Documentation

MN-GFM, version 6.7: 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, and MGGA_MS2

Functionals in the *Gaussian09–version C 01* Program

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Contents

Executive summary

MN-GFM, version 6.7 (Minnesota Gaussian Functional Module, version 6.7) 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, MGGAMS0, MGGAMS1, and MGGAMS2 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**, *in press.*

N12

Peverati, R.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2012**, *in press.*

N12-SX

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

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**, *submitted.*

MN12-SX

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

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.; Xiao, H.; Truhlar, G. D. *Phys. Chem. Chem. Phys.* **2015**, *17*, 12146.

MN15-L

Yu, H. S.; Xiao, H.; Truhlar, G. D. *online ASAP.*

MN15

Yu, H. S.; Xiao, H.; Li, S.; Truhlar, G. D. *submited.*

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

MGGA_MS0, MGGA_MS1, and MGG_AMS2
Sun, J.; Haunschild, R.; Xiao, B.; Bulik, I.; Scuseria, G.; Perdew, J. *Chem. Phys.* **2013**, *138*, 044113.

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.

MGGAMS0   This keyword specifies the MGGAMS0 functional.

MGGAMS1   This keyword specifies the MGGAMS1 functional.

MGGAMS2   This keyword specifies the MGGAMS2 functional.

Package

The source code of *MN-GFM* consists of a single directory, MN-GFM6.7, 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-GFM6.7.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-GFM6.7.tar.gz`

The uncompressed file will be named `MN-GFM6.7.tar`. After extracting the files from the tar file, which can be done with the command:

`tar -xvf MN-GFM6.7.tar`

a new directory, MN-GFM6.7, is created. 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		

The test directory contains the input and output files of 33 test runs.

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

1) Make sure that the officially distributed Gaussian09.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, l1002, l1014, and l1110.

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

Platforms

MN-GFM versions 1.0, 2.0, and 2.0.1 have been 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 versions 4.0 has been 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 versions 4.1 has been 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 versions 4.2 has been 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 versions 4.3 has been 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 versions 5.0 has been tested on the following platforms:
- Sun Fire X4600 Linux Cluster and compiled with the Portland Compiler Suite: Version 10.3

MN-GFM versions 5.1 has been 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 versions 5.2 has been tested on the following platforms:
- HP Proliant BL280c G6 Linux Cluster and compiled with the Portland Compiler Suite: Version 10.9

MN-GFM versions 6.0 has been 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 versions 6.1 has been 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 versions 6.2 has been 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 versions 6.3 has been 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 versions 6.4 has been 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 versions 6.5 has been tested on the following platforms:
- HP Apollo 6000 system and compiled with the Portland Compiler Suite: Version 12.3 (MSI Mesabi)

MN-GFM versions 6.6 has been tested on the following platforms:
- HP Apollo 6000 system and compiled with the Portland Compiler Suite: Version 12.3 (MSI Mesabi)

MN-GFM versions 6.7 has been 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 revsion 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 revsion 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 revsion D01 of *Gaussian 03*.

The M06-HF, M06, and M06-2X functionals have been added to *MN-GFM*. This version was tested with revsion 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 tempeorarily 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 revsion 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 revsion 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 revsion 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 revsion 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. X$\alpha\beta\gamma$) 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, MGGAMS0, MGGAMS1, MGGAMS2, and MGGAMS2h functionals have been added.

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

The MN15-L functionals have been added.

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

The MN15 functionals have been added.

Scaling of M08 correlation functionals

User-Defined Models in Gaussian 09

Gaussian 09 can use any model of the general form:

$$P_2 E_X^{HF} + P_1(P_4 E_X^{Slater} + P_3 \Delta E_x^{semi-local}) + P_6 E_C^{local} + P_5 \Delta E_C^{semi-local} \qquad (1)$$

The only available local exchange method is Slater (S), which should be used when only local exchange is desired. Any combinable semi-local exchange functional and combinable correlation functional may be used.

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.

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

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

where $\varepsilon_C^{LSDA}(r_s, \varsigma)$ is the correlation energy per electron of the uniform electron gas limit, for which we use the parametrization of Perdew and Wang; $H^{PBE}(r_s, \varsigma, t)$ 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.

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

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 M08SO keyword 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

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-121G effective 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 28: GAM geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 28: MN15-L single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 28: MN15-L geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 28: MN15 single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 28: MN15 geometry optimization of H_2O with the 6-31+G(d,p) basis set.

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

Test run 28: OreLYP geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 29: MGGA_MS0 single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 30: MGGA_MS0 geometry optimization of H_2O with the 6-31+G(d,p) basis set.

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

Test run 32: MGGA_MS1 geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Test run 33: MGGA_MS2 single-point calculation on CH_3 with the 6-31+G(d,p) basis set.

Test run 34: MGGA_MS2 geometry optimization of H_2O with the 6-31+G(d,p) basis set.

Reference energies and gradients

Table 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 forces (Hartree/Bohr) for CH_3

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	

MGGAMS0   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

MGGAMS1   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

MGGAMS2   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

Table 2. Reference energies (Hartrees) and forces (Hartree/Bohr) for H_2O

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

	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

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

MGGAMS0 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

MGGAMS1 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

MGGAMS2 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

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.