

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 [Choraman11a]. 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

Sam P. De Visser, Thomas S. Hofer



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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

Introductory Organic Chemistry and Hydrocarbons Caio Lima Firme, 2019-08-28 A novel proposal for teaching organic chemistry based on a broader and simplified use of quantum chemistry theories and notions of some statistical thermodynamic concepts aiming to enrich the learning process of the organic molecular properties and organic reactions A detailed physical chemistry approach to teach organic chemistry for undergraduate students is the main aim of this book A secondary objective is to familiarize undergraduate students with computational chemistry since most of illustrations of optimized geometries plus some topological graphs and information is from quantum chemistry outputs which will also enable students to obtain a deeper understanding of organic chemistry

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

Theoretical Chemistry in Belgium Benoît Champagne, Michael S. Deleuze, Frank De Proft, Tom Leyssens, 2013-10-16 Readers of this volume can take a tour around the research locations in Belgium which are active in theoretical and computational chemistry Selected researchers from Belgium present research highlights of their work Originally published in the journal Theoretical Chemistry Accounts these outstanding contributions are now available in a hardcover print format This volume will be of benefit in particular to those research groups and libraries that have chosen to have only electronic access to the journal It also provides valuable content for all researchers in theoretical chemistry

Fault Analysis in Cryptography Marc Joye, Michael Tunstall, 2012-06-21 In the 1970s researchers noticed that radioactive particles produced by elements naturally present in packaging material could

cause bits to flip in sensitive areas of electronic chips Research into the effect of cosmic rays on semiconductors an area of particular interest in the aerospace industry led to methods of hardening electronic devices designed for harsh environments Ultimately various mechanisms for fault creation and propagation were discovered and in particular it was noted that many cryptographic algorithms succumb to so called fault attacks Preventing fault attacks without sacrificing performance is nontrivial and this is the subject of this book Part I deals with side channel analysis and its relevance to fault attacks The chapters in Part II cover fault analysis in secret key cryptography with chapters on block ciphers fault analysis of DES and AES countermeasures for symmetric key ciphers and countermeasures against attacks on AES Part III deals with fault analysis in public key cryptography with chapters dedicated to classical RSA and RSA CRT implementations elliptic curve cryptosystems and countermeasures using fault detection devices resilient to fault injection attacks lattice based fault attacks on signatures and fault attacks on pairing based cryptography Part IV examines fault attacks on stream ciphers and how faults interact with countermeasures used to prevent power analysis attacks Finally Part V contains chapters that explain how fault attacks are implemented with chapters on fault injection technologies for microprocessors and fault injection and key retrieval experiments on a widely used evaluation board This is the first book on this topic and will be of interest to researchers and practitioners engaged with cryptographic engineering

Theoretical and Computational Chemistry Editor's Pick 2024, 2nd edition Sam P. De Visser, Thomas S. Hofer, 2025-03-31 We are pleased to introduce the collection Frontiers in Chemistry Theoretical and Computational Chemistry Editor s Pick 2024 This collection showcases most well received spontaneous articles from the past couple of years and have been specially handpicked by our Chief Editors The work presented here highlights the broad diversity of research performed across the section and aims to put a spotlight on the main areas of interest All research presented here displays strong advances in theory experiment and methodology with applications to compelling problems This collection aims to further support Frontiers strong community by recognizing highly deserving authors

Accurate Condensed-Phase Quantum Chemistry Fred Manby, 2010-08-02 The theoretical methods of quantum chemistry have matured to the point that accurate predictions can be made and experiments can be understood for a wide range of important gas phase phenomena A large part of this success can be attributed to the maturation of hierarchies of approximation which allow one to approach very high accuracy provided t

Publications of the National Bureau of Standards United States. National Bureau of Standards, 1983

The Interpretation of Quantum Mechanics Roland Omnès, 2018-06-05 The interpretation of quantum mechanics has been controversial since the introduction of quantum theory in the 1920s Although the Copenhagen interpretation is commonly accepted its usual formulation suffers from some serious drawbacks Based mainly on Bohr s concepts the formulation assumes an independent and essential validity of classical concepts running in parallel with quantum ones and leaves open the possibility of their ultimate conflict In this book Roland Omn s examines a number of recent advances which combined lead to a consistent

revision of the Copenhagen interpretation His aim is to show how this interpretation can fit all present experiments to weed out unnecessary or questionable assumptions and to assess the domain of validity where the older statements apply Drawing on the new contributions The Interpretation of Quantum Mechanics offers a complete and self contained treatment of interpretation in nonrelativistic physics in a manner accessible to both physicists and students Although some hard results are included the concepts and mathematical developments are maintained at an undergraduate level This book enables readers to check every step apply the techniques to new problems and make sure that no paradox or obscurity can arise in the theory In the conclusion the author discusses various philosophical implications pertinent to the study of quantum mechanics

Long-Range Dependence and Self-Similarity Vladas Pipiras,Murad S. Taqqu,2017-04-18 A modern and rigorous introduction to long range dependence and self similarity complemented by numerous more specialized up to date topics in this research area *Scientific and Technical Aerospace Reports* , Structure Property Correlations for Nanoporous Materials Abhijit Chatterjee,2010-05-17 Nanoporous materials are critical to various fields of research including ion exchange separation catalysis sensor applications biological molecular isolation and purification In addition they offer new opportunities in such areas as inclusion chemistry guest host synthesis and molecular manipulations and reactions at the nanoscale In St **Nano-Enabled Medical Applications** Lajos P. Balogh,2020-11-23 This book is the second in a series presenting articles that received the most citations in recent years in nanomedicine The series is edited by a prominent nanotechnology researcher and editor in chief of Precision Nanomedicine The theme of the second volume is about nano enabled medical applications The 19 articles collected here have already acquired more than 12 500 citations highlighting the importance and professional recognition of the work of these scientists in nanomedicine The content includes the general overview of the field and a wide variety of applications that have been impossible without nanoscience and nanotechnology

Superhalogens and Superalkalis Pratim Kumar Chattaraj,Ambrish Kumar Srivastava,2024-04-15 Superhalogens and Superalkalis is a comprehensive volume designed as the go to resource on the exciting and evolving topics of these special classes of atomic clusters and the acid salt that results from their interactions The book details how these substances possess not only unusual structures but also unique properties which can be exploited for various applications Superhalogens strong oxidizing capacity resulting from their high electron affinity leads to their applications in the design of superacids organic superconductors and ionic liquids The low ionization energy of superalkalis enables them to act as strong reducing agents making them useful in the design of superbases and alkalides Illustrated throughout this timely book provides an overview of the research and development on these and other aspects of superhalogen and superalkalis Key features Offers a basic introduction of superatoms that is accessible for readers to understand Includes extensive study questions after each chapter Provides a systematic presentation of the existing literature on this increasingly trending topic Presents the latest developments in the field offering readers state of art knowledge This book is a key reference guide for graduate students

postdocs upper level undergraduate students academic professionals and researchers who are interested in this fascinating topic *Applied Mechanics Reviews* ,1969 **Canadian Journal of Chemistry** ,2009 *Uncovering Quantum Field Theory and the Standard Model* Wolfgang Bietenholz,Uwe-Jens Wiese,2024-02-29 This textbook provides an accessible introduction to quantum field theory and the Standard Model of particle physics It adopts a distinctive pedagogical approach with clear intuitive explanations to complement the mathematical exposition The book begins with basic principles of quantum field theory relating them to quantum mechanics classical field theory and statistical mechanics before building towards a detailed description of the Standard Model Its concepts and components are introduced step by step and their dynamical roles and interactions are gradually established Advanced topics of current research are woven into the discussion and key chapters address physics beyond the Standard Model covering subjects such as axions technicolor and Grand Unified Theories This book is ideal for graduate courses and as a reference and inspiration for experienced researchers Additional material is provided in appendices while numerous end of chapter problems and quick questions reinforce the understanding and prepare students for their own research **Novel and Emerging Therapies for the Treatment of Obesity and Related Disorders** Isabel Rodriguez Amado,Marina Romani Perez,Pablo Fuciños,Manuel Gil-Lozano,2024-05-06 Obesity and its associated comorbidities e g type II diabetes and cardiovascular disease represent a serious challenge for healthcare systems worldwide Obesity is a chronic disease characterized by excessive adipose tissue mass resulting from an imbalance between energy intake and expenditure with growing relevance in an increasingly sedentary society Obesity is multifactorial where alterations in the physiology of gastrointestinal hormones playing a key role in the interplay between the gastrointestinal system and the brain and in the gut microbiota contribute to the development of this disorder *Complex Quantum Systems: Analysis Of Large Coulomb Systems* Heinz Siedentop,2013-05-20 This volume is based on lectures given during the program Complex Quantum Systems held at the National University of Singapore s Institute for Mathematical Sciences from 17 February to 27 March 2010 It guides the reader through two introductory expositions on large Coulomb systems to five of the most important developments in the field derivation of mean field equations derivation of effective Hamiltonians alternative high precision methods in quantum chemistry modern many body methods originating from quantum information and the most complex semirelativistic quantum electrodynamics These introductions are written by leaders in their fields amongst them are Volker Bach Rafael Benguria Thomas Chen and Jan Philip Solovej Together they fill a gap between current textbooks and the vast modern literature on complex quantum systems *Laser and Ion Beam Modification of Materials* I. Yamada,H. Ishiwara,E. Kamijo,2013-10-22 Laser and Ion Beam Modification of Materials is a compilation of materials from the proceedings of the symposium U Material Synthesis and Modification by Ion beams and Laser Beams This collection discusses the founding of the KANSAI Science City in Japan and the structures equipment and research projects of two institutions are discussed pertaining to eV MeV ion beams A description of ion beams as used in

materials research and in manufacturing processes along with trends in ion implantation technology in semiconductors is discussed Research into ion beams by China and its industrial uses in non semiconductor area is noted For industrial applications developing technology in terms of high speed large surface modifications and use of high doses is important Thus the development of different ion beam approaches is examined Industrial applications of ion and laser processing are discussed as cluster beams are used in solid state physics and chemistry Mention is made on a high power discharge pumped solid state physics ArF excimer laser as a potential light source for better material processing Under ion beam material processing is nanofabrication using focused ion beams important for research work in mesoscopic systems Progress in the use of ion beam mixing using kinetic energy of ion beams to mingle with pre deposited surface layers of substrate materials has shown promise Advanced materials researchers and scientists as well as academicians in the field of nuclear physics will find this collection helpful

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