Taken from *MN-GSM* version 6.1 User's Manual
October 19, 2006

Density Functional Methods Availble in *Gaussian 03* and *MN-GFM*

The CM2, SM5.42, CM3, and SM5.43 models are parameterized for specific combinations of electronic structure method and basis set (see the "Executive Summary" portion of this manual for a list of electronic structure method and basis set combinations that can be used with these models). The CM4 and SM6 models are designed to be compatible with any density functional, as long as the density functional gives a reasonable electronic energy for the molecule of interest. (CM4 and SM6 are still basis set dependent; currently CM4 and SM6 parameter sets exist for the MIDI!6D, 6-31G(d), 6-31+G(d), and 6-31+G(d,p) basis sets). Likewise, SM6T can be used with any combination of electronic structure method and basis set for which SM6 can. Table 1 lists some commonly used density functionals that can be invoked using a single keyword in *Gaussian 03*. Any of these functionals can also be used with CM4, SM6, and SM6T. For a full list of the functionals available in *Gaussian 03*, see the *Gaussian* user's manual.

In addition to the predefined density functionals available in *Gaussian 03*, user-defined density functional methods can be specified using the Iop(3/76), Iop(3/77), and Iop(3/78) statements. Table 2 lists some previously developed density functionals that can be invoked using these Iop statements. All of the density functionals listed in this table, as well as any other well-behaved user-defined density functional can be used with CM4, SM6, and SM6T. For more information on the above Iop statements, see the *Gaussian* user's manual. For more information on the density functionals listed in Table 2, see http://comp.chem.umn.edu/info/DFT.htm.

MN-GSM can also be used in conjunction with *MN-GFM*, which is a locally modified version of *Gaussian 03* revision D.01 that supports several recently developed density functionals that are not available in the distributed version of *Gaussian 03*. Table 3 lists the density functionals that can be invoked using a single keyword in *MN-GFM*. All of the functionals listed in this table can be used with CM4, SM6, and SM6T. For more information on *MN-GFM* and the density functionals in Table 3, see the *MN-GFM* user's manual.

Table 1. DFT functionals that can be invoked using a single keyword in *Gaussian 03*, listed in chronological order. The HFE keyword must be specified in the $MNGSM namelist when using these or any other DFT functionals in conjunction with *MN-GSM*. For a full list of the density functionals available in *Gaussian 03*, see the *Gaussian* user's manual.

Functional	*Gaussian 03* Keyword[a]	HFE[b]	Reference(s)
BLYP	`BLYP`	0.000	(a) Becke, A. D. *Phys. Rev. A: At., Mol., Opt. Phys.* **1988**, *38*, 3098 (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785.
B3PW91	`B3PW91`	0.200	(a) Becke, A. D. *Phys. Rev. A: At., Mol., Opt. Phys.* **1988**, *38*, 3098 (b) Perdew, J. P. In *Electronic Structure of Solids '91*; Ziesche, P., Eschig, H., Eds.; Akademie Verlag: Berlin, 1991; p 11 (c) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.
B3LYP	`B3LYP`	0.200	(a) Becke, A. D. *Phys. Rev. A: At., Mol., Opt. Phys.* **1988**, *38*, 3098 (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785 (c) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623.
BB95	`BB95`	0.000	(a) Becke, A. D. *Phys. Rev. A: At., Mol., Opt. Phys.* **1988**, *38*, 3098 (b) Becke, A. D. *J. Chem. Phys.* **1996**, *104*, 1040.
B1B95	`B1B95`	0.280	(a) Becke, A. D. *Phys. Rev. A: At., Mol., Opt. Phys.* **1988**, *38*, 3098 (b) Becke, A. D. *J. Chem. Phys.* **1996**, *104*, 1040.
G96LYP	`G96LYP`	0.000	(a) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785 (b) Gill, P. M. W. *Mol. Phys.* **1996**, *89*, 433.
PBE	`PBEPBE`	0.000	Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.* **1996**, *77*, 3865.
B1LYP	`B1LYP`	0.250	(a) Becke, A. D. *Phys. Rev. A: At., Mol., Opt. Phys.* **1988**, *38*, 3098 (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785 (c) Adamo, C.; Barone, V. *Chem. Phys. Lett.* **1997**, *274*, 242.
MPWPW91	`MPWPW91`	0.000	(a) Perdew, J. P. In *Electronic Structure of Solids '91*; Ziesche, P., Eschig, H., Eds.; Akademie Verlag: Berlin, 1991; p 11 (b) Adamo, C.; Barone, V. *J. Chem. Phys.* **1998**, *108*, 664.
MPW1PW91[c]	`MPW1PW91`	0.250	(a) Perdew, J. P. In *Electronic Structure of Solids '91*; Ziesche, P., Eschig, H., Eds.; Akademie Verlag: Berlin, 1991; p 11 (b) Adamo, C.; Barone, V. *J. Chem. Phys.* **1998**, *108*, 664 (c) Lynch, B. J.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2003**, *107*, 1384.

B98	`B98`	0.2198	Schmider, H. L.; Becke, A. D. *J. Chem. Phys.* **1998**, *108*, 9624.
B97-1	`B971`	0.210	Hamprecht, F. A.; Cohen, A. J.; Tozer, D. J.; Handy, N. C. *J. Chem. Phys.* **1998**, *109*, 6264.
PBE1PBE[d]	`PBE1PBE`	0.250	Adamo, C.; Barone, V. *J. Chem. Phys.* **1999**, *110*, 6158.
VSXC	`VSXC`	0.000	Van Voorhis, T.; Scuseria, G. E. *J. Chem. Phys.* **1998**, *109*, 400.
B97-2	`B972`	0.210	Hamprecht, F. A.; Cohen, A. J.; Tozer, D. J.; Handy, N. C. *J. Chem. Phys.* **1998**, *109*, 6264.
τ-HCTHh	`THCTHH`	0.150	Boese, A. D.; Handy, N. C. *J. Chem. Phys.* **2002**, *116*, 9559.
TPSS	`TPSSTPSS`	0.000	Tao, J.; Perdew, J. P.; Staroverov, V. N.; Scuseria, G. E. *Phys. Rev. Lett.* **2003**, *91*, 146401.
X3LYP	`X3LYP`	0.218	(a) Xu, X.; Goddard, W. A. *Proc. Natl. Acad. Sci. U.S.A.* **2004**, *101*, 2673 (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785.
BMK	`BMK`	0.420	Boese, A. D.; Martin, J. M. L. *J. Chem. Phys.* **2004**, *121*, 3405.

[a]This keyword is specified in the *Gaussian 03* route section.
[b]This is the fraction of HFE that is specified in the $MNGSM namelist using the HFE keyword.
[c]Also called mPW0 and MPW25.
[d]Also called PBE0.

Table 2. DFT functionals that can be invoked using the Iop(3/76), Iop(3/77), and Iop(3/78) statements in *Gaussian 03*, listed in chronological order. For most of the functionals in this table, only the Iop(3/76) statement is required. For several other functionals, only the Iop(3/78) statement is required. The HFE keyword must be specified in the $MNGSM namelist when using these or any other DFT functionals in conjunction with *MN-GSM*.

Functional	*Gaussian 03* Keywords[a]	HFE[b]	Reference(s)
MPW1K	`MPWPW91` `Iop(3/76=0572004280)`	0.428	(a) Lynch, B. J.; Fast, P. L.; Harris, M.; Truhlar, D. G. *J. Phys. Chem. A* **2000**, *104*, 4811 (b) Lynch, B. J.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2003**, *107*, 1384..
MPW1N	`MPWPW91` `Iop(3/76=0594004060)`	0.406	(a) Kormos, B. L.; Cramer, C. J. *J. Phys. Org. Chem.* **2002**, *15*, 712 (b) Lynch, B. J.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2003**, *107*, 1384..
MPW1S	`MPWPW91` `Iop(3/76=0940000600)`	0.060	(a) Lynch, B. J.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2003**, *107*, 1384 (b) Lynch, B. J.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2003**, *107*, 1384..
TPSSh	`TPSSTPSS` `Iop(3/76=0900001000)`	0.100	Staroverov, V. N.; Scuseria, G. E.; Tao, J.; Perdew, J. P. *J. Chem. Phys.* **2003**, *119*, 12129.
BB1K	`BB95` `Iop(3/76=0580004200)`	0.420	(a) Becke, A. D. *Phys. Rev. A: At., Mol., Opt. Phys.* **1988**, *38*, 3098 (b) Becke, A. D. *J. Chem. Phys.* **1996**, *104*, 1040 (c) Zhao, Y.; Lynch, B. J.; Truhlar, D. G. *J. Phys. Chem. A* **2004**, *108*, 2715.
MPW1B95	`MPWB95` `Iop(3/76=0690003100)`	0.310	(a) Becke, A. D. *J. Chem. Phys.* **1996**, *104*, 1040 (b) Adamo, C.; Barone, V. *J. Chem. Phys.* **1998**, *108*, 664 (c) Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2004**, *108*, 6908.
MPWB1K	`MPWB95` `Iop(3/76=0560004400)`	0.440	(a) Becke, A. D. *J. Chem. Phys.* **1996**, *104*, 1040 (b) Adamo, C.; Barone, V. *J. Chem. Phys.* **1998**, *108*, 664 (c) Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2004**, *108*, 6908.
TPSS1KCIS	`TPSSKCIS` `Iop(3/76=0870001300)`	0.130	(a) Krieger, J. B.; Chen, J.; Iafrate, G. J.; Savin, A. In *Electron Correlations and Materials Properties*; Gonis, A., Kioussis, N., Eds.; Plenum: New York, 1999, p 463 (b) Tao, J.; Perdew, J. P.; Staroverov, V. N.; Scuseria, G. E. *Phys. Rev. Lett.* **2003**, *91*, 146401 (c) Zhao, Y.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2005**, *7*, 2701.

MPW3LYP	`MPWLYP`
	`Iop(3/76=1000002000)`
	`Iop(3/77=0720008000)`
	`Iop(3/78=0810010000)`
		0.200	Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2004**, *108*, 6908

MPWKCIS1K	`MPWKCIS` `Iop(3/76=0590004100)`	0.410	Zhao, Y.; González-Garcia, N.; Truhlar, D. G. *J. Phys. Chem. A* **2005**, *109*, 2012.
MPW1KCIS	`MPWKCIS` `Iop(3/76=0850001500)`	0.150	Zhao, Y.; González-Garcia, N.; Truhlar, D. G. *J. Phys. Chem. A* **2005**, *109*, 2012.
PBE1KCIS	`PBEKCIS` `Iop(3/76=0780002200)`	0.220	Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2005**, *1*, 415.
PBE1W	`PBEPBE` `Iop(3/78=0740010000)`	0.000	Dahlke, E. E.; Truhlar, D. G. *J. Phys. Chem. B* **2005**, *109*, 15677.
MPWLYP1W	`MPWV5LYP` `Iop(3/78=0880010000)`	0.000	Dahlke, E. E.; Truhlar, D. G. *J. Phys. Chem. B* **2005**, *109*, 15677.
PBELYP1W	`PBEV5LYP` `Iop(3/78=0540010000)`	0.000	Dahlke, E. E.; Truhlar, D. G. *J. Phys. Chem. B* **2005**, *109*, 15677.
TPSSLYP1W	`TPSSV5LYP` `Iop(3/78=0740010000)`	0.000	Dahlke, E. E.; Truhlar, D. G. *J. Phys. Chem. B* **2005**, *109*, 15677.

[a]These keywords are specified in the *Gaussian 03* route section.
[b]This is the fraction of HFE that is specified in the $MNGSM namelist using the HFE keyword.

Table 3. DFT functionals that can be invoked using a single keyword in *MN-GFM*. The HFE keyword must be specified in the $MNGSM namelist when using these or any other DFT functionals in conjunction with *MN-GSM*.

Functional	*MN-GFM* Keyword[a]	HFE[b]	Reference
PW6B95	`PW6B95`	0.280	Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Theory Comput.* **2006**, *2*, 364.
PWB6K	`PWB6K`	0.460	Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Theory Comput.* **2006**, *2*, 364.
M05	`M05`	0.280	Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Theory Comput.* **2006**, *2*, 364.
M05-2X	`M052X`	0.560	Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Theory Comput.* **2006**, *2*, 364.
M06-L	`M06L`	0.000	Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Phys.*, **2006**, In Press.

[a]These keywords are specified in the *MN-GFM* route section.
[b]This is the fraction of HFE that is specified in the $MNGSM namelist using the HFE keyword.