

Erratum: “A note on quantum thermodynamic rate theories” [J. Chem. Phys. 115, 6876 (2001)]

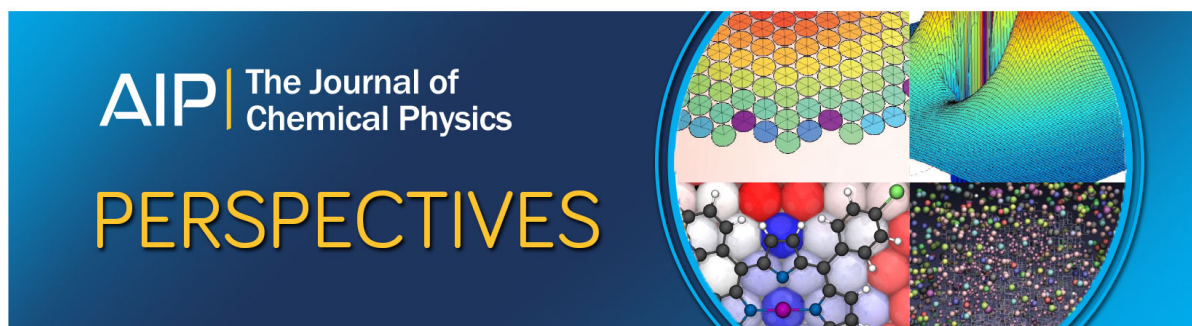
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ERRATA

Erratum: “The ^{19}F – ^1H coupling constants transmitted through covalent, hydrogen bond, and van der Waals interactions” [J. Chem. Phys. 115, 5498 (2001)]

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The caption for Fig. 3 on p. 5502, “The surface of the intermolecular couplings (in Hz) in FHF^- as a function of the fluorine–fluorine distance $R(\text{FF})$ and a difference between proton–fluorine distances (in Å): (a) the ^{19}F – ^1H coupling constant, (b) the ^{19}F – ^{19}F coupling constant,” should be replaced by “The surface of the intermolecular couplings (in

Hz) in FHF^- as a function of the fluorine–fluorine distance $R(\text{FF})$ and a difference between proton–fluorine distances (in Å): (a) the ^{19}F – ^{19}F coupling constant, (b) the ^{19}F – ^1H coupling constant”.

The labels on the vertical axes of the graphs in Fig. 6 on p. 5505 are reversed.

Erratum: “A note on quantum thermodynamic rate theories” [J. Chem. Phys. 115, 6876 (2001)]

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The integral equation (3.3) in Ref. 1 is not a solution of the Wigner–Liouville equation [Eq. (3.1)]. The correct integral equation representation for the Wigner–Liouville equation may be found for example in Eqs. (6) and (7) of Ref. 2. Equation (3.3) given in our paper does give the correct fourth order initial time derivative, including the quantum correction term, but is already incorrect for the fifth order initial time derivative. This error does not detract from the main

result of the paper, which is that the first three initial time derivatives of a coordinate dependent operator are the same in quantum and classical mechanics.

¹E. Pollak and J. Shao, J. Chem. Phys. **115**, 6876 (2001).

²V. S. Filinov, Yu. V. Medvedev, and V. L. Kamskyi, Mol. Phys. **85**, 711 (1995).