

Gaussian 09 Revision D.01 Release Notes

8 June 2013

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Features and Bug Fixes: New D.01

- The capabilities of the fragment-based methods have been substantially expanded:
 - Full automatic IR prediction can now be used (Comment 1)
 - The CCPT2 (Hartree, Molecule) and CCPT2 (Molecule) methods now support automatic fragment computations of automatic frequency and gradient functions.
 - Various computational new methods (D.01) have been added. These methods have been significantly improved.
 - The output has been made more readable.
- Recent and full IR methods can be calculated separately from calculation of the linear potential and normal modes, in addition using a larger basis for those properties as recommended in Comment 1. The keyword **IRMethod** (or **IRMethod**) supports that the linear potential be picked up from the checkpoint file too, from a previous **IR** calculation and new calculation distribution (and the other two linear distributions for full IR) be computed and combined with the linear potential in predicting vibrational and spectra. For full IR provides an example of the two-step **IR** calculation.
- Time-dependent DFT calculations can employ the **Time-Dependent Approximation** via the **TDApprox** keyword.
- An energy compressor specialized for CIP and T-Computation energies via the following new options in **IR**, **IR** and **IR**:

IRMethod=1	Generate initial guess using only active occupied orbitals 1 and higher.
IRMethod=2	Generate initial guess using only the first 10 active occupied orbitals 1-10, the rest use the highest 10 occupied.
IRMethod=3	Generate initial guess using estimated correlation energies (100000 eV).
IRMethod=4	Generate only active having correlation energy (1.00000 eV, 1000-1, and threshold from input, 1000-1, and the threshold for full IR). Hartree.
IRMethod=5	Specify the number of active occupied orbitals having correlation energy is increased.
IRMethod=6	Specify the number of active occupied orbitals having correlation energy is increased.

The default for **IRMethod** when **IR** is the order of the active point group. The default for **IRMethod** is 1 for **IR** and 1 for **IR** and **IR**. Large values may be needed if there are many atoms in the range of interest.
- Several new DFT functionals and new empirical dispersion models have been added:
 - EmpiricalDispersion=GD3**, **GD3** or **GD3B** explicitly request Perdew-Burke-Ernzerhof (Comment 1) or Grimme's [36] dispersion (Comment 1) or **GD3** dispersion (Comment 1).

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Marco Cascella



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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

Advances in Quantum Systems in Chemistry, Physics, and Biology Liliana Mammino, Davide Ceresoli, Jean Maruani, Erkki Brändas, 2020-02-05 This edited multi author book gathers selected peer reviewed contributions based on papers presented at the 23rd International Workshop on Quantum Systems in Chemistry Physics and Biology QSCP XXIII held in Mopani Camp The Kruger National Park South Africa in September 2018 The content is primarily intended for scholars researchers and graduate students working at universities and scientific institutes who are interested in the structure properties dynamics and spectroscopy of atoms molecules biological systems and condensed matter

Structural and Dynamic Aspects of Protein Function and Allostery George Lisi, Ivan Rivalta, Vincenzo Venditti, 2022-03-28

Sense the Real Change: Proceedings of the 20th International Conference on Near Infrared Spectroscopy Xiaoli Chu, Longhai Guo, Yue Huang, Hongfu Yuan, 2022-08-08 This book features selected papers presented at the 20th International Conference on Near Infrared Spectroscopy It discusses the latest progress in the field of near infrared spectroscopy from around the globe including the advances in instrumentation spectral interpretation and Chemometrics In addition it presents potential trends for near infrared spectroscopy in the next decade and highlights developments in

process analytical technology chemical imaging and deep learning It can be used as a reference book for researchers and application personnel engaged in spectroscopy technology Chemometrics analytical instruments on site rapid or on line analysis process control and other fields It will also be useful for undergraduates and postgraduates studying these topics

Metal Nanocluster Chemistry Manzhou Zhu, 2023-01-18 Atomically precise metal nanoclusters occupy the gap between discrete atoms and plasmonic nanomaterials and they offer intriguing physical chemical properties that can be rationalized in terms of their quantum size effects and discrete electronic states The atomically precise nature of their structures lends them well to structure property relationship elucidation making them particularly useful for informing the rational design of nanoclusters with enhanced performance Metal Nanocluster Chemistry Ligand Protected Metal Nanoclusters With Atomic Precision provides a concise introduction to the study of these useful nanoclusters Beginning with an introduction to the fundamental concepts of and prospects for metal nanoclusters the book goes on to highlight synthetic methods for controllable preparation The subsequent chapters then highlight characterization mechanism of size growth and structure evolution and physical chemical properties Later chapters examine theoretical approaches for calculating and evaluating structures and properties They also highlight the assembly of nanocluster building blocks and their practical applications Drawing on the knowledge of its expert author Metal Nanocluster Chemistry is a useful introductory guide to these exciting structures Provides a concise introduction to atomically precise metal nanoclusters ranging from characterization and property investigation to applications Includes insight into both current trends and future potential encouraging and supporting further development Holistically combines physical approaches with theoretical calculation methods

Application of Optimization Algorithms in Chemistry Jorge M. C. Marques, Emilio Martinez-Nunez, William L. Hase, 2020-06-08 This eBook is dedicated to Prof William L Hase who passed away on Monday March 23 2020

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

Advances in the discovery of natural molecules and their analogues against microbial infection-related biofilms Laura Quintieri,Giovanni Lentini,Sridhar Mani,Giuseppantonio Maisetta,2022-12-29 *Carbohydrate-Based Interactions at the Molecular and the Cellular Level* Kieran L. Hudson,2018-05-28 This book offers a clearly written and highly accessible account of two different aspects of carbohydrate chemistry Carbohydrates are an essential component of life and have many important biological functions but the details of how carbohydrates interact with other biomolecules to mediate biological signalling remain unclear Firstly this thesis details innovative methods to mine protein structural data to uncover new features of carbohydrate based interactions It also explains these findings using physical chemistry specifically CH pi interactions associated with the properties of the interacting partners Carbohydrates are also critical for tissue growth and development yet are underexploited in the materials science that underpins much of regenerative medicine As such the second part of this thesis describes a diverse array of techniques ranging from synthetic chemistry and enzymatic synthesis to prepare a wide variety of carbohydrates and materials chemistry to prepare glycosylated hydrogels to cell biology to determine the effects on cellular development for tissue engineering applications

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Sun,Gennady L. Gutsev,2022-12-07 Title List of Documents Made Publicly Available U.S. Nuclear Regulatory Commission,1983

Scientific and Technical Aerospace Reports , 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

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