

Erratum

to the paper

Miscibility and Thermodynamics of Mixing of Different Models of Formamide and Water in Computer Simulation

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by

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Due to an unfortunate mistake, we used the r_{\min} values instead of σ in the calculations with the CHARMM model of formamide. These two values are related to each other as $r_{\min} = \sqrt[6]{2}\sigma/2$. Thus, the interaction parameters reported in Table 3 for the CHARMM model are wrong; the correct parameters are listed in Table 1 of this Erratum.

We have repeated all the calculations concerning the combinations of the CHARMM model of formamide with the SPC/E as well as TIP4P models of water. The composition dependence of the Helmholtz free energy, energy, and entropy of mixing of these models are shown in Figure 1, while that of the D parameter, defined by eq. 1 of the original paper, is shown in Figure 2 of this Erratum. Since F^{mix} is negative, and D is positive in the entire composition range, the correction of the aforementioned unfortunate mistake does not change any of the conclusions of the paper: both of these model combinations reproduce the full miscibility of water and formamide. The experimental U^{mix} data are somewhat better reproduced when the SPC/E water model is used; therefore, the use of the CHARMM model of formamide together with the SPC/E model of water seems to be the best combination when describing the thermodynamics of mixing of formamide and water.

Table 1. Interaction Parameters of the CHARMM model of Formamide.

site	$\sigma/\text{\AA}$	$\epsilon/\text{kJ mol}^{-1}$	q/e
C	3.564	0.293	0.42
O	3.029	0.502	-0.51
H(C)	2.352	0.090	0.08
N	3.296	0.837	-0.69
H	0.400	0.192	0.35

Figure 1. Helmholtz free energy of mixing (top panel), energy of mixing (middle panel), and entropy of mixing (bottom panel) of the CHARMM model of formamide with the SPC/E (red open circles) and TIP4P (blue full circles) models of water. The lines connecting the symbols only serve as guides to the eye. Zero value is indicated by dashed line, experimental data of the energy of mixing is shown by a thick line in the middle panel, the entropy of ideal mixing is shown by dotted line in the bottom panel.

Figure 2. Composition dependence of the parameter D , defined by eq. 1 of the original paper, in mixtures of the SPC/E (red line) and TIP4P (blue line) models of water with the CHARMM model of formamide.

Figure 1.
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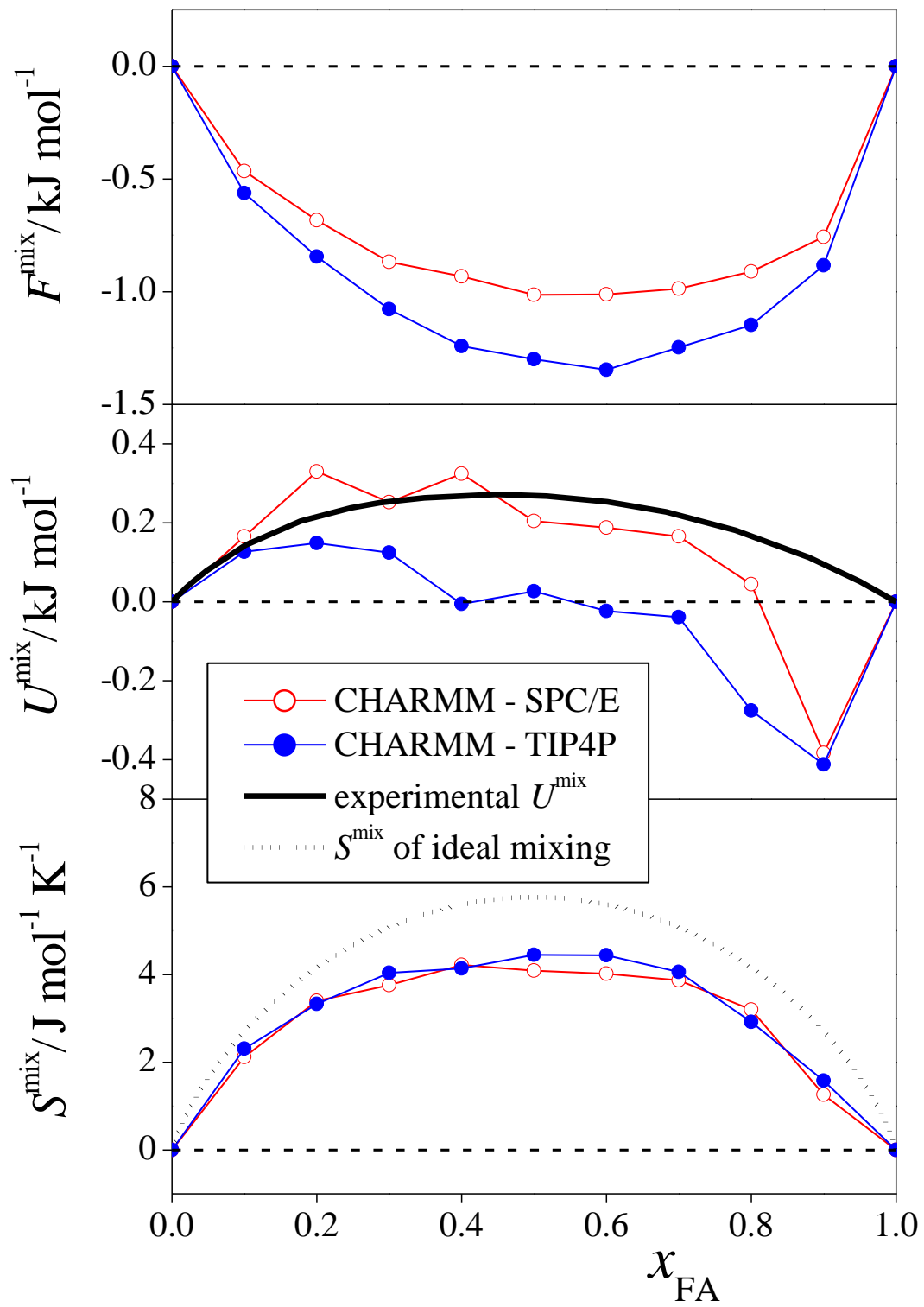


Figure 2
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