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Erratum

# Erratum to: Simulation of weak polyelectrolytes: a comparison between the constant pH and the reaction ensemble method*

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In the final print version of the article formulas (11) and (12) are wrong. The formulas should read in accordance with reference [1]:

$$Z_{\mathrm{pH}} = \sum_{\bar{n}} \binom{N_0}{(1-\bar{n})N_0} x^{N_0(1-\bar{n})} \sum_{i(\bar{n})} \exp(-\beta E_{\mathrm{pot,i}}), \tag{11}$$

as a sum over all degrees of association and over all corresponding configurational microstates $i$ of the system, where $\binom{n}{k} = \frac{n!}{(n-k)!k!}$ is the binomial coefficient. The individual probability for a microstate with a certain degree of association should be

$$p(\bar{n}, E_{\mathrm{pot,\,i}}) = \binom{N_0}{(1-\bar{n})N_0} x^{N_0(1-\bar{n})} \exp(-\beta E_{\mathrm{pot,i}}) \tag{12}$$

with $x = 10^{\mathrm{pH_{in}} - \mathrm{pK}_a}$ and predefined and fixed values for $\mathrm{pH_{in}}$ and $\mathrm{pK}_a$.

## Reference

1. C.E. Reed, W.F. Reed, J. Chem. Phys. **96**, 1609 (1992)

* The online version of the original article can be found at https://doi.org/10.1140/epjst/e2016-60324-3

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