An Improved Slater's Transition State Approximation

Kimihiko Hirao[a,b], Takahito Nakajima[b], and Bun Chan[c]

[a] *Fukui Institute for Fundamental Chemistry, Kyoto University, Takano, Nishihiraki-cho 34-4, Sakyo-ku, Kyoto, 606-8103, Japan*

[b] *RIKEN Center for Computational Science, 7-1-26, Minatojima-minami-machi, Chuo-ku, Kobe, 650-0047, Japan*

[c] *Graduate School of Engineering, Nagasaki University, Bunkyo 1-14, Nagasaki 852-8521, Japan*

Abstract

We have extended Slater's transition state (STS) concept for the approximation of the difference in total energies of the initial and final states. It is simple and is conceptually useful for gaining improved understanding of SCF-type orbital theories. Numerical validation was performed with the valence and the core ionization energies by using Hartree-Fock and Kohn-Sham theory. Particularly, the shifted STS performs well for the core ionization energies of the second period and third period elements.