Second Derivative of Approximately Spin-Projected Energy (AP-hessian) for Diatomic Singlet Diradicals

Yasutaka Kitagawa[1)], Toru Saito[1)], Yasuyuki Nakanishi[1)], Mitsuo Shoji[1)], Kenichi Koizumi[1)], Takashi Kawakami[1)], Mitsutaka Okumura[1)] and Kizashi Yamaguchi[2)]

1) Department of Chemistry, Graduate School of Science, Osaka University, Osaka 560-0043, Japan.

2) Center for Quantum Science and Technology under Extreme Conditions, KYOKUGEN, Osaka University, Osaka 560-8531, Japan.

E-mail: kitagawa@chem.sci.osaka-u.ac.jp

Abstract

A broken-symmetry (BS) method is one of the effective tools for calculations of large poly-radical systems with lower computing costs. However it always suffers from a spin contamination of higher spin states on singlet biradical and low-spin species. For the problem, some spin-projection procedures have been proposed. Very recently, we proposed a new method for the calculation of a spin-projected energy gradient (AP-gradient) based on Yamaguchi's approximately spin-projected (AP) energy expression [1,2]. By using the AP-gradient, one can optimize geometry of singlet biradicals without the spin contamination error.

In this paper, we propose a new method to calculate a second derivative of the AP energy (AP-hessian) for diatomic singlet diradicals. By the method we can eliminate the spin contamination error in the hessian of diradicals even with the BS procedure.

References

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