

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/Haswell 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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L Darling-Hammond



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Advances in Physical Organic Chemistry, 2022-11-22 Advances in Physical Organic Chemistry Volume 56 presents the latest reviews of recent work in physical organic chemistry The book provides a valuable source of information that is ideal not only for physical organic chemists applying their expertise to both novel and traditional problems but also for non specialists across diverse areas who identify a physical organic component in their approach to research Chapters due to be included in this release cover flavin dependent enzyme catalysed reactions coacervates and their properties heavy atom tunnelling machine learning acidity and substituent effects Reviews the application of quantitative and mathematical methods to help readers understand chemical problems Provides the chemical community with authoritative and critical assessments of the many aspects of physical organic chemistry Covers organic organometallic bioorganic enzymes and materials topics Presents the only regularly published resource for reviews in physical organic chemistry Written by authoritative experts who cover a wide range of topics that require a quantitative molecular level understanding of phenomena across a diverse range of disciplines Molecular Modelling and Drug Design Vintner,1994-05-03 This book provides a myriad of fresh ideas and energetic approaches to the newer aspects of everyday drug modelling With contributions from some of the best young talents of today Molecular Modelling and Drug Design encourages a break from old traditions and probes the unexplored avenues of the modelling tool The contributors views act as a gauge to future trends in computer aided drug design an area that continues to expand and play an ever more significant role in drug discovery

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