

MANUAL
Minnesota Functional Module
Version 6.0

Subroutines for evaluating the following exchange-correlation functionals:
GAM, M05, M05-2X, M06, M06-2X, M06-HF, M06-L, M06-SX, M06CR,
M08-HX, M08-SO, M11, M11-L, MN12-L, MN12-SX, MN15, MN15-L, N12, N12-SX,
revM06, revM06-L, revM11, SOGGA, SOGGA11, and SOGGA11-X

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Executive summary

Minnesota Functional Module (abbreviated *MFM*) is a Fortran77 code for evaluating the GAM, M05, M05-2X, M06, M06-2X, M06-HF, M06-L, M06-SX, M06CR, M08-HX, M08-SO, M11, M11-L, MN12-L, MN12-SX, MN15, MN15-L, N12, N12-SX, revM06, revM06-L, revM11, SOGGA, SOGGA11, and SOGGA11-X exchange-correlation functionals for Kohn-Sham density functional theory. The subroutines are in the accompanying tar file.

Literature references

A. Original references for functionals

GAM

Yu, H. S.; Zhang, W.; Verma, P.; He, X.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2015**, *17*, 12146-12160.
doi.org/10.1039/C5CP01425E

M05

Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Phys.* **2005**, *123*, 161103.
doi.org/10.1063/1.2126975

M05-2X

Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Theory Comput.* **2006**, *2*, 364-382.
doi.org/10.1021/ct0502763

M06 and M06-2X

Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215-241.
doi.org/10.1007/s00214-007-0310-x
 Erratum: **2008**, *119*, 525. doi.org/10.1007/s00214-007-0401-8

M06-HF

Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2006**, *110*, 13126-13130.
doi.org/10.1021/jp066479k

M06-L

Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *125*, 194101.
doi.org/10.1063/1.4948728

M06-SX

Wang, Y.; Verma, P.; Zhang, L. J.; Li, Y. Q.; Liu, Z. H.; Truhlar, D.G.; He, X., *Proc. Natl. Acad. Sci. U.S.A.* **2020**, *117*, 2294-2301.
doi.org/10.1073/pnas.1913699117

M06CR

Long, B.; Wang, Y.; Xia, Y.; He, X.; Bao, J.L.; Truhlar, D.G., *J. Am. Chem. Soc.* **2021**, *143*, 8402-8413.
doi.org/10.1021/jacs.1c02029

M08-HX and M08-SO

Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2008**, *4*, 1849-1868.
doi.org/10.1021/ct800246v

M11

Peverati, R.; Truhlar, D. G. *J. Phys. Chem. Lett.* **2011**, *2*, 2810-2817.
doi.org/10.1021/jz201170d

Note that in eqs 21 and 22 of the M11 paper, Y should be $X/100$.

M11-L

Peverati, R.; Truhlar, D. G. *J. Phys. Chem. Lett.* **2012**, *3*, 117-124.
doi.org/10.1021/jz201525m

MN12-L

Peverati, R.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2012**, *14*, 13171-13174.
doi.org/10.1039/c2cp42025b

MN12-SX and N12-SX

Peverati, R.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2012**, *14*, 16187-16191.
doi.org/10.1039/C2CP42576A

MN15

Yu, H. S.; He, X.; Li, S.; Truhlar, D. G. *Chem. Sci.* **2016**, *7*, 50325051.
doi.org/10.1039/C6SC00705h
 Correction: **7**, 6278-6279 (2016). doi.org/10.1039/c6sc90044e

MN15-L

Yu, H. S.; He, X.; Truhlar, D. G. *J. Chem. Theory Comput.* **2016**, *12*, 1280-1293.
doi.org/10.1021/acs.jctc.5b01082

N12

Peverati, R.; Truhlar, D. G. *J. Chem. Theory Comput.* **2012**, *8*, 2310-12319.

doi.org/10.1021/ct3002656

revM06

Wang, Y.; Verma, P.; Jin, X. S.; Truhlar, D. G.; He, X. *Proc. Natl. Acad. Sci. U.S.A.* **2018**, *115*, 10257-10262.

doi.org/10.1073/pnas.1810421115

revM06-L

Wang, Y.; Jin, X. S.; Yu, H. S.; Truhlar, D. G.; He, X. *Proc. Natl. Acad. Sci. U.S.A.* **2017**, *114*, 8487-8492.

doi.org/10.1073/pnas.1705670114

revM11

Verma, P.; Wang, Y.; Ghosh, S.; He, X.; Truhlar, D.G. *J. Phys. Chem. A*, **2019**, *123*, 2966-2990.

doi.org/10.1021/acs.jpca.8b11499

SOGGA

Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2008**, *128*, 184109.

doi.org/10.1063/1.2912068

SOGGA11

Peverati, R.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. Lett.* **2011**, *2*, 1911-1997.

doi.org/10.1021/jz200616w

Note that there is a typo in eq. 3 of the SOGGA11 paper. The correct expression is:

$$g_l^x = \sum_{i=0}^m a_i^x \left(1 - \frac{1}{1 + \frac{m}{k} s^2} \right)^i$$

SOGGA11-X

Peverati, R.; D. G. Truhlar, *J. Chem. Phys.* **2011**, *135*, 191102.

doi.org/10.1063/1.3663871

B. Reviews

“Density Functionals with Broad Applicability in Chemistry,” Y. Zhao and D. G. Truhlar, Accounts of Chemical Research **41**, 157-167 (2008).

doi.org/10.1021/ar700111a

“Applications and Validations of the Minnesota Density Functionals,” Y. Zhao and D. G. Truhlar, Chemical Physics Letters **502**, 1-13 (2011).

doi.org/10.1016/j.cplett.2010.11.060

“Perspective: Kohn-Sham Density Functional Theory Descending a Staircase,” H. S. Yu, S. L. Li, and D. G. Truhlar, Journal of Chemical Physics **145**, article no. 130901 (2016).

doi.org/10.1063/1.4963168

“Status and Challenges of Density Functional Theory,” P. Verma and D. G. Truhlar, Trends in Chemistry **2**, 302-318 (2020).

doi.org/10.1016/j.trechm.2020.02.005

Input and output

INPUT:

RA, RB - Spin densities

D1RA, D1RB - Spin density gradients

TA, TB - τ_σ and τ_β

NGrid - total number of grid points at which the functional is evaluated.

OUTPUT:

F - Functional values on the grids

D1F - First derivatives with respect to RA, RB, GA, GB, TA, TB on the grids

Notes

1. We used Becke's definition (J. Chem. Phys. **104** 1040 (1996)) of τ_σ and τ_β . By this definition they are two times larger than spin kinetic energy densities.
2. The correlation part of all Minnesota functionals uses the local spin density part of the Perdew-Wang-91 correlation functional (J. P. Perdew and Y. Wang, Phys. Rev. B **45**, 13244-13249 (1992)), which is a fit to the correlation energy of a uniform electron gas (lsdac subroutine). Since we are not allowed to distribute the work of others, **users should provide their own subroutine for this LSDA correlation functional**, or they may find help on Kieron Burke's web site at:

<http://www.chem.uci.edu/~kieron/dftold2/pubs/PBE.asc>

<http://www.chem.uci.edu/~kieron/dftold2/pubs/PBESol.html>
3. The correlation part of all M08-class functionals also needs to use the $H(r_s, \zeta, t)$ function in the PBE correlation (PBEH0 subroutine). As for the previous point, we are not allowed to distribute this subroutine and **users should provide their own**, or they may find help on the author's (Kieron Burke) web site at:

<http://www.chem.uci.edu/~kieron/dftold2/pubs/PBE.asc>

<http://www.chem.uci.edu/~kieron/dftold2/pubs/PBESol.html>

4. The correlation parts of the N12, GAM, and N12-SX are obtained from B97-like expansion truncated at the fourth order, with the opposite spin contribution calculated as:

$$E_{cab} = \int d\mathbf{r} e_{cab}^{\text{UEG}} \left\{ \sum_{i=0}^n b_i u_{cab}^i \right\}$$

and the same spin contribution calculated as:

$$E_{css} = \int d\mathbf{r} e_{css}^{\text{UEG}} \left\{ \sum_{i=0}^{n'} c_i u_{css}^i \right\}$$

once again, **users should provide their own subroutine for this**, and use the parameters in Table 1.

Note that there is a typo in the N12 paper, the corrected values for b_i and c_i are shown below.

Table 1. Parameters of the B97-like expansion for the N12, GAM, and N12-SX correlation functionals.

| | N12 | GAM | N12-SX |
|-------|--------------|--------------|--------------|
| b_0 | 1.00000D+00 | 0.860548D+00 | 2.63373D+00 |
| b_1 | 3.24511D+00 | -2.94135D+00 | -1.05450D+00 |
| b_2 | -2.52893D+01 | 15.4176D+00 | -7.29853D-01 |
| b_3 | 1.44407D+01 | -5.99825D+00 | 4.94024D+00 |
| b_4 | 1.96870D+01 | -23.4119D+00 | -7.31760D+00 |
| c_0 | 1.00000D+00 | 0.231765D+00 | 8.33615D-01 |
| c_1 | -5.53170D+00 | 0.575592D+00 | 3.24128D+00 |
| c_2 | 3.07958D+01 | -3.43391D+00 | -1.06407D+01 |
| c_3 | -5.64196D+01 | 5.77281D+00 | -1.60471D+01 |
| c_4 | 3.21250D+01 | 9.52449D+00 | 2.51047D+01 |

5. One needs to add a portion of the Hartree-Fock exchange energy to the total exchange-correlation energy for the M05, M05-2X, M06, M06-2X, M06-HF, M08-HX, M08-SO, SOGGA11-X, MN15, revM06, revM11, and M06CR functionals. See the details in Table 2.

6. The exchange part of M11 and rev M11 requires range-separation with the error function with M11: 42.8% short-range HF exchange, and 100% long-range HF exchange.

The range parameter ω is 0.225 a_0^{-1} .

revM11: 22.5% short-range HF exchange and 100% long-range exchange.

The range parameter ω is 0.40 a_0^{-1} .

7. The exchange part of N12-SX and MN12-SX requires 25% of “screened exchange”, which is: 25% short-range HF exchange and 0% long-range HF exchange. The range parameter μ is 0.11.
8. The exchange part of M06-SX requires 33.5% of “screened exchange”, which is: 33.5% short-range HF exchange and 0% long-range HF exchange. The range parameter μ is 0.10.
9. There is a quick way to implement the M06CR functional in G16. First, make a new copy of the source codes (name the new folder as revG16), then modify the parameters of M06 in G16 source codes and recompile the codes as revG16. When one utilizes the M06 functional in revG16, actually it calls the M06CR functional. In the input file, one simply specifies the functional M06 to get M06CR. The parameters of M06CR are available in the MFM codes (also in the SI of the M06CR paper). One may simply "grep" the parameters of M06 in the original G16 source codes and find out where they are for M06. In addition, the percentage of the HF exchange energy is 0.4041 for M06CR, which needs to be changed accordingly in the following lines of the original source code “utilam.F”,

else if(IMOpt.eq.-27) then

C M06

IMHF = 270000

Remember to run the test file in the MFM manual to make sure you get the same single point energies as the benchmark results of M06CR for CH₃ and H₂O.

Table 2. Hartree-Fock exchange energies in the Minnesota functionals^a

| Functional | Fraction of Hartree-Fock exchange energy |
|---|--|
| GAM, M06-L, M11-L, MN12-L, MN15-L, N12, revM06-L, revM11, SOGGA, SOGGA11 | 0 |
| M05 | 0.28 E^{HFE} |
| M05-2X | 0.56 E^{HFE} |
| M06 | 0.27 E^{HFE} |
| M06-2X | 0.54 E^{HFE} |
| M06-HF | 1.0 E^{HFE} |

| | |
|-----------------|---|
| M06-SX | $0.335 E^{\text{SX}} (\mu = 0.10)$ |
| M06CR | $0.4041 E^{\text{HFE}}$ |
| M08-HX | $0.5223 E^{\text{HFE}}$ |
| M08-SO | $0.5679 E^{\text{HFE}}$ |
| M11 | $0.428 E^{\text{SR-HFE}} + 1.0 E^{\text{LR-HFE}} (\omega = 0.25)$ |
| MN12-SX, N12-SX | $0.25 E^{\text{SX}} (\mu = 0.11)$ |
| MN15 | $0.44 E^{\text{HFE}}$ |
| revM06 | $0.4041 E^{\text{HFE}}$ |
| revM11 | $0.225 E^{\text{SR-HFE}} + 1.0 E^{\text{LR-HFE}} (\omega = 0.40)$ |
| SOGGA11-X | $0.4015 E^{\text{HFE}}$ |

^a E^{HFE} is the Hartree-Fock exchange energy, $E^{\text{SR-HFE}}$ and $E^{\text{LR-HFE}}$ are the short-range and long-range Hartree–Fock exchange energies respectively, and E^{SX} is the short-range Hartree–Fock screened exchange in a screened functional

Reference energies and gradients

Table 3 and 4 present reference energies and forces of CH₃ (open shell, doublet) and H₂O (closed shell, singlet) with the 6-31+G** basis set and a pruned (99,590) grid.

Geometry of CH₃ (in angstroms)

```
*****
C      0.000000  0.000000  0.000000
H      0.000000  1.078000  0.000000
H      0.933000 -0.539000  0.000000
H     -0.933000 -0.539000  0.000000
*****
```

Table 3. Reference energies (E_h) and forces (X,Y,Z, E_h/a_0) for CH₃

| | | | | |
|-----------|----|------------|-----------|----------|
| PW6B95 | E= | -39.888691 | | |
| | C | 0.000000 | 0.000294 | 0.000000 |
| | H | 0.000000 | 0.000371 | 0.000000 |
| | H | 0.000665 | -0.000333 | 0.000000 |
| | H | -0.000665 | -0.000333 | 0.000000 |
| PWB6K | E= | -39.854636 | | |
| | C | 0.000000 | 0.000294 | 0.000000 |
| | H | 0.000000 | -0.002977 | 0.000000 |
| | H | -0.002231 | 0.001342 | 0.000000 |
| | H | 0.002231 | 0.001342 | 0.000000 |
| SOGGA | E= | -39.538835 | | |
| | C | 0.000000 | 0.000313 | 0.000000 |
| | H | 0.000000 | 0.011083 | 0.000000 |
| | H | 0.009947 | -0.005698 | 0.000000 |
| | H | -0.009947 | -0.005698 | 0.000000 |
| SOGGA11 | E= | -39.842525 | | |
| | C | 0.000000 | 0.000229 | 0.000000 |
| | H | 0.000000 | 0.006611 | 0.000000 |
| | H | 0.006004 | -0.003420 | 0.000000 |
| | H | -0.006004 | -0.003420 | 0.000000 |
| SOGGA11-X | E= | -39.831323 | | |
| | C | 0.000000 | 0.000292 | 0.000000 |
| | H | 0.000000 | 0.003387 | 0.000000 |

| | | | | |
|---------|----|------------|-----------|----------|
| | H | 0.003276 | -0.001840 | 0.000000 |
| | H | -0.003276 | -0.001840 | 0.000000 |
| N12 | E= | -39.822945 | | |
| | C | 0.000000 | 0.000149 | 0.000000 |
| | H | 0.000000 | -0.000495 | 0.000000 |
| | H | -0.000108 | 0.000173 | 0.000000 |
| | H | 0.000108 | 0.000173 | 0.000000 |
| N12-SX | E= | -39.823220 | | |
| | C | 0.000000 | 0.000282 | 0.000000 |
| | H | 0.000000 | -0.002663 | 0.000000 |
| | H | -0.001970 | 0.001191 | 0.000000 |
| | H | 0.001970 | 0.001191 | 0.000000 |
| M08-HX | E= | -39.828570 | | |
| | C | 0.000000 | 0.000294 | 0.000000 |
| | H | 0.000000 | 0.003959 | 0.000000 |
| | H | 0.003782 | -0.002126 | 0.000000 |
| | H | -0.003782 | -0.002126 | 0.000000 |
| M11 | E= | -39.805603 | | |
| | C | 0.000000 | 0.000277 | 0.000000 |
| | H | 0.000000 | 0.005260 | 0.000000 |
| | H | 0.004876 | -0.002769 | 0.000000 |
| | H | -0.004876 | -0.002769 | 0.000000 |
| M11-L | E= | -39.827503 | | |
| | C | 0.000000 | 0.000257 | 0.000000 |
| | H | 0.000000 | 0.004995 | 0.000000 |
| | H | 0.004663 | -0.002626 | 0.000000 |
| | H | -0.004663 | -0.002626 | 0.000000 |
| MN12-L | E= | -39.776262 | | |
| | C | 0.000000 | 0.000205 | 0.000000 |
| | H | 0.000000 | 0.001150 | 0.000000 |
| | H | 0.001371 | -0.000678 | 0.000000 |
| | H | 0.001371 | -0.000678 | 0.000000 |
| MN12-SX | E= | -39.802089 | | |
| | C | 0.000000 | 0.000233 | 0.000000 |
| | H | 0.000000 | 0.001712 | 0.000000 |
| | H | 0.001846 | -0.000972 | 0.000000 |
| | H | -0.001846 | -0.000972 | 0.000000 |
| GAM | E= | -39.857257 | | |

| | | | | |
|----------|----|------------|-----------|----------|
| | C | 0.000000 | 0.000306 | 0.000000 |
| | H | 0.000000 | 0.000744 | 0.000000 |
| | H | 0.000994 | -0.000525 | 0.000000 |
| | H | -0.000994 | -0.000525 | 0.000000 |
| MN15-L | E= | -39.790513 | | |
| | C | 0.000000 | 0.000313 | 0.000000 |
| | H | 0.000000 | 0.008751 | 0.000000 |
| | H | 0.007937 | -0.004532 | 0.000000 |
| | H | -0.007937 | -0.004532 | 0.000000 |
| MN15 | E= | -39.780507 | | |
| | C | 0.000000 | 0.000300 | 0.000000 |
| | H | 0.000000 | 0.001890 | 0.000000 |
| | H | 0.001985 | -0.001095 | 0.000000 |
| | H | -0.001985 | -0.001095 | 0.000000 |
| revM06-L | E= | -39.811321 | | |
| | C | 0.000000 | 0.000292 | 0.000000 |
| | H | 0.000000 | 0.002164 | 0.000000 |
| | H | 0.002219 | -0.001228 | 0.000000 |
| | H | -0.002219 | -0.001228 | 0.000000 |
| revM06 | E= | -39.797379 | | |
| | C | 0.000000 | 0.000296 | 0.000000 |
| | H | 0.000000 | 0.002391 | 0.000000 |
| | H | 0.002418 | -0.001343 | 0.000000 |
| | H | -0.002418 | -0.001343 | 0.000000 |
| revM11 | E= | -39.809756 | | |
| | C | 0.000000 | 0.000300 | 0.000000 |
| | H | 0.000000 | 0.003959 | 0.000000 |
| | H | 0.003774 | -0.002130 | 0.000000 |
| | H | -0.003774 | -0.002130 | 0.000000 |
| M06-SX | E= | -39.744493 | | |
| | C | 0.000000 | 0.000295 | 0.000000 |
| | H | 0.000000 | 0.001151 | 0.000000 |
| | H | 0.001343 | -0.000723 | 0.000000 |
| | H | -0.001343 | -0.000723 | 0.000000 |
| M06CR | E= | -39.779107 | | |
| | C | 0.000000 | 0.000309 | 0.000000 |
| | H | 0.000000 | 0.004116 | 0.000000 |
| | H | 0.003913 | -0.002212 | 0.000000 |
| | H | -0.003913 | -0.002212 | 0.000000 |

| | | | | |
|--------|----|------------|-----------|----------|
| PBEsol | E= | -39.586795 | | |
| | C | 0.000000 | 0.000311 | 0.000000 |
| | H | 0.000000 | 0.010513 | 0.000000 |
| | H | 0.009453 | -0.005412 | 0.000000 |
| | H | -0.009453 | -0.005412 | 0.000000 |
| WC06 | E= | -39.673096 | | |
| | C | 0.000000 | 0.000307 | 0.000000 |
| | H | 0.000000 | 0.008746 | 0.000000 |
| | H | 0.007921 | -0.004527 | 0.000000 |
| | H | -0.007921 | -0.004527 | 0.000000 |
| RPBE | E= | -39.847464 | | |
| | C | 0.000000 | 0.000305 | 0.000000 |
| | H | 0.000000 | 0.008991 | 0.000000 |
| | H | 0.008133 | -0.004648 | 0.000000 |
| | H | -0.008133 | -0.004648 | 0.000000 |
| revPBE | E= | -39.831098 | | |
| | C | 0.000000 | 0.000305 | 0.000000 |
| | H | 0.000000 | 0.008874 | 0.000000 |
| | H | 0.008032 | -0.004590 | 0.000000 |
| | H | -0.008032 | -0.004590 | 0.000000 |
| B97-3 | E= | -39.833716 | | |
| | C | 0.000000 | 0.000300 | 0.000000 |
| | H | 0.000000 | 0.002450 | 0.000000 |
| | H | 0.002469 | -0.001375 | 0.000000 |
| | H | -0.002469 | -0.001375 | 0.000000 |

Geometry of H₂O (in Å)

| | | | |
|---|----------|----------|-----------|
| O | 0.000000 | 0.000000 | 0.000000 |
| H | 0.000000 | 0.000000 | 0.956914 |
| H | 0.926363 | 0.000000 | -0.239868 |

Table 4. Reference energies (E_h) and forces (X,Y,Z, E_h/a_0) for H₂O

| | | | | | |
|--------|----|------------|----------|-----------|--|
| M05 | E= | -76.398883 | | | |
| | O | -0.001497 | 0.000000 | -0.001159 | |
| | H | -0.001588 | 0.000000 | 0.003598 | |
| | H | 0.003085 | 0.000000 | -0.002439 | |
| M05-2X | E= | -76.416245 | | | |
| | O | -0.000061 | 0.000000 | -0.000047 | |
| | H | -0.002966 | 0.000000 | 0.003895 | |
| | H | 0.003027 | 0.000000 | -0.003848 | |
| M06 | E= | -76.397702 | | | |
| | O | -0.002239 | 0.000000 | -0.001733 | |
| | H | -0.002242 | 0.000000 | 0.005209 | |
| | H | 0.004481 | 0.000000 | -0.003476 | |
| M06-L | E= | -76.420152 | | | |
| | O | -0.002994 | 0.000000 | -0.002317 | |
| | H | -0.000683 | 0.000000 | 0.003975 | |
| | H | 0.003677 | 0.000000 | -0.001658 | |
| M06-2X | E= | -76.394863 | | | |
| | O | -0.002361 | 0.000000 | -0.001828 | |
| | H | -0.002678 | 0.000000 | 0.005899 | |
| | H | 0.005039 | 0.000000 | -0.004072 | |
| M06-HF | E= | -76.391767 | | | |
| | O | 0.000348 | 0.000000 | 0.000270 | |
| | H | -0.005141 | 0.000000 | 0.006282 | |
| | H | 0.004793 | 0.000000 | -0.006551 | |
| M06-SX | E= | -76.352728 | | | |
| | O | 0.001748 | 0.000000 | 0.001353 | |
| | H | -0.001950 | 0.000000 | 0.000714 | |
| | H | 0.000202 | 0.000000 | -0.002067 | |

| | | | | | |
|-----------|----|------------|----------|-----------|--|
| M06CR | E= | -76.362804 | | | |
| | O | -0.000837 | 0.000000 | -0.000648 | |
| | H | -0.002677 | 0.000000 | 0.004323 | |
| | H | 0.003514 | 0.000000 | -0.003675 | |
| M08-HX | E= | -76.397793 | | | |
| | O | -0.000086 | 0.000000 | -0.000067 | |
| | H | -0.003293 | 0.000000 | 0.004343 | |
| | H | 0.003379 | 0.000000 | -0.004276 | |
| M08-SO | E= | -76.381535 | | | |
| | O | -0.005417 | 0.000000 | -0.004193 | |
| | H | -0.003612 | 0.000000 | 0.010262 | |
| | H | 0.009029 | 0.000000 | -0.006069 | |
| M11 | E= | -76.403933 | | | |
| | O | -0.001641 | 0.000000 | -0.001270 | |
| | H | -0.003892 | 0.000000 | 0.006723 | |
| | H | 0.005533 | 0.000000 | -0.005453 | |
| M11-L | E= | -76.404506 | | | |
| | O | 0.003288 | 0.000000 | 0.002545 | |
| | H | -0.000043 | 0.000000 | -0.003341 | |
| | H | -0.003245 | 0.000000 | 0.000795 | |
| MN12-L | E= | -76.355836 | | | |
| | O | 0.001127 | 0.000000 | 0.000873 | |
| | H | -0.003229 | 0.000000 | 0.003006 | |
| | H | 0.002101 | 0.000000 | -0.003879 | |
| MN12-SX | E= | -76.373687 | | | |
| | O | -0.003107 | 0.000000 | -0.002405 | |
| | H | -0.003170 | 0.000000 | 0.007304 | |
| | H | 0.006277 | 0.000000 | -0.004900 | |
| SOGGA11 | E= | -76.423371 | | | |
| | O | -0.003780 | 0.000000 | -0.002926 | |
| | H | -0.000816 | 0.000000 | 0.004959 | |
| | H | 0.004596 | 0.000000 | -0.002033 | |
| SOGGA11-X | E= | -76.405420 | | | |
| | O | -0.000473 | 0.000000 | -0.000366 | |
| | H | -0.001773 | 0.000000 | 0.002779 | |
| | H | 0.002246 | 0.000000 | -0.002413 | |

| | | | | |
|--|----|------------|----------|-----------|
| N12 | E= | -76.383122 | | |
| | O | 0.003850 | 0.000000 | 0.002980 |
| | H | -0.002507 | 0.000000 | -0.000738 |
| | H | -0.001343 | 0.000000 | -0.002242 |
| N12-SX | E= | -76.385858 | | |
| | O | 0.003032 | 0.000000 | 0.002347 |
| | H | -0.003636 | 0.000000 | 0.001566 |
| | H | 0.000604 | 0.000000 | -0.003913 |
| GAM | E= | -76.402043 | | |
| | O | 0.003354 | 0.000000 | 0.002596 |
| | H | -0.000553 | 0.000000 | -0.002749 |
| | H | -0.002800 | 0.000000 | 0.000154 |
| MN15 | E= | -76.351267 | | |
| | O | -0.005094 | 0.000000 | -0.003943 |
| | H | -0.003620 | 0.000000 | 0.009939 |
| | H | 0.008715 | 0.000000 | -0.005996 |
| MN15-L | E= | -76.347439 | | |
| | O | -0.006624 | 0.000000 | -0.005128 |
| | H | -0.000844 | 0.000000 | 0.007933 |
| | H | 0.007468 | 0.000000 | -0.002805 |
| revM06-L | E= | -76.396983 | | |
| | O | 0.002221 | 0.000000 | 0.001719 |
| | H | -0.000568 | 0.000000 | -0.001561 |
| | H | -0.001654 | 0.000000 | -0.000158 |
| revM11 | E= | -76.400663 | | |
| | O | -0.004213 | 0.000000 | -0.003261 |
| | H | -0.003825 | 0.000000 | 0.009293 |
| | H | 0.008038 | 0.000000 | -0.006032 |
| revM06 | E= | -76.387777 | | |
| | O | 0.000368 | 0.000000 | 0.000285 |
| | H | -0.002491 | 0.000000 | 0.002838 |
| | H | 0.002123 | 0.000000 | -0.003123 |
| M08-HX | E= | -76.132125 | | |
| Exchange-only with 0.5223 E^{HFE} included | O | -0.011250 | 0.000000 | -0.008708 |
| | H | -0.003871 | 0.000000 | 0.016623 |
| | H | 0.015122 | 0.000000 | -0.007915 |

| | | | | |
|--|----|------------|----------|-----------|
| M08-HX | E= | -72.106719 | | |
| Correlation and $0.5223E^{\text{HFE}}$ | O | -0.101534 | 0.000000 | -0.078592 |
| only (no meta exchange) | H | -0.005570 | 0.000000 | 0.112079 |
| | H | 0.107104 | 0.000000 | -0.033487 |
| M08-HX | E= | -67.697943 | | |
| Correlation-only with | O | -0.234053 | 0.000000 | -0.181167 |
| no meta or HF exchange | H | -0.010609 | 0.000000 | 0.255477 |
| | H | 0.244661 | 0.000000 | -0.074310 |

Note: the final three entries in the above table are for developers.

Version history

Version 1, December 31, 2008

Original version

Version 1.1, April 23, 2009

Added SOGGA

Version 1.2, May 14, 2009

Fixed some bugs, added reference energies and forces in the manual

Version 1.3, May 12, 2011

Added SOGGA11

Version 1.4 October 07, 2011

Fixed some bugs, added reference citation for SOGGA11.

Version 1.5 November 07, 2011

Added SOGGA11-X and M11

Version 1.6 December 05, 2011

Added M11-L, fixed some bugs

Version 1.7 April 18, 2012

Added N12, fixed some bugs

Version 1.8 September 05, 2012

Added MN12-L, N12-SX and MN12-SX, fixed some bugs

Version 2.0 January 27, 2016

Added GAM, MN15-L and MN15

Version 3.0 March 16, 2018

Added revM06-L and revM06

Version 4.0 December 1, 2018

Added revM11

Version 5.0 October 6, 2019

Added M06-SX

Version 6.0 February 21, 2022

Added M06CR