2007, Volume 111B

Marat Valiev*, Jie Yang, Joseph A. Adams, Susan S. Taylor, and John H. Weare: Phosphorylation Reaction in cAPK Protein Kinase-Free Energy Quantum Mechanical/Molecular Mechanics Simulations

Page 13455. Reference 63 in this publication was incorrect and has been withdrawn by the authors at the request of Professor Kyte.

10.1021/jp910239g
Published on Web 04/28/2010

2009, Volume 113B

M. Cecchini,* S. V. Krivov, M. Spichty, and M. Karplus*: Calculation of Free-Energy Differences by Confinement Simulations. Application to Peptide Conformers

Page 9728. Equation 24 for the vibrational entropy of a classical harmonic oscillator should be correctly written as

$$S = k_B \sum_{i=1}^{3N-6} \left[1 + \ln\left(\frac{k_B T}{h\omega_i}\right)\right]$$

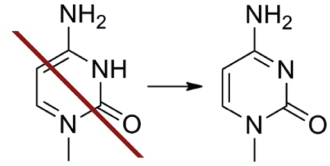
where ω_i is the frequency of the ith normal mode, T is the temperature in Kelvin, h is Plank's constant, and k_B is the Boltzmann constant; the "1" was omitted in the equation. No result presented in the paper is affected by this error because the omitted term cancels out when ΔS is computed. However, the correct determination of both the absolute vibrational entropy and the harmonic free energy strictly requires the use of the corrected equation given here.

10.1021/jp102878c
Published on Web 04/22/2010

2010, Volume 114B

Aymeric Naômé,* Patric Schyman, Aatto Laaksonen, and Daniel P. Vercauteren: Molecular Dynamics Simulation of 8-Oxoguanine Containing DNA Fragments Reveals Altered Hydration and Ion Binding Patterns

Page 4789. After online publication, we noticed an error in Figure 1. The structure of cytosine is obviously wrong and one should read the following:



10.1021/jp103126r
Published on Web 04/26/2010