

Gaussian 09 Revision A.02 Release Notes

5 August 2009

Feature and Usage Notes

- ◆ If CIS frequencies are to be used with the Herzberg-Teller or Franck-Condon-Herzberg-Teller analysis, the CIS frequencies must be done numerically (**Freq=Numer** rather than **Freq**). This is because the transition dipole derivatives are not computed during the analytic force constant evaluation. The corresponding HF frequency calculation on the ground state, which is also required, can be done analytically as usual.
- ◆ CIS and CASSCF frequencies with PCM solvation must also be done numerically using **Freq=Numer**.
- ◆ The linear scaling (FMM-based) algorithms are now Linda-parallel, so Linda parallel jobs on large molecules do not need to specify **NoFMM**, and will run faster with the default algorithms chosen by the program.
- ◆ **Opt=GDIIS** is still present but deprecated; the new default optimization algorithm (**Opt=GEDIIS**) is better than GDIIS for the few cases where GDIIS was better than the G03 default (**Opt=RFO**).
- ◆ Optimizations of large molecules which have many very low frequency vibrational modes with DFT will often proceed more reliably when a larger DFT integration grid is requested (**Int=UltraFine**).
- ◆ Density fitting can be made the default for jobs using pure DFT functionals by adding the **DenFit** keyword to the route section (**-#-**) line in the **Default.Route** file. Fitting is faster than doing the Coulomb term exactly for systems up to several hundred atoms (depending on basis set), but is slower than exact Coulomb using linear scaling techniques (which are turned on automatically with exact Coulomb) for very large systems.
- ◆ The default IRC algorithm has changed; refer to the *User's Guide* for details. The default is to report only the energies and reaction coordinate at each point on the path; if geometrical parameters along the path are desired, these should be defined as redundant internal coordinates via **Geom=ModRedundant** or as input to the IRC code via **IRC(Report=Read)**.
- ◆ The references for variations of the M06 functional were swapped and incomplete. The correct references are: M06HF [Zhao06b,Zhao06c], M062X [Zhao08]. The M05 functionals are also still available: M05 [Zhao05] and M052X [Zhao06].

Missing, Corrected and Updated References

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- Clemente08 F. Clemente, T. Vreven, and M. J. Frisch, in *Quantum Biochemistry*, Ed. C. Matta (Wiley VCH, 2008).
- Collins02 M. A. Collins, "Molecular potential-energy surfaces for chemical reaction dynamics," *Theor. Chem. Acc.*, **108** (2002) 313-24.
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- Izmaylov06 A. F. Izmaylov, G. Scuseria, and M. J. Frisch, "Efficient evaluation of short-range Hartree-Fock exchange in large molecules and periodic systems," *J. Chem. Phys.*, **125** (2006) 104103: 1-8.
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- Zhao05 Y. Zhao, N. E. Schultz, and D. G. Truhlar, "Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions," *J. Chem. Phys.*, **123** (2005) .
- Zhao06 Y. Zhao, N. E. Schultz, and D. G. Truhlar, "Design of density functionals by combining the method of constraint satisfaction with parametrization for thermochemistry, thermochemical kinetics, and noncovalent interactions," *J. Chem. Theory and Comput.*, **2** (2006) 364-82.
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- Zhao06c Y. Zhao and D. G. Truhlar, "Density Functional for Spectroscopy: No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States," *J. Phys. Chem. A*, **110** (2006) 13126-30.

Changes in Usage and Defaults between Gaussian 03 and Gaussian 09

- ◆ There are many changes in the PCM algorithms:
 - ❖ The default surface integration is new and gives continuous potential energy surfaces. It is strongly recommended for all new studies. The route option **SCRF=G03Defaults** restores most of the defaults to those in G03, but should be used only for comparison with previous calculations done using G03.
 - ❖ When using the default IEFPCM solvation method or **SCRF=CPCM**, Gaussian 03 computed and reported non-electrostatic contributions to the solvation energy but did not include these in the energies and they were not included in the energies used for geometry optimizations, frequencies, etc. By default Gaussian 09 does not compute these values at all.
 - ❖ The new SMD solvation model is recommended for absolute solvation energies and other properties for which the non-electrostatic solvation terms are significant. When **SCRF=SMD** is specified, the SMD non-electrostatic terms are included in the basic energies (the SCF energy reported in the "SCF Done" line, correlated energies, etc.) and are included in the geometry optimization and frequency calculations. The non-electrostatic energy is also reported separately.
 - ❖ Absolute solvation energies should be computed by doing a gas-phase optimization and frequency calculation on the system, followed by the same calculations **with SCRF=SMD** or **SCRF=(SMD,Solvent=...)**.
 - ❖ The **SCFVac** PCM input option has been removed. If preliminary gas-phase energy is desired, do this in a separate job step before the solvated calculation.
- ◆ MP and CC calculations now default to a partial transformation (**Tran=IABC**). This is faster on most systems, especially when several processors are used. A full transformation can be requested using **Tran=Full**.
- ◆ The default SCF convergence is 10⁸ on the density for all calculations, including single points.
- ◆ The physical constants used by default are those from the 2006 CODATA tables; those used in Gaussian 03 can be requested via **Constants=1998**.
- ◆ AM1, PM3, and PM3MM by default use the new semi-empirical code, which has proper analytic first and second derivatives but which gives slightly different total energies because it computes the overlap integrals via 6-Gaussian expansions rather than over Slater functions. **AM1=Old** and **Use=L402** both request use of the old (MOPAC 6) code, through the regular links or through link 402, respectively. The new code is strongly recommended except when comparison with results from Gaussian 03 is required.
- ◆ **Stable=Opt** defaults to the usual (L502) SCF procedure for the initial SCF but then uses **SCF=QC** for additional SCF calculations, if they are required.

Changes between Gaussian 09 Revision A.01 and A.02:

- ◆ The logic for handling extra negative eigenvalues of the Hessian during minimizations has been improved.
- ◆ The combination of DFT and General SCF, automatically turned on if DFT is requested along with **Int=DKHSO**, does not work and is now rejected by the route generator.
- ◆ ONIOM input is now checked for divalent link atoms. The position of these atoms is ill-defined unless the distance scale factors are set to 1, and the model is usually poor if the scale factor is forced to be 1. Since this input is normally an error, it is now rejected by Link 101. **IOP(1/132)** can be used to force acceptance of this input, but this is strongly discouraged.
- ◆ Semi-direct integral transformation is the default. This code parallelizes better than the fully direct or in-core algorithms and is similar in speed on a single processor.
- ◆ A bug which caused **ONIOM=InputFiles** to fail when PDB secondary structure information was included in the input has been fixed.

Building from Source Code

- ◆ There are problems with the Solaris/x86_64 compilers. We have been able to build working binaries using a combination of libraries from one compiler version with the compiler itself from another version. This is not supported for customers, but the binary distribution we built is available.
- ◆ Building Gaussian 09 with Linda requires Linda version 8.2; the executables will not build with previous version of Linda.
- ◆ Building on Intel Macs requires a case-sensitive file system. In order to build the ia32 version you must specify:
bsd/bldg09 all mac32
as there is no way for the build script to determine that it is running on a x86 rather than x86_64 machine, and the default is to build for x86_64.

Gaussian 09 User's Reference Errata

- ◆ The following are missing from the list of links (pp. 38-39):
 - L117 Performs IPCM calculations.
 - L610 Numerical integration (for testing integral codes).The following links included in the list are not part of Gaussian 09: L909, L921, L922.
- ◆ The "thresh" keyword described in the discussion of selecting normal mode output on pages 107 and 289 is not available.
- ◆ The reference to **Opt=DiagFull** on page 116 should be **Freq=DiagFull**.

Gaussian 09 IOps Reference Errata

The description of IOps(1/111-113) is incorrect. Here is the corrected version:

IOp(1/111)

L103: Step-size to use with steepest descent when L103 is having trouble.

- N Scale up to RMS step of N/1000 if DXRMS is less.
- 1 Effectively disables the scaling.
- 0 Default (50).
- N Scale up or down to maximum change in a variable of N/1000.

L101: Temperature for thermochemistry.

- 0 Default (standard temperature, unless read in).
- N N/1000 degrees.
- N N/1000000 degrees.

IOp(1/112)

Pressure for thermochemistry.

- 0 Default (1 atmosphere, unless read in).
- N N/1000 atmospheres.
- N N/1000000 atmospheres.

IOp(1/113)

Scale factor for harmonic frequencies for use in thermochemistry and harmonic vibration-rotation analysis.

- 0 Default (1 unless specified by IOp in overlay 7 or read in).
 - N N/1000000.
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Note that IOp(1/114) is not defined.