

Xinhao Zhang

List of Publications by Year in descending order

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125
papers

5,348
citations

76326

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102487

66
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143
all docs

143
docs citations

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times ranked

4564
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|---|------|-----------|
| 1 | Palladium-Catalyzed <i>meta</i> -Selective C–H Bond Activation with a Nitrile-Containing Template: Computational Study on Mechanism and Origins of Selectivity. <i>Journal of the American Chemical Society</i> , 2014, 136, 344-355. | 13.7 | 317 |
| 2 | Computational Organic Chemistry: Bridging Theory and Experiment in Establishing the Mechanisms of Chemical Reactions. <i>Journal of the American Chemical Society</i> , 2015, 137, 1706-1725. | 13.7 | 271 |
| 3 | Role of <i>N</i> -Acyl Amino Acid Ligands in Pd(II)-Catalyzed Remote C–H Activation of Tethered Arenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 894-897. | 13.7 | 263 |
| 4 | Mechanism, Reactivity, and Selectivity in Palladium-Catalyzed Redox-Relay Heck Arylations of Alkenyl Alcohols. <i>Journal of the American Chemical Society</i> , 2014, 136, 1960-1967. | 13.7 | 187 |
| 5 | Copper-Catalyzed Radical 1,4-Difunctionalization of 1,3-Enynes with Alkyl Diacyl Peroxides and <i>N</i> -Fluorobenzenesulfonimide. <i>Journal of the American Chemical Society</i> , 2019, 141, 548-559. | 13.7 | 162 |
| 6 | Ligand-Controlled Remarkable Regio- and Stereodivergence in Intermolecular Hydrosilylation of Internal Alkynes: Experimental and Theoretical Studies. <i>Journal of the American Chemical Society</i> , 2013, 135, 13835-13842. | 13.7 | 135 |
| 7 | Iron-Catalyzed Carboamination of Olefins: Synthesis of Amines and Disubstituted β -Amino Acids. <i>Journal of the American Chemical Society</i> , 2017, 139, 13076-13082. | 13.7 | 131 |
| 8 | Copper-Catalyzed Enantioselective Radical 1,4-Difunctionalization of 1,3-Enynes. <i>Journal of the American Chemical Society</i> , 2020, 142, 18014-18021. | 13.7 | 109 |
| 9 | New Mechanistic Insights on the Selectivity of Transition-Metal-Catalyzed Organic Reactions: The Role of Computational Chemistry. <i>Accounts of Chemical Research</i> , 2016, 49, 1302-1310. | 15.6 | 100 |
| 10 | Metal-Free [2+2+2] Cycloaddition of Ynamides and Nitriles: Mild and Regioselective Synthesis of Fully Substituted Pyridines. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 9704-9708. | 13.8 | 96 |
| 11 | A Combined IMMS/DFT Study on [Pd(MPAA)]-Catalyzed Enantioselective C–H Activation: Relay of Chirality through a Rigid Framework. <i>Chemistry - A European Journal</i> , 2015, 21, 11180-11188. | 3.3 | 94 |
| 12 | Generation of Halomethyl Radicals by Halogen Atom Abstraction and Their Addition Reactions with Alkenes. <i>Journal of the American Chemical Society</i> , 2019, 141, 16643-16650. | 13.7 | 91 |
| 13 | Conversion of Methane to Methanol: Nickel, Palladium, and Platinum (d^{9}) Cations as Catalysts for the Oxidation of Methane by Ozone at Room Temperature. <i>Chemistry - A European Journal</i> , 2010, 16, 11605-11610. | 3.3 | 89 |
| 14 | Synthesis of Indolo[2,1- <i>a</i>]isoquinolines via a Triazene-Directed C–H Annulation Cascade. <i>Journal of Organic Chemistry</i> , 2014, 79, 11863-11872. | 3.2 | 87 |
| 15 | Iron-catalyzed carboazidation of alkenes and alkynes. <i>Nature Communications</i> , 2019, 10, 122. | 12.8 | 83 |
| 16 | Highly Regio- and Stereoselective Hydrosilylation of Internal Thioalkynes under Mild Conditions. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 5632-5635. | 13.8 | 77 |
| 17 | A diversity-oriented synthesis of bioactive benzanilides via a regioselective $C(sp^2)$ -H hydroxylation strategy. <i>Chemical Science</i> , 2016, 7, 2229-2238. | 7.4 | 74 |
| 18 | Rhodium-Catalyzed Regioselective N^2 -Alkylation of Benzotriazoles with Diazo Compounds/Enynones via a Nonclassical Pathway. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 12489-12493. | 13.8 | 73 |

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|----|---|------|-----------|
| 19 | Assembling a Hybrid Pd Catalyst from a Chiral Anionic Co ^{III} Complex and Ligand for Asymmetric C(sp ³)–H Functionalization. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1803-1807. | 13.8 | 73 |
| 20 | Enantioselective Addition of Cyclic Ketones to Unactivated Alkenes Enabled by Amine/Pd(II) Cooperative Catalysis. <i>ACS Catalysis</i> , 2019, 9, 791-797. | 11.2 | 72 |
| 21 | Palladium-catalyzed benzo[d]isoxazole synthesis by C–H activation/[4 + 1] annulation. <i>Chemical Science</i> , 2014, 5, 1574-1578. | 7.4 | 67 |
| 22 | Structure and Chemistry of the Heteronuclear Oxo-Cluster [VPO ₄] ⁺ : A Model System for the Gas-Phase Oxidation of Small Hydrocarbons. <i>Journal of the American Chemical Society</i> , 2013, 135, 3711-3721. | 13.7 | 66 |
| 23 | Iron-catalysed asymmetric carboazidation of styrenes. <i>Nature Catalysis</i> , 2021, 4, 28-35. | 34.4 | 60 |
| 24 | ¹³ C-Amino Butyric Acid (GABA) Synthesis Enabled by Copper-Catalyzed Carboamination of Alkenes. <i>Organic Letters</i> , 2017, 19, 4718-4721. | 4.6 | 59 |
| 25 | Access to N-Substituted α -Pyridones by Catalytic Intermolecular Dearomatization and 1,4-Acyl Transfer. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1980-1984. | 13.8 | 58 |
| 26 | A Combined DFT/IM-MS Study on the Reaction Mechanism of Cationic Ru(II)-Catalyzed Hydroboration of Alkynes. <i>ACS Catalysis</i> , 2017, 7, 1361-1368. | 11.2 | 56 |
| 27 | Diastereo- and Enantioselective Catalytic Radical Oxysulfonylation of Alkenes in α,β -Unsaturated Ketoximes. <i>CheM</i> , 2020, 6, 1692-1706. | 11.7 | 55 |
| 28 | A bioinspired and biocompatible ortho-sulfiliminy phenol synthesis. <i>Nature Communications</i> , 2017, 8, 15912. | 12.8 | 54 |
| 29 | Conjugate Addition vs Heck Reaction: A Theoretical Study on Competitive Coupling Catalyzed by Isoelectronic Metal (Pd(II) and Rh(I)). <i>Journal of Organic Chemistry</i> , 2012, 77, 7487-7496. | 3.2 | 53 |
| 30 | Mechanistic Study on Cu(II)-Catalyzed Oxidative Cross-Coupling Reaction between Arenes and Boronic Acids under Aerobic Conditions. <i>Journal of the American Chemical Society</i> , 2018, 140, 5579-5587. | 13.7 | 52 |
| 31 | A Combined Computational and Experimental Study of Rh-Catalyzed C–H Silylation with Silacyclobutanes: Insights Leading to a More Efficient Catalyst System. <i>Journal of the American Chemical Society</i> , 2021, 143, 3571-3582. | 13.7 | 52 |
| 32 | Bonding in Cationic MCH ₂ ⁺ (M=La, Hf–Rn): A Theoretical Study on Periodic Trends. <i>Chemistry - A European Journal</i> , 2010, 16, 5882-5888. | 3.3 | 51 |
| 33 | Silicon-Containing Formal 4-Electron Four-Membered Ring Systems: Antiaromatic, Aromatic, or Nonaromatic?. <i>Chemistry - A European Journal</i> , 2012, 18, 7516-7524. | 3.3 | 51 |
| 34 | Why does Togni's reagent I exist in the high-energy hypervalent iodine form? Re-evaluation of benziodoxole based hypervalent iodine reagents. <i>Chemical Communications</i> , 2016, 52, 5371-5374. | 4.1 | 50 |
| 35 | Total Synthesis of Incarvilleatone and Incarviditone: Insight into Their Biosynthetic Pathways and Structure Determination. <i>Organic Letters</i> , 2012, 14, 4878-4881. | 4.6 | 46 |
| 36 | Thermal Activation of Methane and Ethene by Bare MO ₂ ⁺ (M=Ge, Sn, and Pb): A Combined Theoretical/Experimental Study. <i>Chemistry - A European Journal</i> , 2011, 17, 9619-9625. | 3.3 | 45 |

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|----|---|------|-----------|
| 37 | Organocatalytic nitrogen transfer to unactivated olefins via transient oxaziridines. <i>Nature Catalysis</i> , 2020, 3, 386-392. | 34.4 | 45 |
| 38 | Ligand-Controlled Reactivity, Selectivity, and Mechanism of Cationic Ruthenium-Catalyzed Hydrosilylations of Alkynes, Ketones, and Nitriles: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 8856-8864. | 3.2 | 44 |
| 39 | Synthetic Study of 1,3-Butadiene-Based IMDA Approach to Construct a [5 ⁺ 7 ⁺ 6] Tricyclic Core and Its Application to the Total Synthesis of C8-epi-Guanacastepene O. <i>Journal of Organic Chemistry</i> , 2006, 71, 6892-6897. | 3.2 | 42 |
| 40 | Computational Studies on the Mechanism of the Copper-Catalyzed sp^3 -C-H Cross-Dehydrogenative Coupling Reaction. <i>ChemPlusChem</i> , 2013, 78, 943-951. | 2.8 | 42 |
| 41 | Enantioselective Formation of Cyano-Bearing All-Carbon Quaternary Stereocenters: Desymmetrization by Copper-Catalyzed N-Arylation. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 9555-9559. | 13.8 | 42 |
| 42 | Reaction of Ta(NMe ₂) ₅ with O ₂ : Formation of Aminoxy and Unusual (Aminomethyl)amide Oxo Complexes and Theoretical Studies of the Mechanistic Pathways. <i>Journal of the American Chemical Society</i> , 2007, 129, 14408-14421. | 13.7 | 41 |
| 43 | An Unusual Exchange between Alkylidyne Alkyl and Bis(alkylidene) Tungsten Complexes Promoted by Phosphine Coordination: A Kinetic, Thermodynamic, and Theoretical Studies. <i>Journal of the American Chemical Society</i> , 2004, 126, 10208-10209. | 13.7 | 40 |
| 44 | A Theoretical Study on the Mechanism of the Reductive Half-Reaction of Xanthine Oxidase. <i>Inorganic Chemistry</i> , 2005, 44, 1466-1471. | 4.0 | 40 |
| 45 | Bonding in cationic MOH n + (M=Al, Hf, Rn; n=2): DFT performances and periodic trends. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 389-399. | 1.4 | 40 |
| 46 | Ir-Catalyzed Regio- and Stereoselective Hydrosilylation of Internal Thioalkynes: A Combined Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2016, 81, 6157-6164. | 3.2 | 40 |
| 47 | Reactions of d ⁰ Group 4 Amides with Dioxygen. Preparation of Unusual Oxo Aminoxy Complexes and Theoretical Studies of Their Formation. <i>Journal of the American Chemical Society</i> , 2005, 127, 5204-5211. | 13.7 | 39 |
| 48 | Hybrid Palladium Catalyst Assembled from Chiral Phosphoric Acid and Thioamide for Enantioselective sp^3 -C-H Arylation. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 12774-12778. | 13.8 | 39 |
| 49 | Ru-Catalyzed Migratory Geminal Semihydrogenation of Internal Alkynes to Terminal Olefins. <i>Journal of the American Chemical Society</i> , 2019, 141, 17441-17451. | 13.7 | 38 |
| 50 | Pd-Catalyzed Asymmetric Intramolecular Aryl C-O Bond Formation with SDP(O) Ligand: Enantioselective Synthesis of (2,3-Dihydrobenzo[1,4]dioxin-2-yl)methanols. <i>Organic Letters</i> , 2015, 17, 840-843. | 4.6 | 37 |
| 51 | A Redox Non-Innocent Ligand Controls the Life Time of a Reactive Quartet Excited State - An MCSCF Study of [Ni(H)(OH)] ⁺ . <i>Journal of the American Chemical Society</i> , 2009, 131, 12634-12642. | 13.7 | 36 |
| 52 | Accurate Calculation, Prediction, and Assignment of ³ He NMR Chemical Shifts of Helium-3-Encapsulated Fullerenes and Fullerene Derivatives. <i>Journal of Organic Chemistry</i> , 2003, 68, 6732-6738. | 3.2 | 35 |
| 53 | Metal-Free Synthesis of 3-Arylquinolin-2-ones from Acrylic Amides via a Highly Regioselective 1,2-Aryl Migration: An Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2016, 81, 4058-4065. | 3.2 | 35 |
| 54 | A Twist of the Twist Mechanism, 2-Iodoxybenzoic Acid (IBX)-Mediated Oxidation of Alcohol Revisited: Theory and Experiment. <i>Organic Letters</i> , 2017, 19, 6502-6505. | 4.6 | 35 |

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|----|--|------|-----------|
| 55 | Rh(II)/Brønsted Acid Catalyzed General and Highly Diastereo- and Enantioselective Propargylation of in Situ Generated Oxonium Ylides and C-Alkynyl N-Boc N,O-Acetals: Synthesis of Polyfunctional Propargylamines. <i>Organic Letters</i> , 2019, 21, 1292-1296. | 4.6 | 35 |
| 56 | A Tungsten Silyl Alkylidyne Complex and Its Bis(alkylidene) Tautomer. Their Interconversion and an Unusual Silyl Migration in Their Reaction with Dioxigen. <i>Organometallics</i> , 2005, 24, 1214-1224. | 2.3 | 33 |
| 57 | A DFT Study on the Mechanism of Hydrosilylation of Unsaturated Compounds with Neutral Hydrido(hydrosilylene)tungsten Complex. <i>Journal of Organic Chemistry</i> , 2008, 73, 820-829. | 3.2 | 33 |
| 58 | Formal Syntheses of (±)-Platensimycin and (±)-Platencin via a Dual-Mode Lewis Acid Induced Cascade Cyclization Approach. <i>Journal of Organic Chemistry</i> , 2013, 78, 7912-7929. | 3.2 | 33 |
| 59 | Chemoselective and Enantioselective Insertion of Furyl Carbene into the N-H Bond of 2-Pyridones. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 16942-16946. | 13.8 | 32 |
| 60 | Exploring an Expedient IMDA Reaction Approach to Construct the Guanacastepene Core. <i>Organic Letters</i> , 2005, 7, 3709-3712. | 4.6 | 30 |
| 61 | Thermal Activation of Methane by Diatomic Metal Oxide Radical Cations: PbO ⁺ as One of the Missing Pieces. <i>ChemCatChem</i> , 2010, 2, 1391-1394. | 3.7 | 30 |
| 62 | N-Heterocyclic Carbene-Catalyzed Four-Component Reaction: Chemoselective C ₂ radical-C ₂ radical Relay Coupling Involving the Homoenate Intermediate. <i>ACS Catalysis</i> , 2021, 11, 10123-10130. | 11.2 | 30 |
| 63 | Unexpected Formation of (Dimethylaminomethylene)methylamide Complexes from the Reactions between Metal Chlorides and Lithium Dimethylamide. <i>Organometallics</i> , 2008, 27, 1338-1341. | 2.3 | 27 |
| 64 | Facile Dissociation of [(LNi ^{II}) ₂ E ₂] Dichalcogenides: Evidence for [LNi ^{II} E ₂] Superselenides and Supertellurides in Solution. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 4551-4554. | 13.8 | 27 |
| 65 | Rhodium-Catalyzed C-N Bond Formation through a Rebound Hydrolysis Mechanism and Application in β-Lactam Synthesis. <i>Organic Letters</i> , 2019, 21, 4124-4127. | 4.6 | 27 |
| 66 | Theoretical studies on the mechanism and stereoselectivity of Rh(Phebox)-catalyzed asymmetric reductive aldol reaction. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5845. | 2.8 | 26 |
| 67 | Metal-Free [2+2+2] Cycloaddition of Ynamides and Nitriles: Mild and Regioselective Synthesis of Fully Substituted Pyridines. <i>Angewandte Chemie</i> , 2016, 128, 9856-9860. | 2.0 | 26 |
| 68 | Directing Effects on the Copper-Catalyzed Site-Selective Arylation of Indoles. <i>Organic Letters</i> , 2018, 20, 6502-6505. | 4.6 | 26 |
| 69 | Mechanistic understanding of catalysis by combining mass spectrometry and computation. <i>Chemical Communications</i> , 2019, 55, 12749-12764. | 4.1 | 25 |
| 70 | Gas-Phase Reactions of Cationic Vanadium-Phosphorus Oxide Clusters with C ₂ H _x (x=4, 6): A DFT-Based Analysis of Reactivity Patterns. <i>Chemistry - A European Journal</i> , 2013, 19, 3017-3028. | 3.3 | 24 |
| 71 | Radical Reactivity, Catalysis, and Reaction Mechanism of Arylcopper(II) Compounds: The Missing Link in Organocopper Chemistry. <i>Journal of the American Chemical Society</i> , 2019, 141, 18341-18348. | 13.7 | 24 |
| 72 | Facile difluoromethylation of aliphatic alcohols with an S-(difluoro-methyl)sulfonium salt: reaction, scope and mechanistic study. <i>Chemical Communications</i> , 2019, 55, 7446-7449. | 4.1 | 24 |

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|----|--|------|-----------|
| 73 | Asymmetric radical carboesterification of dienes. <i>Nature Communications</i> , 2021, 12, 6670. | 12.8 | 24 |
| 74 | Construction of C [∞] C Axial Chirality via Asymmetric Carbene Insertion into Arene C [∞] H Bonds. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 25714-25718. | 13.8 | 23 |
| 75 | Generation of Gas [∞] Phase Nanosized Vanadium Oxide Clusters from a Mononuclear Precursor by Solution Nucleation and Electrospray Ionization. <i>Chemistry - A European Journal</i> , 2010, 16, 1163-1167. | 3.3 | 22 |
| 76 | Mechanistic Study on Pd/Mono-N-protected Amino Acid Catalyzed Vinyl [∞] Vinyl Coupling Reactions: Reactivity and <i>E</i> / <i>Z</i> Selectivity. <i>Organic Letters</i> , 2016, 18, 5240-5243. | 4.6 | 22 |
| 77 | Assembling a Hybrid Pd Catalyst from a Chiral Anionic Co(III) Complex and Ligand for Asymmetric C(sp ³) T _j ETQq1 1,0,784314,rgBT /Ove | 2.0 | 22 |
| 78 | Degradation of atrazine (ATZ) by ammonia/chlorine synergistic oxidation process. <i>Chemical Engineering Journal</i> , 2021, 415, 128841. | 12.7 | 22 |
| 79 | Systematic investigation of the aza-Cope reaction for fluorescence imaging of formaldehyde <i>in vitro</i> and <i>in vivo</i> . <i>Chemical Science</i> , 2021, 12, 13857-13869. | 7.4 | 22 |
| 80 | Isomerization of an N-Heterocyclic Germylene to an Azagermabenzen-1-ylidene and Its Coupling to a Unique Bis(germylene). <i>Organometallics</i> , 2010, 29, 5353-5357. | 2.3 | 21 |
| 81 | Iron(III)-Catalyzed Ortho-Preferred Radical Nucleophilic Alkylation of Electron-Deficient Arenes. <i>Organic Letters</i> , 2017, 19, 6538-6541. | 4.6 | 21 |
| 82 | Ligand [∞] Assisted Palladium(II)/(IV) Oxidation for <i>sp</i> ³ C [∞] H Fluorination. <i>Advanced Synthesis and Catalysis</i> , 2016, 358, 1946-1957. | 4.3 | 20 |
| 83 | Streamlined asymmetric $\hat{\pm}$ -difunctionalization of ynones. <i>Nature Communications</i> , 2018, 9, 375. | 12.8 | 20 |
| 84 | Synthesis of <i>ortho</i> -Phenolic Sulfilimines via an Intermolecular Sulfur Atom Transfer Cascade Reaction. <i>Organic Letters</i> , 2020, 22, 3799-3803. | 4.6 | 19 |
| 85 | Reactivity Pattern in the Room [∞] Temperature Activation of NH ₃ by the Main [∞] Group Atomic Ions Ga ⁺ , Ge ⁺ , As ⁺ and Se ⁺ . <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 1516-1521. | 2.0 | 18 |
| 86 | Reactivities of d ⁰ transition metal complexes toward oxygen: Synthetic and mechanistic studies. <i>Science in China Series B: Chemistry</i> , 2009, 52, 1723-1733. | 0.8 | 17 |
| 87 | N ₂ Activation by a Hafnium Complex: A DFT Study on CO [∞] Assisted Dinitrogen Cleavage and Functionalization. <i>Chemistry - A European Journal</i> , 2010, 16, 12564-12569. | 3.3 | 17 |
| 88 | Enantioselective Synthesis of Chiral Oxygen-Containing Heterocycles Using Copper-Catalyzed Aryl C [∞] O Coupling Reactions via Asymmetric Desymmetrization. <i>Journal of Organic Chemistry</i> , 2017, 82, 1458-1463. | 3.2 | 16 |
| 89 | Ruthenium [∞] Catalyzed Geminal Hydroborative Cyclization of Enynes. <i>Angewandte Chemie - International Edition</i> , 2022, 61, . | 13.8 | 16 |
| 90 | Thermal Activation of Ni [∞] H Bonds by Transition [∞] metal Oxide Cations: Does a Hierarchy Exist in the First Row?. <i>Chemistry - A European Journal</i> , 2011, 17, 3886-3892. | 3.3 | 15 |

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|-----|--|------|-----------|
| 91 | Copper(I)-Catalyzed Intramolecular Asymmetric Double C-Arylation for the Formation of Chiral Spirocyclic Bis-oxindoles. <i>Organic Letters</i> , 2019, 21, 4505-4509. | 4.6 | 15 |
| 92 | A DFT-Based Analysis of the Grossly Varying Reactivity Pattern in Room-Temperature Activation and Dehydrogenation of CH ₄ by Main-Group Atomic M ⁺ (M=Ga, Ge, As, and Se). <i>Chemistry - A European Journal</i> , 2009, 15, 11559-11565. | 3.3 | 14 |
| 93 | Reactions of a tungsten alkylidyne complex with mono-dentate phosphines: Thermodynamic and theoretical studies. <i>Polyhedron</i> , 2013, 58, 30-38. | 2.2 | 14 |
| 94 | Diastereoselective Total Synthesis of (±)-Basiliolide B and (±)-8-Basiliolide B. <i>Journal of Organic Chemistry</i> , 2017, 82, 3463-3481. | 3.2 | 14 |
| 95 | Asymmetric Arylation of Diazoesters with Anisoles Enabled by Cooperative Gold and Phosphoric Acid Catalysis. <i>Organic Letters</i> , 2022, 24, 2809-2814. | 4.6 | 14 |
| 96 | Hybrid Palladium Catalyst Assembled from Chiral Phosphoric Acid and Thioamide for Enantioselective $\text{I}^2\text{C}(\text{sp}^3)\text{-H}$ Arylation. <i>Angewandte Chemie</i> , 2020, 132, 12874-12878. | 2.0 | 13 |
| 97 | An unusual formal migrative cycloaddition of aurone-derived azadienes: synthesis of benzofuran-fused nitrogen heterocycles. <i>Chemical Science</i> , 2021, 12, 7953-7957. | 7.4 | 13 |
| 98 | Rhodium-Catalyzed Regioselective N^2 -Alkylation of Benzotriazoles with Diazo Compounds/Enynes via a Nonclassical Pathway. <i>Angewandte Chemie</i> , 2018, 130, 12669-12673. | 2.0 | 12 |
| 99 | Designing new Togni reagents by computation. <i>Chemical Communications</i> , 2019, 55, 5667-5670. | 4.1 | 12 |
| 100 | Synthesis of Benzofurans and Benzoxazoles through a [3,3]-Sigmatropic Rearrangement: O ⁺ NHAc as a Multitasking Functional Group. <i>Organic Process Research and Development</i> , 2019, 23, 1646-1653. | 2.7 | 12 |
| 101 | Access to N^2 -Substituted P^2 Pyridones by Catalytic Intermolecular Dearomatization and 1,4-Acyl Transfer. <i>Angewandte Chemie</i> , 2019, 131, 2002-2006. | 2.0 | 12 |
| 102 | DFT Studies on the Thermal Activation of Molecular Oxygen by Bare $[\text{Ni}(\text{H})(\text{OH})]^+$. <i>Helvetica Chimica Acta</i> , 2009, 92, 151-164. | 1.6 | 11 |
| 103 | Ligand-Controlled C=O Bond Coupling of Carboxylic Acids and Aryl Iodides: Experimental and Computational Insights. <i>Advanced Synthesis and Catalysis</i> , 2020, 362, 126-132. | 4.3 | 11 |
| 104 | Precise Introduction of the CH_nX_3 (X = F, Cl, Br, I) Moiety to Target Molecules by a Radical Strategy: A Theoretical and Experimental Study. <i>Journal of the American Chemical Society</i> , 2021, 143, 13195-13204. | 13.7 | 11 |
| 105 | Revealing the Iron-Catalyzed I^2 -Methyl Scission of tert-Butoxyl Radicals via the Mechanistic Studies of Carboazidation of Alkenes. <i>Molecules</i> , 2020, 25, 1224. | 3.8 | 10 |
| 106 | Unusual Chemistry of the Complex Mg^{2+} (2-Fluoropyridine) Activated by the Photoexcitation of Mg^{2+} . <i>Journal of the American Chemical Society</i> , 2003, 125, 12351-12357. | 13.7 | 8 |
| 107 | Effects of Aromatic Substitutions on the Photoreactions in Mg^{2+} (C ₆ H _n F ₂ X _{4-n}) (X = F, CH ₃) Complexes: A^{\cdot} Formation and Decomposition of Benzynes Radical Cations. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3356-3366. | 2.5 | 8 |
| 108 | Density Functional Theory Study of the Reaction between d ⁰ Tungsten Alkylidyne Complexes and H ₂ O: Addition versus Hydrolysis. <i>Inorganic Chemistry</i> , 2017, 56, 7111-7119. | 4.0 | 8 |

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|-----|--|-----|-----------|
| 109 | Interaction of peptide backbones and transition metal ions: 1. an IM-MS and DFT study of the binding pattern, structure and fragmentation of Pd(II)/Ni(II)-Polyalanine complexes. <i>International Journal of Mass Spectrometry</i> , 2019, 438, 87-96. | 1.5 | 8 |
| 110 | Computational Study on the Fate of Oxidative Directing Groups in Ru(II), Rh(III), and Pd(II) Catalyzed C-H Functionalization. <i>Journal of Organic Chemistry</i> , 2020, 85, 12594-12602. | 3.2 | 8 |
| 111 | Sulfonium Triggered Alkyne-Azide Click Cycloaddition. <i>Organic Letters</i> , 2022, 24, 1448-1453. | 4.6 | 8 |
| 112 | Isotope-Sensitive Degenerate [1,3]-Hydrogen Migration versus Competitive Enol-Keto Tautomerization. <i>Chemistry - A European Journal</i> , 2009, 15, 11815-11819. | 3.3 | 7 |
| 113 | Computational exploration of reactive fragment for mechanism-based inhibition of xanthine oxidase. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 58-67. | 1.8 | 6 |
| 114 | Fluorine-substitution induced switching of dissociation patterns of C ₆ H ₄ ^{TM+} produced by photoelimination of MgF ₂ from the complexes of Mg ^{TM+} (multifluorobenzene). <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 826-831. | 2.8 | 5 |
| 115 | The reaction of alkyl hydropersulfides (RSSH, R = CH ₃ and ^t Bu) with H ₂ S in the gas phase and in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 537-545. | 2.8 | 4 |
| 116 | Chemo- and Enantioselective Insertion of Furyl Carbene into the N-H Bond of 2-Pyridones. <i>Angewandte Chemie</i> , 2021, 133, 17079-17083. | 2.0 | 3 |
| 117 | Construction of C-C Axial Chirality via Asymmetric Carbene Insertion into Arene C-H Bonds. <i>Angewandte Chemie</i> , 0, , . | 2.0 | 3 |
| 118 | Pyridyne radical cations produced by photodissociation of Mg ^{TM+} (multifluoro-pyridine) complexes: A combined experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 607-615. | 2.8 | 2 |
| 119 | Copper-catalyzed intramolecular asymmetric C-arylation of acyclic β -ester amides: enantioselective formation of chiral oxindoles. <i>Organic Chemistry Frontiers</i> , 2021, 8, 4211-4216. | 4.5 | 2 |
| 120 | Ruthenium-Catalyzed Geminal Hydroborative Cyclization of Enynes. <i>Angewandte Chemie</i> , 0, , . | 2.0 | 2 |
| 121 | Gaseous Ni ⁺ complexes with BINOL derivatives and chiral esters in the gas phase: an experimental and theoretical investigation. <i>Collection of Czechoslovak Chemical Communications</i> , 2009, 74, 255-273. | 1.0 | 1 |
| 122 | Front Cover Picture: Ligand-Assisted Palladium(II)/(IV) Oxidation for sp ³ C-H Fluorination (<i>Adv. Synth. Tj ETQq0 0 0 rgBT /Overlock 10 T</i>) | 4.3 | 0 |
| 123 | Innentitelbild: Access to N-Substituted 2-Pyridones by Catalytic Intermolecular Dearomatization and 1,4-Acyl Transfer (<i>Angew. Chem. 7/2019</i>). <i>Angewandte Chemie</i> , 2019, 131, 1866-1866. | 2.0 | 0 |
| 124 | InnenrÄ¼cktitelbild: Assembling a Hybrid Pd Catalyst from a Chiral Anionic Co ^{III} Complex and Ligand for Asymmetric C(sp ³) ³ -H Functionalization (<i>Angew. Chem. 6/2019</i>). <i>Angewandte Chemie</i> , 2019, 131, 1863-1863. | 2.0 | 0 |
| 125 | Copper-catalyzed asymmetric intramolecular C-arylation with ureas as the additives: highly enantioselective formation of spirooxindoles. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 7480-7484. | 2.8 | 0 |