



# Organic and Inorganic Chemistry

Professor: Mrs. Jocelyn Soriano Diesta



## WEEK 1: PREVIEW OF DESCRIPTIVE AND THEORETICAL CHEMISTRY

### CHEMISTRY

- study of matter and the changes it undergoes.
- does not only investigate the qualities of matter, but also how and why it changes.
- often called the "central science."
  - It is central because a basic knowledge of chemistry is essential to our way of life. Without it, we would be living shorter lives in what we would consider primitive conditions.

### FIVE MAIN BRANCHES OF CHEMISTRY

#### 1. PHYSICAL CHEMISTRY

- Study of the physical properties of molecules, and their relation to the ways in which molecules and atoms are put together.

#### 2. ANALYTICAL CHEMISTRY

- Study involving how we analyze the chemical components of samples.

#### 3. ORGANIC CHEMISTRY

- Study of carbon-containing compounds.

#### 4. INORGANIC CHEMISTRY

- Study of elements and compounds other than carbon or hydrocarbons.

#### 5. BIOCHEMISTRY

- Study of chemical processes in living organisms.

### SIGNIFICANCE

- Everything in our environment is made of matter. Chemistry is significant in our civilization because it affects our basic needs for food, clothing, shelter, health, energy, and clean air, water, and soil, among other things.
- Chemistry lies at the heart of many matters of public concern: improvement of health care, conservation of natural resources, protection of the environment, and provision of our daily needs for food, clothing, and shelter.
- Using chemistry, we have discovered pharmaceutical chemicals that enhance health and prolong lives. We have increased food production through the use of fertilizers and pesticides, and we have developed plastics and other materials used in almost every facet of our lives, from electronics to sporting equipment to building construction.
- Chemical discoveries and their applications have played a pivotal role in the advancement of humankind and will continue to have a profound impact on health, the environment, industry, agriculture, science, and technology.

Community  
Health  
Environment  
Medicine  
Industry  
Sciences  
Technology  
Research  
You



### CONCERNS

- Chemistry is about more than discovery—the science and art of matter involve both creation and destruction.

- It is a scientific study that plays a pivotal role in our understanding of synthetic and physical phenomena and, as follows, both the material and natural world.
- Throughout history, chemists have come together to work with other skilled experts in their fields for a single reason: **to solve grand challenges in society.**
- Unfortunately, some chemicals can harm our health or the environment. As educated citizens and consumers, it is in our best interest to understand the profound effects, both positive and negative, that chemicals have on our lives and to strike an informed balance about their uses.

### CONTRIBUTION OF CHEMISTRY TO SOCIETY

- Source of knowledge and skills
- Field of communication
- Transportation
- Sophisticated equipments / Materials
- Increases the agricultural product
- Crimes (provide evidences to solve it)
- Environmental sanitation
- Supply to Food
- Development of life-saving medicines
- Innovation of technologies
- Entertainment

### THE SCIENTIFIC METHOD

- Used by scientists to search for answers to questions and solutions to problems.
- Consists of making observations, formulation hypotheses, and designing experiments; lead to additional observations, hypotheses, and experiments in repeated cycles.

### STEPS IN THE SCIENTIFIC METHOD

#### STEP 1: MAKE OBSERVATIONS

- Can be qualitative and quantitative.

#### STEP 2: FORMULATE A HYPOTHESIS

- Scientists begin by forming a hypothesis, a tentative explanation for the observations.
- May not be correct, but puts into a form that can be tested.
- Suitable experiments can be designed to choose between two alternatives.

#### STEP 3: DESIGN AND PERFORM EXPERIMENTS

- After a formulating a hypothesis, scientists conduct experiments to test its validity.
- Experiments are systematic observations or measurements, made under controlled conditions (in which a single variable changes)

#### STEP 4: ACCEPT OR MODIFY THE HYPOTHESIS

- After experimenting, it enables scientists to determine whether the hypothesis is valid
- If it is not, the hypothesis must be modified

#### STEP 5: DEVELOPMENT INTO A LAW AND/OR THEORY

- More experimental data are then collected and analyzed, and scientists may think that the results are dependable to merit being summarized in a law.
- Law is a verbal or mathematical description of a phenomenon that allows for general predictions.

# Lecture Notes On Theoretical Chemistry

**Ferdinand G. Wiechmann**



## **Lecture Notes On Theoretical Chemistry:**

Lecture-notes on Theoretical Chemistry Ferdinand Gerhard Wiechmann, 1895      **Lecture-Notes on Theoretical Chemistry** Ferdinand G. Wiechmann, 2019-12-11      **Lecture-notes on Theoretical Chemistry (Classic Reprint)** Ferdinand G. Wiechmann, 2017-11-26

Excerpt from Lecture Notes on Theoretical Chemistry The study of theoretical chemistry has not in general met with that recognition and appreciation which is warranted by the interest and importance attaching to this branch of chemical science Seeking For an explanation it appears that to many this study presents considerable difficulty on account of the number and variety of themes frequently exhibiting no organic connection to which the attention of the student is invited About the Publisher Forgotten Books publishes hundreds of thousands of rare and classic books Find more at [www.forgottenbooks.com](http://www.forgottenbooks.com) This book is a reproduction of an important historical work Forgotten Books uses state of the art technology to digitally reconstruct the work preserving the original format whilst repairing imperfections present in the aged copy In rare cases an imperfection in the original such as a blemish or missing page may be replicated in our edition We do however repair the vast majority of imperfections successfully any imperfections that remain are intentionally left to preserve the state of such historical works      **LECTURE-NOTES ON THEORETICAL C** Ferdinand Gerhard 1858-1919 Wiechmann, 2016-08-29 This work has been selected by scholars as being culturally important and is part of the knowledge base of civilization as we know it This work was reproduced from the original artifact and remains as true to the original work as possible Therefore you will see the original copyright references library stamps as most of these works have been housed in our most important libraries around the world and other notations in the work This work is in the public domain in the United States of America and possibly other nations Within the United States you may freely copy and distribute this work as no entity individual or corporate has a copyright on the body of the work As a reproduction of a historical artifact this work may contain missing or blurred pages poor pictures errant marks etc Scholars believe and we concur that this work is important enough to be preserved reproduced and made generally available to the public We appreciate your support of the preservation process and thank you for being an important part of keeping this knowledge alive and relevant      **Lecture Notes in Quantum Chemistry II** Björn O. Roos, 2012-12-06 The first volume of Lecture Notes in Quantum Chemistry Lecture Notes in Chemistry 58 Springer Verlag Berlin 1992 contained a compilation of selected lectures given at the two first European Summer Schools in Quantum Chemistry ESQC held in southern Sweden in August 1989 and 1991 respectively The notes were written by the teachers at the school and covered a large range of topics in ab initio quantum chemistry After the third summer school held in 1993 it was decided to put together a second volume with additional material Important lecture material was excluded in the first volume and has now been added Such added topics are integrals and integral derivatives SCF theory coupled cluster theory relativity in quantum chemistry and density functional theory One chapter in the present volume contains the exercise

material used at the summer school and in addition solutions to all the exercises It is the hope of the authors that the two volumes will find good use in the scientific community as textbooks for students who are interested in learning more about modern methodology in molecular quantum chemistry The books will be used as teaching material in the European Summer Schools in Quantum Chemistry which are presently planned Lund in July 1994 Bjorn Roos NOTES ON HARTREE FOCK THEORY AND RELATED TOPICS JanAlmlof Department of Chemistry University of Minnesota Minneapolis MN 55455 USA Contents 1 Introduction 2 The Born Oppenheimer Approximation 3 Determinant Wavefunctions and the Pauli Principle 4 Expectation Values With a Determinant Wavefunction Lecture Notes in Quantum Chemistry Björn O. Roos, 2012-12-06

Quantum Chemistry is the course material of a European Summer School in Quantum Chemistry organized by Björn O. Roos It consists of lectures by outstanding scientists who participate in the education of students and young scientists The book has a wider appeal as additional reading for University courses Contents P. A. Malmquist Mathematical Tools in Quantum Chemistry J. Olsen The Method of Second Quantization P. R. Taylor Molecular Symmetry and Quantum Chemistry B. O. Roos The Multiconfigurational MC Self Consistent Field SCF Theory P. E. M. Siegbahn The Configuration Interaction Method T. Helgaker Optimization of Minima and Saddle Points P. R. Taylor Accurate Calculations and Calibration U. Wahlgren Effective Core Potential Method Theoretical Chemistry and Physics of Heavy and Superheavy Elements U. Kaldor, Stephen Wilson, 2013-06-29

Quantum mechanics provides the fundamental theoretical apparatus for describing the structure and properties of atoms and molecules in terms of the behaviour of their fundamental components electrons and nucleons For heavy atoms and molecules containing them the electrons can move at speeds which represent a substantial fraction of the speed of light and thus relativity must be taken into account Relativistic quantum mechanics therefore provides the basic formalism for calculating the properties of heavy atom systems The purpose of this book is to provide a detailed description of the application of relativistic quantum mechanics to the many body problem in the theoretical chemistry and physics of heavy and superheavy elements Recent years have witnessed a continued and growing interest in relativistic quantum chemical methods and the associated computational algorithms which facilitate their application This interest is fuelled by the need to develop robust yet efficient theoretical approaches together with efficient algorithms which can be applied to atoms in the lower part of the Periodic Table and more particularly molecules and molecular entities containing such atoms Such relativistic theories and computational algorithms are an essential ingredient for the description of heavy element chemistry becoming even more important in the case of superheavy elements They are destined to become an indispensable tool in the quantum chemist's armoury Indeed since relativity influences the structure of every atom in the Periodic Table relativistic molecular structure methods may replace in many applications the non relativistic techniques widely used in contemporary research *Chemistry, Quantum Mechanics and Reductionism* H. Primas, 2013-11-11

The purpose of this book is to provide a deeper insight into the modern theories of molecular matter It incorporates the most important developments which have

taken place during the last decades and reflects the modern trend to abstraction At the present state of the art we have acquired a fairly good knowledge of how to compute small molecules using the methods of quantum chemistry Yet in spite of many statements to the contrary and many superficial discussions the theoretical basis of chemistry and biology is not safely in our hands It is all but impossible to summarize the modern developments of the theory of matter in nontechnical language But I hope that I can give some feeling for the problems the intellectual excitements and the worries of some theoreticians I know very well that such an enterprise is a dangerous adventure and that one says that a clever scientist should take care of his reputation by barricading himself behind the safe wall of his speciality This volume is not meant to be a textbook in many respects it has complementary goals For good and bad reasons most textbooks ignore the historical and philosophical aspects and go ahead on the basis of crude simplifications many even lie like the devil and do not shrink from naive indoctrination Some sections of this book can be read as commentaries on our standard texts they are intended to stir the waters with controversy

**Theoretical Chemistry** Henry Eyring, Douglas W. Henderson, 2013-10-22 Theoretical Chemistry Advances and Perspectives Volume 5 covers articles concerning all aspects of theoretical chemistry The book discusses the mean spherical approximation for simple electrolyte solutions the representation of lattice sums as Mellin transformed products of theta functions and the evaluation of two dimensional lattice sums by number theoretic means The text also describes an application of contour integration a lattice model of quantum fluid as well as the computational aspects of chemical equilibrium in complex systems Chemists and physicists will find the book useful

Practical Aspects of Computational Chemistry IV Jerzy Leszczynski, Manoj K. Shukla, 2016-05-17 The editors of this volume have compiled an important book that is a useful vehicle for important computational research in the development of theoretical methodologies and their practical applications Themes include new methodologies state of the art computational algorithms and hardware as well as new applications This volume Practical Aspects of Computational Chemistry IV is part of a continuous effort by the editors to document recent progress made by eminent researchers Most of these chapters have been collected from invited speakers from the annual international meeting Current Trends in Computational Chemistry organized by Jerzy Leszczynski one of the editors of the current volume This conference series has become an exciting platform for eminent Theoretical Computational Chemists to discuss their recent findings and is regularly honored by the presence of Nobel laureates Certainly it is not possible to cover all topics related to the Computational Chemistry in a single volume but we hope that the recent contributions in the latest volume of this collection adequately highlight this important scientific area

*Trends in Applied Theoretical Chemistry* L.A. Montero, Y.G. Smeyers, 2012-12-06 The present volume gathers a series of selected and updated contributions presented at the International Symposium on Applied Theoretical Chemistry held in Havana Cuba July 2-6 1990 This Symposium was intended to illustrate current applications of Theoretical Chemistry in different fields of Physical Chemistry Theoretical Chemistry has become a powerful tool of investigation in all areas of Chemistry Biochemistry and

Physical Chemistry The plenary lectures given in the Symposium were classified into four topics Atom Surface Interactions Chemical Reaction Mechanisms Molecular Structure and Properties and Molecular Spectroscopy We retain the same division in this volume Over 60 scientists from Cuba Finland France Germany Great Britain Hungary Italy Spain Sweden USA USSR and Venezuela participated in the Conference Twenty plenary lectures were given by distinguished members of the international scientific community Furthermore a large number of posters were presented by younger experts in various fields of Theoretical Chemistry This International Symposium was organized by the Faculty of Chemistry of the University of Havana and the Cuban Chemical Society It was an opportunity to bring together in Havana several outstanding scientists from various countries of the world Havana is worldwide renown for its wonderful climate the hospitality of its inhabitants and the proximity of beautiful touring resorts

*An Outline of the theory of solution and its results* John Livingston Rutgers Morgan, 1897      **Annual Catalogue of the Officers and Students for the Year ... with Announcements for the Year ...** Montana School of Mines, 1917      **A Subject Index of the Modern Works Added to the Library of the British Museum in the Years 1880-[95]: 1891-1895** British Museum. Dept. of Printed Books, 1897      A Course on the Stresses in Bridge and Roof Trusses, Arched Ribs and Suspension Bridges William Hubert Burr, 1902      New Theoretical Concepts for Understanding Organic Reactions Juan Bertrán, Imre G. Csizmadia, 2012-12-06

People who attended the NATO Advanced Study Institute ASI entitled NEW THEORETICAL CONCEPTS FOR UNDERSTANDING ORGANIC REACTIONS held at Sant Feliu de Guixols on the Costa Brava of Spain had a unique experience They have seen the evolution of the field from qualitative arguments through the generation of Potential Energy Surfaces PES to the use of PES in molecular dynamics The excellent lectures that were dedicated to the various aspects of Potential Energy Surfaces clearly revealed a colossal amount of material that represents our current understanding of the overall problem It is our hope that the present volume will recreate the excitement in the readers that we all experienced during the meeting in Spain One can say without too much exaggeration that chemistry has become and exercise on potential energy surfaces PES Structural position of the energy minima spectroscopic vicinity around the minima and reactivity reaction path along the surface properties may be determined from the analysis of PES New theoretical tools together with recent developments in computer technology and programming have allowed to obtain a better knowledge of these surfaces and to extract further chemical information from them so new horizons have been added to Theoretical Organic Chemistry

**The American Catalog**, 1896      The Pharmaceutical Era, 1894      Practical Aspects of Computational Chemistry I Jerzy Leszczynski, Manoj Shukla, 2012-01-13

Practical Aspects of Computational Chemistry I An Overview of the Last Two Decades and Current Trends gathers the advances made within the last 20 years by well known experts in the area of theoretical and computational chemistry and physics The title itself reflects the celebration of the twentieth anniversary of the Conference on Current Trends in Computational Chemistry CCTCC to which all authors have participated and contributed to its success This volume poses and

answers important questions of interest to the computational chemistry community and beyond What is the historical background of the Structural Chemistry Is there any way to avoid the problem of intruder state in the multi reference formulation What is the recent progress on multi reference coupled cluster theory Starting with a historical account of structural chemistry the book focuses on the recent advances made in promising theories such as many body Brillouin Wigner theory multireference state specific coupled cluster theory relativistic effect in chemistry linear and nonlinear optical properties of molecules solution to Kohn Sham problem electronic structure of solid state materials development of model core potential quantum Monte Carlo method nano and molecular electronics dynamics of photodimerization and excited states intermolecular interactions hydrogen bonding and non hydrogen bonding interactions conformational flexibility metal cations in zeolite catalyst and interaction of nucleic acid bases with minerals Practical Aspects of Computational Chemistry I An Overview of the Last Two Decades and Current Trends is aimed at theoretical and computational chemists physical chemists materials scientists and particularly those who are eager to apply computational chemistry methods to problem of chemical and physical importance This book will provide valuable information to undergraduate graduate and PhD students as well as to established researchers

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