

***MN-GFM:***  
**Minnesota Gaussian Functional Module**  
Incorporating the PW6B95, PWB6K, M05, M05-2X, M06-L, M06-HF, M06, and M06-2X  
Functionals in the *Gaussian03.D01* Program

**Documentation**

Version 3.0

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## Executive summary

*MN-GFM*, version 3.0 (Minnesota Gaussian Functional Module, version 3.0) is a module for incorporation of the PW6B95, PWB6K, M05, M05-2X, M06-L, M06-HF, M06, and M06-2X DFT methods into revision D01 of the *Gaussian 03* code.

## Licensing

*Gaussian 03.D01* is licensed by Gaussian, Inc. The modified *Gaussian* source code is not available for distribution except by Gaussian, Inc. Gaussian, Inc. plans to incorporate these capabilities into a future version of *Gaussian03*. This package is a vehicle for transmitting these changes to Gaussian, Inc. and for local use by the developers of the modified code.

## Literature references – For functionals

### PW6B95 and PWB6K

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

### M05

Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Phys.* **2005**, *123*, 161103.

### M05-2X

Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Theory Comput.* **2006**, *2*, 364.

### M06-L

Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *125*, 194101.

### M06-HF

Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2006**, *110*, 13126.

### M06 and M06-2X

Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2007**, submitted.

## Literature references – For applications

### Application of PW6B95 and PWB6K

Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2005**, *109*, 6624.

Zhao, Y.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2005**, *7*, 2701.

Zhao, Y.; Tishchenko, O.; Truhlar, D. G. *J. Phys. Chem. B* **2005**, *109*, 19046.

Application of M05 and M05-2X

Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2006**, *110*, 5121.

Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2006**, *110*, 10478.

Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2006**, *2*, 1009.

Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *124*, 224105.

Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2007**, in press.

## Usage

*MN-GFM* allows users to perform calculations with five DFT functionals developed in the Truhlar group. The keywords for setting up these calculations are described here.

### *Required Keywords*

**pw6b95** This keyword specifies the PW6B95 functional.

**pw6k** This keyword specifies the PWB6K functional.

**m05** This keyword specifies the M05 functional.

**m052x** This keyword specifies the M05-2X functional

**m06L** This keyword specifies the M06-L functional

**m06hf** This keyword specifies the M06-HF functional

**m06** This keyword specifies the M06 functional

**m062x** This keyword specifies the M06-2X functional

### **Package**

The source code of *MN-GFM* consists of a single directory, MNGFM3.0, 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-GFM3.0.tar.gz*. It contains the necessary subroutines to run *MN-GFM* with *Gaussian 03 D01*, and it also contains a directory for test runs.

To uncompress, enter

```
gunzip MN-GFM3.0.tar.gz
```

The uncompressed file will be named *MN-GFM3.0.tar*. After extracting the files from the tar file, which can be done with the command:

```
tar -xvf MN-GFM3.0.tar
```

a new directory, *MN-GFM3.0*, is created. This directory contains all the files included in the package, as follows

<i>MN-GFM-build-Altix</i>	<i>bc95ss.F</i>	<i>loclxc.F</i>	<i>m5x.F</i>	<i>nameex.F</i>
<i>MN-GFM-build-IBM</i>	<i>xcfunc.F</i>	<i>gau-cpp</i>	<i>m5c.F</i>	<i>mpw97.F</i>
<i>prcpta.F</i>	<i>bc95.F</i>	<i>getdft.F</i>	<i>m5css.F</i>	<i>nameco.F</i>
<i>putprc.F</i>	<i>m6x.F</i>	<i>mvs.F</i>	<i>doc/</i>	<i>test/</i>

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

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

- 1) Make sure that the officially distributed *Gaussian03.D01* is properly installed. Make sure that the *\$g03root* environment variable is properly set and the *\$g03root/g03/bsd/g03.login* file has been sourced. The *\$g03root* environment variable is the location of the *Gaussian 03* directory structure on a given machine (for example, */usr/local/g03.d01/* could be the location).

Note: The *MN-GFM* code will modify the installation of *Gaussian* in the *\$g03root* directory. *MN-GFM* modifies the following 16 links in this directory: 11, 1121, 1301, 1401, 1502, 1508, 1510, 1608, 1703, 1801, 1913, 1914, 1916, 11002, 11014, and 11110.

- 2) Go to the *MN-GFM3.0* directory. There are two install scripts in the *MN-GFM3.0* directory; one is for the SGI Altix computer, called *MN-GFM-build-Altix*, and the other one is for the SP or Regatta machines of IBM, called *MN-GFM-build-IBM*. Running one of the install scripts (according to the type of machine you use) accomplishes 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 3.0 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

## 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*.

### ***MN-GFM-v.3.0*** (12-11-06)

Authors: Y. Zhao and D. G. Truhlar

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

## Test Runs

Test run 1: PW6B95 single-point calculation on H<sub>2</sub>O with the 6-311+G(2df,2p) basis set.

Test run 2: Unrestricted PWB6K force calculation on CH<sub>3</sub> with the 6-31+G(d,p) basis set.

Test run 3: M05 single-point calculation on CH<sub>3</sub>SH with the 6-31+G(d,p) basis set.

Test run 4: M05-2X geometry optimization and frequency calculation for H<sub>2</sub>O with the 6-31+G(d,p) basis set.

Test run 5: Unrestricted M05 geometry optimization of SiH<sub>4</sub><sup>+</sup> with the 6-311+G(3d2f,2df,2p) basis set.

Test run 6: M05 geometry optimization of Cu<sub>2</sub> (closed shell singlet) with the CEP-121G effective core potential.

Test run 7: M06-L geometry optimization and frequencies calculations of F<sub>2</sub> with the 6-311+G(2df,2p) basis set.

Test run 8: M06-HF TDDFT calculation of the NH<sub>3</sub>...F<sub>2</sub> complex with the 6-31+G(d,p) basis set.

Test run 9: M06 optimization of HF with the 6-311+G(2df,2p) basis set.

Test run 10: M06-2X single-point calculation on OH<sup>-</sup> with the 6-311+G(2df,2p) basis set.

## 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>.