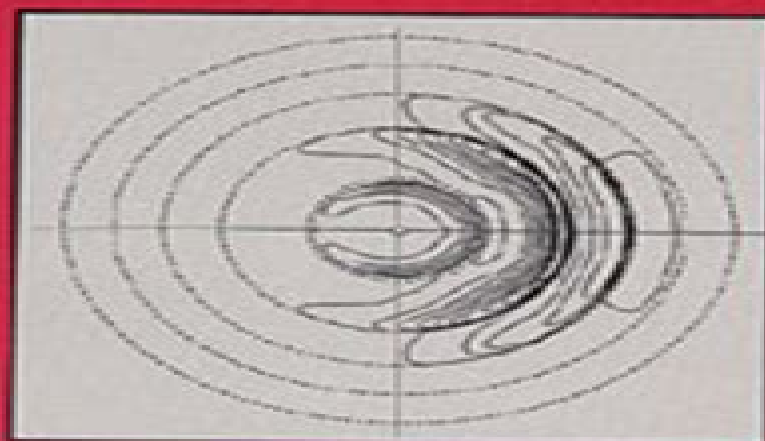


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**An Introductory Guide to Computational Methods for the Solution of Physics Problems** George Rawitscher,Victo dos Santos Filho,Thiago Carvalho Peixoto,2018-10-24 This monograph presents fundamental aspects of modern spectral and other computational methods which are not generally taught in traditional courses It emphasizes concepts as errors convergence stability order and efficiency applied to the solution of physical problems The spectral methods consist in expanding the function to be calculated into a set of appropriate basis functions generally orthogonal polynomials and the respective expansion coefficients are obtained via collocation equations The main advantage of these methods is that they simultaneously take into account all available information rather than only the information available at a limited number of mesh points They require more complicated matrix equations than those obtained in finite difference methods However the elegance speed and accuracy of the spectral methods more than compensates for any such drawbacks During the course of the monograph the authors examine the usually rapid convergence of the spectral expansions and the improved accuracy that results when nonequispaced support points are used in contrast to the equispaced points used in finite difference methods In particular they demonstrate the enhanced accuracy obtained in the solution of integral equations The monograph includes an informative introduction to old and new computational methods with numerous practical examples while at the same time pointing out the errors that each of the available algorithms introduces into the specific solution It is a valuable resource for undergraduate students as an introduction to the field and for graduate students wishing to compare the available computational methods In addition the work develops the criteria required for students to select the most suitable method to solve the particular scientific problem that they are confronting

*Books in Series, 1876-1949* R.R. Bowker Company,1982

**Intermolecular and Surface Forces** Jacob N. Israelachvili,2011-07-22 Intermolecular and Surface Forces describes the role of various intermolecular and interparticle forces in determining the properties of simple systems such as gases liquids and solids with a special focus on more complex colloidal polymeric and biological systems The book provides a thorough foundation in theories and concepts of intermolecular forces allowing researchers and students to recognize which forces are important in any particular system as well as how to control these forces This third edition is expanded into three sections and contains five new chapters over the previous edition Starts from the basics and builds up to more complex systems Covers all aspects of intermolecular and interparticle forces both at the fundamental and applied levels Multidisciplinary approach bringing together and unifying phenomena from different fields This new edition has an expanded Part III and new chapters on non equilibrium dynamic

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*Molecular Physical Chemistry* José J. C. Teixeira-Dias,2017-01-16 This is the physical chemistry textbook for students with an affinity for computers It offers basic and advanced knowledge for students in the second year of chemistry masters studies and beyond In seven chapters the book presents thermodynamics chemical kinetics quantum mechanics and molecular structure including an introduction to quantum chemical calculations molecular symmetry and crystals The application of physical chemical knowledge and problem solving is demonstrated in a chapter on water treating both the water molecule as well as water in condensed phases Instead of a traditional textbook top down approach this book presents the subjects on the basis of examples exploring and running computer programs Mathematica discussing the results of molecular orbital calculations performed using Gaussian on small molecules and turning to suitable reference works to obtain thermodynamic data Selected Mathematica codes are explained at the end of each chapter and cross referenced with the text enabling students to plot functions solve equations fit data normalize probability functions manipulate matrices and test physical models In addition the book presents clear and step by step explanations and provides detailed and complete answers to all exercises In this way it creates an active learning environment that can prepare students for pursuing their own research projects further down the road Students who are not yet familiar with Mathematica or Gaussian will find a valuable introduction to computer based problem solving in the molecular sciences Other computer applications can alternatively be used For every chapter learning goals are clearly listed in the beginning so that readers can easily spot the highlights and a glossary in the end of the chapter offers a quick look up of important terms      Modern Physical Chemistry G.H. Duffey,2013-11-11 In this new textbook on physical chemistry fundamentals are introduced simply yet in more depth than is common Topics are arranged in a progressive pattern with simpler theory early and more complicated theory later General principles are induced from key experimental results Some mathematical background is supplied where it would be helpful Each chapter includes worked out examples and numerous references Extensive problems review and discussion questions are included for each chapter More detail than is common is devoted to the nature of work and heat and how they differ Introductory Caratheodory theory and the standard integrating factor for dGrev are carefully developed The fundamental role played by uncertainty and symmetry in quantum mechanics is emphasized In chemical kinetics various methods for determined rate laws are presented The key mechanisms are detailed Considerable statistical mechanics and reaction rate theory are then surveyed Professor Duffey has given us a most readable easily followed text in physical chemistry      Applying Maths in the Chemical and Biomolecular Sciences Godfrey Beddard,2009-09-03 Godfrey Beddard is

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