May 17, 2010

Unpublished erratum for

"Statistical Thermodynamics of Bond Torsional Modes: Tests of Separable, Almost-Separable, and Improved Pitzer–Gwinn Approximations" B. A. Ellingson, V. A. Lynch, S. L. Mielke, and D. G. Truhlar, Journal of Chemical Physics **125**, 84305/1-17 (2006).

In eqs. (33) and (36) the upper bounds on the summations were not explicitly stated; correct results can be obtained by setting both to M, the total number of wells, rather than to P, the number of distinct wells. However, in computations it is more convenient to sum over only distinct wells, and we note that one can equivalently write the correct equations by summing over $j = 1, 2, \ldots, P$ distinct wells in eqs. (33) and (36) if one replaces $Q_{\mathrm{FR},j}$ by $\sigma Q_{\mathrm{FR},j}$ in eq. (34).

The example (H_2O_2) treated in the paper has $\sigma = 1$, and therefore $M = P$, so the ambiguity in the upper limit did not cause any numerical errors.

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