Explanation for MOHLYP and MOHLYP2 density functionals

Both MOHLYP[1] and MOHLYP2[2] functionals take scaled OptX exchange functional and scaled LYP correlation functional, but they use different scaling factors.

The functional form of the gradient enhancement for the OptX exchange functional[3] used in OLYP is

$$F(s) = 1.05151 - \frac{b}{C_F}\frac{\gamma s^2}{(1+\gamma s^2)}$$

where $\gamma = 0.006$, $b = 1.4317$, C_F is from the LDA, and s is the reduced gradient.

MOHLYP functional

The MOHLYP functional replaces 1.05151 by 1.0 to restore the uniform electron gas (UEG) limit, and changes b from 1.4317 to 1.292. MOHLYP functional only scale the non-local term of the LYP correlation functional[4] by a factor 0.5. Because IOp(3/77) functions differently in different revisions of *G03* program at least for OptX exchange functional, we should use different IOp(3/77) for different revisions of *G03* program.

MOHLYP keyword

Gaussian version	keyword
G03 B.05 and C.01	OV5LYP IOp(3/77=1292010000) IOp(3/78=0500010000)
G03 D.01 and E.01	OV5LYP IOp(3/77=0902409510) IOp(3/78=0500010000)
G09 A.02	OV5LYP IOp(3/77=0902409510) IOp(3/78=0500010000)

Note: IOp(3/77=0902409510) is obtained by: 1.292/1.4317 = 0.9024 and 1.0/1.05151 = 0.9510. Because 0.9024 and 0.9510 have some round off errors, G03 B.05 and C.01 may give slightly different total energies than those obtained by G03 D.01 and the later versions.

MOHLYP2 functional

The MOHLYP2 functional only changes the *b* from 1.4317 to 1.8497564 for the OptX exchange functional, and scale both local and non-local terms of LYP correlation functional by a factor 0.5. The keywords used for Gaussian program are given in the below table.

MOHLYP2 keyword

Gaussian version	keyword
G03 B.05 and C.01	OV5LYP IOp(3/77=1849810515) IOp(3/78=0500005000)
G03 D.01 and E.01	OV5LYP IOp(3/77=1292010000) IOp(3/78=0500005000)
G09 A.02	OV5LYP IOp(3/77=1292010000) IOp(3/78=0500005000)

Note: Also due to the round off error introduced by different IOp(3/77), G03 B.05 and C.01 may give slightly different total energies than those obtained by G03 D.01 and the later versions.

Reference:

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(3) Handy, N. C.; Cohen, A. J. *Mol. Phys.* **2001**, *99*, 403.
(4) Lee, C. T.; Yang, W. T.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.