

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

$$U = -(\mathcal{E} + \frac{1}{2}\mathcal{L})^T \mathcal{M}.$$

Equation (54) should read

$$p_{\alpha_1 \cdots \alpha_n \beta_m \cdots \beta_1}^{(n,m)} = \sum_{i=1}^N \sum_{j=1}^N \sum_{h=0}^n (h!/n!) \sum_{P(n,h)} r_{i,\alpha_1} \cdots r_{i,\alpha_{n-h}} \{ (m!)^{-1} B_{ij, \alpha_{n-h+1} \cdots \alpha_n}^{(h,0)} r_{j,\beta_m} \cdots r_{j,\beta_1} \\ + \sum_{k=1}^m [(k-1)!/(m-1)!] \sum_{P(m-1,k-1)} B_{ij, \alpha_{n-h+1} \cdots \alpha_n \beta_m \cdots \beta_{m-k+1}}^{(h,k)} r_{j,\beta_{m-k}} \cdots r_{j,\beta_1} \}.$$

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

$$\beta = \frac{1}{6} p_{\alpha\beta\gamma}^{(1,2)} \epsilon_{\gamma\beta\alpha}$$

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.