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Relaxation and Dynamic Processes; 5.1 Introduction and Survey of Theoretical Approaches; 5.2 The Master Equation; 5.3 Spectral Density Functions; 5.4 Relaxation Mechanisms; 5.5 Nuclear Overhauser Effect; 5.6 Chemical Exchange Effects in NMR Spectroscopy; References; 6 Experimental 1H NMR Methods; 6.1 Assessment of the 1D 1H Spectrum; 6.2 COSY-Type Experiments; 6.3 Multiple-Quantum Filtered COSY; 6.4 Multiple-Quantum Spectroscopy; 6.5 TOCSY; 6.6 Cross-Relaxation NMR Experiments; 6.7 1H 3D Experiments; References 7 Heteronuclear NMR Experiments7.1 Heteronuclear Correlation NMR Spectroscopy; 7.2 Heteronuclear-Edited NMR Spectroscopy; 7.3 13C-13C Correlations: The HCCH-COSY and HCCH-TOCSY Experiments; 7.4 3D Triple-Resonance Experiments; 7.5 Measurement of Scalar Coupling Constants; 7.6 Measurement of Residual Dipolar Coupling Constants; References; 8 Experimental NMR Relaxation Methods; 8.1 Pulse Sequences and Experimental Methods; 8.2 Picosecond-Nanosecond Dynamics; 8.3 Microsecond-Second Dynamics; References; 9 Larger Proteins and Molecular Interactions; 9.1 Larger Proteins 9.2 Intermolecular Interactions9.3 Methods for Rapid Data Acquisition; References; 10 Sequential Assignment, Structure Determination, and Other Applications; 10.1 Resonance Assignment Strategies; 10.2 Three-Dimensional Solution Structures; 10.3 Conclusion; References; Table of Symbols; List of Figures; List of Tables; Suggested Reading; Biomolecular NMR Spectroscopy; NMR Spectroscopy; Quantum Mechanics; Index; Spin-1/2 Product Operator Equations; Table of Constants

Sommario/riassunto

Protein NMR Spectroscopy combines a comprehensive theoretical treatment of NMR spectroscopy with an extensive exposition of the experimental techniques applicable to proteins and other biological macromolecules in solution. Beginning with simple theoretical models and experimental techniques, Protein NMR Spectroscopy develops the complete repertoire of theoretical principles and experimental techniques necessary for understanding and implementing the most sophisticated NMR experiments.Important new techniques and applications of NMR spectroscopy have emerged since the f

2. Record Nr. UNINA9911004739403321

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1. Coupled T-H-M-C Processes in Radioactive Waste Disposal Systems; Theme 1-1 DECOVALEX III/BENCHPAR Projects- Task 1
Chapter 9. The FEBEX benchmark test. Case definition and comparison of different modelling approachesChapter 10. Modelling the response of the bentonite in the FEBEX heater experiment; Chapter 11. THM simulation of the full-scale in-situ engineered barrier system experiment in Grimsel Test Site in Switzeriand; Chapter 12. Hydromechanical response of jointed host granitic rock during excavation of the FEBEX tunnel; Chapter 13. Analyses of coupled hydrological-mechanical effects during drilling of the FEBEX tunnel at Grimsel; Chapter 14. Thermomechanical model for compacted bentonite
Chapter 15. A fully coupled three-dimensional THM analysis of the FEBEX in situ test with the ROCMAS code: Prediction of THM behavior in a bentonite barrierChapter 16. A discrete approach to modelling hydromechanical rock response of FEBEX tunnel excavation (Grimsel Underground Research Laboratory, Switzerland); Theme 1-2 DECOVALEX III/BENCHPAR Projects- Task 2; Chapter 17. Measuring thermal, hydrological, mechanical, and chemical responses in the Yucca Mountain Drift Scale Test
Chapter 18. Analysis of stress and moisture induced changes in fractured rock permeability at the Yucca Mountain Drift Scale TestChapter 19. Thermal-mechanical modeling of a large-scale heater test; Chapter 20. Numerical simulation of thermal-hydrological processes observed at the Drift-Scale Heater Test at Yucca Mountain, Nevada; Chapter 21. THM analysis of a heating test in a fractured tuff; Chapter 22. Comparative analyses of predicted and measured displacements during the heating phase of the Yucca Mountain Drift Scale Test; Theme 1-3 DECOVALEX III/BENCHPAR Projects- Task 3: BMT1/WP2
Chapter 23. Building confidence in the mathematical models by calibration with a T-H-M field experiment

Sommario/riassunto

Among the most important and exciting current steps forward in geo-engineering is the development of coupled numerical models. They represent the basic physics of geo-engineering processes which can include the effects of heat, water, mechanics and chemistry. Such models provide an integrating focus for the wide range of geo-engineering disciplines. The articles within this volume were originally presented at the inaugural GeoProc conference held in Stockholm and contain a collection of unusually high quality information not available elsewhere in an edited and coherent form. This coll