

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	1
Feature and Usage Notes: Rev D.01	1
Feature and Usage Notes: Rev C	5
Feature and Usage Notes: Rev B	6
Feature and Usage Notes: Rev A	7
New, Updated/Corrected and Omitted References	7
Citation Corrections	8
Errata to the Printed Gaussian 09 User's Reference	8
Errata to the Printed Gaussian 09 I/Os Reference	9
Building from Source Code	9
Corrections to Deprecated Features:	9
*Bug fixes between Gaussian 09 Revisions E.01 and D.01:	9
Bug Fixes between Gaussian 09 Revisions D.01 and C.01:	10
Bug Fixes and Minor Changes between Gaussian 09 Revisions C.01 and B.01:	11
Bug Fixes and Minor Changes between Gaussian 09 Revisions B.01 and A.02:	13
Bug Fixes and Minor Changes between Gaussian 09 Revision A.02 and A.01:	13
Changes in Usage and Defaults between Gaussian 09 and Gaussian 03	13

*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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RJ Shavelson



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Table of Contents Gaussian 09 Revision E 01 Release Notes

1. Understanding the eBook Gaussian 09 Revision E 01 Release Notes
 - The Rise of Digital Reading Gaussian 09 Revision E 01 Release Notes
 - Advantages of eBooks Over Traditional Books
2. Identifying Gaussian 09 Revision E 01 Release Notes
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Gaussian 09 Revision E 01 Release Notes
 - User-Friendly Interface
4. Exploring eBook Recommendations from Gaussian 09 Revision E 01 Release Notes
 - Personalized Recommendations
 - Gaussian 09 Revision E 01 Release Notes User Reviews and Ratings
 - Gaussian 09 Revision E 01 Release Notes and Bestseller Lists

5. Accessing Gaussian 09 Revision E 01 Release Notes Free and Paid eBooks
 - Gaussian 09 Revision E 01 Release Notes Public Domain eBooks
 - Gaussian 09 Revision E 01 Release Notes eBook Subscription Services
 - Gaussian 09 Revision E 01 Release Notes Budget-Friendly Options
6. Navigating Gaussian 09 Revision E 01 Release Notes eBook Formats
 - ePub, PDF, MOBI, and More
 - Gaussian 09 Revision E 01 Release Notes Compatibility with Devices
 - Gaussian 09 Revision E 01 Release Notes Enhanced eBook Features
7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Gaussian 09 Revision E 01 Release Notes
 - Highlighting and Note-Taking Gaussian 09 Revision E 01 Release Notes
 - Interactive Elements Gaussian 09 Revision E 01 Release Notes
8. Staying Engaged with Gaussian 09 Revision E 01 Release Notes
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Gaussian 09 Revision E 01 Release Notes
9. Balancing eBooks and Physical Books Gaussian 09 Revision E 01 Release Notes
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Gaussian 09 Revision E 01 Release Notes
10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
11. Cultivating a Reading Routine Gaussian 09 Revision E 01 Release Notes
 - Setting Reading Goals Gaussian 09 Revision E 01 Release Notes
 - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Gaussian 09 Revision E 01 Release Notes
 - Fact-Checking eBook Content of Gaussian 09 Revision E 01 Release Notes
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning

- Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
- Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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