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ADDITION/CORRECTION

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Correction to "Charge Asymmetries in Hydration of Polar Solutes"

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Our previous work reported calculated hydration free energies for a variety of artificial polar ring-shaped solutes as a function of water model (TIP3P,[1] TIP4P-Ew,[2] and TIP5P-E[3]). We also examined the asymmetry (the difference between hydration free energies of solutes with a large positive charge, versus those with a large negative charge) as a function of water model. However, all free energies and asymmetries computed with the TIP4P-Ew water model were affected by a bug in the GROMACS simulation package affecting four-point water models, as noted in an erratum on one of our previous papers.[4]

Here, we repeated all of the calculations for the TIP4P-Ew water model, and we provide the new results. Specifically, Figure 6 of the original work, which showed TIP4P-Ew asymmetries along with those from the other two models, is corrected by Figure 1 here. Additionally, the previous Supporting Information contained a table of all computed hydration free energies. Here, we provide an updated Table 1 correcting the TIP4P-Ew results that appeared in the previous table (Supporting Information Table 2).

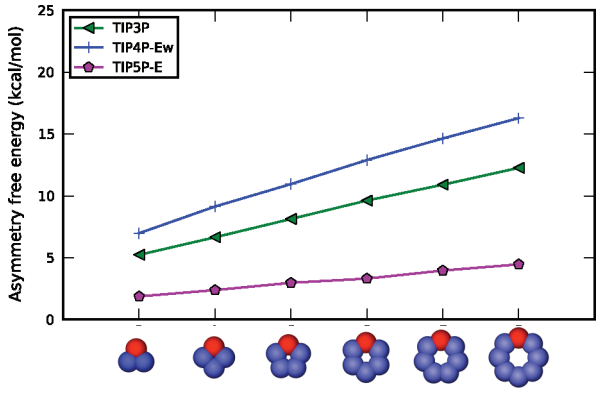

Figure 1. Asymmetries for the distributed scheme,with different water models. Shown, as a function of bracelets size, are asymmetries for bracelets with distributed charges, for TIP3P (triangles), TIP4P-Ew (plus symbols), and TIP5P-E (pentagons). In each case, the asymmetry increases monotonically with the size of the bracelet. Cartoon representations at the bottom are for the negative case. Red atoms are negative and blue are positive, with color intensity denoting the charge magnitude. Lines are a guide for the eye. Only the TIP4P-Ew results are updated from the original.

The new results do not affect any of the conclusions from our previous work—trends in asymmetries and hydration free energies are still the same.

In addition to the above corrections, Dr. Mobley is now listed as the corresponding author on the paper as the calculations were repeated in his lab, and Janene R. Baker has been added as a co-author as she was responsible for repeating the calculations.

Table 1. Hydration Free Energies for Different Bracelets[a]

geometry	radius scale factor	P-bracelet	N-bracelet
triangle	1.0	−14.19 ± 0.13	−21.18 ± 0.15
square	1.0	−13.55 ± 0.14	−22.69 ± 0.16
pentagon	1.0	−14.52 ± 0.14	−25.48 ± 0.18
hexagon	1.0	−15.82 ± 0.15	−28.72 ± 0.20
heptagon	1.0	−17.34 ± 0.16	−31.99 ± 0.22
octagon	1.0	−18.92 ± 0.18	−35.21 ± 0.24

[a] Shown are all computed hydration free energies in TIP4P-Ew for bracelets of different geometries, for both P- and N-bracelets. The radius scale factor column denotes the scaling factor applied to Lennard-Jones radii for the calculation. These use the distributed charge scheme, as described in the previous work.

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