Figure S1: Overlap of ranges onto the last range. The figure aims to show pictorially how the running averages and standard deviations of the volume and potential energy of the system in the activity calculations were judged to be equilibrated. Shown by the circles and bars are the average and standard deviation of a window of time. The ranges are projected onto the last range shown rightmost and when these ranges overlap (shown numerically above) by greater than 95% over the previous 40 ns simulation window, the simulation was judged to be converged.

Figure S2: Autocorrelation curve of $dU/d\lambda$ over time. The autocorrelation curve as a function of time was defined as,

$$R(t) = \frac{1}{n-t} \sum_{i=1}^{n-t} \left[ (dU/d\lambda)_i - \langle dU/d\lambda \rangle \right] \cdot \left[ (dU/d\lambda)_{i+t} - \langle dU/d\lambda \rangle \right]$$

when the time step has a even gap (1 ps in this case) and $n$ is the longest time. A plot of a typical normalized autocorrelation curve (i.e. $R(t)/R(0)$) is shown. This was from the simulation of NaCl at 0.037 $m$ NaCl at $\lambda=0.5$. The results suggest that the autocorrelation clearly decays earlier than 1 ps.
Figure S3. Correlation the diffusion coefficients of ions ($D_i$) with the diffusion coefficients of water ($D_w$) and water-ion residence time ($\tau_{w-i}$). It was found empirically that $D_i$ and $D_w/\tau_{w-i}^{1/2}$ have a roughly linear relationship. The charts are illustrated using water-model specific ions (A) and Smith-Dang-Garrett ions (B). The units of the diffusion coefficient and the residence time are $10^{-5}$ cm$^2$/s and ps, respectively. The diffusion coefficients of the various waters are 5.19 (TIP3P)$^{56}$, 2.49 (SPC/E)$^{56}$, and 2.4 (TIP4P$_{EW}$)$^{11}$. The shape of individual data indicates water models. Circles, squares and diamonds denote TIP3P, TIP4P$_{EW}$, and SPC/E water, respectively. When the points are fit into lines using least-squares method, the lines were $y = 0.809x - 0.522$ ($R^2 = 0.9389$) for (A) and $y = 0.834x - 0.492$ ($R^2 = 0.8463$) for (B).
Table S1. Contributions to the chemical potential and the activity coefficients of KCl and NaCl solutions at various concentrations calculated with the TIP3P-specific ion parameters of Joung & Cheatham. The volume (V) values represent the average of all the TI windows with units of Å$^3$. The excess chemical potential ($\mu$excess), which is equivalent to the hydration free energy of the inserted particle, calculated by TI are divided by three perturbations as described in the methods section of the main text. $\mu_{vdw}$ is the excess chemical potential involved with turning on van der Waals interactions and $\mu_{elec1}$ and $\mu_{elec2}$ are involved with turning on cationic charge interaction and anion charge interaction, respectively. $\mu_{elec}$ is the sum over all the electric excess chemical potentials. $\Delta\mu$ is the difference from the most dilute solution where the activity coefficient is defined to be unity. In this table, we empirically assumed that there is 0.10 kcal/mol difference in the hydration free energies between the most diluted solution and 0.037 m solution in this calculation. $m$ denotes molality and the unit of energy is kcal/mol.

| $m$ | $-kT\ln(m)$ | $-kT\ln(V)$ | $kT\ln(N)$ | $\mu_{elec1}$ | $\mu_{elec2}$ | $\mu_{elec}$ | $\mu_{vdw}$ | $\mu_{excess}$ | $\mu_{total}$ | $\Delta\mu$ | $\gamma$ |
|-----|--------------|--------------|-------------|---------------|---------------|--------------|-------------|--------------|--------------|-------------|--------|
| NaCl |              |              |             |               |               |              |              |              |              |              |        |
| 0.037 | 1.95        | -6.35        | 0.00        | -90.26        | -94.29        | -184.55      | 6.93         | -177.62      | -182.02      | -0.10       | 0.85   |
| 0.111 | 1.30        | -6.35        | 0.65        | -90.26        | -94.37        | -184.62      | 6.96         | -177.66      | -182.06      | -0.14       | 0.79   |
| 0.186 | 1.00        | -6.35        | 0.95        | -90.24        | -94.42        | -184.66      | 7.01         | -177.65      | -182.05      | -0.13       | 0.80   |
| 0.298 | 0.72        | -6.35        | 1.23        | -90.23        | -94.50        | -184.73      | 7.07         | -177.67      | -182.07      | -0.15       | 0.78   |
| 0.486 | 0.43        | -6.35        | 1.52        | -90.18        | -94.61        | -184.79      | 7.13         | -177.65      | -182.06      | -0.14       | 0.79   |
| 0.713 | 0.20        | -6.35        | 1.74        | -90.13        | -94.75        | -184.89      | 7.25         | -177.63      | -182.04      | -0.12       | 0.82   |
| 0.982 | 0.01        | -6.35        | 1.93        | -90.08        | -94.91        | -184.99      | 7.37         | -177.62      | -182.03      | -0.11       | 0.83   |
| 1.489 | -0.24       | -6.35        | 2.17        | -90.01        | -95.15        | -185.15      | 7.60         | -177.55      | -181.96      | -0.04       | 0.93   |
| 2.006 | -0.41       | -6.35        | 2.34        | -89.90        | -95.41        | -185.31      | 7.80         | -177.51      | -181.92      | 0.00        | 0.99   |
| 2.495 | -0.54       | -6.34        | 2.46        | -89.89        | -95.59        | -185.48      | 8.00         | -177.48      | -181.91      | 0.01        | 1.02   |
| 2.992 | -0.65       | -6.34        | 2.57        | -89.82        | -95.80        | -185.62      | 8.22         | -177.40      | -181.82      | 0.10        | 1.18   |
| 4.017 | -0.82       | -6.34        | 2.73        | -89.84        | -96.09        | -185.93      | 8.59         | -177.34      | -181.78      | 0.14        | 1.27   |
| 4.998 | -0.95       | -6.34        | 2.85        | -89.94        | -96.36        | -186.30      | 8.92         | -177.38      | -181.83      | 0.09        | 1.17   |
| KCl |              |              |             |               |               |              |              |              |              |              |        |
| 0.037 | 1.95        | -6.35        | 0.00        | -72.44        | -94.29        | -166.73      | 7.13         | -159.60      | -164.00      | -0.10       | 0.85   |
| 0.111 | 1.30        | -6.35        | 0.65        | -72.49        | -94.31        | -166.80      | 7.16         | -159.64      | -164.04      | -0.15       | 0.78   |
| 0.186 | 1.00        | -6.35        | 0.95        | -72.53        | -94.32        | -166.84      | 7.21         | -159.64      | -164.04      | -0.15       | 0.78   |
| 0.298 | 0.72        | -6.35        | 1.23        | -72.59        | -94.34        | -166.93      | 7.26         | -159.67      | -164.08      | -0.18       | 0.74   |
| 0.487 | 0.43        | -6.35        | 1.52        | -72.69        | -94.35        | -167.04      | 7.36         | -159.68      | -164.09      | -0.19       | 0.72   |
| 0.716 | 0.20        | -6.35        | 1.74        | -72.82        | -94.37        | -167.20      | 7.48         | -159.72      | -164.13      | -0.23       | 0.68   |
| 0.989 | 0.01        | -6.35        | 1.93        | -72.97        | -94.39        | -167.35      | 7.60         | -159.75      | -164.17      | -0.27       | 0.63   |
| 1.502 | -0.24       | -6.35        | 2.17        | -73.25        | -94.36        | -167.61      | 7.85         | -159.76      | -164.18      | -0.28       | 0.62   |
| 1.991 | -0.41       | -6.35        | 2.33        | -73.53        | -94.35        | -167.88      | 8.07         | -159.82      | -164.24      | -0.35       | 0.56   |
| 2.493 | -0.54       | -6.35        | 2.45        | -73.82        | -94.29        | -168.12      | 8.26         | -159.85      | -164.29      | -0.39       | 0.52   |
Table S2. Diffusion coefficients of the alkali and halide ions in water. Diffusion coefficients were measured from three different simulations each with different volumes for the periodic unit cell to allow correction for finite size effects as per Yeh & Hummer, 2004 (as described in the main text). $V$ indicates the volume of the periodic unit cell in $10^3 \, \text{Å}^3$. $D_{\text{cation}}$ and $D_{\text{anion}}$ are diffusion coefficients of the cations and the anions, respectively. $D_{\text{cor}}$ are the corrected diffusion coefficients calculated using the individual diffusion coefficients. The unit of the diffusion coefficients is $10^{-5} \, \text{cm}^2/\text{s}$. The data follows on the next few pages for various different sets of ion parameters and water models.
A) TIP3P water / TIP3P-compatible ions at 1 m solution

| Solute | Set 1  | Set 2  | Set 3  | $D_{corr}$ |
|--------|--------|--------|--------|------------|
| LiCl   | V      |        |        |            |
| $D_{cation}$ | 1.86 ± 0.12 | 1.95 ± 0.11 | 2.00 ± 0.10 | 2.31        |
| $D_{anion}$  | 2.37 ± 0.12 | 2.46 ± 0.10 | 2.54 ± 0.09 | 2.89        |
| LiBr   | V      |        |        |            |
| $D_{cation}$ | 1.99 ± 0.13 | 2.10 ± 0.11 | 2.14 ± 0.09 | 2.48        |
| $D_{anion}$  | 2.64 ± 0.07 | 2.74 ± 0.05 | 2.79 ± 0.03 | 3.14        |
| LiI    | V      |        |        |            |
| $D_{cation}$ | 2.10 ± 0.12 | 2.19 ± 0.10 | 2.26 ± 0.09 | 2.60        |
| $D_{anion}$  | 2.84 ± 0.02 | 2.95 ± 0.03 | 3.02 ± 0.05 | 3.40        |
| NaF    | V      |        |        |            |
| $D_{cation}$ | 1.60 ± 0.12 | 1.68 ± 0.11 | 1.72 ± 0.10 | 2.01        |
| $D_{anion}$  | 1.66 ± 0.11 | 1.73 ± 0.10 | 1.77 ± 0.09 | 2.02        |
| NaCl   | V      |        |        |            |
| $D_{cation}$ | 1.73 ± 0.12 | 1.85 ± 0.09 | 1.90 ± 0.08 | 2.28        |
| $D_{anion}$  | 2.51 ± 0.11 | 2.58 ± 0.09 | 2.63 ± 0.08 | 2.90        |
| NaBr   | V      |        |        |            |
| $D_{cation}$ | 1.79 ± 0.10 | 1.88 ± 0.09 | 1.94 ± 0.07 | 2.30        |
| $D_{anion}$  | 2.60 ± 0.07 | 2.73 ± 0.04 | 2.78 ± 0.03 | 3.22        |
| NaF    | V      |        |        |            |
| $D_{cation}$ | 1.84 ± 0.11 | 1.96 ± 0.07 | 2.01 ± 0.06 | 2.42        |
| $D_{anion}$  | 2.78 ± 0.02 | 2.92 ± 0.03 | 2.97 ± 0.04 | 3.42        |
| KF     | V      |        |        |            |
| $D_{cation}$ | 2.44 ± 0.10 | 2.57 ± 0.07 | 2.60 ± 0.06 | 2.98        |
| $D_{anion}$  | 1.75 ± 0.10 | 1.87 ± 0.08 | 1.90 ± 0.08 | 2.26        |
| KCl    | V      |        |        |            |
| $D_{cation}$ | 2.69 ± 0.08 | 2.80 ± 0.05 | 2.82 ± 0.04 | 3.14        |
| $D_{anion}$  | 2.61 ± 0.09 | 2.75 ± 0.06 | 2.78 ± 0.05 | 3.18        |
| KBr    | V      |        |        |            |
| $D_{cation}$ | 2.74 ± 0.06 | 2.84 ± 0.03 | 2.89 ± 0.02 | 3.24        |
| $D_{anion}$  | 2.73 ± 0.04 | 2.84 ± 0.02 | 2.91 ± 0.01 | 3.29        |
| KI     | V      |        |        |            |
| $D_{cation}$ | 2.83 ± 0.05 | 2.92 ± 0.02 | 2.97 ± 0.01 | 3.28        |
| $D_{anion}$  | 2.93 ± 0.04 | 3.02 ± 0.06 | 3.08 ± 0.07 | 3.41        |
| RbF    | V      |        |        |            |
| $D_{cation}$ | 2.58 ± 0.04 | 2.64 ± 0.03 | 2.71 ± 0.01 | 2.98        |
| $D_{anion}$  | 2.57 ± 0.04 | 2.63 ± 0.03 | 2.70 ± 0.01 | 3.23        |
| RbCl   | V      |        |        |            |
| $D_{cation}$ | 2.79 ± 0.02 | 2.91 ± 0.01 | 2.96 ± 0.03 | 3.36        |
| $D_{anion}$  | 2.66 ± 0.08 | 2.76 ± 0.06 | 2.83 ± 0.04 | 3.20        |
| RbBr   | V      |        |        |            |
| $D_{cation}$ | 2.83 ± 0.01 | 2.94 ± 0.02 | 3.02 ± 0.04 | 3.42        |
| $D_{anion}$  | 2.78 ± 0.03 | 2.89 ± 0.00 | 2.95 ± 0.02 | 3.33        |
| RbI    | V      |        |        |            |
| $D_{cation}$ | 2.96 ± 0.02 | 3.03 ± 0.04 | 3.10 ± 0.05 | 3.39        |
| $D_{anion}$  | 2.93 ± 0.04 | 3.05 ± 0.07 | 3.10 ± 0.08 | 3.49        |
| CsF    | V      |        |        |            |
| $D_{cation}$ | 2.61 ± 0.02 | 2.69 ± 0.03 | 2.76 ± 0.04 | 3.08        |
| $D_{anion}$  | 1.77 ± 0.10 | 1.87 ± 0.08 | 1.93 ± 0.07 | 2.28        |
| CsCl   | V      |        |        |            |
| $D_{cation}$ | 2.85 ± 0.05 | 2.97 ± 0.07 | 3.02 ± 0.08 | 3.40        |
| $D_{anion}$  | 2.67 ± 0.08 | 2.81 ± 0.05 | 2.83 ± 0.04 | 3.21        |
| CsBr   | V      |        |        |            |
| $D_{cation}$ | 2.87 ± 0.06 | 3.02 ± 0.08 | 3.06 ± 0.10 | 3.51        |
| $D_{anion}$  | 2.79 ± 0.02 | 2.91 ± 0.01 | 2.96 ± 0.02 | 3.36        |
| CsI    | V      |        |        |            |
| $D_{cation}$ | 3.00 ± 0.08 | 3.09 ± 0.10 | 3.17 ± 0.12 | 3.51        |
| $D_{anion}$  | 2.97 ± 0.05 | 3.06 ± 0.08 | 3.11 ± 0.09 | 3.42        |
B) TIP4P$\text{EW}$ water / TIP4P$\text{EW}$ -compatible ions at 1 m solution

| Solute | V | Set 1 | Set 2 | Set 3 | $D_{\text{cor}}$ |
|--------|---|-------|-------|-------|-----------------|
| LiCl   | 15.35 ± 0.05 | 30.72 ± 0.07 | 46.08 ± 0.08 | 1.30 |
|        | 0.97 ± 0.22 | 1.04 ± 0.23 | 1.07 ± 0.23 | 1.62 |
|        | 1.31 ± 0.23 | 1.36 ± 0.23 | 1.41 ± 0.22 | 1.67 |
| LiBr   | 15.51 ± 0.05 | 31.03 ± 0.07 | 46.54 ± 0.08 | 1.31 |
|        | 1.00 ± 0.23 | 1.07 ± 0.22 | 1.09 ± 0.23 | 1.67 |
|        | 1.38 ± 0.23 | 1.43 ± 0.23 | 1.47 ± 0.23 | 1.75 |
| LiI    | 15.76 ± 0.05 | 31.53 ± 0.06 | 47.31 ± 0.08 | 1.32 |
|        | 1.05 ± 0.23 | 1.11 ± 0.23 | 1.14 ± 0.22 | 1.75 |
|        | 1.46 ± 0.24 | 1.52 ± 0.24 | 1.55 ± 0.23 | 1.98 |
| NaF    | 14.77 ± 0.05 | 29.56 ± 0.07 | 44.33 ± 0.08 | 0.95 |
|        | 0.75 ± 0.18 | 0.79 ± 0.18 | 0.81 ± 0.18 | 1.05 |
|        | 0.83 ± 0.23 | 0.86 ± 0.19 | 0.90 ± 0.19 | 1.05 |
| NaCl   | 15.21 ± 0.04 | 30.44 ± 0.06 | 45.65 ± 0.08 | 1.12 |
|        | 0.85 ± 0.18 | 0.90 ± 0.18 | 0.93 ± 0.18 | 1.17 |
|        | 1.31 ± 0.22 | 1.36 ± 0.22 | 1.38 ± 0.22 | 1.67 |
| NaBr   | 15.37 ± 0.04 | 30.74 ± 0.07 | 46.11 ± 0.08 | 1.20 |
|        | 0.86 ± 0.18 | 0.92 ± 0.18 | 0.96 ± 0.18 | 1.31 |
|        | 1.37 ± 0.22 | 1.44 ± 0.22 | 1.46 ± 0.22 | 1.76 |
| KF     | 14.94 ± 0.05 | 29.88 ± 0.07 | 44.84 ± 0.08 | 1.32 |
|        | 1.31 ± 0.20 | 1.36 ± 0.20 | 1.38 ± 0.19 | 1.53 |
|        | 0.92 ± 0.19 | 0.97 ± 0.19 | 0.98 ± 0.19 | 1.72 |
| KCl    | 15.39 ± 0.05 | 30.78 ± 0.07 | 46.18 ± 0.08 | 1.70 |
|        | 1.47 ± 0.19 | 1.52 ± 0.20 | 1.55 ± 0.19 | 1.70 |
|        | 1.41 ± 0.21 | 1.46 ± 0.22 | 1.50 ± 0.21 | 1.70 |
| KBr    | 15.54 ± 0.04 | 31.09 ± 0.06 | 46.63 ± 0.08 | 1.75 |
|        | 1.49 ± 0.19 | 1.55 ± 0.19 | 1.57 ± 0.19 | 1.74 |
|        | 1.49 ± 0.21 | 1.53 ± 0.21 | 1.57 ± 0.20 | 1.75 |
| KI     | 15.79 ± 0.05 | 31.59 ± 0.06 | 47.38 ± 0.08 | 1.82 |
|        | 1.53 ± 0.20 | 1.57 ± 0.20 | 1.62 ± 0.18 | 1.82 |
|        | 1.53 ± 0.22 | 1.58 ± 0.22 | 1.65 ± 0.20 | 1.88 |
| RbF    | 15.00 ± 0.05 | 29.99 ± 0.06 | 45.00 ± 0.08 | 1.22 |
|        | 1.41 ± 0.20 | 1.48 ± 0.20 | 1.51 ± 0.19 | 1.75 |
|        | 0.92 ± 0.19 | 0.99 ± 0.19 | 1.01 ± 0.18 | 1.88 |
| RbCl   | 15.45 ± 0.05 | 30.91 ± 0.07 | 46.37 ± 0.08 | 1.93 |
|        | 1.57 ± 0.19 | 1.65 ± 0.18 | 1.68 ± 0.18 | 1.75 |
|        | 1.43 ± 0.22 | 1.50 ± 0.21 | 1.53 ± 0.20 | 1.75 |
| RbBr   | 15.60 ± 0.05 | 31.22 ± 0.06 | 46.83 ± 0.08 | 1.96 |
|        | 1.61 ± 0.19 | 1.66 ± 0.18 | 1.72 ± 0.17 | 1.80 |
|        | 1.50 ± 0.21 | 1.55 ± 0.21 | 1.59 ± 0.20 | 1.80 |
| RbI    | 15.85 ± 0.05 | 31.71 ± 0.06 | 47.57 ± 0.08 | 1.96 |
|        | 1.65 ± 0.19 | 1.72 ± 0.18 | 1.74 ± 0.17 | 1.96 |
|        | 1.56 ± 0.22 | 1.64 ± 0.21 | 1.66 ± 0.21 | 1.90 |
| CsF    | 15.09 ± 0.05 | 30.19 ± 0.07 | 45.30 ± 0.08 | 1.79 |
|        | 1.51 ± 0.19 | 1.56 ± 0.20 | 1.60 ± 0.19 | 1.79 |
|        | 0.94 ± 0.19 | 1.01 ± 0.18 | 1.03 ± 0.18 | 1.22 |
| CsCl   | 15.56 ± 0.05 | 31.11 ± 0.06 | 46.67 ± 0.08 | 1.83 |
|        | 1.64 ± 0.19 | 1.71 ± 0.18 | 1.77 ± 0.17 | 2.05 |
|        | 1.45 ± 0.21 | 1.52 ± 0.21 | 1.56 ± 0.20 | 2.05 |
| CsBr   | 15.71 ± 0.05 | 31.42 ± 0.06 | 47.14 ± 0.08 | 1.83 |
|        | 1.68 ± 0.17 | 1.74 ± 0.17 | 1.78 ± 0.16 | 2.00 |
|        | 1.51 ± 0.21 | 1.59 ± 0.19 | 1.60 ± 0.20 | 2.17 |
| CsI    | 15.96 ± 0.05 | 31.92 ± 0.06 | 47.89 ± 0.08 | 1.98 |
|        | 1.71 ± 0.18 | 1.78 ± 0.17 | 1.86 ± 0.15 | 1.98 |
|        | 1.56 ± 0.21 | 1.63 ± 0.20 | 1.69 ± 0.19 | 1.98 |
C) SPC/E water / SPC/E-compatible ions at 1 m solution

| Solute  | V       | D_{cation} | D_{anion} | D_{cor} |
|---------|---------|------------|-----------|---------|
| LiCl    | 15.28 ± 0.04 | 1.08 ± 0.21 | 1.36 ± 0.21 | 1.30 ± 0.21 ± 0.08 |
|         |         | 1.12 ± 0.21 | 1.41 ± 0.21 | 1.61 ± 0.21 ± 0.08 |
| LiBr    | 15.44 ± 0.05 | 1.10 ± 0.21 | 1.41 ± 0.21 | 1.38 ± 0.21 ± 0.08 |
|         |         | 1.16 ± 0.21 | 1.48 ± 0.21 | 1.77 ± 0.21 ± 0.08 |
| LiI     | 15.71 ± 0.04 | 1.13 ± 0.22 | 1.51 ± 0.23 | 1.47 ± 0.21 ± 0.08 |
| NaF     | 14.75 ± 0.04 | 0.89 ± 0.18 | 0.89 ± 0.18 | 1.2 ± 0.18 ± 0.07 |
| NaCl    | 15.20 ± 0.04 | 0.98 ± 0.18 | 0.98 ± 0.18 | 1.34 ± 0.18 ± 0.08 |
| NaBr    | 15.35 ± 0.04 | 1.03 ± 0.18 | 1.03 ± 0.18 | 1.66 ± 0.18 ± 0.08 |
| NaI     | 15.71 ± 0.04 | 1.05 ± 0.19 | 1.05 ± 0.19 | 1.8 ± 0.19 ± 0.08 |
| KF      | 14.89 ± 0.05 | 1.46 ± 0.20 | 0.95 ± 0.17 | 1.81 ± 0.20 ± 0.08 |
| KCl     | 15.35 ± 0.04 | 1.64 ± 0.20 | 1.64 ± 0.20 | 1.8 ± 0.20 ± 0.08 |
| KBr     | 15.50 ± 0.04 | 1.66 ± 0.19 | 1.66 ± 0.19 | 1.77 ± 0.19 ± 0.08 |
| KI      | 15.76 ± 0.04 | 1.71 ± 0.19 | 1.71 ± 0.19 | 1.99 ± 0.19 ± 0.08 |
| RbF     | 14.96 ± 0.04 | 1.50 ± 0.19 | 0.96 ± 0.17 | 1.86 ± 0.18 ± 0.08 |
| RbCl    | 15.41 ± 0.04 | 1.69 ± 0.19 | 1.69 ± 0.19 | 1.85 ± 0.18 ± 0.08 |
| RbBr    | 15.57 ± 0.04 | 1.60 ± 0.20 | 1.60 ± 0.20 | 1.72 ± 0.18 ± 0.08 |
| Rbl     | 15.82 ± 0.04 | 1.72 ± 0.19 | 1.72 ± 0.19 | 2.0 ± 0.18 ± 0.08 |
| CsF     | 15.07 ± 0.04 | 1.69 ± 0.19 | 1.69 ± 0.19 | 2.13 ± 0.18 ± 0.08 |
| CsCl    | 15.54 ± 0.04 | 1.55 ± 0.19 | 1.55 ± 0.19 | 2.0 ± 0.18 ± 0.08 |
| CsBr    | 15.69 ± 0.04 | 1.66 ± 0.19 | 1.66 ± 0.19 | 2.13 ± 0.18 ± 0.08 |
| CsI     | 15.94 ± 0.04 | 1.74 ± 0.16 | 1.74 ± 0.16 | 1.86 ± 0.17 ± 0.08 |
(Table S2 continued)

D) TIP3P water / Smith-Dang-Garrett ions at 1 m solution

| Solute | Set 1    | Set 2    | Set 3    | D_{corr} |
|--------|----------|----------|----------|----------|
| LiCl   | V        | 15.49 ± 0.04 | 31.00 ± 0.05 | 46.50 ± 0.06 |
|        | D_{cation} | 2.01 ± 0.13 | 2.13 ± 0.10 | 2.16 ± 0.09 | 2.53 |
|        | D_{anion}   | 2.70 ± 0.10 | 2.82 ± 0.08 | 2.87 ± 0.07 | 3.27 |
| LiF    | V        | 15.98 ± 0.04 | 31.97 ± 0.05 | 47.96 ± 0.06 |
|        | D_{cation} | 2.14 ± 0.12 | 2.26 ± 0.09 | 2.32 ± 0.08 | 2.73 |
|        | D_{anion}   | 2.90 ± 0.02 | 3.04 ± 0.04 | 3.10 ± 0.05 | 3.56 |
| NaF    | V        | 15.10 ± 0.10 | 30.29 ± 0.17 | 45.32 ± 0.21 |
|        | D_{cation} | 1.09 ± 0.10 | 1.04 ± 0.07 | 1.18 ± 0.07 | 1.27 |
|        | D_{anion}   | 1.18 ± 0.09 | 1.10 ± 0.07 | 1.24 ± 0.06 | 1.27 |
| NaCl   | V        | 15.44 ± 0.03 | 30.89 ± 0.05 | 46.35 ± 0.06 |
|        | D_{cation} | 1.77 ± 0.11 | 1.85 ± 0.09 | 1.91 ± 0.08 | 2.22 |
|        | D_{anion}   | 2.69 ± 0.10 | 2.75 ± 0.09 | 2.81 ± 0.07 | 3.08 |
| NaI    | V        | 15.92 ± 0.03 | 31.85 ± 0.05 | 47.78 ± 0.06 |
|        | D_{cation} | 1.85 ± 0.11 | 1.98 ± 0.07 | 2.04 ± 0.06 | 2.48 |
|        | D_{anion}   | 2.87 ± 0.02 | 2.97 ± 0.02 | 3.04 ± 0.04 | 3.42 |
| KF     | V        | 15.12 ± 0.04 | 30.25 ± 0.05 | 45.39 ± 0.06 |
|        | D_{cation} | 2.63 ± 0.09 | 2.71 ± 0.07 | 2.73 ± 0.07 | 2.97 |
|        | D_{anion}   | 1.82 ± 0.10 | 1.92 ± 0.08 | 1.96 ± 0.07 | 2.26 |
| KCl    | V        | 15.66 ± 0.04 | 31.32 ± 0.05 | 46.99 ± 0.06 |
|        | D_{cation} | 2.88 ± 0.07 | 2.96 ± 0.05 | 3.02 ± 0.03 | 3.30 |
|        | D_{anion}   | 2.81 ± 0.09 | 2.90 ± 0.06 | 2.95 ± 0.05 | 3.26 |
| KI     | V        | 16.13 ± 0.03 | 32.27 ± 0.05 | 48.40 ± 0.06 |
|        | D_{cation} | 2.98 ± 0.05 | 3.12 ± 0.01 | 3.17 ± 0.01 | 3.59 |
|        | D_{anion}   | 2.94 ± 0.04 | 3.08 ± 0.07 | 3.13 ± 0.08 | 3.59 |
| RbF    | V        | 15.17 ± 0.04 | 30.35 ± 0.05 | 45.53 ± 0.06 |
|        | D_{cation} | 2.62 ± 0.05 | 2.75 ± 0.03 | 2.80 ± 0.01 | 3.20 |
|        | D_{anion}   | 1.80 ± 0.10 | 1.95 ± 0.07 | 1.98 ± 0.06 | 2.43 |
| RbCl   | V        | 15.71 ± 0.04 | 31.44 ± 0.05 | 47.16 ± 0.06 |
|        | D_{cation} | 2.92 ± 0.01 | 2.99 ± 0.02 | 3.04 ± 0.03 | 3.31 |
|        | D_{anion}   | 2.80 ± 0.08 | 2.89 ± 0.05 | 2.97 ± 0.03 | 3.34 |
| RbI    | V        | 16.19 ± 0.03 | 32.38 ± 0.05 | 48.57 ± 0.06 |
|        | D_{cation} | 2.99 ± 0.02 | 3.10 ± 0.05 | 3.14 ± 0.06 | 3.50 |
|        | D_{anion}   | 2.90 ± 0.03 | 3.04 ± 0.06 | 3.10 ± 0.08 | 3.57 |
| CsF    | V        | 15.28 ± 0.04 | 30.57 ± 0.05 | 45.87 ± 0.06 |
|        | D_{cation} | 2.75 ± 0.03 | 2.86 ± 0.04 | 2.88 ± 0.05 | 3.19 |
|        | D_{anion}   | 1.83 ± 0.11 | 1.95 ± 0.08 | 1.98 ± 0.06 | 2.36 |
| CsCl   | V        | 15.83 ± 0.04 | 31.67 ± 0.05 | 47.52 ± 0.06 |
|        | D_{cation} | 2.94 ± 0.05 | 3.03 ± 0.07 | 3.10 ± 0.09 | 3.44 |
|        | D_{anion}   | 2.82 ± 0.06 | 2.90 ± 0.05 | 2.96 ± 0.02 | 3.25 |
| CsI    | V        | 16.31 ± 0.03 | 32.62 ± 0.05 | 48.94 ± 0.06 |
|        | D_{cation} | 2.96 ± 0.07 | 3.13 ± 0.10 | 3.17 ± 0.11 | 3.64 |
|        | D_{anion}   | 2.83 ± 0.03 | 3.02 ± 0.07 | 3.06 ± 0.08 | 3.62 |
(Table S2 continued)

E) TIP4P$_{ EW }$ water / Smith-Dang-Garrett ions at 1 m solution

| Solute | Set 1 | Set 2 | Set 3 | $D_{ cor }$ |
|--------|-------|-------|-------|------------|
| LiCl   | V     | 15.28 ± 0.05 | 30.57 ± 0.07 | 45.87 ± 0.09 |
|        | $D_{cation}$ | 1.14 ± 0.21 | 1.77 ± 0.21 | 1.22 ± 0.20 | 1.39 |
|        | $D_{anion}$ | 1.40 ± 0.22 | 1.45 ± 0.22 | 1.48 ± 0.22 | 1.66 |
| LiI    | V     | 15.75 ± 0.05 | 31.51 ± 0.07 | 47.26 ± 0.08 |
|        | $D_{cation}$ | 1.23 ± 0.21 | 1.27 ± 0.21 | 1.30 ± 0.21 | 1.46 |
|        | $D_{anion}$ | 1.51 ± 0.24 | 1.59 ± 0.23 | 1.62 ± 0.23 | 1.86 |
| NaF    | V     | 14.77 ± 0.05 | 29.54 ± 0.07 | 44.33 ± 0.09 |
|        | $D_{cation}$ | 0.77 ± 0.18 | 0.84 ± 0.18 | 0.85 ± 0.18 | 1.06 |
|        | $D_{anion}$ | 0.78 ± 0.18 | 0.84 ± 0.18 | 0.86 ± 0.18 | 1.04 |
| NaCl   | V     | 15.26 ± 0.04 | 30.52 ± 0.06 | 45.79 ± 0.08 |
|        | $D_{cation}$ | 0.91 ± 0.19 | 0.97 ± 0.19 | 1.00 ± 0.18 | 1.20 |
|        | $D_{anion}$ | 1.34 ± 0.22 | 1.39 ± 0.23 | 1.44 ± 0.22 | 1.64 |
| NaI    | V     | 15.71 ± 0.04 | 31.44 ± 0.06 | 47.16 ± 0.08 |
|        | $D_{cation}$ | 0.98 ± 0.19 | 1.04 ± 0.19 | 1.06 ± 0.18 | 1.24 |
|        | $D_{anion}$ | 1.49 ± 0.23 | 1.54 ± 0.24 | 1.57 ± 0.23 | 1.75 |
| KF     | V     | 14.97 ± 0.05 | 29.95 ± 0.07 | 44.92 ± 0.08 |
|        | $D_{cation}$ | 1.49 ± 0.21 | 1.53 ± 0.21 | 1.56 ± 0.21 | 1.72 |
|        | $D_{anion}$ | 0.91 ± 0.18 | 0.96 ± 0.18 | 0.99 ± 0.18 | 1.17 |
| KCl    | V     | 15.50 ± 0.05 | 31.03 ± 0.06 | 46.54 ± 0.08 |
|        | $D_{cation}$ | 1.65 ± 0.21 | 1.70 ± 0.21 | 1.73 ± 0.20 | 1.92 |
|        | $D_{anion}$ | 1.49 ± 0.21 | 1.55 ± 0.21 | 1.57 ± 0.20 | 1.76 |
| KI     | V     | 15.96 ± 0.04 | 31.93 ± 0.06 | 47.91 ± 0.08 |
|        | $D_{cation}$ | 1.69 ± 0.20 | 1.74 ± 0.20 | 1.77 ± 0.20 | 1.96 |
|        | $D_{anion}$ | 1.52 ± 0.22 | 1.59 ± 0.21 | 1.64 ± 0.21 | 1.89 |
| RbF    | V     | 15.02 ± 0.05 | 30.06 ± 0.07 | 45.10 ± 0.08 |
|        | $D_{cation}$ | 1.52 ± 0.21 | 1.56 ± 0.21 | 1.60 ± 0.20 | 1.77 |
|        | $D_{anion}$ | 0.91 ± 0.19 | 0.98 ± 0.18 | 0.99 ± 0.18 | 1.21 |
| RbCl   | V     | 15.57 ± 0.05 | 31.15 ± 0.07 | 46.73 ± 0.08 |
|        | $D_{cation}$ | 1.67 ± 0.21 | 1.72 ± 0.19 | 1.76 ± 0.19 | 1.97 |
|        | $D_{anion}$ | 1.48 ± 0.21 | 1.54 ± 0.21 | 1.57 ± 0.20 | 1.75 |
| RbI    | V     | 16.03 ± 0.05 | 32.06 ± 0.06 | 48.10 ± 0.08 |
|        | $D_{cation}$ | 1.69 ± 0.19 | 1.74 ± 0.19 | 1.78 ± 0.18 | 1.97 |
|        | $D_{anion}$ | 1.51 ± 0.22 | 1.59 ± 0.21 | 1.62 ± 0.20 | 1.88 |
| CsF    | V     | 15.15 ± 0.04 | 30.31 ± 0.07 | 45.46 ± 0.08 |
|        | $D_{cation}$ | 1.57 ± 0.22 | 1.62 ± 0.21 | 1.65 ± 0.21 | 1.84 |
|        | $D_{anion}$ | 0.93 ± 0.18 | 0.97 ± 0.18 | 1.01 ± 0.18 | 1.17 |
| CsCl   | V     | 15.70 ± 0.05 | 31.40 ± 0.06 | 47.12 ± 0.08 |
|        | $D_{cation}$ | 1.67 ± 0.21 | 1.76 ± 0.19 | 1.79 ± 0.19 | 2.08 |
|        | $D_{anion}$ | 1.51 ± 0.20 | 1.57 ± 0.20 | 1.58 ± 0.20 | 1.76 |
| CsI    | V     | 16.16 ± 0.04 | 32.33 ± 0.06 | 48.50 ± 0.08 |
|        | $D_{cation}$ | 1.69 ± 0.20 | 1.77 ± 0.19 | 1.79 ± 0.18 | 2.04 |
|        | $D_{anion}$ | 1.50 ± 0.22 | 1.59 ± 0.21 | 1.63 ± 0.20 | 1.90 |
(Table S2 continued)

F) SPC/E water / Smith-Dang-Garrett ions at 1 m solution

| Solute | Set 1     | Set 2     | Set 3     | $D_{cor}$ |
|--------|-----------|-----------|-----------|-----------|
| LiCl   | 15.35 ± 0.04  | 30.70 ± 0.06  | 46.05 ± 0.07 |           |
|        | $D_{cation}$ | 1.05 ± 0.21  | 1.10 ± 0.22  | 1.15 ± 0.21 | 1.38 |
|        | $D_{anion}$  | 1.39 ± 0.22  | 1.46 ± 0.21  | 1.51 ± 0.20 | 1.78 |
| LiI    | 15.83 ± 0.04  | 31.67 ± 0.06  | 47.51 ± 0.07 |           |
|        | $D_{cation}$ | 1.13 ± 0.22  | 1.19 ± 0.22  | 1.22 ± 0.21 | 1.43 |
|        | $D_{anion}$  | 1.57 ± 0.22  | 1.64 ± 0.21  | 1.67 ± 0.22 | 1.90 |
| NaF    | 14.75 ± 0.05  | 29.51 ± 0.07  | 44.27 ± 0.08 |           |
|        | $D_{cation}$ | 0.89 ± 0.18  | 0.92 ± 0.18  | 0.96 ± 0.18 | 1.12 |
|        | $D_{anion}$  | 0.85 ± 0.17  | 0.90 ± 0.17  | 0.92 ± 0.17 | 1.07 |
| NaCl   | 15.26 ± 0.04  | 30.53 ± 0.06  | 45.81 ± 0.08 |           |
|        | $D_{cation}$ | 1.04 ± 0.18  | 1.10 ± 0.18  | 1.12 ± 0.18 | 1.31 |
|        | $D_{anion}$  | 1.40 ± 0.22  | 1.48 ± 0.20  | 1.51 ± 0.21 | 1.76 |
| NaI    | 15.73 ± 0.04  | 31.48 ± 0.06  | 47.22 ± 0.07 |           |
|        | $D_{cation}$ | 1.11 ± 0.19  | 1.17 ± 0.18  | 1.21 ± 0.18 | 1.42 |
|        | $D_{anion}$  | 1.57 ± 0.21  | 1.64 ± 0.21  | 1.69 ± 0.20 | 1.94 |
| KF     | 14.94 ± 0.05  | 29.89 ± 0.06  | 44.84 ± 0.08 |           |
|        | $D_{cation}$ | 1.57 ± 0.20  | 1.63 ± 0.21  | 1.66 ± 0.20 | 1.84 |
|        | $D_{anion}$  | 0.95 ± 0.18  | 1.01 ± 0.17  | 1.04 ± 0.17 | 1.24 |
| KCl    | 15.49 ± 0.04  | 30.99 ± 0.06  | 46.49 ± 0.08 |           |
|        | $D_{cation}$ | 1.77 ± 0.21  | 1.83 ± 0.20  | 1.85 ± 0.20 | 2.05 |
|        | $D_{anion}$  | 1.51 ± 0.20  | 1.59 ± 0.19  | 1.63 ± 0.19 | 1.89 |
| KI     | 15.96 ± 0.04  | 31.92 ± 0.06  | 47.90 ± 0.07 |           |
|        | $D_{cation}$ | 1.86 ± 0.19  | 1.91 ± 0.19  | 1.93 ± 0.19 | 2.10 |
|        | $D_{anion}$  | 1.64 ± 0.20  | 1.71 ± 0.19  | 1.73 ± 0.18 | 1.96 |
| RbF    | 14.99 ± 0.04  | 30.00 ± 0.06  | 45.00 ± 0.08 |           |
|        | $D_{cation}$ | 1.57 ± 0.21  | 1.63 ± 0.20  | 1.66 ± 0.20 | 1.85 |
|        | $D_{anion}$  | 0.94 ± 0.18  | 1.02 ± 0.16  | 1.04 ± 0.17 | 1.29 |
| RbCl   | 15.55 ± 0.05  | 31.11 ± 0.06  | 46.68 ± 0.07 |           |
|        | $D_{cation}$ | 1.76 ± 0.19  | 1.83 ± 0.19  | 1.85 ± 0.18 | 2.06 |
|        | $D_{anion}$  | 1.53 ± 0.19  | 1.59 ± 0.19  | 1.61 ± 0.19 | 1.81 |
| RbI    | 16.02 ± 0.04  | 32.04 ± 0.06  | 48.07 ± 0.07 |           |
|        | $D_{cation}$ | 1.81 ± 0.18  | 1.90 ± 0.17  | 1.93 ± 0.17 | 2.20 |
|        | $D_{anion}$  | 1.60 ± 0.20  | 1.69 ± 0.19  | 1.72 ± 0.18 | 2.00 |
| CsF    | 15.10 ± 0.04  | 30.22 ± 0.06  | 45.34 ± 0.07 |           |
|        | $D_{cation}$ | 1.61 ± 0.21  | 1.66 ± 0.20  | 1.69 ± 0.20 | 1.88 |
|        | $D_{anion}$  | 0.97 ± 0.17  | 1.02 ± 0.17  | 1.04 ± 0.17 | 1.22 |
| CsCl   | 15.67 ± 0.04  | 31.35 ± 0.06  | 47.03 ± 0.07 |           |
|        | $D_{cation}$ | 1.76 ± 0.19  | 1.86 ± 0.18  | 1.86 ± 0.18 | 2.12 |
|        | $D_{anion}$  | 1.52 ± 0.20  | 1.60 ± 0.19  | 1.63 ± 0.18 | 1.89 |
| CsI    | 16.14 ± 0.04  | 32.29 ± 0.06  | 48.44 ± 0.07 |           |
|        | $D_{cation}$ | 1.79 ± 0.19  | 1.86 ± 0.17  | 1.91 ± 0.16 | 2.17 |
|        | $D_{anion}$  | 1.60 ± 0.19  | 1.67 ± 0.18  | 1.70 ± 0.18 | 1.93 |
Table S3: Characteristic radii in radial distribution functions (RDF) of the cation-anion, water-cation, and water-anion interactions. The RDFs were measured from the ~1 m solution simulations with each specified alkali-halide salt. \( r_{\text{max1}} \): radius of the first peak, \( r_{\text{p}} \): upper boundary of \( R \) state, \( r_{\text{min1}} \): radius of the first minimum, \( r_{\text{p}} \): lower boundary of \( P \) state, \( r_{\text{max2}} \): radius of the second peak, \( N \): Number of coordination at \( r_{\text{min1}} \). The unit of the distances is Ångströms. Note that the peak values were estimated at points where the first derivatives of Bézier curve fits to the raw RDF data were zero. The data follows on the next few pages.
### A) TIP3P + TIP3P-compatible ions

| Salt    | $r_{\text{max}1}$ | $r_R$  | $r_{\text{min}1}$ | $r_P$  | $r_{\text{max}2}$ | $N$  |
|---------|--------------------|--------|--------------------|--------|--------------------|------|
| Cation-Anion RDF |                      |        |                    |        |                    |      |
| LiF     | 1.93               | 2.43   | 2.66               | 2.94   | 4.11               | 0.10 |
| NaF     | 2.30               | 2.57   | 3.02               | 3.50   | 4.54               | 0.15 |
| KF      | 2.66               | 2.86   | 3.40               | 3.86   | 4.50               | 0.17 |
| RbF     | 2.82               | 3.09   | 3.55               | 4.00   | 4.61               | 0.15 |
| CsF     | 2.99               | 3.27   | 3.72               | 4.18   | 4.76               | 0.15 |
| LiCl    | 2.31               | 2.59   | 3.11               | 3.75   | 4.66               | 0.32 |
| NaCl    | 2.72               | 3.05   | 3.56               | 4.09   | 5.06               | 0.11 |
| KCl     | 3.08               | 3.42   | 3.99               | 4.50   | 5.34               | 0.25 |
| RbCl    | 3.26               | 3.60   | 4.18               | 4.67   | 5.46               | 0.26 |
| CsCl    | 3.44               | 3.79   | 4.40               | 4.91   | 5.64               | 0.31 |
| LiBr    | 2.44               | 2.72   | 3.18               | 3.83   | 4.81               | 0.08 |
| NaBr    | 2.86               | 3.20   | 3.72               | 4.25   | 5.21               | 0.09 |
| KBr     | 3.23               | 3.58   | 4.16               | 4.70   | 5.53               | 0.26 |
| RbBr    | 3.58               | 3.98   | 4.59               | 5.06   | 5.91               | 0.34 |
| CsBr    | 3.63               | 3.86   | 3.77               | 3.95   | 5.02               | 0.01 |
| LiI     | 3.07               | 3.42   | 3.93               | 4.51   | 5.44               | 0.05 |
| KI      | 3.43               | 3.80   | 4.38               | 4.94   | 5.80               | 0.23 |
| RbI     | 3.60               | 3.98   | 4.59               | 5.15   | 5.98               | 0.27 |
| CsI     | 3.78               | 4.19   | 4.84               | 5.37   | 6.20               | 0.36 |
| Water-Cation RDF |                      |        |                    |        |                    |      |
| LiF     | 1.97               | 2.20   | 2.47               | 3.27   | 4.32               | 4.18 |
| NaF     | 2.37               | 2.67   | 3.18               | 3.71   | 4.63               | 5.71 |
| KF      | 2.76               | 3.06   | 3.34               | 3.95   | 5.05               | 7.29 |
| RbF     | 2.92               | 3.24   | 3.48               | 4.21   | 5.27               | 8.29 |
| CsF     | 3.11               | 3.44   | 4.10               | 4.66   | 5.54               | 9.68 |
| LiCl    | 1.97               | 2.20   | 2.76               | 3.39   | 4.31               | 3.85 |
| NaCl    | 2.37               | 2.69   | 3.21               | 3.71   | 4.62               | 5.73 |
| KCl     | 2.75               | 3.06   | 3.62               | 4.13   | 4.99               | 6.93 |
| RbCl    | 2.92               | 3.23   | 3.82               | 4.34   | 5.19               | 7.86 |
| CsCl    | 3.11               | 3.43   | 4.08               | 4.59   | 5.53               | 9.16 |
| LiBr    | 1.96               | 2.20   | 2.77               | 3.42   | 4.31               | 4.13 |
| NaBr    | 2.37               | 2.69   | 3.21               | 3.91   | 4.82               | 5.76 |
| KBr     | 2.75               | 3.06   | 3.62               | 4.13   | 4.99               | 6.89 |
| RbBr    | 3.10               | 3.43   | 4.07               | 4.58   | 5.49               | 9.00 |
| CsBr    | 1.96               | 2.20   | 2.78               | 3.43   | 4.31               | 4.22 |
| LiI     | 2.37               | 2.69   | 3.21               | 3.71   | 4.62               | 5.80 |
| KI      | 2.75               | 3.06   | 3.62               | 4.14   | 4.99               | 6.89 |
| RbI     | 2.92               | 3.23   | 3.83               | 4.34   | 5.18               | 7.78 |
| CsI     | 3.10               | 3.43   | 4.07               | 4.57   | 5.46               | 8.89 |
| Water-Anion RDF |                      |        |                    |        |                    |      |
| LiF     | 2.63               | 2.88   | 3.39               | 3.83   | 4.56               | 6.60 |
| NaF     | 2.63               | 2.88   | 3.32               | 3.75   | 4.54               | 6.34 |
| KF      | 2.63               | 2.89   | 3.34               | 3.73   | 4.54               | 6.33 |
| RbF     | 2.63               | 2.90   | 3.34               | 3.74   | 4.54               | 6.33 |
| CsF     | 2.63               | 2.90   | 3.34               | 3.74   | 4.54               | 6.33 |
| LiCl    | 3.14               | 3.45   | 3.97               | 4.27   | 5.06               | 8.05 |
| NaCl    | 3.13               | 3.41   | 3.87               | 4.23   | 5.01               | 7.56 |
| KCl     | 3.13               | 3.40   | 3.85               | 4.19   | 4.95               | 7.28 |
| RbCl    | 3.13               | 3.41   | 3.85               | 4.19   | 4.95               | 7.26 |
| CsCl    | 3.13               | 3.41   | 3.85               | 4.19   | 4.95               | 7.22 |
| LiBr    | 3.29               | 3.58   | 4.05               | 4.38   | 5.12               | 8.02 |
| NaBr    | 3.29               | 3.57   | 4.03               | 4.37   | 5.12               | 7.95 |
| KBr     | 3.29               | 3.56   | 4.01               | 4.32   | 5.04               | 7.64 |
| RbBr    | 3.29               | 3.56   | 4.01               | 4.32   | 5.04               | 7.64 |
| CsBr    | 3.29               | 3.56   | 4.01               | 4.32   | 5.04               | 7.64 |
| LiI     | 3.50               | 3.76   | 4.24               | 4.54   | 5.22               | 8.30 |
| KI      | 3.50               | 3.78   | 4.25               | 4.56   | 5.22               | 8.43 |
| RbI     | 3.50               | 3.77   | 4.23               | 4.53   | 5.14               | 8.08 |
| CsI     | 3.50               | 3.77   | 4.23               | 4.52   | 5.14               | 7.98 |
### B) TIP4P$_{EW}$ + TIP4P$_{EW}$-compatible ions

| Salt     | $r_{\text{max}1}$ | $r_r$ | $r_{\text{min}1}$ | $r_p$ | $r_{\text{max}2}$ | $N$  |
|--------|-----------------|------|-----------------|------|-----------------|-----|
| LiF    | 2.00            | 2.49 | 2.74            | 3.09 | 4.07            | 0.07|
| NaF    | 2.38            | 2.58 | 2.92            | 3.38 | 4.66            | 0.01|
| KF     | 2.73            | 2.93 | 3.29            | 3.76 | 4.37            | 0.07|
| RbF    | 2.90            | 3.11 | 3.42            | 3.92 | 4.50            | 0.07|
| CsF    | 2.56            | 2.61 | 3.62            | 4.10 | 4.62            | 0.12|
| LiCl   | 2.36            | 2.62 | 3.00            | 3.52 | 4.54            | 0.02|
| NaCl   | 2.77            | 3.05 | 3.48            | 3.99 | 4.86            | 0.03|
| KCl    | 3.11            | 3.39 | 3.89            | 4.42 | 5.07            | 0.15|
| RbCl   | 3.28            | 3.61 | 4.08            | 4.54 | 5.21            | 0.19|
| CsCl   | 3.42            | 3.76 | 4.31            | 4.74 | 5.33            | 0.28|
| LiBr   | 2.48            | 3.01 | 3.13            | 3.19 | 4.68            | 0.01|
| NaBr   | 2.91            | 3.23 | 3.65            | 4.18 | 5.07            | 0.03|
| KBr    | 3.24            | 3.57 | 4.08            | 4.56 | 5.29            | 0.19|
| RbBr   | 3.41            | 3.74 | 4.28            | 4.73 | 5.43            | 0.24|
| CsBr   | 3.55            | 3.90 | 4.52            | 4.98 | 5.55            | 0.37|
| LiI    | 2.69            | 2.93 | 3.26            | 3.84 | 4.89            | 0.00|
| NaI    | 3.12            | 3.45 | 3.88            | 4.44 | 5.27            | 0.03|
| KI     | 3.44            | 3.78 | 4.30            | 4.85 | 5.58            | 0.19|
| RbI    | 3.62            | 3.98 | 4.55            | 5.02 | 5.71            | 0.28|
| CsI    | 3.74            | 4.14 | 4.79            | 5.15 | 5.91            | 0.41|

#### Water-Cation RDF

| Salt     | $r_{\text{max}1}$ | $r_r$ | $r_{\text{min}1}$ | $r_p$ | $r_{\text{max}2}$ | $N$  |
|--------|-----------------|------|-----------------|------|-----------------|-----|
| LiF    | 1.92            | 2.17 | 2.85            | 3.19 | 4.16            | 4.25|
| NaF    | 2.34            | 2.68 | 3.18            | 3.65 | 4.45            | 5.89|
| KF     | 2.71            | 3.02 | 3.57            | 4.02 | 4.77            | 6.89|
| RbF    | 2.87            | 3.18 | 3.73            | 4.22 | 4.93            | 7.78|
| CsF    | 3.03            | 3.35 | 3.93            | 4.38 | 5.08            | 8.64|
| LiCl   | 1.92            | 2.14 | 2.65            | 3.30 | 4.16            | 4.02|
| NaCl   | 2.34            | 2.68 | 3.19            | 3.67 | 4.46            | 5.86|
| KCl    | 2.71            | 3.02 | 3.55            | 4.04 | 4.78            | 6.77|
| RbCl   | 2.87            | 3.18 | 3.73            | 4.21 | 4.93            | 7.50|
| CsCl   | 3.03            | 3.34 | 3.91            | 4.36 | 5.07            | 8.17|
| LiBr   | 1.92            | 2.14 | 2.65            | 3.29 | 4.16            | 4.04|
| NaBr   | 2.34            | 2.68 | 3.19            | 3.65 | 4.46            | 5.73|
| KBr    | 2.71            | 3.02 | 3.54            | 4.04 | 4.79            | 6.68|
| RbBr   | 2.87            | 3.19 | 3.78            | 4.21 | 4.93            | 7.41|
| CsBr   | 3.03            | 3.35 | 3.91            | 4.37 | 5.07            | 8.02|
| LiI    | 1.92            | 2.14 | 2.65            | 3.30 | 4.16            | 4.05|
| NaI    | 2.34            | 2.68 | 3.19            | 3.66 | 4.47            | 5.84|
| KI     | 2.71            | 3.03 | 3.55            | 4.04 | 4.79            | 6.67|
| RbI    | 2.87            | 3.19 | 3.73            | 4.20 | 4.94            | 7.32|
| CsI    | 3.03            | 3.35 | 3.92            | 4.39 | 5.08            | 7.94|

#### Water-Anion RDF

| Salt     | $r_{\text{max}1}$ | $r_r$ | $r_{\text{min}1}$ | $r_p$ | $r_{\text{max}2}$ | $N$  |
|--------|-----------------|------|-----------------|------|-----------------|-----|
| LiF    | 2.69            | 2.94 | 3.40            | 3.82 | 4.50            | 6.60|
| NaF    | 2.69            | 2.96 | 3.37            | 3.76 | 4.49            | 6.26|
| KF     | 2.69            | 2.95 | 3.37            | 3.76 | 4.50            | 6.20|
| RbF    | 2.69            | 2.95 | 3.37            | 3.77 | 4.50            | 6.18|
| CsF    | 2.69            | 2.96 | 3.37            | 3.76 | 4.50            | 6.15|
| LiCl   | 3.16            | 3.43 | 3.85            | 4.20 | 4.86            | 6.96|
| NaCl   | 3.16            | 3.43 | 3.85            | 4.20 | 4.86            | 7.02|
| KCl    | 3.16            | 3.42 | 3.84            | 4.18 | 4.85            | 6.85|
| RbCl   | 3.16            | 3.43 | 3.84            | 4.17 | 4.85            | 6.81|
| CsCl   | 3.15            | 3.43 | 3.84            | 4.18 | 4.85            | 6.72|
| LiBr   | 3.31            | 3.58 | 3.99            | 4.33 | 4.97            | 7.18|
| NaBr   | 3.31            | 3.58 | 3.99            | 4.32 | 4.96            | 7.20|
| KBr    | 3.31            | 3.57 | 3.98            | 4.30 | 4.95            | 7.06|
| RbBr   | 3.31            | 3.57 | 3.98            | 4.31 | 4.94            | 7.01|
| CsBr   | 3.31            | 3.57 | 3.97            | 4.29 | 4.94            | 6.84|
| LiI    | 3.52            | 3.78 | 4.19            | 4.51 | 5.11            | 7.48|
| NaI    | 3.52            | 3.78 | 4.19            | 4.50 | 5.10            | 7.59|
| KI     | 3.52            | 3.77 | 4.18            | 4.50 | 5.07            | 7.37|
| RbI    | 3.52            | 3.77 | 4.18            | 4.48 | 5.07            | 7.30|
| CsI    | 3.51            | 3.77 | 4.17            | 4.47 | 5.06            | 7.11|
C) SPC/E and SPC/E-compatible ions

| Salt | $r_{\text{max}1}$ | $r_g$ | $r_{\text{min}1}$ | $r_P$ | $r_{\text{max}2}$ | $N$ |
|------|-----------------|------|-----------------|------|-----------------|----|
|      |                 |      |                 |      |                 |    |
| LiF  | 3.93            | 4.59 | 4.94            | 5.53 | 6.06            | 0.02 |
| NaF  | 2.40            | 2.65 | 2.98            | 3.44 | 4.46            | 0.02 |
| KF   | 2.75            | 3.05 | 3.37            | 3.83 | 4.45            | 0.09 |
| RbF  | 2.85            | 3.11 | 3.52            | 3.95 | 4.55            | 0.12 |
| CsF  | 2.88            | 3.13 | 3.63            | 4.07 | 4.62            | 0.22 |
| LiCl | 2.45            | 2.71 | 3.01            | 3.62 | 4.61            | 0.00 |
| NaCl | 2.82            | 3.11 | 3.51            | 4.04 | 4.96            | 0.02 |
| KCl  | 3.15            | 3.47 | 3.93            | 4.41 | 5.15            | 0.12 |
| RbCl | 3.28            | 3.62 | 4.11            | 4.53 | 5.25            | 0.19 |
| CsCl | 3.24            | 3.61 | 4.27            | 4.74 | 5.36            | 0.55 |
| LiBr | 2.57            | 2.74 | 3.10            | 3.74 | 4.75            | 0.00 |
| NaBr | 2.96            | 3.25 | 3.67            | 4.25 | 5.12            | 0.02 |
| KBr  | 3.28            | 3.62 | 4.09            | 4.59 | 5.36            | 0.14 |
| RbBr | 3.41            | 3.75 | 4.27            | 4.77 | 5.49            | 0.22 |
| CsBr | 3.37            | 3.76 | 4.46            | 4.92 | 5.59            | 0.61 |
| LiI  | 2.78            | 3.08 | 3.20            | 3.33 | 4.98            | 0.00 |
| NaI  | 3.18            | 3.49 | 3.89            | 4.45 | 5.35            | 0.02 |
| KI   | 3.48            | 3.84 | 4.33            | 4.89 | 5.68            | 0.15 |
| RbI  | 3.61            | 3.95 | 4.55            | 5.02 | 5.82            | 0.25 |
| CsI  | 3.57            | 4.00 | 4.74            | 5.23 | 5.93            | 0.72 |

| Salt | $r_{\text{max}1}$ | $r_g$ | $r_{\text{min}1}$ | $r_P$ | $r_{\text{max}2}$ | $N$ |
|------|-----------------|------|-----------------|------|-----------------|----|
|      |                 |      |                 |      |                 |    |
| LiF  | 1.98            | 2.23 | 2.79            | 3.37 | 4.24            | 4.40 |
| NaF  | 2.38            | 2.68 | 3.18            | 3.66 | 4.48            | 5.85 |
| KF   | 2.75            | 3.05 | 3.57            | 4.09 | 4.83            | 7.59 |
| RbF  | 2.89            | 3.20 | 3.78            | 4.26 | 5.00            | 8.09 |
| CsF  | 2.96            | 3.27 | 3.86            | 4.36 | 5.05            | 8.16 |
| LiCl | 1.98            | 2.22 | 2.78            | 3.39 | 4.24            | 4.22 |
| NaCl | 2.38            | 2.68 | 3.19            | 3.67 | 4.50            | 5.83 |
| KCl  | 2.75            | 3.05 | 3.59            | 4.09 | 4.82            | 7.06 |
| RbCl | 2.89            | 3.20 | 3.77            | 4.24 | 4.95            | 7.77 |
| CsCl | 2.96            | 3.27 | 3.83            | 4.31 | 4.98            | 7.32 |
| LiBr | 1.98            | 2.22 | 2.79            | 3.40 | 4.24            | 4.22 |
| NaBr | 2.38            | 2.68 | 3.19            | 3.67 | 4.50            | 5.82 |
| KBr  | 2.75            | 3.04 | 3.59            | 4.10 | 4.83            | 7.01 |
| RbBr | 2.89            | 3.20 | 3.77            | 4.25 | 4.98            | 7.83 |
| CsBr | 2.96            | 3.26 | 3.83            | 4.32 | 5.00            | 7.16 |
| LiI  | 1.98            | 2.22 | 2.78            | 3.39 | 4.24            | 4.18 |
| NaI  | 2.38            | 2.69 | 3.19            | 3.68 | 4.50            | 5.82 |
| KI   | 2.75            | 3.04 | 3.59            | 4.08 | 4.83            | 6.98 |
| RbI  | 2.89            | 3.20 | 3.77            | 4.25 | 4.96            | 7.63 |
| CsI  | 2.96            | 3.26 | 3.83            | 4.32 | 5.03            | 6.91 |

| Salt | $r_{\text{max}1}$ | $r_g$ | $r_{\text{min}1}$ | $r_P$ | $r_{\text{max}2}$ | $N$ |
|------|-----------------|------|-----------------|------|-----------------|----|
|      |                 |      |                 |      |                 |    |
| LiF  | 2.68            | 2.95 | 3.38            | 3.81 | 4.56            | 6.60 |
| NaF  | 2.68            | 2.95 | 3.39            | 3.82 | 4.56            | 6.42 |
| KF   | 2.68            | 2.95 | 3.39            | 3.84 | 4.56            | 6.35 |
| RbF  | 2.68            | 2.95 | 3.39            | 3.83 | 4.56            | 6.32 |
| CsF  | 2.68            | 2.95 | 3.38            | 3.82 | 4.56            | 6.19 |
| LiCl | 3.14            | 3.42 | 3.86            | 4.25 | 4.95            | 7.15 |
| NaCl | 3.14            | 3.42 | 3.86            | 4.26 | 4.95            | 7.20 |
| KCl  | 3.14            | 3.42 | 3.85            | 4.25 | 4.94            | 7.06 |
| RbCl | 3.14            | 3.41 | 3.85            | 4.25 | 4.93            | 6.99 |
| CsCl | 3.13            | 3.41 | 3.83            | 4.21 | 4.93            | 6.50 |
| LiBr | 3.28            | 3.57 | 4.00            | 4.37 | 5.06            | 7.39 |
| NaBr | 3.28            | 3.57 | 4.00            | 4.38 | 5.06            | 7.44 |
| KBr  | 3.28            | 3.56 | 3.99            | 4.38 | 5.04            | 7.28 |
| RbBr | 3.28            | 3.56 | 3.99            | 4.37 | 5.05            | 7.29 |
| CsBr | 3.28            | 3.55 | 3.97            | 4.33 | 5.03            | 6.66 |
| LiI  | 3.50            | 3.78 | 4.21            | 4.57 | 5.22            | 7.65 |
| NaI  | 3.50            | 3.77 | 4.21            | 4.58 | 5.22            | 7.81 |
| KI   | 3.50            | 3.77 | 4.21            | 4.57 | 5.20            | 7.69 |
| RbI  | 3.50            | 3.77 | 4.20            | 4.55 | 5.19            | 7.54 |
| CsI  | 3.50            | 3.76 | 4.18            | 4.53 | 5.16            | 6.89 |
### D) TIP3P + Smith-Dang-Garret ions

| Salt   | $r_{\text{max}}^1$ | $r_{R}$ | $r_{\text{min}}^1$ | $r_{P}$ | $r_{\text{max}}^2$ | $N$ |
|--------|---------------------|---------|---------------------|---------|---------------------|-----|
|        |                     |         |                     |         |                     |     |
| Cation-Anion RDF |
| NaF    | 2.34                | 2.67    | 3.26                | 3.83    | 4.64                | 1.97|
| KF     | 2.78                | 3.06    | 3.57                | 4.03    | 4.67                | 0.20|
| RbF    | 2.88                | 3.17    | 3.66                | 4.17    | 4.74                | 0.17|
| CsF    | 3.08                | 3.34    | 3.82                | 4.27    | 4.92                | 0.15|
| LiCl   | 2.43                | 2.71    | 3.15                | 3.68    | 4.77                | 0.06|
| NaCl   | 2.82                | 3.18    | 3.69                | 4.19    | 5.17                | 0.10|
| KCl    | 3.23                | 3.60    | 4.22                | 4.75    | 5.54                | 0.39|
| RbCl   | 3.32                | 3.70    | 4.35                | 4.85    | 5.68                | 0.44|
| CsCl   | 3.49                | 3.89    | 4.59                | 5.05    | 5.88                | 0.51|
| LiI    | 2.81                | 3.22    | 3.31                | 3.45    | 5.16                | 0.00|
| NaI    | 3.23                | 3.60    | 4.04                | 4.62    | 5.55                | 0.03|
| KI     | 3.59                | 3.99    | 4.64                | 5.23    | 6.02                | 0.38|
| RbI    | 3.67                | 4.10    | 4.79                | 5.32    | 6.18                | 0.48|
| CsI    | 3.83                | 4.25    | 5.07                | 5.59    | 6.42                | 0.64|
|        |                     |         |                     |         |                     |     |
| Water-Cation RDF |
| NaF    | 2.38                | 2.64    | 3.08                | 3.60    | 4.90                | 3.93|
| KF     | 2.83                | 3.13    | 3.71                | 4.24    | 5.14                | 7.51|
| RbF    | 2.93                | 3.24    | 3.84                | 4.36    | 5.28                | 8.10|
| CsF    | 3.11                | 3.44    | 4.09                | 4.62    | 5.59                | 9.33|
| LiCl   | 1.97                | 2.22    | 2.80                | 3.44    | 4.32                | 4.25|
| NaCl   | 2.37                | 2.68    | 3.20                | 3.70    | 4.62                | 5.76|
| KCl    | 2.82                | 3.13    | 3.70                | 4.22    | 5.06                | 6.99|
| RbCl   | 2.93                | 3.24    | 3.82                | 4.33    | 5.16                | 7.41|
| CsCl   | 3.11                | 3.44    | 4.06                | 4.55    | 5.42                | 8.46|
| LiI    | 1.97                | 2.22    | 2.80                | 3.45    | 4.32                | 4.31|
| NaI    | 2.37                | 2.69    | 3.21                | 3.71    | 4.62                | 5.83|
| KI     | 2.82                | 3.14    | 3.71                | 4.23    | 5.07                | 6.93|
| RbI    | 2.92                | 3.24    | 3.83                | 4.34    | 5.18                | 7.27|
| CsI    | 3.11                | 3.44    | 4.06                | 4.59    | 5.42                | 8.05|
|        |                     |         |                     |         |                     |     |
| Water-Anion RDF |
| NaF    | 2.70                | 2.88    | 3.58                | 4.29    | 4.78                | 5.72|
| KF     | 2.70                | 2.97    | 3.41                | 3.80    | 4.63                | 6.63|
| RbF    | 2.70                | 2.97    | 3.41                | 3.80    | 4.62                | 6.66|
| CsF    | 2.70                | 2.97    | 3.42                | 3.81    | 4.63                | 6.70|
| LiCl   | 3.24                | 3.52    | 3.99                | 4.33    | 5.07                | 7.93|
| NaCl   | 3.24                | 3.51    | 3.99                | 4.34    | 5.09                | 7.96|
| KCl    | 3.24                | 3.51    | 3.95                | 4.27    | 4.98                | 7.40|
| RbCl   | 3.24                | 3.51    | 3.95                | 4.25    | 4.98                | 7.32|
| CsCl   | 3.24                | 3.51    | 3.95                | 4.26    | 5.00                | 7.22|
| LiI    | 3.64                | 3.90    | 4.38                | 4.67    | 5.26                | 8.76|
| NaI    | 3.64                | 3.91    | 4.39                | 4.68    | 5.26                | 8.90|
| KI     | 3.63                | 3.89    | 4.37                | 4.62    | 5.13                | 8.45|
| RbI    | 3.64                | 3.90    | 4.36                | 4.61    | 5.12                | 8.25|
| CsI    | 3.64                | 3.89    | 4.35                | 4.62    | 5.14                | 7.94|
## E) TIP4P<sub>EW</sub> + Smith-Dang-Garret ions

| Salt   | \( r_{\text{max}1} \) | \( r_{R} \) | \( r_{\text{min}1} \) | \( r_{P} \) | \( r_{\text{max}2} \) | \( N \) |
|--------|------------------|-------|------------------|-------|------------------|-----|
|        | Cation-Anion RDF |       | Water-Cation RDF |       | Water-Anion RDF  |     |
| NaF    | 2.32             | 2.59  | 3.01             | 3.41  | 4.10             | 0.21|
| KF     | 2.81             | 3.05  | 3.43             | 3.86  | 4.47             | 0.11|
| RbF    | 2.92             | 3.13  | 3.51             | 4.03  | 4.55             | 0.11|
| CsF    | 3.13             | 3.35  | 3.66             | 4.20  | 4.71             | 0.10|
| LiCl   | 2.43             | 2.68  | 3.13             | 3.71  | 4.67             | 0.07|
| NaCl   | 2.82             | 3.13  | 3.63             | 4.12  | 4.96             | 0.11|
| KCl    | 3.24             | 3.57  | 4.20             | 4.65  | 5.26             | 0.42|
| RbCl   | 3.33             | 3.70  | 4.32             | 4.75  | 5.37             | 0.46|
| CsCl   | 3.51             | 3.91  | 4.57             | 4.95  | 5.54             | 0.53|
| LiI    | 2.82             | 2.94  | 3.31             | 4.07  | 5.07             | 0.00|
| NaI    | 3.22             | 3.58  | 4.04             | 4.56  | 5.42             | 0.06|
| KI     | 3.58             | 3.99  | 4.67             | 5.12  | 5.84             | 0.56|
| RbI    | 3.67             | 4.08  | 4.84             | 5.33  | 5.93             | 0.69|
| CsI    | 3.84             | 4.29  | 5.11             | 5.45  | 6.12             | 0.86|

### Water-Cation RDF

| Salt   | \( r_{\text{max}1} \) | \( r_{R} \) | \( r_{\text{min}1} \) | \( r_{P} \) | \( r_{\text{max}2} \) | \( N \) |
|--------|------------------|-------|------------------|-------|------------------|-----|
| NaF    | 2.40             | 2.70  | 3.19             | 3.67  | 4.48             | 5.74|
| KF     | 2.85             | 3.16  | 3.70             | 4.18  | 4.90             | 7.48|
| RbF    | 2.95             | 3.26  | 3.82             | 4.29  | 4.99             | 7.97|
| CsF    | 3.13             | 3.45  | 4.04             | 4.48  | 5.15             | 8.98|
| LiCl   | 2.00             | 2.29  | 2.90             | 3.48  | 4.24             | 4.48|
| NaCl   | 2.39             | 2.72  | 3.22             | 3.69  | 4.50             | 5.80|
| KCl    | 2.85             | 3.16  | 3.69             | 4.17  | 4.90             | 6.87|
| RbCl   | 2.95             | 3.26  | 3.80             | 4.29  | 4.98             | 7.25|
| CsCl   | 3.13             | 3.45  | 4.02             | 4.45  | 5.12             | 8.13|
| LiI    | 2.00             | 2.28  | 2.90             | 3.50  | 4.24             | 4.54|
| NaI    | 2.39             | 2.72  | 3.22             | 3.70  | 4.51             | 5.85|
| KI     | 2.85             | 3.16  | 3.70             | 4.18  | 4.92             | 6.60|
| RbI    | 2.94             | 3.26  | 3.81             | 4.28  | 5.01             | 6.82|
| CsI    | 3.13             | 3.45  | 4.02             | 4.46  | 5.17             | 7.45|

### Water-Anion RDF

| Salt   | \( r_{\text{max}1} \) | \( r_{R} \) | \( r_{\text{min}1} \) | \( r_{P} \) | \( r_{\text{max}2} \) | \( N \) |
|--------|------------------|-------|------------------|-------|------------------|-----|
| NaF    | 2.68             | 2.91  | 3.33             | 3.77  | 4.49             | 6.21|
| KF     | 2.68             | 2.93  | 3.35             | 3.74  | 4.48             | 6.28|
| RbF    | 2.68             | 2.93  | 3.35             | 3.75  | 4.49             | 6.27|
| CsF    | 2.68             | 2.94  | 3.35             | 3.74  | 4.49             | 6.27|
| LiCl   | 3.22             | 3.48  | 3.92             | 4.26  | 4.89             | 7.31|
| NaCl   | 3.22             | 3.48  | 3.90             | 4.26  | 4.89             | 7.23|
| KCl    | 3.22             | 3.47  | 3.88             | 4.21  | 4.86             | 6.75|
| RbCl   | 3.22             | 3.47  | 3.88             | 4.22  | 4.86             | 6.71|
| CsCl   | 3.22             | 3.48  | 3.88             | 4.22  | 4.87             | 6.63|
| LiI    | 3.61             | 3.86  | 4.27             | 4.56  | 5.15             | 7.76|
| NaI    | 3.61             | 3.86  | 4.28             | 4.58  | 5.14             | 7.89|
| KI     | 3.61             | 3.84  | 4.25             | 4.54  | 5.06             | 7.20|
| RbI    | 3.61             | 3.84  | 4.24             | 4.53  | 5.06             | 6.97|
| CsI    | 3.61             | 3.84  | 4.24             | 4.53  | 5.08             | 6.74|
(Table S3 continued)
F) SPC/E + Smith-Dang-Garret ions

| Salt  | $r_{\text{max}1}$ | $r_R$ | $r_{\text{min}1}$ | $r_P$ | $r_{\text{max}2}$ | $N$  |
|-------|------------------|------|------------------|------|----------------|-----|
|       | Cation-Anion RDF |      |                  |      |                |     |
| NaF   | 2.32             | 2.60 | 3.04             | 3.47 | 4.22           | 0.21|
| KF    | 2.80             | 3.08 | 3.49             | 3.93 | 4.54           | 0.15|
| RbF   | 2.91             | 3.18 | 3.59             | 4.05 | 4.62           | 0.15|
| CsF   | 2.64             | 2.69 | 3.76             | 4.21 | 4.76           | 0.14|
| LiCl  | 2.44             | 2.96 | 3.09             | 3.16 | 4.68           | 0.02|
| NaCl  | 2.82             | 3.18 | 3.65             | 4.13 | 5.04           | 0.08|
| KCl   | 3.24             | 3.61 | 4.20             | 4.64 | 5.39           | 0.39|
| RbCl  | 3.33             | 3.72 | 4.34             | 4.75 | 5.47           | 0.47|
| CsCl  | 3.50             | 3.90 | 4.59             | 4.98 | 5.62           | 0.53|
| LiI   | 2.83             | 3.23 | 3.34             | 3.44 | 5.07           | 0.00|
| NaI   | 3.23             | 3.56 | 4.04             | 4.64 | 5.47           | 0.04|
| KI    | 3.58             | 4.00 | 4.67             | 5.14 | 5.91           | 0.50|
| RbI   | 3.67             | 4.10 | 4.83             | 5.29 | 6.05           | 0.60|
| CsI   | 3.83             | 4.29 | 5.11             | 5.63 | 6.32           | 0.80|
|       | Water-Cation RDF |      |                  |      |                |     |
| NaF   | 2.38             | 2.66 | 3.16             | 3.67 | 4.49           | 5.58|
| KF    | 2.83             | 3.14 | 3.70             | 4.18 | 4.92           | 7.51|
| RbF   | 2.93             | 3.24 | 3.83             | 4.31 | 5.02           | 8.11|
| CsF   | 3.12             | 3.44 | 4.11             | 4.55 | 5.21           | 9.58|
| LiCl  | 1.97             | 2.20 | 2.74             | 3.35 | 4.22           | 4.11|
| NaCl  | 2.38             | 2.68 | 3.19             | 3.67 | 4.50           | 5.70|
| KCl   | 2.83             | 3.13 | 3.68             | 4.16 | 4.89           | 6.90|
| RbCl  | 2.93             | 3.24 | 3.81             | 4.29 | 4.97           | 7.36|
| CsCl  | 3.12             | 3.44 | 4.06             | 4.48 | 5.12           | 8.52|
| LiI   | 1.97             | 2.19 | 2.73             | 3.37 | 4.22           | 4.11|
| NaI   | 2.37             | 2.68 | 3.19             | 3.68 | 4.51           | 5.74|
| KI    | 2.83             | 3.13 | 3.69             | 4.18 | 4.92           | 6.68|
| RbI   | 2.93             | 3.24 | 3.81             | 4.29 | 5.01           | 7.03|
| CsI   | 3.12             | 3.44 | 4.05             | 4.50 | 5.17           | 7.84|
|       | Water-Anion RDF  |      |                  |      |                |     |
| NaF   | 2.69             | 2.93 | 3.37             | 3.89 | 4.57           | 6.40|
| KF    | 2.69             | 2.95 | 3.39             | 3.83 | 4.57           | 6.43|
| RbF   | 2.69             | 2.95 | 3.39             | 3.84 | 4.57           | 6.43|
| CsF   | 2.69             | 2.95 | 3.39             | 3.84 | 4.57           | 6.42|
| LiCl  | 3.23             | 3.51 | 3.95             | 4.33 | 5.02           | 7.45|
| NaCl  | 3.23             | 3.50 | 3.95             | 4.34 | 5.02           | 7.50|
| KCl   | 3.23             | 3.49 | 3.92             | 4.31 | 4.99           | 7.01|
| RbCl  | 3.23             | 3.49 | 3.92             | 4.29 | 4.99           | 6.91|
| CsCl  | 3.23             | 3.49 | 3.92             | 4.30 | 4.99           | 6.83|
| LiI   | 3.62             | 3.89 | 4.32             | 4.66 | 5.29           | 8.03|
| NaI   | 3.62             | 3.89 | 4.33             | 4.67 | 5.29           | 8.17|
| KI    | 3.62             | 3.87 | 4.30             | 4.63 | 5.22           | 7.56|
| RbI   | 3.62             | 3.87 | 4.29             | 4.62 | 5.22           | 7.37|
| CsI   | 3.61             | 3.87 | 4.28             | 4.61 | 5.23           | 7.04|
Table S4: Cluster populations from various ion and water models.
N indicates the number of cations and anions in the clusters. Sub-indices ‘+’
denotes cation and ‘-’ denotes anion. Cluster populations are expressed in terms
of molar fraction ($X$), molality ($m$) and molarity ($M$). Next to each population
shows the standard deviation. The data follow on the next few pages.

A) TIP3P + TIP3P-compatible ions

| $N_+$ | $N_-$ | $X$       | $M$       | $m$       |
|-------|-------|-----------|-----------|-----------|
| LiCl  |       |           |           |           |
| 0 1   |       | 4.153E-01 | 2.798E-02 | 6.721E-01 | 4.529E-02 | 6.947E-01 | 4.681E-02 |
| 1 0   | 4.211E-01 | 2.331E-02 | 6.814E-01 | 3.773E-02 | 7.043E-01 | 3.899E-02 |
| 1 1   | 1.396E-01 | 4.713E-02 | 2.259E-01 | 7.627E-02 | 2.336E-01 | 7.883E-02 |
| 1 2   | 1.170E-02 | 1.628E-02 | 1.893E-02 | 2.634E-02 | 1.957E-02 | 2.722E-02 |
| 2 1   | 6.584E-03 | 1.101E-02 | 1.066E-02 | 1.781E-02 | 1.101E-02 | 1.841E-02 |
| 2 2   | 4.389E-03 | 9.996E-03 | 7.102E-03 | 1.618E-02 | 7.342E-03 | 1.672E-02 |
| 3 1   | 4.364E-05 | 1.011E-03 | 7.062E-05 | 1.637E-03 | 7.299E-05 | 1.692E-03 |
| 2 3   | 9.908E-04 | 4.649E-03 | 1.603E-03 | 7.524E-03 | 1.657E-03 | 7.777E-03 |
| 3 2   | 2.708E-04 | 2.440E-03 | 4.383E-04 | 3.948E-03 | 4.530E-04 | 4.081E-03 |
| 3 3   | 1.693E-05 | 6.142E-04 | 2.740E-05 | 9.940E-04 | 2.832E-05 | 1.027E-03 |
| LiBr  |       |           |           |           |
| 0 1   | 4.795E-01 | 1.360E-02 | 8.815E-01 | 2.502E-02 | 9.196E-01 | 2.608E-02 |
| 1 0   | 4.809E-01 | 1.337E-02 | 8.841E-01 | 2.461E-02 | 9.223E-01 | 2.565E-02 |
| 1 1   | 3.744E-02 | 2.627E-02 | 6.883E-02 | 4.829E-02 | 7.181E-02 | 5.038E-02 |
| 1 2   | 1.763E-03 | 5.633E-03 | 3.242E-03 | 1.036E-02 | 3.382E-03 | 1.080E-02 |
| 2 1   | 3.533E-04 | 2.634E-03 | 6.495E-04 | 4.843E-03 | 6.776E-04 | 5.053E-03 |
| 2 2   | 6.727E-05 | 1.166E-03 | 1.237E-04 | 2.143E-03 | 1.290E-04 | 2.236E-03 |
| LiI   |       |           |           |           |
| 0 1   | 4.981E-01 | 4.270E-03 | 9.344E-01 | 8.104E-03 | 9.916E-01 | 8.501E-03 |
| 1 0   | 4.981E-01 | 4.272E-03 | 9.344E-01 | 8.106E-03 | 9.916E-01 | 8.503E-03 |
| 1 1   | 3.799E-03 | 8.540E-03 | 7.126E-03 | 1.602E-02 | 7.562E-03 | 1.700E-02 |
| 2 1   | 7.692E-07 | 1.216E-04 | 1.443E-06 | 2.282E-04 | 1.531E-06 | 2.421E-04 |
Table S4 continued.

A) TIP3P + TIP3P-compatible ions

|     | NaF     |          |          |          |          |          |
|-----|---------|----------|----------|----------|----------|----------|
| 0   | 1       | 4.641E-01| 1.990E-02| 8.565E-01| 3.674E-02| 8.562E-01| 3.670E-02|
| 1   | 0       | 4.672E-01| 1.866E-02| 8.622E-01| 3.446E-02| 8.620E-01| 3.443E-02|
| 1   | 1       | 5.734E-02| 3.261E-02| 1.058E-01| 6.018E-02| 1.056E-01| 6.016E-02|
| 1   | 2       | 5.656E-03| 1.110E-02| 1.044E-02| 2.048E-02| 1.043E-02| 2.047E-02|
| 2   | 1       | 3.377E-03| 8.320E-03| 6.233E-03| 1.535E-02| 6.231E-03| 1.535E-02|
| 1   | 3       | 3.117E-04| 2.543E-03| 5.752E-04| 4.692E-03| 5.750E-04| 4.691E-03|
| 2   | 2       | 1.311E-03| 5.180E-03| 2.420E-03| 9.559E-03| 2.419E-03| 9.556E-03|
| 3   | 1       | 7.079E-05| 1.212E-03| 1.306E-04| 2.237E-03| 1.306E-04| 2.237E-03|

|     | NaCl    |          |          |          |          |          |
|-----|---------|----------|----------|----------|----------|----------|
| 0   | 1       | 4.733E-01| 1.634E-02| 8.690E-01| 3.003E-02| 8.933E-01| 3.084E-02|
| 1   | 0       | 4.732E-01| 1.686E-02| 8.688E-01| 3.097E-02| 8.931E-01| 3.181E-02|
| 1   | 1       | 4.871E-02| 3.026E-02| 8.942E-02| 5.555E-02| 9.192E-02| 5.711E-02|
| 1   | 2       | 2.060E-03| 6.310E-03| 3.781E-03| 1.158E-02| 3.887E-03| 1.191E-02|
| 2   | 1       | 2.068E-03| 6.388E-03| 3.796E-03| 1.173E-02| 3.902E-03| 1.205E-02|
| 1   | 3       | 1.766E-05| 6.093E-04| 3.243E-05| 1.119E-03| 3.334E-05| 1.150E-03|
| 2   | 2       | 4.585E-04| 3.039E-03| 8.418E-04| 5.579E-03| 8.654E-04| 5.735E-03|
| 3   | 1       | 4.442E-05| 9.685E-04| 8.155E-05| 1.778E-03| 8.383E-05| 1.828E-03|

|     | NaBr    |          |          |          |          |          |
|-----|---------|----------|----------|----------|----------|----------|
| 0   | 1       | 4.791E-01| 1.444E-02| 8.819E-01| 2.661E-02| 9.158E-01| 2.761E-02|
| 1   | 0       | 4.786E-01| 1.459E-02| 8.811E-01| 2.688E-02| 9.150E-01| 2.789E-02|
| 1   | 1       | 3.952E-02| 2.716E-02| 7.275E-02| 4.999E-02| 7.555E-02| 5.192E-02|
| 1   | 2       | 1.066E-03| 4.617E-03| 1.963E-03| 8.499E-03| 2.038E-03| 8.826E-03|
| 2   | 1       | 1.416E-03| 5.252E-03| 2.607E-03| 9.668E-03| 2.708E-03| 1.004E-02|
| 1   | 3       | 5.291E-06| 3.282E-04| 9.740E-06| 6.041E-04| 1.011E-05| 6.273E-04|
| 2   | 2       | 2.117E-04| 2.070E-03| 3.897E-04| 3.811E-03| 4.047E-04| 3.957E-03|
| 3   | 1       | 4.251E-05| 9.316E-04| 7.825E-05| 1.715E-03| 8.126E-05| 1.781E-03|

|     | NaI     |          |          |          |          |          |
|-----|---------|----------|----------|----------|----------|----------|
| 0   | 1       | 4.884E-01| 1.040E-02| 9.022E-01| 1.923E-02| 9.530E-01| 2.028E-02|
| 1   | 0       | 4.883E-01| 1.055E-02| 9.020E-01| 1.952E-02| 9.527E-01| 2.059E-02|
| 1   | 1       | 2.250E-02| 2.020E-02| 4.156E-02| 3.731E-02| 4.390E-02| 3.941E-02|
| 2   | 1       | 4.424E-04| 2.959E-03| 8.172E-04| 5.467E-03| 8.632E-04| 5.774E-03|
| 1   | 3       | 1.043E-05| 4.571E-04| 1.926E-05| 8.443E-04| 2.034E-05| 8.919E-04|
| 2   | 2       | 4.530E-05| 9.477E-04| 8.367E-05| 1.751E-03| 8.838E-05| 1.849E-03|
| 3   | 1       | 3.961E-06| 2.801E-04| 7.316E-06| 5.173E-04| 7.728E-06| 5.464E-04|
Table S4 continued

A) TIP3P + TIP3P-compatible ions

|      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|
| KF   |      |      |      |      |      |      |      |
| 0 1  | 4.569E-01 | 2.116E-02 | 8.283E-01 | 3.838E-02 | 8.353E-01 | 3.868E-02 |
| 1 0  | 4.599E-01 | 1.973E-02 | 8.337E-01 | 3.580E-02 | 8.407E-01 | 3.608E-02 |
| 1 1  | 7.453E-02 | 3.698E-02 | 1.351E-01 | 6.705E-02 | 1.363E-01 | 6.761E-02 |
| 1 2  | 5.197E-03 | 1.024E-02 | 9.422E-03 | 1.857E-02 | 9.501E-03 | 1.873E-02 |
| 2 1  | 2.519E-03 | 7.198E-03 | 4.567E-03 | 1.305E-02 | 4.605E-03 | 1.316E-02 |
| 1 3  | 1.373E-04 | 1.705E-03 | 2.490E-04 | 3.091E-03 | 2.511E-04 | 3.117E-03 |
| 2 2  | 7.571E-04 | 4.007E-03 | 1.373E-03 | 7.265E-03 | 1.384E-03 | 7.326E-03 |
| 3 1  | 9.176E-06 | 4.376E-04 | 1.664E-05 | 7.934E-04 | 1.678E-05 | 8.000E-04 |
| KCl  |      |      |      |      |      |      |      |
| 0 1  | 4.423E-01 | 2.415E-02 | 7.447E-01 | 4.067E-02 | 7.728E-01 | 4.219E-02 |
| 1 0  | 4.411E-01 | 2.407E-02 | 7.426E-01 | 4.053E-02 | 7.706E-01 | 4.205E-02 |
| 1 1  | 9.543E-02 | 4.151E-02 | 1.607E-01 | 6.989E-02 | 1.667E-01 | 7.252E-02 |
| 1 2  | 7.771E-03 | 1.293E-02 | 1.308E-02 | 2.177E-02 | 1.358E-02 | 2.259E-02 |
| 2 1  | 8.793E-03 | 1.349E-02 | 1.480E-02 | 2.272E-02 | 1.536E-02 | 2.357E-02 |
| 1 3  | 2.525E-04 | 2.366E-03 | 4.252E-04 | 3.983E-04 | 4.142E-04 | 4.133E-03 |
| 2 2  | 2.973E-03 | 8.112E-03 | 5.005E-03 | 1.366E-02 | 5.194E-03 | 1.417E-02 |
| 3 1  | 3.476E-04 | 2.756E-03 | 5.853E-04 | 4.640E-04 | 6.074E-04 | 4.814E-03 |
| KBr  |      |      |      |      |      |      |      |
| 0 1  | 4.402E-01 | 2.509E-02 | 7.300E-01 | 4.162E-02 | 7.652E-01 | 4.362E-02 |
| 1 0  | 4.381E-01 | 2.565E-02 | 7.266E-01 | 4.255E-02 | 7.616E-01 | 4.459E-02 |
| 1 1  | 1.001E-01 | 4.351E-02 | 1.660E-01 | 7.216E-02 | 1.740E-01 | 7.564E-02 |
| 1 2  | 7.630E-03 | 1.274E-02 | 1.265E-02 | 2.113E-02 | 1.326E-02 | 2.215E-02 |
| 2 1  | 9.117E-03 | 1.398E-02 | 1.512E-02 | 2.319E-02 | 1.585E-02 | 2.431E-02 |
| 1 3  | 2.036E-04 | 2.130E-03 | 3.377E-04 | 3.533E-04 | 3.540E-04 | 3.703E-03 |
| 2 2  | 3.130E-03 | 8.337E-03 | 5.190E-03 | 1.383E-02 | 5.440E-03 | 1.449E-02 |
| 3 1  | 4.265E-04 | 3.056E-03 | 7.073E-04 | 5.069E-03 | 7.413E-04 | 5.313E-03 |
| KI   |      |      |      |      |      |      |      |
| 0 1  | 4.460E-01 | 2.348E-02 | 7.399E-01 | 3.896E-02 | 7.886E-01 | 4.151E-02 |
| 1 0  | 4.447E-01 | 2.412E-02 | 7.378E-01 | 4.003E-02 | 7.863E-01 | 4.265E-02 |
| 1 1  | 9.223E-02 | 4.140E-02 | 1.530E-01 | 6.867E-02 | 1.631E-01 | 7.319E-02 |
| 1 2  | 6.384E-03 | 1.160E-02 | 1.059E-02 | 1.924E-02 | 1.129E-02 | 2.050E-02 |
| 2 1  | 7.385E-03 | 1.251E-02 | 1.225E-02 | 2.075E-02 | 1.306E-02 | 2.211E-02 |
| 1 3  | 1.888E-04 | 2.053E-03 | 3.132E-04 | 3.406E-03 | 3.338E-04 | 3.630E-03 |
| 2 2  | 2.220E-03 | 6.896E-03 | 3.682E-03 | 1.144E-02 | 3.924E-03 | 1.219E-02 |
| 3 1  | 2.683E-04 | 2.457E-03 | 4.451E-04 | 4.076E-03 | 4.744E-04 | 4.344E-03 |
Table S4 continued

A) TIP3P + TIP3P-compatible ions

|   | RbF | RbCl | RbBr | Rbl |
|---|-----|------|------|-----|
| 0 | 1   | 4.608E-01 | 1.966E-02 | 8.397E-01 | 3.585E-02 | 8.497E-01 | 3.626E-02 |
| 1 | 0   | 4.625E-01 | 1.898E-02 | 8.429E-01 | 3.461E-02 | 8.529E-01 | 3.500E-02 |
| 1 | 1   | 7.053E-02 | 3.586E-02 | 1.285E-01 | 6.535E-02 | 1.301E-01 | 6.613E-02 |
| 1 | 2   | 3.612E-03 | 8.628E-03 | 6.583E-03 | 1.572E-02 | 6.616E-03 | 1.591E-02 |
| 2 | 1   | 1.956E-03 | 6.406E-03 | 3.565E-03 | 1.168E-02 | 3.607E-03 | 1.181E-02 |
| 1 | 3   | 4.991E-05 | 1.027E-03 | 9.096E-05 | 1.871E-03 | 9.204E-05 | 1.894E-03 |
| 2 | 2   | 4.993E-04 | 3.241E-03 | 9.099E-04 | 5.906E-03 | 9.207E-04 | 5.976E-03 |
| 3 | 1   | 6.422E-06 | 3.711E-04 | 1.170E-05 | 6.763E-04 | 1.184E-05 | 6.843E-04 |
|   | RbCl |      |      |      |      |      |      |
| 0 | 1   | 4.365E-01 | 2.556E-02 | 7.255E-01 | 4.250E-02 | 7.555E-01 | 4.424E-02 |
| 1 | 0   | 4.362E-01 | 2.572E-02 | 7.250E-01 | 4.276E-02 | 7.549E-01 | 4.451E-02 |
| 1 | 1   | 1.057E-01 | 4.444E-02 | 1.756E-01 | 7.386E-02 | 1.829E-01 | 7.691E-02 |
| 1 | 2   | 8.333E-03 | 1.349E-02 | 1.385E-02 | 2.242E-02 | 1.442E-02 | 2.334E-02 |
| 2 | 1   | 8.626E-03 | 1.342E-02 | 1.434E-02 | 2.230E-02 | 1.493E-02 | 2.322E-02 |
| 1 | 3   | 2.315E-04 | 2.280E-03 | 3.848E-04 | 3.790E-03 | 4.007E-04 | 3.947E-03 |
| 2 | 2   | 3.087E-03 | 8.193E-03 | 5.131E-03 | 1.362E-02 | 5.342E-03 | 1.418E-02 |
| 3 | 1   | 2.865E-04 | 2.526E-03 | 4.761E-04 | 4.198E-03 | 4.958E-04 | 4.371E-03 |
|   | RbBr |      |      |      |      |      |      |
| 0 | 1   | 4.339E-01 | 2.615E-02 | 7.080E-01 | 4.268E-02 | 7.447E-01 | 4.488E-02 |
| 1 | 0   | 4.324E-01 | 2.653E-02 | 7.056E-01 | 4.329E-02 | 7.421E-01 | 4.553E-02 |
| 1 | 1   | 1.098E-01 | 4.539E-02 | 1.791E-01 | 7.407E-02 | 1.884E-01 | 7.790E-02 |
| 1 | 2   | 8.747E-03 | 1.357E-02 | 1.427E-02 | 2.214E-02 | 1.501E-02 | 2.329E-02 |
| 2 | 1   | 9.892E-03 | 1.444E-02 | 1.614E-02 | 2.356E-02 | 1.698E-02 | 2.478E-02 |
| 1 | 3   | 2.210E-04 | 2.216E-03 | 3.606E-04 | 3.615E-03 | 3.793E-04 | 3.802E-03 |
| 2 | 2   | 3.431E-03 | 8.689E-03 | 5.599E-03 | 1.418E-02 | 5.889E-03 | 1.491E-02 |
| 3 | 1   | 3.831E-04 | 2.914E-03 | 6.251E-04 | 4.755E-03 | 6.575E-04 | 5.002E-03 |
|   | Rbl  |      |      |      |      |      |      |
| 0 | 1   | 4.354E-01 | 2.577E-02 | 7.009E-01 | 4.149E-02 | 7.496E-01 | 4.436E-02 |
| 1 | 0   | 4.340E-01 | 2.617E-02 | 6.985E-01 | 4.214E-02 | 7.471E-01 | 4.505E-02 |
| 1 | 1   | 1.073E-01 | 4.456E-02 | 1.727E-01 | 7.173E-02 | 1.847E-01 | 7.671E-02 |
| 1 | 2   | 8.512E-03 | 1.369E-02 | 1.370E-02 | 2.204E-02 | 1.465E-02 | 2.357E-02 |
| 2 | 1   | 9.535E-03 | 1.416E-02 | 1.535E-02 | 2.280E-02 | 1.641E-02 | 2.438E-02 |
| 1 | 3   | 2.612E-04 | 2.414E-03 | 4.204E-04 | 3.886E-03 | 4.496E-04 | 4.156E-03 |
| 2 | 2   | 3.364E-03 | 8.699E-03 | 5.415E-03 | 1.400E-02 | 5.791E-03 | 1.497E-02 |
| 3 | 1   | 3.522E-04 | 2.833E-03 | 5.670E-04 | 4.559E-03 | 6.063E-04 | 4.876E-03 |
Table S4 continued

A) TIP3P + TIP3P-compatible ions

|        | CsF       | CsCl       | CsBr       | CsI       |
|--------|-----------|------------|------------|-----------|
|        | 0 1       | 4.596E-01  | 2.013E-02  | 8.313E-01 | 3.644E-02 | 8.460E-01 | 3.706E-02 |
|        | 1 0       | 4.616E-01  | 1.926E-02  | 8.349E-01 | 3.486E-02 | 8.496E-01 | 3.545E-02 |
|        | 1 1       | 7.267E-02  | 3.669E-02  | 1.314E-01 | 6.637E-02 | 1.338E-01 | 6.753E-02 |
|        | 1 2       | 3.698E-03  | 8.698E-03  | 6.689E-03 | 1.573E-02 | 6.806E-03 | 1.601E-02 |
|        | 2 1       | 1.839E-03  | 6.157E-03  | 3.326E-03 | 1.114E-02 | 3.384E-03 | 1.133E-02 |
|        | 1 3       | 4.892E-05  | 1.015E-03  | 8.849E-05 | 1.837E-03 | 9.005E-05 | 1.869E-03 |
|        | 2 2       | 4.945E-04  | 3.220E-03  | 8.945E-04 | 5.825E-03 | 9.102E-04 | 5.927E-03 |
|        | 3 1       | 4.694E-06  | 3.166E-04  | 8.491E-06 | 5.727E-04 | 8.641E-06 | 5.828E-04 |
|        | CsCl      | 0 1       | 4.250E-01  | 2.791E-02  | 6.847E-01 | 4.498E-02 | 7.171E-01 | 4.710E-02 |
|        | 1 0       | 4.267E-01  | 2.727E-02  | 6.874E-01 | 4.394E-02 | 7.199E-01 | 4.601E-02 |
|        | 1 1       | 1.207E-01  | 4.736E-02  | 1.945E-01 | 7.629E-02 | 2.037E-01 | 7.990E-02 |
|        | 1 2       | 1.129E-02  | 1.556E-02  | 1.819E-02 | 2.506E-02 | 1.905E-02 | 2.625E-02 |
|        | 2 1       | 9.887E-03  | 1.455E-02  | 1.593E-02 | 2.344E-02 | 1.668E-02 | 2.455E-02 |
|        | 1 3       | 4.148E-04  | 3.100E-03  | 6.683E-04 | 4.994E-03 | 6.999E-04 | 5.230E-03 |
|        | 2 2       | 4.198E-03  | 9.761E-03  | 6.763E-03 | 1.573E-02 | 7.083E-03 | 1.647E-02 |
|        | 3 1       | 2.923E-04  | 2.599E-03  | 4.709E-04 | 4.187E-03 | 4.932E-04 | 4.385E-03 |
|        | CsBr      | 0 1       | 4.186E-01  | 2.956E-02  | 6.546E-01 | 4.623E-02 | 6.925E-01 | 4.890E-02 |
|        | 1 0       | 4.190E-01  | 2.937E-02  | 6.551E-01 | 4.593E-02 | 6.930E-01 | 4.858E-02 |
|        | 1 1       | 4.289E-01  | 4.926E-02  | 2.016E-01 | 7.702E-02 | 2.133E-01 | 8.148E-02 |
|        | 1 2       | 1.244E-02  | 1.668E-02  | 1.945E-02 | 2.609E-02 | 2.058E-02 | 2.760E-02 |
|        | 2 1       | 1.228E-02  | 1.641E-02  | 1.921E-02 | 2.565E-02 | 2.032E-02 | 2.714E-02 |
|        | 1 3       | 4.684E-04  | 3.313E-03  | 7.325E-04 | 5.181E-03 | 7.749E-04 | 5.481E-03 |
|        | 2 2       | 5.470E-03  | 1.126E-02  | 8.554E-03 | 1.761E-02 | 9.049E-03 | 1.863E-02 |
|        | 3 1       | 4.566E-04  | 3.268E-03  | 7.140E-04 | 5.111E-03 | 7.553E-04 | 5.406E-03 |
|        | CsI       | 0 1       | 4.150E-01  | 3.002E-02  | 6.303E-01 | 4.560E-02 | 6.780E-01 | 4.904E-02 |
|        | 1 0       | 4.145E-01  | 2.976E-02  | 6.296E-01 | 4.521E-02 | 6.773E-01 | 4.862E-02 |
|        | 1 1       | 1.325E-01  | 4.988E-02  | 2.012E-01 | 7.576E-02 | 2.164E-01 | 8.149E-02 |
|        | 1 2       | 1.371E-02  | 1.723E-02  | 2.082E-02 | 2.617E-02 | 2.239E-02 | 2.815E-02 |
|        | 2 1       | 1.380E-02  | 1.751E-02  | 2.097E-02 | 2.660E-02 | 2.255E-02 | 2.861E-02 |
|        | 1 3       | 6.267E-04  | 3.817E-03  | 9.518E-04 | 5.798E-03 | 1.024E-03 | 6.236E-03 |
|        | 2 2       | 6.243E-03  | 1.202E-02  | 9.482E-03 | 1.826E-02 | 1.020E-02 | 1.964E-02 |
|        | 3 1       | 6.611E-04  | 3.926E-03  | 1.004E-03 | 5.963E-03 | 1.080E-03 | 6.414E-03 |
Table S4 continued

B) TIP4P\textsubscript{EW} + TIP4P\textsubscript{EW}-compatible ions

| $N_+$ | $N_-$ | $X$  | $M$       | $m$       |
|-------|-------|------|-----------|-----------|
| LiCl  |       |      |           |           |
| 0     | 1     | 4.938E-01| 1.069E-02| 9.493E-01| 2.062E-02| 9.749E-01| 2.111E-02|
| 1     | 0     | 4.938E-01| 1.069E-02| 9.493E-01| 2.062E-02| 9.749E-01| 2.111E-02|
| 1     | 1     | 1.230E-02| 2.139E-02| 2.364E-02| 4.111E-02| 2.428E-02| 4.222E-02|
| LiBr  |       |      |           |           |
| 0     | 1     | 4.963E-01| 7.128E-03| 9.493E-01| 1.373E-02| 9.846E-01| 1.414E-02|
| 1     | 0     | 4.963E-01| 7.128E-03| 9.493E-01| 1.373E-02| 9.846E-01| 1.414E-02|
| 1     | 1     | 7.350E-03| 1.426E-02| 1.406E-02| 2.727E-02| 1.458E-02| 2.828E-02|
| LiI   |       |      |           |           |
| 0     | 1     | 4.991E-01| 3.031E-03| 9.444E-01| 5.956E-03| 9.957E-01| 6.045E-03|
| 1     | 0     | 4.991E-01| 3.031E-03| 9.444E-01| 5.956E-03| 9.957E-01| 6.045E-03|
| 1     | 1     | 1.744E-03| 6.061E-03| 3.301E-03| 1.147E-02| 3.480E-03| 1.209E-02|
| NaF   |       |      |           |           |
| 0     | 1     | 4.970E-01| 5.449E-03| 9.992E-01| 1.111E-02| 9.871E-01| 1.082E-02|
| 1     | 0     | 4.970E-01| 5.454E-03| 9.992E-01| 1.112E-02| 9.871E-01| 1.083E-02|
| 1     | 1     | 5.600E-05| 1.038E-03| 1.126E-04| 2.087E-03| 1.112E-04| 2.062E-03|
| 2     | 1     | 1.381E-02| 1.506E-02| 2.673E-02| 2.916E-02| 2.719E-02| 2.966E-02|
| 2     | 2     | 1.654E-04| 1.787E-03| 3.202E-04| 3.458E-03| 3.258E-04| 3.519E-03|
| NaCl  |       |      |           |           |
| 0     | 1     | 4.929E-01| 7.722E-03| 9.542E-01| 1.504E-02| 9.708E-01| 1.521E-02|
| 1     | 0     | 4.929E-01| 7.799E-03| 9.541E-01| 1.519E-02| 9.707E-01| 1.536E-02|
| 1     | 1     | 1.301E-02| 1.506E-02| 2.673E-02| 2.916E-02| 2.719E-02| 2.966E-02|
| 2     | 1     | 6.554E-05| 1.122E-03| 1.318E-04| 2.256E-03| 1.302E-04| 2.229E-03|
| NaBr  |       |      |           |           |
| 0     | 1     | 4.924E-01| 8.394E-03| 9.428E-01| 1.615E-02| 9.688E-01| 1.651E-02|
| 1     | 0     | 4.923E-01| 8.644E-03| 9.425E-01| 1.662E-02| 9.685E-01| 1.700E-02|
| 1     | 1     | 1.493E-02| 1.665E-02| 2.858E-02| 3.187E-02| 2.937E-02| 3.275E-02|
| 2     | 1     | 2.021E-04| 1.982E-03| 3.870E-04| 3.794E-03| 3.977E-04| 3.898E-03|
| 2     | 2     | 1.051E-04| 1.440E-03| 2.012E-04| 2.757E-03| 2.068E-04| 2.833E-03|
| NaI   |       |      |           |           |
| 0     | 1     | 4.933E-01| 7.981E-03| 9.310E-01| 1.514E-02| 9.723E-01| 1.573E-02|
| 1     | 0     | 4.932E-01| 8.110E-03| 9.307E-01| 1.538E-02| 9.720E-01| 1.598E-02|
| 1     | 1     | 1.312E-02| 1.571E-02| 2.476E-02| 2.964E-02| 2.586E-02| 3.095E-02|
| 2     | 1     | 1.224E-04| 1.563E-03| 2.310E-04| 2.951E-03| 2.412E-04| 3.081E-03|
| 2     | 2     | 2.772E-04| 2.302E-03| 5.231E-04| 4.345E-03| 5.463E-04| 4.537E-03|
### B) TIP4P<sub>EW</sub> + TIP4P<sub>EW</sub>-compatible ions

|       | KF      | KCl      | KBr      | KI      |
|-------|---------|----------|----------|---------|
| 0 1   | 4.825E-01 | 1.330E-02 | 9.313E-01 | 2.573E-02 |
| 1 0   | 4.830E-01 | 1.311E-02 | 9.322E-01 | 2.536E-02 |
| 1 1   | 3.311E-02 | 2.562E-02 | 6.390E-02 | 4.945E-02 |
| 1 2   | 9.269E-04 | 4.190E-03 | 1.789E-03 | 8.088E-03 |
| 2 1   | 4.598E-04 | 3.026E-02 | 8.876E-04 | 5.840E-03 |
| 1 3   | 4.000E-06 | 2.828E-04 | 3.860E-06 | 3.857E-04 |
| 3 1   | 2.000E-06 | 2.000E-04 | 3.860E-06 | 3.857E-04 |
|       | 4.830E-01 | 1.311E-02 | 9.322E-01 | 2.536E-02 |
| 1 0   | 4.830E-01 | 1.311E-02 | 9.322E-01 | 2.536E-02 |
| 1 1   | 3.311E-02 | 2.562E-02 | 6.390E-02 | 4.945E-02 |
| 1 2   | 9.269E-04 | 4.190E-03 | 1.789E-03 | 8.088E-03 |
| 2 1   | 4.598E-04 | 3.026E-02 | 8.876E-04 | 5.840E-03 |
| 1 3   | 4.000E-06 | 2.828E-04 | 3.860E-06 | 3.857E-04 |
| 3 1   | 2.000E-06 | 2.000E-04 | 3.860E-06 | 3.857E-04 |
|       | 4.830E-01 | 1.311E-02 | 9.322E-01 | 2.536E-02 |
| 1 0   | 4.830E-01 | 1.311E-02 | 9.322E-01 | 2.536E-02 |
| 1 1   | 3.311E-02 | 2.562E-02 | 6.390E-02 | 4.945E-02 |
| 1 2   | 9.269E-04 | 4.190E-03 | 1.789E-03 | 8.088E-03 |
| 2 1   | 4.598E-04 | 3.026E-02 | 8.876E-04 | 5.840E-03 |
| 1 3   | 4.000E-06 | 2.828E-04 | 3.860E-06 | 3.857E-04 |
| 3 1   | 2.000E-06 | 2.000E-04 | 3.860E-06 | 3.857E-04 |
|       | 4.830E-01 | 1.311E-02 | 9.322E-01 | 2.536E-02 |
| 1 0   | 4.830E-01 | 1.311E-02 | 9.322E-01 | 2.536E-02 |
| 1 1   | 3.311E-02 | 2.562E-02 | 6.390E-02 | 4.945E-02 |
| 1 2   | 9.269E-04 | 4.190E-03 | 1.789E-03 | 8.088E-03 |
| 2 1   | 4.598E-04 | 3.026E-02 | 8.876E-04 | 5.840E-03 |
| 1 3   | 4.000E-06 | 2.828E-04 | 3.860E-06 | 3.857E-04 |
| 3 1   | 2.000E-06 | 2.000E-04 | 3.860E-06 | 3.857E-04 |
|       | 4.830E-01 | 1.311E-02 | 9.322E-01 | 2.536E-02 |
| 1 0   | 4.830E-01 | 1.311E-02 | 9.322E-01 | 2.536E-02 |
| 1 1   | 3.311E-02 | 2.562E-02 | 6.390E-02 | 4.945E-02 |
| 1 2   | 9.269E-04 | 4.190E-03 | 1.789E-03 | 8.088E-03 |
| 2 1   | 4.598E-04 | 3.026E-02 | 8.876E-04 | 5.840E-03 |
| 1 3   | 4.000E-06 | 2.828E-04 | 3.860E-06 | 3.857E-04 |
| 3 1   | 2.000E-06 | 2.000E-04 | 3.860E-06 | 3.857E-04 |
### Table S4 continued

#### B) TIP4P<sub>Ew</sub> + TIP4P<sub>Ew</sub>-compatible ions

|    | RbF   | RbCl   | RbBr   | Rbl   |
|----|-------|--------|--------|-------|
| 0 1| 4.809E-01 1.354E-02 9.221E-01 2.602E-02 | 4.815E-01 1.304E-02 9.233E-01 2.506E-02 | 4.892E-02 1.593E-02 9.292E-01 2.605E-02 | 3.554E-05 1.900E-04 5.763E-05 1.490E-03 |
| 1 0| 3.602E-02 2.551E-02 6.906E-02 4.892E-02 | 3.602E-02 2.551E-02 6.906E-02 4.892E-02 | 3.602E-02 2.551E-02 6.906E-02 4.892E-02 | 3.602E-02 2.551E-02 6.906E-02 4.892E-02 |
| 1 1| 1.034E-03 4.595E-03 1.982E-03 8.809E-03 | 1.034E-03 4.595E-03 1.982E-03 8.809E-03 | 1.034E-03 4.595E-03 1.982E-03 8.809E-03 | 1.034E-03 4.595E-03 1.982E-03 8.809E-03 |
| 1 2| 4.432E-04 2.966E-03 8.498E-04 5.687E-03 | 4.432E-04 2.966E-03 8.498E-04 5.687E-03 | 4.432E-04 2.966E-03 8.498E-04 5.687E-03 | 4.432E-04 2.966E-03 8.498E-04 5.687E-03 |
| 2 1| 6.970E-04 8.896E-05 1.854E-03 8.922E-05 | 6.970E-04 8.896E-05 1.854E-03 8.922E-05 | 6.970E-04 8.896E-05 1.854E-03 8.922E-05 | 6.970E-04 8.896E-05 1.854E-03 8.922E-05 |
| 2 2| 4.830E-01 1.304E-02 9.233E-01 2.506E-02 | 4.830E-01 1.304E-02 9.233E-01 2.506E-02 | 4.830E-01 1.304E-02 9.233E-01 2.506E-02 | 4.830E-01 1.304E-02 9.233E-01 2.506E-02 |
| 3 1| 1.057E-04 1.507E-03 1.849E-04 2.637E-04 | 1.057E-04 1.507E-03 1.849E-04 2.637E-04 | 1.057E-04 1.507E-03 1.849E-04 2.637E-04 | 1.057E-04 1.507E-03 1.849E-04 2.637E-04 |
| 3 2| 5.300E-05 1.081E-03 9.273E-05 1.561E-03 | 5.300E-05 1.081E-03 9.273E-05 1.561E-03 | 5.300E-05 1.081E-03 9.273E-05 1.561E-03 | 5.300E-05 1.081E-03 9.273E-05 1.561E-03 |
| 3 3| 1.057E-04 1.507E-03 1.849E-04 2.637E-04 | 1.057E-04 1.507E-03 1.849E-04 2.637E-04 | 1.057E-04 1.507E-03 1.849E-04 2.637E-04 | 1.057E-04 1.507E-03 1.849E-04 2.637E-04 |
| 3 4| 3.554E-05 1.900E-04 5.763E-05 1.490E-03 | 3.554E-05 1.900E-04 5.763E-05 1.490E-03 | 3.554E-05 1.900E-04 5.763E-05 1.490E-03 | 3.554E-05 1.900E-04 5.763E-05 1.490E-03 |
### Table S4 continued

#### B) TIP4P\textsubscript{EW} + TIP4P\textsubscript{EW}-compatible ions

|       | CsF         | CsCl         | CsBr         | Csl          |
|-------|-------------|--------------|--------------|--------------|
|       |             |              |              |              |
|       | 0 1 4.697E-01  1.721E-02  8.743E-01  3.207E-02  8.825E-01  3.234E-02 |
|       | 1 0 4.708E-01  1.667E-02  8.763E-01  3.108E-02  8.845E-01  3.133E-02 |
|       | 1 1 5.580E-02  3.215E-02  1.039E-01  5.984E-02  1.048E-01  6.040E-02 |
|       | 1 2 2.217E-03  6.637E-03  4.126E-03  1.235E-02  4.165E-03  1.247E-02 |
|       | 1 2 1.208E-03  4.955E-03  2.249E-03  9.222E-03  2.270E-03  9.309E-03 |
|       | 2 1 2.411E-04  2.323E-03  4.487E-04  4.323E-03  4.530E-04  4.364E-03 |
|       |             |              |              |              |
|       | 0 1 4.289E-01  2.744E-02  7.053E-01  4.513E-02  7.336E-01  4.692E-02 |
|       | 1 0 4.308E-01  2.711E-02  7.083E-01  4.459E-02  7.367E-01  4.636E-02 |
|       | 1 1 1.184E-01  4.754E-02  7.816E-02  2.026E-01  8.129E-02  |
|       | 1 2 9.302E-03  1.420E-02  1.529E-01  5.984E-02  1.048E-01  6.040E-02 |
|       | 2 1 1.208E-03  4.955E-03  2.249E-03  9.222E-03  2.270E-03  9.309E-03 |
|       | 1 3 2.388E-04  2.323E-03  4.126E-03  1.235E-02  4.165E-03  1.247E-02 |
|       | 2 2 2.411E-04  2.323E-03  4.487E-04  4.323E-03  4.530E-04  4.364E-03 |
|       |             |              |              |              |
|       | 0 1 4.086E-01  3.127E-02  6.305E-01  4.826E-02  6.623E-01  5.068E-02 |
|       | 1 0 4.100E-01  3.093E-02  6.327E-01  4.774E-02  6.646E-01  5.013E-02 |
|       | 1 1 1.437E-01  5.324E-02  2.217E-01  8.215E-02  2.329E-01  8.629E-02 |
|       | 1 2 1.462E-02  1.767E-02  2.256E-02  2.726E-02  2.370E-02  2.864E-02 |
|       | 2 1 1.333E-02  1.727E-02  2.056E-02  2.665E-02  2.160E-02  2.800E-02 |
|       | 1 3 3.938E-04  3.055E-03  6.077E-04  4.714E-03  6.383E-04  4.952E-03 |
|       | 2 2 6.105E-03  1.203E-02  9.420E-03  1.857E-02  9.895E-03  1.951E-02 |
|       | 3 1 3.170E-04  2.724E-03  4.892E-04  4.203E-03  5.139E-04  4.415E-03 |
|       | 2 3 1.057E-03  5.001E-03  1.631E-03  7.716E-03  1.714E-03  8.106E-03 |
|       | 3 2 1.104E-03  5.202E-03  1.703E-03  8.027E-03  1.789E-03  8.432E-03 |
|       | 3 3 4.444E-04  3.280E-03  6.857E-04  5.061E-03  7.203E-04  5.316E-03 |
|       |             |              |              |              |
|       | 0 1 4.017E-01  3.297E-02  5.949E-01  4.884E-02  6.349E-01  5.211E-02 |
|       | 1 0 4.005E-01  3.331E-02  5.932E-01  4.935E-02  6.331E-01  5.265E-02 |
|       | 1 1 1.502E-01  5.385E-02  2.225E-01  7.976E-02  2.374E-01  8.512E-02 |
|       | 1 2 1.669E-02  1.934E-02  2.471E-02  2.864E-02  2.638E-02  3.057E-02 |
|       | 2 1 1.749E-02  1.999E-02  2.590E-02  2.960E-02  2.764E-02  3.159E-02 |
|       | 1 3 7.303E-04  4.210E-03  1.082E-03  6.235E-03  1.154E-03  6.654E-03 |
|       | 2 2 8.199E-03  1.391E-02  1.214E-02  2.060E-02  1.296E-02  2.199E-02 |
|       | 3 1 6.588E-04  4.035E-03  9.756E-04  5.975E-03  1.041E-03  6.377E-03 |
|       | 2 3 1.021E-03  5.012E-03  1.512E-03  7.423E-03  1.613E-03  7.922E-03 |
|       | 3 2 1.360E-03  5.754E-03  2.014E-03  8.521E-03  2.150E-03  9.094E-03 |
|       | 3 3 8.710E-04  4.637E-03  1.290E-03  6.867E-03  1.377E-03  7.329E-03 |
### C) SPC/E + SPC/E-compatible ions

| $N$ | $N$ | $X$ | $M$ | $m$ |
|-----|-----|-----|-----|-----|
|     |     |     | LiCl |     |
| 0   | 1   | 4.991E-01 | 2.802E-03 | 9.741E-01 | 5.719E-03 | 9.955E-01 | 5.589E-03 |
| 1   | 0   | 4.991E-01 | 2.802E-03 | 9.741E-01 | 5.719E-03 | 9.955E-01 | 5.589E-03 |
| 1   | 1   | 1.840E-03 | 5.604E-03 | 3.591E-03 | 1.094E-02 | 3.670E-03 | 1.118E-02 |
|     |     |     | LiBr |     |
| 0   | 1   | 4.995E-01 | 2.119E-03 | 9.656E-01 | 4.416E-03 | 9.971E-01 | 4.230E-03 |
| 1   | 0   | 4.995E-01 | 2.119E-03 | 9.656E-01 | 4.416E-03 | 9.971E-01 | 4.230E-03 |
| 1   | 1   | 1.006E-03 | 4.238E-03 | 1.944E-03 | 8.194E-03 | 2.008E-03 | 8.461E-03 |
|     |     |     | LiF  |     |
| 0   | 1   | 4.946E-01 | 7.008E-03 | 9.910E-01 | 1.415E-02 | 9.778E-01 | 1.385E-02 |
| 1   | 0   | 4.947E-01 | 6.810E-03 | 9.912E-01 | 1.376E-02 | 9.779E-01 | 1.346E-02 |
| 1   | 1   | 1.054E-02 | 1.355E-02 | 2.111E-02 | 2.714E-02 | 2.083E-02 | 2.678E-02 |
| 1   | 2   | 1.232E-04 | 1.548E-03 | 2.469E-04 | 3.101E-03 | 2.436E-04 | 3.060E-03 |
| 2   | 1   | 3.480E-05 | 8.196E-04 | 6.974E-05 | 1.642E-03 | 6.880E-05 | 1.620E-03 |
|     |     |     | NaF  |     |
| 0   | 1   | 4.950E-01 | 6.843E-03 | 9.635E-01 | 1.340E-02 | 9.794E-01 | 1.354E-02 |
| 1   | 0   | 4.950E-01 | 6.935E-03 | 9.635E-01 | 1.358E-02 | 9.793E-01 | 1.372E-02 |
| 1   | 1   | 9.857E-03 | 1.362E-02 | 1.919E-02 | 2.652E-02 | 1.950E-02 | 2.695E-02 |
| 1   | 2   | 2.900E-05 | 7.482E-04 | 5.644E-05 | 1.456E-03 | 5.737E-05 | 1.480E-03 |
| 2   | 1   | 6.833E-05 | 1.153E-03 | 1.330E-04 | 2.244E-03 | 1.352E-04 | 2.281E-03 |
|     |     |     | NaCl |     |
| 0   | 1   | 4.942E-01 | 7.330E-03 | 9.502E-01 | 1.418E-02 | 9.759E-01 | 1.448E-02 |
| 1   | 0   | 4.941E-01 | 7.379E-03 | 9.501E-01 | 1.428E-02 | 9.757E-01 | 1.457E-02 |
| 1   | 1   | 1.141E-02 | 1.433E-02 | 2.193E-02 | 2.755E-02 | 2.252E-02 | 2.830E-02 |
| 1   | 2   | 1.073E-04 | 1.443E-03 | 2.062E-04 | 2.774E-03 | 2.118E-04 | 2.848E-03 |
| 2   | 1   | 1.710E-04 | 1.815E-03 | 3.287E-04 | 3.489E-03 | 3.376E-04 | 3.583E-03 |
|     |     |     | NaBr |     |
| 0   | 1   | 4.948E-01 | 6.969E-03 | 9.372E-01 | 1.328E-02 | 9.786E-01 | 1.378E-02 |
| 1   | 0   | 4.948E-01 | 6.993E-03 | 9.373E-01 | 1.332E-02 | 9.786E-01 | 1.383E-02 |
| 1   | 1   | 1.022E-02 | 1.384E-02 | 1.936E-02 | 2.621E-02 | 2.021E-02 | 2.736E-02 |
| 1   | 2   | 5.788E-05 | 1.055E-03 | 1.096E-04 | 1.999E-03 | 1.145E-04 | 2.087E-03 |
| 2   | 1   | 4.484E-05 | 9.340E-04 | 8.493E-05 | 1.769E-03 | 8.868E-05 | 1.847E-03 |
| 2   | 2   | 9.804E-06 | 4.383E-04 | 1.857E-05 | 8.302E-04 | 1.939E-05 | 8.669E-04 |
### Table S4 continued

#### C) SPC/E + SPC/E-compatible ions

|       | KF         | KCl         | KBr         | KI         |
|-------|------------|-------------|-------------|------------|
| 0 1   | 4.778E-01  | 1.447E-02   | 9.166E-01   | 2.780E-02  |
| 1 0   | 4.785E-01  | 1.418E-02   | 9.178E-01   | 2.725E-02  |
| 1 1   | 4.192E-02  | 2.763E-02   | 8.041E-02   | 5.301E-02  |
| 1 2   | 1.170E-03  | 4.799E-03   | 2.244E-03   | 9.206E-03  |
| 2 1   | 5.352E-04  | 3.246E-03   | 1.027E-03   | 6.227E-03  |
| 1 3   | 3.961E-06  | 2.801E-04   | 7.598E-06   | 5.372E-04  |
| 2 2   | 8.180E-05  | 1.291E-03   | 1.569E-04   | 2.477E-03  |

|       |            |            |            |
|-------|------------|------------|------------|
| 0 1   | 4.690E-01  | 1.758E-02   | 8.552E-01   | 3.208E-02  |
| 1 0   | 4.689E-01  | 1.781E-02   | 8.550E-01   | 3.251E-02  |
| 1 1   | 5.716E-02  | 3.340E-02   | 1.042E-01   | 6.090E-02  |
| 1 2   | 2.157E-03  | 6.542E-03   | 3.933E-03   | 1.193E-02  |
| 2 1   | 2.164E-03  | 6.632E-03   | 3.945E-03   | 1.209E-02  |
| 1 3   | 1.646E-05  | 5.820E-04   | 3.002E-05   | 1.061E-03  |
| 2 2   | 4.718E-04  | 3.091E-03   | 8.603E-04   | 5.635E-03  |
| 3 1   | 6.806E-05  | 1.183E-03   | 1.241E-04   | 2.157E-03  |
| 3 2   | 2.344E-05  | 7.071E-04   | 4.275E-05   | 1.289E-03  |
| 3 3   | 4.211E-06  | 2.977E-04   | 7.678E-06   | 5.429E-04  |

|       |            |            |            |
|-------|------------|------------|------------|
| 0 1   | 4.648E-01  | 1.837E-02   | 8.301E-01   | 3.283E-02  |
| 1 0   | 4.638E-01  | 1.902E-02   | 8.283E-01   | 3.399E-02  |
| 1 1   | 6.459E-02  | 3.437E-02   | 1.153E-01   | 6.138E-02  |
| 1 2   | 2.587E-03  | 7.164E-03   | 4.621E-03   | 1.279E-02  |
| 2 1   | 3.389E-03  | 8.127E-03   | 6.052E-03   | 1.452E-02  |
| 1 3   | 2.657E-05  | 7.370E-04   | 4.745E-05   | 1.316E-03  |
| 2 2   | 6.564E-04  | 3.729E-03   | 1.172E-03   | 6.659E-03  |
| 3 1   | 7.924E-05  | 1.301E-03   | 1.415E-04   | 2.324E-03  |
| 3 2   | 1.482E-05  | 5.602E-04   | 2.647E-05   | 1.001E-03  |
| 3 3   | 7.686E-05  | 1.279E-03   | 1.373E-04   | 2.284E-03  |

|       |            |            |            |
|-------|------------|------------|------------|
| 0 1   | 4.637E-01  | 1.947E-02   | 8.132E-01   | 3.418E-02  |
| 1 0   | 4.629E-01  | 1.935E-02   | 8.117E-01   | 3.395E-02  |
| 1 1   | 6.653E-02  | 3.558E-02   | 1.167E-01   | 6.239E-02  |
| 1 2   | 2.636E-03  | 7.513E-03   | 4.623E-03   | 1.317E-02  |
| 2 1   | 3.357E-03  | 8.184E-03   | 5.887E-03   | 1.435E-02  |
| 1 3   | 5.215E-05  | 1.042E-03   | 9.145E-05   | 1.828E-03  |
| 2 2   | 6.066E-04  | 3.549E-03   | 1.064E-03   | 6.223E-03  |
| 3 1   | 1.009E-04  | 1.502E-03   | 1.770E-04   | 2.634E-03  |
| 3 2   | 2.449E-05  | 7.388E-04   | 4.295E-05   | 1.296E-03  |
| 3 3   | 6.618E-06  | 3.821E-04   | 1.161E-05   | 6.700E-04  |

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Table S4 continued

C) SPC/E + SPC/E-compatible ions

|       | 0   | 1   | 4.699E-01 | 1.725E-02 | 8.828E-01 | 3.245E-02 | 8.832E-01 | 3.243E-02 |
|-------|-----|-----|------------|-----------|-----------|-----------|-----------|-----------|
| 1     | 0   | 4.707E-01 | 1.675E-02 | 8.843E-01 | 3.150E-02 | 8.848E-01 | 3.148E-02 |
| 1     | 1   | 5.607E-02 | 3.230E-02 | 1.054E-01 | 6.068E-02 | 1.054E-01 | 6.071E-02 |
| 1     | 2   | 1.994E-03 | 6.560E-03 | 3.747E-03 | 1.233E-02 | 3.749E-03 | 1.233E-02 |
| 2     | 1   | 1.199E-03 | 4.919E-03 | 2.253E-03 | 9.242E-03 | 2.254E-03 | 9.247E-03 |
| 2     | 2   | 1.654E-04 | 1.854E-03 | 3.107E-04 | 3.484E-03 | 3.109E-04 | 3.486E-03 |

|       | 0   | 1   | 4.707E-01 | 1.725E-02 | 8.828E-01 | 3.245E-02 | 8.832E-01 | 3.243E-02 |
|-------|-----|-----|------------|-----------|-----------|-----------|-----------|-----------|
| 1     | 0   | 4.521E-01 | 2.164E-02 | 7.901E-01 | 3.784E-02 | 8.145E-01 | 3.899E-02 |
| 1     | 1   | 8.379E-02 | 3.844E-02 | 1.464E-01 | 6.718E-02 | 1.510E-01 | 6.926E-02 |
| 1     | 2   | 4.630E-03 | 9.682E-03 | 3.747E-03 | 1.233E-02 | 3.749E-03 | 1.233E-02 |
| 2     | 1   | 5.152E-03 | 1.046E-02 | 9.005E-03 | 2.254E-03 | 9.247E-03 |
| 2     | 3   | 9.386E-05 | 1.441E-03 | 1.710E-03 | 2.518E-03 | 1.763E-03 | 2.595E-03 |
| 3     | 1   | 8.345E-05 | 1.334E-03 | 1.458E-03 | 2.332E-03 | 1.503E-03 | 2.404E-03 |
| 3     | 2   | 1.808E-04 | 1.978E-03 | 3.160E-04 | 3.457E-03 | 3.258E-04 | 3.564E-03 |
| 3     | 3   | 4.858E-05 | 1.035E-03 | 8.490E-05 | 8.752E-05 | 1.864E-03 |

|       | 0   | 1   | 4.707E-01 | 1.725E-02 | 8.828E-01 | 3.245E-02 | 8.832E-01 | 3.243E-02 |
|-------|-----|-----|------------|-----------|-----------|-----------|-----------|-----------|
| 1     | 0   | 4.453E-01 | 2.403E-02 | 7.560E-01 | 4.092E-02 | 7.892E-01 | 4.258E-02 |
| 1     | 1   | 9.312E-02 | 4.198E-02 | 1.585E-01 | 7.146E-02 | 1.651E-01 | 7.440E-02 |
| 1     | 2   | 6.126E-03 | 1.152E-02 | 1.043E-02 | 1.961E-02 | 1.086E-02 | 2.042E-02 |
| 2     | 1   | 6.721E-03 | 1.188E-02 | 1.144E-02 | 2.022E-02 | 1.191E-02 | 2.105E-02 |
| 2     | 3   | 1.528E-04 | 1.822E-03 | 2.602E-04 | 3.102E-03 | 2.709E-04 | 3.230E-03 |
| 3     | 1   | 1.743E-03 | 6.211E-03 | 2.967E-03 | 1.057E-02 | 3.089E-03 | 1.101E-02 |
| 3     | 2   | 2.089E-04 | 2.124E-03 | 3.557E-04 | 3.616E-03 | 3.703E-04 | 3.765E-03 |
| 3     | 3   | 1.758E-04 | 1.959E-03 | 2.993E-04 | 3.335E-03 | 3.116E-04 | 3.472E-03 |
| 3     | 4   | 3.155E-04 | 2.660E-03 | 5.371E-04 | 4.529E-03 | 5.592E-04 | 4.715E-03 |
| 3     | 5   | 4.058E-05 | 9.561E-04 | 6.909E-05 | 1.628E-03 | 7.193E-05 | 1.695E-03 |

|       | 0   | 1   | 4.415E-01 | 2.471E-02 | 7.292E-01 | 4.079E-02 | 7.907E-01 | 4.245E-02 |
|-------|-----|-----|------------|-----------|-----------|-----------|-----------|-----------|
| 1     | 0   | 4.406E-01 | 2.525E-02 | 7.278E-01 | 4.173E-02 | 7.703E-01 | 4.415E-02 |
| 1     | 1   | 9.837E-02 | 4.318E-02 | 1.625E-01 | 7.132E-02 | 7.549E-02 |
| 1     | 2   | 7.407E-03 | 1.254E-02 | 1.223E-02 | 2.071E-02 | 1.295E-02 | 2.192E-02 |
| 2     | 1   | 7.992E-03 | 1.272E-02 | 1.320E-02 | 2.102E-02 | 1.397E-02 | 2.225E-02 |
| 2     | 3   | 2.776E-03 | 2.470E-03 | 4.585E-04 | 4.080E-03 | 4.853E-04 | 4.319E-03 |
| 3     | 1   | 3.108E-03 | 2.611E-03 | 5.134E-04 | 4.314E-03 | 5.435E-04 | 4.566E-03 |
| 3     | 2   | 2.502E-04 | 2.377E-03 | 4.134E-04 | 3.927E-03 | 4.375E-04 | 4.156E-03 |
| 3     | 3   | 3.802E-04 | 2.959E-03 | 6.281E-04 | 4.888E-03 | 6.648E-04 | 5.174E-03 |
| 3     | 4   | 7.908E-05 | 1.356E-03 | 1.306E-04 | 2.240E-03 | 1.383E-04 | 2.371E-03 |
| 4     | 3   | 5.346E-05 | 1.114E-03 | 8.830E-05 | 1.840E-03 | 9.347E-05 | 1.948E-03 |
Table S4 continued

|       | CsF                  |                 | CsCl                  |                 | CsBr                  |                 | CsI                  |                 |
|-------|----------------------|-----------------|-----------------------|-----------------|-----------------------|-----------------|----------------------|-----------------|
| C)     | SPC/E + SPC/E-compatible ions |                 |                       |                 |                       |                 |                       |                 |
|       |                      | CsF             |                       | CsCl            |                       | CsBr            |                       | CsI             |
|       |                      |                 |                       |                 |                       |                 |                       |                 |
| 0 1   | 4.422E-01            | 2.426E-02       | 7.791E-01             | 4.277E-02       | 7.853E-01             | 4.308E-02       |                       |                 |
| 0 2   | 4.450E-01            | 2.301E-02       | 7.841E-01             | 4.057E-02       | 7.903E-01             | 4.087E-02       |                       |                 |
| 0 3   | 1.015E-01            | 4.341E-02       | 1.789E-01             | 7.648E-02       | 1.803E-01             | 7.708E-02       |                       |                 |
| 1 0   | 6.214E-03            | 1.147E-02       | 1.095E-02             | 2.020E-02       | 1.104E-02             | 2.036E-02       |                       |                 |
| 1 1   | 3.809E-03            | 8.841E-03       | 6.710E-03             | 1.558E-02       | 6.763E-03             | 1.570E-02       |                       |                 |
| 1 2   | 2.104E-02            | 2.201E-02       | 2.984E-02             | 3.068E-02       | 3.101E-02             | 3.188E-02       |                       |                 |
| 2 0   | 3.717E-01            | 3.940E-02       | 5.182E-01             | 5.494E-02       | 5.385E-01             | 5.709E-02       |                       |                 |
| 2 1   | 3.762E-01            | 3.691E-02       | 5.244E-01             | 5.146E-01       | 5.450E-01             | 5.347E-02       |                       |                 |
| 2 2   | 3.762E-01            | 3.691E-02       | 5.244E-01             | 5.146E-01       | 5.450E-01             | 5.347E-02       |                       |                 |
| 2 3   | 3.655E-01            | 9.276E-03       | 4.691E-03             | 1.293E-02       | 4.875E-03             | 1.344E-02       |                       |                 |
| 3 2   | 2.155E-03            | 7.561E-03       | 3.004E-03             | 1.054E-02       | 3.122E-03             | 1.095E-02       |                       |                 |
| 3 3   | 2.104E-02            | 2.201E-02       | 2.984E-02             | 3.068E-02       | 3.101E-02             | 3.188E-02       |                       |                 |
| 3 4   | 2.104E-02            | 2.201E-02       | 2.984E-02             | 3.068E-02       | 3.101E-02             | 3.188E-02       |                       |                 |
| 4 3   | 2.104E-02            | 2.201E-02       | 2.984E-02             | 3.068E-02       | 3.101E-02             | 3.188E-02       |                       |                 |
| 4 4   | 2.104E-02            | 2.201E-02       | 2.984E-02             | 3.068E-02       | 3.101E-02             | 3.188E-02       |                       |                 |
Table S4 continued

D) TIP3P + Smith-Dang-Garret ions

| $N_1$ | $N_2$ | $X$   | $M$     | $m$     |
|-------|-------|-------|---------|---------|
| LiCl  |       |       |         |         |
| 0     | 1     | 4.859E-01 | 1.226E-02 | 9.102E-01 | 2.300E-02 | 9.432E-01 | 2.379E-02 |
| 1     | 0     | 4.859E-01 | 1.354E-02 | 9.102E-01 | 2.539E-02 | 9.432E-01 | 2.628E-02 |
| 1     | 1     | 2.696E-02 | 2.424E-02 | 5.050E-02 | 4.540E-02 | 5.233E-02 | 4.705E-02 |
| 1     | 2     | 6.003E-04 | 3.368E-03 | 1.125E-03 | 6.309E-03 | 1.165E-03 | 6.538E-03 |
| 2     | 1     | 6.415E-04 | 3.566E-03 | 1.202E-03 | 6.679E-03 | 1.245E-03 | 6.921E-03 |
| LiI   |       |       |         |         |
| 0     | 1     | 4.997E-01 | 1.647E-03 | 9.338E-01 | 3.309E-03 | 9.980E-01 | 3.289E-03 |
| 1     | 0     | 4.997E-01 | 1.647E-03 | 9.338E-01 | 3.309E-03 | 9.980E-01 | 3.289E-03 |
| 1     | 1     | 5.851E-04 | 3.293E-03 | 1.093E-03 | 6.154E-03 | 1.168E-03 | 6.578E-03 |
| NaF   |       |       |         |         |
| 0     | 1     | 4.425E-01 | 5.838E-02 | 3.401E-01 | 4.489E-02 | 3.435E-01 | 4.532E-02 |
| 1     | 0     | 4.076E-01 | 5.868E-02 | 3.132E-01 | 4.512E-02 | 3.164E-01 | 4.555E-02 |
| 1     | 1     | 6.701E-02 | 6.677E-02 | 5.150E-02 | 6.450E-02 | 5.202E-02 | 5.182E-02 |
| 2     | 1     | 7.805E-02 | 1.835E-02 | 5.998E-02 | 1.140E-02 | 6.058E-02 | 1.424E-02 |
| 2     | 2     | 9.205E-03 | 1.971E-02 | 7.074E-03 | 1.514E-02 | 7.145E-03 | 1.529E-02 |
| 3     | 1     | 6.415E-04 | 3.566E-03 | 1.202E-03 | 6.679E-03 | 1.245E-03 | 6.921E-03 |
| 3     | 2     | 9.205E-03 | 1.971E-02 | 7.074E-03 | 1.514E-02 | 7.145E-03 | 1.529E-02 |
| 4     | 1     | 6.278E-04 | 4.062E-03 | 1.165E-03 | 6.538E-03 | 1.183E-03 | 6.952E-03 |
| 4     | 2     | 9.205E-03 | 1.971E-02 | 7.074E-03 | 1.514E-02 | 7.145E-03 | 1.529E-02 |
| 7     | 6     | 7.307E-04 | 4.714E-03 | 5.615E-03 | 3.622E-03 | 5.672E-03 | 3.659E-03 |
| 7     | 7     | 2.137E-03 | 8.291E-03 | 1.642E-03 | 6.371E-03 | 1.659E-03 | 6.435E-03 |
| 7     | 8     | 9.983E-04 | 6.079E-03 | 7.672E-04 | 4.672E-03 | 7.749E-04 | 4.719E-03 |
| 11    | 10    | 2.370E-03 | 9.151E-03 | 8.216E-03 | 7.038E-03 | 1.839E-03 | 7.103E-03 |
| 11    | 11    | 2.752E-03 | 1.048E-02 | 2.115E-03 | 8.042E-03 | 2.136E-03 | 8.123E-03 |
| 14    | 15    | 7.155E-04 | 5.577E-03 | 5.499E-04 | 4.286E-03 | 5.554E-04 | 4.329E-03 |
| 18    | 15    | 1.668E-03 | 8.958E-03 | 1.282E-03 | 8.801E-03 | 2.707E-03 | 8.889E-03 |
| 17    | 17    | 6.059E-04 | 5.594E-03 | 4.656E-04 | 4.299E-03 | 4.703E-04 | 4.342E-03 |
| 19    | 16    | 1.183E-03 | 7.935E-03 | 9.093E-04 | 6.098E-03 | 9.184E-04 | 6.159E-03 |
| 19    | 17    | 3.469E-03 | 1.332E-02 | 2.666E-03 | 1.023E-02 | 2.693E-03 | 1.034E-02 |
| 20    | 16    | 1.392E-03 | 8.978E-03 | 1.070E-03 | 6.899E-03 | 1.080E-03 | 6.969E-03 |
| 19    | 18    | 1.983E-03 | 1.034E-02 | 1.524E-03 | 7.946E-03 | 1.539E-03 | 8.026E-03 |
| 20    | 17    | 1.950E-03 | 1.041E-02 | 1.498E-03 | 7.998E-03 | 1.513E-03 | 8.079E-03 |
| 20    | 18    | 6.526E-04 | 6.248E-03 | 5.015E-04 | 4.802E-03 | 5.065E-04 | 4.850E-03 |
| 19    | 20    | 2.694E-03 | 1.290E-02 | 2.070E-03 | 9.917E-03 | 2.091E-03 | 1.002E-02 |
| 20    | 19    | 3.170E-03 | 1.388E-02 | 2.436E-03 | 1.067E-02 | 2.460E-03 | 1.078E-02 |
| 19    | 21    | 3.230E-03 | 1.474E-02 | 2.482E-03 | 1.133E-02 | 2.507E-03 | 1.144E-02 |
| 20    | 20    | 3.360E-03 | 1.462E-02 | 2.582E-03 | 1.123E-02 | 2.608E-03 | 1.135E-02 |
| 19    | 22    | 1.373E-03 | 1.003E-02 | 1.055E-03 | 7.704E-03 | 1.066E-03 | 7.782E-03 |
| 21    | 20    | 1.188E-03 | 9.144E-03 | 9.129E-04 | 7.027E-03 | 9.221E-04 | 7.097E-03 |
Table S4 continued

D) TIP3P + Smith-Dang-Garret ions

|       | NaCl       |       |       |       |       |       |       |
|-------|------------|-------|-------|-------|-------|-------|-------|
|       |            | 0     | 1     | 2     | 3     | 4     | 5     |
| 0     | 1.479E-02  | 8.771E-01 | 2.757E-02 | 9.059E-01 | 2.845E-02 |
| 1     | 1.539E-02  | 8.757E-01 | 2.834E-02 | 9.045E-01 | 2.924E-02 |
| 2     | 1.479E-02  | 8.771E-01 | 2.757E-02 | 9.059E-01 | 2.845E-02 |
| 3     | 1.479E-02  | 8.771E-01 | 2.757E-02 | 9.059E-01 | 2.845E-02 |
| 4     | 1.479E-02  | 8.771E-01 | 2.757E-02 | 9.059E-01 | 2.845E-02 |

|       | NaI        |       |       |       |       |       |       |
|-------|------------|-------|-------|-------|-------|-------|-------|
|       |            | 0     | 1     | 2     | 3     | 4     | 5     |
| 0     | 9.067E-01  | 1.694E-02 | 9.653E-01 | 1.800E-02 |
| 1     | 9.068E-01  | 1.674E-02 | 9.655E-01 | 1.778E-02 |
| 2     | 1.794E-02  | 3.089E-02 | 3.310E-02 | 3.289E-02 | 3.524E-02 |
| 3     | 1.914E-02  | 1.794E-02 | 3.089E-02 | 3.310E-02 | 3.524E-02 |

|       | KF         |       |       |       |       |       |       |
|-------|------------|-------|-------|-------|-------|-------|-------|
|       |            | 0     | 1     | 2     | 3     | 4     | 5     |
| 0     | 2.312E-02  | 7.986E-01 | 4.108E-02 | 8.078E-01 | 4.153E-02 |
| 1     | 2.158E-02  | 8.040E-01 | 3.835E-02 | 8.132E-01 | 3.877E-02 |
| 2     | 1.201E-02  | 1.207E-02 | 2.133E-02 | 1.221E-02 | 2.158E-02 |
| 3     | 1.611E-04  | 1.879E-03 | 2.861E-04 | 3.338E-03 | 3.736E-03 |

|       | KCl        |       |       |       |       |       |       |
|-------|------------|-------|-------|-------|-------|-------|-------|
|       |            | 0     | 1     | 2     | 3     | 4     | 5     |
| 0     | 3.108E-02  | 6.319E-01 | 4.767E-02 | 6.618E-01 | 4.991E-02 |
| 1     | 3.175E-02  | 6.278E-01 | 4.870E-02 | 6.575E-01 | 5.099E-02 |
| 2     | 1.816E-02  | 1.515E-01 | 7.056E-02 | 1.532E-01 | 7.136E-02 |
| 3     | 1.265E-02  | 1.517E-01 | 7.056E-02 | 1.532E-01 | 7.136E-02 |
| 4     | 1.634E-02  | 1.933E-02 | 2.506E-02 | 2.964E-02 | 3.104E-02 |

|       | KCl        |       |       |       |       |       |       |
|-------|------------|-------|-------|-------|-------|-------|-------|
|       |            | 0     | 1     | 2     | 3     | 4     | 5     |
| 0     | 3.115E-03  | 6.306E-04 | 4.778E-03 | 6.603E-04 | 5.003E-03 |
| 1     | 3.115E-03  | 6.306E-04 | 4.778E-03 | 6.603E-04 | 5.003E-03 |
| 2     | 1.265E-02  | 1.517E-01 | 7.056E-02 | 1.532E-01 | 7.136E-02 |
| 3     | 1.265E-02  | 1.517E-01 | 7.056E-02 | 1.532E-01 | 7.136E-02 |
| 4     | 1.634E-02  | 1.933E-02 | 2.506E-02 | 2.964E-02 | 3.104E-02 |
| 5     | 1.634E-02  | 1.933E-02 | 2.506E-02 | 2.964E-02 | 3.104E-02 |
Table S4 continued

D) TIP3P + Smith-Dang-Garret ions

|        |        |        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|        |        |        |        |        |        |        |        |        |
|        |        |        |        |        |        |        |        |        |
| **KI** |        |        |        |        |        |        |        |        |
| 0 1    | 4.135E-01 | 2.989E-02 | 6.191E-01 | 4.476E-02 | 6.678E-01 | 4.827E-02 |
| 1 0    | 4.095E-01 | 3.124E-02 | 6.131E-01 | 4.678E-02 | 6.613E-01 | 5.045E-02 |
| 1 1    | 1.341E-01 | 5.086E-02 | 2.008E-01 | 7.615E-02 | 2.166E-01 | 8.214E-02 |
| 1 2    | 1.433E-02 | 1.715E-02 | 2.145E-02 | 2.568E-02 | 2.314E-02 | 2.770E-02 |
| 2 1    | 1.649E-02 | 1.891E-02 | 2.469E-02 | 2.831E-02 | 2.663E-02 | 3.053E-02 |
| 1 3    | 4.071E-04 | 3.068E-03 | 6.095E-04 | 4.593E-03 | 6.574E-04 | 4.954E-03 |
| 2 2    | 6.990E-03 | 1.243E-02 | 1.047E-02 | 1.862E-02 | 1.129E-02 | 2.008E-02 |
| 3 1    | 9.179E-04 | 4.665E-03 | 1.374E-03 | 6.985E-03 | 1.482E-03 | 7.535E-03 |
| 2 3    | 1.116E-03 | 5.076E-03 | 1.670E-03 | 7.600E-03 | 1.802E-03 | 8.198E-03 |
| 3 2    | 1.496E-03 | 6.030E-03 | 2.239E-03 | 9.028E-03 | 2.416E-03 | 9.739E-03 |
| 3 3    | 6.234E-04 | 3.912E-03 | 9.334E-04 | 5.856E-03 | 1.007E-03 | 6.317E-03 |
| 4 3    | 1.170E-04 | 1.706E-03 | 1.752E-04 | 2.555E-03 | 1.890E-04 | 2.756E-03 |
| **RbF** |        |        |        |        |        |        |        |        |
| 0 1    | 4.554E-01 | 2.174E-02 | 8.181E-01 | 3.907E-02 | 8.301E-01 | 3.962E-02 |
| 1 0    | 4.583E-01 | 2.043E-02 | 8.233E-01 | 3.672E-02 | 8.353E-01 | 3.724E-02 |
| 1 1    | 7.757E-02 | 3.841E-02 | 1.393E-01 | 6.901E-02 | 1.414E-01 | 7.002E-02 |
| 1 2    | 5.162E-03 | 1.053E-02 | 9.274E-03 | 1.891E-02 | 9.410E-03 | 1.919E-02 |
| 2 1    | 2.547E-03 | 7.069E-03 | 4.575E-03 | 1.270E-02 | 4.642E-03 | 1.289E-02 |
| 1 3    | 1.228E-04 | 1.610E-03 | 2.206E-04 | 2.893E-03 | 2.238E-04 | 2.935E-03 |
| 2 2    | 7.793E-04 | 4.041E-03 | 1.400E-03 | 7.259E-03 | 1.421E-03 | 7.366E-03 |
| **RbCl** |        |        |        |        |        |        |        |        |
| 0 1    | 4.001E-01 | 3.415E-02 | 5.903E-01 | 5.040E-02 | 6.204E-01 | 5.296E-02 |
| 1 0    | 3.972E-01 | 3.416E-02 | 5.861E-01 | 5.040E-02 | 6.159E-01 | 5.297E-02 |
| 1 1    | 1.478E-01 | 5.451E-02 | 2.181E-01 | 8.043E-02 | 2.292E-01 | 8.453E-02 |
| 1 2    | 1.696E-02 | 1.995E-02 | 2.502E-02 | 2.944E-02 | 2.630E-02 | 3.094E-02 |
| 2 1    | 1.851E-02 | 2.013E-02 | 2.731E-02 | 2.970E-02 | 2.871E-02 | 3.121E-02 |
| 1 3    | 9.492E-03 | 4.807E-03 | 1.401E-03 | 7.093E-03 | 1.472E-03 | 7.454E-03 |
| 2 2    | 1.021E-02 | 1.563E-02 | 2.306E-02 | 1.583E-02 | 2.424E-02 | 2.424E-02 |
| 3 1    | 1.119E-03 | 5.147E-03 | 1.651E-03 | 7.594E-03 | 1.735E-03 | 7.981E-03 |
| 2 3    | 1.958E-03 | 7.180E-03 | 2.889E-03 | 1.059E-02 | 3.037E-03 | 1.113E-02 |
| 3 2    | 2.435E-03 | 7.761E-03 | 3.592E-03 | 1.145E-02 | 3.776E-03 | 1.204E-02 |
| 2 4    | 2.083E-04 | 2.404E-03 | 3.074E-04 | 3.547E-03 | 3.230E-04 | 3.727E-03 |
| 3 3    | 1.212E-03 | 5.459E-03 | 1.788E-03 | 8.054E-03 | 1.879E-03 | 8.465E-03 |
| 4 2    | 2.787E-04 | 2.765E-03 | 4.112E-04 | 4.080E-03 | 4.322E-04 | 4.288E-03 |
| 3 4    | 2.721E-04 | 2.649E-03 | 4.015E-04 | 3.909E-03 | 4.219E-04 | 4.108E-03 |
| 4 3    | 3.500E-04 | 2.988E-03 | 5.165E-04 | 4.409E-03 | 5.428E-04 | 4.634E-03 |
| 4 4    | 1.425E-04 | 1.919E-03 | 2.102E-04 | 2.831E-03 | 2.209E-04 | 2.975E-03 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 0  | 1  | 3.920E-01 | 3.541E-02 | 5.481E-01 | 4.952E-02 | 5.933E-01 | 5.359E-02 |
| 1  | 0  | 3.895E-01 | 3.525E-02 | 5.446E-01 | 4.929E-02 | 5.894E-01 | 5.334E-02 |
| 1  | 1  | 1.545E-01 | 5.615E-02 | 2.160E-01 | 7.851E-02 | 2.338E-01 | 8.496E-02 |
| 1  | 2  | 2.030E-02 | 2.181E-02 | 2.838E-02 | 3.050E-02 | 3.072E-02 | 3.301E-02 |
| 2  | 1  | 2.048E-02 | 2.184E-02 | 2.863E-02 | 3.053E-02 | 3.099E-02 | 3.305E-02 |
| 1  | 3  | 7.973E-04 | 4.397E-03 | 1.115E-03 | 6.149E-03 | 1.207E-03 | 6.655E-03 |
| 2  | 2  | 2.815E-03 | 8.347E-03 | 3.936E-03 | 1.167E-02 | 4.281E-03 | 1.263E-02 |
| 2  | 4  | 2.271E-04 | 2.430E-03 | 3.175E-04 | 3.397E-03 | 3.437E-04 | 3.677E-03 |
| 3  | 3  | 1.410E-03 | 6.134E-03 | 1.972E-03 | 8.577E-03 | 2.135E-03 | 9.284E-03 |
| 4  | 2  | 2.617E-04 | 2.622E-03 | 3.659E-04 | 3.666E-03 | 3.960E-04 | 3.969E-03 |
| 4  | 3  | 4.545E-04 | 3.459E-03 | 6.356E-04 | 6.836E-04 | 5.235E-04 | 5.381E-03 |
| 5  | 4  | 1.215E-04 | 1.812E-03 | 1.699E-04 | 2.533E-03 | 1.839E-04 | 2.742E-03 |
|   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |
| 0  | 1  | 4.623E-01 | 1.927E-02 | 8.366E-01 | 3.489E-02 | 8.551E-01 | 3.564E-02 |
| 1  | 0  | 4.640E-01 | 1.831E-02 | 8.397E-01 | 3.316E-02 | 8.584E-01 | 3.387E-02 |
| 1  | 1  | 6.791E-02 | 3.488E-02 | 1.229E-01 | 6.311E-02 | 1.256E-01 | 6.451E-02 |
| 1  | 2  | 3.353E-03 | 8.298E-03 | 6.068E-03 | 1.502E-02 | 6.202E-03 | 1.535E-02 |
| 2  | 1  | 1.835E-02 | 3.488E-02 | 1.229E-01 | 6.311E-02 | 1.256E-01 | 6.451E-02 |
| 2  | 2  | 4.401E-04 | 3.056E-03 | 7.964E-04 | 5.531E-04 | 8.141E-04 | 5.653E-03 |
|   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |
| 0  | 1  | 3.813E-01 | 3.557E-02 | 5.348E-01 | 4.990E-02 | 5.663E-01 | 5.283E-02 |
| 1  | 0  | 3.830E-01 | 3.487E-02 | 5.373E-01 | 4.892E-02 | 5.689E-01 | 5.179E-02 |
| 1  | 1  | 1.670E-01 | 5.764E-02 | 2.342E-01 | 8.085E-02 | 2.480E-01 | 8.561E-02 |
| 1  | 2  | 2.198E-02 | 2.290E-02 | 3.083E-02 | 3.212E-02 | 3.265E-02 | 3.402E-02 |
| 2  | 1  | 2.212E-02 | 2.244E-02 | 3.103E-02 | 3.148E-02 | 3.266E-02 | 3.333E-02 |
| 2  | 2  | 1.106E-03 | 5.350E-03 | 1.552E-03 | 7.505E-03 | 1.643E-03 | 7.947E-03 |
| 3  | 1  | 7.221E-04 | 4.320E-03 | 1.013E-03 | 6.060E-03 | 1.073E-03 | 6.417E-03 |
| 2  | 3  | 3.229E-03 | 9.000E-03 | 4.529E-03 | 1.262E-02 | 4.796E-03 | 1.337E-02 |
| 3  | 2  | 2.526E-03 | 8.190E-03 | 3.543E-03 | 1.149E-02 | 3.752E-03 | 1.216E-02 |
| 2  | 4  | 4.342E-04 | 3.382E-03 | 6.090E-04 | 4.743E-04 | 6.449E-04 | 5.023E-03 |
| 3  | 3  | 1.749E-03 | 7.023E-03 | 2.454E-03 | 9.851E-03 | 2.598E-03 | 1.043E-02 |
| 4  | 2  | 2.412E-04 | 2.500E-03 | 3.384E-04 | 3.507E-03 | 3.583E-04 | 3.714E-03 |
| 3  | 4  | 5.377E-04 | 3.870E-03 | 7.542E-04 | 5.428E-03 | 7.986E-04 | 5.748E-03 |
| 4  | 3  | 4.063E-04 | 3.371E-03 | 5.699E-04 | 4.728E-03 | 6.035E-04 | 5.007E-03 |
| 4  | 4  | 2.701E-04 | 2.723E-03 | 3.788E-04 | 3.819E-03 | 4.011E-04 | 4.044E-03 |
| 5  | 4  | 1.222E-04 | 1.923E-03 | 1.715E-04 | 2.697E-03 | 1.816E-04 | 2.856E-03 |
Table S4 continued

D) TIP3P + Smith-Dang-Garret ions

|   | Csl |   |   |   |   |   |   |   |   |
|---|-----|---|---|---|---|---|---|---|---|
| 0 | 1   | 3.587E-01 | 4.174E-02 | 4.448E-01 | 5.176E-02 | 4.850E-01 | 5.644E-02 |   |   |
| 1 | 0   | 3.556E-01 | 4.377E-02 | 4.409E-01 | 5.428E-02 | 4.808E-01 | 5.919E-02 |   |   |
| 1 | 1   | 1.804E-01 | 6.325E-02 | 2.237E-01 | 7.843E-02 | 2.440E-01 | 8.553E-02 |   |   |
| 1 | 2   | 2.888E-02 | 2.693E-02 | 3.581E-02 | 3.339E-02 | 3.905E-02 | 3.642E-02 |   |   |
| 2 | 1   | 2.975E-02 | 2.766E-02 | 3.689E-02 | 3.430E-02 | 4.023E-02 | 3.740E-02 |   |   |
| 1 | 3   | 1.518E-03 | 6.404E-03 | 1.883E-03 | 7.941E-03 | 2.053E-03 | 8.660E-03 |   |   |
| 2 | 2   | 2.230E-02 | 2.392E-02 | 2.765E-02 | 2.965E-02 | 3.015E-02 | 3.234E-02 |   |   |
| 3 | 1   | 1.824E-03 | 7.150E-03 | 2.261E-03 | 8.866E-03 | 2.466E-03 | 9.669E-03 |   |   |
| 2 | 3   | 5.381E-03 | 1.194E-02 | 6.672E-03 | 1.481E-02 | 7.276E-03 | 1.615E-02 |   |   |
| 3 | 2   | 5.761E-03 | 1.291E-02 | 7.143E-03 | 1.601E-02 | 7.790E-03 | 1.746E-02 |   |   |
| 2 | 4   | 5.274E-04 | 3.837E-03 | 6.540E-03 | 4.758E-03 | 7.132E-03 | 5.189E-03 |   |   |
| 3 | 3   | 3.881E-03 | 1.053E-02 | 4.812E-03 | 1.305E-02 | 5.248E-03 | 1.424E-02 |   |   |
| 4 | 2   | 8.622E-04 | 5.014E-03 | 1.069E-03 | 6.217E-03 | 1.166E-03 | 6.780E-03 |   |   |
| 3 | 4   | 9.601E-04 | 5.235E-03 | 1.191E-03 | 6.491E-03 | 1.298E-03 | 7.078E-03 |   |   |
| 4 | 3   | 1.057E-03 | 5.484E-03 | 1.310E-03 | 6.800E-03 | 1.429E-03 | 7.416E-03 |   |   |
| 3 | 5   | 2.432E-04 | 2.646E-03 | 3.015E-04 | 3.281E-03 | 3.288E-04 | 3.578E-03 |   |   |
| 4 | 4   | 8.023E-04 | 4.792E-03 | 9.948E-04 | 5.941E-03 | 1.085E-03 | 6.479E-03 |   |   |
| 5 | 3   | 2.298E-04 | 2.601E-03 | 2.851E-04 | 3.225E-03 | 3.109E-04 | 3.517E-03 |   |   |
| 4 | 5   | 2.412E-04 | 2.677E-03 | 2.991E-04 | 3.319E-03 | 3.262E-04 | 3.620E-03 |   |   |
| 5 | 4   | 3.608E-04 | 3.272E-03 | 4.473E-04 | 4.058E-03 | 4.878E-04 | 4.425E-03 |   |   |
| 5 | 5   | 1.918E-04 | 2.414E-03 | 2.378E-04 | 2.994E-03 | 2.594E-04 | 3.265E-03 |   |   |
| 6 | 4   | 1.026E-04 | 1.795E-03 | 1.273E-04 | 2.225E-03 | 1.388E-04 | 2.427E-03 |   |   |
| 6 | 5   | 1.243E-04 | 2.000E-03 | 1.542E-04 | 2.479E-03 | 1.681E-04 | 2.704E-03 |   |   |
Table S4 continued

| $N_+$ | $N_-$ | $X$ | $M$ | $m$ |
|-------|-------|-----|-----|-----|
| LiCl  |       |     |     |     |
| 0     | 1     | 4.819E-01 | 1.358E-02 | 9.088E-01 | 2.566E-02 | 9.289E-01 | 2.617E-02 |
| 1     | 0     | 4.81E-01  | 1.379E-02 | 9.082E-01 | 2.606E-02 | 9.283E-01 | 2.657E-02 |
| 1     | 1     | 3.61E-02  | 2.716E-02 | 6.822E-02 | 5.121E-02 | 6.973E-02 | 5.235E-02 |
| 2     | 1     | 2.83E-04  | 2.358E-03 | 5.337E-04 | 4.447E-03 | 5.455E-04 | 4.546E-03 |
| Lil   |       |     |     |     |
| 0     | 1     | 4.99E-01  | 2.470E-03 | 9.464E-01 | 4.975E-03 | 9.968E-01 | 4.931E-03 |
| 1     | 0     | 4.99E-01  | 2.470E-03 | 9.464E-01 | 4.975E-03 | 9.968E-01 | 4.931E-03 |
| 1     | 1     | 1.18E-03  | 4.94E-03  | 2.234E-03 | 9.364E-03 | 2.353E-03 | 9.862E-03 |
| NaF   |       |     |     |     |
| 0     | 1     | 4.56E-01  | 2.182E-02 | 8.259E-01 | 3.949E-02 | 8.158E-01 | 3.898E-02 |
| 1     | 0     | 4.52E-01  | 2.188E-02 | 8.175E-01 | 3.959E-02 | 8.076E-01 | 3.908E-02 |
| 1     | 1     | 7.19E-02  | 3.770E-02 | 1.301E-01 | 6.817E-02 | 1.285E-01 | 6.734E-02 |
| 2     | 1     | 5.44E-03  | 1.011E-02 | 9.848E-03 | 1.828E-02 | 9.729E-02 | 1.806E-02 |
| 2     | 2     | 3.60E-03  | 9.363E-03 | 6.513E-03 | 1.693E-02 | 6.433E-03 | 1.673E-02 |
| 3     | 1     | 1.11E-03  | 4.763E-03 | 2.019E-03 | 8.614E-03 | 1.994E-03 | 8.509E-03 |
| 2     | 3     | 5.91E-04  | 3.614E-03 | 1.069E-03 | 6.536E-03 | 1.056E-03 | 6.456E-03 |
| 3     | 2     | 7.40E-04  | 4.050E-03 | 1.339E-03 | 7.324E-03 | 1.322E-03 | 7.235E-03 |
| 3     | 3     | 1.75E-04  | 1.929E-03 | 3.171E-04 | 3.489E-03 | 3.133E-04 | 3.447E-03 |
| 4     | 2     | 2.04E-05  | 6.464E-04 | 3.698E-05 | 1.169E-03 | 3.653E-05 | 1.155E-03 |
| 3     | 4     | 4.25E-06  | 3.009E-04 | 7.695E-06 | 5.441E-04 | 7.602E-06 | 5.375E-04 |
| 4     | 3     | 1.87E-05  | 6.247E-04 | 3.391E-05 | 1.130E-03 | 3.349E-05 | 1.116E-03 |
| NaCl  |       |     |     |     |
| 0     | 1     | 4.72E-01  | 1.532E-02 | 8.735E-01 | 2.836E-02 | 8.913E-01 | 2.890E-02 |
| 1     | 0     | 4.71E-01  | 1.585E-02 | 8.718E-01 | 2.933E-02 | 8.896E-01 | 2.989E-02 |
| 1     | 1     | 5.19E-02  | 2.884E-02 | 9.594E-02 | 5.330E-02 | 9.790E-02 | 5.439E-02 |
| 1     | 2     | 1.30E-03  | 5.22E-03  | 2.406E-03 | 9.659E-03 | 2.455E-03 | 9.856E-03 |
| 2     | 1     | 1.96E-03  | 6.291E-03 | 3.622E-03 | 1.162E-02 | 3.696E-03 | 1.186E-02 |
| 2     | 2     | 1.79E-04  | 1.926E-03 | 3.314E-04 | 3.559E-03 | 3.381E-04 | 3.631E-03 |
| 3     | 1     | 5.17E-05  | 1.034E-03 | 9.565E-05 | 1.911E-03 | 9.760E-05 | 1.950E-03 |
| 3     | 2     | 1.52E-04  | 1.802E-03 | 2.816E-04 | 3.330E-03 | 2.873E-04 | 3.398E-03 |
| NaI   |       |     |     |     |
| 0     | 1     | 4.85E-01  | 1.270E-02 | 8.944E-01 | 2.347E-02 | 9.400E-01 | 2.461E-02 |
| 1     | 0     | 4.84E-01  | 1.313E-02 | 8.935E-01 | 2.425E-02 | 9.391E-01 | 2.543E-02 |
| 1     | 1     | 2.87E-02  | 2.468E-02 | 5.295E-02 | 4.550E-02 | 5.565E-02 | 4.782E-02 |
| 1     | 2     | 3.83E-04  | 2.738E-03 | 7.077E-04 | 5.048E-03 | 7.438E-04 | 5.305E-03 |
| 2     | 1     | 8.57E-04  | 4.098E-03 | 1.580E-03 | 7.555E-03 | 1.660E-03 | 7.939E-03 |
| 2     | 2     | 9.64E-05  | 1.390E-03 | 1.778E-04 | 2.562E-03 | 1.869E-04 | 2.692E-03 |
| 3     | 2     | 2.00E-06  | 2.00E-04  | 3.687E-06 | 3.687E-04 | 3.875E-06 | 3.874E-04 |
Table S4 continued

E) TIP4P<sub>EW</sub> + Smith-Dang-Garret ions

|       | KF       | KCl      | KI       |
|-------|----------|----------|----------|
|       |         |          |          |
| 0  1  | 4.726E-01 | 1.666E-02 | 8.923E-01 | 3.150E-02 | 8.932E-01 | 3.148E-02 |
| 1  0  | 4.736E-01 | 1.609E-02 | 8.943E-01 | 3.043E-02 | 8.952E-01 | 3.041E-02 |
| 1  1  | 5.065E-02 | 3.087E-02 | 9.564E-02 | 5.828E-02 | 9.574E-02 | 5.835E-02 |
| 1  2  | 2.024E-03 | 6.368E-03 | 3.822E-03 | 1.202E-02 | 3.826E-03 | 1.204E-02 |
| 2  1  | 9.898E-04 | 4.462E-03 | 1.869E-03 | 8.425E-03 | 1.871E-03 | 8.434E-03 |
| 2  2  | 1.496E-04 | 1.783E-03 | 2.825E-04 | 3.367E-03 | 2.827E-04 | 3.370E-03 |
| 0  1  | 4.039E-01 | 3.283E-02 | 6.127E-01 | 4.981E-02 | 6.355E-01 | 5.165E-02 |
| 1  0  | 3.991E-01 | 3.290E-02 | 6.055E-01 | 4.992E-02 | 6.280E-01 | 5.177E-02 |
| 1  1  | 1.474E-01 | 5.381E-02 | 2.236E-01 | 8.163E-02 | 2.319E-01 | 8.467E-02 |
| 1  2  | 1.490E-02 | 1.873E-02 | 2.260E-02 | 2.842E-02 | 2.344E-02 | 2.947E-02 |
| 2  1  | 1.889E-02 | 2.085E-02 | 2.865E-02 | 3.162E-02 | 2.972E-02 | 3.280E-02 |
| 2  2  | 4.604E-04 | 3.404E-03 | 6.984E-04 | 5.164E-03 | 7.244E-04 | 5.356E-03 |
| 2  3  | 9.898E-04 | 4.095E-03 | 6.984E-04 | 5.164E-03 | 7.244E-04 | 5.356E-03 |
| 3  1  | 6.741E-04 | 4.095E-03 | 1.023E-03 | 6.212E-03 | 1.061E-03 | 6.443E-03 |
| 3  2  | 1.857E-03 | 6.623E-03 | 2.818E-03 | 1.005E-02 | 2.922E-03 | 1.042E-02 |
| 3  3  | 1.989E-03 | 7.075E-03 | 3.017E-03 | 1.073E-02 | 3.130E-03 | 1.113E-02 |
| 4  2  | 1.335E-04 | 1.814E-03 | 2.026E-04 | 2.751E-03 | 2.101E-04 | 2.853E-03 |
| 4  3  | 7.478E-04 | 4.276E-03 | 1.134E-03 | 6.486E-03 | 1.176E-03 | 6.727E-03 |
| 4  4  | 2.029E-04 | 2.483E-03 | 3.078E-04 | 3.766E-03 | 3.192E-04 | 3.907E-03 |
| 4  5  | 1.606E-04 | 2.035E-03 | 2.436E-04 | 3.088E-03 | 2.526E-04 | 3.203E-03 |
| 5  3  | 2.452E-04 | 2.483E-03 | 3.720E-04 | 3.767E-03 | 3.858E-04 | 3.907E-03 |
| 5  4  | 3.022E-04 | 2.963E-03 | 4.077E-04 | 3.997E-03 | 4.353E-04 | 4.267E-03 |
| 5  5  | 3.890E-04 | 3.288E-03 | 5.248E-04 | 4.435E-03 | 5.603E-04 | 4.735E-03 |
| 6  4  | 7.822E-04 | 4.540E-03 | 1.055E-03 | 6.124E-03 | 1.127E-03 | 6.539E-03 |
| 6  5  | 4.298E-04 | 3.507E-03 | 5.797E-04 | 4.730E-03 | 6.190E-04 | 5.050E-03 |
| 7  5  | 1.777E-04 | 1.818E-03 | 1.588E-04 | 2.452E-03 | 1.695E-04 | 2.618E-03 |
| 8  5  | 1.048E-04 | 1.747E-03 | 1.414E-04 | 2.357E-03 | 1.509E-04 | 2.517E-03 |
| 9  5  | 1.683E-04 | 2.170E-03 | 2.270E-04 | 2.927E-03 | 2.424E-04 | 3.125E-03 |
| 10 5  | 1.010E-04 | 1.734E-03 | 1.362E-04 | 2.338E-03 | 1.454E-04 | 2.497E-03 |
Table S4 continued

| E) TIP4P\textsubscript{EW} + Smith-Dang-Garret ions | \text{RbF} | \text{RbCl} | \text{RbI} |
|--------------------------------------------------|--------|--------|--------|
| 0 1 4.723E-01 1.627E-02 8.879E-01 3.064E-02 8.924E-01 3.075E-02 | 3.902E-01 3.526E-02 5.752E-01 5.198E-02 5.990E-01 5.412E-02 | 3.907E-01 3.594E-02 5.759E-01 5.298E-02 5.997E-01 5.516E-02 |
| 0 1 4.731E-01 1.603E-02 8.894E-01 3.019E-02 8.940E-01 3.030E-02 | 1.633E-01 5.812E-02 2.407E-01 8.567E-02 2.507E-01 8.921E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 |
| 1 1 5.176E-02 3.104E-02 9.731E-02 5.835E-02 9.780E-02 5.865E-02 | 1.855E-02 2.105E-02 2.734E-02 3.102E-02 2.847E-02 3.230E-02 | 1.567E-04 2.946E-04 3.368E-03 2.961E-04 3.386E-03 |
| 1 2 5.755E-03 3.200E-03 1.082E-02 3.216E-03 1.087E-02 | 1.633E-01 5.812E-02 2.407E-01 8.567E-02 2.507E-01 8.921E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 |
| 2 1 9.308E-04 4.282E-03 1.750E-03 8.051E-03 1.759E-03 8.091E-03 | 1.633E-01 5.812E-02 2.407E-01 8.567E-02 2.507E-01 8.921E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 |
| 2 2 1.567E-04 3.104E-02 9.731E-02 5.835E-02 9.780E-02 5.865E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 |
| 3 1 6.148E-04 3.910E-03 9.061E-03 3.216E-03 9.436E-03 6.001E-03 | 1.633E-01 5.812E-02 2.407E-01 8.567E-02 2.507E-01 8.921E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 |
| 3 2 4.499E-04 3.301E-03 6.630E-03 4.866E-03 6.904E-03 5.066E-03 | 1.633E-01 5.812E-02 2.407E-01 8.567E-02 2.507E-01 8.921E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 |
| 3 3 1.064E-03 5.175E-03 1.569E-03 3.719E-03 3.846E-03 | 1.633E-01 5.812E-02 2.407E-01 8.567E-02 2.507E-01 8.921E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 |
| 3 4 2.432E-04 2.946E-04 3.368E-03 2.961E-04 3.386E-03 | 1.633E-01 5.812E-02 2.407E-01 8.567E-02 2.507E-01 8.921E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 |
| 4 3 1.059E-03 3.154E-03 1.103E-03 2.430E-03 | 1.633E-01 5.812E-02 2.407E-01 8.567E-02 2.507E-01 8.921E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 |
| 4 4 3.693E-03 3.719E-04 3.846E-03 | 1.633E-01 5.812E-02 2.407E-01 8.567E-02 2.507E-01 8.921E-02 | 1.937E-02 2.160E-02 2.855E-02 3.184E-02 2.973E-02 3.316E-02 |
Table S4 continued

E) TIP4P\textsubscript{EW} + Smith-Dang-Garret ions

|       | CsF     |       |       |       |       |       |       |
|-------|---------|-------|-------|-------|-------|-------|-------|
|       | 0       | 1     | 4.743E-01 | 1.616E-02 | 8.884E-01 | 3.031E-02 | 9.000E-01 | 3.066E-02 |
|       | 1       | 0     | 4.751E-01 | 1.559E-02 | 8.899E-01 | 2.925E-02 | 9.015E-01 | 2.959E-02 |
|       | 1       | 1     | 4.820E-02 | 3.031E-02 | 9.028E-02 | 5.678E-02 | 9.145E-02 | 5.752E-02 |
|       | 1       | 2     | 1.500E-03 | 5.450E-03 | 2.810E-03 | 1.021E-02 | 2.846E-03 | 1.034E-02 |
|       | 2       | 1     | 7.578E-04 | 3.902E-03 | 1.419E-03 | 7.309E-03 | 1.438E-03 | 7.404E-03 |
|       | CsCl    |       |       |       |       |       |       |       |
|       | 0       | 1     | 3.681E-01 | 3.860E-02 | 5.115E-01 | 3.860E-02 | 5.370E-01 | 5.631E-02 |
|       | 1       | 0     | 3.727E-01 | 3.882E-02 | 5.179E-01 | 5.395E-02 | 5.438E-01 | 5.664E-02 |
|       | 1       | 1     | 1.889E-01 | 6.309E-02 | 8.767E-01 | 2.757E-01 | 9.205E-02 | 2.713E-02 |
|       | 2       | 1     | 2.453E-02 | 3.299E-02 | 3.409E-02 | 3.334E-02 | 3.579E-02 | 3.501E-02 |
|       | 3       | 1     | 9.552E-04 | 4.970E-03 | 6.906E-03 | 1.327E-03 | 7.254E-03 | 7.251E-03 |
|       | CsI     |       |       |       |       |       |       |       |
|       | 0       | 1     | 3.111E-01 | 3.860E-02 | 3.299E-01 | 3.860E-02 | 5.370E-01 | 5.631E-02 |
|       | 1       | 0     | 3.116E-01 | 4.797E-02 | 3.304E-01 | 5.087E-02 | 5.371E-01 | 5.497E-02 |
|       | 1       | 1     | 2.129E-01 | 7.550E-02 | 2.258E-01 | 2.398E-01 | 8.005E-02 | 8.652E-02 |
|       | 2       | 1     | 3.713E-02 | 3.328E-02 | 3.937E-02 | 3.528E-02 | 4.254E-02 | 3.813E-02 |
|       | 3       | 1     | 3.752E-02 | 3.245E-02 | 3.978E-02 | 3.440E-02 | 4.299E-02 | 3.718E-02 |
|       | 4       | 1     | 3.978E-04 | 7.893E-03 | 3.341E-03 | 1.097E-02 | 3.508E-03 | 1.152E-02 |
|       | 5       | 1     | 2.526E-03 | 9.060E-03 | 2.678E-03 | 2.846E-03 | 2.784E-03 | 3.691E-03 |
|       | 6       | 1     | 1.059E-02 | 1.817E-02 | 1.122E-02 | 1.927E-02 | 1.213E-02 | 2.082E-02 |
|       | 3       | 2     | 9.871E-03 | 1.785E-02 | 1.047E-02 | 1.893E-02 | 1.131E-02 | 2.046E-02 |
|       | 4       | 2     | 7.884E-04 | 5.076E-03 | 8.359E-04 | 5.382E-03 | 9.034E-04 | 5.816E-03 |
|       | 5       | 3     | 9.293E-03 | 1.739E-02 | 9.853E-03 | 1.844E-02 | 1.065E-02 | 1.993E-02 |
|       | 4       | 4     | 8.657E-04 | 5.275E-03 | 9.179E-04 | 5.593E-03 | 9.920E-04 | 6.045E-03 |
|       | 5       | 4     | 3.232E-03 | 1.040E-02 | 3.427E-03 | 1.103E-02 | 3.704E-03 | 1.192E-02 |
|       | 6       | 4     | 3.293E-03 | 1.065E-02 | 3.491E-03 | 1.129E-02 | 3.773E-03 | 1.221E-02 |
|       | 5       | 5     | 5.413E-04 | 4.374E-03 | 5.739E-04 | 4.638E-03 | 6.203E-04 | 5.012E-03 |
|       | 6       | 5     | 3.173E-03 | 1.051E-02 | 3.364E-03 | 1.115E-02 | 3.636E-03 | 1.205E-02 |
|       | 7       | 5     | 1.498E-03 | 7.080E-03 | 1.588E-03 | 7.506E-03 | 1.716E-03 | 8.112E-03 |
|       | 6       | 6     | 8.679E-04 | 5.429E-03 | 9.201E-04 | 5.756E-03 | 9.944E-04 | 6.220E-03 |
|       | 7       | 6     | 1.047E-03 | 5.984E-03 | 1.110E-03 | 6.344E-03 | 1.200E-03 | 6.856E-03 |
|       | 8       | 6     | 3.626E-04 | 3.643E-03 | 3.845E-04 | 3.863E-03 | 4.155E-04 | 4.175E-03 |
|       | 9       | 6     | 3.587E-04 | 3.600E-03 | 3.803E-04 | 3.817E-03 | 4.110E-04 | 4.125E-03 |
Table S4 continued

F) SPC/E + Smith-Dang-Garret ions

| Nₐ | Nᵦ | X   | M    | m    |
|----|----|-----|------|------|
| LiCl | 0  | 1   | 4.944E-01 | 7.305E-03 | 9.521E-01 | 1.415E-02 | 9.770E-01 | 1.444E-02 |
|     | 1  | 0   | 4.944E-01 | 7.305E-03 | 9.521E-01 | 1.415E-02 | 9.770E-01 | 1.444E-02 |
|     | 1  | 1   | 1.119E-02 | 1.461E-02 | 2.155E-02 | 2.813E-02 | 2.211E-02 | 2.887E-02 |
| LiI  | 0  | 1   | 4.997E-01 | 1.643E-03 | 9.425E-01 | 3.407E-03 | 9.980E-01 | 3.281E-03 |
|     | 1  | 0   | 4.997E-01 | 1.643E-03 | 9.425E-01 | 3.407E-03 | 9.980E-01 | 3.281E-03 |
|     | 1  | 1   | 5.906E-04 | 3.285E-03 | 1.114E-03 | 6.197E-03 | 1.179E-03 | 6.561E-03 |
| NaF  | 0  | 1   | 4.506E-01 | 2.147E-02 | 8.140E-01 | 3.881E-02 | 8.030E-01 | 3.826E-02 |
|     | 1  | 0   | 4.486E-01 | 2.172E-02 | 8.104E-01 | 3.926E-02 | 7.994E-01 | 3.870E-02 |
|     | 1  | 1   | 8.273E-02 | 3.809E-02 | 1.494E-01 | 6.881E-02 | 1.474E-01 | 6.788E-02 |
|     | 1  | 2   | 6.726E-03 | 1.189E-02 | 1.215E-02 | 2.148E-02 | 1.198E-02 | 2.119E-02 |
|     | 2  | 1   | 8.858E-03 | 1.206E-02 | 1.660E-02 | 2.179E-02 | 1.578E-02 | 2.150E-02 |
|     | 2  | 2   | 2.224E-03 | 6.597E-03 | 4.017E-03 | 1.92E-03  | 3.963E-03 | 1.176E-02 |
|     | 2  | 3   | 1.409E-04 | 1.800E-03 | 2.546E-04 | 3.251E-03 | 2.512E-04 | 3.207E-03 |
|     | 3  | 2   | 4.255E-06 | 3.099E-04 | 7.686E-06 | 5.435E-04 | 7.583E-06 | 5.361E-04 |
|     | 3  | 3   | 5.444E-05 | 1.088E-03 | 9.834E-05 | 1.964E-03 | 9.702E-05 | 1.938E-03 |
| NaCl | 0  | 1   | 4.805E-01 | 1.364E-02 | 9.008E-01 | 2.561E-02 | 9.196E-01 | 2.610E-02 |
|     | 1  | 0   | 4.791E-01 | 1.412E-02 | 8.981E-01 | 2.652E-02 | 9.168E-01 | 2.703E-02 |
|     | 1  | 1   | 3.699E-02 | 2.595E-02 | 6.935E-02 | 4.866E-02 | 7.079E-02 | 4.967E-02 |
|     | 1  | 2   | 7.393E-04 | 3.795E-03 | 1.386E-03 | 7.114E-03 | 1.415E-03 | 7.262E-03 |
|     | 2  | 1   | 2.317E-03 | 6.757E-03 | 4.344E-03 | 1.267E-02 | 4.434E-03 | 1.293E-02 |
|     | 1  | 3   | 6.270E-05 | 1.124E-03 | 1.75E-04  | 2.108E-03 | 1.200E-04 | 2.152E-03 |
|     | 2  | 2   | 2.343E-04 | 2.182E-03 | 4.392E-04 | 4.091E-03 | 4.483E-04 | 4.176E-03 |
|     | 3  | 1   | 6.122E-06 | 3.534E-04 | 1.148E-05 | 6.626E-04 | 1.172E-05 | 6.763E-04 |
|     | 2  | 3   | 1.458E-05 | 5.510E-04 | 2.734E-05 | 1.033E-03 | 2.791E-05 | 1.054E-03 |
|     | 3  | 2   | 1.004E-05 | 4.489E-04 | 1.882E-05 | 8.416E-04 | 1.921E-05 | 8.591E-04 |
|     | 3  | 3   | 2.245E-05 | 6.765E-04 | 4.208E-05 | 1.268E-03 | 4.296E-05 | 1.295E-03 |
| NaI  | 0  | 1   | 4.902E-01 | 9.375E-03 | 9.123E-01 | 1.750E-02 | 9.601E-01 | 1.836E-02 |
|     | 1  | 0   | 4.900E-01 | 9.528E-03 | 9.119E-01 | 1.779E-02 | 9.597E-01 | 1.866E-02 |
|     | 1  | 1   | 1.949E-02 | 1.862E-02 | 3.628E-02 | 3.466E-02 | 3.818E-02 | 3.647E-02 |
|     | 1  | 2   | 8.387E-05 | 1.276E-03 | 1.561E-04 | 2.376E-03 | 1.643E-04 | 2.500E-03 |
|     | 2  | 1   | 2.867E-04 | 2.348E-03 | 5.337E-04 | 4.370E-03 | 5.616E-04 | 4.599E-03 |
|     | 2  | 2   | 1.961E-06 | 1.961E-04 | 3.649E-06 | 3.649E-04 | 3.841E-06 | 3.840E-04 |
Table S4 continued

F) SPC/E + Smith-Dang-Garret ions

|   | KF       | KCl      | KI       |
|---|----------|----------|----------|
| 0 | 1 4.617E-01 1.974E-02 8.533E-01 3.652E-02 8.528E-01 3.646E-02 |
| 1 | 0 4.628E-01 1.932E-02 8.554E-01 3.574E-02 8.548E-01 3.569E-02 |
| 1 | 1 6.992E-02 3.660E-02 1.292E-01 6.765E-02 1.292E-01 6.760E-02 |
| 1 | 2 3.107E-03 8.058E-03 5.743E-03 1.489E-02 5.739E-03 1.488E-02 |
| 2 | 1 1.979E-03 6.333E-03 3.657E-03 1.171E-02 3.655E-03 1.170E-02 |
| 2 | 2 5.003E-04 3.237E-03 9.248E-04 5.984E-03 9.242E-04 5.980E-03 |
|   | KCl      | KCl      | KCl      |
| 0 | 1 4.097E-01 3.064E-02 6.340E-01 4.743E-02 6.569E-01 4.913E-02 |
| 1 | 0 4.059E-01 3.186E-02 6.282E-01 4.932E-02 6.509E-01 5.109E-02 |
| 1 | 1 1.422E-01 5.118E-02 2.201E-01 7.921E-02 2.880E-01 8.207E-02 |
| 1 | 2 1.263E-02 1.667E-02 1.954E-02 2.579E-02 2.025E-02 2.672E-02 |
| 2 | 1 1.589E-02 1.919E-02 2.459E-02 2.970E-02 2.548E-02 3.077E-02 |
| 1 | 3 4.504E-04 3.288E-03 6.970E-04 5.089E-03 7.221E-04 5.272E-03 |
| 2 | 2 8.519E-03 1.391E-02 1.318E-02 2.153E-02 1.366E-02 2.231E-02 |
| 3 | 1 5.555E-04 3.621E-03 8.597E-04 5.603E-03 8.907E-04 5.805E-03 |
| 2 | 3 1.200E-03 5.462E-03 1.858E-03 8.453E-03 1.925E-03 8.758E-03 |
| 3 | 2 1.487E-03 5.926E-03 2.301E-03 9.171E-03 2.384E-03 9.502E-03 |
| 3 | 3 7.653E-04 4.288E-03 1.184E-03 6.637E-03 1.227E-03 6.877E-03 |
| 4 | 2 1.090E-04 1.623E-03 1.686E-04 2.512E-03 1.747E-04 2.602E-03 |
| 3 | 4 1.381E-04 1.865E-03 2.138E-04 2.886E-03 2.215E-04 2.990E-03 |
| 4 | 3 1.466E-04 1.890E-03 2.266E-04 2.925E-03 2.350E-04 3.031E-03 |
|   | KI       | KI       | KI       |
| 0 | 1 3.893E-01 3.657E-02 5.448E-01 5.118E-02 5.816E-01 5.463E-02 |
| 1 | 0 3.852E-01 3.827E-02 5.390E-01 5.356E-02 5.754E-01 5.716E-02 |
| 1 | 1 1.571E-01 5.760E-02 2.199E-01 8.061E-02 2.347E-01 8.605E-02 |
| 1 | 2 2.001E-02 2.231E-02 2.800E-02 3.123E-02 2.988E-02 3.333E-02 |
| 2 | 1 2.149E-02 2.287E-02 3.008E-02 3.201E-02 3.211E-02 3.417E-02 |
| 1 | 3 8.061E-04 4.455E-03 1.128E-03 6.235E-03 1.204E-03 6.655E-03 |
| 2 | 2 1.399E-02 1.858E-02 1.958E-02 2.601E-02 2.090E-02 2.776E-02 |
| 3 | 1 1.389E-03 5.913E-03 1.944E-03 8.275E-03 2.075E-03 8.833E-03 |
| 2 | 3 2.668E-03 8.154E-03 3.733E-03 1.141E-02 3.985E-03 1.218E-02 |
| 3 | 2 4.066E-03 1.011E-02 5.691E-03 1.415E-02 6.074E-03 1.510E-02 |
| 2 | 4 2.690E-04 2.713E-03 3.765E-04 3.796E-03 4.019E-04 4.052E-03 |
| 3 | 3 1.936E-02 7.237E-03 2.710E-03 1.013E-02 2.893E-03 1.081E-02 |
| 4 | 2 3.495E-04 3.042E-03 4.891E-04 4.256E-03 5.220E-04 4.543E-03 |
| 3 | 4 3.798E-04 3.163E-03 5.315E-04 4.426E-03 5.673E-04 4.724E-03 |
| 4 | 3 4.654E-04 3.487E-03 6.513E-04 4.880E-03 6.953E-04 5.209E-03 |
| 4 | 4 2.386E-04 2.524E-03 3.339E-04 3.533E-03 3.564E-04 3.771E-03 |
Table S4 continued

F) SPC/E + Smith-Dang-Garret ions

|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| RbF |   |   |   |   |   |   |   |
| 0  | 1 | 4.619E-01 | 1.973E-02 | 8.520E-01 | 3.643E-02 | 8.544E-01 | 3.650E-02 |
| 1  | 0 | 4.632E-01 | 1.890E-02 | 8.545E-01 | 3.489E-02 | 8.569E-01 | 3.495E-02 |
| 1  | 1 | 7.016E-02 | 3.610E-02 | 1.294E-01 | 6.659E-02 | 1.298E-01 | 6.678E-02 |
| 1  | 2 | 2.765E-03 | 7.604E-03 | 5.101E-03 | 1.403E-02 | 5.115E-03 | 1.407E-02 |
| 2  | 1 | 1.460E-03 | 5.488E-03 | 2.693E-03 | 1.012E-02 | 2.700E-03 | 1.015E-02 |
| 2  | 2 | 4.249E-04 | 2.961E-03 | 7.838E-04 | 5.463E-03 | 7.860E-04 | 5.478E-03 |
| RbCl |   |   |   |   |   |   |   |
| 0  | 1 | 3.920E-01 | 3.486E-02 | 5.762E-01 | 5.125E-02 | 5.994E-01 | 5.331E-02 |
| 1  | 0 | 3.909E-01 | 3.299E-02 | 5.746E-01 | 4.850E-02 | 5.977E-01 | 5.044E-02 |
| 1  | 1 | 1.584E-01 | 5.683E-02 | 2.326E-01 | 8.354E-02 | 2.423E-01 | 8.690E-02 |
| 1  | 2 | 1.908E-02 | 2.048E-02 | 2.805E-02 | 3.010E-02 | 2.918E-02 | 3.131E-02 |
| 2  | 1 | 1.974E-02 | 2.114E-02 | 2.902E-02 | 3.107E-02 | 3.019E-02 | 3.232E-02 |
| 2  | 2 | 6.437E-04 | 3.988E-03 | 9.462E-04 | 6.082E-03 | 9.843E-04 | 6.098E-03 |
| 2  | 3 | 1.130E-02 | 1.663E-02 | 1.662E-02 | 2.445E-02 | 1.728E-02 | 2.543E-02 |
| 3  | 1 | 9.021E-04 | 4.639E-03 | 1.326E-03 | 6.818E-03 | 1.379E-03 | 7.093E-03 |
| 2  | 3 | 2.200E-03 | 7.486E-03 | 3.233E-03 | 1.101E-02 | 3.363E-03 | 1.145E-02 |
| 3  | 2 | 2.147E-03 | 7.243E-03 | 3.156E-03 | 1.065E-02 | 3.283E-03 | 1.107E-02 |
| 3  | 3 | 1.273E-03 | 5.689E-03 | 1.871E-03 | 8.363E-03 | 1.946E-03 | 8.699E-03 |
| 3  | 4 | 3.748E-04 | 3.097E-03 | 5.509E-04 | 4.553E-03 | 5.730E-04 | 4.736E-03 |
| 4  | 3 | 2.917E-04 | 2.747E-03 | 4.288E-04 | 4.038E-03 | 4.460E-04 | 4.201E-03 |
| 4  | 4 | 2.707E-04 | 2.659E-03 | 3.979E-04 | 3.909E-03 | 4.139E-04 | 4.066E-03 |
| RbI |   |   |   |   |   |   |   |
| 0  | 1 | 3.681E-01 | 4.018E-02 | 4.807E-01 | 5.247E-02 | 5.150E-01 | 5.621E-02 |
| 1  | 0 | 3.625E-01 | 4.042E-02 | 4.733E-01 | 5.278E-02 | 5.071E-01 | 5.654E-02 |
| 1  | 1 | 1.794E-01 | 6.125E-02 | 2.343E-01 | 7.998E-02 | 2.510E-01 | 8.568E-02 |
| 1  | 2 | 2.518E-02 | 2.541E-02 | 3.286E-02 | 3.319E-02 | 3.522E-02 | 3.555E-02 |
| 2  | 1 | 2.646E-02 | 2.590E-02 | 3.455E-02 | 3.382E-02 | 3.702E-02 | 3.623E-02 |
| 1  | 3 | 9.830E-04 | 5.190E-03 | 1.284E-03 | 6.777E-03 | 1.375E-03 | 7.261E-03 |
| 2  | 2 | 1.776E-02 | 2.100E-02 | 2.319E-02 | 2.742E-02 | 2.484E-02 | 2.938E-02 |
| 3  | 1 | 1.916E-03 | 7.404E-03 | 2.502E-03 | 9.668E-03 | 2.680E-03 | 1.036E-02 |
| 2  | 3 | 4.385E-03 | 1.080E-02 | 5.726E-03 | 1.410E-02 | 6.134E-03 | 1.511E-02 |
| 3  | 2 | 5.458E-03 | 1.175E-02 | 7.127E-03 | 1.534E-02 | 7.636E-03 | 1.643E-02 |
| 2  | 4 | 3.578E-04 | 3.142E-03 | 4.673E-04 | 4.104E-03 | 5.006E-04 | 4.396E-03 |
| 3  | 3 | 3.550E-03 | 9.897E-03 | 4.636E-03 | 1.292E-02 | 4.966E-03 | 1.385E-02 |
| 4  | 2 | 6.237E-04 | 4.202E-03 | 8.145E-04 | 5.487E-03 | 8.726E-04 | 5.878E-03 |
| 3  | 4 | 7.315E-04 | 4.515E-03 | 9.553E-04 | 5.895E-03 | 1.023E-03 | 6.316E-03 |
| 4  | 3 | 9.407E-04 | 5.134E-03 | 1.228E-03 | 6.704E-03 | 1.316E-03 | 7.182E-03 |
| 4  | 4 | 6.224E-04 | 4.144E-03 | 8.128E-04 | 5.412E-03 | 8.708E-04 | 5.798E-03 |
| 5  | 4 | 2.101E-04 | 2.440E-03 | 2.744E-04 | 3.186E-03 | 2.939E-04 | 3.413E-03 |
Table S4 continued

F) SPC/E + Smith-Dang-Garret ions

|        | CsF          |           |           |           |           |           |           |           |           |
|--------|--------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |

CsCl

|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|--------|--------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |

CsI

|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|--------|--------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |
|        |              | 0         | 1         | 2         | 3         | 4         | 5         | 6         | 7         |

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Table S5. Association constants of cation-anion pairs at 1 \( m \).
A) Ion concentrations listed in Table S4 were used to calculate the constants in terms of both molar and molal concentration. B) Association constants were calculated using Fuoss’ Gurney radii to define free ions and ion pairs. The radii used are listed in Table 2 of Fuoss’ article.\(^53\)

A)  

| Salt        | \( K_M (M^-) \)  | \( K_m (m^-) \)  |
|-------------|------------------|------------------|
| **TIP3P / TIP3P-compatible ions** |                  |                  |
| LiCl        | 0.493 ± 0.172    | 0.477 ± 0.166    |
| LiBr        | 0.0883 ± 0.0621  | 0.0847 ± 0.0595  |
| LiI         | 0.00816 ± 0.0183 | 0.00769 ± 0.0173 |
| NaF         | 0.143 ± 0.0819   | 0.143 ± 0.0820   |
| NaCl        | 0.118 ± 0.0738   | 0.115 ± 0.0718   |
| NaBr        | 0.0936 ± 0.0645  | 0.0902 ± 0.0621  |
| NaI         | 0.0511 ± 0.0459  | 0.0484 ± 0.0434  |
| KF          | 0.196 ± 0.0979   | 0.194 ± 0.0971   |
| KCl         | 0.290 ± 0.128    | 0.280 ± 0.124    |
| KBr         | 0.313 ± 0.138    | 0.299 ± 0.132    |
| KI          | 0.280 ± 0.128    | 0.263 ± 0.120    |
| RbF         | 0.182 ± 0.0930   | 0.179 ± 0.0919   |
| RbCl        | 0.334 ± 0.143    | 0.321 ± 0.137    |
| RbBr        | 0.359 ± 0.151    | 0.341 ± 0.144    |
| RbI         | 0.353 ± 0.150    | 0.330 ± 0.140    |
| CsF         | 0.189 ± 0.0963   | 0.186 ± 0.0946   |
| CsCl        | 0.413 ± 0.166    | 0.394 ± 0.159    |
| CsBr        | 0.470 ± 0.186    | 0.444 ± 0.175    |
| CsI         | 0.507 ± 0.198    | 0.471 ± 0.184    |
| **TIP4P\(_{\text{EW}}\) / TIP4P\(_{\text{EW}}\)-compatible ions** |                  |                  |
| LiCl        | 0.0262 ± 0.0456  | 0.0255 ± 0.0444  |
| LiBr        | 0.0156 ± 0.0303  | 0.0150 ± 0.0292  |
| LiI         | 0.00370 ± 0.0129 | 0.00351 ± 0.0122 |
| NaF         | 0.0118 ± 0.0216  | 0.0120 ± 0.0218  |
| NaCl        | 0.0294 ± 0.0320  | 0.0289 ± 0.0315  |
| NaBr        | 0.0322 ± 0.0359  | 0.0313 ± 0.0349  |
| NaI         | 0.0286 ± 0.0342  | 0.0274 ± 0.0328  |
| KF          | 0.0736 ± 0.0570  | 0.0737 ± 0.0571  |
| KCl         | 0.177 ± 0.0943   | 0.172 ± 0.0916   |
| KBr         | 0.224 ± 0.106    | 0.216 ± 0.102    |
| KI          | 0.241 ± 0.113    | 0.228 ± 0.107    |
| RbF         | 0.0811 ± 0.0576  | 0.0809 ± 0.0574  |
| RbCl        | 0.235 ± 0.112    | 0.227 ± 0.108    |
| RbBr        | 0.306 ± 0.131    | 0.293 ± 0.126    |
| RbI         | 0.366 ± 0.154    | 0.345 ± 0.146    |
| CsF         | 0.136 ± 0.0784   | 0.134 ± 0.0777   |
| CsCl        | 0.390 ± 0.160    | 0.375 ± 0.154    |
| CsBr        | 0.556 ± 0.214    | 0.529 ± 0.204    |
| CsI         | 0.630 ± 0.238    | 0.591 ± 0.223    |
|                | SPC/E / SPC/E-compatible ions | TIP3P / Smith-Dang-Garrett ions | TIP4P_Ew / Smith-Dang-Garrett ions |
|----------------|-------------------------------|---------------------------------|-----------------------------------|
| LiCl           | 0.00378 ± 0.0115 0.00370 ± 0.0113 | 0.0610 ± 0.0549 0.0588 ± 0.0529 | 0.0827 ± 0.0621 0.0809 ± 0.0608 |
| LiBr           | 0.00208 ± 0.00879 0.00202 ± 0.00851 | NaF 0.483 ± 0.491 0.479 ± 0.486 | NaF 0.193 ± 0.102 0.195 ± 0.103 |
| LiI            | 0.000556 ± 0.00466 0.000529 ± 0.00444 | NaCl 0.105 ± 0.0680 0.101 ± 0.0658 | NaCl 0.126 ± 0.0702 0.123 ± 0.0688 |
| NaF            | 0.0215 ± 0.0276 0.0218 ± 0.0280 | NaI 0.0376 ± 0.0403 0.0353 ± 0.0378 | NaI 0.0663 ± 0.0570 0.063 ± 0.0542 |
| NaCl           | 0.0207 ± 0.0286 0.0203 ± 0.0281 | KF 0.236 ± 0.111 0.233 ± 0.110 | KF 0.120 ± 0.0733 0.120 ± 0.0732 |
| NaBr           | 0.0243 ± 0.0305 0.0237 ± 0.0297 | KCl 0.515 ± 0.204 0.492 ± 0.195 | KCl 0.603 ± 0.231 0.581 ± 0.223 |
| NaI            | 0.0220 ± 0.0298 0.0211 ± 0.0286 | KBr 0.177 ± 0.0951 0.168 ± 0.0902 | KBr 0.135 ± 0.0780 0.135 ± 0.0780 |
| KF             | 0.0956 ± 0.0631 0.0959 ± 0.0634 | RbF 0.234 ± 0.109 0.227 ± 0.105 | RbF 0.207 ± 0.103 0.204 ± 0.102 |
| KCl            | 0.143 ± 0.0836 0.139 ± 0.0815 | RbCl 0.306 ± 0.137 0.289 ± 0.129 | RbCl 0.630 ± 0.245 0.600 ± 0.233 |
| KBr            | 0.168 ± 0.0898 0.162 ± 0.0866 | RbCl 0.275 ± 0.126 0.265 ± 0.121 | RbCl 0.724 ± 0.279 0.669 ± 0.258 |
| KI             | 0.177 ± 0.0951 0.168 ± 0.0902 | CsF 0.293 ± 0.127 0.290 ± 0.126 | CsF 0.175 ± 0.0904 0.171 ± 0.0884 |
| RbF            | 0.135 ± 0.0780 0.135 ± 0.0780 | CsCl 0.900 ± 0.335 0.866 ± 0.322 | CsCl 0.815 ± 0.301 0.770 ± 0.284 |
| RbCl           | 0.234 ± 0.109 0.227 ± 0.105 | CsBr 1.07 ± 0.407 1.020 ± 0.388 | CsBr 1.14 ± 0.444 1.05 ± 0.407 |
| RbBr           | 0.275 ± 0.126 0.265 ± 0.121 | CsI 1.18 ± 0.500 1.110 ± 0.469 | CsI 0.114 ± 0.072 0.113 ± 0.071 |
| Rbl            | 0.306 ± 0.137 0.289 ± 0.129 |                  |                  |
| Salt     | $K_M (M^{-1})$ | $K_m (m^{-1})$ |
|----------|----------------|----------------|
| **SPC/E / Smith-Dang-Garrett ions** |
| LiCl     | 0.0238 ± 0.0310 | 0.0232 ± 0.0302 |
| LiI      | 0.00125 ± 0.00698 | 0.00118 ± 0.00659 |
| NaF      | 0.227 ± 0.105 | 0.230 ± 0.107 |
| NaCl     | 0.0857 ± 0.0602 | 0.0840 ± 0.0590 |
| NaI      | 0.0436 ± 0.0417 | 0.0414 ± 0.0396 |
| KF       | 0.177 ± 0.0933 | 0.177 ± 0.0933 |
| KCl      | 0.553 ± 0.208 | 0.533 ± 0.200 |
| KI       | 0.749 ± 0.293 | 0.701 ± 0.274 |
| RbF      | 0.178 ± 0.0921 | 0.177 ± 0.0918 |
| RbCl     | 0.703 ± 0.267 | 0.676 ± 0.256 |
| RbI      | 1.03 ± 0.387 | 0.961 ± 0.361 |
| CsF      | 0.177 ± 0.0906 | 0.175 ± 0.0897 |
| CsCl     | 0.982 ± 0.358 | 0.937 ± 0.342 |
| CsI      | 1.61 ± 0.657 | 1.49 ± 0.609 |

| Salt     | $K_M (M^{-1})$ | $K_m (m^{-1})$ |
|----------|----------------|----------------|
| **TIP3P / TIP3P-compatible ions** |
| LiCl     | 1.44 ± 0.560 | 1.39 ± 0.542 |
| LiBr     | 0.850 ± 0.323 | 0.815 ± 0.309 |
| LiI      | 0.751 ± 0.285 | 0.708 ± 0.268 |
| NaF      | 1.14 ± 0.452 | 1.14 ± 0.452 |
| NaCl     | 0.980 ± 0.379 | 0.953 ± 0.369 |
| NaBr     | 0.929 ± 0.358 | 0.895 ± 0.345 |
| NaI      | 0.843 ± 0.326 | 0.798 ± 0.309 |
| KCl      | 0.354 ± 0.149 | 0.341 ± 0.143 |
| KBr      | 0.374 ± 0.157 | 0.357 ± 0.150 |
| KI       | 0.341 ± 0.146 | 0.320 ± 0.137 |
| RbF      | 0.214 ± 0.103 | 0.211 ± 0.102 |
| RbCl     | 0.109 ± 0.0698 | 0.105 ± 0.0670 |
| RbBr     | 0.112 ± 0.0715 | 0.106 ± 0.0679 |
| RbI      | 0.113 ± 0.0722 | 0.105 ± 0.0675 |
| CsF      | 0.649 ± 0.239 | 0.637 ± 0.235 |
| CsCl     | 0.142 ± 0.0810 | 0.135 ± 0.0773 |
| CsBr     | 0.154 ± 0.0862 | 0.145 ± 0.0815 |
| CsI      | 0.171 ± 0.0915 | 0.159 ± 0.0851 |

| Salt     | $K_M (M^{-1})$ | $K_m (m^{-1})$ |
|----------|----------------|----------------|
| **TIP4P_{EW} / TIP4P_{EW}-compatible ions** |
| LiCl     | 0.969 ± 0.366 | 0.944 ± 0.357 |
| LiBr     | 0.918 ± 0.335 | 0.885 ± 0.323 |
| LiI      | 0.872 ± 0.326 | 0.827 ± 0.309 |
| NaF      | 1.30 ± 0.506 | 1.31 ± 0.512 |
| NaCl     | 1.03 ± 0.390 | 1.01 ± 0.383 |
| NaBr     | 1.02 ± 0.382 | 0.989 ± 0.372 |
| NaI      | 0.916 ± 0.348 | 0.877 ± 0.334 |
| KCl      | 0.283 ± 0.128 | 0.275 ± 0.125 |
| KBr      | 0.321 ± 0.136 | 0.309 ± 0.131 |
|       | SPC/E / SPC/E-compatible ions       | TIP3P / Smith-Dang-Garrettions | TIP4P/Ew / Smith-Dang-Garrettions |
|-------|-------------------------------------|-------------------------------|-----------------------------------|
| KI    | 0.340 ± 0.144 0.322 ± 0.136        |                               |                                   |
| RbF   | 0.132 ± 0.0770 0.132 ± 0.0768      |                               |                                   |
| RbCl  | 0.0608 ± 0.0517 0.0589 ± 0.0500    |                               |                                   |
| RbBr  | 0.0841 ± 0.0605 0.0806 ± 0.0580    |                               |                                   |
| RbI   | 0.102 ± 0.0688 0.0966 ± 0.0649     |                               |                                   |
| CsF   | 0.806 ± 0.293 0.799 ± 0.291        |                               |                                   |
| CsCl  | 0.135 ± 0.0795 0.130 ± 0.0764      |                               |                                   |
| CsBr  | 0.187 ± 0.0960 0.178 ± 0.0914      |                               |                                   |
| CsI   | 0.224 ± 0.109 0.210 ± 0.102        |                               |                                   |
| LiCl  | 0.877 ± 0.339 0.858 ± 0.332        |                               |                                   |
| LiBr  | 0.804 ± 0.300 0.779 ± 0.290        |                               |                                   |
| LiI   | 0.785 ± 0.296 0.748 ± 0.282        |                               |                                   |
| NaF   | 1.21 ± 0.490 1.22 ± 0.497          |                               |                                   |
| NaCl  | 0.882 ± 0.334 0.868 ± 0.328        |                               |                                   |
| NaBr  | 0.916 ± 0.354 0.892 ± 0.345        |                               |                                   |
| NaI   | 0.837 ± 0.319 0.802 ± 0.306        |                               |                                   |
| KCl   | 0.225 ± 0.108 0.219 ± 0.105        |                               |                                   |
| KBr   | 0.249 ± 0.114 0.240 ± 0.110        |                               |                                   |
| KI    | 0.250 ± 0.119 0.237 ± 0.113        |                               |                                   |
| RbF   | 0.180 ± 0.0925 0.180 ± 0.0925      |                               |                                   |
| RbCl  | 0.0655 ± 0.0520 0.0636 ± 0.0505    |                               |                                   |
| RbBr  | 0.0820 ± 0.0605 0.0787 ± 0.0581    |                               |                                   |
| RbI   | 0.0913 ± 0.0644 0.0862 ± 0.0608    |                               |                                   |
| CsF   | 1.12 ± 0.402 1.11 ± 0.399          |                               |                                   |
| CsCl  | 0.576 ± 0.222 0.554 ± 0.214        |                               |                                   |
| CsBr  | 0.665 ± 0.255 0.633 ± 0.243        |                               |                                   |
| CsI   | 0.739 ± 0.303 0.693 ± 0.284        |                               |                                   |
| LiCl  | 0.742 ± 0.277 0.716 ± 0.267        |                               |                                   |
| LiI   | 0.673 ± 0.256 0.629 ± 0.240        |                               |                                   |
| NaF   | 1.42 ± 1.10 1.41 ± 1.09            |                               |                                   |
| NaCl  | 0.872 ± 0.337 0.844 ± 0.326        |                               |                                   |
| NaI   | 0.731 ± 0.280 0.687 ± 0.263        |                               |                                   |
| KCl   | 0.559 ± 0.219 0.533 ± 0.209        |                               |                                   |
| KI    | 0.564 ± 0.219 0.523 ± 0.203        |                               |                                   |
| RbF   | 0.221 ± 0.108 0.218 ± 0.106        |                               |                                   |
| RbCl  | 0.128 ± 0.0775 0.121 ± 0.0737      |                               |                                   |
| RbI   | 0.146 ± 0.0839 0.135 ± 0.0775      |                               |                                   |
| CsF   | 0.520 ± 0.199 0.508 ± 0.195        |                               |                                   |
| CsCl  | 0.193 ± 0.0984 0.183 ± 0.0929      |                               |                                   |
| CsBr  | 0.273 ± 0.126 0.250 ± 0.115        |                               |                                   |
| CsI   | 0.925 ± 0.352 0.881 ± 0.335        |                               |                                   |
| Salt      | $K_M (M^{-1})$ | $K_m (m^{-1})$ |
|-----------|----------------|----------------|
| LiCl      | 1.44           | 1.39           | 0.969 ± 0.366 | 0.944 ± 0.357 |
| LiBr      | 0.850          | 0.815          | 0.918 ± 0.335 | 0.885 ± 0.323 |
| LiI       | 0.751          | 0.708          | 0.872 ± 0.326 | 0.827 ± 0.309 |
| NaF       | 1.14           | 1.14           | 0.687 ± 0.259 | 0.662 ± 0.249 |
| NaCl      | 0.980          | 0.953          | 0.969 ± 0.374 | 0.907 ± 0.350 |
| NaBr      | 0.929          | 0.895          | 0.917 ± 0.358 | 0.850 ± 0.309 |
| NaI       | 0.843          | 0.798          | 0.843 ± 0.326 | 0.815 ± 0.309 |
| KCl       | 0.354          | 0.341          | 0.697 ± 0.124 | 0.662 ± 0.104 |
| KBr       | 0.374          | 0.357          | 0.374 ± 0.156 | 0.346 ± 0.144 |
| KI        | 0.341          | 0.320          | 0.341 ± 0.146 | 0.313 ± 0.137 |
| RbF       | 0.214          | 0.211          | 0.214 ± 0.103 | 0.209 ± 0.104 |
| RbCl      | 0.109          | 0.105          | 0.109 ± 0.0698 | 0.105 ± 0.0670 |
| RbBr      | 0.112          | 0.106          | 0.112 ± 0.0715 | 0.106 ± 0.0679 |
| Rbl       | 0.113          | 0.105          | 0.113 ± 0.0722 | 0.105 ± 0.0675 |
| CsF       | 0.649          | 0.637          | 0.649 ± 0.239 | 0.637 ± 0.235 |
| CsCl      | 0.142          | 0.135          | 0.142 ± 0.0810 | 0.135 ± 0.0773 |
| CsBr      | 0.154          | 0.145          | 0.154 ± 0.0862 | 0.145 ± 0.0815 |
| CsI       | 0.171          | 0.159          | 0.171 ± 0.0915 | 0.159 ± 0.0851 |

**B)**
|       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|
| NaF   | 1.30  | ± 0.506 | 1.31  | ± 0.512 |
| NaCl  | 1.03  | ± 0.390 | 1.01  | ± 0.383 |
| NaBr  | 1.02  | ± 0.382 | 0.989 | ± 0.372 |
| NaI   | 0.916 | ± 0.348 | 0.877 | ± 0.334 |
| KCl   | 0.283 | ± 0.128 | 0.275 | ± 0.125 |
| KBr   | 0.321 | ± 0.136 | 0.309 | ± 0.131 |
| KI    | 0.340 | ± 0.144 | 0.322 | ± 0.136 |
| RbF   | 0.132 | ± 0.0770 | 0.132 | ± 0.0768 |
| RbCl  | 0.0608 | ± 0.0517 | 0.0589 | ± 0.0500 |
| RbBr  | 0.0841 | ± 0.0605 | 0.0806 | ± 0.0580 |
| RbI   | 0.102 | ± 0.0688 | 0.0966 | ± 0.0649 |
| CsF   | 0.806 | ± 0.293 | 0.799 | ± 0.291 |
| CsCl  | 0.135 | ± 0.0795 | 0.130 | ± 0.0764 |
| CsBr  | 0.187 | ± 0.0960 | 0.178 | ± 0.0914 |
| CsI   | 0.224 | ± 0.109 | 0.210 | ± 0.102 |

**SPC/E / SPC/E-compatible ions**

|       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|
| LiCl  | 0.877 | ± 0.339 | 0.858 | ± 0.332 |
| LiBr  | 0.804 | ± 0.300 | 0.779 | ± 0.290 |
| LiI   | 0.785 | ± 0.296 | 0.748 | ± 0.282 |
| NaF   | 1.21  | ± 0.490 | 1.22  | ± 0.497 |
| NaCl  | 0.882 | ± 0.334 | 0.868 | ± 0.328 |
| NaBr  | 0.916 | ± 0.354 | 0.892 | ± 0.345 |
| NaI   | 0.837 | ± 0.319 | 0.802 | ± 0.306 |
| KCl   | 0.225 | ± 0.108 | 0.219 | ± 0.105 |
| KBr   | 0.249 | ± 0.114 | 0.240 | ± 0.110 |
| KI    | 0.250 | ± 0.119 | 0.237 | ± 0.113 |
| RbF   | 0.180 | ± 0.0925 | 0.180 | ± 0.0925 |
| RbCl  | 0.0655 | ± 0.0520 | 0.0636 | ± 0.0505 |
| RbBr  | 0.0820 | ± 0.0605 | 0.0787 | ± 0.0581 |
| RbI   | 0.0913 | ± 0.0644 | 0.0862 | ± 0.0608 |
| CsF   | 1.12  | ± 0.402 | 1.11  | ± 0.399 |
| CsCl  | 0.576 | ± 0.222 | 0.554 | ± 0.214 |
| CsBr  | 0.665 | ± 0.255 | 0.633 | ± 0.243 |
| CsI   | 0.739 | ± 0.303 | 0.693 | ± 0.284 |

**TIP3P / Smith-Dang-Garrettions**

|       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|
| LiCl  | 0.742 | ± 0.277 | 0.716 | ± 0.267 |
| LiI   | 0.673 | ± 0.256 | 0.629 | ± 0.240 |
| NaF   | 1.42  | ± 1.10  | 1.41  | ± 1.09  |
| NaCl  | 0.872 | ± 0.337 | 0.844 | ± 0.326 |
| NaI   | 0.731 | ± 0.280 | 0.687 | ± 0.263 |
| KCl   | 0.559 | ± 0.219 | 0.533 | ± 0.209 |
| KI    | 0.564 | ± 0.219 | 0.523 | ± 0.203 |
| RbF   | 0.221 | ± 0.108 | 0.218 | ± 0.106 |
| RbCl  | 0.128 | ± 0.0775 | 0.121 | ± 0.0737 |
| RbI   | 0.146 | ± 0.0839 | 0.135 | ± 0.0775 |
| CsF   | 0.520 | ± 0.199 | 0.508 | ± 0.195 |
| CsCl  | 0.193 | ± 0.0984 | 0.183 | ± 0.0929 |
| CsI   | 0.273 | ± 0.126 | 0.250 | ± 0.115 |
|                | TIP4P<sub>EW</sub> / Smith-Dang-Garrettions | SPC/E / Smith-Dang-Garrettions |
|----------------|---------------------------------------------|---------------------------------|
| LiCl           | 0.970 ± 0.355 0.949 ± 0.348                 | 0.821 ± 0.310 0.800 ± 0.302     |
| LiI            | 0.762 ± 0.291 0.724 ± 0.276                 | 0.760 ± 0.282 0.718 ± 0.267     |
| NaF            | 2.02 ± 0.887 2.04 ± 0.898                   | 1.77 ± 0.758 1.80 ± 0.769       |
| NaCl           | 1.21 ± 0.457 1.19 ± 0.448                   | 0.985 ± 0.391 0.965 ± 0.383     |
| NaI            | 0.925 ± 0.352 0.881 ± 0.335                 | 0.792 ± 0.300 0.752 ± 0.285     |
| KCl            | 0.687 ± 0.259 0.662 ± 0.249                 | 0.618 ± 0.228 0.597 ± 0.220     |
| KI             | 0.969 ± 0.374 0.907 ± 0.350                 | 0.796 ± 0.309 0.746 ± 0.290     |
| RbF            | 0.170 ± 0.0909 0.170 ± 0.0904               | 0.214 ± 0.103 0.214 ± 0.103     |
| RbCl           | 0.112 ± 0.0712 0.107 ± 0.0684               | 0.212 ± 0.0738 0.117 ± 0.0709   |
| RbI            | 0.209 ± 0.104 0.195 ± 0.0973                | 0.182 ± 0.0955 0.170 ± 0.0891   |
| CsF            | 0.678 ± 0.252 0.669 ± 0.249                 | 0.750 ± 0.264 0.743 ± 0.261     |
| CsCl           | 0.174 ± 0.0924 0.166 ± 0.0880               | 0.189 ± 0.0968 0.181 ± 0.0923   |
| CsI            | 0.374 ± 0.156 0.346 ± 0.144                 | 0.338 ± 0.148 0.313 ± 0.137     |
Table S6. The calculated residence times of alkali cation-halide anion, water-alkali cation, and water-halide anions (in ps).

A) Cation-Anion

| Water-model specific Ions | Smith-Dang-Garrett Ions |
|---------------------------|-------------------------|
|                           | TIP3P                   | TIP4P_EW               | SPC/E               |
|                           | Li⁺  | Na⁺  | K⁺   | Rb⁺  | Cs⁺  | Li⁺  | Na⁺  | K⁺   | Rb⁺  | Cs⁺  | Li⁺  | Na⁺  | K⁺   | Rb⁺  | Cs⁺  |
| F⁻                          | -    | 51.3 | 10.1 | 7.0  | 5.7  | F⁻    | -    | 297.2| 8.5  | 6.9  | 4.6  |
| Cl⁻                         | 404.2| 32.7 | 13.3 | 9.8  | 8.7  | Cl⁻   | 54.7 | 15.5 | 14.5 | 13.7 | 12.5 |
| Br⁻                         | 164.0| 23.4 | 13.3 | 10.2 | 9.5  | Br⁻   | 45.2 | 19.0 | 13.8 | 13.7 | 12.4 |
| I⁻                          | 38.9 | 11.7 | 11.2 | 9.9  | 10.2 | I⁻    | 8.4  | 5.7  | 12.5 | 14.3 | 16.9 |

B) Water-Cation

| Water-model specific Ions | Smith-Dang-Garrett Ions |
|---------------------------|-------------------------|
|                           | TIP3P                   | TIP4P_EW               | SPC/E               |
|                           | Li⁺  | Na⁺  | K⁺   | Rb⁺  | Cs⁺  | Li⁺  | Na⁺  | K⁺   | Rb⁺  | Cs⁺  | Li⁺  | Na⁺  | K⁺   | Rb⁺  | Cs⁺  |
| F⁻                          | -    | 8.4  | 4.9  | 5.1  | 8.5  | F⁻    | -    | 52.7 | 6.7  | 5.8  | -    | 19.1 | 19.0 | 19.0 |
| Cl⁻                         | 20.6 | 5.7  | 6.5  | 7.0  | 18.2 | Cl⁻   | 57.4 | 15.5 | 14.5 | 14.7 | 13.8 |
| Br⁻                         | 23.3 | 6.3  | 7.2  | 8.3  | 20.9 | Br⁻   | 41.4 | 9.9  | 17.6 | 21.4 | 21.0 |
| I⁻                          | 9.3  | 4.9  | 6.9  | 8.9  | 24.7 | I⁻    | 5.8  | 6.7  | 17.0 | 19.1 | 23.9 |
### C) Water-Anion

|                | Li⁺ | Na⁺ | K⁺ | Rb⁺ | Cs⁺ | Avg  | Li⁺ | Na⁺ | K⁺ | Rb⁺ | Cs⁺ | Avg  |
|----------------|-----|-----|----|-----|-----|------|-----|-----|----|-----|-----|------|
| **TIP3P**      |     |     |    |     |     |      |     |     |    |     |     |      |
| F⁻             | -   | 16.2| 16.1| 16.3| 16.5| 16.3 | F⁻  | -   | 14.2| 10.8| 10.9| 11.0| 11.7 |
| Cl⁻            | 10.1| 6.6 | 6.3 | 6.4 | 6.5 | 7.2  | Cl⁻ | 5.3 | 5.1 | 4.8 | 4.8 | 4.9 | 5.0  |
| Br⁻            | 6.5 | 5.7 | 5.4 | 5.4 | 5.5 | 5.7  | Br⁻ | 3.8 | 3.8 | 3.6 | 3.5 | 3.6 | 3.7  |
| I⁻             | 4.7 | 4.6 | 4.4 | 4.4 | 4.4 | 4.5  | I⁻  | 3.8 | 3.8 | 3.6 | 3.5 | 3.6 | 3.7  |
| **TIP4P**      |     |     |    |     |     |      |     |     |    |     |     |      |
| F⁻             | -   | 19.0| 18.5| 18.5| 18.5| 18.6 | F⁻  | -   | 19.6| 19.0| 19.1| 19.2| 19.2 |
| Cl⁻            | 8.5 | 8.4 | 8.0 | 8.0 | 8.0 | 8.2  | Cl⁻ | 7.8 | 7.8 | 7.3 | 7.4 | 7.5 | 7.5  |
| Br⁻            | 7.4 | 7.3 | 6.9 | 6.9 | 6.9 | 7.1  | Br⁻ | 5.5 | 5.6 | 5.2 | 5.1 | 5.2 | 5.3  |
| I⁻             | 6.2 | 6.1 | 5.9 | 5.8 | 5.7 | 5.9  | I⁻  | 5.5 | 5.6 | 5.2 | 5.1 | 5.2 | 5.3  |
| **SPC/E**      |     |     |    |     |     |      |     |     |    |     |     |      |
| F⁻             | -   | 17.7| 17.2| 17.7| 17.8| 17.6 | F⁻  | -   | 18.0| 17.4| 17.6| 18.0| 17.8 |
| Cl⁻            | 8.6 | 8.5 | 8.2 | 8.2 | 8.0 | 8.3  | Cl⁻ | 7.9 | 7.8 | 7.3 | 7.3 | 7.5 | 7.5  |
| Br⁻            | 7.5 | 7.5 | 7.3 | 7.2 | 7.0 | 7.3  | Br⁻ | 5.7 | 5.7 | 5.2 | 5.2 | 5.2 | 5.4  |
| I⁻             | 6.3 | 6.2 | 6.0 | 5.9 | 5.8 | 6.0  | I⁻  | 5.7 | 5.7 | 5.2 | 5.2 | 5.2 | 5.4  |