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spin dynamics basics of nuclear magnetic resonance second edition is a comprehensive and modern introduction which focuses on those essential principles and concepts needed for a thorough understanding of the subject rather than the practical aspects the quantum theory of nuclear magnets is presented within a strong physical framework supported by figures the book assumes only a basic knowledge of complex numbers and matrices and provides the reader with numerous worked examples and exercises to encourage understanding with the explicit aim of carefully developing the subject from the beginning the text starts with coverage of quarks and nucleons and progresses through to a detailed explanation of several important nmr experiments including nmr imaging cosy noesy and trosy completely revised and updated the second edition features new material on the properties and distributions of isotopes chemical shift anisotropy and quadrupolar interactions pake patterns spin echoes slice selection in nmr imaging and a complete new chapter on the nmr spectroscopy of quadrupolar nuclei new appendices have been included on euler angles and coherence selection by field gradients as in the first edition all material is heavily supported by graphics much of which is new to this edition written for undergraduates and postgraduate students taking a first course in nmr

spectroscopy and for those needing an up to date account of the subject this multi disciplinary book will appeal to chemical physical material life medical earth and environmental scientists the detailed physical insights will also make the book of interest for experienced spectroscopists and nmr researchers an accessible and carefully written introduction designed to help students to fully understand this complex and dynamic subject takes a multi disciplinary approach focusing on basic principles and concepts rather than the more practical aspects presents a strong pedagogical approach throughout with emphasis placed on individual spins to aid understanding includes numerous worked examples problems further reading and additional notes praise from the reviews of the first edition this is an excellent book that many teachers of nmr spectroscopy will cherish it deserves to be a classic among nmr spectroscopy texts nmr in biomedicine i strongly recommend this book to everyone it is probably the best modern comprehensive description of the subject angewandte chemie international edition

this volume explores the application of high performance computing hpc technologies to computational drug discovery cdd and biomedicine the first section collects cdd approaches that together with hpc can revolutionize and automate drug discovery process such as knowledge graphs natural language processing nlp bayesian optimization automated virtual screening platforms alchemical free energy workflows fragment molecular orbitals fmo hpc adapted molecular dynamic simulation md hpc and the potential of cloud computing for drug discovery the second section delves into computational algorithms and workflows for biomedicine featuring an hpc framework to assess drug induced arrhythmic risk digital patient applications relevant to the clinic virtual human simulations cellular and whole body blood flow modeling for stroke treatments prediction of the femoral bone strength from ct data and many more subjects written for the highly successful methods in molecular biology series chapters include introductions to their respective topics lists of the necessary software and tools step by step and readily reproducible modeling protocols and tips on troubleshooting and avoiding known pitfalls authoritative and practical high performance computing for drug discovery and biomedicine allows a diverse audience including computer scientists computational and medicinal chemists biologists clinicians pharmacologists and drug designers to navigate the complex landscape of what is currently possible and to understand the challenges and future directions of hpc based technologies

selected articles on quantum chemistry classical and quantum electrodynamics path integrals and operator calculus liquid helium quantum gravity and computer theory

governments face increasingly serious seemingly intractable management challenges this book brings together scholars thought leaders and government executives to address the future of government operations and provide government leaders with practical actionable insights on how best to manage and lead through uncertain and disruptive times

for courses in metallurgy and materials science co authored by kenneth g budinski and michael k budinski his son with over 50 years of combined industry experience in the field this practical understandable introduction to engineering materials theory and industry standard selection practices provides students with the working knowledge to 1 make an informed selection of materials

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