

# 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

# Gaussian 09 Revision E 01 Release Notes

**Wenbin Ji**



**Gaussian 09 Revision E 01 Release Notes:**

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In a fast-paced world fueled by information and interconnectivity, the spellbinding force of linguistics has acquired newfound prominence. Its capacity to evoke emotions, stimulate contemplation, and stimulate metamorphosis is really astonishing. Within the pages of "**Gaussian 09 Revision E 01 Release Notes**," an enthralling opus penned by a very acclaimed wordsmith, readers embark on an immersive expedition to unravel the intricate significance of language and its indelible imprint on our lives. Throughout this assessment, we shall delve into the book's central motifs, appraise its distinctive narrative style, and gauge its overarching influence on the minds of its readers.

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