

## Chemistry – Unit 5 Worksheet 2

1. An old (pre-1987) penny is nearly pure copper. If such a penny has a mass of 3.3 g, how many moles of copper atoms would be in one penny?

$$3.3 \text{ g} \times \frac{1 \text{ mole}}{63.5 \text{ g}} = 5.2 \times 10^{-2} \text{ mol or } 0.052 \text{ mol}$$

2. Four nails have a total mass of 4.42 grams. How many moles of iron atoms do they contain?

$$4.42 \text{ g} \times \frac{1 \text{ mole}}{55.8 \text{ g}} = 7.92 \times 10^{-2} \text{ mol or } 0.0792 \text{ mol}$$

3. A raindrop has a mass of 0.050 g. How many moles of water does a raindrop contain?

$$0.050 \text{ g} \times \frac{1 \text{ mole}}{18.0 \text{ g}} = 2.78 \times 10^{-3} \text{ mol} \rightarrow 2.8 \times 10^{-3} \text{ mol}$$

4. What mass of water would you need to have 15.0 moles of H<sub>2</sub>O?

$$15.0 \text{ moles} \times \frac{18.0 \text{ g}}{1 \text{ mole}} = 2.70 \times 10^2 \text{ g}$$

5. One box of Morton's Salt contains 737 grams. How many moles of sodium chloride is this?

$$737 \text{ g} \times \frac{1 \text{ mole}}{58.5 \text{ g}} = 12.6 \text{ mol}$$

Na	23.0
Cl	35.5
	<hr/> 58.5 g

6. A chocolate chip cookie recipe calls for 0.050 moles of baking soda (sodium bicarbonate). How many grams should the chef mass out?

$$0.050 \text{ moles} \times \frac{84.0 \text{ g}}{1 \text{ mole}} = 4.2 \text{ g}$$

Na	23.0
H	1.0
C	12.0
O	48.0
	<hr/> 84.0

7. Rust is iron(III) oxide. The owner of a 1959 Cadillac convertible wants to restore it by removing the rust with oxalic acid, but he needs to know how many moles of rust will be involved in the reaction. How many moles of iron(III) oxide are contained in 2.50 kg of rust?

$$2.50 \text{ kg} \times \frac{1000 \text{ g}}{1 \text{ kg}} \times \frac{1 \text{ mole}}{159.6 \text{ g}} = 15.7 \text{ mol Fe}_2\text{O}_3$$

Fe	111.6
O	48.0
	<hr/> 159.6

# Modeling Chemistry Unit 1ws1

**Peter Comba**



## **Modeling Chemistry Unit 1ws1:**

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**Practical Chemistry Unit 1**, 1987

**Chemical Modeling**

Alan Hinchliffe, 1999-10-26 Chemical Modeling From Atoms to Liquids examines materials in terms of the basic properties of atoms molecules and polymer chains In particular the interactions between these fundamental building blocks and the intermolecular and intramolecular potentials are examined Fundamental theories of the constituent particles are covered introducing and developing classical mechanics and quantum mechanics from basics These theories are then applied to modeling developing models from both classical mechanics and quantum mechanics The book aims to make this subject both appealing and relevant whilst avoiding excessive mathematical rigour Carefully structured the text starts by introducing classical quantum and statistical mechanics before moving on to cover the modeling of solids gases and liquids To bring the subject alive many real life examples and applications have been included This book brings together the often scattered and diffuse background information that is essential for a full understanding of chemical modeling FEATURES Assumes no prior knowledge of modeling Brings together all the background information that a reader needs to know to fully understand modeling Develops classical and quantum mechanical theories from basics Avoids unnecessary mathematical rigour Includes a detailed mathematical Toolbox as a ready reference Includes brief descriptions and web addresses of key software packages CONTENTS Introduction Acknowledgements Software Packages Describing Macroscopic Systems Thermodynamics R sum of Classical Mechanics Modeling Simple Solids I Introduction to Quantum Mechanics Electric Multipoles Polarizabilities and Intermolecular Forces Some Statistical Ideas Applications of the Boltzmann Distribution Modeling Simple Solids II Molecular Mechanics Molecular Dynamics and Monte Carlo Techniques The Ideal Monatomic Gas Quantum Gases Introduction to Statistical Thermodynamics Modeling Atoms Diatomics Quantum Modeling of Larger Systems Describing Electron Correlation The Band Theory of Solids Modeling Polymeric Materials Modeling Liquids Appendices Suggestions for Further Reading Index

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Applying Molecular and Materials Modeling Phillip Westmoreland, Peter A. Kollman, Anne M. Chaka, Peter T. Cummings, Keiji Morokuma, Matthew Neurock, Ellen B. Stechel, Priya Vashishta, 2002-10-31 Computational molecular and materials modeling has emerged to deliver solid technological impacts in the chemical pharmaceutical and materials industries It is not the all predictive science fiction that discouraged early adopters in the 1980s Rather it is proving a valuable aid to designing and developing new products and

processes People create not computers and these tools give them qualitative relations and quantitative properties that they need to make creative decisions With detailed analysis and examples from around the world Applying Molecular and Materials Modeling describes the science applications and infrastructures that have proven successful Computational quantum chemistry molecular simulations informatics desktop graphics and high performance computing all play important roles At the same time the best technology requires the right practitioners the right organizational structures and most of all a clearly understood blend of imagination and realism that propels technological advances This book is itself a powerful tool to help scientists engineers and managers understand and take advantage of these advances **Molecular Modeling**

**Basics** Jan H. Jensen, 2010-04-26 Molecular modeling is becoming an increasingly important part of chemical research and education as computers become faster and programs become easier to use The results however have not become easier to understand Addressing the need for a workshop oriented book Molecular Modeling Basics provides the fundamental theory needed to understand Modeling of Molecular Properties Peter Comba, 2011-10-05 Molecular modeling encompasses applied theoretical approaches and computational techniques to model structures and properties of molecular compounds and materials in order to predict and or interpret their properties The modeling covered in this book ranges from methods for small chemical to large biological molecules and materials With its comprehensive coverage of important research fields in molecular and materials science this is a must have for all organic inorganic and biochemists as well as materials scientists interested in applied theoretical and computational chemistry The 28 chapters written by an international group of experienced theoretically oriented chemists are grouped into four parts Theory and Concepts Applications in Homogeneous Catalysis Applications in Pharmaceutical and Biological Chemistry and Applications in Main Group Organic and Organometallic Chemistry The various chapters include concept papers tutorials and research reports **Introducing Molecular Modeling Into the Undergraduate Chemistry Curriculum** Warren J. Hehre, Janet E. Nelson, 1997

*Chemical Applications of Molecular Modelling* Jonathan M. Goodman, 1998 This book explores the molecular modeling enabling the nonspecialist to appreciate the power as well as the limitations of the computational tools available and giving a background to the methods used and how they were developed It also provides examples of how molecular modeling has been used to address chemical questions commonly asked by the experimental chemist and includes practical examples and case studies 143 illus *Chemistry, 4e and Molecular Modeling Kit to Accompany Organic Chemistry, 7e Print Set* Allan Blackman, 2019-11-12 This print pack contains Chemistry 4th Edition Molecular Modeling Kit to accompany Organic Chemistry 7th Edition Print Set **Introductory Chemistry** Darrell D. Ebbing, Albert E. Richardson, 1995 *Introductory Chemistry* Charles H. Corwin, 2005 For one semester courses in Basic Chemistry Introduction to Chemistry and Preparatory Chemistry and the first term of Allied Health Chemistry This text is carefully crafted to help students learn chemical skills and concepts more effectively Corwin covers math and problem solving early in the text he builds student confidence and

skills through innovative problem solving pedagogy and technology formulated to meet student needs      **Using Modeling to Gain a Better Understanding of Chemistry Concepts** Elisabeth Knierim,2018      Molecular Modeling of Inorganic Compounds, Includes CD-ROM with Tutorial Peter Comba,Trevor W. Hambley,2001-03-12 In many branches of chemistry Molecular Modeling is a well established and powerful tool for the investigation of complex structures The second completely revised and enlarged edition of this highly recognized book shows how this method can be successfully applied to inorganic and coordination compounds The first part of the book gives a general introduction to Molecular Modeling which will be of use for chemists in all areas The second part discusses numerous carefully selected examples chosen to illustrate the wide range of applicability of molecular modeling to metal complexes and the approaches being taken to dealing with some of the difficulties involved While the general outline is similar to that of the first edition many of the examples chosen for discussion reflect the changes of the past five years In the third part the reader learns how to apply Molecular Modeling to a new system and how to interpret the results The accompanying software features 20 tutorial lessons based on examples from the literature and the book itself The authors take special care to highlight possible pitfalls and offer advice on how to avoid them Therefore this book will be invaluable to everyone working in or entering the field      **Molecular Modeling** Hans-Dieter Höltje,Wolfgang Sippl,Didier Rognan,Gerd Folkers,2008-02-26 Ideal for beginners this book explains the basics of modeling in a competent yet easily understandable way Following complete sections on the modeling of small molecules protein modeling and chemogenomics completely worked out examples show the way to the reader s first modeling experiment This new third edition features a new chapter on chemogenomics reflecting the trend towards chemical biology as well as the protein modeling example being completely rewritten for a better feel of modeling complex biomolecules The authors are experienced university teachers who regularly hold courses on molecular modeling making this a tried and tested text for teachers It is equally valuable for experts since it is the only book to evaluate the strengths and limitations of the molecular modeling techniques and software currently available      *Chemistry* Nicholas Derry,Nick Derry,Lanna Derry,2000-01

**Molecular Modeling Workbook** Hehre,2003-08      *Molecular Modelling: Principles And Applications, 2/E* Leach,2009-09      **Handbook of Materials Modeling** Wanda Andreoni,2018      Molecular Modeling Hans-Dieter Höltje,Gerd Folkers,2008-07-11 Written by experienced experts in molecular modeling this books describes the basics to the extent that is necessary if one wants to be able to reliably judge the results from molecular modeling calculations Its main objective is the description of the various pitfalls to be avoided Without unnecessary overhead it leads the reader from simple calculations on small molecules to the modeling of proteins and other relevant biomolecules A textbook for beginners as well as an invaluable reference for all those dealing with molecular modeling in their daily work

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