

# Gaussian 09 Revision C.01 Release Notes

7 October 2011

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## Features and Usage Notes: Rev C.01

- ◆ Changes to optimization algorithms and options:
  - ❖ The selection of modes to include when stepping down from a region of wrong curvature during an optimization has been improved. This can also now be controlled by route options:
    - Opt=NoDownHill** Don't try to go downhill; just take an RFO-like step.
    - Opt=NGoDown=m** Mix at most  $m$  eigenvectors in taking a downhill step. The default is 3.
  - ❖ Linear bends are handled more reliably, and included in internal coordinate more frequently, than before. This avoids many optimization problems involving nearly linear angles becoming exactly linear.
  - ❖ The connectivities of reactant and product are now merged in generating the internal coordinates for the TS during QST2 and QST3 optimizations.
  - ❖ The maximum number of steps allowed ever in an optimization (i.e., include later restarts) can be reduced. This is sometimes useful for very large systems in order to reduce memory and disk usage.
  - ❖ The program now checks if the standard orientation of a molecule has flipped by 180 degrees during an optimization and avoids the flip. This avoids jumps when animating optimizations, IRCs, etc. in GaussView and improves SCF convergence.
  - ❖ The memory allocation for generation of internal coordinates is now proportional to the amount of memory provided by **%Mem**. This allows jobs with very large numbers of atoms or internal coordinates which previously failed to run if enough memory is provided.
  - ❖ By default, internal coordinates for potential hydrogen bonds are not generated automatically. Bond coordinates are still added to connect otherwise disjoint fragments, so coordinates for hydrogen bonds which connect fragments will still be included.
- ◆ Single-point BD calculations now default to frozen-core, with the core orbitals uncorrelated but updated using the BD Fock matrix. The previous default was to leave the core orbitals unchanged from the HF values, or from the orbitals read in with **BD=Read**. The new default produces energies which are independent of the choice of starting orbitals. Gradients with BD still require and defaults to full rather than frozen-core. The **OldFCBD** keyword requests the old-style frozen-core.
- ◆ On some machines fully direct integral transformation and fully direct MP2 are chosen if there is a large amount of memory, but the semi-direct algorithms are faster. **Tran=SemiDirect** in the **Default.Route** file now forces the semi-direct algorithm for MP2 as well as the transformation in higher level post-SCF calculations. Note that all method keywords such as **MP2** are ignored in the **Default.Route** file, because otherwise they would force that model in all calculations.
- ◆ **Output=Wfn** and **Output=Wfx** with post-SCF methods now default to **Density=Current** and **Pop=NOAB**, both of which are necessary for the post-SCF density to be stored in the **.wfn/.wfx** file. Problems with the orientation of the forces in these files and in generating them with ROHF wavefunctions and/or linearly dependent basis sets have also been fixed.
- ◆ Several customers have used the file generated for COSMORS as input to their local simulation programs, so this capability has been put back into G09.
- ◆ **Polar=Gamma** has been added as more descriptive option for requesting second hyperpolarizabilities. It is synonym for **Polar=(DCSHG,Cubic)**.
- ◆ The **RevTPSS** exchange and correlation functionals have been added.
- ◆ **SDD** now defaults to more recent basis sets for actinides; **OldSDD** requests the previous default.

- ◆ **TB** and **TW** can now be used to specify memory and disk allocations in units of terabytes and terawords, respectively.
- ◆ The **Direct** option is available for SAC-CI. This requests an integral-direct algorithm suitable for larger molecules.
- ◆ A **%OldChk** Link0 command has been added. The contents of the checkpoint file specified by **%OldChk** are copied to the checkpoint file of the current job step at the start of the job step. This allows data to be picked up from a previous calculation without destroying anything on the checkpoint file from it.
- ◆ Diffuse (**aug-**) functions were added for cc-pVDZ for the first transition row.
- ◆ A Windows64 version is now available.

#### Feature and Usage Notes: Rev B

- ◆ NewZMat now writes out secondary structure information, if present, with **-opdb**.
- ◆ NewZMat can now merge data from two input files. Either two text files or an input and a checkpoint file can be merged.
- ◆ **Polar=(Cubic,DCSHG)** can now be used to numerically differentiate frequency-dependent hyperpolarizabilities (betas) to produce second hyperpolarizabilities (gammas). These polarizabilities are now printed in the standard coordinate systems (i.e., with components of beta along and perpendicular to the dipole moment).
- ◆ WfnX files, used by the newer versions of AIMPAC, can now be written via **Output=WfnX**.
- ◆ Performance for very large MM systems (>20K atoms) has been improved, especially when range limits are applied to the Coulomb and Van der Waals terms. There is a new route option, **Geom=Huge**, which turns off various actions, useful in QM calculations but unnecessary and expensive with enormous MM runs.
- ◆ **MaxDisk** can now be specified in the **Default.Route** file.
- ◆ The Hu, Lu, and Wang charge fitting model (*JCTC* **3** (2007) 1004-13) is now available via **Pop=HLY**. The authors only parametrized the atomic densities required for the model for the first 18 elements. An alternative version, **Pop=HLYGAt**, uses the HLY fitting scheme but with Gaussian's standard atomic densities, which are available for the entire periodic table. For systems which can be done either way, the difference in atomic charges is usually between 1% and 5%.
- ◆ The SCVS method of Todd Keith, which scales the molecule in order to make the virial condition satisfied exactly, has been added.

#### Feature and Usage Notes: Rev A

- ◆ 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)**.

#### Missing, Corrected and Updated References

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].

Boese02      A. D. Boese and N. C. Handy, "New exchange-correlation density functionals: The role of the kinetic-energy density," *J. Chem. Phys.*, **116** (2002) 9559-69.

- Cammi00a R. Cammi, C. Cappelli, S. Corni, and J. Tomasi, "On the calculation of infrared intensities in solution within the polarizable continuum model," *J. Phys. Chem. A*, **104** (2000) 9874-79.
- 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.
- Fukui81 K. Fukui, "The path of chemical-reactions — The IRC approach," *Acc. Chem. Res.*, **14** (1981) 363-68.
- Henderson09 T. M. Henderson, A. F. Izmaylov, G. Scalmani, and G. E. Scuseria, "Can short-range hybrids describe long-range-dependent properties?" *J. Chem. Phys.*, **131** (2009) 044108.
- 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.
- Marenich09 A. V. Marenich, C. J. Cramer, and D. G. Truhlar, "Universal solvation model based on solute electron density and a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions," *J. Phys. Chem. B*, **113** (2009) 6378-96.
- 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.
- Zhao06a Y. Zhao and D. G. Truhlar, "A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions," *J. Chem. Phys.*, **125** (2006) 194101: 1-18.
- 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.

#### 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:

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#### 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.

### 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.

### Corrections to Deprecated Features:

- ◆ Problems with setting non-integer nuclear charges in **Message** input have been corrected. There is now a **ZNuc** function in **Message** input which changes the nuclear charge but not the atomic number.

### Bug Fixes and Minor Changes between Gaussian 09 Revisions B.01 and C.01:

- ◆ The memory required by very large ONIOM(MO:MM) and pure MM frequency calculations has been reduced.
- ◆ The definition of improper torsions in the Amber force field is dependent on the ordering of atoms in the molecule. Calculations in the Amber program on typical proteins are consistent because of the standard ordering of atoms within residues and residues within a PDB file, but for general molecules produced with GaussView the results depend on the order of atoms in an arbitrary way. G09 has been changed to average over the 6 possible orders of atoms in an Amber improper torsion, making the results slightly different than the standard Amber force field, but making the energy independent of permutations of atoms in the molecule.
- ◆ Printing during **Pop=MK** with **IOp33** increased has been restored to include the data required for RESP charge fitting. However, G09 can now generate the data file for AnteChamber directly, by setting **IOp(6/50=1)** in the **Pop=MK** job, and this is the recommended method for generating input for RESP.
- ◆ A bug in CIS frequencies with PCM solvation was fixed.
- ◆ **MaxDisk** in a **Default.Route** file now applies to all steps of a compound job; previously, only the first step was defaulted properly.
- ◆ A bug which prevented reading AlpB parameters for AM1 was fixed.
- ◆ Convergence during SCVS calculations is now checked more carefully.
- ◆ **Pop=SaveBio** in **Stable=Opt** jobs caused the stability calculation to be wrong or fail. This now works properly, saving the biorthogonal orbitals only after the wavefunction has been made stable.
- ◆ External point charges now work with symmetry turned on.
- ◆ A bug in TD-DFT gradients with frozen core was fixed.
- ◆ Print statements for NMR shielding were fixed to work with more than 999 atoms.
- ◆ A bug in DFTB using interpolated (not analytic) parameters with d functions was fixed.
- ◆ A rare problem with uncompleted write statements on slow file systems was fixed.
- ◆ Problems with some combinations of charge and multiplicity in fragments during **Guess=Fragment** calculations were fixed.
- ◆ Printing of Coriolis terms during **Freq=VibRot** was restored.
- ◆ Some memory allocation problems for PBC calculations with large unit cells were fixed.
- ◆ Inconsistencies in how the geometry was modified in some cases by **Symm=Loose** were fixed.
- ◆ A bug in the ROMP4 triples energy when **NoSymm** was specified was fixed.
- ◆ An ominous sounding but unnecessary warning from the CBS extrapolation was turned off.
- ◆ ONIOM(MO:MM) jobs which do microiterations and which fail to finish are now restartable.
- ◆ A bug in reading ECPs with ONIOM when the same ECP was placed on multiple centers was fixed.

- ◆ The combination of **IRC** and **Freq**, which did the frequency calculation at the last point of the IRC rather than the TS, is now rejected.
- ◆ Several unsupported combinations of Douglas-Kroll-Hess with properties now generate an error message rather than incorrect answers.
- ◆ A bug in generating the default (Harris) initial guess when using ECPs on charged species was fixed. The quality of the initial guess when using ECPs has also been improved.
- ◆ Several defaults for whether to use FMM and other integral options have been updated for better performance on current models of CPU.
- ◆ **Formchk** now writes -1 rather than \*\*\*\*\* to the formatted checkpoint file if the value exceeds  $10^{13}-1$ . This allows **unfchk** and other utilities to process the resulting **fchk** file.
- ◆ A bug affecting **Geom=Check** after numerical frequencies when using ONIOM was fixed.
- ◆ The combination of **BD** or **W1BD** with **SCRF**, which does not work correctly, is now rejected by the route generator.
- ◆ A new version of the ATLAS BLAS library is used on most platforms. This fixes several problems when using very large amounts of memory. However, in the event of any lingering problems of this type, **IOP1=NoAssem** can now be specified on the route line to turn off use of the ATLAS matrix multiplication routines.
- ◆ A problem in reported transition moments between excited states computed in SAC-CI jobs was fixed.
- ◆ Empirical dispersion with DFT and ghost atoms now runs. Empirical dispersion and PBC now produced an error message, since it is not implemented.
- ◆ **Opt Freq** with **ROHF/RODFT** now works correctly, doing **Freq=Numer** with the restricted open-shell wavefunction in the second job step.
- ◆ Franck-Condon calculations now function correctly for forbidden transitions.
- ◆ The route generator rejects the combination of **TD** and double-hybrid DFT methods, which never worked (previously, TD was done based on only the SCF part of the double-hybrid).
- ◆ **IRC=(RCFRC,GradientOnly)** calculations now correctly use the Hessian from the checkpoint file.
- ◆ A memory allocation bug for very large systems, which could cause a failure with the message "NIJ > Max2 in MMCore," was fixed.
- ◆ The **External** keyword functions correctly in the Windows version. Consult **g09\tests\com\test726.gjf** for an example of using it.
- ◆ A problem with the G09W front-end writing out multi-step jobs when the **--Link1--** lines were truncated was fixed.

#### Bug Fixes and Minor Changes between Gaussian 09 Revisions A.02 and B.01:

- ◆ A bug in MP2 frequencies with PCM was fixed.
- ◆ An updated version of the SAC-CI code is included. This includes a new integral-direct algorithm, specified with **SACCI=(Direct, ...)**, which is much faster for large systems.
- ◆ The **ExtraOverlay** route keyword did not function in Revision A.02; this has been corrected.
- ◆ **Opt Freq TD** calculations now run both job steps properly.
- ◆ Problems with the dummy basis set used with Molecular Mechanics for systems that are highly charged or have very high spin were fixed.
- ◆ The free-format input routines have been generalized in order to make data from newer DFTB parameter files acceptable. These files still require some modification to be used with G09.
- ◆ The full tensors for ECD using TDDFT (including the quadrupole component) are now printed.
- ◆ The use of IOps to specify user-selected ranges for integrals has been updated in order to make it more general.
- ◆ The default algorithm for optimizations when minimizing in a region of incorrect curvature has been improved.
- ◆ The initial guess for AM1 and PM6 has been improved.
- ◆ More analysis of input ONIOM and MM parameters with respect to secondary structure is now done (by default for systems with <10,000 atoms when secondary structure information is available). The net MM charges on residues and average distances between residues are reported.
- ◆ Various performance improvements, including ones for larger numbers of SMP processors and for SCF frequency calculations.

### Bug Fixes and Minor 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.

### 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  $10^8$  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.