

October 27, 2009

Unpublished erratum for:

“The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights,” J. Zheng, Y. Zhao, and D. G. Truhlar, *Journal of Chemical Theory and Computation* **5**, 808-821 (2009).
<http://dx.doi.org/10.1021/ct800568m>

The MOHLYP density functional in this paper is not the same as the original MOHLYP potential. The one in this paper will henceforth be called MOHLYP2, and the original one is called MOHLYP.

Whereas MOHLYP changes two parameters of the OPTX exchange functional (1.05151 to 1 and 1.4317 to 1.292), MOHLYP2 changes only one (1.4317 to 1.8497564). Furthermore, MOHLYP scales the gradient-correction part of the LYP correlation functional by 0.5, whereas MOHLYP2 scales the entire LYP correlation functional by 0.5.