

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

Jörg Rösgen\* and Ruby Jackson-Atogi

*J. Am. Chem. Soc.*, **2012**, *134* (7), 3590–3597. DOI: 10.1021/ja211530n

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

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

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 ( $v$ ) 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.<sup>1</sup> 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<sup>2</sup> in calculating eq 26. It is given by  $1 + (Z_{\text{HS}} - 1)B_2/4$ , where  $Z_{\text{HS}}$  is the hard-sphere equation of state<sup>3</sup> and  $B_2$  the second virial coefficient for hard ellipsoids.<sup>4</sup>

## REFERENCES

- (1) Auton, M.; Bolen, D.; Rösgen, J. *Proteins* **2008**, *73*, 802–813.
- (2) Vega, C. *Mol. Phys.* **1997**, *92*, 651–665.
- (3) Carnahan, N. F.; Starling, K. E. *J. Chem. Phys.* **1969**, *51*, 635–636.
- (4) Singh, G.; Kumar, B. *J. Chem. Phys.* **1996**, *105*, 2429–2435.

Published: August 14, 2012