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Kenneth M. Benjamin, Andrew J. Schultz, and David A. Kofke*: Fourth and Fifth Virial Coefficients of Polarizable Water

Page 7810. We recently reported virial coefficients computed for a polarizable model of water. We have learned of errors in parts of the equations we presented for the fourth and fifth virial coefficients as written for polarizable molecular interaction models.

In eq 7, giving the expression for ΔB_4 , the term $\delta_{(ijk)}^{(b)}$ should be replaced by the following:

$$\delta_{(ijk)l}^{(b)} = -(e_{ijk} - e_{ij}e_{ik}e_{jk})(f_{il} + f_{jl} + f_{kl} + 1) \quad (1)$$

Then, in eq 8 for ΔB_5 , three corrections are needed. In the term $\Delta_{12345}^{(a)}$, the e_{ij} functions should be multiplied, not summed:

$$\Delta_{12345}^{(a)} = e_{12345} - e_{12}e_{13}e_{14}e_{15}e_{23}e_{24}e_{25}e_{34}e_{35}e_{45} \quad (2)$$

the term for $\delta_{(ijkl)m}^{(b)}$ should be preceded by a minus sign:

$$\delta_{(ijkl)m}^{(b)} = -(e_{ijkl} - e_{ij}e_{ik}e_{il}e_{jk}e_{jl}e_{kl})(f_{im} + f_{jm} + f_{km} + f_{lm} + 1) \quad (3)$$

and the terms for $\delta_{(ij)(kl)m}$ should be replaced by

$$\delta_{(ij)(kl)m} = -(e_{ijm}e_{klm} - e_{ij}e_{im}e_{jm}e_{kl}e_{km}e_{lm}) \quad (4)$$

Also, in connection with this term, the sum (c) is taken over all unique ways of forming two pairs (ij) and (kl) (the original work incorrectly indicated (km)).

All of the virial coefficients presented in the paper were computed using the correct formulas, so no revision of the tabulated results is required.

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