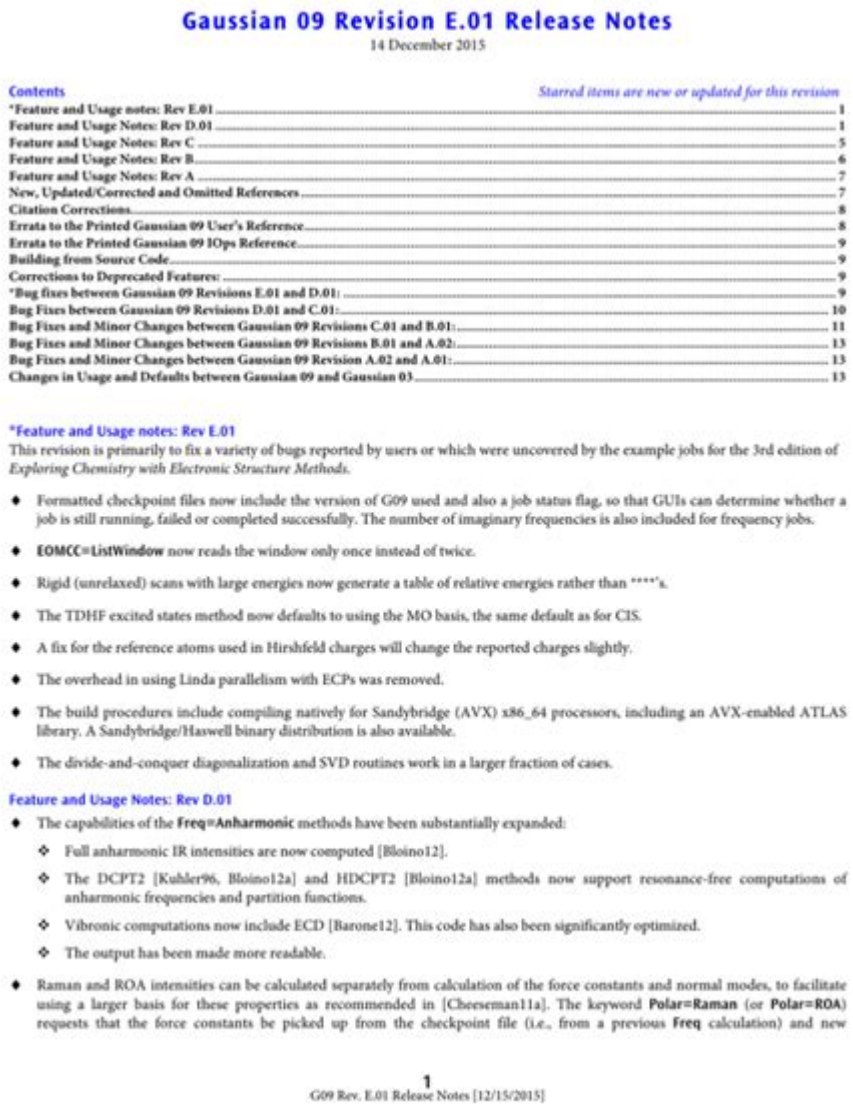
Gaussian 09 Revision E 01 Release Notes



Gaussian 09 Revision E.01 Release Notes

14 December 2015

Contents *Starred items are new or updated for this revision*

*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.
- **EOMCC=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 ****'s.
- 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 [Cheeseman11a]. 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

The Gaussian 09 software suite, a cornerstone in computational chemistry, has undergone various revisions to enhance its capabilities and performance. The Revision E.01 release is a significant update that introduces multiple improvements, bug fixes, and new features aimed at providing a more robust and user-friendly experience for researchers in the field of theoretical chemistry. This article will delve into the details of the Gaussian 09 Revision E.01 release notes, highlighting the enhancements made, the issues addressed, and the implications for users.

Overview of Gaussian 09

Gaussian is a software package that allows scientists to perform quantum

mechanical calculations on molecular systems. It is widely used in fields such as chemistry, biology, and materials science to predict molecular properties, simulate chemical reactions, and explore potential energy surfaces. Gaussian 09, which is the ninth major release of the software, has been a vital tool for researchers since its introduction.

Key Features of Gaussian 09 Revision E.01

The Revision E.01 update builds upon the established functionalities of Gaussian 09, adding new features and improving existing ones. Below are the key features introduced in this release:

1. Enhanced Computational Methods

- New Methods: The E.01 revision incorporates new methods that improve the accuracy of calculations. Among them are:
- Time-Dependent Density Functional Theory (TDDFT) enhancements.
- Improvements to wavefunction-based methods like Coupled Cluster (CC) and Møller-Plesset perturbation theory (MP).

- Optimized Algorithms: Several algorithms have been optimized for better performance, especially in large-scale computations. The improvements in these algorithms lead to reduced computational time and resource usage.

2. Improved User Interface

- Graphical User Interface (GUI): The GUI has been updated for better usability. Users can now access features more intuitively, making it easier to set up and execute calculations.

- Documentation and Help Resources: Comprehensive documentation has been provided to aid users in navigating new features and methods. The help resources have been expanded to include tutorials and examples.

3. Bug Fixes and Stability Improvements

- Resolved Issues: Several bugs from previous versions have been addressed in this release, leading to increased stability. Notable fixes include:
- Correction of issues related to input file parsing which previously caused unexpected terminations.
- Resolved memory leaks that could occur during long calculations.

- Performance Enhancements: Many of the underlying routines have been optimized, resulting in faster execution times for a variety of tasks.

New Features and Functionalities

In addition to the enhancements mentioned above, the Revision E.01 release

includes several new features that expand the capabilities of Gaussian 09.

1. Improved Solvation Models

Gaussian 09 E.01 introduces new solvation models that allow for more accurate simulations of molecular systems in solvent environments. These models provide researchers with better tools for studying reaction mechanisms and molecular interactions in solution.

2. Expanded Basis Set Options

The release includes additional basis sets, particularly for transition metals and heavier elements, which are essential for accurate electronic structure calculations. Users can now utilize these basis sets to achieve better results in their simulations.

3. Advanced Visualization Tools

The new version of Gaussian 09 also features enhanced visualization tools that facilitate the analysis of molecular orbitals, electron density plots, and potential energy surfaces. These tools aid researchers in interpreting their results more effectively.

Compatibility and System Requirements

As with any software update, it is crucial to understand the system requirements and compatibility aspects of Gaussian 09 Revision E.01.

1. Supported Platforms

Gaussian 09 E.01 is compatible with various operating systems, including:

- Windows
- Linux
- macOS

Users should ensure that their system meets the following requirements:

- A minimum of 4 GB of RAM (8 GB or more is recommended for larger calculations).
- A multi-core processor for optimal performance.
- Adequate disk space for installation and computational data.

2. Integration with Other Software

The new release continues to support integration with various third-party

software, enhancing its capabilities in computational workflows. This includes compatibility with software for molecular visualization, data analysis, and workflow management.

Installation and Upgrade Instructions

To ensure a smooth transition to Gaussian 09 Revision E.01, users should follow the installation and upgrade instructions carefully.

1. Installation Process

- Download: Obtain the latest version of Gaussian 09 Revision E.01 from the official Gaussian website.
- Installation: Follow the provided installation guide, which includes step-by-step instructions for various operating systems.

- Configuration: After installation, configure the software according to your system settings and preferences.

2. Upgrading from Previous Versions

For users upgrading from earlier versions of Gaussian 09, it is recommended to:

- Backup important data and files before proceeding with the upgrade.
- Follow the upgrade instructions outlined in the documentation, ensuring that all previous configurations are properly migrated.

Conclusion

The Gaussian 09 Revision E.01 release represents a significant step forward in the capabilities and performance of one of the most widely used computational chemistry software packages. With its enhanced computational methods, improved user interface, new features, and bug fixes, users can expect a more efficient and robust experience. As computational chemistry continues to evolve, updates like this ensure that Gaussian remains at the forefront, providing researchers with the tools they need to explore the intricacies of molecular systems. By embracing the innovations in this release, users can enhance their research outcomes and contribute effectively to the advancement of scientific knowledge.

Frequently Asked Questions

What are the main enhancements introduced in Gaussian 09 Revision E.01?

Gaussian 09 Revision E.01 includes improvements in computational efficiency,

enhanced algorithms for geometry optimizations, and support for new functionals in DFT calculations.

How does Gaussian 09 Revision E.01 improve parallel processing capabilities?

The revision introduces better load balancing across processors, allowing for more efficient memory usage and reduced computation times in parallel jobs.

Are there any new features related to molecular dynamics in Gaussian 09 Revision E.01?

Yes, the revision adds new features for molecular dynamics simulations, including improved algorithms for temperature control and enhanced sampling techniques.

What bug fixes are included in the Gaussian 09 Revision E.01 release notes?

The release notes detail several bug fixes related to energy calculations, issues with certain input formats, and corrections to output file formatting.

Does Gaussian 09 Revision E.01 support any new quantum chemistry methods?

Yes, it adds support for the latest developments in multi-reference methods and improved implementations of coupled cluster theories.

What improvements have been made to the user interface in Gaussian 09 Revision E.01?

The user interface has been enhanced for better usability, including improved visualization tools and easier navigation for setting up calculations.

How can users access the updated documentation for Gaussian 09 Revision E.01?

Updated documentation can be accessed through the official Gaussian website or directly within the software, which includes comprehensive guides and examples.

Are there any compatibility issues with previous versions when upgrading to Gaussian 09 Revision E.01?

Most users should experience smooth transitions; however, it is recommended to review the release notes for any specific compatibility concerns with older input files.

What types of systems or platforms does Gaussian 09 Revision E.01 support?

Gaussian 09 Revision E.01 supports a variety of platforms, including Windows, Linux, and macOS, ensuring broad accessibility for users across different systems.

Gaussian 09 Revision E 01 Release Notes

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