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Corrigendum to

"A thermodynamic model of mixed organic–inorganic aerosols to predict activity coefficients" published in Atmos. Chem. Phys., 8, 4559-4593, 2008

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The authors would like to report three corrections regarding the article "A thermodynamic model of mixed organic–inorganic aerosols to predict activity coefficients" by Zuend et al. (2008).

(1) On page 4565, text below Eq. (17), the expression for the average value M_{av} has been stated incorrectly as the average molar mass of the solvent mixture. Instead, M_{av} represents the average molar mass of the solvent main groups k, $M_{\mathrm{av}} = \sum_k x'_k M_k$, with the M_k being calculated from the specific subgroup molar masses, M_t, and relative molar abundances of the subgroups present in the mixture making up the main group contribution of k. That is, $M_k = \sum_{t(k)} \frac{X'_{t(k)}}{x'_{k(t)}} M_{t(k)}$, with $X'_{t(k)}$ the mole fraction of subgroup t in the electrolyte-free (solvent) subgroup mixture associated with main group k (denoted as $t(k)$) and $x'_{k(t)}$ the mole fraction (electrolyte-free basis) of main group k comprising subgroups t ($x'_{k(t)} = \sum_{t(k)} X'_{t(k)}$). M_{av} could also be calculated directly using the subgroup contributions: $M_{\mathrm{av}} = \sum_t X'_t M_t$ (but the M_k are required anyways in Eq. 17). M_{av} is used in Eqs. (17), (19), and (20) of the article. We note that reported AIOMFAC model results were unaffected by the incorrectly stated expression for M_{av} since our model implementation was coded using the correct expression.

(2) The values of the density (ρ_w) and the relative static permittivity (ϵ_w) of pure water at 298.15 K, used in Eqs. (11) and (12), have not been specified in the article. The values used in the AIOMFAC model implementation are: $\rho_w = 997\,\mathrm{kg\,m^{-3}}$ and $\epsilon_w = 78.54$ (dimensionless).

(3) There is a typo in Table 5 on page 4573 with regard to the value of the fitted binary cation-anion MR interaction parameter $c^{(1)}_{c,a}$ for Mg^{2+}, Cl^-. The correct value is: $c^{(1)}_{Mg^{2+},Cl^-} = 0.078654\,\mathrm{kg^2\,mol^{-2}}$.

In addition, we note that some of the interaction parameters reported in Table 5 and all values of Table 6 have been revised in the extended AIOMFAC parameterization by Zuend et al. (2011) and additional organic groups and inorganic ions have been introduced; see Sect. 5.1 in Zuend et al. (2011).

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References

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