Reparameterization of PM6 Applied to Through-bond and Through-space Magnetic Interactions

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Semi-empirical molecular orbital (SE-MO) approaches to quantum chemistry were developed to simplify and speed up calculations by replacing integrals with an optimum set of parameters. These methods including MNDO, AM1, PM3, and PM6 [1,2] are now applied to a range of chemical and biological problems because the SE-MO calculations are much faster than density functional theory (DFT) ones. However, their performance for open-shell systems seems to be uncertain though these methods may be reliable for closed-shell species. It was found that the standard spin-unrestricted SE-MO methods including UAM1, UPM3 and UPM6 are likely to overestimate the spin polarization (spin contamination) effect and thus they significantly underperform UDFT. For this reason, we performed a reparameterization of PM6 (called rPM6) so that we can compute open-shell species as accurate as possible [3, 4]. Its application to a variety of molecules which exhibit either through-bond or through-space magnetic interactions will be presented.

[1] W. Thiel, WIRES: Comput. Mol. Sci. 4, 145 (2014).
[2] J. J. P. Stewart, J. Mol. Model. 13, 1173 (2007).
[3] T. Saito, Y. Kitagawa, Y. Takano, J. Phys. Chem. A 120, 8750 (2016)
[4] T. Saito et al., *submitted*.