Eur. Phys. J. Special Topics **228**, 2779 (2019)

https://doi.org/ 10.1140/epjst/e2019-900073-7

THE EUROPEAN PHYSICAL JOURNAL SPECIAL TOPICS

Erratum

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

Eur. Phys. J. Special Topics 226, 725–736 (2017), https://doi.org/10.1140/epjst/e2016-60324-3

Jonas Landsgesell[a], Christian Holm, and Jens Smiatek[b]

Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany

Received 16 April 2019
Published online 21 May 2019

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 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

[a] e-mail: jlandsgesell@icp.uni-stuttgart.de
[b] e-mail: smiatek@icp.uni-stuttgart.de