

Correction to Volume Exclusion and H-Bonding Dominate the Thermodynamics and Solvation of Trimethylamine-N-oxide in Aqueous Urea

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The following three corrections do not affect the results, discussion, figures, and conclusions in our paper: Page 3596. Eq 26 in the original paper should read

$$a_{SS} = \frac{1 + \eta(4 + \eta(2 - \eta)^2)}{(1 - \eta)^4}$$

where $\eta = cv$ is the packing fraction of the hard-sphere, c its molarity, and v its molar volume.

Second, in a one-component gas, the volume of the particles (ν) is not given by the partial molar volume but by the van der Waals volume. It equals the volume of spheres with radii of 1.4, 2.33, and 2.66 Å for water, urea, and TMAO, respectively. Third, the shape of TMAO was previously approximated by a hard-sphere. However, an ellipsoid with semiaxes with a ratio of 1:1.6:1.8 is a better approximation for TMAO dihydrate. Then, we must use an equation of state for ellipsoids 2 in calculating eq 26. It is given by $1 + (Z_{HS} - 1)B_2/4$, where Z_{HS} is the hard-sphere equation of state 3 and B_2 the second virial coefficient for hard ellipsoids. 4

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