

# Gaussian 09 Revision E.01 Release Notes

14 December 2015

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## \*Feature and Usage notes: Rev E.01

This revision is primarily to fix a variety of bugs reported by users or which were uncovered by the example jobs for the 3rd edition of *Exploring Chemistry with Electronic Structure Methods*.

- Formatted checkpoint files now include the version of G09 used and also a job status flag, so that GUIs can determine whether a job is still running, failed or completed successfully. The number of imaginary frequencies is also included for frequency jobs.
- **LOMCC=ListWindow** now reads the window only once instead of twice.
- Rigid (unrelaxed) scans with large energies now generate a table of relative energies rather than "\*\*\*\*".
- The TDHF excited states method now defaults to using the MO basis, the same default as for CIS.
- A fix for the reference atoms used in Hirshfeld charges will change the reported charges slightly.
- The overhead in using Linda parallelism with ECPs was removed.
- The build procedures include compiling natively for Sandybridge (AVX) x86\_64 processors, including an AVX-enabled ATLAS library. A Sandybridge/Hawell binary distribution is also available.
- The divide-and-conquer diagonalization and SVD routines work in a larger fraction of cases.

## Feature and Usage Notes: Rev D.01

- The capabilities of the **Freq=Anharmonic** methods have been substantially expanded:
  - ◊ Full anharmonic IR intensities are now computed [Bloino12].
  - ◊ The DCPT2 [Kuhler96, Bloino12a] and HDCPT2 [Bloino12a] methods now support resonance-free computations of anharmonic frequencies and partition functions.
  - ◊ Vibronic computations now include ECD [Barone12]. This code has also been significantly optimized.
  - ◊ The output has been made more readable.
- Raman and ROA intensities can be calculated separately from calculation of the force constants and normal modes, to facilitate using a larger basis for these properties as recommended in [Chosenman11a]. The keyword **Polar=Raman** (or **Polar=ROA**) requests that the force constants be picked up from the checkpoint file (i.e., from a previous **Freq** calculation) and new

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**Michael Brown**



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