# Michael B Hall

## List of Publications by Year in Descending Order



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| 348 papers | 13,334 citations | 59 h-index | 97 g-index |
| 367 ext. papers | 14,058 ext. citations | 8.2 avg, IF | 6.64 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 348 | Separation, speciation, and mechanism of astatine and bismuth extraction from nitric acid into 1-octanol and methyl anthranilate. *Separation and Purification Technology*, **2021**, 282, 120088 | 8.3 | 1 |
| 347 | Protonating metal-metal bonds: Changing the metal-metal interaction from bonding, to nonbonding, and to antibonding. *Polyhedron*, **2021**, 212, 115585 | 2.7 | 1 |
| 346 | Nickel-Borolide Complexes and Their Complex Electronic Structure. *Inorganic Chemistry*, **2021**, 60, 16160-16167 | 5.1 | 1 |
| 345 | Computational Investigation of Dichloromethane Ligand Substitution in the Enantiopure Cation [(η5-C5H5)Re(NO)(PPh3)(ClCH2Cl)]+, a Functional Equivalent of a Chiral Lewis Acid. *Organometallics*, **2021**, 40, 742-759 | 3.8 | 1 |
| 344 | Self-Assembled Nickel-4 Supramolecular Squares and Assays for HER Electrocatalysts Derived Therefrom. *Inorganic Chemistry*, **2021**, 60, 7051-7061 | 5.1 | |
| 343 | Unsupported Lanthanide-Transition Metal Bonds: Ionic vs Polar Covalent?. *Inorganic Chemistry*, **2021**, 60, 9394-9401 | 5.1 | 7 |
| 342 | Efficient Redox-Neutral Photocatalytic Formate to Carbon Monoxide Conversion Enabled by Long-Range Hot Electron Transfer from Mn-Doped Quantum Dots. *Journal of the American Chemical Society*, **2021**, 143, 10292-10300 | 16.4 | 6 |
| 341 | Macrocyclic Complexes Derived from Four cis-L Pt Corners and Four Butadiynediyl Linkers; Syntheses, Electronic Structures, and Square versus Skew Rhombus Geometries. *Chemistry - A European Journal*, **2021**, 27, 10021-10039 | 4.8 | 1 |
| 340 | Platinum(II) alkyl complexes of chelating dibridgehead diphosphines P((CH))P ( = 14, 18, 22); facile / isomerizations interconverting gyroscope and parachute like adducts. *Dalton Transactions*, **2021**, 50, 12457-12477 | 4.3 | 1 |
| 339 | Toward Frameworks with Multiple Aligned and Interactive Fe(CO) Rotators: Syntheses and Structures of Diiron Complexes Linked by Two -Diaxial Diphosphine Ligands ArP(CH)PAr. *Inorganic Chemistry*, **2021**, 60, 3314-3330 | 5.1 | 0 |
| 338 | Syntheses, Structures, Reactivities, and Basicities of Quinolinyl and Isoquinolinyl Complexes of an Electron Rich Chiral Rhenium Fragment and Their Electrophilic Addition Products. *Chemistry - A European Journal*, **2021**, 27, 13399-13417 | 4.8 | 0 |
| 337 | A computational study of hydrogen bonding motifs in halide, tetrafluoroborate, hexafluorophosphate, and tetraarylborate salts of chiral cationic ruthenium and cobalt guanidinobenzimidazole hydrogen bond donor catalysts; acceptor properties of the BArf anion. *Polyhedron*, **2020**, 187, 114618 | 2.7 | 10 |
| 336 | Role of aromatic amino acids in amyloid self-assembly. *International Journal of Biological Macromolecules*, **2020**, 156, 949-959 | 7.9 | 21 |
| 335 | Astatine partitioning between nitric acid and conventional solvents: indication of covalency in ketone complexation of AtO. *Chemical Communications*, **2020**, 56, 9004-9007 | 5.8 | 5 |
| 334 | Stacking interactions of resonance-assisted hydrogen-bridged rings and C-aromatic rings. *Physical Chemistry Chemical Physics*, **2020**, 22, 13721-13728 | 3.6 | 5 |
| 333 | Electrocatalytic Hydrogen Evolution and Oxidation with Rhenium Tris(thiolate) Complexes: A Competition between Rhenium and Sulfur for Electrons and Protons. *ACS Catalysis*, **2020**, 10, 3778-3789 | 13.1 | 14 |
| 332 | What Is Special about Aromatic-Aromatic Interactions? Significant Attraction at Large Horizontal Displacement. *ACS Central Science*, **2020**, 6, 420-425 | 16.8 | 23 |

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| 331 | Silylation of Pyridine, Picolines, and Quinoline with a Zinc Catalyst. *ACS Omega*, **2020**, 5, 1528-1539 | 3.9 | 6 |
| 330 | Full Conformational Analyses of the Ultrafast Isomerization in Penta-coordinated Ru(SC(CF))(CO)(PPh): One Compound, Two Crystal Structures, Three CO Frequencies, 24 Stereoisomers, and 48 Transition States. *Inorganic Chemistry*, **2020**, 59, 11757-11769 | 5.1 | 1 |
| 329 | Controlling P□/C□H Bond Cleavage in Nickel Bis(diphosphine) Complexes: Reactivity Scope, Mechanism, and Computations. *Organometallics*, **2020**, 39, 3306-3314 | 3.8 | 3 |
| 328 | Invoking Side-Chain Functionality for the Mediation of Regioselectivity during Ring-Opening Polymerization of Glucose Carbonates. *Journal of the American Chemical Society*, **2020**, 142, 16974-16981 | 16.4 | 15 |
| 327 | Computational Investigations of Enantioselection in Carbon□Carbon Bond Forming Reactions of Ruthenium Guanidinobenzimidazole Second Coordination Sphere Hydrogen Bond Donor Catalysts. *Organometallics*, **2020**, 39, 1149-1162 | 3.8 | 15 |
| 326 | Controlling O Reactivity in Synthetic Analogues of [NiFeS]- and [NiFeSe]-Hydrogenase Active Sites. *Journal of the American Chemical Society*, **2019**, 141, 15338-15347 | 16.4 | 10 |
| 325 | Oxygen uptake in complexes related to [NiFeS]- and [NiFeSe]-hydrogenase active sites. *Chemical Science*, **2019**, 10, 1368-1373 | 9.4 | 21 |
| 324 | Influence of chelate ring type on chelate-chelate and chelate-aryl stacking: the case of nickel bis(dithiolene). *Physical Chemistry Chemical Physics*, **2019**, 21, 1198-1206 | 3.6 | 5 |
| 323 | M□ssbauer Spectroscopy and Theoretical Studies of Iron Bimetallic Complexes Showing Electrocatalytic Hydrogen Evolution. *Inorganic Chemistry*, **2019**, 58, 7069-7077 | 5.1 | 7 |
| 322 | Stacking interaction potential energy surfaces of square-planar metal complexes containing chelate rings. *Advances in Inorganic Chemistry*, **2019**, 159-189 | 2.1 | 4 |
| 321 | Triisopropylsilyl (TIPS) Alkynes as Building Blocks for Syntheses of Platinum Triisopropylsilylpolyynyl and Diplatinum Polyynediyl Complexes. *Organometallics*, **2019**, 38, 3294-3310 | 3.8 | 7 |
| 320 | Stacking Interactions of Resonance-Assisted Hydrogen-Bridged Rings. A Systematic Study of Crystal Structures and Quantum-Chemical Calculations. *Crystal Growth and Design*, **2019**, 19, 5619-5628 | 3.5 | 6 |
| 319 | Photoinduced Terminal Hydride of [FeFe]-Hydrogenase Biomimetic Complexes. *Inorganic Chemistry* , **2019**, 58, 13737-13741 | 5.1 | 3 |
| 318 | Study of stacking interactions between two neutral tetrathiafulvalene molecules in Cambridge Structural Database crystal structures and by quantum chemical calculations. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2019**, 75, 1-7 | 1.8 | 6 |
| 317 | Theoretical Analysis of Competing Pathways for Carbon-Hydrogen Activation of Cyclopentadienyl-Triphenylphosphine-Iridium in Benzene. *Inorganic Chemistry*, **2019**, 58, 16553-16558 | 5.1 | |
| 316 | Origin of Shielding and Deshielding Effects in NMR Spectra of Organic Conjugated Polyynes. *Organic Letters*, **2019**, 21, 753-757 | 6.2 | 14 |
| 315 | Recent computational studies on transition-metal carbon□hydrogen bond activation of alkanes. *International Journal of Quantum Chemistry*, **2018**, 118, e25605 | 2.1 | 4 |
| 314 | Nickel Fluorocarbene Metathesis with Fluoroalkenes. *Angewandte Chemie*, **2018**, 130, 5874-5878 | 3.6 | 7 |

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| 313 | Nickel Fluorocarbene Metathesis with Fluoroalkenes. *Angewandte Chemie - International Edition*, **2018**, 57, 5772-5776 | 16.4 | 17 |
| 312 | Influence of metal ion on chelate aryl stacking interactions. *International Journal of Quantum Chemistry*, **2018**, 118, e25629 | 2.1 | 7 |
| 311 | Unraveling the Role of a Flexible Tetradentate Ligand in the Aerobic Oxidative Carbon-Carbon Bond Formation with Palladium Complexes: A Computational Mechanistic Study. *Journal of the American Chemical Society*, **2018**, 140, 3929-3939 | 16.4 | 10 |
| 310 | Probing the Carbon-Hydrogen Activation of Alkanes Following Photolysis of Tp'Rh(CNR)(carbodiimide): A Computational and Time-Resolved Infrared Spectroscopic Study. *Journal of the American Chemical Society*, **2018**, 140, 1842-1854 | 16.4 | 20 |
| 309 | Cyanide Docking and Linkage Isomerism in Models for the Artificial [FeFe]-Hydrogenase Maturation Process. *Journal of the American Chemical Society*, **2018**, 140, 9904-9911 | 16.4 | 5 |
| 308 | Structure and Magnetization Dynamics of Dy Fe and Dy Ru Bonded Complexes. *Angewandte Chemie*, **2018**, 130, 8276-8280 | 3.6 | 3 |
| 307 | Structure and Magnetization Dynamics of Dy-Fe and Dy-Ru Bonded Complexes. *Angewandte Chemie - International Edition*, **2018**, 57, 8144-8148 | 16.4 | 29 |
| 306 | Stacking of cyclopentadienyl organometallic sandwich and half-sandwich compounds. Strong interactions of sandwiches at large offsets. *CrystEngComm*, **2018**, 20, 4506-4514 | 3.3 | 8 |
| 305 | Tuning Reactivity of Bioinspired [NiFe]-Hydrogenase Models by Ligand Design and Modeling the CO Inhibition Process. *ACS Catalysis*, **2018**, 8, 10658-10667 | 13.1 | 35 |
| 304 | Structural and Electronic Responses to the Three Redox Levels of Fe(NO)N S -Fe(NO). *Chemistry - A European Journal*, **2018**, 24, 16003-16008 | 4.8 | 7 |
| 303 | Cobalt Pincer Complexes in Catalytic C-H Borylation: The Pincer Ligand Flips Rather Than Dearomatizes. *ACS Catalysis*, **2018**, 8, 10606-10618 | 13.1 | 26 |
| 302 | Towards understanding of lanthanide-transition metal bonding: investigations of the first Ce-Fe bonded complex. *Chemical Communications*, **2018**, 54, 10893-10896 | 5.8 | 25 |
| 301 | Comparisons of MNSvs. bipyridine as redox-active ligands to manganese and rhenium in (L-L)M'(CO)Cl complexes. *Dalton Transactions*, **2017**, 46, 5175-5182 | 4.3 | 10 |
| 300 | Noncovalent bonding: Stacking interactions of chelate rings of transition metal complexes. *Coordination Chemistry Reviews*, **2017**, 345, 318-341 | 23.2 | 71 |
| 299 | The Distinctive Electronic Structures of Rhenium Tris(thiolate) Complexes, an Unexpected Contrast to the Valence Isoelectronic Ruthenium Tris(thiolate) Complexes. *Inorganic Chemistry*, **2017**, 56, 583-593 | 5.1 | 10 |
| 298 | Interplay of hemilability and redox activity in models of hydrogenase active sites. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E9775-E9782 | 11.5 | 33 |
| 297 | A matrix of heterobimetallic complexes for interrogation of hydrogen evolution reaction electrocatalysts. *Chemical Science*, **2017**, 8, 8291-8300 | 9.4 | 38 |
| 296 | Molybdenum Trihydride Complexes: Computational Model of Oxidatively Induced Reductive Elimination of Dihydrogen. *Inorganic Chemistry*, **2017**, 56, 9653-9659 | 5.1 | 2 |

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| 295 | Biomimetics of [NiFe]-Hydrogenase: Nickel- or Iron-Centered Proton Reduction Catalysis?. *Journal of the American Chemical Society*, **2017**, 139, 18065-18070 | 16.4 | 50 |
| 294 | Unexpected Importance of Aromatic-Aliphatic and Aliphatic Side Chain-Backbone Interactions in the Stability of Amyloids. *Chemistry - A European Journal*, **2017**, 23, 11046-11053 | 4.8 | 9 |
| 293 | Methane Activations by Titanium Neopentylidene Complexes: Electronic Resilience and Steric Control. *Inorganic Chemistry*, **2017**, 56, 9264-9272 | 5.1 | 5 |
| 292 | Interactions of Aromatic Residues in Amyloids: A Survey of Protein Data Bank Crystallographic Data. *Crystal Growth and Design*, **2017**, 17, 6353-6362 | 3.5 | 10 |
| 291 | Hemilabile Bridging Thiolates as Proton Shuttles in Bioinspired H Production Electrocatalysts. *Journal of the American Chemical Society*, **2016**, 138, 12920-12927 | 16.4 | 64 |
| 290 | The Rich Structural Chemistry Displayed by the Carbon Monoxide as a Ligand to Metal Complexes. *Structure and Bonding*, **2016**, 199-248 | 0.9 | 6 |
| 289 | Innenrücktitelbild: Flexible Zirconium Metal-Organic Frameworks as Bioinspired Switchable Catalysts (Angew. Chem. 36/2016). *Angewandte Chemie*, **2016**, 128, 11079-11079 | 3.6 | |
| 288 | Facile P-C/C-H Bond-Cleavage Reactivity of Nickel Bis(diphosphine) Complexes. *Chemistry - A European Journal*, **2016**, 22, 9493-7 | 4.8 | 3 |
| 287 | The stacking interactions of bipyridine complexes: the influence of the metal ion type on the strength of interactions. *Journal of Molecular Modeling*, **2016**, 22, 30 | 2 | 5 |
| 286 | Two-State Reactivity in Low-Valent Iron-Mediated C-H Activation and the Implications for Other First-Row Transition Metals. *Journal of the American Chemical Society*, **2016**, 138, 3715-30 | 16.4 | 108 |
| 285 | Flexible Zirconium Metal-Organic Frameworks as Bioinspired Switchable Catalysts. *Angewandte Chemie - International Edition*, **2016**, 55, 10776-80 | 16.4 | 143 |
| 284 | Cyanide-bridged iron complexes as biomimetics of tri-iron arrangements in maturases of the H cluster of the di-iron hydrogenase. *Chemical Science*, **2016**, 7, 3710-3719 | 9.4 | 17 |
| 283 | Carbon-hydrogen bond activation by a titanium neopentylidene complex. *Journal of Coordination Chemistry*, **2016**, 69, 1759-1768 | 1.6 | 7 |
| 282 | Molybdenum Trihydride Complexes: Computational Determinations of Hydrogen Positions and Rearrangement Mechanisms. *Inorganic Chemistry*, **2015**, 54, 6380-5 | 5.1 | 6 |
| 281 | Carbon–Hydrogen Bond Activation in Bis(2,6-dimethylbenzenethiolato)tris(trimethylphosphine)ruthenium(II): Ligand Dances and Solvent Transformations. *Organometallics*, **2015**, 34, 3129-3140 | 3.8 | 4 |
| 280 | Host-guest behavior of a heavy-atom heterocycle Re4(CO)16(μ-SbPh2)2(μ-H)2 obtained from a palladium-assisted ring opening dimerization of Re2(CO)8(μ-SbPh2)(μ-H). *Inorganic Chemistry*, **2015**, 54, 3536-44 | 5.1 | 6 |
| 279 | Addition of ethylene to a π-conjugated two-dimensional nickel-based organometallic framework with implications for olefin separation. *Journal of Molecular Modeling*, **2015**, 21, 107 | 2 | 9 |
| 278 | Regioselectivity in ligand substitution reactions on diiron complexes governed by nucleophilic and electrophilic ligand properties. *Inorganic Chemistry*, **2015**, 54, 3523-35 | 5.1 | 11 |

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| 277 | Understanding the Effects of Bidentate Directing Groups: A Unified Rationale for sp(2) and sp(3) C-H Bond Activations. *Journal of Organic Chemistry*, **2015**, 80, 4672-82 | 4.2 | 52 |
| 276 | Role of the chemically non-innocent ligand in the catalytic formation of hydrogen and carbon dioxide from methanol and water with the metal as the spectator. *Journal of the American Chemical Society*, **2015**, 137, 12330-42 | 16.4 | 49 |
| 275 | Understanding the Radical Nature of an Oxidized Ruthenium Tris(thiolate) Complex and Its Role in the Chemistry. *Journal of the American Chemical Society*, **2015**, 137, 15616-9 | 16.4 | 11 |
| 274 | Influence of the density functional and basis set on the relative stabilities of oxygenated isomers of diiron models for the active site of [FeFe]-hydrogenase. *Journal of Chemical Theory and Computation*, **2015**, 11, 205-14 | 6.4 | 13 |
| 273 | A reduced 2Fe2S cluster probe of sulfur-hydrogen versus sulfur-gold interactions. *Angewandte Chemie - International Edition*, **2015**, 54, 11102-6 | 16.4 | 9 |
| 272 | A Reduced 2Fe2S Cluster Probe of Sulfur–Hydrogen versus Sulfur–Gold Interactions. *Angewandte Chemie*, **2015**, 127, 11254-11258 | 3.6 | 1 |
| 271 | Computational Mechanistic Studies on Reactions of Transition Metal Complexes with Noninnocent Pincer Ligands: Aromatization–Dearomatization or Not. *ACS Catalysis*, **2015**, 5, 1895-1913 | 13.1 | 67 |
| 270 | Origins of Selective C(sp2)–H Activation Using Transition Metal Complexes with N,N-Bidentate Directing Groups: A Combined Theoretical–Experimental Study. *ACS Catalysis*, **2014**, 4, 649-656 | 13.1 | 44 |
| 269 | Mechanism of the formation of carboxylate from alcohols and water catalyzed by a bipyridine-based ruthenium complex: a computational study. *Journal of the American Chemical Society*, **2014**, 136, 383-95 | 16.4 | 79 |
| 268 | Carbon-hydrogen activation of cycloalkanes by cyclopentadienylcarbonylrhodium--a lifetime enigma. *Journal of the American Chemical Society*, **2014**, 136, 8614-25 | 16.4 | 28 |
| 267 | Computational study of the cycloaddition reactivity of the osmium silylyne. *Inorganica Chimica Acta*, **2014**, 422, 40-46 | 2.7 | 3 |
| 266 | Computational exploration of alternative catalysts for olefin purification: cobalt and copper analogues inspired by nickel bis(dithiolene) electrocatalysis. *Inorganic Chemistry*, **2014**, 53, 9679-91 | 5.1 | 17 |
| 265 | Theoretical investigation on the mechanism of FeCl3-catalysed cross-coupling reaction of alcohols with alkenes. *Molecular Physics*, **2014**, 112, 2107-2113 | 1.7 | 1 |
| 264 | Uptake of one and two molecules of 1,3-butadiene by platinum bis(dithiolene): a theoretical study. *Inorganic Chemistry*, **2014**, 53, 9692-702 | 5.1 | 15 |
| 263 | Intramolecular iron-mediated C-H bond heterolysis with an assist of pendant base in a [FeFe]-hydrogenase model. *Journal of the American Chemical Society*, **2014**, 136, 16817-23 | 16.4 | 34 |
| 262 | Redox active iron nitrosyl units in proton reduction electrocatalysis. *Nature Communications*, **2014**, 5, 3684 | 17.4 | 47 |
| 261 | Theoretical investigation on the reaction of HS+ with CH3NH2. *Chemical Papers*, **2014**, 68, | 1.9 | 1 |
| 260 | Ambidentate thiocyanate and cyanate ligands in dinitrosyl iron complexes. *Inorganic Chemistry*, **2013**, 52, 2119-24 | 5.1 | 32 |

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| 259 | Understanding Pd-Pd bond length variation in (PNP)Pd-Pd(PNP) dimers. *Inorganic Chemistry*, **2013**, 52, 2317-22 | 5.1 | 12 |
| 258 | The mechanism of addition of aldehydes to germene in different solvents: A DFT study. *Journal of Organometallic Chemistry*, **2013**, 748, 8-12 | 2.3 | 3 |
| 257 | Comparative insight into electronic properties and reactivities toward C-H bond activation by iron(IV)-nitrido, iron(IV)-oxo, and iron(IV)-sulfido complexes: a theoretical investigation. *Inorganic Chemistry*, **2013**, 52, 2684-96 | 5.1 | 19 |
| 256 | Apparent anti-Woodward-Hoffmann addition to a nickel bis(dithiolene) complex: the reaction mechanism involves reduced, dimetallic intermediates. *Inorganic Chemistry*, **2013**, 52, 3711-23 | 5.1 | 27 |
| 255 | A mechanism for the addition of ethylene to nickel bis-dithiolene. *International Journal of Quantum Chemistry*, **2013**, 113, 1621-1625 | 2.1 | 11 |
| 254 | Stacking interactions of Ni(acac) chelates with benzene: calculated interaction energies. *ChemPhysChem*, **2013**, 14, 1797-800 | 3.2 | 14 |
| 253 | Carbon monoxide induced reductive elimination of disulfide in an N-heterocyclic carbene (NHC)/thiolate dinitrosyl iron complex (DNIC). *Journal of the American Chemical Society*, **2013**, 135, 8423-30 | 16.4 | 24 |
| 252 | Analysis of an alternative to the H-atom abstraction mechanism in methane C-H bond activation by nonheme iron(IV)-oxo oxidants. *Dalton Transactions*, **2013**, 42, 10260-70 | 4.3 | 13 |
| 251 | Investigating the electronic structure of the Atox1 copper(I) transfer mechanism with density functional theory. *Inorganic Chemistry*, **2013**, 52, 10387-93 | 5.1 | 4 |
| 250 | The osmium-silicon triple bond: synthesis, characterization, and reactivity of an osmium silylyne complex. *Journal of the American Chemical Society*, **2013**, 135, 11780-3 | 16.4 | 50 |
| 249 | Measuring the internal energies of species emitted from hypervelocity nanoprojectile impacts on surfaces using recalibrated benzylpyridinium probe ions. *Journal of Chemical Physics*, **2013**, 138, 214301 | 3.9 | 16 |
| 248 | The effect of the axial ligand on distinct reaction tunneling for methane hydroxylation by nonheme iron(IV)-oxo complexes. *Physical Chemistry Chemical Physics*, **2012**, 14, 12863-74 | 3.6 | 16 |
| 247 | The mechanism of alkene addition to a nickel bis(dithiolene) complex: the role of the reduced metal complex. *Journal of the American Chemical Society*, **2012**, 134, 4481-4 | 16.4 | 40 |
| 246 | □Cleavage of Phenyl Groups from GePh3 Ligands in Iridium Carbonyl Cluster Complexes. A Mechanism and Its Role in the Synthesis of Bridging Germylene Ligands. *Organometallics*, **2012**, 31, 2621-2630 | 3.8 | 12 |
| 245 | Bonding and Reactivity in the Electronically Unsaturated Hydrogen-Bridged Dimer [Ru3(CO)8(□-CMe)(□H)2(□-H)]2. *Organometallics*, **2012**, 31, 50-53 | 3.8 | 4 |
| 244 | Computational insights into uranium complexes supported by redox-active □diimine ligands. *Inorganic Chemistry*, **2012**, 51, 2058-64 | 5.1 | 22 |
| 243 | Structural and spectroscopic features of mixed valent Fe(II)Fe(I) complexes and factors related to the rotated configuration of diiron hydrogenase. *Journal of the American Chemical Society*, **2012**, 134, 13089-102 | 16.4 | 73 |
| 242 | Computational studies on ethylene addition to nickel bis(dithiolene). *Journal of Physical Chemistry A*, **2012**, 116, 476-82 | 2.8 | 35 |

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| 241 | Comparison of the FeO(2+) and FeS(2+) complexes in the cyanide and isocyanide ligand environment for methane hydroxylation. *Journal of Computational Chemistry*, **2012**, 33, 1448-57 | 3.5 | 3 |
| 240 | Diruthenium Naphthalene and Anthracene Complexes Containing a Doubly Linked Dicyclopentadienyl Ligand. *Organometallics*, **2012**, 31, 4838-4848 | 3.8 | 14 |
| 239 | Modeling structures and vibrational frequencies for dinitrosyl iron complexes (DNICs) with density functional theory. *Inorganic Chemistry*, **2011**, 50, 8532-40 | 5.1 | 37 |
| 238 | Observation of inductive effects that cause a change in the rate-determining step for the conversion of rhenium azides to imido complexes. *Inorganic Chemistry*, **2011**, 50, 10505-14 | 5.1 | 15 |
| 237 | Self-assembly of dinitrosyl iron units into imidazolate-edge-bridged molecular squares: characterization including M□ssbauer spectroscopy. *Journal of the American Chemical Society*, **2011**, 133, 20426-34 | 16.4 | 39 |
| 236 | Density Functional Calculations on Protonation of the [FeFe]-Hydrogenase Model Complex Fe2(□pdt)(CO)4(PMe3)2 and Subsequent Isomerization Pathways. *European Journal of Inorganic Chemistry*, **2011**, 2011, 1080-1093 | 2.3 | 36 |
| 235 | Computational Investigations into Hydrogen-Atom Abstraction from Rhodium Hydride Complexes by Methyl Radicals in Aqueous Solution. *European Journal of Inorganic Chemistry*, **2011**, 2011, 4901-4905 | 2.3 | 1 |
| 234 | Combined experimental and theoretical investigation into C-H activation of cyclic alkanes by Cp'Rh(CO)2 (Cp' = □5-C5H5 or □5-C5Me5). *Dalton Transactions*, **2011**, 40, 1751-7 | 4.3 | 17 |
| 233 | cis-Dithiolatonickel as metalloligand to dinitrosyl iron units: the di-metallic structure of Ni(□SR)[Fe(NO)2] and an unexpected, abbreviated metalloadamantyl cluster, Ni2(□SR)4[Fe(NO)2]3. *Dalton Transactions*, **2011**, 40, 6047-53 | 4.3 | 17 |
| 232 | Tetrarhena-heterocycle from the palladium-catalyzed dimerization of Re2(CO)8(□SbPh2)(□H) exhibits an unusual host-guest behavior. *Journal of the American Chemical Society*, **2011**, 133, 12994-7 | 16.4 | 138 |
| 231 | Computational investigation of the concerted dismutation of chlorite ion by water-soluble iron porphyrins. *Inorganic Chemistry*, **2011**, 50, 7928-30 | 5.1 | 18 |
| 230 | Carbon□Bromine Bond Formation through a Nickel-Centered Spin-Crossing Mechanism. *Organometallics*, **2011**, 30, 6365-6371 | 3.8 | 18 |
| 229 | Allyl Ligand Reactivity in Tantalum(V) Compounds: Experimental and Computational Evidence for Allyl Transfer to the Formamidinate Ligand infac-Ta(NMe2)3(□1-allyl)[iPrNC(H)NiPr] via a Metallo-Claisen Rearrangement. *Organometallics*, **2011**, 30, 5832-5843 | 3.8 | 5 |
| 228 | Theoretical study on the reaction of PH+ with H2O. *Computational and Theoretical Chemistry*, **2011**, 966, 328-333 | 2 | |
| 227 | Unexpected □oxo five-member ring intermediates for oxygen atom transfer between osmium complexes. *Journal of Coordination Chemistry*, **2010**, 63, 2846-2853 | 1.6 | |
| 226 | Understanding the factors affecting the activation of alkane by Cp'Rh(CO)2 (Cp' = Cp or Cp*). *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 20178-83 | 11.5 | 32 |
| 225 | Mechanism of water splitting and oxygen-oxygen bond formation by a mononuclear ruthenium complex. *Journal of the American Chemical Society*, **2010**, 132, 120-30 | 16.4 | 125 |
| 224 | Thermal decomposition pathways of hydroxylamine: theoretical investigation on the initial steps. *Journal of Physical Chemistry A*, **2010**, 114, 9262-9 | 2.8 | 36 |

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| 223 | Crystallographic evidence of a base-free uranium(IV) terminal oxo species. *Inorganic Chemistry*, **2010**, 49, 7620-2 | 5.1 | 68 |
| 222 | Ortho-Metalation Dynamics and Ligand Fluxionality in the Conversion of Os3(CO)10(dppm) to HOs3(CO)8[PhP(C6H4-2,1)CH2PPh2]: Experimental and DFT Evidence for the Participation of Agostic CH and Aryl Intermediates at an Intact Triosmium Cluster. *Organometallics*, **2010**, 29, 4041-4057 | 3.8 | 28 |
| 221 | Origins of the selectivity for borylation of primary over secondary C-H bonds catalyzed by Cp*-rhodium complexes. *Journal of the American Chemical Society*, **2010**, 132, 3078-91 | 16.4 | 97 |
| 220 | Potential hydrogen bottleneck in nickel-iron hydrogenase. *Inorganic Chemistry*, **2010**, 49, 6378-80 | 5.1 | 28 |
| 219 | Density functional study of the thermodynamics of hydrogen production by tetrairon hexathiolate, Fe4[MeC(CH2S)3]2(CO)8, a hydrogenase model. *Inorganic Chemistry*, **2010**, 49, 5737-47 | 5.1 | 20 |
| 218 | Density functional theory applied to a difference in pathways taken by the enzymes cytochrome P450 and superoxide reductase: spin States of ferric hydroperoxo intermediates and hydrogen bonds from water. *Inorganic Chemistry*, **2010**, 49, 188-98 | 5.1 | 14 |
| 217 | Mechanism of electrocatalytic hydrogen production by a di-iron model of iron-iron hydrogenase: a density functional theory study of proton dissociation constants and electrode reduction potentials. *Dalton Transactions*, **2010**, 39, 3093-104 | 4.3 | 65 |
| 216 | Analysis of a pentacoordinate iron dicarbonyl as synthetic analogue of the Hmd or mono-iron hydrogenase active site. *Chemistry - A European Journal*, **2010**, 16, 3083-9 | 4.8 | 67 |
| 215 | Oxygen atom transfer catalysis: Ligand effects on the key reaction barrier in molybdenum (VI) dioxo systems. *Journal of Molecular Catalysis A*, **2010**, 324, 15-23 | | 11 |
| 214 | Generalized molecular orbital theory: Ground state and ionization potentials of water and dinitrogen. *International Journal of Quantum Chemistry*, **2009**, 16, 195-203 | 2.1 | |
| 213 | Density functional theory study of the mechanism for Ni(NHC)2 catalyzed dehydrogenation of ammoniaborane for chemical hydrogen storage. *Journal of Organometallic Chemistry*, **2009**, 694, 2831-2838 | 2.3 | 34 |
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