

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/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

Gaussian 09 Revision E 01 Release Notes

Clifford Lane



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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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web because a mattanza is the catch of an entire school of fish dozens of tuna may be captured the ambience of bloody water and particularly large fish which may be compared to cattle or large game leaves one with a singular impression

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web mattanza s f dallo spagn matanza uccisione der di matar uccidere fase finale della pesca del tonno particolarmente cruenta e impressionante durante la quale i tonni pervenuti nella tonnara e giunti nell ultimo compartimento