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Titolo	Spin states in biochemistry and inorganic chemistry : influence on structure and reactivity / / edited by Marcel Swart and Miquel Costas
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Descrizione fisica	1 online resource (684 p.)
Disciplina	612/01524
Soggetti	Nuclear spin Free radicals (Chemistry) Biochemistry Chemistry, Inorganic Spin (Física nuclear) Radicals lliures (Química) Bioquímica Química inorgànica
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Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Title page; Copyright; Dedication; About the Editors; Marcel Swart; Miquel Costas; List of Contributors; Foreword; Acknowledgments; 1 General Introduction to Spin States; 1.1 Introduction; 1.2 Experimental Chemistry: Reactivity, Synthesis and Spectroscopy; 1.3 Computational Chemistry: Quantum Chemistry and Basis Sets; References; 2 Application of Density Functional and Density Functional Based Ligand Field Theory to Spin States; 2.1 Introduction; 2.2 What Is the Problem with Theory?; 2.3 Validation and Application Studies; 2.4 Concluding Remarks; Acknowledgments; References 3 Ab Initio Wavefunction Approaches to Spin States3.1 Introduction and Scope; 3.2 Wavefunction-Based Methods for Spin States; 3.3 Spin Crossover; 3.4 Magnetic Coupling; 3.5 Spin States in Biochemical and

Biomimetic Systems; 3.6 Two-State Reactivity; 3.7 Concluding Remarks; References; 4 Experimental Techniques for Determining Spin States; 4.1 Introduction; 4.2 Magnetic Measurements; 4.3 EPR Spectroscopy; 4.4 Mossbauer Spectroscopy; 4.5 X-ray Spectroscopic Techniques; 4.6 NMR Spectroscopy; 4.7 Other Techniques; 4.A Appendix; References; 5 Molecular Discovery in Spin Crossover; 5.1 Introduction
5.2 Theoretical Background5.3 Thermal SCO Systems: Fe(II); 5.4 SCO in Non-d6 Systems; 5.5 Computational Methods; 5.6 Outlook; References; 6 Multiple Spin-State Scenarios in Organometallic Reactivity; 6.1 Introduction; 6.2 "Spin-Forbidden" Reactions and Two-State Reactivity; 6.3 Spin-State Changes in Transition Metal Complexes; 6.4 Spin-State Changes in Catalysis; 6.5 Concluding Remarks; References; 7 Principles and Prospects of Spin-States Reactivity in Chemistry and Bioinorganic Chemistry; 7.1 Introduction; 7.2 Spin-States Reactivity
7.3 Prospects of Two-State Reactivity and Multi-State Reactivity7.4 Concluding Remarks; Acknowledgement; Note Added in Proof; References; 8 Multiple Spin-State Scenarios in Gas-Phase Reactions; 8.1 Introduction; 8.2 Experimental Methods for the Investigation of Metal-Ion Reactions; 8.3 Multiple State Reactivity: Reactions of Metal Cations with Methane; 8.4 Effect of the Oxidation State: Reactions of Metal Hydride Cations with Methane; 8.5 Two-State Reactivity: Reactions of Metal Oxide Cations; 8.6 Effect of Ligands; 8.7 Effect of Noninnocent Ligands; 8.8 Concluding Remarks; References
9 Catalytic Function and Mechanism of Heme and Nonheme Iron(IV)-Oxo Complexes in Nature9.1 Introduction; 9.2 Cytochrome P450 Enzymes; 9.3 Nonheme Iron Dioxygenases; 9.4 Conclusions; 9.5 Acknowledgments; References; 10 Terminal Metal-Oxo Species with Unusual Spin States; 10.1 Introduction; 10.2 Bonding; 10.3 Case Studies; 10.4 Reactivity; 10.5 Summary; Note Added in Proof; References; 11 Multiple Spin Scenarios in Transition-Metal Complexes Involving Redox Non-Innocent Ligands; 11.1 Introduction; 11.2 Survey of Non-Innocent Ligands; 11.3 Identification of Non-Innocent Ligands
11.4 Selected Examples of Biological and Chemical Systems Involving Non-Innocent Ligands

2. Record Nr.	UNINA9910822072303321
Autore	Young Paul G. <1950->
Titolo	Promoting positive behaviors : an elementary principal's guide to structuring the learning environment / / Paul G. Young ; foreword by Gail Connelly ; cover designer, Michael Dubowé
Pubbl/distr/stampa	Thousand Oaks, California : , : Corwin Press : , : National Association of Elementary School Principals, , 2008 ©2008
ISBN	1-4522-9487-9 1-4522-9799-1
Descrizione fisica	1 online resource (136 p.)
Disciplina	371.5
Soggetti	School discipline - United States School management and organization - United States School principals - United States
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Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	""Cover""; ""Contents""; ""Foreword""; ""Acknowledgments""; ""About the Author""; ""Introduction""; ""Purpose of This Book""; ""Overview of the Contents""; ""Chapter 1 - Beginnings: The Day and the Year""; ""Introduction""; ""1.1 Plan for Effective Morning Playground Supervision""; ""1.2 Allow Recess in the Morning""; ""1.3 Form and Train a Safety Patrol""; ""1.4 Teach Expectations to Students While Lining up after the Bell Sounds""; ""1.5 Build Relationships with Parents""; ""1.6 Teach Children to Move Quietly through the Hallways""; ""1.7 Lock the Doors"" ""1.8 Structure Homeroom Activities""""1.9 Provide Universal Breakfast in the Classroom""; ""1.10 Make Morning Announcements""; ""1.11 Check Book Bags and Homework Planners""; ""1.12 Do the Shirts and the Pants Touch?""; ""1.13 No Talking during Emergency Drills""; ""1.14 Establish a Student Council""; ""1.15 Establish Student Incentives and Recognitions""; ""1.16 Empower Staff to Develop Schedules""; ""1.17 Learn all Students' Names""; ""1.18 Establish an Effective Intervention Assistance Process""; ""1.19 Structure Effective Meetings""

""1.20 Check Mail and Messages at Least Three Times Daily""""1.21 Establish the Schedule and Goals for the Day""; ""Concluding thoughts""; ""Explanation of the Structural Analysis and Assessment Checklists""; ""Checklist 1a€?Beginnings: Structural Analysis and Assessment""; ""Chapter 2 - Early Focus on Learning and Instruction""; ""Introduction""; ""2.1 Escort Students to and from Special Classes""; ""2.2 Establish Procedures for Restroom Breaks""; ""2.3 Practice Entering and Leaving Assemblies""; ""2.4 Develop a Substitute Handbook""; ""2.5 Time on Task""
""2.6 Establish Inclusion Practices""""2.7 Establish Procedures for Referring Students to the Office""; ""2.8 Fully Utilize Volunteer Services""; ""2.9 Teach a Code of Conduct""; ""2.10 Common, Grade-Level Planning Increases Student Achievement""; ""Concluding thoughts""; ""Checklist 2a€?Learning and Instruction: Structural Analysis and Assessment""; ""Chapter 3 - Midpoints of the Day and the Year""; ""Introduction""; ""3.1 Equip Yourself for Playground Supervision""; ""3.2 Teach Manners and Hygiene""; ""3.3 Facilitate Efficient Food Serving Lines""
""3.4 Schedule Recess First, Eat Afterward""""3.5 Speak with Inside Voices""; ""3.6 Practice Forming Lines""; ""3.7 Structure Playground Games""; ""3.8 Monitor Studentsa€? Behavior and Eating Habits""; ""3.9 Establish Procedures for Indoor Recess Supervision""; ""3.10 Take Pictures and Use Recorders""; ""3.11 Establish Contingency Plans for Crisis Supervision""; ""3.12 Teach Children to Speak in Complete Sentences""; ""3.13 Develop a Conflict Mediation Program"";
""Concluding thoughts""; ""Checklist 3a€?Midpoints: Structural Analysis and Assessment""
""Chapter 4 - The Second Half of the Day and the Year""

Sommario/riassunto

This practical handbook helps educators create processes that communicate expectations, promote positive student behaviors, reduce schoolwide management problems, build relationships with parents, and increase student achievement.

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Autore	Panda Dhabaleswar K
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Disciplina	004.6 004.11
Soggetti	Computer engineering Computer networks Computer vision Microprogramming Computer input-output equipment Operating systems (Computers) Database management Computer Engineering and Networks Computer Vision Control Structures and Microprogramming Input/Output and Data Communications Operating Systems Database Management System
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Session I – File Systems, Storage and Communication -- A BeeGFS-based Caching File System for Data-intensive Parallel Computing -- Multiple HPC Environments-Aware Container Image Configuration Workflow for Large-Scale All-to-All Protein-Protein Docking Calculations -- DAOS: A Scale-out High Performance Storage Stack for

Storage Class Memory -- Cloud Platform Optimization for HPC --
Session II – Applications and Scheduling -- swGBDT: Efficient Gradient
Boosted Decision Tree on Sunway Many-core Processor -- Numerical
Simulations of Serrated Propellers to Reduce Noise -- High-
performance Computing in Maritime and Offshore Applications --
Correcting Job Walltime in a Resource-Constrained Environment.

Sommario/riassunto

This open access book constitutes the refereed proceedings of the 6th Asian Supercomputing Conference, SCFA 2020, which was planned to be held in February 2020, but unfortunately, the physical conference was cancelled due to the COVID-19 pandemic. The 8 full papers presented in this book were carefully reviewed and selected from 22 submissions. They cover a range of topics including file systems, memory hierarchy, HPC cloud platform, container image configuration workflow, large-scale applications, and scheduling.