Delta G_{sim} + \Delta G_{fs} + \Delta G_{press} + \Delta G_{surf}, \tag{S2}$$

with

$$\Delta G_{press} = N_A k_B T \ln p_1/p_0 = 1.9 \text{ kcal/mol}, \tag{S3}$$

$$\Delta G_{surf} = -z \times 12.1415 \text{ kcal/mol}, \tag{S4}$$

and

$$\Delta G_{fs} = -z^2 \frac{N_A e^2}{4\pi\epsilon_0} \frac{1}{2L} \left[\frac{\xi_{Ew}}{\epsilon_r} + \left(1 - \frac{1}{\epsilon_r}\right) \left(\frac{4\pi}{3} \left(\frac{R}{L}\right)^2 - \frac{16\pi^2}{45} \left(\frac{R}{L}\right)^5 \right) \right], \tag{S5}$$

where z is the ion valency, N_A is the Avogadros constant, k_B the Boltzmann constant, e the electron charge, ϵ_0 the dielectric permitivity of vacuum, ϵ_r the dielectric permitivity of the water model used, $\xi_{Ew} = 2.837297$ the Wigner potential, L the box side length, and R the Ion-Oxygen Distance. For a full derivation of the finite-size effects the reader is referred to refs. 2–4.

We note here that the Mamatkulov 2013 paper had several typos in equation (S5). Namely, ϵ_0 was squared and $(1 - 1/\epsilon_r)$ was written with a plus instead of a minus and in the last term a multiplicative factor of 2 was missing. These errors were found to only be textual, whereas the results reported in the SI could be reproduced without any problem using the form as described above. Furthermore, if the factor in the last term of equation (S5) would have been used wrong, this was confirmed to have a negligible effect as was also stated by Hummer et al.[3].

SII. ELECTRONIC CHARGE CORRECTION

The Electronic Charge Correction was proposed amongst others by Leontyev at al.[5,6] in order to account for the electronic contribution to the dielectric constant in non-polarizable force fields. In this approach the charges are scaled following $q_{eff} = q/\sqrt{\epsilon_{el}}$, in order to account for the electric screening by the medium. In the case of the TIP4P/2005 water model, this factor is described as $\epsilon_{el} = 1/0.85^2$.[7–9] Here we show that the approach from Leontyev et al. and that of simply scaling the hydration free energy by ϵ_{el}, are in fact similar.

Starting at the definition for the solvation energy proposed by Leontyev et al.,

$$\Delta G_{solv} = \Delta G_{MD} + \Delta G_{el} \tag{S6}$$

with

$$\Delta G_{MD} = \frac{q^2}{2R\epsilon_{el}} \left(1 - \frac{1}{\epsilon_{MD}}\right) \tag{S7}$$

and

$$\Delta G_{el} = \frac{q^2}{2R} \left(1 - \frac{1}{\epsilon_{el}}\right). \tag{S8}$$

Combining (S7) and (S8), it can be shown that

$$\Delta G_{el} = \Delta G_{MD} \left[\frac{\epsilon_{el}}{1 - \frac{1}{\epsilon_{MD}}} \left(1 - \frac{1}{\epsilon_{el}}\right)\right]. \tag{S9}$$

In the limit of $\epsilon_{MD} >> 1$, (S9) can be simplified to

$$\Delta G_{el} = \Delta G_{MD} \left[\frac{\epsilon_{el}}{1 - 0} \left(1 - \frac{1}{\epsilon_{el}}\right)\right] = \Delta G_{MD} \left(\epsilon_{el} - 1\right). \tag{S10}$$

Inserting (S10) into (S6), then yields

$$\Delta G_{solv} = \Delta G_{MD} + \Delta G_{MD} \left(\epsilon_{el} - 1\right) = \Delta G_{MD} \epsilon_{el}. \tag{S11}$$

SIII. VERIFICATION

Our simulation and analysis protocol was verified by reproducing the results from Smith and Dang, Benavides, Joung and Cheatham and Mamatkulov, as shown in figures S1a-S1c. Li et al. only provided error estimates and not the values themselves. However, based on the succesful verification of our strategy with the other results, the reproduction of the results from Li et al. is believed to be accurate. The results from the Hydration Free Energy

calculations are shown on the left and for the Ion-Oxygen Distance calculations on the right in figures S1a-S1c.

For the SD and Benavides ions, the single ion ΔG_{solv} were combined following $\Delta G^{\mathrm{NaCl}} = \Delta G^{\mathrm{Na^+}} + \Delta G^{\mathrm{Cl^-}}$ to form the ion pair ΔG_{solv} reported in the original papers. It is found that this approach predicts an ion pair ΔG_{solv} below the reported value by 3 % for the SD ions and 8 % for the Benavides ions. The reason for this discrepancy is unknown as no corrections were applied to either results and finite size effects have been shown to be negligible above 500 water molecules. We consider the possibility that the strategy involved to compute the ΔG_{solv} is responsible, as neither Smith and Dang nor Benavides, used Thermodynamic Integration (TI). Furthermore, the fact that for the SD and Benavides ions, ion pairs were simulated, thus not considering alchemical simulations with a charge imbalance, may play a role. The Joung and Cheatham results could be reproduced with errors below 1 %. The Mamatkulov results first needed to be transformed as described in their publication and above in this SI. Once corrected, we were able to also reproduce the Mamatkulov results for ΔG_{solv} with errors below 1 %.

In terms of the r_{IO}, we were able to reproduce the results from Smith and Dang and Benavides with errors below 2 %, and for the JC ions the differences found were always below 1 %. The Mamatkulov ions showed the largest differences, with errors up to 2 % for the Ca^{2+} ion. The reason for the larger error discrepancy between our results and the Mamatkulov results is unknown. One possible explanation we see is the use of a larger simulation box by Mamatkulov et al, which contained 2,180 water molecules with 19 cations and 38 anions from which the radial pair distribution function was obtained. Hence, the simulation conditions, at a finite molarity compared to infinite dilution were different. However, the effect did not appear to influence the results of the Benavides NaCl, which was reported at a 1 M molarity. Finite size effects can be shown to not be the origin of the discrepancy with simulations we performed with 66, 523 and 4,179 water molecules, in which the r_{IO} remained 2.36, 2.37 and 2.36, respectively.

Concluding the verification, our simulation and analysis procedure is shown to reproduce results from the literature. Differences have been shown to occur when comparing single ion and ion pair ΔG_{solv} results. These have been attributed to differences in the strategy to compute the ΔG_{solv}, but no definite factor could be identified. The r_{IO} could be reproduced very well, also when comparing inifinite dilution to finite molarity systems, the differences

remained below 2 %.

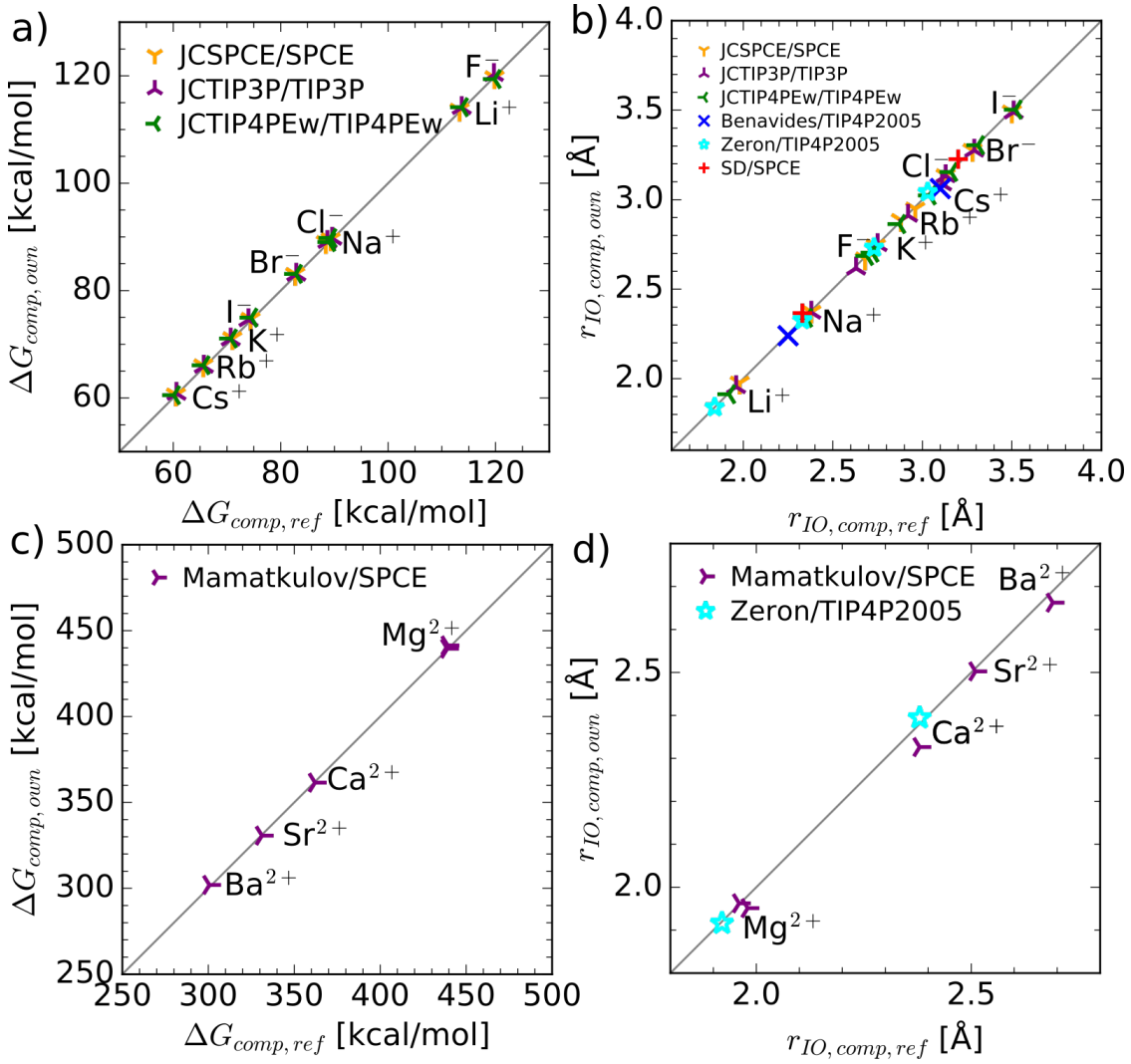

FIG. S1. Results from reproducing reported values by Smith and Dang, Benavides and Joung and Cheatham (a) and (b), and Mamatkulov (c) and (d).

SIV. ACTIVITY COEFFICIENTS

At low concentrations the activity coefficient can be obtained combining equation (6) with the Debye hückel limiting law

$$\ln \gamma = \frac{z_i^2 q^2 k}{8\pi\varepsilon_0\varepsilon_r k_B T}, \tag{S12}$$

using the chemical potential and molality from the simulation in equation (6) and obtaining $\ln\gamma$ from equation (S12). In equation (S12), z_i is the charge of a single ion in electrons, q is

the electron charge in Coulombs, k is the inverse of the Debye length (see equation (S13)), ε_0 is the vacuum dielectric, ε_r is the water model dielectric, k_B is the Boltzmann constant, and T is the temperature. The dielectric constants ε_r for TIP4P/Ew and TIP4P/2005 were set to 62.9 and 60 respectively[7,10]. Finite system size corrections for the activity coefficients have been proposed by Young et al.[11], but deemed not representative in this case as the expected uncertainties, exceed the finite system size corrections.

$$k^2 = \frac{2Iq}{\varepsilon_0 \varepsilon_r k_B T} \tag{S13}$$

TABLE SI. Fitting parameters for equation (6).

	A	B	b	C	D
JCTIP4PEw/TIP4PEw	0.710762	2.206544	0.141916	-0.033628	0.004114
JCTIP4PEw/TIP4P2005	0.762910	0.000000	0.466863	-0.039372	0.002355
Benavides/TIP4P2005	0.468522	2.702357	-0.029320	0.023978	-0.002292

TABLE SII. Chemical potentials and activity coefficients of NaCl for the JCTIP4PEw/TIP4PEw case. Units in mol/kg Å^3 and kJ/mol.

N_w	N_i	m	vol	μ	μ_{ex}	$\mu^\dagger$	$\ln\gamma$
1110	1	0.0500	33381.5000	-410.1114	-745.2973	-393.9866	-0.2584
555	1	0.1000	16692.3000	-406.7317	-745.3520	-393.9866	-0.2695
555	5	0.5001	16756.6000	-399.0320	-745.6088	-393.9866	-0.3252
555	10	1.0002	16869.8000	-394.9808	-744.9590	-393.9866	-0.2008
555	20	2.0003	17120.0000	-391.4275	-744.7676	-393.9866	-0.1769
555	40	4.0006	17731.4000	-386.7194	-743.3205	-393.9866	0.0801
555	60	6.0009	18487.0000	-382.1755	-740.5790	-393.9866	0.5916

TABLE SIII. Chemical potentials and activity coefficients of NaCl for the JCTIP4PEw/TIP4P2005 case. Units in mol/kg Å^3 and kJ/mol.

N_w	N_i	m	vol	μ	μ_{ex}	$\mu^\dagger$	$\ln\gamma$
1110	1	0.0500	33318.6000	-409.0650	-744.2603	-391.7671	-0.4951
555	1	0.1000	16652.0000	-406.2755	-744.9078	-391.7671	-0.6253
555	5	0.5001	16732.0000	-398.6816	-745.2656	-391.7671	-0.7023
555	10	1.0002	16847.5000	-395.0369	-745.0216	-391.7671	-0.6600
555	20	2.0003	17113.3000	-391.9570	-745.2990	-391.7671	-0.7316
555	40	4.0006	17767.4000	-386.3589	-742.9499	-391.7671	-0.2951
555	60	6.0009	18551.0000	-382.6366	-741.0230	-391.7671	0.0506

TABLE SIV. Chemical potentials and activity coefficients of NaCl for the Benavides/TIP4P2005 case. Units in mol/kg Å^3 and kJ/mol.

N_w	N_i	m	vol	μ	μ_{ex}	$\mu^\dagger$	$\ln\gamma$
1110	1	0.0500	33313.2000	-226.2906	-561.4867	-210.4177	-0.2076
555	1	0.1000	16654.4000	-222.9176	-561.5492	-210.4177	-0.2201
555	5	0.5001	16774.7000	-215.0569	-561.6283	-210.4177	-0.2432
555	10	1.0002	16939.2000	-211.8100	-561.7678	-210.4177	-0.2811
555	20	2.0003	17265.2000	-208.5399	-561.8382	-210.4177	-0.3144
555	40	4.0006	17973.5000	-203.7772	-560.3111	-210.4177	-0.0464
555	60	6.0009	18726.7000	-201.0781	-559.4178	-210.4177	0.0928

SV. ADDITIONAL GRAPHS

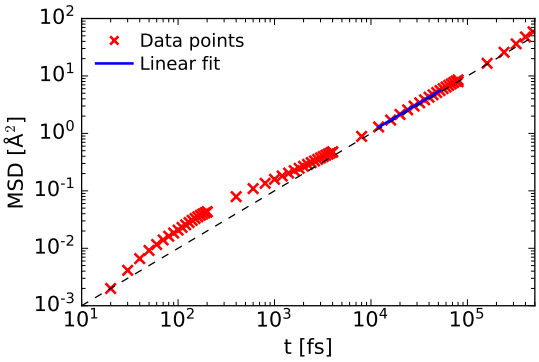

FIG. S2. MSD obtained for a single SD Na^+ ion in TIP4P/2005 water. Ballistic regime is found at at $t < 10$, and linear regime at $t > 10$ ps. Linear regression was done from 10 to 50 ps obtaining the slope. Coefficients of determination for the regression were above 0.999 for all simulations.

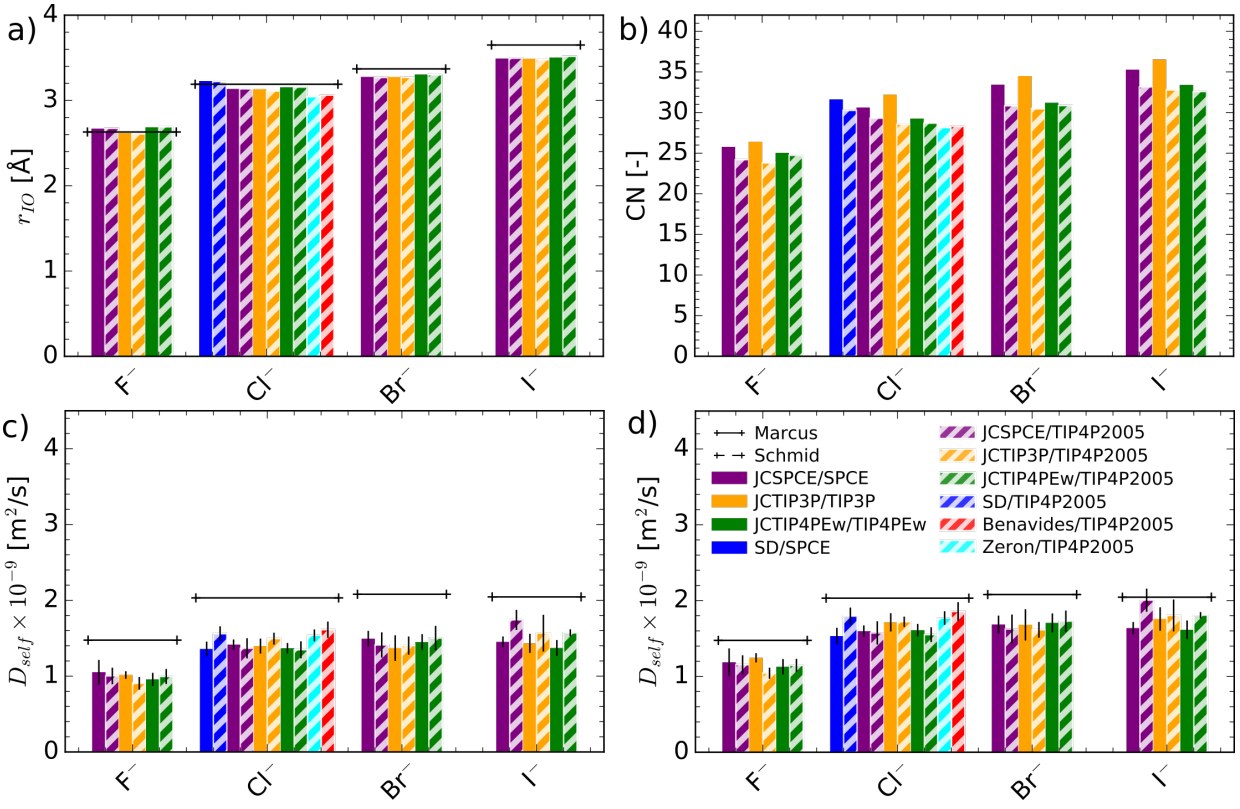

FIG. S3. Radius of second hydration (a), coordination number of the second hydration shell (b), scaled diffusion coefficient by $\eta_{\text{model}}/\eta_{\text{exp}}$ (c) scaled diffusion coefficient by $Di, \text{exp}/Di, \text{model}$ (b) for monovalent anions.

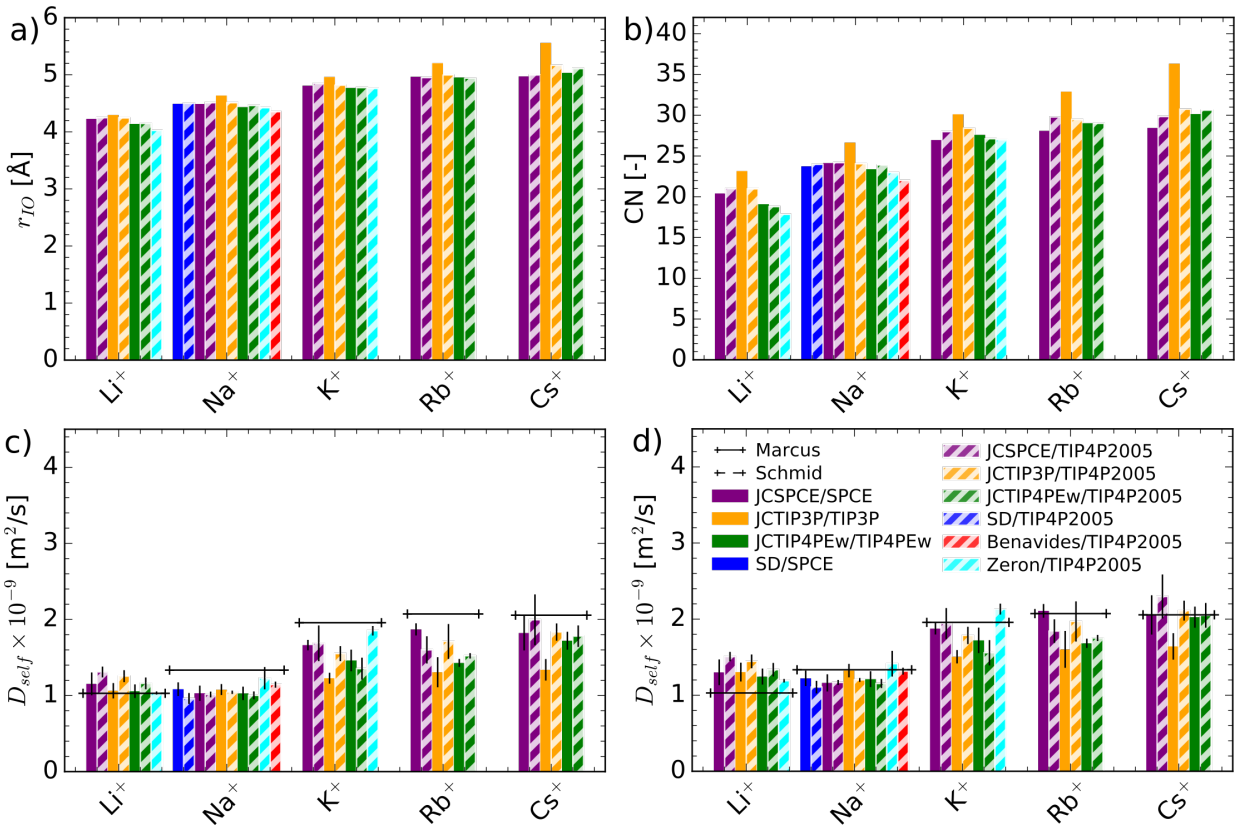

FIG. S4. Radius of second hydration (a), coordination number of the second hydration shell (b), scaled diffusion coefficient by $\eta_{\mathrm{model}}/\eta_{\mathrm{exp}}$ (c) scaled diffusion coefficient by $Di, \mathrm{exp}/Di, \mathrm{model}$ (b) for monovalent cations.

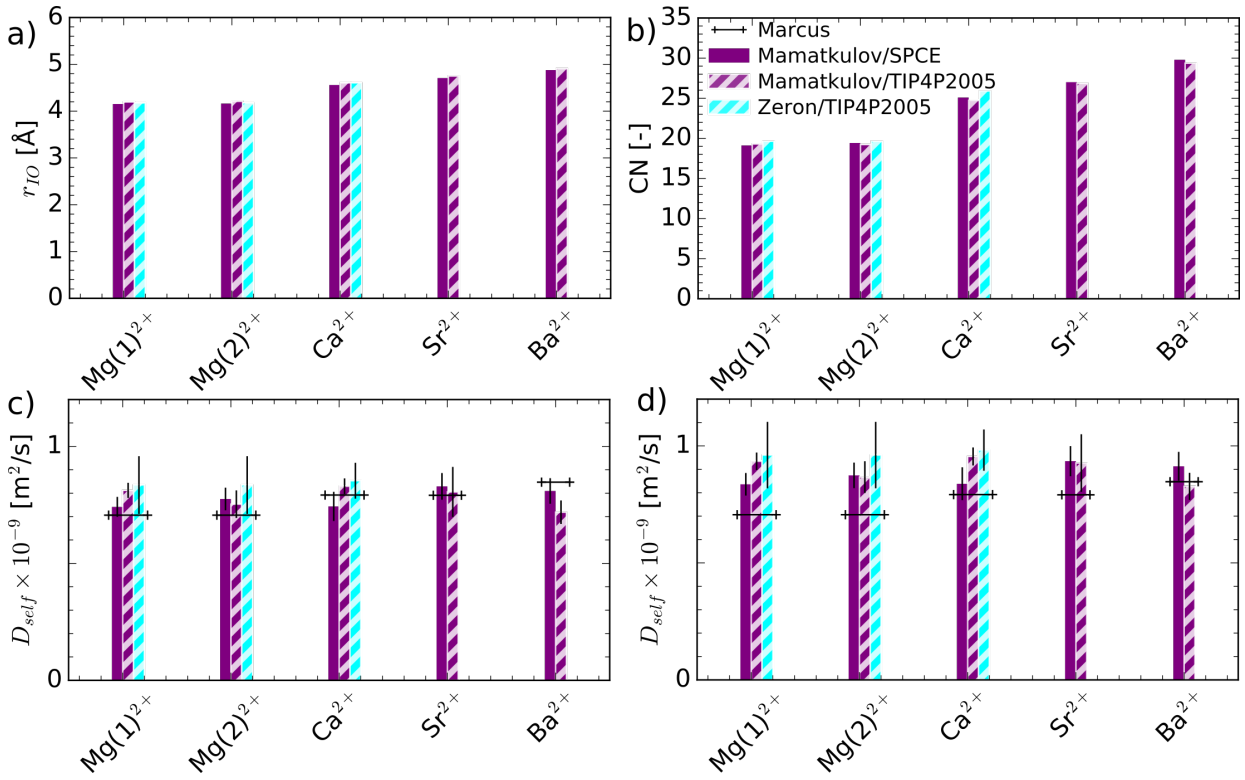

FIG. S5. Radius of second hydration (a), coordination number of the second hydration shell (b), scaled diffusion coefficient by $\eta_{\text{model}}/\eta_{\text{exp}}$ (c) scaled diffusion coefficient by $Di, \text{exp}/Di, \text{model}$ (b) for divalent cations

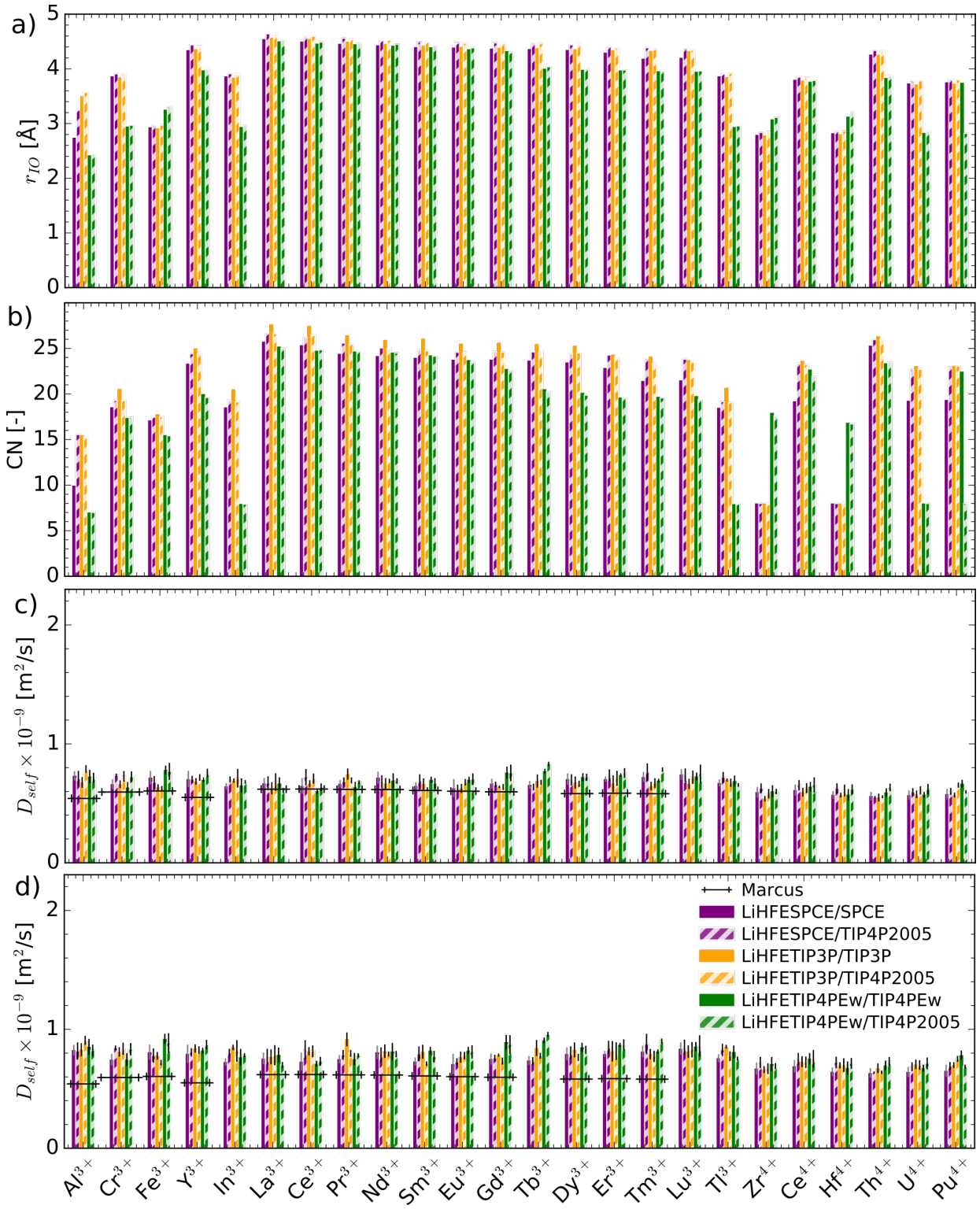

FIG. S6. Radius of second hydration (a), coordination number of the second hydration shell (b), scaled diffusion coefficient by $\eta_{\text{model}}/\eta_{\text{exp}}$ (c) scaled diffusion coefficient by $Di, \text{exp}/Di, \text{model}$ (b) for trivalent cations optimized for ΔG_{solv}.

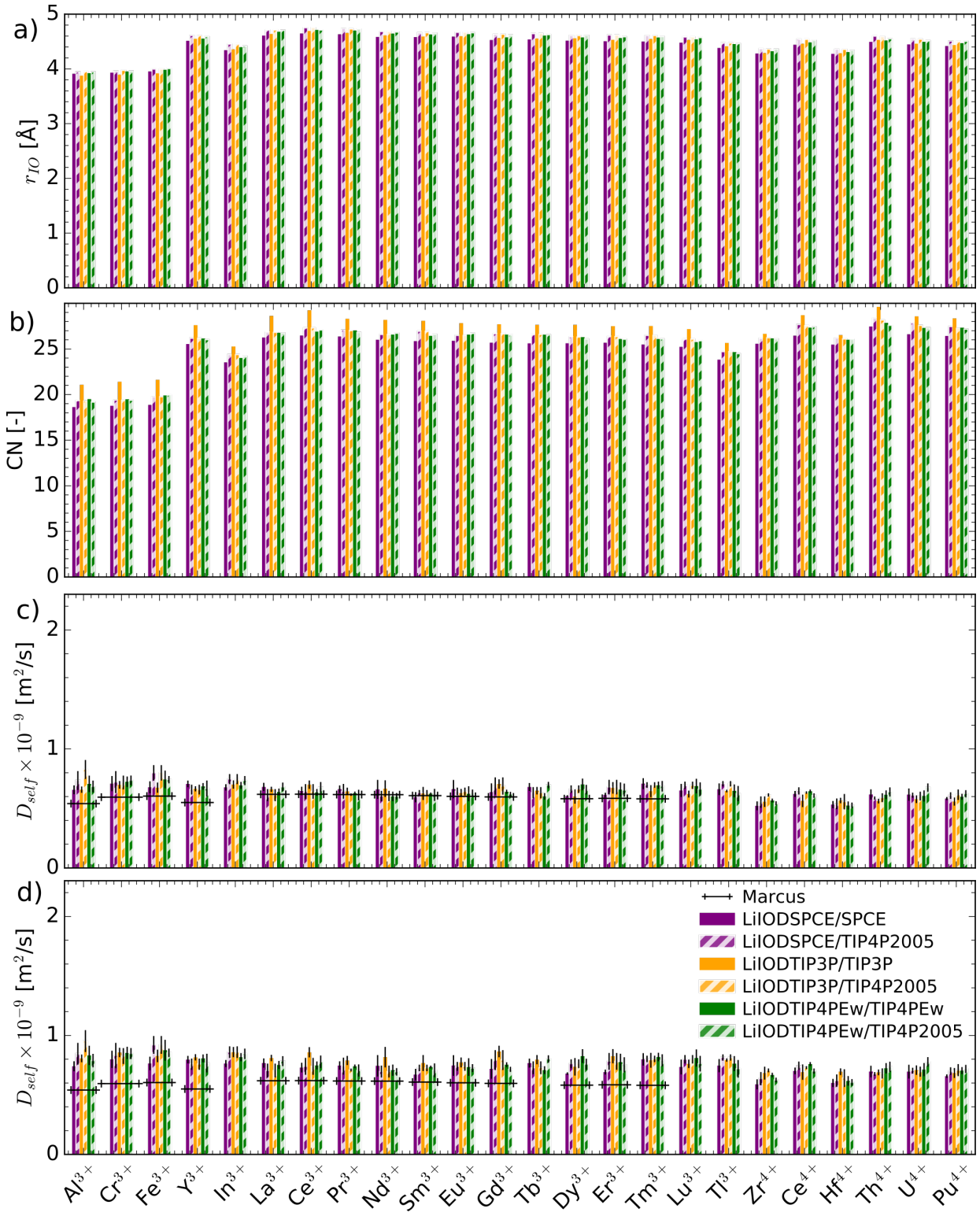

FIG. S7. Radius of second hydration (a), coordination number of the second hydration shell (b), scaled diffusion coefficient by $\eta_{\text{model}}/\eta_{\text{exp}}$ (c) scaled diffusion coefficient by $Di, \text{exp}/Di, \text{model}$ (b) for trivalent cations optimized for r_{IO}.

SVI. ADDITIONAL TABLES

TABLE SV. ΔG_{solv} obtained for monovalent ions for different water models. Units are in kcal/mol.

	TIP4P /2005	SPC/E own	SPC/E ref[12]	TIP4P /2005	TIP3P own	TIP3P ref[12]	TIP4P /2005	TIP4P/Ew own	TIP4P/Ew ref[12]	Schmid[13]	Marcus[14]
		JCSPCE			JCTIP3P			JCTIP4PEw			
Li^+	107.9	113.6	113.3	106.3	114.0	113.7	112.6	114.2	113.7	113.8	113.5
Na^+	86.2	89.0	88.4	84.4	89.1	88.7	88.4	89.0	89.0	88.7	87.2
K^+	69.5	71.1	71.0	67.2	70.9	70.7	70.4	71.1	70.7	71.2	70.5
Rb^+	64.5	66.0	65.6	62.9	65.9	65.7	65.6	66.1	65.6	66.0	65.7
Cs^+	59.0	60.6	60.5	57.6	60.8	60.6	60.2	60.5	60.1	60.5	59.8
F^-	123.7	119.7	119.8	129.3	120.2	119.7	121.2	119.4	119.8	119.7	111.1
Cl^-	91.7	89.5	89.3	94.4	89.7	89.6	90.0	89.8	89.2	89.1	81.3
Br^-	85.0	83.0	82.7	86.8	83.0	82.9	83.8	83.1	82.8	82.7	75.3
I^-	75.6	74.7	74.4	77.3	74.5	74.0	75.3	75.0	74.5	74.3	65.7
		SD									
Na^+	85.1	87.5	182.0							88.7	87.2
Cl^-	90.4	88.3	182.0							89.1	81.3
		Benavides									
Na^+	68.2									88.7	87.2
Cl^-	66.5									89.1	81.3
		Zeron									
Li^+	90.3									113.8	113.5
Na^+	63.7									88.7	87.2
K^+	51.3									71.2	70.5
Cl^-	67.7									89.1	81.3

TABLE SVI. r_{IO} obtained for monovalent ions for different water models. Units are in Å.

	TIP4P /2005	SPC/E own	SPC/E ref[12]	TIP4P /2005	TIP3P own	TIP3P ref[12]	TIP4P /2005	TIP4P/Ew own	TIP4P/Ew ref[12]	Marcus[14]
		JCSPCE			JCTIP3P			JCTIP4PEw		
Li^+	2.03(0)	1.98(0)	1.98	1.99(0)	1.95(0)	1.96	1.92(0)	1.91(0)	1.92	2.08
Na^+	2.40(1)	2.37(0)	2.38	2.40(0)	2.37(0)	2.38	2.35(1)	2.34(0)	2.35	2.36
K^+	2.77(1)	2.74(1)	2.74	2.77(0)	2.75(0)	2.75	2.72(1)	2.70(0)	2.72	2.80
Rb^+	2.90(1)	2.88(1)	2.88	2.94(1)	2.91(1)	2.92	2.87(0)	2.86(0)	2.87	2.89
Cs^+	2.98(0)	2.95(0)	2.96	3.12(0)	3.09(1)	3.11	3.04(0)	3.02(1)	3.04	3.14
F^-	2.67(0)	2.67(1)	2.68	2.61(0)	2.62(0)	2.63	2.69(1)	2.69(0)	2.69	2.63
Cl^-	3.14(0)	3.14(0)	3.13	3.11(0)	3.13(1)	3.13	3.16(1)	3.15(1)	3.16	3.19
Br^-	3.27(0)	3.28(0)	3.28	3.27(1)	3.28(0)	3.29	3.30(0)	3.30(1)	3.31	3.37
I^-	3.49(0)	3.49(0)	3.50	3.48(0)	3.49(1)	3.51	3.52(1)	3.50(1)	3.52	3.65
		SD								
Na^+	2.40(1)	2.37(0)	2.33							2.36
Cl^-	3.22(0)	3.23(1)	3.20							3.19

	TIP4P/2005 own	TIP4P/2005 ref[8] (1m)	Marcus[14]
	Benavides		
Na^+	2.24(0)	2.25	2.36
Cl^-	3.06(1)	3.10	3.19

	TIP4P/2005 own	TIP4P/2005 ref[9]	Marcus[14]
	Zeron		
Li^+	1.84(0)	1.84(12m)	2.08
Na^+	2.33(1)	2.33(6m)	2.36
K^+	2.73(1)	2.73(4.5m)	2.80
Cl^-	3.04(1)	3.03-3.05 (4.5-12m)	3.19

TABLE SVII. CNs obtained for monovalent ions for different water models.

	TIP4P /2005	SPC/E own	TIP4P /2005	TIP3P own	TIP4P /2005	TIP4P/Ew own		
	JCSPCE				JCTIP3P		JCTIP4PEw	
Li^+	4.93(2)	4.23(2)		4.59(1)	4.23(1)		4.06(1)	4.04(0)
Na^+	5.96(0)	5.82(1)		5.94(3)	5.84(2)		5.92(1)	5.88(1)
K^+	7.13(7)	7.01(6)		7.10(4)	7.06(6)		6.91(4)	6.87(4)
Rb^+	7.67(4)	7.87(13)		7.85(12)	7.92(21)		7.60(4)	7.58(3)
Cs^+	7.83(7)	7.97(17)		8.99(27)	9.19(31)		8.34(7)	8.29(13)
F^-	6.11(1)	6.31(2)		6.02(1)	6.38(1)		6.10(2)	6.14(2)
Cl^-	6.65(3)	6.99(5)		6.72(4)	7.31(1)		6.72(4)	6.77(0)
Br^-	6.82(3)	7.18(9)		6.85(5)	7.69(5)		6.87(6)	6.99(5)
I^-	7.12(10)	7.44(8)		7.05(5)	8.04(12)		7.06(3)	7.17(4)

	SD	
Na^+	5.94(1)	5.77(1)
Cl^-	6.84(3)	7.23(9)

	TIP4P/2005 own	TIP4P/2005 ref[8] (1m)
	Benavides	
Na^+	5.31(2)	5.30
Cl^-	5.91(5)	5.80

	TIP4P/2005 own	TIP4P/2005 ref[9]
	Zeron	
Li^+	4.00(0)	4.00(12m)
Na^+	5.53(1)	5.40(6m)
K^+	6.81(8)	6.50(4.5m)
Cl^-	5.79(4)	5.8-6.2 (4.5-12m)

TABLE SVIII. $D_{i,\mathrm{self}}$ obtained for monovalent ions for different water models. Units in 10^{-5} cm^2/s = 10^{-9} m^2/s.

	TIP4P /2005	SPC/E own	TIP4P /2005	TIP3P own	TIP4P /2005	TIP4P/Ew own	Marcus[14]
	JCSPCE		JCTIP3P		JCTIP4PEw		
Li^+	1.36(7)	1.41(18)	1.31(8)	2.95(28)	1.21(8)	1.30(11)	1.03
Na^+	1.06(4)	1.26(12)	1.09(2)	2.99(20)	1.04(5)	1.26(11)	1.33
K^+	1.76(23)	2.03(8)	1.61(10)	3.40(20)	1.41(15)	1.80(17)	1.96
Rb^+	1.67(17)	2.28(10)	1.78(24)	3.62(55)	1.58(4)	1.75(6)	2.07
Cs^+	2.08(32)	2.22(28)	1.91(12)	3.71(39)	1.85(15)	2.11(14)	2.06
F^-	1.04(11)	1.28(20)	0.94(8)	2.82(14)	1.04(10)	1.18(11)	1.48
Cl^-	1.42(14)	1.73(8)	1.56(8)	3.87(27)	1.40(11)	1.68(9)	2.03
Br^-	1.47(17)	1.82(13)	1.46(12)	3.80(47)	1.56(16)	1.78(13)	2.08
I^-	1.81(14)	1.77(9)	1.63(23)	3.97(35)	1.63(5)	1.68(13)	2.04
	SD						
Na^+	1.00(7)	1.32(11)					1.33
Cl^-	1.62(10)	1.66(12)					2.03

	TIP4P/2005 own	TIP4P/2005 ref[8]	Marcus[14]
	Benavides		
Na^+	1.19(4)	1.20	1.33
Cl^-	1.68(11)	1.60	2.03

	TIP4P/2005 own	TIP4P/2005 ref[9] (0.5m)	Marcus[14]
	Zeron		
Li^+	1.08(2)	0.92	1.03
Na^+	1.28(15)	1.22	1.33
K^+	1.93(6)	1.70	1.96
Cl^-	1.60(8)	1.23-1.45	2.03

TABLE SIX. ΔG_{solv} obtained for divalent ions in SPC/E and TIP4P/2005 water. Units in kcal/mol.

	TIP4P/2005	SPC/E own	SPC/E ref[15]	Marcus[14]
		Mamatkulov		
	TIP4P/2005	SPC/E	ref	Marcus
$Mg(1)^{2+}$	415.0	439.5	439.1	439.3
$Mg(2)^{2+}$	413.2	441.4	439.3	439.3
Ca^{2+}	344.0	361.5	362.1	362.1
Sr^{2+}	316.8	330.7	331.3	331.3
Ba^{2+}	289.4	302.0	300.7	300.7
		Zeron		
	TIP4P/2005			Marcus[14]
Mg^{2+}	345.4			439.3
Ca^{2+}	270.7			362.1

TABLE SX. r_{IO} obtained for divalent ions in SPC/E and TIP4P/2005 water. Units in Å.

	TIP4P/2005	SPC/E own	SPC/E ref[15]	Marcus[14]
		Mamatkulov		
$Mg(1)^{2+}$	1.99(0)	1.95(0)	1.98	2.09
$Mg(2)^{2+}$	1.98(0)	1.96(0)	1.96	2.09
Ca^{2+}	2.36(0)	2.33(0)	2.38	2.41
Sr^{2+}	2.53(0)	2.50(0)	2.51	2.64
Ba^{2+}	2.70(0)	2.66(0)	2.69	2.75
	TIP4P/2005 own	TIP4P/2005 ref[9]		Marcus[14]
		Zeron		
Mg^{2+}	1.92(0)	1.92(5m)		2.09
Ca^{2+}	2.39(0)	2.38(6m)		2.41

TABLE SXI. CNs obtained for divalent ions in SPC/E and TIP4P/2005 water.

	TIP4P/2005	SPC/E own	SPC/E ref[15]
		Mamatkulov	
$Mg(1)^{2+}$	6.00(0)	6.00(0)	
$Mg(2)^{2+}$	6.00(0)	6.00(0)	
Ca^{2+}	7.61(3)	7.21(2)	
Sr^{2+}	8.06(1)	7.99(1)	
Ba^{2+}	8.81(4)	8.45(3)	
	TIP4P/2005 own	TIP4P/2005 ref[9]	
		Zeron	
Mg^{2+}	6.00(0)	6(5m)	
Ca^{2+}	7.44(3)	7.1(6m)	

TABLE SXII. $D_{i,\mathrm{self}}$ obtained for divalent ions in SPC/E and TIP4P/2005 water. Units in 10^{-5} $\mathrm{cm}^2/\mathrm{s} = 10^{-9}$ m^2/s.

	TIP4P/2005	SPC/E own	SPC/E ref[15]	Marcus[14]
		Mamatkulov		
$Mg(1)^{2+}$	0.85(3)	0.91(5)		0.71
$Mg(2)^{2+}$	0.78(6)	0.95(6)		0.71
Ca^{2+}	0.86(3)	0.91(8)		0.79
Sr^{2+}	0.84(11)	1.01(7)		0.79
Ba^{2+}	0.75(5)	0.99(7)		0.85

	TIP4P/2005 own	TIP4P/2005 ref[9] (0.5m)		Marcus[14]
		Zeron		
Mg^{2+}	0.87(13)	0.64		0.71
Ca^{2+}	0.89(8)	0.63		0.79

TABLE SXIII. ΔG_{solv} obtained for tri- and quadrivalent ions for different water models. Units in kcal/mol.

	TIP4P/2005	SPC/E	TIP4P/2005	TIP3P	TIP4P/2005	TIP4P/Ew	Marcus
	LiHFESPCE		LiHFETIP3P		LiHFETIP4PEw		
Al^{3+}	994.2	1077.5	998.2	1076.3	1060.9	1083.3	1081.5
Cr^{3+}	906.7	968.5	904.9	966.1	954.4	971.3	958.4
Fe^{3+}	957.1	1032.5	961.4	1033.0	996.7	1015.4	1019.4
Y^{3+}	776.4	817.3	777.0	822.7	815.9	827.2	824.6
In^{3+}	899.9	965.3	903.9	962.9	948.5	964.4	951.2
La^{3+}	717.4	754.0	718.1	755.4	743.9	753.8	751.7
Ce^{3+}	728.5	766.3	728.3	766.6	756.4	767.1	764.8
Pr^{3+}	736.9	776.6	737.8	777.3	765.6	775.6	775.6
Nd^{3+}	744.6	785.7	745.3	785.5	773.2	782.5	783.9
Sm^{3+}	753.2	795.3	755.3	796.4	778.9	790.1	794.7
Eu^{3+}	759.8	802.0	760.9	804.2	788.3	799.6	803.1
Gd^{3+}	762.7	805.1	764.0	806.8	792.6	803.1	806.6
Tb^{3+}	767.8	810.1	768.5	812.2	799.6	810.6	812.6
Dy^{3+}	772.6	814.9	773.9	817.2	807.2	819.0	818.6
Er^{3+}	782.9	830.4	785.8	829.7	831.0	842.1	835.3
Tm^{3+}	787.9	834.2	790.3	836.1	836.4	848.4	840.1
Lu^{3+}	788.2	834.1	790.0	834.8	837.1	848.3	840.1
Tl^{3+}	897.8	963.5	901.5	960.6	945.2	962.4	948.9
Zr^{4+}	1527.1	1640.1	1535.4	1642.1	1602.0	1632.9	1622.8
Ce^{4+}	1378.3	1465.8	1383.4	1465.8	1457.5	1482.9	1462.7
Hf^{4+}	1566.9	1686.1	1574.8	1685.3	1627.2	1658.1	1664.7
Th^{4+}	1314.0	1391.9	1316.2	1390.8	1370.5	1391.4	1389.8
U^{4+}	1483.3	1587.7	1487.5	1585.5	1562.4	1591.8	1567.9
Pu^{4+}	1440.1	1542.0	1444.6	1539.3	1505.7	1528.7	1520.1

TABLE SXIV. ΔG_{solv} obtained for tri- and quadrivalent ions for different water models. Units in kcal/mol.

	TIP4P/2005	SPC/E	TIP4P/2005	TIP3P	TIP4P/2005	TIP4P/Ew	Marcus
	LiIODSPCE		LiIODTIP3P		LiIODTIP4PEw		
Al^{3+}	860.5	917.4	860.2	912.9	866.6	878.7	1081.5
Cr^{3+}	834.4	888.5	834.4	883.6	840.0	852.6	958.4
Fe^{3+}	809.5	860.4	809.5	856.0	816.3	827.5	1019.4
Y^{3+}	726.4	764.0	726.4	763.8	730.5	739.3	824.6
In^{3+}	775.8	819.4	775.8	819.3	779.0	789.4	951.2
La^{3+}	689.0	723.9	689.0	723.8	693.6	701.0	751.7
Ce^{3+}	681.6	716.1	681.6	715.6	685.9	694.1	764.8
Pr^{3+}	683.6	718.4	684.4	719.0	687.6	696.3	775.6
Nd^{3+}	703.0	736.3	703.0	737.9	704.8	714.6	783.9
Sm^{3+}	709.6	742.7	709.6	745.0	711.9	720.8	794.7
Eu^{3+}	706.8	741.4	706.8	743.3	710.5	718.4	803.1
Gd^{3+}	720.0	756.9	720.0	757.5	723.0	732.1	806.6
Tb^{3+}	717.3	753.6	717.3	754.7	720.9	729.8	812.6
Dy^{3+}	723.6	761.6	723.6	761.7	727.6	736.9	818.6
Er^{3+}	726.2	764.7	726.2	764.1	730.0	739.8	835.3
Tm^{3+}	726.6	763.8	726.6	764.2	730.8	739.7	840.1
Lu^{3+}	731.1	769.9	731.1	769.5	734.6	744.5	840.1
Tl^{3+}	758.0	799.9	758.0	799.2	761.8	772.4	948.9
Zr^{4+}	1286.0	1359.2	1287.9	1356.1	1294.9	1314.7	1622.8
Ce^{4+}	1199.9	1262.0	1203.6	1263.1	1211.0	1227.1	1462.7
Hf^{4+}	1297.1	1372.4	1297.5	1369.1	1307.0	1326.5	1664.7
Th^{4+}	1189.4	1250.1	1191.4	1250.8	1199.8	1215.4	1389.8
U^{4+}	1200.5	1262.3	1203.8	1264.1	1211.4	1227.0	1567.9
Pu^{4+}	1212.8	1274.6	1214.1	1275.4	1221.2	1237.0	1520.1

TABLE SXV. r_{IO} obtained for tri- and quadrivalent ions for different water models. Units in Å.

	TIP4P/2005	SPC/E	TIP4P/2005	TIP3P	TIP4P/2005	TIP4P/Ew	Marcus
	LiHFESPCE		LiHFETIP3P		LiHFETIP4PEw		
Al^{3+}	1.35(0)	1.33(0)	1.25(0)	1.28(0)	1.09(0)	1.08(0)	1.88
Cr^{3+}	1.82(0)	1.79(0)	1.81(0)	1.78(0)	1.54(0)	1.53(0)	1.96
Fe^{3+}	1.54(0)	1.51(0)	1.53(0)	1.49(0)	1.31(0)	1.32(0)	2.03
Y^{3+}	2.19(0)	2.16(0)	2.17(0)	2.14(0)	1.99(0)	1.98(0)	2.36
In^{3+}	1.83(0)	1.80(0)	1.83(0)	1.79(0)	1.55(0)	1.54(0)	2.15
La^{3+}	2.42(0)	2.39(0)	2.42(0)	2.39(0)	2.31(0)	2.30(0)	2.52
Ce^{3+}	2.38(0)	2.34(0)	2.37(0)	2.34(0)	2.28(0)	2.26(0)	2.55
Pr^{3+}	2.33(0)	2.30(0)	2.33(0)	2.30(0)	2.25(0)	2.23(0)	2.54
Nd^{3+}	2.31(0)	2.28(0)	2.31(0)	2.27(0)	2.21(0)	2.20(0)	2.47
Sm^{3+}	2.29(0)	2.25(0)	2.28(0)	2.24(0)	2.15(0)	2.14(0)	2.44
Eu^{3+}	2.27(0)	2.23(0)	2.26(0)	2.22(0)	2.11(0)	2.10(0)	2.45
Gd^{3+}	2.26(0)	2.22(0)	2.25(0)	2.21(0)	2.06(0)	2.06(0)	2.39
Tb^{3+}	2.24(0)	2.21(0)	2.23(0)	2.20(0)	2.02(0)	2.01(0)	2.40
Dy^{3+}	2.22(0)	2.19(0)	2.20(0)	2.17(0)	2.01(0)	1.99(0)	2.37
Er^{3+}	2.13(0)	2.11(0)	2.13(0)	2.09(0)	1.96(0)	1.94(0)	2.36
Tm^{3+}	2.12(0)	2.04(0)	2.09(1)	2.07(0)	1.95(0)	1.93(0)	2.36
Lu^{3+}	2.12(0)	2.04(1)	2.09(0)	2.07(0)	1.95(0)	1.93(0)	2.34
Tl^{3+}	1.83(0)	1.80(0)	1.83(0)	1.79(0)	1.56(0)	1.55(0)	2.23
Zr^{4+}	1.55(0)	1.52(0)	1.54(0)	1.51(0)	1.37(0)	1.37(0)	2.19
Ce^{4+}	1.91(0)	1.88(0)	1.91(0)	1.87(0)	1.82(0)	1.80(0)	2.42
Hf^{4+}	1.50(0)	1.47(0)	1.49(0)	1.46(0)	1.22(0)	1.27(0)	2.16
Th^{4+}	2.17(0)	2.13(0)	2.16(0)	2.12(0)	1.93(0)	1.91(0)	2.45
U^{4+}	1.79(0)	1.75(0)	1.78(0)	1.74(0)	1.51(0)	1.49(0)	2.42
Pu^{4+}	1.84(0)	1.80(0)	1.83(0)	1.79(0)	1.58(0)	1.73(0)	2.39

TABLE SXVI. r_{IO} obtained for tri- and quadrivalent ions for different water models. Units in Å.

	TIP4P/2005	SPC/E	TIP4P/2005	TIP3P	TIP4P/2005	TIP4P/Ew	Marcus
	LiIODSPCE		LiIODTIP3P		LiIODTIP4PEw		
Al^{3+}	1.90(0)	1.87(0)	1.90(0)	1.87(0)	1.89(0)	1.88(0)	1.88
Cr^{3+}	1.95(0)	1.92(0)	1.95(0)	1.92(0)	1.94(0)	1.93(0)	1.96
Fe^{3+}	2.00(0)	1.97(0)	2.00(0)	1.97(0)	1.99(0)	1.98(0)	2.03
Y^{3+}	2.38(0)	2.35(0)	2.38(0)	2.35(0)	2.36(0)	2.35(0)	2.36
In^{3+}	2.19(0)	2.16(0)	2.19(0)	2.16(0)	2.16(0)	2.15(0)	2.15
La^{3+}	2.52(0)	2.49(0)	2.52(0)	2.48(0)	2.51(0)	2.49(0)	2.52
Ce^{3+}	2.54(0)	2.51(0)	2.54(0)	2.51(0)	2.53(0)	2.52(0)	2.55
Pr^{3+}	2.54(0)	2.50(0)	2.53(0)	2.50(0)	2.52(0)	2.51(0)	2.54
Nd^{3+}	2.48(0)	2.45(0)	2.48(0)	2.44(0)	2.47(0)	2.45(0)	2.47
Sm^{3+}	2.46(0)	2.42(0)	2.46(0)	2.42(0)	2.44(0)	2.43(0)	2.44
Eu^{3+}	2.47(0)	2.44(0)	2.47(0)	2.43(0)	2.45(0)	2.44(0)	2.45
Gd^{3+}	2.41(0)	2.39(0)	2.41(0)	2.38(0)	2.40(0)	2.39(0)	2.39
Tb^{3+}	2.43(0)	2.39(0)	2.43(0)	2.39(0)	2.41(0)	2.40(0)	2.40
Dy^{3+}	2.40(0)	2.36(0)	2.40(0)	2.36(0)	2.38(0)	2.37(0)	2.37
Er^{3+}	2.39(0)	2.35(0)	2.39(0)	2.35(0)	2.37(0)	2.35(0)	2.36
Tm^{3+}	2.39(0)	2.35(0)	2.39(0)	2.35(0)	2.36(0)	2.35(0)	2.36
Lu^{3+}	2.36(0)	2.33(0)	2.36(0)	2.33(0)	2.34(0)	2.33(0)	2.34
Tl^{3+}	2.27(0)	2.24(0)	2.27(0)	2.23(0)	2.26(0)	2.24(0)	2.23
Zr^{4+}	2.22(0)	2.19(0)	2.22(0)	2.18(0)	2.20(0)	2.19(0)	2.19
Ce^{4+}	2.42(0)	2.38(0)	2.41(0)	2.37(0)	2.39(0)	2.38(0)	2.42
Hf^{4+}	2.20(0)	2.17(0)	2.20(0)	2.16(0)	2.18(0)	2.17(0)	2.16
Th^{4+}	2.46(0)	2.42(0)	2.45(0)	2.42(0)	2.42(0)	2.41(0)	2.45
U^{4+}	2.42(0)	2.38(0)	2.41(0)	2.37(0)	2.39(0)	2.38(0)	2.42
Pu^{4+}	2.39(0)	2.36(0)	2.39(0)	2.35(0)	2.37(0)	2.35(0)	2.39

TABLE SXVII. CNs obtained for tri- and quadrivalent ions for different water models.

	TIP4P/2005	SPC/E	TIP4P/2005	TIP3P	TIP4P/2005	TIP4P/Ew
	LiHFESPCE		LiHFETIP3P		LiHFETIP4PEw	
Al^{3+}	5.00(0)	5.00(0)	5.15(2)	5.03(0)	2.00(0)	2.00(0)
Cr^{3+}	6.00(0)	6.00(0)	6.00(0)	6.00(0)	4.00(0)	4.00(0)
Fe^{3+}	4.00(0)	4.00(0)	4.00(0)	4.00(0)	5.05(0)	5.02(0)
Y^{3+}	8.55(3)	8.07(3)	8.61(3)	8.56(4)	6.00(0)	6.00(0)
In^{3+}	6.00(0)	6.00(0)	6.00(0)	6.00(0)	4.00(0)	4.00(0)
La^{3+}	9.00(0)	8.99(0)	8.99(0)	9.00(0)	8.08(1)	8.09(0)
Ce^{3+}	8.96(1)	8.89(1)	8.96(2)	8.98(1)	8.00(0)	8.01(0)
Pr^{3+}	8.99(4)	8.15(1)	8.62(34)	8.98(4)	8.00(0)	8.00(0)
Nd^{3+}	8.06(1)	8.02(0)	8.05(1)	8.06(0)	7.98(2)	7.99(1)
Sm^{3+}	8.01(0)	8.00(0)	8.01(0)	8.00(0)	8.69(3)	8.57(3)
Eu^{3+}	8.00(0)	8.00(0)	8.00(0)	8.00(0)	8.64(4)	8.66(1)
Gd^{3+}	8.00(0)	8.00(0)	8.00(0)	8.00(0)	6.42(3)	7.85(8)
Tb^{3+}	8.00(1)	8.00(0)	7.99(1)	7.99(1)	6.01(0)	6.01(0)
Dy^{3+}	8.00(2)	7.99(1)	8.03(2)	7.99(1)	6.00(0)	6.00(0)
Er^{3+}	8.74(3)	8.35(4)	8.74(1)	8.76(2)	6.00(0)	6.00(0)
Tm^{3+}	8.72(3)	6.58(5)	8.23(15)	8.67(4)	6.00(0)	6.00(0)
Lu^{3+}	8.67(6)	6.59(7)	8.21(8)	8.72(2)	6.00(0)	6.00(0)
Tl^{3+}	6.00(0)	6.00(0)	6.00(0)	6.00(0)	4.00(0)	4.00(0)
Zr^{4+}	4.00(0)	4.00(0)	4.00(0)	4.00(0)	4.80(1)	4.63(3)
Ce^{4+}	6.00(0)	6.00(0)	6.00(0)	6.00(0)	6.00(0)	6.00(0)
Hf^{4+}	4.00(0)	4.00(0)	4.00(0)	4.00(0)	5.05(2)	5.02(1)
Th^{4+}	8.00(0)	7.99(0)	7.99(1)	8.00(0)	6.00(0)	6.00(0)
U^{4+}	6.00(0)	6.00(0)	6.00(0)	6.00(0)	4.00(0)	4.00(0)
Pu^{4+}	6.00(0)	6.00(0)	6.00(0)	6.00(0)	4.00(0)	6.00(0)

TABLE SXVIII. CNs obtained for tri- and quadrivalent ions for different water models.

	TIP4P/2005	SPC/E	TIP4P/2005	TIP3P	TIP4P/2005	TIP4P/Ew
	LiIODSPCE		LiIODTIP3P		LiIODTIP4PEw	
Al^{3+}	6.00(0)	6.00(0)	6.00(0)	6.00(0)	6.00(0)	6.00(0)
Cr^{3+}	6.00(0)	6.00(0)	6.00(0)	6.00(0)	6.00(0)	6.00(0)
Fe^{3+}	6.00(0)	6.00(0)	6.00(0)	6.00(0)	6.00(0)	6.00(0)
Y^{3+}	8.98(1)	8.93(1)	8.98(1)	8.99(0)	8.96(1)	8.96(1)
In^{3+}	8.55(3)	8.06(4)	8.55(3)	7.97(6)	8.60(1)	8.54(3)
La^{3+}	9.01(0)	9.00(0)	9.01(0)	9.03(0)	9.01(0)	9.01(0)
Ce^{3+}	9.10(1)	9.03(1)	9.10(1)	9.22(1)	9.03(1)	9.04(1)
Pr^{3+}	9.06(1)	9.01(0)	9.05(0)	9.13(1)	9.02(0)	9.02(0)
Nd^{3+}	9.00(0)	9.00(0)	9.00(0)	9.00(0)	9.00(0)	9.00(0)
Sm^{3+}	9.00(0)	9.00(0)	9.00(0)	9.00(0)	9.00(0)	9.00(0)
Eu^{3+}	9.00(0)	9.00(0)	9.00(0)	9.00(0)	9.00(0)	9.00(0)
Gd^{3+}	8.99(0)	8.99(0)	8.99(0)	9.00(0)	8.98(0)	8.98(1)
Tb^{3+}	9.00(0)	8.99(0)	9.00(0)	9.00(0)	8.99(0)	8.99(0)
Dy^{3+}	8.98(1)	8.96(1)	8.98(1)	8.99(0)	8.97(1)	8.97(1)
Er^{3+}	8.98(0)	8.93(1)	8.98(0)	8.98(1)	8.96(2)	8.95(1)
Tm^{3+}	8.98(1)	8.91(1)	8.98(1)	8.98(0)	8.96(2)	8.95(1)
Lu^{3+}	8.98(1)	8.78(5)	8.98(1)	8.99(1)	8.97(2)	8.95(2)
Tl^{3+}	8.00(0)	8.00(0)	8.00(0)	8.00(0)	8.00(0)	8.00(0)
Zr^{4+}	8.00(0)	8.00(0)	8.00(0)	8.00(0)	8.00(0)	8.00(0)
Ce^{4+}	9.11(1)	9.07(1)	9.07(1)	9.14(1)	9.01(1)	9.01(0)
Hf^{4+}	8.00(0)	8.00(0)	8.00(0)	8.00(0)	8.00(0)	8.00(0)
Th^{4+}	9.94(1)	9.87(1)	9.91(2)	9.96(1)	9.14(1)	9.22(1)
U^{4+}	9.11(1)	9.08(1)	9.06(1)	9.15(1)	9.01(0)	9.01(0)
Pu^{4+}	9.01(0)	9.00(0)	9.01(0)	9.01(0)	9.00(0)	9.00(0)

TABLE SXIX. $D_{i,\mathrm{self}}$ obtained for tri- and quadrivalent ions for different water models. Units in 10^{-5} cm^2/s = 10^{-9} m^2/s.

	TIP4P/2005	SPC/E	TIP4P/2005	TIP3P	TIP4P/2005	TIP4P/Ew	Marcus
	LiHFESPCE		LiHFETIP3P		LiHFETIP4PEw		
Al^{3+}	0.74(7)	0.89(5)	0.82(3)	1.87(12)	0.75(4)	0.89(7)	0.54
Cr^{3+}	0.76(2)	0.81(5)	0.76(5)	1.83(9)	0.75(5)	0.78(6)	0.60
Fe^{3+}	0.71(5)	0.87(7)	0.65(2)	1.76(7)	0.80(7)	0.96(4)	0.60
Y^{3+}	0.73(3)	0.86(8)	0.75(3)	1.90(8)	0.79(4)	0.86(2)	0.55
In^{3+}	0.73(3)	0.78(3)	0.74(8)	1.92(5)	0.71(2)	0.80(7)	
La^{3+}	0.70(6)	0.82(5)	0.71(8)	1.74(14)	0.63(2)	0.82(6)	0.62
Ce^{3+}	0.75(7)	0.79(8)	0.74(4)	1.84(8)	0.66(3)	0.74(3)	0.62
Pr^{3+}	0.71(4)	0.81(4)	0.72(3)	2.07(13)	0.71(1)	0.78(5)	0.62
Nd^{3+}	0.71(6)	0.87(6)	0.72(2)	1.85(13)	0.72(2)	0.85(7)	0.62
Sm^{3+}	0.72(6)	0.79(4)	0.64(2)	1.83(13)	0.70(4)	0.86(3)	0.61
Eu^{3+}	0.66(3)	0.77(9)	0.70(3)	1.73(11)	0.73(5)	0.86(3)	0.60
Gd^{3+}	0.69(2)	0.81(5)	0.66(3)	1.77(3)	0.79(7)	0.93(6)	0.60
Tb^{3+}	0.66(3)	0.80(4)	0.70(2)	1.91(15)	0.87(2)	0.95(3)	
Dy^{3+}	0.73(5)	0.86(6)	0.69(3)	1.87(14)	0.75(3)	0.89(4)	0.58
Er^{3+}	0.77(5)	0.86(3)	0.74(7)	1.84(20)	0.79(4)	0.91(2)	0.59
Tm^{3+}	0.79(8)	0.88(5)	0.70(4)	1.79(10)	0.82(2)	0.85(2)	0.58
Lu^{3+}	0.77(6)	0.91(6)	0.75(6)	1.84(12)	0.78(8)	0.89(4)	
Tl^{3+}	0.75(5)	0.82(4)	0.70(4)	1.93(4)	0.68(2)	0.84(6)	
Zr^{4+}	0.65(4)	0.73(5)	0.61(4)	1.50(7)	0.62(2)	0.74(6)	
Ce^{4+}	0.68(5)	0.75(6)	0.65(4)	1.65(10)	0.68(7)	0.79(5)	
Hf^{4+}	0.65(4)	0.70(4)	0.63(5)	1.58(6)	0.65(4)	0.70(6)	
Th^{4+}	0.58(1)	0.68(4)	0.58(1)	1.52(9)	0.66(3)	0.73(4)	
U^{4+}	0.62(3)	0.69(5)	0.63(4)	1.60(9)	0.64(5)	0.70(3)	
Pu^{4+}	0.62(3)	0.70(5)	0.68(2)	1.58(6)	0.62(1)	0.82(4)	

TABLE SXX. $D_{i,\mathrm{self}}$ obtained for tri- and quadrivalent ions for different water models. Units in 10^{-5} cm^2/s = 10^{-9} m^2/s.

	TIP4P/2005	SPC/E	TIP4P/2005	TIP3P	TIP4P/2005	TIP4P/Ew	Marcus
	LiIODSPCE		LiIODTIP3P		LiIODTIP4PEw		
Al^{3+}	0.77(8)	0.80(5)	0.86(8)	1.82(7)	0.71(5)	0.87(8)	0.54
Cr^{3+}	0.75(10)	0.87(8)	0.75(6)	1.94(9)	0.77(4)	0.89(5)	0.60
Fe^{3+}	0.83(7)	0.83(6)	0.83(7)	1.87(12)	0.77(3)	0.91(9)	0.60
Y^{3+}	0.69(4)	0.86(3)	0.69(4)	1.84(6)	0.69(7)	0.84(3)	0.55
In^{3+}	0.78(4)	0.83(3)	0.78(4)	1.94(10)	0.76(4)	0.85(4)	
La^{3+}	0.64(5)	0.83(4)	0.64(5)	1.83(6)	0.71(4)	0.78(4)	0.62
Ce^{3+}	0.67(6)	0.79(4)	0.67(6)	1.94(10)	0.70(5)	0.78(4)	0.62
Pr^{3+}	0.67(6)	0.81(4)	0.64(1)	1.78(9)	0.64(5)	0.77(2)	0.62
Nd^{3+}	0.63(5)	0.81(10)	0.63(5)	1.85(19)	0.63(3)	0.74(5)	0.62
Sm^{3+}	0.66(2)	0.73(5)	0.66(2)	1.74(15)	0.64(5)	0.77(1)	0.61
Eu^{3+}	0.67(3)	0.81(9)	0.67(3)	1.75(9)	0.66(3)	0.77(8)	0.60
Gd^{3+}	0.72(8)	0.78(9)	0.72(8)	1.96(11)	0.65(2)	0.79(2)	0.60
Tb^{3+}	0.66(5)	0.83(4)	0.66(5)	1.80(9)	0.73(3)	0.74(3)	
Dy^{3+}	0.69(3)	0.74(1)	0.69(3)	1.66(17)	0.69(4)	0.86(6)	0.58
Er^{3+}	0.71(6)	0.75(2)	0.71(6)	1.87(14)	0.68(6)	0.81(7)	0.59
Tm^{3+}	0.73(2)	0.87(6)	0.73(2)	1.79(14)	0.72(5)	0.85(4)	0.58
Lu^{3+}	0.72(3)	0.80(7)	0.72(3)	1.72(8)	0.69(6)	0.85(8)	
Tl^{3+}	0.74(2)	0.81(6)	0.74(2)	1.79(3)	0.65(7)	0.80(7)	
Zr^{4+}	0.58(5)	0.64(5)	0.64(1)	1.54(12)	0.57(2)	0.70(2)	
Ce^{4+}	0.67(3)	0.76(3)	0.66(1)	1.56(15)	0.63(2)	0.79(2)	
Hf^{4+}	0.56(5)	0.65(4)	0.58(7)	1.57(6)	0.55(2)	0.64(4)	
Th^{4+}	0.61(1)	0.75(5)	0.62(4)	1.56(5)	0.67(4)	0.76(5)	
U^{4+}	0.64(2)	0.75(6)	0.63(4)	1.60(9)	0.70(4)	0.74(6)	
Pu^{4+}	0.63(3)	0.71(2)	0.64(5)	1.55(9)	0.65(3)	0.74(3)	

TABLE SXXI. Finite Concentration data for TIP4PEw optimized JCTIP4PEw LiCl.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20166.21	33494(1)	2.37	0.002(1)
555	4	10167.89	16811(0)	3.58	0.002(0)
555	8	10337.44	16964(0)	2.37	0.018(12)
555	16	10676.57	17264(1)	2.37	0.038(9)
555	32	11354.81	17901(1)	2.36	0.095(21)

TABLE SXXII. Finite Concentration data for TIP4PEw optimized JCTIP4PEw NaCl.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20230.41	33426(1)	2.78	0.006(3)
555	4	10232.08	16750(1)	2.78	0.014(5)
555	8	10465.84	16834(1)	2.76	0.022(3)
555	16	10933.36	17032(0)	2.76	0.042(4)
555	32	11868.41	17507(1)	2.76	0.094(7)

TABLE SXXIII. Finite Concentration data for TIP4PEw optimized JCTIP4PEw KCl.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20294.84	33502(1)	3.10	0.036(5)
555	4	10296.52	16829(0)	3.09	0.074(10)
555	8	10594.71	16987(1)	3.12	0.119(6)
555	16	11191.09	17340(1)	3.11	0.220(9)
555	32	12383.86	18132(1)	3.09	0.406(9)

TABLE SXXIV. Finite Concentration data for TIP4P2005 optimized JCTIP4PEw LiCl.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20166.21	33429(1)	3.61	0.002(0)
555	4	10167.89	16788(1)	3.61	0.002(0)
555	8	10337.44	16936(1)	2.36	0.021(12)
555	16	10676.57	17247(1)	2.35	0.046(15)
555	32	11354.81	17907(1)	2.36	0.112(26)

TABLE SXXV. Finite Concentration data for TIP4P2005 optimized JCTIP4PEw NaCl.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20230.41	33365(1)	2.76	0.008(3)
555	4	10232.08	16723(1)	2.79	0.013(5)
555	8	10465.84	16816(0)	2.77	0.018(2)
555	16	10933.36	17021(1)	2.77	0.048(6)
555	32	11868.41	17527(1)	2.77	0.104(11)

TABLE SXXVI. Finite Concentration data for TIP4P2005 optimized JCTIP4PEw KCl.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20294.84	33448(1)	3.12	0.037(9)
555	4	10296.52	16799(0)	3.09	0.065(10)
555	8	10594.71	16967(0)	3.11	0.113(10)
555	16	11191.09	17342(0)	3.11	0.223(7)
555	32	12383.86	18155(1)	3.11	0.405(10)

[H]

TABLE SXXVII. Finite Concentration data for TIP4P2005 optimized Zeron LiCl.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20166.21	33425(1)	3.61	0.002(0)
555	4	10167.89	16776(1)	3.61	0.003(0)
555	8	10337.44	16913(1)	3.61	0.007(0)
555	16	10676.57	17193(0)	3.61	0.012(0)
555	32	11354.81	17736(0)	3.61	0.024(0)

TABLE SXXVIII. Finite Concentration data for TIP4P2005 optimized Zeron NaCl.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20230.41	33401(1)	2.82	0.006(1)
555	4	10232.08	16764(1)	2.81	0.010(2)
555	8	10465.84	16889(1)	2.83	0.020(1)
555	16	10933.36	17158(0)	2.83	0.041(2)
555	32	11868.41	17722(0)	2.84	0.080(2)

TABLE SXXIX. Finite Concentration data for TIP4P2005 optimized Zeron KCl.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20294.84	33473(1)	3.32	0.032(4)
555	4	10296.52	16828(1)	3.26	0.031(4)
555	8	10594.71	17026(1)	3.26	0.073(4)
555	16	11191.09	17422(1)	3.30	0.149(5)
555	32	12383.86	18267(1)	3.26	0.267(3)

TABLE SXXX. Finite Concentration data for SPCE optimized Mamatkulov $MgCl_2$.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20377.47	33346(1)	0.00	0.000(0)
555	4	10379.15	16739(1)	2.43	0.250(0)
555	8	10759.97	16898(0)	2.43	0.500(0)
555	16	11521.60	17270(1)	2.43	1.006(5)
555	32	13044.89	18100(1)	2.43	1.694(7)

TABLE SXXXI. Finite Concentration data for SPCE optimized Mamatkulov $CaCl_2$.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20440.56	33388(1)	3.41	0.000(0)
555	4	10442.24	16766(0)	3.28	0.000(0)
555	8	10886.15	16956(1)	2.65	0.108(47)
555	16	11773.97	17419(3)	2.65	0.348(68)
555	32	13549.62	18613(8)	2.65	0.769(93)

TABLE SXXXII. Finite Concentration data for TIP4P2005 optimized Mamatkulov $MgCl_2$.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20377.47	33421(1)	3.61	0.000(0)
555	4	10379.15	16812(0)	2.42	0.500(0)
555	8	10759.97	17014(1)	2.42	0.625(0)
555	16	11521.60	17458(1)	2.43	1.125(0)
555	32	13044.89	18475(1)	2.43	1.775(4)

TABLE SXXXIII. Finite Concentration data for TIP4P2005 optimized Mamatkulov $CaCl_2$.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20440.56	33420(1)	2.67	0.029(18)
555	4	10442.24	16788(2)	2.66	0.092(57)
555	8	10886.15	16956(1)	2.66	0.024(16)
555	16	11773.97	17508(3)	2.66	0.505(46)
555	32	13549.62	18949(8)	2.67	1.532(52)

TABLE SXXXIV. Finite Concentration data for TIP4P2005 optimized Zeron $MgCl_2$.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20377.47	33435(1)	3.60	0.000(0)
555	4	10379.15	16786(0)	3.60	0.000(0)
555	8	10759.97	16944(1)	3.61	0.000(0)
555	16	11521.60	17280(1)	3.61	0.000(0)
555	32	13044.89	17989(1)	3.61	0.000(0)

TABLE SXXXV. Finite Concentration data for TIP4P2005 optimized Zeron $CaCl_2$.

Nw	Ni	mass [g/mol]	volume [Å^3]	r_{ca} [Å]	CIPca
1110	4	20440.56	33429(1)	2.70	0.002(1)
555	4	10442.24	16785(1)	3.61	0.000(0)
555	8	10886.15	16959(1)	3.61	0.000(0)
555	16	11773.97	17329(1)	3.60	0.001(0)
555	32	13549.62	18227(1)	3.61	0.002(0)

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