Manual

MN-GFM, version 6.11: Minnesota Gaussian Functional Module

Incorporating the PW6B95, PWB6K, SOGGA, SOGGA11, SOGGA11-X, N12, N12-SX, M08-HX, M08-SO, M11, M11-L, MN12-L, MN12-SX, PBEsol, WC06, RPBE, revPBE, B97-3, B86, GAM, MN15-L, MN15, OreLYP, MGGA_MS0, MGGA_MS1, MGGA_MS2, MGGA_MS2h, revM06-L, revM06, revM11, and M06-SX

Functionals in the *Gaussian09–version C01* Program

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Contents

Executive summary

MN-GFM, version 6.11 (Minnesota Gaussian Functional Module, version 6.11) is a module for incorporation of the PW6B95, PWB6K, SOGGA, SOGGA11, SOGGA11-X, N12, N12-SX, M08-HX, M08-SO, M11, M11-L, MN12-L, MN12-SX, PBEsol, WC06, RPBE, revPBE, B97-3, B86, GAM, MN15-L, MN15, OreLYP, MGGA_MS0, MGGA_MS1, MGGA_MS2, MGGA_MS2h, revM06-L, revM06, revM11, and M06-SX DFT methods into revision C01 of the *Gaussian 09* code.

Licensing

Gaussian 09.C01 is licensed by Gaussian, Inc. The modified *Gaussian* source code is not available for distribution except by Gaussian, Inc. This package is for local use by the developers of the modified code and users of the code covered by the University of Minnesota site license.

Literature references – original references for functionals

PW6B95 and PWB6K

Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2005**, *109*, 5656.

SOGGA

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

SOGGA11

Peverati, R.; Zhao, Y.; D. G. Truhlar, *J. Phys. Chem. Lett*. **2011**, *2*, 1991.

SOGGA11-X

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

N12

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

N12-SX

Peverati, R.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2012**, *14*, 16187

M08-HX and M08-SO

Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2008**, *4*, 1849.

M11

Peverati, R.; Truhlar, D. G. *J. Phys. Chem. Lett*. **2011**, *2*, 2810.

M11-L

Peverati, R.; Truhlar, D. G. *J. Phys. Chem. Lett.* **2012**, *3*, 117.

MN12-L

Peverati, R.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2012**, *14*, 13171

MN12-SX

Peverati, R.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2012**, *14*, 16187.

PBEsol

Perdew, J. et al. *Phys. Rev. Lett.* **2008**, *100*, 136406.

WC06

Wu, Z.; Cohen, R. E. *Phys. Rev. B* **2006**, *73*, 235116. See also Zhao, Y.; Truhlar, D. G. *Phys. Rev. B* **2008**, *78*, 197101.

RPBE

Hammer B.; Hansen L. B.; Norskov, J. K. *Phys. Rev. B* **1999**, *59,* 7413.

revPBE

Zhang, Y; Yang W. *Phys. Rev. Lett.* **1998**, *80*, 890.

B97-3

Keal, T. W.; Tozer D. J. *J. Chem. Phys.* **2005**, *123*, 121103.

B86 (also known as Xαβγ)

Becke, A. D. *J. Chem. Phys.* **1986**, *84*, 4524.

GAM

Yu, H. S.; Zhang, W.; Verma, P.; He, X.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2015**, *17*, 12146.

MN15-L

Yu, H. S.; He, X.; Truhlar, D. G. *J. Chem. Theory Comput.* **2016**, *12*, 1280.

MN15

Yu, H. S.; He, X.; Li, S.; Truhlar, D. G. *Chem. Sci.* **2016**, *7*, 5032.

OreLYP
Thakkar, A. J.; McCarthy, S. P. *J. Chem. Phys.* **2009**, *131*, 134109.

MGGA_MS0, MGGA_MS1, MGGA_MS2 and MGGA_MS2h
Sun, J.; Haunschild, R.; Xiao, B.; Bulik, I.; Scuseria, G.; Perdew, J. *J. Chem. Phys.* **2013**, *138*, 044113.

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.

revM06
Wang, Y.; Verma, P.; Jin, X. S.; Truhlar, D. G.; He, X. *Proc. Natl. Acad. Sci. U.S.A.*, **2018**, 115, 10257.

revM11
Verma, P.; Wang, Y.; Ghosh, S.; He, X.; Truhlar, D. G. *J. Phys. Chem. A*, **2019**, 123, 2966

M06-SX
Wang, Y.; Verma, P.; Zhang, L. J.; Li, Y. Q.; Liu, Z. H.; Truhlar, D.G.; He, X., **2019**, submitted.

Usage

MN-GFM allows users to perform calculations with additional DFT functionals (developed by the Truhlar group and by other groups). The keywords for setting up these calculations are described here.

Required Keywords

pw6b95 This keyword specifies the PW6B95 functional.

pwb6k This keyword specifies the PWB6K functional.

sogga This keyword specifies the SOGGA functional.

sogga11 This keyword specifies the SOGGA11 functional.

sogga11x This keyword specifies the SOGGA11-X functional.

n12 This keyword specifies the N12 functional.

n12sx This keyword specifies the N12-SX functional.

m08hx This keyword specifies the M08-HX functional.

m08so This keyword specifies the M08-SO functional.

m11 This keyword specifies the M11 functional.

m11l This keyword specifies the M11-L functional.

mn12l This keyword specifies the MN12-L functional.

mn12sx This keyword specifies the MN12-SX functional.

pbesol This keyword specifies the PBEsol functional.

wc06 This keyword specifies the WC06 functional.

rpbe This keyword specifies the RPBE functional.

revpbe This keyword specifies the revPBE functional.

b973 This keyword specifies the B97-3 functional.

b86 This keyword specifies the B86 exchange functional. It can be combined with any correlation functional (a reasonable combination is with PW91 correlation by using the b86pw91 keyword)

GAMGAM This keyword specifies the GAM functional.

MN15L This keyword specifies the MN15-L functional.

MN15 This keyword specifies the MN15 functional.

OreLYP This keyword specifies the OreLYP functional.

MGGAMS0betaPBE This keyword specifies the MGGA_MS0 functional.

MGGAMS1betaPBE This keyword specifies the MGGA_MS1 functional.

MGGAMS2betaPBE This keyword specifies the MGGA_MS2 functional.

MGGAMS2HbetaPBE This keyword specifies the MGGA_MS2h functional.

revM06L This keyword specifies the revM06-L functional.

revM06 This keyword specifies the revM06 functional.

revM11 This keyword specifies the revM11 functional.

M06SX This keyword specifies the M06-SX functional.

Package

The source code of *MN-GFM* consists of a single directory, MN-GFM6.11, in which the implemented and modified subroutines necessary to run *MN-GFM* reside.

Installing *MN-GFM*

The *MN-GFM* code is a compressed tar file named `MN-GFM6.11.tar.gz`. It contains the necessary subroutines to run *MN-GFM* with *Gaussian 09 C01*, and it also contains a directory for test runs.

To uncompress, enter `gunzip MN-GFM6.11.tar.gz`

The uncompressed file will be named `MN-GFM6.11.tar`. After extracting the files from the tar file, which can be done with the command:

```
tar -xvf MN-GFM6.11.tar
```

This creates a new directory, MN-GFM6.11. This directory contains all the files included in the package, as follows:

MN-GFM-build	exwcor.F	getdft.F	loclxc.F	m11x1.F	mpbeh0.F
nameco.F	ndxc1g.F	pwbc.F	revnum.F	sodfGG.F	sogga.F
sogga11x.F	wc06.F	xcgetw.F	cfunc.F	exwex.F	ixctyc.F
m11c.F	mn12x.F	n12x.F	nameex.F	pbesolc.F	pwbcss.F
rpbe.F	sodfRG.F	sogga1.F	sogga11x1.F	wc061.F	xfunc.F
doc	gaucite.F	ixctyx.F	m11x.F	mn12x1.F	n12x1.F
namexc.F	prcdft.F	pwbx.F	rpbe1.F	sodfRR.F	sogga11c.F
test	xcfunc.F	GAMx.F	MGGAMSx1.F	MGGAMSx.F	mn16x1.F
MN16c.F	GAMx1.F	revExWCor.f			
revHCTHx.F	revVSC.F	revVSX.F			

The Test directory contains the input and output files of 49 test runs. The ExtraTest directory contains the input and output files of 60 test runs for GAM, MN15, MN15-L, M08-HX, and PW6B95.

The following steps need to be taken to properly install *MN-GFM*:

1) Make sure that the officially distributed *Gaussian 09*.C01 is properly installed. Make sure that the $g09root environment variable is properly set and the $g09root/g09/bsd/g09.login file has been sourced. The $g09root environment variable is the location of the *Gaussian 09* directory structure on a given machine (for example, /usr/local/g09.C01/ could be the location).

   Note: The MN-GFM code will modify the installation of *Gaussian* in the $g09root directory. MN-GFM modifies the following 16 links in this directory: l1, l121, l301, l401, l502, l508, l510, l608, l703, l801, l913, l914, l916, l11002, l11014, and l11110.

2) Go to the MN-GFM directory. There is one install script in the MN-GFM directory, called MN-GFM-build. Run the install script to accomplish the installation.

Platforms

MN-GFM versions 1.0, 2.0, and 2.0.1 were tested on the following platforms:

- IBM SP with WinterHawk+ nodes with 375 MHz Power3 processors running the AIX version 5.2 operating system and compiled with the XL Fortran compiler version 9.1
- IBM pSeries 690 and pSeries 655 Nodes (Power 4 processors) running AIX version 5.2 and compiled with the XL Fortran compiler version 9.1
- SGI Altix 3700 running the Linux SuSE 9.0 operating system and compiled with the Intel Fortran compiler version 8.1

MN-GFM version 4.0 was tested on the following platforms:

- IBM pSeries 690 and pSeries 655 Nodes (Power 4 processors) running AIX version 5.2 and compiled with the XL Fortran compiler version 9.1
- SGI Altix 3700 running the Linux SuSE 9.0 operating system and compiled with the Intel Fortran compiler version 8.1
- IBM Blade285 running the Linux operating system and compiled with the PathScale(TM) EKOPath™ Compiler Suite: Version 2.5

MN-GFM version 4.1 was tested on the following platforms:

- IBM pSeries 690 and pSeries 655 Nodes (Power 4 processors) running AIX version 5.2 and compiled with the XL Fortran compiler version 9.1
- SGI Altix 3700 running the Linux SuSE 9.0 operating system and compiled with the Intel Fortran compiler version 8.1
- IBM Blade285 running the Linux operating system and compiled with the PathScale(TM) EKOPath™ Compiler Suite: Version 2.5

MN-GFM version 4.2 was tested on the following platforms:

- IBM Blade285 running the Linux operating system and compiled with the PathScale(TM) EKOPath™ Compiler Suite: Version 2.5

MN-GFM version 4.3 was tested on the following platforms:

- IBM Blade285 running the Linux operating system and compiled with the PathScale(TM) EKOPath™ Compiler Suite: Version 2.5
- IBM Calhoun running the Linux operating system and compiled with the Intel Compiler version 11.0

MN-GFM version 5.0 was tested on the following platforms:

- Sun Fire X4600 Linux Cluster and compiled with the Portland Compiler Suite: Version 10.3

MN-GFM version 5.1 was tested on the following platforms:

- Sun Fire X4600 Linux Cluster and compiled with the Portland Compiler Suite: Version 10.3
- HP Proliant BL280c G6 Linux Cluster and compiled with the Portland Compiler Suite: Version 10.9

MN-GFM version 5.2 was tested on the following platforms:

- HP Proliant BL280c G6 Linux Cluster and compiled with the Portland Compiler Suite: Version 10.9

MN-GFM version 6.0 was tested on the following platforms:

- HP Proliant BL280c G6 Linux Cluster and compiled with the Portland Compiler Suite: Version 11.0 (MSI Itasca)
- SGI Altix XE 1300 Linux cluster and compiled with the Portland Compiler Suite: Version 11.0 (MSI Calhoun)
- Sun Fire X4600 Linux Cluster and compiled with the Portland Compiler Suite: Version 10.3 and Version 11.0 (MSI Elmo)

MN-GFM version 6.1 was tested on the following platforms:

- HP Proliant BL280c G6 Linux Cluster and compiled with the Portland Compiler Suite: Version 11.0 (MSI Itasca)
- SGI Altix XE 1300 Linux cluster and compiled with the Portland Compiler Suite: Version 11.0 (MSI Calhoun)
- Sun Fire X4600 Linux Cluster and compiled with the Portland Compiler Suite: Version 10.3 and Version 11.0 (MSI Elmo)

MN-GFM version 6.2 was tested on the following platforms:

- HP Proliant BL280c G6 Linux Cluster and compiled with the Portland Compiler Suite: Version 11.0 (MSI Itasca)
- SGI Altix XE 1300 Linux cluster and compiled with the Portland Compiler Suite: Version 11.0 (MSI Calhoun)
- Sun Fire X4600 Linux Cluster and compiled with the Portland Compiler Suite: Version 10.3 and Version 11.0 (MSI Elmo)

MN-GFM version 6.3 was tested on the following platforms:

- HP Proliant BL280c G6 Linux Cluster and compiled with the Portland Compiler Suite: Version 12.3 (MSI Itasca)
- Constellation of SGI systems and compiled with the Portland Compiler Suite: Version 11.7 (MSI Koronis)

MN-GFM version 6.4 was tested on the following platforms:

- HP Proliant BL280c G6 Linux Cluster and compiled with the Portland Compiler Suite: Version 12.3 (MSI Itasca)

MN-GFM version 6.5 was tested on the following platforms:

- HP Apollo 6000 system and compiled with the Portland Compiler Suite: Version 12.3 (MSI Mesabi)

MN-GFM version 6.6 was tested on the following platforms:

- HP Apollo 6000 system and compiled with the Portland Compiler Suite: Version 12.3 (MSI Mesabi)

MN-GFM version 6.7 was tested on the following platforms:

- HP Apollo 6000 system and compiled with the Portland Compiler Suite: Version 12.3 (MSI Mesabi)

MN-GFM version 6.8 was tested on the following platforms:

- HP Apollo 6000 system and compiled with the Portland Compiler Suite: Version 12.3 (MSI Mesabi)

MN-GFM version 6.9 was tested on the following platforms:

- HP Apollo 6000 system and compiled with the Portland Compiler Suite: Version 12.3 (MSI Mesabi)

MN-GFM version 6.10 was tested on the following platforms:

- HP Apollo 6000 system and compiled with the Portland Compiler Suite: Version 12.3 (MSI Mesabi)

MN-GFM version 6.11 was tested on the following platforms:

- HP Apollo 6000 system and compiled with the Portland Compiler Suite: Version 12.3 (MSI Mesabi)

Revision history and version summaries

MN-GFM-v.1.0 (02-21-06)
Authors: Y. Zhao and D. G. Truhlar

The first version of *MN-GFM*. This version contains PW6B95, PWB6K, M05, and M05-2X. This version was tested with revision D01 of *Gaussian 03*.

MN-GFM-v.2.0 (08-02-06)
Authors: Y. Zhao and D. G. Truhlar

The M06-L functional has been added to *MN-GFM*. This version was tested with revision D01 of *Gaussian 03*.

MN-GFM-v.2.0.1 (09-05-06)
Authors: Y. Zhao and D. G. Truhlar

An error in the M06-L functional has been fixed. This version was tested with revision D01 of *Gaussian 03*.

The M06-HF, M06, and M06-2X functionals have been added to *MN-GFM*. This version was tested with revision D01 of *Gaussian 03*.

MN-GFM-v.3.1 *(12-11-06)*
Authors: Y. Zhao and D. G. Truhlar

This version was sent to Michael Frisch on Dec. 31, 2008. It is a special stripped down version that has only the M06 family. See the 3.1 manual for further details.

MN-GFM-v.4.0 (12-31-08)
Authors: Y. Zhao and D. G. Truhlar

The SOGGA, M08-HX, and M08-SO functionals have been added to *MN-GFM, and* PW6B95, PWB6K, which were temporarily removed in the 3.1 version that we sent to Michael Frisch, have been restored to MN-GFM. Note that since M05 and M05-2X are already added to *Gaussian03*, they are no longer included in MN-GFM. Version 4.0 was tested with revision E01 of *Gaussian 03*.

MN-GFM-v.4.1 (12-31-08)
Authors: Y. Zhao and D. G. Truhlar

The PBEsol and WC06 functionals have been added to *MN-GFM*. *MN-GFM* Version 4.1 was tested with revision E01 of *Gaussian 03*.

MN-GFM-v.4.2 (08-10-09)
Authors: Y. Zhao and D. G. Truhlar

The RPBE and revPBE functionals have been added to *MN-GFM*. *MN-GFM* Version 4.2 was tested with revision E01 of *Gaussian 03.*

MN-GFM-v.4.3 (09-09-09)
Authors: Y. Zhao and D. G. Truhlar

The B97-3 functional has been added to *MN-GFM*. *MN-GFM* Version 4.3 was tested with revision E01 of *Gaussian 03.*

MN-GFM-v.5.0 (11-07-10)
Authors: K. Yang and D. G. Truhlar

The functionals in M06 family have been removed from MN-GFM Version 5.0 since they are implemented in *Gaussian 09*. The other functionals in MN-GFM Version 4.3 have been incorporated in revision A02 of *Gaussian 09*.

The **IOp(3/78)** option has been implemented for M08-type correlation functionals.

MN-GFM-v.5.2 (05-11-11)
Authors: R. Peverati and D. G. Truhlar

The SOGGA11 functional has been added to *MN-GFM*. *MN-GFM.* Version 5.2 was tested with revision A02 of *Gaussian 09.*

MN-GFM-v.6.0 (10-26-11)
Authors: R. Peverati and D. G. Truhlar

The SOGGA11-X, M11, and M11-L functionals have been added to *MN-GFM*.
MN-GFM Version 6.0 was tested with revision C01 of *Gaussian 09.*

MN-GFM-v.6.1 (02-07-12)
Authors: R. Peverati and D. G. Truhlar

Fixed some bugs (in particular, second derivatives of SOGGA11s and M11s)

MN-GFM-v.6.2 (02-20-12)
Authors: R. Peverati and D. G. Truhlar

The Becke 86 functional (a.k.a. Xαβγ) exchange functional has been added.

MN-GFM-v.6.3 (06-20-12)
Authors: R. Peverati and D. G. Truhlar

The N12 and MN12-L functionals have been added.

MN-GFM-v.6.4 (09-XX-12)

Authors: R. Peverati and D. G. Truhlar

The N12-SX and MN12-SX functionals have been added.

MN-GFM-v.6.5 (05-XX-15)
Authors: Xiao He, Haoyu Yu, and D. G. Truhlar

The GAM. OreLYP, MGGA_MS0, MGGA_MS1, MGGA_MS2, and MGGA_MS2h functionals have been added.

MN-GFM-v.6.6 (11-XX-15)
Authors: Haoyu Yu and D. G. Truhlar

The MN15-L functional has been added.

MN-GFM-v.6.7 (12-XX-15)
Authors: Haoyu Yu and D. G. Truhlar

The MN15 functional has been added.

MN-GFM-v.6.8 (02-23-17)
Authors: Xiao He and D. G. Truhlar

The revM06-L functional has been added.

MN-GFM-v.6.9 (11-26-18)
Authors: Xiao He, Ying Wang, Pragya Verma and D. G. Truhlar

The revM06 functional has been added.

MN-GFM-v.6.10 (12-02-18)
Authors: Xiao He, Pragya Verma, Ying Wang and D. G. Truhlar

The revM11 functional has been added.

MN-GFM-v.6.11 (10-06-19)
Authors: Xiao He, Ying Wang, Pragya Verma and D. G. Truhlar

The M06-SX functional has been added.

Scaling of exchange-correlation functionals

User-Defined Models in Gaussian 09

Gaussian 09 can use any model of the general form:

$$P_2E_X^{HF} + P_1(P_4E_X^{Slater} + P_3\Delta E_x^{semi\text{-}local}) + P_6E_C^{local} + P_5\Delta E_C^{semi\text{-}local} \quad (1)$$

Any combinable semi-local exchange functional and combinable correlation functional may be used. The only available local exchange method is called Slater (S) by *Gaussian* , but actually it is the Gáspár-Kohn-Sham exchange, which is 2/3 as large as Slater's.

The values of the six parameters are specified with various non-standard options (**IOps**) to the program:

- **IOp(3/76=*mmmmmnnnnn*)** sets P_1 to *mmmmm*/10000 and P_2 to *nnnnn*/10000. P_1 is usually set to either 1.0 or 0.0, depending on whether an exchange functional is desired or not, and any scaling is accomplished using P_3 and P_4.
- **IOp(3/77=*mmmmmnnnnn*)** sets P_3 to *mmmmm*/10000 and P_4 to *nnnnn*/10000.
- **IOp(3/78=*mmmmmnnnnn*)** sets P_5 to *mmmmm*/10000 and P_6 to *nnnnn*/10000.

Note that all values must be expressed using five digits, adding any necessary leading zeros, and by default each P_i = 1.0.For example, **IOp(3/76=0560004400)** sets P_1 to 0.56 and P_2 to 0.44. By combining this IOp with the MPWB95 keyword, we actually specify the MPWB1K functional (Note that P_3, P_4, P_5, and P_6 are equal to 1.0 by default if **IOp(3/77)** and **IOp(3/78)** are not specified).

P_5 and P_6 from **IOp(3/78)** are used to scale the local and semilocal part of the correlation functional (Eq 1). However, P_5 and P_6 are implemented differently in MN-GFM for M08 functionals.

Scaling of M08-type correlation functionals

The functional form of the M08-type correlation functional is given by

$$E_C^{M08} = \int d\mathbf{r}\rho\varepsilon_C^{LSDA}(r_s,\varsigma)f_3(w)d\mathbf{r} + \int d\mathbf{r}\rho H^{PBE}(r_s,\varsigma,t)f_4(w)d\mathbf{r} \quad (2)$$

where $\varepsilon_C^{\mathrm{LSDA}}(r_s,\varsigma)$ is the correlation energy per electron of the uniform electron gas limit, for which we use the parametrization of Perdew and Wang; $H^{\mathrm{PBE}}(r_s,\varsigma,t)$ is the PBE gradient correction for the correlation, and $f_3(w)$ and $f_4(w)$ are the kinetic-energy-density enhancement factors for correlation.

In our implementation, we used P_5 and P_6 to scale the two terms in Eq 2, i.e.

$$E_C^{M08} = P_6\int d\mathbf{r}\rho\varepsilon_C^{LSDA}(r_s,\varsigma)f_3(w)d\mathbf{r} + P_5\int d\mathbf{r}\rho H^{PBE}(r_s,\varsigma,t)f_4(w)d\mathbf{r} \quad (3)$$

If **IOp(3/78)** is not specified, P_5 and P_6 are set to be 1.0 by default. Combining **IOp(3/78=0500005000)** and M08HX keyword in MN-GFM, sets P_5 to 0.5 and P_6 to 0.5, i.e. it specifies a non-standard M08-HX functional with the total M08-HX correlation energy scaled by 0.5. Combining **IOp(3/78=0900008000)** with the keyword M08SO specifies a non-standard M08-SO functional with P_5 = 0.9 and P_6 = 0.8 in Eq 3.

Note: The limit of P_5 and P_6 is 0 – 9.9999 (same as P_1, P_2, P_3, and P_4). One should not use IOp(3/76=0000000000) or (IOp(3/77=0000000000) or (IOp(3/78=0000000000) to set the values of the parameters for any density functionals in G09. *Gaussian* interprets this not as a request to set the parameters to zero but rather as IOp(3/78=0), which means to use default value of 1.0 for the parameters.

Test Runs in the Test directory

Test run 1: PW6B95 single-point calculation on H_2O with the 6-311+G(2df,2p) basis set.

Test run 2: PWB6K force calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 3: SOGGA geometry optimization of Cu_2 (closed shell singlet) with the CEP-121Geffective core potential.

Test run 4: M08-SO single-point calculation on NH_3 with the 6-311+G(2df,2p) basis set.

Test run 5: M08-HX single-point calculation on H_2S with the 6-31+G(d,p) basis set.

Test run 6: PBEsol single-point calculation on H_2O with the 6-311+G(2df,2p) basis set.

Test run 7: WC06 single-point calculation on H_2O with the 6-311+G(2df,2p) basis set.

Test run 8: RPBE single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set.

Test run 9: revPBE single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set.

Test run 10: B97-3 single-point calculation on H_2O with the 6-311+G(2df,2p) basis set.

Test run 11: A non-standard M08-SO single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set and **IOp(3/78=0900008000)** to scale the M08-SO correlation.

Test run 12: SOGGA11 single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set.

Test run 13: SOGGA11 geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 14: SOGGA11-X single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set.

Test run 15: SOGGA11-X geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 16: M11 single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set.

Test run 17: M11 geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 18: M11-L single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set.

Test run 19: M11-L geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 20: N12 single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set.

Test run 21: N12 geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 22: MN12-L single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set.

Test run 23: MN12-L geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 24: N12-SX single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set.

Test run 25: N12-SX geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 26: MN12-SX single-point calculation on CH_3 with the 6-311+G(2df,2p) basis set.

Test run 27: MN12-SX geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 28: GAM single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 29: GAM single-point calculation on H_2O with the 6-31+G(d,p) basis set.

Test run 30: MN15-L single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 31: MN15-L single-point calculation on H_2O with the 6-31+G(d,p) basis set.

Test run 32: MN15 single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 33: MN15 single-point calculation on H_2O with the 6-31+G(d,p) basis set.

Test run 34: OreLYP single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 35: OreLYP single-point calculation on H_2O with the 6-31+G(d,p) basis set.

Test run 36: MGGA_MS0 single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 37: MGGA_MS0 single-point calculation on H_2O with the 6-31+G(d,p) basis set.

Test run 38: MGGA_MS1 single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 39: MGGA_MS1 single-point calculation on H_2O with the 6-31+G(d,p) basis set.

Test run 40: MGGA_MS2 single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 41: MGGA_MS2 single-point calculation on H_2O with the 6-31+G(d,p) basis set.

Test run 42: revM06-L geometry optimization of CH_3 with the 6-31+G(d,p) basis set.

Test run 43: revM06-L geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 44: revM06 geometry optimization of CH_3 with the 6-31+G(d,p) basis set.

Test run 45: revM06 geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 46: revM11 geometry optimization of CH_3 with the 6-31+G(d,p) basis set.

Test run 47: revM11 geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 48: M06-SX geometry optimization of CH_3 with the 6-31+G(d,p) basis set.

Test run 49: M06-SX geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Reference energies and gradients

Tables 1 and 2 present reference energies and forces of CH_3 (open shell, doublet) and H_2O (closed shell, singlet) with the 6-31+G** basis set and a pruned (99, 590) grid.

Geometry of CH_3 (in angstrom)

```
**********************************************************
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
**********************************************************
```

Geometry of H_2O (in angstrom)

```
**********************************************************
O     0.000000    0.000000     0.000000
H     0.000000    0.000000     0.956914
H     0.926363    0.000000    -0.239868
**********************************************************
```

Table 1. Reference energies (hartrees) and gradients (hartree/bohr)

PW6B95	E=	-39.888691			
			Forces		
		X	Y	Z	
	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			
			Forces		
		X	Y	Z	
	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			
			Forces		
		X	Y	Z	
	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			
			Forces		
		X	Y	Z	
	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			
			Forces		
		X	Y	Z	
	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

Forces

	X	Y	Z
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

Forces

	X	Y	Z
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

Forces

	X	Y	Z
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

Forces

	X	Y	Z
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

Forces

	X	Y	Z
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

	Forces		
	X	Y	Z
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

	Forces		
	X	Y	Z
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

PBEsol E= -39.586795

	Forces		
	X	Y	Z
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

	Forces		
	X	Y	Z
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

	Forces		
	X	Y	Z
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

			Forces	
		X	Y	Z
	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			
			Forces		
		X	Y	Z	
	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	

GAM	E=	-39.857392			
			Forces		
		X	Y	Z	
	C	0.000000	0.000306	0.000000	
	H	0.000000	0.000704	0.000000	
	H	0.000994	-0.000525	0.000000	
	H	-0.000994	-0.000525	0.000000	

MN15-L	E=	-39.790513			
			Forces		
		X	Y	Z	
	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			
			Forces		
		X	Y	Z	
	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	

OreLYP	E=	-39.823827			
			Forces		
		X	Y	Z	
	C	0.000000	0.000303	0.000000	
	H	0.000000	0.007580	0.000000	
	H	0.006910	-0.003942	0.000000	

	H	-0.006910	-0.003942	0.000000

MGGA_MS0 E= -39.878368

	Forces		
	X	Y	Z
C	0.000000	0.000314	0.000000
H	0.000000	0.001498	0.000000
H	0.001661	-0.000906	0.000000
H	-0.001661	-0.000906	0.000000

MGGA_MS1 E= -39.869479

	Forces		
	X	Y	Z
C	0.000000	0.000314	0.000000
H	0.000000	0.002843	0.000000
H	0.002824	-0.001579	0.000000
H	-0.002824	-0.001579	0.000000

MGGA_MS2 E= -39.874393

	Forces		
	X	Y	Z
C	0.000000	0.000320	0.000000
H	0.000000	0.003008	0.000000
H	0.002975	-0.001664	0.000000
H	-0.002975	-0.001664	0.000000

revM06-L E= -39.811321

	Forces		
	X	Y	Z
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

	Forces		
	X	Y	Z
C	0.000000	0.000295	0.000000
H	0.000000	0.002390	0.000000
H	0.002418	-0.001343	0.000000
H	-0.002418	-0.001343	0.000000

revM11 E= -39.809756

	Forces		
	X	Y	Z
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

	Forces		
	X	Y	Z
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

Table 2. Reference energies (hartrees) and gradients (hartree/bohr)

PW6B95	E=	-76.511732		
			Forces	
		X	Y	Z
	O	-0.000549	0.000000	-0.000425
	H	-0.002113	0.000000	0.003297
	H	0.002662	0.000000	-0.002872
PWB6K	E=	-76.457380		
			Forces	
		X	Y	Z
	O	0.007242	0.000000	0.005606
	H	-0.002399	0.000000	-0.004382
	H	-0.004843	0.000000	-0.001224
SOGGA	E=	-76.028293		
			Forces	
		X	Y	Z
	O	-0.014319	0.000000	-0.011083
	H	-0.001961	0.000000	0.017325
	H	0.016280	0.000000	-0.006242
SOGGA11	E=	-76.423371		
			Forces	
		X	Y	Z
	O	-0.003780	0.000000	-0.002926
	H	-0.000816	0.000000	0.004959
	H	0.004596	0.000000	-0.002033
SOGGA11-X	E=	-76.405414		
			Forces	
		X	Y	Z
	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		
			Forces	
		X	Y	Z
	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

Forces

	X	Y	Z
O	0.003032	0.000000	0.002347
H	-0.003636	0.000000	0.001566
H	0.000604	0.000000	-0.003913

M08-HX E= -76.397793

Forces

	X	Y	Z
O	-0.000086	0.000000	-0.000067
H	-0.003293	0.000000	0.004343
H	0.003379	0.000000	-0.004277

M11 E= -76.403935

Forces

	X	Y	Z
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

Forces

	X	Y	Z
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

Forces

	X	Y	Z
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

Forces

X	Y	Z

	O	-0.003107	0.000000	-0.002405
	H	-0.003170	0.000000	0.007304
	H	0.006277	0.000000	-0.004900

PBEsol E= -76.087952

	Forces		
	X	Y	Z
O	-0.014345	0.000000	-0.011103
H	-0.002052	0.000000	0.017468
H	0.016396	0.000000	-0.006365

WC06 E= -76.216737

	Forces		
	X	Y	Z
O	-0.012857	0.000000	-0.009952
H	-0.002037	0.000000	0.015913
H	0.014895	0.000000	-0.005961

RPBE E= -76.427997

	Forces		
	X	Y	Z
O	-0.014386	0.000000	-0.011135
H	-0.001130	0.000000	0.016320
H	0.015516	0.000000	-0.005185

revPBE E= -76.408566

	Forces		
	X	Y	Z
O	-0.014131	0.000000	-0.010938
H	-0.001242	0.000000	0.016202
H	0.015374	0.000000	-0.005264

B97-3 E= -76.412895

	Forces		
	X	Y	Z
O	-0.001394	0.000000	-0.001079
H	-0.001939	0.000000	0.003945
H	0.003333	0.000000	-0.002867

GAM	E=	-76.402043		
			Forces	
		X	Y	Z
	O	0.003354	0.000000	0.002596
	H	-0.000553	0.000000	-0.002749
	H	-0.002800	0.000000	0.0001537
MN15-L	E=	-76.347439		
			Forces	
		X	Y	Z
	O	-0.006624	0.000000	-0.005128
	H	-0.000844	0.000000	0.007933
	H	-0.007468	0.000000	-0.002805
MN15	E=	-76.351267		
			Forces	
		X	Y	Z
	O	-0.005094	0.000000	-0.003943
	H	-0.003620	0.000000	0.009939
	H	0.008715	0.000000	-0.005996
OreLYP	E=	-76.405631		
			Forces	
		X	Y	Z
	O	-0.010362	0.000000	-0.008020
	H	-0.001027	0.000000	0.012031
	H	0.011389	0.000000	-0.004010
MGGA_MS0	E=	-76.445031		
			Forces	
		X	Y	Z
	O	-0.005886	0.000000	-0.004556
	H	-0.000830	0.000000	0.007152
	H	0.006716	0.000000	-0.002596
MGGA_MS1	E=	-76.432232		
			Forces	
		X	Y	Z
	O	-0.007404	0.000000	-0.005731
	H	-0.000762	0.000000	0.008632
	H	0.008166	0.000000	-0.002901

MGGA_MS2	E=	-76.440246		
		Forces		
		X	Y	Z
	O	-0.008542	0.000000	-0.006612
	H	-0.000575	0.000000	0.009567
	H	0.009118	0.000000	-0.002955

revM06-L	E=	-76.396983		
		Forces		
		X	Y	Z
	O	0.002221	0.000000	0.001719
	H	-0.000568	0.000000	-0.001561
	H	-0.001654	0.000000	-0.000158

revM06	E=	-76.387777		
		Forces		
		X	Y	Z
	O	0.000368	0.000000	0.000285
	H	-0.002491	0.000000	-0.002838
	H	-0.002123	0.000000	-0.003123

revM11	E=	-76.400663		
		Forces		
		X	Y	Z
	O	-0.004213	0.000000	-0.003261
	H	-0.003825	0.000000	0.009293
	H	0.008038	0.000000	-0.006032

M06-SX	E=	-76.352728		
		Forces		
		X	Y	Z
	O	0.001748	0.000000	0.001353
	H	-0.001950	0.000000	0.000714
	H	0.000202	0.000000	-0.002067

Extra Test runs for five Minnesota Functionals: (in the ExtraTest directory)

GAM, M08-HX, MN15, MN15-L, and PW6B95.

In the following five tables we include some extra tests for GAM, M08-HX, MN15, MN15-L, and PW6B95 functionals.

Table 1. Absolute energies (Unit: au) of three species that are involved in the following reaction and reaction barrier heights with Def2-QZVP basis sets (BH in unit: kcal/mol).
"H + N2O -> OH + N2"

Name	GAM	M08-HX	MN15	MN15-L	PW6B95
H	-0.501102876	-0.502236425	-0.499179655	-0.496287756	-0.501564496
N2O	-184.7517925	-184.6781003	-184.6407886	-184.65572	-184.9649287
TS1	-185.2275756	-185.1519042	-185.1146363	-185.12336	-185.4426571
BH	15.89	17.84	15.9	17.98	14.96

Table 2. Harmonic Frequencies of Ethanol Calculated by MP2 and by GAM, M08-HX, MN15, MN15-L, and PW6B95 with 6-31+G(d,p) basis set and Ultrafine Integration Grids (units: cm^{-1})

MP2	GAM	M08-HX	MN15	MN15-L	PW6B95
3779.3	3892.9	3922.7	3912.7	3922.3	3901.9
3220.4	3172.8	3141.9	3169.8	3135.8	3169.3
3209.8	3171.1	3139.9	3165.8	3134.5	3163.9
3118.3	3072.5	3047.6	3080.5	3033.5	3082.6
3103.1	3042.6	3031.9	3066.2	3001.5	3061.9
3060.8	3003.5	2991.1	3030.7	2962.0	3027.7
1597.9	1505.5	1524.1	1516.7	1527.7	1538.6
1566.1	1479.4	1495.4	1486.8	1498.9	1511.7
1549.3	1460.3	1478.6	1467.1	1480.6	1493.2
1509.0	1440.9	1455.6	1442.5	1457.1	1460.0
1454.6	1374.4	1395.7	1384.4	1392.0	1406.6
1335.6	1283.5	1300.7	1287.0	1298.9	1306.7
1311.1	1264.3	1262.8	1231.5	1279.7	1265.0
1221.9	1161.3	1178.4	1169.6	1180.5	1185.4
1144.6	1097.9	1133.2	1135.9	1124.3	1124.7
1077.6	1045.2	1047.6	1033.9	1046.6	1047.8
935.7	898.8	916.9	913.6	912.7	915.4
846.3	809.1	817.3	805.7	805.6	820.8
425.8	420.9	417.8	408.6	415.7	415.5
313.0	289.3	262.5	285.2	306.8	288.6
263.4	242.5	218.4	243.1	248.3	243.1

Table 3. Bond length (BL) of Pt2 calculated by GAM, M08-HX, MN15, MN15-L, and PW6B95 with Def2-QZVP basis sets (units: Å)

Name	GAM	M08-HX	MN15	MN15-L	PW6B95
BL	2.37	2.30	2.29	2.30	2.31

Table 4. Absolute energies (Unit: au) of Cu, Cl, and CuCl and bond dissociation energy (BDE) of CuCl calculated by GAM, M08-HX, MN15, MN15-L, and PW6B95 with Def2-QZVP basis sets (unit: kcal/mol).

Name	GAM	M08-HX	MN15	MN15-L	PW6B95
Cu	-1641.477741	-1640.47167	-1640.843284	-1640.511627	-1641.384795
Cl	-460.1502716	-460.1465668	-460.1265813	-460.1368764	-460.5168649
CuCl	-2101.75797	-2100.759612	-2101.108714	-2100.791991	-2102.038129
BDE	81.55	88.71	87.13	90.04	85.64

Table 5. Absolute energies (Unit: au) of Ag and Ag_2 and bond dissociation energy (BDE) of Ag_2 calculated by GAM, M08-HX, MN15, MN15-L, and PW6B95 with jun-cc-pVTZ-PP basis sets (using ECP) (unit: kcal/mol).

Name	GAM	M08-HX	MN15	MN15-L	PW6B95
Cu	-147.509708	-146.8242144	-146.6199003	-146.3861615	-146.995186
Cl	-295.0809159	-293.7068318	-293.3055556	-292.8387762	-294.0507743
BDE	38.59	36.65	41.26	41.70	37.90

Table 6. Absolute energies (Unit: au) of Zr and Zr_2 and bond dissociation energy (BDE) of Ag_2 calculated by GAM, M08-HX, MN15, MN15-L, and PW6B95 with cc-pVTZ-DK basis sets (using DKH) (unit: kcal/mol).

Name	GAM	M08-HX	MN15	MN15-L	PW6B95
Cu	-3600.202193	-3598.117481	-3600.222402	-3599.811976	-3599.300783
Cl	-7200.511957	-7196.319888	-7200.543006	-7199.730702	-7198.705334
BDE	67.50	53.29	61.62	66.99	65.12

Further information

If and when needed, updated information will be made available at the University of Minnesota Computational Chemistry Web site: http://comp.chem.umn.edu/MN-GFM.