Erratum: A multipole interaction theory of electric polarization of atomic and molecular assemblies [J. Chem. Phys. 83, 809 (1985)]

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Erratum: A multipole interaction theory of electric polarization of atomic and molecular assemblies [J. Chem. Phys. 83, 809 (1985)]

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The second equality of Eq. (25) should read

$$U=-(\mathscr{E}+\tfrac{1}{2}\mathscr{F})^{T}\mathscr{M}\ .$$

Equation (54) should read

$$p^{(n,m)}_{\alpha_1\cdots\alpha_n\beta_m\cdots\beta_1}=\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{h=0}^{n}(h!/n!)\sum_{P(n,h)}r_{i,\alpha_1}\cdots r_{i,\alpha_{n-h}}\{(m!)^{-1}B^{(h,0)}_{ij,\alpha_{n-h+1}\cdots\alpha_n}r_{j,\beta_m}\cdots r_{j,\beta_1}$$

$$+\sum_{k=1}^{m}[(k-1)!/(m-1)!]\sum_{P(m-1,k-1)}B^{(h,k)}_{ij,\alpha_{n-h+1}\cdots\alpha_n\beta_m\cdots\beta_{m-k+1}}r_{j,\beta_{m-k}}\cdots r_{j,\beta_1}\}\ .$$

A clarification of the notation for tensor component indices in Eq. (54) is needed. For consistency with the notation on the left-hand side, $\alpha_p\cdots\alpha_q$ denotes a sequence of α_i in ascending order of the subscripts i; hence, if $p>q$, there are no indices in the sequence, corresponding to zero tensor rank. Likewise, the notation $\beta_p\cdots\beta_q$ denotes a sequence of β_i in descending order of i; hence, if $p<q$, the corresponding tensor rank is zero.

Equation (55) should read

$$\beta=\tfrac{1}{6}p^{(1,2)}_{\alpha\beta\gamma}\epsilon_{\gamma\beta\alpha}$$

in accordance with the cited reference. The error in the paper amounts to a reversal of the sign of β. The error was not committed in the numerical calculations.

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