

Coordination Chemistry Reviews 238-239 (2003) 415-417



www.elsevier.com/locate/ccr

Subject Index of Volumes 238–239

π Acceptor bridges

Effects of the bridging ligands on the molecular and electronic structure of Fe₂(CO)₉ derivatives 333

Accurate X-ray diffraction

Chemical bonding in transition metal carbonyl clusters: complementary analysis of theoretical and experimental electron densities. 383

Activation energy

Fundamental properties of small molecule models of Fe-only hydrogenase: computations relative to the definition of an entatic state in the active site 255

Activation parameters

Thermal and optical electron transfer involving transition metal complexes: insights from theory and computation 167

Binuclear iron carbonyls

Effects of the bridging ligands on the molecular and electronic structure of Fe₂(CO)₉ derivatives 333

Bonding analysis

Towards a rigorously defined quantum chemical analysis of the chemical bond in donor-acceptor complexes 55

Bond theory

The importance of interligand interactions to structure and reactivity of coordinatively unsaturated ruthenium and iron half-sandwich complexes—application of the TSC concept II 363

Bridging carbonyl ligands

Chemical bonding in transition metal carbonyl clusters: complementary analysis of theoretical and experimental electron densities. 383

Broken symmetry

Density functional methods applied to metalloenzymes 211

Carbon-hydrogen bond activation

De Novo design in organometallic chemistry: stabilizing iridium(V) 315

Catalytic cycle

Density functional methods applied to metalloenzymes 211

π -Cation interaction

Density functional methods applied to metalloenzymes 211

Christian Klixbull Jørgensen

Christian Klixbull Jørgensen (1931–2001): inorganic spectroscopist extraordinaire 3

Complementary

Fit and misfit between ligands and metal ions 21

Computational bioinorganic chemistry

Modeling the spin-dependent properties of open-shell Fe(III)-containing systems: towards a computational description of nitrile hydratase 291

Computational coordination chemistry

Double perturbation theory: a powerful tool in computational coordination chemistry 83

Coordination chemistry

The importance of interligand interactions to structure and reactivity of coordinatively unsaturated ruthenium and iron half-sandwich complexes—application of the TSC concept II 363

Understanding the reactivity of transition metal complexes involving multiple spin states 347

Coordination compounds

DFT calculations of molecular magnetic properties of coordination compounds 187

Density functional

Density functional methods applied to metalloenzymes 211 Density functional theory

De Novo design in organometallic chemistry: stabilizing iridium(V) 315

Modeling the spin-dependent properties of open-shell Fe(III)-containing systems: towards a computational description of nitrile hydratase 291

DFT

Inorganic and bioinorganic molecular mechanics modeling—the problem of the force field parameterization 9

DFT calculations

DFT calculations of molecular magnetic properties of coordination compounds 187

DFT studies

Molecular orbital and DFT studies on water exchange mechanisms of metal ions 233

Dioxygen chemistry

How iron-containing proteins control dioxygen chemistry: a detailed atomic level description via accurate quantum chemical and mixed quantum mechanics/molecular mechanics calculations 267

Donor-acceptor bonds

Towards a rigorously defined quantum chemical analysis of the chemical bond in donor-acceptor complexes 55

Double perturbation theory

Double perturbation theory: a powerful tool in computational coordination chemistry 83

Elasticity

Fit and misfit between ligands and metal ions 21

Electroabsorption spectroscopy

Theory of electroabsorption spectroscopy in poly-nuclear Ru complexes 127

Electron density distribution

Chemical bonding in transition metal carbonyl clusters: complementary analysis of theoretical and experimental electron densities, 383

Electronic Coupling Elements

Thermal and optical electron transfer involving transition metal complexes: insights from theory and computation 167

Electronic spectroscopy

Electronic spectroscopy and photoreactivity in transition metal complexes 143

Electron transfer

Density functional methods applied to metalloenzymes 211

Thermal and optical electron transfer involving transition metal

Elsevier Science B.V. doi:10.1016/S0010-8545(03)00044-4

complexes: insights from theory and computation 167

Electrostatics

Density functional methods applied to metalloenzymes 211 Energy partitioning

Towards a rigorously defined quantum chemical analysis of the chemical bond in donor-acceptor complexes 55

Energy surfaces

Thermal and optical electron transfer involving transition metal complexes: insights from theory and computation 167

Entatic state

Fit and misfit between ligands and metal ions 21

Fe(III) complexes

Modeling the spin-dependent properties of open-shell Fe(III)-containing systems: towards a computational description of nitrile hydratase 291

Flexibility

Fit and misfit between ligands and metal ions 21

Force field development

Inorganic and bioinorganic molecular mechanics modeling—the problem of the force field parameterization 9

Half-sandwich complexes

The importance of interligand interactions to structure and reactivity of coordinatively unsaturated ruthenium and iron half-sandwich complexes—application of the TSC concept II 363

H atom transfer

Density functional methods applied to metalloenzymes 211

Inorganic chemistry

Christian Klixbull Jørgensen (1931–2001): inorganic spectroscopist extraordinaire 3

Iridium complexes

De Novo design in organometallic chemistry: stabilizing iridium(V) 315

Iron

The importance of interligand interactions to structure and reactivity of coordinatively unsaturated ruthenium and iron half-sandwich complexes—application of the TSC concept II 363

Iron-containing proteins

How iron-containing proteins control dioxygen chemistry: a detailed atomic level description via accurate quantum chemical and mixed quantum mechanics/molecular mechanics calculations 267

Iron-oxo enzymes

Density functional methods applied to metalloenzymes 211 Ir(V) intermediates

De Novo design in organometallic chemistry: stabilizing iridium(V)

Main group complexes

Towards a rigorously defined quantum chemical analysis of the chemical bond in donor-acceptor complexes 55

Metalloproteins

Inorganic and bioinorganic molecular mechanics modeling—the problem of the force field parameterization 9

Metal-metal bonding, MO calculations

Effects of the bridging ligands on the molecular and electronic structure of Fe₂(CO)₉ derivatives 333

Metal-metal bonds

Chemical bonding in transition metal carbonyl clusters: complementary analysis of theoretical and experimental electron densities. 383

Methane monooxygenase

Density functional methods applied to metalloenzymes 211

Minimum energy crossing point

Understanding the reactivity of transition metal complexes involving multiple spin states 347

Mixed quantum mechanics/molecular mechanics calculations

How iron-containing proteins control dioxygen chemistry: a detailed atomic level description via accurate quantum chemical and mixed quantum mechanics/molecular mechanics calculations 267

Molecular magnetic properties

DFT calculations of molecular magnetic properties of coordination compounds 187

Molecular orbital

Molecular orbital and DFT studies on water exchange mechanisms of metal ions 233

Molecular properties

Double perturbation theory: a powerful tool in computational coordination chemistry 83

NIR-vis spectra

Theory of electroabsorption spectroscopy in poly-nuclear Ru complexes 127

Nitrile hydratase

Modeling the spin-dependent properties of open-shell Fe(III)-containing systems: towards a computational description of nitrile hydratase 291

NMR studies

Fundamental properties of small molecule models of Fe-only hydrogenase: computations relative to the definition of an entatic state in the active site 255

Organometallic chemistry

Understanding the reactivity of transition metal complexes involving multiple spin states 347

Organometallic complexes

Fundamental properties of small molecule models of Fe-only hydrogenase: computations relative to the definition of an entatic state in the active site 255

Organometallic reaction mechanisms

De Novo design in organometallic chemistry: stabilizing iridium(V) 315

Oxidative addition

De Novo design in organometallic chemistry: stabilizing iridium(V)

Photoreactivity

Electronic spectroscopy and photoreactivity in transition metal complexes 143

Poisson-Boltzmann

Density functional methods applied to metalloenzymes 211

Poly-nuclear Ru complexes

Theory of electroabsorption spectroscopy in poly-nuclear Ru complexes 127

Preorganization

Fit and misfit between ligands and metal ions 21

Proton transfer

Density functional methods applied to metalloenzymes 211

OM/MM

Inorganic and bioinorganic molecular mechanics modeling—the problem of the force field parameterization 9

QM/MM calculations

Modeling the spin-dependent properties of open-shell Fe(III)-containing systems: towards a computational description of nitrile hydratase 291

Quantum chemistry

Electronic spectroscopy and photoreactivity in transition metal complexes 143

Redox

Density functional methods applied to metalloenzymes 211 Ribonucleotide reductase

Density functional methods applied to metalloenzymes 211 Ruthenium

The importance of interligand interactions to structure and reactivity of coordinatively unsaturated ruthenium and iron half-sandwich complexes—application of the TSC concept II 363

Second-order energy derivatives

Double perturbation theory: a powerful tool in computational coordination chemistry 83

Solvent effects

Modeling the spin-dependent properties of open-shell Fe(III)-containing systems: towards a computational description of nitrile hydratase 291

Spectroscopist

Christian Klixbull Jørgensen (1931–2001): inorganic spectroscopist extraordinaire 3

Spin acceleration

Understanding the reactivity of transition metal complexes involving multiple spin states 347

Spin crossover

Understanding the reactivity of transition metal complexes involving multiple spin states 347

Spin-dependent properties

Modeling the spin-dependent properties of open-shell Fe(III)-containing systems: towards a computational description of nitrile hydratase 291

Stark spectroscopy

Theory of electroabsorption spectroscopy in poly-nuclear Ru complexes 127

Through-space interactions

The importance of interligand interactions to structure and reactivity of coordinatively unsaturated ruthenium and iron half-sandwich complexes—application of the TSC concept II 363

Transition metal carbonyl clusters

Chemical bonding in transition metal carbonyl clusters: complementary analysis of theoretical and experimental electron densities. 383

Transition metal complexes

Electronic spectroscopy and photoreactivity in transition metal complexes 143

Towards a rigorously defined quantum chemical analysis of the chemical bond in donor-acceptor complexes 55

Two-state reactivity

Understanding the reactivity of transition metal complexes involving multiple spin states 347

Validation

Inorganic and bioinorganic molecular mechanics modeling—the problem of the force field parameterization 9

Water exchange mechanisms

Molecular orbital and DFT studies on water exchange mechanisms of metal ions 233

Wavepacket dynamics

Electronic spectroscopy and photoreactivity in transition metal complexes 143