

### Chapter 1: Stoichiometry

Q4.

Sol:  $\text{CaCO}_3 \rightarrow \text{CaO} + \text{CO}_2$

Since 1 mole of  $\text{CaCO}_3$  produces 1 mole of  $\text{CaO}$ , So

1 mole of  $\text{CaO}$  will produce 1 mole of  $\text{CaCO}_3$ .

$\therefore$  1 mole of  $\text{CaO}$   $\rightarrow$  1 mole of  $\text{CaCO}_3$ .

Sol:  $\text{BaCl}_2 \rightarrow \text{BaSO}_4$

Given:

5 moles of  $\text{BaCl}_2$  contains 1 mole of  $\text{Ba}$  & 10 moles of  $\text{Cl}$  & each form 1 mole of  $\text{BaSO}_4$ ,  $\therefore$  since 1 mole of  $\text{BaSO}_4$  contains 1 mole of  $\text{Ba}$

Sol:  $2 \text{Na} \rightarrow \text{Na}_2\text{O}$

5 moles  $\text{O}_2$  given

$\therefore$  2 moles produces 1 mole of  $\text{Na}_2\text{O}$

$\therefore$  5  $\rightarrow$   $\frac{5}{2}$

$\therefore$  5  $\rightarrow$   $\frac{5}{2} \times 2 = 5$  moles of  $\text{Na}_2\text{O}$ .

Q1.

Ans:  $\text{Ca} + \frac{1}{2} \text{O}_2 \rightarrow \text{CaO}$  (balanced chemical equation)

Wt. of  $\text{Ca} = 40 \text{ g/mole}$

So, moles of  $\text{Ca} = \frac{80}{40} = 2 \text{ moles}$

From above balanced chemical equation, 1 moles of  $\text{Ca}$  reacts with  $\frac{1}{2}$  moles of  $\text{O}_2$ .

Wt. of  $\text{O}_2$  with which 80g of  $\text{Ca}$  react  $= \frac{1}{2} \times 32 = 16 \text{ g}$

Ans.

Q2.

Sol:  $\text{NaCl} \rightarrow \text{NaCl}$

50 gm

If we have not balanced the chemical equation, then we have to apply P.M.C. rule or g-equivalent rule.

By P.M.C. rule Cl atom

Mass of Cl atom in the reactant = Mass of Cl atom in the product

So, mass of moles of  $\text{NaCl} = \text{Wt.} = 2 \times \text{mass of moles of } \text{Cl}_2 = 71 \text{ g}$

$\frac{71}{50} = 1.4$  moles of  $\text{Cl}_2$

moles of  $\text{Cl}_2 = \frac{71}{71}$

# Modern Approach To Chemical Calculations Solutions

**William Jay Hale**



## Modern Approach To Chemical Calculations Solutions:

Physical Chemistry of Electrolyte Solutions Josef Barthel, H. Krienke, Werner Kunz, W. Kunz, 1998-04 The aim and purpose of this book is a survey of our actual basic knowledge of electrolyte solutions It is meant for chemical engineers looking for an introduction to this field of increasing interest for various technologies and for scientists wishing to have access to the broad field of modern electrolyte chemistry

*Thermodynamics of Solutions* Eli Ruckenstein, Ivan L. Shulgin, 2009-06-17 This book consists of a number of papers regarding the thermodynamics and structure of multicomponent systems that we have published during the last decade Even though they involve different topics and different systems they have something in common which can be considered as the signature of the present book First these papers are concerned with difficult or very nonideal systems i e systems with very strong interactions e g hyd gen bonding between components or systems with large differences in the partial molar v umes of the components e g the aqueous solutions of proteins or systems that are far from normal conditions e g critical or near critical mixtures Second the conventional th modynamic methods are not sufficient for the accurate treatment of these mixtures Last but not least these systems are of interest for the pharmaceutical biomedical and related ind tries In order to meet the thermodynamic challenges involved in these complex mixtures we employed a variety of traditional methods but also new methods such as the fluctuation t ory of Kirkwood and Buff and ab initio quantum mechanical techniques The Kirkwood Buff KB theory is a rigorous formalism which is free of any of the proximations usually used in the thermodynamic treatment of multicomponent systems This theory appears to be very fruitful when applied to the above mentioned difficult systems

A Problem-Solving Approach to Aquatic Chemistry James N. Jensen, 2023-01-05 A Problem Solving Approach to Aquatic Chemistry Enables civil and environmental engineers to understand the theory and application of aquatic equilibrium chemistry The second edition of A Problem Solving Approach to Aquatic Chemistry provides a detailed introduction to aquatic equilibrium chemistry calculation methods for systems at equilibrium applications of aquatic chemistry and chemical kinetics The text directly addresses two required ABET program outcomes in environmental engineering chemistry including stoichiometry equilibrium and kinetics and material and energy balances fate and transport of substances in and between air water and soil phases The book is very student centered with each chapter beginning with an introduction and ending with a summary that reviews the chapter s main points To aid in reader comprehension important terms are defined in context and key ideas are summarized Many thought provoking discussion questions worked examples and end of chapter problems are also included Each part of the text begins with a case study a portion of which is addressed in each subsequent chapter illustrating the principles of that chapter In addition each chapter has an Historical Note exploring connections with the people and cultures connected to topics in the text A Problem Solving Approach to Aquatic Chemistry includes Fundamental concepts such as concentration units thermodynamic basis of equilibrium and manipulating equilibria Solutions of chemical equilibrium problems including setting up the problems and

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**Handbook of Computational Chemistry** Jerzy Leszczynski, 2012-01-14 This handbook is a guide to current methods of computational chemistry explaining their limitations and advantages and providing examples of their applications The first part outlines methods the balance of volumes present numerous important applications

**Exploring Chemical Concepts Through Theory and Computation** Shubin Liu, 2024-12-23 Deep theoretical resource on the essence of chemistry explaining a variety of important concepts including redox states and bond types Exploring Chemical Concepts Through Theory and Computation provides a comprehensive account of how the three widely used theoretical frameworks of valence bond theory molecular orbital theory and density functional theory along with a variety of important chemical concepts can between them describe and efficiently and reliably predict key chemical parameters and phenomena By comparing the three main theoretical frameworks readers will become competent in choosing the right modeling approach for their task The authors go beyond a simple comparison of existing algorithms to show how data driven theories can explain why chemical compounds behave the way they do thus promoting a deeper understanding of the essence of chemistry The text is contributed to by top theoretical and computational chemists who have turned computational chemistry into today's data driven and application oriented science Exploring Chemical Concepts Through Theory and Computation discusses topics including Orbital based approaches density based approaches chemical bonding partial charges atoms in molecules oxidation states aromaticity and antiaromaticity and acidity and basicity Electronegativity hardness softness HSAB sigma hole interactions charge transport and energy transfer and homogeneous and heterogeneous catalysis Electrophilicity nucleophilicity cooperativity frustration homochirality and energy decomposition Chemical concepts in solids excited states spectroscopy and machine learning and catalysis and machine learning as well as key connections between related concepts Aimed at both novice and experienced computational theoretical and physical chemists Exploring Chemical Concepts Through Theory and Computation is an essential reference to gain a deeper more advanced holistic understanding of the field of chemistry as a whole

**Computational Approaches for Studying Enzyme Mechanism Part A**, 2016-08-04 Computational Approaches for Studying Enzyme Mechanism Part A is the first of two volumes in the Methods in Enzymology

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**The Calculations of General Chemistry, with Definitions, Explanations, and Problems** William Jay Hale,1920

Physics, Chemistry and Application of Nanostructures Viktor Evgen'evich Borisenko,2013 This book presents invited reviews and original short notes of recent results obtained in studies concerning the fabrication and application of nanostructures which hold great promise for the next generation of electronic optoelectronic and energy conversion devices Covering exciting and relatively new topics such as fast progressing nanoelectronics and optoelectronics molecular electronics and spintronics nanophotonics nanosensorics and nanoenergetics as well as nanotechnology and quantum processing of information this book gives readers a more complete understanding of the practical uses of nanotechnology and nanostructures

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*Mathematical Modeling of Biological Processes* Avner Friedman, Chiu-Yen Kao, 2014-09-19 This book on mathematical modeling of biological processes includes a wide selection of biological topics that demonstrate the power of mathematics and computational codes in setting up biological processes with a rigorous and predictive framework Topics include enzyme dynamics spread of disease harvesting bacteria competition among live species neuronal oscillations transport of neurofilaments in axon cancer and cancer therapy and granulomas Complete with a description of the biological background and biological question that requires the use of mathematics this book is developed for graduate students and advanced undergraduate students with only basic knowledge of ordinary differential equations and partial differential equations background in biology is not required Students will gain knowledge on how to program with MATLAB without previous programming experience and how to use codes in order to test biological hypothesis

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**Thermodynamics and Kinetics of Water-Rock Interaction** Eric H.

Oelkers, Jacques Schott, 2018-12-17 Volume 70 of Reviews in Mineralogy and Geochemistry represents an extensive review of

the material presented by the invited speakers at a short course on Thermodynamics and Kinetics of Water Rock Interaction held prior to the 19th annual V M Goldschmidt Conference in Davos Switzerland June 19 21 2009 Contents Thermodynamic Databases for Water Rock Interaction Thermodynamics of Solid Solution Aqueous Solution Systems Mineral Replacement Reactions Thermodynamic Concepts in Modeling Sorption at the Mineral Water Interface Surface Complexation Modeling Mineral Fluid Equilibria at the Molecular Scale The Link Between Mineral Dissolution Precipitation Kinetics and Solution Chemistry Organics in Water Rock Interactions Mineral Precipitation Kinetics Towards an Integrated Model of Weathering Climate and Biospheric Processes Approaches to Modeling Weathered Regolith Fluid Rock Interaction A Reactive Transport Approach Geochemical Modeling of Reaction Paths and Geochemical Reaction Networks



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