

# Mu-Hyun Baik

## List of Publications by Year in Descending Order

**Source:** <https://exaly.com/author-pdf/6622190/mu-hyun-baik-publications-by-year.pdf>  
**Version:** 2024-04-09

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.  
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

|                    |                         |               |                 |
|--------------------|-------------------------|---------------|-----------------|
| 235<br>papers      | 8,467<br>citations      | 52<br>h-index | 80<br>g-index   |
| 257<br>ext. papers | 9,852<br>ext. citations | 11<br>avg, IF | 6.43<br>L-index |

| #   | Paper   | IF   | Citations |
|-----|---|------|-----------|
| 235 | Rearrangements of the Chrysanthenol Core: Application to a Formal Synthesis of Xishacorene B. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 20482-20490  | 16.4 | 1         |
| 234 | Switching Chemoselectivity Based on the Ring Size: How to Make Ring-Fused Indoles Using Transition-Metal-Mediated Cross-Coupling. <i>ACS Catalysis</i> , <b>2021</b> , 11, 12821-12832  | 13.1 | 0         |
| 233 | Reaction of a Molybdenum Bis(dinitrogen) Complex with Carbon Dioxide: A Combined Experimental and Computational Investigation. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 7708-7718   | 5.1  | 1         |
| 232 | Protecting Benzylic C-H Bonds by Deuteration Doubles the Operational Lifetime of Deep-Blue Ir-Phenylimidazole Dopants in Phosphorescent OLEDs. <i>Advanced Optical Materials</i> , <b>2021</b> , 9, 2100630   | 8.1  | 17        |
| 231 | Mechanistic Study of Metal-Ligand Cooperativity in Mn(II)-Catalyzed Hydroborations: Hemilabile SNS Ligand Enables Metal Hydride-Free Reaction Pathway. <i>ACS Catalysis</i> , <b>2021</b> , 11, 9043-9051   | 13.1 | 9         |
| 230 | Calculation-Assisted Stereochemical Analysis of Securingine A. <i>Bulletin of the Korean Chemical Society</i> , <b>2021</b> , 42, 486-488   | 1.2  | 1         |
| 229 | Diastereoselective Rhodium-Catalyzed [(3+2+2)] Carbocyclization Reactions with Tethered Alkynylidenecyclopropanes: Synthesis of the Tremulane Sesquiterpene Natural Products. <i>Asian Journal of Organic Chemistry</i> , <b>2021</b> , 10, 2174-2183                           | 3    | 0         |
| 228 | Purely organic phosphorescent organic light emitting diodes using alkyl modified phenoselenazine. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 8233-8238  | 7.1  | 5         |
| 227 | The mechanism behind enhanced reactivity of unsaturated phosphorus(v) electrophiles towards thiols. <i>Chemical Science</i> , <b>2021</b> , 12, 8141-8148   | 9.4  | 1         |
| 226 | Ruthenium(ii)-catalyzed regioselective direct C4- and C5-diamidation of indoles and mechanistic studies. <i>Chemical Science</i> , <b>2021</b> , 12, 11427-11437  | 9.4  | 4         |
| 225 | Ni-Catalyzed Intermolecular C(sp <sup>3</sup> )-H Amidation Tuned by Bidentate Directing Groups. <i>ACS Catalysis</i> , <b>2021</b> , 11, 3067-3072   | 13.1 | 7         |
| 224 | Controlled Regulation of the Nitrile Activation of a Peroxocobalt(III) Complex with Redox-Inactive Lewis Acidic Metals. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 11382-11392  | 16.4 | 4         |
| 223 | Phosphorus-Atom Transfer from Phosphaethynolate to an Alkylidyne. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 24411-24417  | 16.4 | 1         |
| 222 | Experimental and Computational Studies on the Ruthenium-Catalyzed Dehydrative C-H Coupling of Phenols with Aldehydes for the Synthesis of 2-Alkylphenol, Benzofuran, and Xanthene Derivatives. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 13428-13440 | 16.4 | 5         |
| 221 | Chiral Brønsted acid-controlled intermolecular asymmetric [2 + 2] photocycloadditions. <i>Nature Communications</i> , <b>2021</b> , 12, 5735  | 17.4 | 9         |
| 220 | Copper-Catalyzed Enantiotopic-Group-Selective Allylation of $\alpha$ -Diborylalkanes. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 1069-1077  | 16.4 | 16        |
| 219 | Understanding the mechanism of direct visible-light-activated [2 + 2] cycloadditions mediated by Rh and Ir photocatalysts: combined computational and spectroscopic studies. <i>Chemical Science</i> , <b>2021</b> , 12, 9673-9681  | 9.4  | 7         |

|     |  |      |    |
|-----|--|------|----|
| 218 | Allene C(sp)-H Activation and Alkenylation Catalyzed by Palladium.. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 21705-21712   | 16.4 | 2  |
| 217 | Naphthalene diimide as a two-electron anolyte for aqueous and neutral pH redox flow batteries. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 11218-11223  | 13   | 14 |
| 216 | Ancillary ligand increases the efficiency of heteroleptic Ir-based triplet emitters in OLED devices. <i>Nature Communications</i> , <b>2020</b> , 11, 2292   | 17.4 | 13 |
| 215 | Multifaceted examination of multielectron transfer reactions. <i>Inorganica Chimica Acta</i> , <b>2020</b> , 510, 119746-7   | 16.7 | 14 |
| 214 | Supramolecular Fullerene Tetramers Concocted with Porphyrin Boxes Enable Efficient Charge Separation and Delocalization. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 12596-12601            | 16.4 | 16 |
| 213 | Dual Mode Radiative Transition from a Phenoselenazine Derivative and Electrical Switching of the Emission Mechanism. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 5591-5600                      | 6.4  | 13 |
| 212 | ZnMe-Mediated, Direct Alkylation of Electron-Deficient N-Heteroarenes with 1,1-Diborylalkanes: Scope and Mechanism. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 13235-13245                 | 16.4 | 17 |
| 211 | C-H/C-C Functionalization Approach to N-Fused Heterocycles from Saturated Azacycles. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 13041-13050  | 16.4 | 12 |
| 210 | The Mechanism of Rhodium-Catalyzed Allylic C-H Amination. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 5842-5851   | 16.4 | 34 |
| 209 | Scope and mechanism of nitrile dihydroboration mediated by a $\beta$ -diketiminato manganese hydride catalyst. <i>Chemical Communications</i> , <b>2020</b> , 56, 3959-3962  | 5.8  | 21 |
| 208 | Oxidation of Cymantrene-Tagged Tamoxifen Analogues: Effect of Diphenyl Functionalization on the Redox Mechanism. <i>Organometallics</i> , <b>2020</b> , 39, 679-687  | 3.8  | 3  |
| 207 | Optical and Fluorescent Dual Sensing of Aminoalcohols by in Situ Generation of BODIPY-like Chromophore. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 4975-4979                               | 16.4 | 14 |
| 206 | Minimalistic Principles for Designing Small Molecules with Multiple Reactivities against Pathological Factors in Dementia. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 8183-8193            | 16.4 | 10 |
| 205 | Nickel-Catalyzed Anionic Cross-Coupling Reaction of Lithium Sulfonimidoyl Alkylidene Carbenoids With Organolithiums. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 2914-2926                             | 4.8  | 4  |
| 204 | Peroxo-cobalt(III) species activates nitriles via a superoxo-cobalt(II) diradical state. <i>Dalton Transactions</i> , <b>2020</b> , 49, 2819-2826  | 4.3  | 2  |
| 203 | Unexpected Selectivity of Intramolecular [3+2] Cycloaddition of Trimethylenemethane (TMM) Diyl toward Total Synthesis of Conidiogenone B. <i>European Journal of Organic Chemistry</i> , <b>2020</b> , 2020, 609-617 | 3.2  | 3  |
| 202 | Direct Stereoconvergent Allylation of Chiral Alkylcopper Nucleophiles with Racemic Allylic Phosphates. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 2592-2596   | 4.8  | 5  |
| 201 | Electro-inductive effect: Electrodes as functional groups with tunable electronic properties. <i>Science</i> , <b>2020</b> , 370, 214-219  | 33.3 | 34 |

|     |  |      |    |
|-----|--|------|----|
| 200 | The electronic structure of a $\mu$ -diketiminato manganese hydride dimer. <i>Dalton Transactions</i> , <b>2020</b> , 49, 14463-14474  | 4.3  | 3  |
| 199 | Ligand-Controlled Product Selectivity in Electrochemical Carbon Dioxide Reduction Using Manganese Bipyridine Catalysts. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 4265-4275   | 16.4 | 57 |
| 198 | Designing a Planar Chiral Rhodium Indenyl Catalyst for Regio- and Enantioselective Allylic C-H Amidation. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 13996-14004   | 16.4 | 52 |
| 197 | Reductive activation of Pd-precatalysts via decarboxylation of pivalate in direct C-H arylation reactions. <i>Chemical Communications</i> , <b>2020</b> , 56, 13868-13871  | 5.8  | 5  |
| 196 | Gigantic Porphyrinic Cages. <i>CheM</i> , <b>2020</b> , 6, 3374-3384   | 16.2 | 28 |
| 195 | Cu(I)-Catalyzed Enantioselective [5 + 1] Cycloaddition of N-Aromatic Compounds and Alkynes via Chelating-Assisted 1,2-Deareomative Addition. <i>ACS Catalysis</i> , <b>2020</b> , 10, 10905-10913  | 13.1 | 7  |
| 194 | Multiple reactivities of flavonoids towards pathological elements in Alzheimer's disease: structure-activity relationship. <i>Chemical Science</i> , <b>2020</b> , 11, 10243-10254   | 9.4  | 7  |
| 193 | Tebbe-like and Phosphonioalkylidene and -alkylidyne Complexes of Scandium. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 10143-10152  | 16.4 | 8  |
| 192 | Chemo- and regioselective click reactions through nickel-catalyzed azide-alkyne cycloaddition. <i>Organic and Biomolecular Chemistry</i> , <b>2020</b> , 18, 3374-3381   | 3.9  | 13 |
| 191 | Efficient Cobalt Catalyst for Ambient-Temperature Nitrile Dihydroboration, the Elucidation of a Chelate-Assisted Borylation Mechanism, and a New Synthetic Route to Amides. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 15327-15337 | 16.4 | 31 |
| 190 | Harnessing Secondary Coordination Sphere Interactions That Enable the Selective Amidation of Benzylic C-H Bonds. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 15356-15366  | 16.4 | 35 |
| 189 | Visible light induced alkene aminopyridylation using N-aminopyridinium salts as bifunctional reagents. <i>Nature Communications</i> , <b>2019</b> , 10, 4117   | 17.4 | 72 |
| 188 | Conversion of methane to ethylene using an Ir complex and phosphorus ylide as a methylene transfer reagent. <i>Chemical Communications</i> , <b>2019</b> , 55, 1927-1930   | 5.8  | 5  |
| 187 | CuH-Catalyzed Enantioselective Alkylation of Indole Derivatives with Ligand-Controlled Regiodivergence. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 3901-3909   | 16.4 | 70 |
| 186 | Selective C-C bond formation from rhodium-catalyzed C-H activation reaction of 2-arylpyridines with 3-aryl-2-azirines. <i>Chemical Science</i> , <b>2019</b> , 10, 2678-2686   | 9.4  | 13 |
| 185 | Site-Selective Functionalization of Pyridinium Derivatives via Visible-Light-Driven Photocatalysis with Quinolinone. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 9239-9248  | 16.4 | 59 |
| 184 | Dynamic Kinetic Resolution of Alkenyl Cyanohydrins Derived from $\alpha$ -Unsaturated Aldehydes: Stereoselective Synthesis of $\beta$ -Tetrasubstituted Olefins. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 11770-11774            | 16.4 | 8  |
| 183 | Enantioselective [2+2] Cycloadditions of Cinnamate Esters: Generalizing Lewis Acid Catalysis of Triplet Energy Transfer. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 9543-9547  | 16.4 | 78 |

|     |   |       |    |
|-----|---|-------|----|
| 182 | Site-Selective 1,1-Difunctionalization of Unactivated Alkenes Enabled by Cationic Palladium Catalysis. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 10048-10059   | 16.4  | 55 |
| 181 | Living Polymerization Caught in the Act: Direct Observation of an Arrested Intermediate in Metathesis Polymerization. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 10039-10047  | 16.4  | 21 |
| 180 | Design and Optimization of Catalysts Based on Mechanistic Insights Derived from Quantum Chemical Reaction Modeling. <i>Chemical Reviews</i> , <b>2019</b> , 119, 6509-6560  | 68.1  | 71 |
| 179 | Catalytic Cascade Reaction To Access Cyclopentane-Fused Heterocycles: Expansion of Pd-TMM Cycloaddition. <i>Organic Letters</i> , <b>2019</b> , 21, 3998-4002   | 6.2   | 13 |
| 178 | Maximizing Property Tuning of Phosphorus Corrole Photocatalysts through a Trifluoromethylation Approach. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 6184-6198   | 5.1   | 20 |
| 177 | Carbon Dioxide-Catalyzed Stereoselective Cyanation Reaction. <i>ACS Catalysis</i> , <b>2019</b> , 9, 6006-6011  | 13.1  | 13 |
| 176 | The Mechanism of Copper-Catalyzed Trifunctionalization of Terminal Allenes. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 9456-9463   | 4.8   | 6  |
| 175 | Aldehyde Carboxylation: A Concise DFT Mechanistic Study and a Hypothetical Role of CO <sub>2</sub> in the Origin of Life. <i>Synlett</i> , <b>2019</b> , 30, 987-996  | 2.2   | 4  |
| 174 | One metal is enough: a nickel complex reduces nitrate anions to nitrogen gas. <i>Chemical Science</i> , <b>2019</b> , 10, 4767-4774   | 9.4   | 21 |
| 173 | Stereoinversion of Unactivated Alcohols by Tethered Sulfonamides. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 1741-1745   | 3.6   | 9  |
| 172 | Ruthenium catalyzes the synthesis of $\beta$ -butenolides fused with cyclohexanones. <i>Chemical Communications</i> , <b>2019</b> , 55, 2940-2943   | 5.8   | 12 |
| 171 | Schrock vs Fischer carbenes: A quantum chemical perspective. <i>Advances in Inorganic Chemistry</i> , <b>2019</b> , 385-443   | 2.1   | 4  |
| 170 | Disrotatory Ring-Opening of Furans Gives Stereocontrol. <i>Journal of Organic Chemistry</i> , <b>2019</b> , 84, 11061-11067   | 10.67 | 3  |
| 169 | Positive shift in corrole redox potentials leveraged by modest $\mu$ CF-substitution helps achieve efficient photocatalytic C-H bond functionalization by group 13 complexes. <i>Dalton Transactions</i> , <b>2019</b> , 48, 12279-12286                      | 4.3   | 14 |
| 168 | Enantioselective Intermolecular Excited-State Photoreactions Using a Chiral Ir Triplet Sensitizer: Separating Association from Energy Transfer in Asymmetric Photocatalysis. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 13625-13634 | 16.4  | 71 |
| 167 | Mechanism of Palladium-Catalyzed C $\equiv$ N Coupling with 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) as a Base. <i>ACS Catalysis</i> , <b>2019</b> , 9, 6851-6856   | 13.1  | 11 |
| 166 | Regioselective Oxidation of C-H Bonds in Unactivated Alkanes by a Vanadium Superoxo Catalyst Bound to a Supramolecular Host. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 16250-16255   | 5.1   | 2  |
| 165 | How bulky ligands control the chemoselectivity of Pd-catalyzed -arylation of ammonia. <i>Chemical Science</i> , <b>2019</b> , 11, 1017-1025   | 9.4   | 10 |

|     |  |      |     |
|-----|--|------|-----|
| 164 | Brønsted acid catalysis of photosensitized cycloadditions. <i>Chemical Science</i> , <b>2019</b> , 11, 856-861   | 9.4  | 25  |
| 163 | How Many O-Donor Groups in Enterobactin Does It Take to Bind a Metal Cation?. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 6955-6962  | 4.8  | 2   |
| 162 | Gold(I)-Catalyzed Hydroxy Group Assisted C(sp)-H Alkylation of Enaminones with Diazo Compounds To Access 3-Alkyl Chromones. <i>Organic Letters</i> , <b>2019</b> , 21, 335-339                                       | 6.2  | 35  |
| 161 | Dimerization Strategies for the Synthesis of High-Order Securinega Alkaloids. <i>Journal of Organic Chemistry</i> , <b>2019</b> , 84, 1398-1406  | 4.2  | 6   |
| 160 | Directing Foldamer Self-Assembly with a Cyclopropanoyl Cap. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 2226-2233  | 4.8  | 1   |
| 159 | Stereoinversion of Unactivated Alcohols by Tethered Sulfonamides. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 1727-1731   | 16.4 | 34  |
| 158 | Reductive Carbocyclization of Homoallylic Alcohols to syn-Cyclobutanes by a Boron-Catalyzed Dual Ring-Closing Pathway. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 2722-2726                                       | 3.6  | 8   |
| 157 | Room temperature olefination of methane with titanium-carbon multiple bonds. <i>Chemical Science</i> , <b>2018</b> , 9, 3376-3385  | 9.4  | 12  |
| 156 | Selective formation of $\beta$ -lactams via C-H amidation enabled by tailored iridium catalysts. <i>Science</i> , <b>2018</b> , 359, 1016-1021   | 33.3 | 188 |
| 155 | Catalytic Asymmetric Dearomatization by Visible-Light-Activated [2+2] Photocycloaddition. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 6350-6354  | 3.6  | 33  |
| 154 | Catalytic Asymmetric Dearomatization by Visible-Light-Activated [2+2] Photocycloaddition. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 6242-6246   | 16.4 | 99  |
| 153 | Unusual solvent polarity dependent excitation relaxation dynamics of a bis[p-ethynylthiobenzoato]Pd-linked bis[(porphinato)zinc] complex. <i>Molecular Systems Design and Engineering</i> , <b>2018</b> , 3, 275-284 | 4.6  | 1   |
| 152 | Designing Redox-Stable Cobalt Polypyridyl Complexes for Redox Flow Batteries: Spin-Crossover Delocalizes Excess Charge. <i>Advanced Energy Materials</i> , <b>2018</b> , 8, 1702897                                  | 21.8 | 26  |
| 151 | Understanding the Origin of the Regioselectivity in Cyclopolymerizations of Diynes and How to Completely Switch It. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 834-841                     | 16.4 | 19  |
| 150 | Reductive Carbocyclization of Homoallylic Alcohols to syn-Cyclobutanes by a Boron-Catalyzed Dual Ring-Closing Pathway. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 2692-2696                | 16.4 | 23  |
| 149 | Palladium-Catalyzed Divergent Arylation of Triazolopyridines: A Computational Study. <i>Chemistry - an Asian Journal</i> , <b>2018</b> , 13, 2505-2510   | 4.5  | 2   |
| 148 | Scorpionate Catalysts for Coupling CO and Epoxides to Cyclic Carbonates: A Rational Design Approach for Organocatalysts. <i>Journal of Organic Chemistry</i> , <b>2018</b> , 83, 9370-9380                           | 4.2  | 43  |
| 147 | Amphiphile self-assembly dynamics at the solution-solid interface reveal asymmetry in head/tail desorption. <i>Chemical Communications</i> , <b>2018</b> , 54, 10076-10079   | 5.8  | 7   |



|     |   |      |     |
|-----|---|------|-----|
| 146 | One-pot bifunctionalization of unactivated alkenes, P(O)H compounds, and N-methoxypyridinium salts for the construction of $\pi$ -pyridyl alkylphosphonates. <i>Organic Chemistry Frontiers</i> , <b>2018</b> , 5, 2595-2603  | 5.2  | 15  |
| 145 | Experimental and Computational Study of the (Z)-Selective Formation of Trisubstituted Olefins and Benzo-Fused Oxacycles from the Ruthenium-Catalyzed Dehydrative C-H Coupling of Phenols with Ketones. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 10289-10296 | 16.4 | 17  |
| 144 | C-H Bond Addition across a Transient Uranium-Nitrido Moiety and Formation of a Parent Uranium Imido Complex. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 11335-11340   | 16.4 | 32  |
| 143 | Conjugate Addition of Perfluoroarenes to $\pi$ -Unsaturated Carbonyls Enabled by an Alkoxide-Hydrosilane System: Implication of a Radical Pathway. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 9659-9668   | 16.4 | 13  |
| 142 | Oxidation of Cymantrene Analogues of Ferrocifen: Electrochemical, Spectroscopic, and Computational Studies of the Parent Complex 1,1'-Diphenyl-2-cymantrenylbutene. <i>Organometallics</i> , <b>2018</b> , 37, 1910-1918  | 3.8  | 6   |
| 141 | Stereoselective construction of sterically hindered oxaspirocycles chiral bidentate directing group-mediated C(sp)-O bond formation. <i>Chemical Science</i> , <b>2018</b> , 9, 1473-1480   | 9.4  | 23  |
| 140 | Iridium-catalysed arylation of C-H bonds enabled by oxidatively induced reductive elimination. <i>Nature Chemistry</i> , <b>2018</b> , 10, 218-224  | 17.6 | 109 |
| 139 | Living Metathesis and Metallotropy Polymerization Gives Conjugated Polyenyne from Multialkynes: How to Design Sequence-Specific Cascades for Polymers. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 16320-16329   | 16.4 | 9   |
| 138 | Catalytic Borylation of Methane: Combining Computational and High-Throughput Screening Approaches to Discover a New Catalyst <b>2018</b> , 337-369  |      | 1   |
| 137 | Pitfalls in Computational Modeling of Chemical Reactions and How To Avoid Them. <i>Organometallics</i> , <b>2018</b> , 37, 3228-3239  | 3.8  | 75  |
| 136 | Palladium-Catalyzed Divergent Cyclopropanation by Regioselective Solvent-Driven C(sp <sup>3</sup> )-H Bond Activation. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 15460-15464   | 16.4 | 14  |
| 135 | Visible-Light-Induced Pyridylation of Remote C(sp <sup>3</sup> )-H Bonds by Radical Translocation of N-Alkoxypyridinium Salts. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 15517-15522   | 16.4 | 98  |
| 134 | Activation of the Basal Plane in Two Dimensional Transition Metal Chalcogenide Nanostructures. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 13663-13671   | 16.4 | 24  |
| 133 | Copper-Mediated Amination of Aryl C-H Bonds with the Direct Use of Aqueous Ammonia via a Disproportionation Pathway. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 14350-14356   | 16.4 | 56  |
| 132 | Visible-Light-Induced Pyridylation of Remote C(sp <sup>3</sup> )-H Bonds by Radical Translocation of N-Alkoxypyridinium Salts. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 15743-15748  | 3.6  | 35  |
| 131 | Rational Design of a Catalyst for the Selective Monoborylation of Methane. <i>ACS Catalysis</i> , <b>2018</b> , 8, 10021-10031  | 13.0 | 18  |
| 130 | Mechanistic study of styrene aziridination by iron(IV) nitrides. <i>Chemical Science</i> , <b>2018</b> , 9, 8542-8552   | 9.4  | 12  |
| 129 | Thermodynamic kinetic control in substituent redistribution reactions of silylium ions steered by the counteranion. <i>Chemical Science</i> , <b>2018</b> , 9, 5600-5607  | 9.4  | 25  |

|     |  |      |     |
|-----|--|------|-----|
| 128 | Rationally Designing Regiodivergent Dipolar Cycloadditions: Frontier Orbitals Show How To Switch between [5 + 3] and [4 + 2] Cycloadditions. <i>ACS Catalysis</i> , <b>2018</b> , 8, 6353-6361   | 13.1 | 20  |
| 127 | Structural elucidation of a mononuclear titanium methyldiene. <i>Chemical Communications</i> , <b>2017</b> , 53, 3415-3417   | 5.3  | 21  |
| 126 | Mechanistic Investigation of Bis(imino)pyridine Manganese Catalyzed Carbonyl and Carboxylate Hydrosilylation. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 4901-4915   | 16.4 | 75  |
| 125 | Important role of ancillary ligand in the emission behaviours of blue-emitting heteroleptic Ir(III) complexes. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 4480-4487  | 7.1  | 15  |
| 124 | Synthesis and reactivity of a mononuclear non-haem cobalt(IV)-oxo complex. <i>Nature Communications</i> , <b>2017</b> , 8, 14839   | 17.4 | 94  |
| 123 | Intramolecular Oxyl Radical Coupling Promotes O-O Bond Formation in a Homogeneous Mononuclear Mn-based Water Oxidation Catalyst: A Computational Mechanistic Investigation. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 4436-4446                                 | 5.1  | 26  |
| 122 | 3,5-Diarylimidazo[1,2-a]pyridines as Color-Tunable Fluorophores. <i>Journal of Organic Chemistry</i> , <b>2017</b> , 82, 4352-4361   | 4.2  | 16  |
| 121 | The mechanism of selective catalytic reduction of NO on Cu-SSZ-13 - a computational study. <i>Dalton Transactions</i> , <b>2017</b> , 46, 369-377  | 4.3  | 6   |
| 120 | Chemoselective Coupling of 1,1-Bis[(pinacolato)boryl]alkanes for the Transition-Metal-Free Borylation of Aryl and Vinyl Halides: A Combined Experimental and Theoretical Investigation. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 976-984 | 16.4 | 48  |
| 119 | Enantioselective Excited-State Photoreactions Controlled by a Chiral Hydrogen-Bonding Iridium Sensitizer. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 17186-17192   | 16.4 | 112 |
| 118 | Asymmetric Synthesis of (-)-6'-Fluoro-aristeromycin via Stereoselective Electrophilic Fluorination. <i>Organic Letters</i> , <b>2017</b> , 19, 5732-5735   | 6.2  | 7   |
| 117 | Computer-aided rational design of Fe(III)-catalysts for the selective formation of cyclic carbonates from CO <sub>2</sub> and internal epoxides. <i>Catalysis Science and Technology</i> , <b>2017</b> , 7, 4375-4387  | 5.5  | 24  |
| 116 | Regiodivergent Conjugate Addition Controlled by Rhodium(I) and Palladium(II) Catalysts: A Combined Computational and Experimental Study. <i>Advanced Synthesis and Catalysis</i> , <b>2017</b> , 359, 3160-3175  | 5.6  | 7   |
| 115 | Room-Temperature Ring-Opening of Quinoline, Isoquinoline, and Pyridine with Low-Valent Titanium. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 12804-12814  | 16.4 | 16  |
| 114 | Ligand-controlled Regiodivergent C-H Alkenylation of Pyrazoles and its Application to the Synthesis of Indazoles. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 16480-16484  | 3.6  | 7   |
| 113 | Ligand-controlled Regiodivergent C-H Alkenylation of Pyrazoles and its Application to the Synthesis of Indazoles. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 16262-16266   | 16.4 | 33  |
| 112 | A new and selective cycle for dehydrogenation of linear and cyclic alkanes under mild conditions using a base metal. <i>Nature Chemistry</i> , <b>2017</b> , 9, 1126-1132  | 17.6 | 37  |
| 111 | Effects of varying the 6-position oxidation state of hexopyranoses: a systematic comparative computational analysis of 48 monosaccharide stereoisomers. <i>Journal of Molecular Modeling</i> , <b>2017</b> , 23, 214   | 2    | 3   |



|     |   |      |     |
|-----|---|------|-----|
| 110 | The Electronic Structure of [Mn(V)O]: What is the Connection between Oxo Radical Character, Physical Oxidation State, and Reactivity?. <i>ACS Catalysis</i> , <b>2016</b> , 6, 7202-7216  | 13.1 | 25  |
| 109 | Mechanistic Studies of Bismuth(V)-Mediated Thioglycoside Activation Reveal Differential Reactivity of Anomers. <i>Journal of Organic Chemistry</i> , <b>2016</b> , 81, 5949-62  | 4.2  | 14  |
| 108 | Factors Affecting the Production of Aromatic Immonium Ions in MALDI 157 nm Photodissociation Studies. <i>Journal of the American Society for Mass Spectrometry</i> , <b>2016</b> , 27, 834-46                                       | 3.5  | 6   |
| 107 | Catalytic borylation of methane. <i>Science</i> , <b>2016</b> , 351, 1424-7   | 33.3 | 108 |
| 106 | Glassy carbon electrodes deliver unpredictable reduction potentials for platinum(IV) antitumor prodrugs. <i>Polyhedron</i> , <b>2016</b> , 103, 28-34   | 2.7  | 9   |
| 105 | Methionine Ligand Interaction in a Blue Copper Protein Characterized by Site-Selective Infrared Spectroscopy. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 7187-93  | 16.4 | 15  |
| 104 | Mechanism of Rh-Catalyzed Oxidative Cyclizations: Closed versus Open Shell Pathways. <i>Accounts of Chemical Research</i> , <b>2016</b> , 49, 1263-70   | 24.3 | 27  |
| 103 | Why is the Ir(III)-Mediated Amido Transfer Much Faster Than the Rh(III)-Mediated Reaction? A Combined Experimental and Computational Study. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 14020-14029        | 16.4 | 116 |
| 102 | How a [Co(IV) a bond and a half O](2+) fragment oxidizes water: involvement of a biradicaloid [Co(II)-(O?)](2+) species in forming the O-O bond. <i>ChemSusChem</i> , <b>2015</b> , 8, 844-52                                       | 8.3  | 39  |
| 101 | Computational and spectroscopic characterization of key intermediates of the Selective Catalytic Reduction cycle of NO on zeolite-supported Cu catalyst. <i>Inorganica Chimica Acta</i> , <b>2015</b> , 430, 132-143                | 2.7  | 14  |
| 100 | Carbon Dioxide Promoted H(+) Reduction Using a Bis(imino)pyridine Manganese Electrocatalyst. <i>Inorganic Chemistry</i> , <b>2015</b> , 54, 4475-82   | 5.1  | 41  |
| 99  | Addition of Si-H and B-H bonds and redox reactivity involving low-coordinate nitrido-vanadium complexes. <i>Inorganic Chemistry</i> , <b>2015</b> , 54, 3068-77   | 5.1  | 18  |
| 98  | The origin of the ligand-controlled regioselectivity in Rh-catalyzed [(2 + 2) + 2] carbocyclizations: steric stereoelectronic effects. <i>Chemical Science</i> , <b>2015</b> , 6, 6896-6900   | 9.4  | 8   |
| 97  | Complete Switch of Selectivity in the C-H Alkenylation and Hydroarylation Catalyzed by Iridium: The Role of Directing Groups. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 13448-51                         | 16.4 | 109 |
| 96  | Cyclo-P[Complexes of Vanadium: Redox Properties and Origin of the $\delta$ P NMR Chemical Shift. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 15247-61  | 16.4 | 35  |
| 95  | Mechanism of redox-active ligand-assisted nitrene-group transfer in a Zr(IV) complex: direct ligand-to-ligand charge transfer preferred. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 1780-9                           | 4.8  | 8   |
| 94  | Intramolecular ring-opening from a CO-derived nucleophile as the origin of selectivity for 5-substituted oxazolidinone from the (salen)Cr-catalyzed [aziridine + CO] coupling. <i>Chemical Science</i> , <b>2015</b> , 6, 1293-1300 | 9.4  | 38  |
| 93  | How a redox-innocent metal promotes the formal reductive elimination of biphenyl using redox-active ligands. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 4308-14  | 4.8  | 11  |

|    |  |      |    |
|----|--|------|----|
| 92 | A computational study of the mechanism of the [(salen)Cr + DMAP]-catalyzed formation of cyclic carbonates from CO <sub>2</sub> and epoxide. <i>Chemical Communications</i> , <b>2014</b> , 50, 2676-8  | 5.8  | 56 |
| 91 | Switching the enantioselectivity in catalytic [4 + 1] cycloadditions by changing the metal center: principles of inverting the stereochemical preference of an asymmetric catalysis revealed by DFT calculations. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 9414-23 | 16.4 | 16 |
| 90 | Binary role of an ylide in formation of a terminal methyldene complex of niobium. <i>Chemical Communications</i> , <b>2014</b> , 50, 6267-9  | 5.8  | 25 |
| 89 | Understanding intrinsically irreversible, non-Nernstian, two-electron redox processes: a combined experimental and computational study of the electrochemical activation of platinum(IV) antitumor prodrugs. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 8992-9000    | 16.4 | 48 |
| 88 | [(Salcen)Cr(III) + Lewis base]-catalyzed synthesis of N-aryl-substituted oxazolidinones from epoxides and aryl isocyanates. <i>Chemical Communications</i> , <b>2014</b> , 50, 15187-90  | 5.8  | 39 |
| 87 | Synthesis and structural characterization of hexacoordinate silicon, germanium, and titanium complexes of the E. coli siderophore enterobactin. <i>Chemistry - A European Journal</i> , <b>2013</b> , 19, 10536-42   | 4.8  | 35 |
| 86 | A four-coordinate thionitrosyl complex of vanadium. <i>Chemical Communications</i> , <b>2013</b> , 49, 2768-70   | 5.8  | 14 |
| 85 | Understanding the competitive dehydroalkoxylation and dehydrogenation of ethers with TiCl <sub>4</sub> multiple bonds. <i>Chemical Science</i> , <b>2013</b> , 4, 2543   | 9.4  | 10 |
| 84 | Studies of iron-mediated Pauson-Khand reactions of 1,1-disubstituted-allenylsilanes: mechanistic implications for a reactive three-membered iron metallacycle. <i>Chemical Science</i> , <b>2013</b> , 4, 238-247  | 9.4  | 15 |
| 83 | Understanding intermolecular C-F bond activation by a transient titanium neopentylidyne: experimental and theoretical studies on the competition between 1,2-CF bond addition and [2 + 2]-cycloaddition/fluoride elimination. <i>Dalton Transactions</i> , <b>2013</b> , 42, 4163-74           | 4.3  | 12 |
| 82 | Epitope fluctuations in the human papillomavirus are under dynamic allosteric control: a computational evaluation of a new vaccine design strategy. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 18458-68  | 16.4 | 16 |
| 81 | The mechanism of O-O bond formation in Tanaka's water oxidation catalyst. <i>Angewandte Chemie - International Edition</i> , <b>2012</b> , 51, 1221-4  | 16.4 | 37 |
| 80 | Stereoselective rhodium-catalyzed [3 + 2 + 1] carbocyclization of alkenylidenecyclopropanes with carbon monoxide: theoretical evidence for a trimethylenemethane metallacycle intermediate. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 20569-72                      | 16.4 | 86 |
| 79 | The mechanism of guanine alkylation by nitrogen mustards: a computational study. <i>Journal of Organic Chemistry</i> , <b>2012</b> , 77, 5914-21   | 4.2  | 61 |
| 78 | A planar three-coordinate vanadium(II) complex and the study of terminal vanadium nitrides from N <sub>2</sub> : a kinetic or thermodynamic impediment to N-N bond cleavage?. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 13035-45                                    | 16.4 | 65 |
| 77 | The Mechanism of O-O Bond Formation in Tanaka's Water Oxidation Catalyst. <i>Angewandte Chemie</i> , <b>2012</b> , 124, 1247-1250  | 3.6  | 13 |
| 76 | Room temperature dehydrogenation of ethane to ethylene. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 10700-3   | 16.4 | 77 |
| 75 | 1,2-CF bond activation of perfluoroarenes and alkylidene isomers of titanium. DFT analysis of the C-F bond activation pathway and rotation of the titanium alkylidene moiety. <i>Journal of Organometallic Chemistry</i> , <b>2011</b> , 696, 4138-4146  | 2.3  | 9  |

|    |   |      |    |
|----|---|------|----|
| 74 | Ring-slippage and multielectron redox properties of Fe/Ru/Os-bis(arene) complexes: does hapticity change really cause potential inversion?. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 18234-42   | 16.4 | 13 |
| 73 | Computational Studies: Cisplatin <b>2011</b> ,  |      | 1  |
| 72 | Methane activation and exchange by titanium-carbon multiple bonds. <i>Chemical Science</i> , <b>2011</b> , 2, 1457  | 9.4  | 61 |
| 71 | Redox properties of Tanaka's water oxidation catalyst: redox noninnocent ligands dominate the electronic structure and reactivity. <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 5946-57   | 5.1  | 34 |
| 70 | Die E.-coli-Siderophore Enterobactin und Salmochelin bilden sechsfach koordinierte Siliciumkomplexe bei physiologischen pH-Werten. <i>Angewandte Chemie</i> , <b>2011</b> , 123, 4317-4321  | 3.6  | 4  |
| 69 | The E. coli siderophores enterobactin and salmochelin form six-coordinate silicon complexes at physiological pH. <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 4230-3  | 16.4 | 20 |
| 68 | Conformational and electronic consequences in crafting extended, $\pi$ -conjugated, light-harvesting macrocycles. <i>Chemistry - A European Journal</i> , <b>2011</b> , 17, 14539-51  | 4.8  | 17 |
| 67 | Computationally designed and experimentally confirmed diastereoselective rhodium-catalyzed Pauson-Khand reaction at room temperature. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 7621-3   | 16.4 | 40 |
| 66 | Improving usability and accessibility of cheminformatics tools for chemists through cyberinfrastructure and education. <i>In Silico Biology</i> , <b>2011</b> , 11, 41-60   | 2    | 2  |
| 65 | Two-electron redox energetics in ligand-bridged dinuclear molybdenum and tungsten complexes. <i>Inorganic Chemistry</i> , <b>2010</b> , 49, 4611-9  | 5.1  | 20 |
| 64 | Synthetic and Mechanistic Studies of the Ring Opening and Denitrogenation of Pyridine and Picolines by Ti $\equiv$ C Multiple Bonds <i>Organometallics</i> , <b>2010</b> , 29, 5409-5422  | 3.8  | 18 |
| 63 | Torsionally responsive C <sub>3</sub> -symmetric azo dyes: azo-hydrazone tautomerism, conformational switching, and application for chemical sensing. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 12133-44   | 16.4 | 86 |
| 62 | Intermolecular C-H bond activation of benzene and pyridines by a vanadium(III) alkylidene including a stepwise conversion of benzene to a vanadium-benzynes complex. <i>Chemical Science</i> , <b>2010</b> , 1, 351   | 9.4  | 58 |
| 61 | DFT Studies on the Thermal Activation of Molecular Oxygen by Bare [Ni(H)(OH)] <sup>+</sup> . <i>Helvetica Chimica Acta</i> , <b>2009</b> , 92, 151-164  | 2    | 10 |
| 60 | Spin crossover-coupled electron transfer of [M(tacn)(2)](3+/2+) complexes (tacn = 1,4,7-triazacyclononane; M = Cr, Mn, Fe, Co, Ni). <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 6189-97  | 16.4 | 39 |
| 59 | ESI-MS, DFT, and synthetic studies on the H(2)-mediated coupling of acetylene: insertion of C=X bonds into rhodacyclopentadienes and Brønsted acid cocatalyzed hydrogenolysis of organorhodium intermediates. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 16054-62 | 16.4 | 75 |
| 58 | A redox non-innocent ligand controls the life time of a reactive quartet excited state - an MCSCF study of [Ni(H)(OH)] <sup>+</sup> . <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 12634-42   | 16.4 | 32 |
| 57 | A Transient Vanadium(III) Neopentylidene Complex. Redox Chemistry and Reactivity of the V $\equiv$ CHtBu Functionality. <i>Organometallics</i> , <b>2009</b> , 28, 843-852  | 3.8  | 43 |

|    |  |      |     |
|----|--|------|-----|
| 56 | Computational Studies: Cisplatin <b>2009</b> ,   |      | 1   |
| 55 | Inorganic Models for Two-Electron Redox Chemistry in Biological Systems. <i>ACS Symposium Series</i> , <b>2009</b> , 151-166   | 0.4  | 3   |
| 54 | Understanding and predicting distorted T- versus Y-geometries for neutral chromous complexes supported by a sterically encumbering beta-diketiminato ligand. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 17351-61                     | 16.4 | 30  |
| 53 | Pi*-pi* bonding interactions generated by halogen oxidation of zirconium(IV) redox-active ligand complexes. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 4364-74   | 16.4 | 82  |
| 52 | The mechanism of water oxidation catalysis promoted by [tpyRu(IV)=O]2L3+: a computational study. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 16231-40   | 16.4 | 77  |
| 51 | The mechanism of the rhodium(I)-catalyzed [2 + 2 + 1] carbocyclization reaction of dienes and CO: a computational study. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 5821-30  | 16.4 | 28  |
| 50 | The effect of one valence electron: contrasting (PNP)Ni(CO) with (PNP)Ni(NO) to understand the half-bent NiNO unit. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 3888-92   | 5.1  | 15  |
| 49 | Why does cyanide pretend to be a weak field ligand in [Cr(CN)5]3-?. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 4413-20   | 5.1  | 13  |
| 48 | Dendritic molecular switch: chiral folding and helicity inversion. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 16812-22   | 16.4 | 52  |
| 47 | Lewis acid stabilized methyldiene and oxoscandium complexes. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 14438-9  | 16.4 | 94  |
| 46 | Computational study of the binding of CuII to Alzheimer's amyloid-beta peptide: do Abeta42 and Abeta40 bind copper in identical fashion?. <i>Journal of Biological Inorganic Chemistry</i> , <b>2008</b> , 13, 1197-204  | 3.7  | 26  |
| 45 | Mechanistic insight into the diastereoselective rhodium-catalyzed Pauson-Khand reaction: role of coordination number in stereocontrol. <i>Angewandte Chemie - International Edition</i> , <b>2008</b> , 47, 342-5  | 16.4 | 42  |
| 44 | Cyanide: a strong-field ligand for ferrohemes and hemoproteins?. <i>Angewandte Chemie - International Edition</i> , <b>2008</b> , 47, 10144-6  | 16.4 | 39  |
| 43 | Mechanistic Insight into the Diastereoselective Rhodium-Catalyzed Pauson-Khand Reaction: Role of Coordination Number in Stereocontrol. <i>Angewandte Chemie</i> , <b>2008</b> , 120, 348-351   | 3.6  | 11  |
| 42 | Cyanide: A Strong-Field Ligand for Ferrohemes and Hemoproteins?. <i>Angewandte Chemie</i> , <b>2008</b> , 120, 10298-10300   | 3.6  | 10  |
| 41 | Intermolecular C-H bond activation reactions promoted by transient titanium alkylidynes. Synthesis, reactivity, kinetic, and theoretical studies of the Ti[triple bond]C linkage. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 8781-93 | 16.4 | 101 |
| 40 | Bifunctional binding of cisplatin to DNA: why does cisplatin form 1,2-intrastrand cross-links with ag but not with GA?. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 5023-30   | 16.4 | 77  |
| 39 | Synthesis, structure, and properties of low-spin manganese(III)-poly(pyrazolyl)borate complexes. <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 2596-603   | 5.1  | 22  |

|    |  |      |     |
|----|--|------|-----|
| 38 | A Co <sub>2</sub> N <sub>2</sub> diamond-core resting state of cobalt(I): a three-coordinate CoI synthon invoking an unusual pincer-type rearrangement. <i>Angewandte Chemie - International Edition</i> , <b>2006</b> , 45, 3291-5  | 16.4 | 94  |
| 37 | cis,cis-[(bpy) <sub>2</sub> RuVO]2O <sub>4</sub> <sup>+</sup> catalyzes water oxidation formally via in situ generation of radicaloid RuIV-O*. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 7476-85  | 16.4 | 159 |
| 36 | Studies of the generation and pericyclic behavior of cyclic pentadienyl carbanions. Alkylation reactions as an efficient route to functionalized cis-bicyclo[3.3.0]octenes. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 12339-48                            | 16.4 | 24  |
| 35 | Evidence for spontaneous resolution of icosahedral proline. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 15988-9   | 16.4 | 14  |
| 34 | Chirally directed formation of nanometer-scale proline clusters. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 10833-9  | 16.4 | 30  |
| 33 | Room temperature ring-opening metathesis of pyridines by a transient Ti[triple bond]C linkage. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 6798-9   | 16.4 | 71  |
| 32 | What difference one double bond makes: Electronic structure of saturated and unsaturated n-heterocyclic carbene ligands in Grubbs 2nd generation-type catalysts. <i>Journal of Organometallic Chemistry</i> , <b>2006</b> , 691, 5505-5512   | 2.3  | 17  |
| 31 | Direct nitric oxide detection in aqueous solution by copper(II) fluorescein complexes. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 14364-73   | 16.4 | 237 |
| 30 | Copper clusters built on bulky amidinate ligands: spin delocalization via superexchange rather than direct metal-metal bonding. <i>Chemical Communications</i> , <b>2005</b> , 1043-5  | 5.8  | 25  |
| 29 | Alpha,beta-(C-C-C) agostic bonds in transition metal based olefin metathesis catalyses. <i>Dalton Transactions</i> , <b>2005</b> , 2982-4  | 4.3  | 50  |
| 28 | A facile approach to a d <sup>4</sup> RuN: moiety. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 5330-1   | 16.4 | 74  |
| 27 | Intermolecular C-H bond activation promoted by a titanium alkylidyne. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 16016-7   | 16.4 | 119 |
| 26 | Diastereoselective intermolecular rhodium-catalyzed [4 + 2 + 2] carbocyclization reactions: computational and experimental evidence for the intermediacy of an alternative metallacycle intermediate. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 1602-3    | 16.4 | 43  |
| 25 | A unique approach to metal-induced Bergman cyclization: long-range enediyne activation by ligand-to-metal charge transfer. <i>Angewandte Chemie - International Edition</i> , <b>2005</b> , 44, 592-5  | 16.4 | 29  |
| 24 | DL-Proline. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2005</b> , 61, o506-8   |      | 42  |
| 23 | Theoretical investigation of the metal-metal interaction in dimolybdenum complexes with bridging hydride and methyl ligands. <i>Polyhedron</i> , <b>2004</b> , 23, 2879-2900   | 2.7  | 47  |
| 22 | Electronic structure of the water-oxidation catalyst [(bpy) <sub>2</sub> (OHx)RuORu(OHy)(bpy) <sub>2</sub> ] <sup>z+</sup> : weak coupling between the metal centers is preferred over strong coupling. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 13222-3 | 16.4 | 62  |
| 21 | Dioxygen activation in methane monooxygenase: a theoretical study. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 2978-90  | 16.4 | 114 |



|    |   |      |     |
|----|---|------|-----|
| 20 | Hydrogen Transfer between Ligands: A Density Functional Study of the Rearrangement of $M(\eta^5-C_7H_8)_2$ into $M(\eta^5-C_7H_7)(\eta^5-C_7H_9)$ [ $M = Mo, Mo^+, Zr$ ]. <i>Organometallics</i> , <b>2004</b> , 23, 2658-2669              | 3.8  | 7   |
| 19 | Terminal vanadium-neopentylidyne complexes and intramolecular cross-metathesis reactions to generate azametallacyclohexatrienes. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 10506-7                               | 16.4 | 59  |
| 18 | Terminal and four-coordinate vanadium(IV) phosphinidene complexes. A pseudo Jahn-Teller effect of second order stabilizing the V-P multiple bond. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 1924-5               | 16.4 | 72  |
| 17 | Terminal Acetylenes React to Increase Unsaturation in $[(tBu_2PCH_2SiMe_2)_2N]Re(H)_4$ . <i>Organometallics</i> , <b>2004</b> , 23, 4934-4943   | 3.8  | 13  |
| 16 | Proton as the simplest of all catalysts for [2 + 2] cycloadditions: DFT study of acid-catalyzed imine metathesis. <i>Journal of Organic Chemistry</i> , <b>2004</b> , 69, 6173-84   | 4.2  | 9   |
| 15 | Kinetics and thermodynamics of H. transfer from $(\eta^5-C_5R_5)Cr(CO)_3H$ ( $R = Ph, Me, H$ ) to methyl methacrylate and styrene. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 10093-102                           | 16.4 | 50  |
| 14 | cis-[Pt(NH <sub>3</sub> ) <sub>2</sub> (L)] <sup>2+/+</sup> (L = Cl, H <sub>2</sub> O, NH <sub>3</sub> ) binding to purines and CO: does pi-back-donation play a role?. <i>Inorganic Chemistry</i> , <b>2003</b> , 42, 8615-7               | 5.1  | 16  |
| 13 | Theoretical study of cisplatin binding to purine bases: why does cisplatin prefer guanine over adenine?. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 14082-92  | 16.4 | 229 |
| 12 | Mechanistic studies on the hydroxylation of methane by methane monooxygenase. <i>Chemical Reviews</i> , <b>2003</b> , 103, 2385-419   | 68.1 | 407 |
| 11 | Peripheral heme substituents control the hydrogen-atom abstraction chemistry in cytochromes P450. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2003</b> , 100, 6998-7002                     | 11.5 | 138 |
| 10 | Hydroxylation of methane by non-heme diiron enzymes: molecular orbital analysis of C-H bond activation by reactive intermediate Q. <i>Journal of the American Chemical Society</i> , <b>2002</b> , 124, 14608-15                            | 16.4 | 61  |
| 9  | Ab initio quantum calculation of the diabatic coupling matrix elements for the self-exchange redox couples $M(Cp)_2^{0/+}$ ( $M = Fe, Co$ ; $Cp = C_5H_5$ ). <i>Inorganic Chemistry</i> , <b>2002</b> , 41, 5926-7                          | 5.1  | 10  |
| 8  | Theoretical study on the stability of N-glycosyl bonds: why does N7-platination not promote depurination?. <i>Journal of the American Chemical Society</i> , <b>2002</b> , 124, 4495-503  | 16.4 | 84  |
| 7  | Computing Redox Potentials in Solution: Density Functional Theory as A Tool for Rational Design of Redox Agents. <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 7407-7412  | 2.8  | 319 |
| 6  | Density functional theory study of redox pairs: 2. Influence of solvation and ion-pair formation on the redox behavior of cyclooctatetraene and nitrobenzene. <i>Journal of the American Chemical Society</i> , <b>2002</b> , 124, 11167-81 | 16.4 | 47  |
| 5  | Theoretical studies of diiron(II) complexes that model features of the dioxygen-activating centers in non-heme diiron enzymes. <i>Israel Journal of Chemistry</i> , <b>2001</b> , 41, 173-186   | 3.4  | 8   |
| 4  | Using Density Functional Theory To Design DNA Base Analogues with Low Oxidation Potentials. <i>Journal of Physical Chemistry B</i> , <b>2001</b> , 105, 6437-6444   | 3.4  | 69  |
| 3  | Synthesis, structure, and electronic properties of monomeric and dimeric trispyrazolylborate platinum(II) hydride complexes. <i>Inorganic Chemistry</i> , <b>2001</b> , 40, 4726-32   | 5.1  | 38  |



- |   |  |      |    |
|---|--|------|----|
| 2 | An experimental and computational analysis of the formation of the terminal nitrido complex (eta3-Cp*)2Mo(N)(N3) by elimination of N2 from Cp*2Mo(N3)2: the barrier to elimination is strongly influenced by the exo versus endo configuration of the azide ligand. <i>Journal of the American Chemical Society</i> , <b>2001</b> , 123, 10111-2 | 16.4 | 19 |
| 1 | Density Functional Theory Study of Redox Pairs. 1. Dinuclear Iron Complexes That Undergo Multielectron Redox Reactions Accompanied by a Reversible Structural Change. <i>Journal of the American Chemical Society</i> , <b>2000</b> , 122, 9143-9154   | 16.4 | 52 |