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

Eli Pollak, and Jiushu Shao

Citation: The Journal of Chemical Physics **116**, 1748 (2002); doi: 10.1063/1.1429650
View online: https://doi.org/10.1063/1.1429650
View Table of Contents: http://aip.scitation.org/toc/jcp/116/4
Published by the American Institute of Physics

ERRATA

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

Magdalena Pecul and Joanna Sadlej
Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland

Jerzy Leszczynski
Computational Center for Molecular Structure and Interactions, Department of Chemistry, Jackson State University, Jackson, Mississippi 39217

[DOI: 10.1063/1.1429246]

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(FF) and a difference between proton–fluorine distances (in Å): (a) the $^{19}F-^{1}H$ 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(FF) and a difference between proton–fluorine distances (in Å): (a) the $^{19}F-^{19}F$ coupling constant, (b) the $^{19}F-^{1}H$ 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)]

Eli Pollak
Chemical Physics Department, Weizmann Institute of Science, 76100 Rehovot, Israel

Jiushu Shao
School of Chemical Sciences, University of Illinois, Urbana, Illinois 61801

[DOI: 10.1063/1.1429650]

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.

[1] E. Pollak and J. Shao, J. Chem. Phys. **115**, 6876 (2001).
[2] V. S. Filinov, Yu. V. Medvedev, and V. L. Kamskyi, Mol. Phys. **85**, 711 (1995).

