Erratum: General polarizability and hyperpolarizability estimators for the path-integral Monte Carlo method applied to small atoms, ions, and molecules at finite temperatures
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Juha Tiihonen, Ilkka Kylänpää, and Tapio T. Rantala
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In our recent work we derived field-free estimators for static polarizabilities and hyperpolarizabilities for the path-integral Monte Carlo method. Our derivation contained some unconventional practices of notation and sign. For example, we had replaced $F_\alpha F_\beta$ with $F_{\alpha\beta}$, etc., whereas the latter is commonly used for a field gradient, i.e., $F_{\alpha\beta} = (\nabla F_\alpha)_\beta$. Also, in Eqs. (5)–(9) there were some sign errors in contrast to Ref. [1]. However, these signs cancel out in either case, leaving the resulting estimators and the data unaffected. The correct way to write the equations would be the following:

$$E^{(1)} = E^{(0)} - \mu_\alpha F_\alpha - \frac{1}{2} \alpha_{\alpha\beta} F_\alpha F_\beta - \frac{1}{6} \beta_{\alpha\beta\gamma} F_\alpha F_\beta F_\gamma - \frac{1}{24} \gamma_{\alpha\beta\gamma\delta} F_\alpha F_\beta F_\gamma F_\delta - \dots, \quad (5)$$

$$\mu_\alpha = - \lim_{F \rightarrow 0} \frac{\partial}{\partial F_\alpha} E^{(1)}, \quad (6)$$

$$\alpha_{\alpha\beta} = - \lim_{F \rightarrow 0} \frac{\partial}{\partial F_\alpha} \frac{\partial}{\partial F_\beta} E^{(1)} = \lim_{F \rightarrow 0} \frac{\partial}{\partial F_\beta} \mu_\alpha, \quad (7)$$

$$\beta_{\alpha\beta\gamma} = - \lim_{F \rightarrow 0} \frac{\partial}{\partial F_\alpha} \frac{\partial}{\partial F_\beta} \frac{\partial}{\partial F_\gamma} E^{(1)} = \lim_{F \rightarrow 0} \frac{\partial}{\partial F_\gamma} \alpha_{\alpha\beta}, \quad (8)$$

$$\gamma_{\alpha\beta\gamma\delta} = - \lim_{F \rightarrow 0} \frac{\partial}{\partial F_\alpha} \frac{\partial}{\partial F_\beta} \frac{\partial}{\partial F_\gamma} \frac{\partial}{\partial F_\delta} E^{(1)} = \lim_{F \rightarrow 0} \frac{\partial}{\partial F_\delta} \beta_{\alpha\beta\gamma}. \quad (9)$$

Furthermore, we want to publish one more nonvanishing property that was left out in the original article. Namely, $\beta_{yyy} = 1.12(14)$ for H_3^+ in the adiabatic (fixed-nuclei) simulation.

[1] A. D. Buckingham, in *Advances in Chemical Physics: Intermolecular Forces*, edited by J. O. Hirschfelder, Advances in Chemical Physics Vol. 12 (Wiley, Hoboken, NJ, 2007), pp. 107–142.