

# Erratum: “Towards an accurate description of anharmonic infrared spectra in solution within the polarizable continuum model: Reaction field, cavity field and nonequilibrium effects” [J. Chem. Phys. 135, 104505 (2011)]

Cite as: J. Chem. Phys. 135, 149901 (2011); <https://doi.org/10.1063/1.3653267>

Submitted: 29 September 2011 . Accepted: 29 September 2011 . Published Online: 14 October 2011

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## Erratum: “Towards an accurate description of anharmonic infrared spectra in solution within the polarizable continuum model: Reaction field, cavity field and nonequilibrium effects” [J. Chem. Phys. 135, 104505 (2011)]

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(Received 29 September 2011; accepted 29 September 2011; published online 14 October 2011)

[doi:10.1063/1.3653267]

A few errors occurred in the Appendix of the article<sup>1</sup> (APPENDIX: NONEQUILIBRIUM FREE ENERGY DERIVATIVES).

Equation (A16)

$$\mathcal{G}^{x,neq}[\rho^0] = \frac{1}{2}(\mathbf{q}_d^\dagger \mathbf{V}^x[\rho^0] + \mathbf{q}_d^{x,\dagger} \mathbf{V}[\rho^0]) + \frac{1}{2}(\mathbf{q}_{in}^\dagger \mathbf{V}^x[\rho^0] + \mathbf{q}_{in}^{x,\dagger} \mathbf{V}[\rho^0])$$

should be replaced by

$$\mathcal{G}^{x,neq}[\rho^0] = \frac{1}{2}(\mathbf{q}_d^\dagger \mathbf{V}^x[\rho^0] + \mathbf{q}_d^{x,\dagger} \mathbf{V}[\rho^0]) + \mathbf{q}_{in}^\dagger \mathbf{V}^x[\rho^0]$$

and Eq. (A18)

$$\mathcal{G}^{x,neq}[\rho^0] = (\mathbf{q}_d^{x,\dagger} + \mathbf{q}_{in}^\dagger) \mathbf{V} = \mathbf{q}^\dagger \mathbf{V}$$

should be replaced by

$$\mathcal{G}^{x,neq}[\rho^0] = (\mathbf{q}_d^\dagger + \mathbf{q}_{in}^\dagger) \mathbf{V}^x[\rho^0] = \mathbf{q}^\dagger \mathbf{V}^x[\rho^0].$$

<sup>1</sup>C. Cappelli, F. Lipparini, J. Bloino, and V. Barone, *J. Chem. Phys.* **135**, 104505 (2011).

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