

# ***Gaussian 98 Release Notes***

## *Revisions A.11.2 and A.11.3*

This document lists changes to and additional information about *Gaussian 98* functionality since the *Gaussian 98 User's Reference* was prepared. The final section gives information about building/running on specific OS's.

*Starred items are added or modified for this release. New items start on page 2.*

### ***Table of Contents***

#### General Program Topics:

➤ *Changes in Revision A.11.2 and A.11.3 .....	2
➤ Changes in Revision A.10/A.11 .....	2
➤ Required Citation for <i>Gaussian 98</i> Revision A.10 and Later .....	2
➤ New and Fixed Features .....	3
➤ NBO Dimensions.....	3
➤ Time-Dependant DFT Changes.....	3
➤ Counterpoise Corrections .....	3
➤ Interface to COSMO-RS.....	4
➤ Updated Input Sections Ordering Table .....	4
➤ Insignificant Output Change with Revision A.4 and Later .....	5
➤ Default Memory.....	5
➤ Additional Basis Sets.....	6
➤ Selecting the Numerical Integration Weighting Scheme.....	6
➤ IRCMax Description.....	6
➤ MaxDisk is Obeyed.....	8
➤ Additional Option to Polar .....	8
➤ Anisotropic Hyperfine Coupling Constants .....	8
➤ SCRF PCM and IPCM Model Availability .....	8
➤ Trajectory Availability .....	8
➤ ZINDO References .....	9
➤ Cube Output Format Clarifications .....	9
➤ Optimization Microiterations.....	9
➤ New formchk Option .....	9
➤ Basis Set Clarifications.....	9
➤ New CBS Method: CBS-QB3 .....	9
➤ Modified CBS-4 Model and New Keywords .....	9
➤ New Printing Options for Geom and NMR.....	9
➤ G3 Methods Added.....	10
➤ New Redundant Internal Coordinates Generation Scheme for Weakly-Bound Complexes .....	10
➤ Change to Charge Generation for Molecular Mechanics Methods .....	10
➤ Longer Link 0 Commands Supported .....	10
➤ Other Minor Corrections/Clarifications to the Printed Manual .....	10
➤ Unavailable Features.....	11
➤ Updated References .....	11
➤ New References Cited in This Document .....	11
System-Specific Information.....	13
➤ Operating System and Software Requirements.....	13
➤ *Correct Compiler for Sun Systems .....	13
➤ Checkpoint Files for 64-bit Integer Versions .....	13
➤ *Building IBM RS/6000 Versions .....	13
➤ System Configuration and Memory Requirements Under UniCOS.....	14
➤ *Fortran Compiler and Libraries for Building the Intel Linux Version .....	14
➤ Windows Version is NOT Parallel-Enabled.....	15
➤ Alpha Linux Version Compiler.....	15
➤ Building Fujitsu VPP300/VPP700/VX Versions .....	15

---

➤ **\*Changes in Revision A.11.2 and A.11.3**

- ◆ With A.11.3, there are changes in the Linux for Intel build procedure. See the System-Specific section for more information.
- ◆ Fujitsu PrimePower systems are now supported.
- ◆ There are now separate normal and Linda-enabled G98 binaries for Red Hat 6.2 and 7.2 (i.e., 4 versions). Similarly, there are also separate versions of the `blas-f2c.a` library for the two Red Hat versions. They are both included on the G98 source-code version distribution CD in the `/intel` top-level directory.
- ◆ Building the program on IA-64 systems requires the 6.0 beta version of the Intel compiler (build 20011129 as of this writing). The compiler can be obtained by sending email to [joe.wolf@intel.com](mailto:joe.wolf@intel.com).

---

➤ **Changes in Revision A.10/A.11**

- ◆ The required citation has changed (see below).
- ◆ The 64-bit integer version is now the standard in the Hitachi and Hewlett-Packard environments as well as for SGI R10000, Sun, IBM Power 3, and Compaq Tru-64 systems. See the system specific section of this document for more information about the implications of this change.
- ◆ The makefile has been updated to work with most recent Compaq Alpha compilers.
- ◆ Network parallel calculations may be performed on Compaq Alpha Linux systems via the Linda environment.
- ◆ Sorting routines now use full 64-bit addresses, so disk space limitations on 64-bit machines are removed.
- ◆ NEC systems no longer need to spawn separate subprocesses for each link. The NEC version now requires Super-UX Version 11.1.
- ◆ IBM Power 3 executables now use 64-bit pointers as well as integers. There are now four available IBM binary formats: Power 1 (32-bit), Power 2 (32-bit), Power 3 under AIX 4.3 (64-bit), and Power 3 under AIX 5.1 (64-bit). See the system-specific section for information on building in the various IBM environments, as *this procedure has changed significantly*. Note also that the correct compatible version of Linda must be used with each environment in order to run in parallel.

---

➤ **Required Citation for *Gaussian 98* Revision A.10 and Later**

The required citation for Revision A.10 and later is different from the one for all earlier *Gaussian 98* revisions (replace *x* with the integer corresponding to your version of the program):

Gaussian 98 (Revision A.1x), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, P. Salvador, J. J. Dannenberg, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2001.

---

## ➤ New and Fixed Features

The following features have been added and/or fixed in Revision A.10:

- ◆ The **PBE1PBE** (hybrid) and **PBEPBE** (pure) functionals have been added [29-30].
- ◆ MP2 frequencies may be computed in the presence of an external electric field (i.e., **MP2 Freq Field=...**).
- ◆ The **Freq=Numer Polar Field=...** keyword combination is now valid.
- ◆ The **IRC(StepSize=n)** now sets the convergence criteria correctly instead of making them too loose.
- ◆ By default, **SCI-PCM** now turns off charge compensation (as was the case in *Gaussian 94*).
- ◆ The selection of internal coordinates has been improved for optimizations, resulting in better behavior for systems like weakly-bound complexes.
- ◆ The printing of transition densities between excited states using the Time Dependant DFT and HF methods is disabled because not all terms are currently computed. The ground-to-excited state transition densities are correct and are still printed.
- ◆ The incorrect exponent for N in the D95 basis has been corrected (results in a 10 microhartree energy change for the atom).
- ◆ The special atom types O\_3\_z, P\_3+5, P\_3+q, S\_3+4, S\_3+6, and W\_3+6 in the Dreiding/UFF force fields are now given the correct values. Previously, they were given the default parameters (e.g. O\_3's for O\_3\_z).
- ◆ The PM3 parameter for Li has been updated per reference [31].

---

## ➤ NBO Dimensions

NBO is now dimensioned for 200 atoms and 10000 basis functions.

---

## ➤ Time-Dependant DFT Changes

- ◆ The TD DFT procedures for pure DFT now does the symmetric problem (a faster algorithm).
- ◆ The initial guess for TD DFT does not use improved virtual orbitals (IVOs).
- ◆ Using **TD=Read** to read an initial guess from a calculation on using a pure functional may now be use for a subsequent hybrid DFT functional calculation.
- ◆ **CIS(Add=n)** and **TD(Add=n)** now imply the **Read** option as well (they were meaningless without it).

---

## ➤ Counterpoise Corrections

Counterpoise corrections may be computed using the **Counterpoise** keyword (which can be used on an energy calculation, optimization or frequency calculation). The facility cannot be used with ECPs or a general basis set.

The **Counterpoise** keyword takes an integer value specifying the number of fragments or monomers in the molecular structure. The facility also requires an additional integer to be placed at the end of each atom specification indicating which fragment/monomer it is part of. Here are examples using a Z-matrix (left) and Cartesian coordinates (right):

# MP2/6-31G Counterpoise=2 Opt

Counterpoise with Z-matrix

```
0,1,0,3,1,2
O,0.0,0.0,0.0,1          structures begin here
O,1,ROO,2
X,1,1.,2,X3O
H,1,RO1H,3,HOX3,2,90.,0,1
H,1,RO1H,3,HOX3,2,-90.,0,1
X,2,1.,1,52.5,3,180.,0
H,2,RO2H1,6,H7OX,1,180.,0,2
H,2,RO2H2,6,H8OX,1,0.,0,2
```

Z-matrix variables...

# MP2/6-31G Counterpoise=2 Opt

Counterpoise with Cartesian

```
0,1
1 0.00 0.00 0.92 1
9 0.17 0.00 2.73 2
1 0.77 0.00 3.43 2
9 0.00 0.00 0.00 1
```

Note that the Z-matrix input requires a 0 after the dihedral angle value/variable (to indicate that the final angle is a dihedral) prior to the fragment number. Also, the first atom in the Z-matrix must be given in Cartesian coordinates.

Clearly, using Cartesian coordinates for such jobs makes specifying fragment numbers in the input much more straightforward.

The preceding Z-matrix also illustrates the use of fragment-specific charge and spin multiplicity specifications. The format of the corresponding input line in this case is:

*molecule-charge, molecule-spin multiplicity, frag. 1-charge, frag.1 multiplicity, frag. 2 charge, frag. 2 multiplicity*

---

## ➤ Interface to COSMO-RS

G98 Revision A.10 and higher can carry out a PCM calculation using Klamt's form of the conductor reaction field (COSMO) and generate the input data for the COSMO-RS solubility programs.

The **SCRF=COSMORS** keyword requests a conductor PCM calculation (CPCM) using atomic radii and other parameters as suggested by Klamt for his models. The name of the text file to write with input data for COSMO-RS is read from the input stream, after the geometry, basis set and other data.

Only single-point calculations are possible with COSMORS option. These calculations will typically be done as single-point solvated calculations using **SCRF=CPCM** optimized geometries.

Here is a sample input file:

```
# B3LYP/6-311+G(2d,2p) SCF=(Tight) SCRF=COSMORS
Water generating COSMO-RS input
0 1
o
h,1,r
h,1,r,2,a
r .96
a 104.5
water.cosmo
```

This produces the data file **water.cosmo**.

COSMO-RS is distributed as COSMOtherm by COSMOlogic GmbH, [www.cosmologic.de](http://www.cosmologic.de).

---

## ➤ Updated Input Sections Ordering Table

This table from the introduction to chapter 3 of the manual has been updated. The new table is printed below:

*Gaussian 98 Input Section Ordering*

<i>Section</i>	<i>Keywords</i>	<i>Final blank-line?</i>
Link 0 commands	<b>% commands</b>	no
Route Section (# lines)	<b>all</b>	yes
Extra Overlays	<b>ExtraOverlays</b>	yes
Title section	<b>all</b>	yes
Molecule specification	<b>all</b>	yes
Modifications to coordinates	<b>Opt=ModRedundant</b>	yes
Connectivity specifications	<b>Geom=Connect or ModConnect</b>	yes
2nd title <sup>†</sup> and molecule specification	<b>Opt=QST2 or QST3</b>	yes
Modifications to 2nd set of coordinates	<b>Opt=ModRedun and QST2 or QST3</b>	yes
Connectivity specifications for 2nd set of coordinates	<b>Geom=Connect or ModConnect and Opt=ModRedun and QST2 or QST3</b>	yes

<i>Section</i>	<i>Keywords</i>	<i>Final blank-line?</i>
3rd title <sup>†</sup> and initial TS structure	<b>Opt=QST3</b>	yes
Modifications to 3rd set of coordinates	<b>Opt=(ModRedun, QST3)</b>	yes
Connectivity specifications for 3rd set of coordinates	<b>Geom=Connect or ModConnect</b> <b>Opt=(ModRedun, QST3)</b>	yes
Initial force constants (Cartesian)	<b>Opt=FCCards</b>	yes
Accuracy of energy & forces	<b>Opt=ReadError</b>	no
Trajectory input (multiple sections depending on options selected)	<b>Trajectory</b>	yes
Atomic masses	<b>IRC=ReadIsotopes</b>	yes
Basis set specification	<b>Gen, ExtraBasis</b>	yes
Basis set alterations	<b>Message</b>	yes
ECP specification	<b>ExtraBasis, Pseudo=Cards</b>	yes
Background charge distribution	<b>Charge</b>	yes
Finite field coefficients	<b>Field=Read</b>	yes
Symmetry types to combine	<b>Guess=LowSymm</b>	no
Orbital specifications <sup>‡</sup>	<b>Guess=Cards</b>	yes
Orbital alterations <sup>‡</sup>	<b>Guess=Alter</b>	yes
Solvation model parameters	<b>SCRF</b>	no
PCM solvation model input	<b>SCRF=(PCM,Read)</b>	yes
Weights for CAS state averaging	<b>CASSCF=StateAverage</b>	no
States of interest for spin orbit coupling	<b>CASSCF=Spin</b>	no
# orbitals/GVB pair	<b>GVB</b>	no
Alternate atomic radii	<b>Pop=ReadRadii or ReadAtRadii</b>	yes
Data for electrostatic properties	<b>Prop=Read or Opt</b>	yes
Cube filename (& spec. for Cards option)	<b>Cube</b>	yes
NBO input	<b>Pop=NBORoad</b>	no
Orbital freezing information	<b>ReadWindow option</b>	yes
OVGF orbitals to refine	<b>R/UOVGF IOp(9/11=100)</b>	yes
Temperature, pressure, atomic masses	<b>Freq=ReadIsotopes</b>	no
PROAIMS wavefunction filename	<b>Output=WFN</b>	no

<sup>†</sup> A blank line also separates the second or third title section from the corresponding molecule specification.

<sup>‡</sup> UHF jobs use separate  $\alpha$  and  $\beta$  sections (themselves separated by a blank line).

## ➤ Insignificant Output Change with Revision A.4 and Later

The reported number of primitive gaussians will differ between revisions A.4 and later and previous revisions. Note that this change has no effect on the results of the calculation since it is an arbitrary, completely informational statistic not used in any actual computation. Previously, this value indicated the number of AO components of gaussian primitives in terms of pure d functions if you were using pure contracted functions in the calculation. Now, it always counts Cartesians regardless of the types of contracted functions in use.

## ➤ Default Memory

The default memory amount in G98 is 6MW.

---

## ➤ Additional Basis Sets

The **EPR-II** and **EPR-III** basis sets of Barone [1] are included in *Gaussian 98*. They are optimized for the computation of hyperfine coupling constants by DFT methods (particularly B3LYP). EPR-II is a double zeta basis set with a single set of polarization functions and an enhanced s part: (6,1)/[4,1] for H and (10,5,1)/[6,2,1] for B to F. EPR-III is a triple-zeta basis set including diffuse functions, double d-polarizations and a single set of f-polarization functions. Also in this case the s-part is improved to better describe the nuclear region: (6,2)/[4,2] for H and (11,7,2,1)/[7,4,2,1] for B to F. The basis sets are available for H, B, C, N, O and F.

---

## ➤ Selecting the Numerical Integration Weighting Scheme

The following options to select the numerical integration weighting scheme have been added to the **Integral** keyword:

**SSWeights**      Use the weighting scheme of Scuseria and Stratman [3] for the numerical integration for DFT calculations. This is the default.

**BWeights**      Use the weighting scheme of Becke for numerical integration. This was the default in *Gaussian 94*.

---

## ➤ IRCMax Description

The description of the **IRCMax** keyword has been updated:

### DESCRIPTION

Performs an IRCMax calculation using the methods of Petersson and coworkers [4-12]. Taking a transition structure as its input, this calculation type finds the maximum energy along a specified reaction path.

### REQUIRED INPUT

**IRCMax** requires two model chemistries as its options, separated by a colon: **IRCMax(model2:model1)**. Here is an example route section:

```
# IRCMax(B3LYP/6-31G(d,p):HF/6-31G(d,p))
```

This calculation will find the point on the HF/6-31G(d,p) reaction path where the B3LYP/6-31G(d,p) energy is at its maximum.

The **Zero** option will produce the data required for zero curvature variational transition state theory (ZC-VTST) [5, 6, 9-12]. Consider the following route:

```
# IRCMax(MP2/6-31G(d):HF/3-21G(d),Zero,Stepsize=10)
```

This job will start from the HF/3-21G(d) TS and search along the HF/3-21G(d) IRC with a stepsize of 0.1 amu<sup>1/2</sup> bohr until the maximum of the MP2/6-31G(d) energy (including the HF/3-21G(d) ZPE) is bracketed. The position along the HF/3-21G(d) IRC for this MP2/6-31G(d) TS will then be optimized. The output includes all quantities required for the calculation of reaction rates using the ZC-VTST version of absolute rate theory: TS moments of inertia, all real vibrational frequencies (HF/3-21G(d)), the imaginary frequency for tunneling (fit to MP2/6-31G(d) + ZPE), and the total MP2/6-31G(d) + ZPE energy of the TS.

### ZC-VTST OPTIONS

**Zero**              Include the zero-point energy in the IRCMax computation.

### PATH SELECTION OPTIONS

**Forward**          Follow the path only in the forward direction.

**Reverse**          Follow the path only in the reverse direction.

<b>ReadVector</b>	Read in the vector to follow. The format is Z-matrix (FFF(I), I=1,NVAR), read as (8F10.6).
<b>MaxPoints=N</b>	Number of points along the reaction path to examine (in each direction if both are being considered). The default is 6.
<b>StepSize=N</b>	Step size along the reaction path, in units of 0.01 amu <sup>-1/2</sup> -Bohr. The default is 10.
<b>MaxCyc=N</b>	Sets the maximum number of steps in each geometry optimization. The default is 20.
<b>Freq</b>	Calculate the projected vibrational frequencies for motion perpendicular to the path, for each optimized point on the path [13]. This option is valid only for reaction paths in mass-weighted internal coordinates.

#### COORDINATE SYSTEM SELECTION OPTIONS

<b>MassWeighted</b>	Follow the path in mass-weighted internal (Z-matrix) coordinates (which is equivalent to following the path in mass-weighted Cartesian coordinates). <b>MW</b> is a synonym for <b>MassWeighted</b> . This is the default.
<b>Internal</b>	Follow the path in internal (Z-matrix) coordinates without mass weighting.
<b>Cartesian</b>	Follow the path in Cartesian coordinates without mass weighting.

#### ISOTOPE SPECIFICATION OPTION

<b>ReadIsotopes</b>	Specify alternate isotopes (the defaults are the most abundant isotopes). This information appears in a separate input section having the format:
---------------------	---

*isotope mass for atom 1*  
*isotope mass for atom 2*  
 ...  
*isotope mass for atom n*

where the lines hold the isotope masses for the various atoms in the molecule, arranged in the same order as they appeared in the molecule specification section. If integers are used to specify the atomic masses, the program will automatically use the corresponding actual exact mass (e.g., 18 specifies O<sup>18</sup>, and *Gaussian 98* uses the value 17.99916).

#### CONVERGENCE-RELATED OPTION

<b>VeryTight</b>	Tightens the convergence criteria used in the optimization at each point along the path. This option is necessary if a very small step size along the path is requested.
------------------	--

#### OPTIONS FOR GENERATING INITIAL FORCE CONSTANTS

<b>CalcFC</b>	Specifies that the force constants be computed at the first point
<b>CalcAll</b>	Specifies that the force constants be computed at every point.
<b>FCCards</b>	Reads the Cartesian forces and force constants from the input stream after the molecule specifications. This option can be used to read force constants recovered from the Quantum Chemistry Archive using its internal <b>FCList</b> command. The format for this input is:  <i>Energy</i> (format D24.16) <i>Cartesian forces</i> (lines of format 6F12.8) <i>Force constants</i> (lines of format 6F12.8)

The force constants are in lower triangular form:  $((F(J,I), J=1,I), I=1, NAt3)$ , where *NAt3* is the number of Cartesian coordinates. If both **FCCards** and **ReadIsotopes** are specified, the masses of the atoms are input before the energy, Cartesian gradients and the Cartesian force constants.

Note that the **RCFC** option is not supported with IRCMax.

#### RESTART OPTION

**Restart** Restarts an IRC calculation which did not complete, or restarts an IRC calculation which did complete, but for which additional points along the path are desired.

#### AVAILABILITY

Analytic gradients are required for the IRC portion of the calculation (*model1* above). Any non-compound energy method and basis set may be used for *model2*.

#### RELATED KEYWORDS

**IRC, Opt, Freq**

---

### ➤ **MaxDisk is Obeyed**

MP3, MP4, QCISD, CCSD, QCISD(T), and CCSD(T) calculations all now look at **MaxDisk**. If the calculation can be done using a full integral transformation while keeping disk usage under **MaxDisk**, this is done; if not, a partial transformation is done and some terms are computed in the AO basis. Since MP2 obeys MaxDisk as much as possible, the **Stingy**, **NoStingy** and **VeryStingy** options are not needed.

Thus, it is *crucial* for a value for MaxDisk to be specified explicitly for these types of jobs, either within the route section or via a system wide setting in the **Default.Route** file. If **MaxDisk** is left unset, the program now assumes that disk is abundant and performs a full transformation by default, in contrast to G94 where a partial transformation was the default in such cases. If **MaxDisk** is not set and sufficient disk space is not available for a full transformation, the job will fail (where it may have worked in G94).

---

### ➤ **Additional Option to Polar**

The **Polar** keyword has an additional option:

**Analytic** Compute polarizability and hyperpolarizability analytically. This is possible for RHF and UHF for which it is the default. The polarizability is always computed during analytic frequency calculations.

---

### ➤ **Anisotropic Hyperfine Coupling Constants**

The **Prop** keyword now supports the **EPR** option:

**EPR** Compute the anisotropic hyperfine coupling constants [1, 14, 15].

---

### ➤ **SCRF PCM and IPCM Model Availability**

The PCM models are available for HF, DFT, MP2, MP3, MP4(SDQ), QCISD, CCD, CID, and CISD energies and HF and DFT gradients.

---

### ➤ **Trajectory Availability**

Trajectory calculations may be performed at the MP2 level as well as the methods listed in the manual.



---

## ➤ ZINDO References

References for the ZINDO method are now provided [16-24].

---

## ➤ Cube Output Format Clarifications

The norm of the density gradient and the Laplacian are also scalar (i.e., one value per point), and are written out in the same manner. Density+gradient grids are similar, but with two writes for each row (of lengths  $N_3$  and  $3*N_3$ ).

Note that all cube files are formatted; requests for unformatted cube files are currently ignored.

---

## ➤ Optimization Microiterations

The use of microiterations in geometry optimizations is the default for MM optimizations and ONIOM optimizations with an MM component. Use the **Opt=NoMicro** option to turn off microiterations.

---

## ➤ New formchk Option

The command **formchk -c** causes the molecular mechanics atom types to appear in the formatted checkpoint file as strings rather than integers.

---

## ➤ Basis Set Clarifications

The **SDD** basis set keyword consists of D95 up to Ar and then a variety of Stuttgart potentials for  $Z > 18$  (see the manual). The **SDDall** keyword selects Stuttgart potentials for  $Z > 2$ . The **SDD**, **SHF**, **SDF**, **MHF**, **MDF**, **MWB** forms may be used to specify these basis sets/potentials within **Gen** basis input. Note that the number of core electrons must be specified following the form (e.g., **MDF28** for the MDF potential replacing 28 core electrons).

The Midi! basis set (keyword **MidiX**) is now implemented for H, C-F, Si-Cl, I and Br.

---

## ➤ New CBS Method: CBS-QB3

The **CBS-QB3** keyword may be used to select the CBS-QB3 method [25]. The CBS-QB3 method has been updated to use the new and more stable Minimal Population localization procedure. This will cause small differences in the CBS-QB3 energy computed with pre-A.7 versions of *Gaussian 98*, but it is more reliable for large molecules. The **CBS-QB30** keyword requests the CBS-QB3 model with the earlier localization scheme, if comparison with previous results is necessary.

---

## ➤ Modified CBS-4 Model and New Keywords

The CBS-4 model chemistry has been updated with both the new localization procedure (discussed in the preceding item) and improved empirical parameters. The new version **CBS-4M** (**M** referring to the use of Minimal Population localization) is recommended for new studies; the **CBS-40** keyword requests the earlier parametrization. Since these can give significantly different results the previous CBS-4 keyword prints an error message rather than defaulting to either version.

---

## ➤ New Printing Options for Geom and NMR

The **Geom=PrintInputOrient** option has been added to include the table giving the cartesian coordinates in the input orientation. By default, this table is printed for smaller molecules but omitted for large ones. The **NMR=PrintEigenvectors** option has been added to display the eigenvectors of the shielding tensor for each atom.

---

### ➤ G3 Methods Added

The recently published **G3** [26] and **G3MP2** [27] methods have been added, along with the variants using B3LYP structures and frequencies, **G3B3** and **G3MP2B3** [28] (using these keywords).

---

### ➤ New Redundant Internal Coordinates Generation Scheme for Weakly-Bound Complexes

The generation of redundant internal coordinates for weakly bound complexes has been updated. The **HBond** and **AllHBond** keywords never did what the documentation suggested (and they have been removed); what is done in revision A.7 and higher is to include Hydrogen bonds automatically. In addition, in connecting different fragments which are only weakly bound (hydrogen-bonded and otherwise), all pairs of atoms with one atom in each fragment having distance within a factor of 1.3 of the closest pair have their distances added to the internal coordinates. If at least 3 such pairs are found, then no angles or dihedrals involving both fragments are added. However, if only 1 or two pairs of atoms are close, then the related angles and dihedrals are added in order to ensure a complete coordinate system. As usual, the **ModRedundant** option can be used to add or remove any coordinates manually.

---

### ➤ Change to Charge Generation for Molecular Mechanics Methods

Beginning in Revision A.7, no charges are assigned to atoms by default when using any molecular mechanics force field. Options are available to estimate charges at the initial point using the QEq algorithm under control of the following options for any of the mechanics keywords:

**QEq** Assign charges to all atoms.

**UnTyped** Assign charges only to those atoms for which the user did not specify a particular type in the input.

**UnCharged** Assign charges for all atoms which have charge zero (i.e., all atoms which were untyped or which were given a type but not a charge in the input).

---

### ➤ Longer Link 0 Commands Supported

Link 0 commands (% lines) can now be up to 500 characters long.

---

### ➤ Other Minor Corrections/Clarifications to the Printed Manual

- ◆ The **IRC** keyword supports a **CalcAll** option.
- ◆ The only valid separator between the various methods for an **IRCM** calculation is a colon. In particular, a double slash (//) will not work.
- ◆ The **Density** is ignored when used with **ZINDO**.
- ◆ Defaults for the **FMM** keyword have been set.
- ◆ The default algorithm for optimizations without gradients is **EF**.
- ◆ **Charge** obeys the **Units** keyword, contrary to manual.
- ◆ The example job in the **ONIOM** discussion uses the **Amber** MM method without specifying atom types in the molecule specification. This will generate an error since **Amber** always requires that explicit atom types be input. Changing **Amber** to **UFF** in this job will make the example run correctly.
- ◆ The DFT keyword **G961LYP** is not implemented.
- ◆ The keyword sequence **MP2 NMR=GIAO** is broken and performs only an MP2 energy calculation. Use **MP2 NMR** to perform a GIAO NMR calculation at the MP2 level.
- ◆ **Int=NoSComp** may be used to turn off symmetry blocking of MO 2-electron integrals. **NoSymmComp** is a synonym for **NoSComp**.
- ◆ The **BiMolecularReactant** and **BiMolecularProduct** options to the **Opt** keyword are not implemented. The **BiMolecular** option is provided, however.
- ◆ **Opt(StepSize=n)** does not work. One must use **IOp(1/8=n)** instead.

---

## ➤ Unavailable Features

A few features documented in the manual will not appear *Gaussian 98*:

- ◆ The Becke96 gradient-corrected exchange functional (accordingly, B1B96 is also deferred).
- ◆ The B1PW91 functional is not implemented.
- ◆ Support for compound energy methods with **IRCM**ax.
- ◆ Support for the **Phase**, **Freq** and **Downhill** options to **IRC**.

---

## ➤ Updated References

The following reference citations have been updated/corrected:

- 123 C. Peng, P. Y. Ayala, H. B. Schlegel and M. J. Frisch, "Using redundant internal coordinates to optimize geometries and transition states," *J. Comp. Chem.* **17**, 49 (1996).
- 132 S. Dapprich, I. Komaromi, K. S. Byun, K. Morokuma and M. J. Frisch, "A New ONIOM Implementation in Gaussian 98. Part I. The Calculation of Energies, Gradients, Vibrational Frequencies and Electric Field Derivatives," *J. Mol. Str. (Theochem)* **461-462**, 1 (1999). [replaces manual references 132 and 133]
- 146 R. E. Stratmann, J. C. Burant, G. E. Scuseria and M. J. Frisch, *J. Chem. Phys.* **106**, 10175 (1997).
- 319 C. Adamo and V. Barone, *Chem. Phys. Lett.* **274**, 242 (1997).

---

## ➤ New References Cited in This Document

- 1 V. Barone, in *Recent Advances in Density Functional Methods, Part I*, Ed. D. P. Chong (World Scientific Publ. Co., Singapore, 1996).
- 3 E. Stratmann, G. E. Scuseria and M. J. Frisch, *Chem. Phys. Lett.* **257**, 213 (1996).
- 4 D. K. Malick, G. A. Petersson and J. A. Montgomery Jr., "Transition States for Chemical Reactions. I. Geometry and Barrier Height," *J. Chem. Phys.* **108**, 5704 (1998).
- 5 B. C. Garrett, D. G. Truhlar, R. S. Grev and A. D. Magnusson, "Improved treatment of threshold contributions in variational transition state theory," *J. Phys. Chem.* **84** (1980).
- 6 G. A. Petersson, "Complete Basis Set Thermochemistry and Kinetics," in *Computational Thermochemistry*, Ed. K. K. Irikura and D. J. Frurip (Amer. Chem. Soc., Washington, DC, 1998) 237.
- 7 M. Schwartz, P. Marshall, R. J. Berry, C. J. Ehlers and G. A. Petersson, "Computational Study of the Kinetics of Hydrogen Abstraction from Fluoromethanes by the Hydroxyl Radical," *J. Phys. Chem.*, submitted (1998).
- 8 G. A. Petersson, D. K. Malick, W. G. Wilson, J. W. Ochterski, J. A. Montgomery Jr. and M. J. Frisch, "Calibration and comparison of the G2, CBS, and DFT methods for computational thermochemistry," *J. Chem. Phys.*, **109**, 10570 (1998).
- 9 H. Eyring, "The activated complex in chemical reactions," *J. Chem Phys.* **3**, 107 (1935).
- 10 D. G. Truhlar, "Adiabatic Theory of Chemical Reactions," *J. Chem. Phys.* **53**, 2041 (1970).
- 11 D. G. Truhlar and A. Kuppermann, "Exact tunneling calculations," *J. Am. Chem. Soc.* **93**, 1840 (1971).
- 12 R. T. Skodje, D. G. Truhlar and B. C. Garrett, "Vibrationally adiabatic models for reactive tunneling," *J. Chem. Phys.* **77**, 5955 (1982).
- 13 A. G. Baboul and H. B. Schlegel, "Improved Method for Calculating Projected Frequencies along a Reaction Path," *J. Chem. Phys.* (1997).
- 14 N. Rega, M. Cossi and V. Barone, *J. Chem. Phys.* **105**, 11060 (1996).
- 15 V. Barone, *Chem. Phys. Lett.* **262**, 201 (1996).
- 16 A. D. Bacon and M. C. Zerner, "An Intermediate Neglect of Differential Overlap Theory for Transition Metal Complexes: Fe, Co, and Cu Chlorides," *Theo. Chim. Acta* **53**, 21 (1979).
- 17 W. P. Anderson, W. D. Edwards and M. C. Zerner, "Calculated Spectra of Hydrated Ions of the First Transition-Metal Series," *Inorganic Chem.* **25**, 2728 (1986).
- 18 M. C. Zerner, G. H. Lowe, R. F. Kirchner and U. T. Mueller-Westerhoff, "An Intermediate Neglect of Differential Overlap Technique for Spectroscopy of Transition-Metal Complexes. Ferrocene," *J. Am. Chem. Soc.* **102**, 589 (1980).
- 19 J. E. Ridley and M. C. Zerner, "An Intermediate Neglect of Differential Overlap Technique for Spectroscopy: Pyrrole and the Azines," *Theo. Chim. Acta.* **32**, 111 (1973).

- 20 J. E. Ridley and M. C. Zerner, "Triplet states via Intermediate Neglect of Differential Overlap: Benzene, Pyridine, and the Diazines," *Theo. Chim. Acta.* **42**, 223 (1976).
- 21 M. A. Thompson and M. C. Zerner, "The Electronic Structure and Spectroscopy of the Photosynthetic Reaction Center from Rhodospseudomonas viridis," *J. Am. Chem. Soc.* **113**, 8210 (1991).
- 22 M. C. Zerner, "Semi Empirical Molecular Orbital Methods," in *Reviews of Computational Chemistry*, Ed. K. B. Lipkowitz and D. B. Boyd (VCH Publishing, New York, 1991), vol. 2, 313.
- 23 M. C. Zerner, P. Correa de Mello and M. Hehenberger, "On the Convergence of the Self Consistent Field Method to Excited States," *Int. J. Quant. Chem.* **21**, 251 (1982).
- 24 L. K. Hanson, J. Fajer, M. A. Thompson and M. C. Zerner, "Environmental Effects on the Properties of Bacteriachlorophylls in Photosynthetic Reaction Centers: Theoretical Models," *J. Amer. Chem. Soc.* **109**, 4728 (1987).
- 25 J. A. Montgomery Jr, M. J. Frisch, J. W. Ochterski and G. A. Petersson, "A complete basis set model chemistry. VI. Use of density functional geometries and frequencies.," *J. Chem. Phys.* **110**, 2822 (1999).
- 26 L.A. Curtiss, K. Raghavachari, P.C. Redfern, V. Rassolov and J.A. Pople, *J. Chem. Phys.*, **109**, 7764 (1998).
- 27 L.A. Curtiss, P.C. Redfern, K. Raghavachari, V. Rassolov and J.A. Pople, *J. Chem. Phys.*, **110**, 4703 (1999).
- 28 A.G. Baboul, L.A. Curtiss, P.C. Redfern, and K. Raghavachari, *J. Chem. Phys.*, **110**, 7650 (1999).
- 29 J.P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.* **77** (1996) 3865.
- 30 J.P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.* **78** (1997) 1396.
- 31 E. Anders, R. Koch, and P. Freunsch, *J. Comp. Chem.* **14** (1993) 1301.

# System-Specific Information

---

## ➤ Operating System and Software Requirements

Be sure to check the Gaussian web site regularly for information about required operating system and compiler revision levels for systems upon which you want to build the program. Any patches required by specific hardware and/or operating system levels are also listed here. You can go directly to this page with the URL: [www.gaussian.com/g98\\_req.htm](http://www.gaussian.com/g98_req.htm).

---

## ➤ \*Correct Compiler for Sun Systems

Sun users should be using the **cc** command from `/opt/SUNWspro/bin` and not from `/usr/ucb`. Be sure that the first directory is included in your path and that it appears in it before `/usr/ucb`.

---

## ➤ Checkpoint Files for 64-bit Integer Versions: SGI R10000, Sun, IBM Power 3, Hitachi, Hewlett-Packard, Compaq Tru-64

By default, the SGI R10000, Sun and AIX Power 3 versions are built using 64-bit integers. This removes the previous limits of 16 GB of main memory and 16 GB disk space imposed in previous versions, but means that checkpoint files from earlier revisions of *Gaussian 98* cannot be used directly by Revision A.8 or higher in the case of SGI, Sun and IBM or by Revision A.10 in the case of Hitachi and Hewlett-Packard.

To convert old IBM, Sun or SGI checkpoint files, use the copy of **formchk** or **chkmove** from revision A.6 to convert them to formatted files, then use **unfchk** or **chkmove** from A.8 to convert them back to binary form. In the case of Hitachi, use the copy of **formchk** or **chkmove** from revision A.9 or earlier to convert old binary checkpoint files to formatted files, then use **unfchk** or **chkmove** from A.10 to convert them back to binary form

---

## ➤ \*Building IBM RS/6000 Versions

The procedure for compiling *Gaussian 98* from source code on IBM RS/6000 systems has been changed for A.10. Because of difficulties with IBM's ESSL library, we have switched to the public-domain ATLAS libraries for turned matrix operation subroutines. Since building ATLAS can be cumbersome, we have included the ATLAS libraries on the G98 source CD, in the `/atlas` top-level directory.

The G98 makefile expects to find the two ATLAS libraries in `/usr/local/lib`. Thus, before compiling G98, the appropriate versions of the libraries should be copied to this location. If a different location is chosen for these libraries, then the file `g98/bsd/rs6k.make` must be edited to reflect the change. The libraries provided are:

<code>power1-4.3-libatlas.a</code>	<code>power3-4.3-libatlas.a</code>
<code>power1-4.3-libf77blas.a</code>	<code>power3-4.3-libf77blas.a</code>
<code>power2-4.3-libatlas.a</code>	<code>power3-5.1-libatlas.a</code>
<code>power2-4.3-libf77blas.a</code>	<code>power3-5.1-libf77blas.a</code>

Note that G98 is built as a 64-bit program for the Power 3 machines, and that AIX 4.3 and AIX 5.1 have different and incompatible binary formats for 64-bit programs. Consequently, there are four pairs of libraries:

<code>power1-4.3*</code>	Use with Power 1 machines and either AIX 4.3 or AIX 5.1 (32-bit version).
<code>power2-4.3*</code>	Use with Power 2 machines and either AIX 4.3 or AIX 5.1 (32-bit version).
<code>power3-4.3*</code>	Use with Power 3 machines and AIX 4.3 only (64-bit version).
<code>power3-5.1*</code>	Use with Power 3 machines and AIX 5.1 only (64-bit version).

For example, for a Power 3 machine running AIX 4.3, execute the following commands (the percent sign is the C shell prompt and should not be typed):

```
% cp /CDROM/atlas/power3-4.3-libf77blas.a /usr/local/lib/libf77blas.a
% cp /CDROM/atlas/power3-4.3-libatlas.a /usr/local/lib/libatlas.a
```

where /CDROM should be replaced with the path to the CDROM drive.

Once the proper libraries are copied, the program can be built as follows (the percent sign is the C shell prompt and should not be typed):

*Power 3 systems:*

```
% cd $g98root/g98
% source bsd/g98.login
% bsd/bldg98 >& g98_build.log
```

*Power 2 systems:*

```
% cd $g98root/g98
% source bsd/g98.login
% bsd/bldg98 all ibmp2 >& g98_build.log
```

*Power 1 systems:*

```
% cd $g98root/g98
% source bsd/g98.login
% bsd/bldg98 all ibmp1 >& g98_build.log
```

---

## ➤ System Configuration and Memory Requirements Under UniCOS

Process and job memory limits should be set to 0; otherwise, the default memory used will be 90% of all available memory (rather than 4MB as in other versions of *Gaussian 98*). This can be done by giving input similar to the following to **udbgen**:

```
update:username:pmemlim[b]:0:jmemlim[b]:0:jmemlim[i]:0:
```

G98 takes more fixed memory on UniCOS systems. When running in NQS batch queues, make sure that the NQS batch memory limit is at least 6 million words larger than the value desired or specified for **%Mem**.

---

## ➤ \*Fortran Compiler and Libraries for Building the Intel Linux Version

The Intel Linux version requires the Portland Group Fortran compiler (see [www.pgroup.com](http://www.pgroup.com)).

The procedure for compiling *Gaussian 98* from source code on Intel Linux systems has been changed for A.11.3. We use the public-domain ATLAS libraries for turned matrix operation subroutines. Since building ATLAS can be cumbersome, we have included the ATLAS libraries on the G98 source CD, in the /atlas top-level directory.

The G98 makefile expects to find the two ATLAS libraries in /usr/local/lib. Thus, before compiling G98, the appropriate versions of the libraries should be copied to this location. If a different location is chosen for these libraries, then the file g98/bsd/i386.make must be edited to reflect the change. The libraries provided are:

```
PIII-RH7-libatlas.a
PIII-RH7-libf77blas.a
```

These libraries can be used with any Linux version (we've tested with Red Hat 6 as well), and with the Pentium 4 as well. You can install the libraries from the CD using the following commands (the percent sign is the C shell prompt and should not be typed):

```
% cp /CDROM/atlas/PIII-RH7-libf77blas.a /usr/local/lib/libf77blas.a
% cp /CDROM/atlas/PIII-RH7-libatlas.a /usr/local/lib/libatlas.a
```

where /CDROM should be replaced with the path to the CDROM drive.

Once the proper libraries are copied, the program can be built as follows:

```
% cd $g98root/g98
% source bsd/g98.login
% bsd/bldg98 >& g98_build.log
```

---

➤ **Windows Version is NOT Parallel-Enabled**

Do not set the Windows environment variable **MKL\_NPROCS** to a value greater than 1 in an attempt to make the program run in parallel. This will result in the program still using only a single processor, but a significant amount of gratuitous overhead will be expended anyway.

---

➤ **Alpha Linux Version Compiler**

The Linux version of the program for the Compaq Alpha platform must be built using the Compaq Fortran compiler. GNU compilers will not work.

---

➤ **Building Fujitsu VPP300/VPP700/VX Versions**

By default, the Fujitsu version of the *Gaussian 98* makefile (**\$g98root/g98/bsd/fujitsu.make**) is configured to build the VPP800/VPP5000 version of the code. VX/VPP300/VPP700/VX users must edit this file according to the instructions contained within it.