Yoshihito Shiota

List of Publications by Year
in descending order

187 papers	6,742 citations	57719 44 h-index	76872 74 g-index
197 all docs	197 docs citations	197 times ranked	6182 citing authors

#	Article	IF	Citations
1	Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds. Journal of Chemical Theory and Computation, 2013, 9, 3872-3877.	2.3	312
2	Methane-to-Methanol Conversion by First-Row Transition-Metal Oxide Ions:Â ScO+, TiO+, VO+, CrO+, MnO+, FeO+, CoO+, NiO+, and CuO+. Journal of the American Chemical Society, 2000, 122, 12317-12326.	6.6	262
3	Intrinsic reaction coordinate analysis of the conversion of methane to methanol by an ironâ€“oxo species: A study of crossing seams of potential energy surfaces. Journal of Chemical Physics, 1999, 111, 538-545.	1.2	191
4	Methaneâˆ'Methanol Conversion by MnO+, FeO+, and CoO+:Â A Theoretical Study of Catalytic Selectivity. Journal of the American Chemical Society, 1998, 120, 564-572.	6.6	164
5	A light-induced spin crossover actuated single-chain magnet. Nature Communications, 2013, 4, .	5.8	162
6	Methane selective oxidation to methanol by metal-exchanged zeolites: a review of active sites and their reactivity. Catalysis Science and Technology, 2019, 9, 1744-1768.	2.1	148
7	Conversion of Methane to Methanol at the Mononuclear and Dinuclear Copper Sites of Particulate Methane Monooxygenase (pMMO):Â A DFT and QM/MM Study. Journal of the American Chemical Society, 2006, 128, 9873-9881.	6.6	146
8	Direct Conversion of Methane to Methanol by Metal-Exchanged ZSM-5 Zeolite (Metal = Fe, Co, Ni, Cu). ACS Catalysis, 2016, 6, 8321-8331.	5.5	141
9	Direct Methaneâˆ'Methanol and Benzeneâˆ'Phenol Conversions on Feâˆ'ZSM-5 Zeolite:â€‰ Theoretical Predictions on the Reaction Pathways and Energetics. Journal of Physical Chemistry B, 2000, 104, 734-740.	1.2	139
10	Rutheniumâ€Catalyzed Selective and Efficient Oxygenation of Hydrocarbons with Water as an Oxygen Source. Angewandte Chemie - International Edition, 2008, 47, 5772-5776.	7.2	133
11	Roles of Zeolite Confinement and Cuâ€“Oâ€“Cu Angle on the Direct Conversion of Methane to Methanol by [Cu₂(Î¼-O)]²⁺-Exchanged AEI, CHA, AFX, and MFI Zeolites. ACS Catalysis, 2017, 7, 3741-3751.	5.5	129
12	Catalytic Mechanism of Dopamine Î²-Monooxygenase Mediated by Cu(III)âˆ'Oxo. Inorganic Chemistry, 2006, 45, 3034-3041.	1.9	123
13	Abstraction of the Hydrogen Atom of Methane by Ironâˆ'Oxo Species:Â The Concerted Reaction Path Is Energetically More Favorable. Organometallics, 1998, 17, 2825-2831.	1.1	119
14	Reaction Paths for the Conversion of Methane to Methanol Catalyzed by FeO⁺. Chemistry - A European Journal, 1997, 3, 1160-1169.	1.7	114
15	Molecular motor-driven abrupt anisotropic shape change in a single crystal of a Ni complex. Nature Chemistry, 2014, 6, 1079-1083.	6.6	111
16	A ferromagnetically coupled Fe42 cyanide-bridged nanocage. Nature Communications, 2015, 6, 5955.	5.8	104
17	Methane Partial Oxidation over [Cu₂(Î¼-O)]²⁺ and [Cu₃(Î¼-O)₃]²⁺ Active Species in Large-Pore Zeolites. ACS Catalysis, 2018, 8, 1500-1509.	5.5	104
18	Comparison of the Reactivity of Bis(Î¼-oxo)Cu^{II}Cu^{III} and Cu^{III}Cu^{III} Species to Methane. Inorganic Chemistry, 2009, 48, 838-845.	1.9	102

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19	A Theoretical Study of the Dynamic Behavior of Alkane Hydroxylation by a Compound I Model of Cytochrome P450. Journal of the American Chemical Society, 2001, 123, 9806-9816.	6.6	97
20	A spinâ€œorbit coupling study on the spin inversion processes in the direct methane-to-methanol conversion by FeO+. Journal of Chemical Physics, 2003, 118, 5872-5879.	1.2	97
21	Reaction Pathway for the Direct Benzene Hydroxylation by Ironâˆ’Oxo Species. Journal of the American Chemical Society, 1999, 121, 147-153.	6.6	91
22	Metalâˆ’Ligand Cooperation in H₂ Production and H₂O Decomposition on a Ru(II) PNN Complex: The Role of Ligand Dearomatizationâˆ’Aromatization. Journal of the American Chemical Society, 2009, 131, 13584-13585.	6.6	90
23	Multiâ€Step Spin Crossover Accompanied by Symmetry Breaking in an Fe^{III} Complex: Crystallographic Evidence and DFT Studies. Chemistry - A European Journal, 2013, 19, 12948-12952.	1.7	89
24	Theoretical Overview of Methane Hydroxylation by Copperâ€œOxygen Species in Enzymatic and Zeolitic Catalysts. Accounts of Chemical Research, 2018, 51, 2382-2390.	7.6	85
25	Computational Exploration of the Catalytic Mechanism of Dopamine Î²-Monooxygenase:Â Modeling of Its Mononuclear Copper Active Sites. Inorganic Chemistry, 2005, 44, 4226-4236.	1.9	82
26	Reversible Electron Transfer in a Linear {Fe₂Co} Trinuclear Complex Induced by Thermal Treatment and Photoirraditaion. Angewandte Chemie - International Edition, 2012, 51, 4367-4370.	7.2	81
27	Does the Hydroperoxo Species of Cytochrome P450 Participate in Olefin Epoxidation with the Main Oxidant, Compound I? Criticism from Density Functional Theory Calculations. Bulletin of the Chemical Society of Japan, 2003, 76, 721-732.	2.0	77
28	Specific Enhancement of Catalytic Activity by a Dicopper Core: Selective Hydroxylation of Benzene to Phenol with Hydrogen Peroxide. Angewandte Chemie - International Edition, 2017, 56, 7779-7782.	7.2	77
29	A Lowâ€Spin Ruthenium(IV)â€œOxo Complex: Does the Spin State Have an Impact on the Reactivity?. Angewandte Chemie - International Edition, 2010, 49, 8449-8453.	7.2	76
30	Homogeneous Photocatalytic Water Oxidation with a Dinuclear Co^{III}â€œPyridylmethylamine Complex. Inorganic Chemistry, 2016, 55, 1154-1164.	1.9	73
31	Quantum Chemical Approach to the Mechanism for the Biological Conversion of Tyrosine to Dopaquinone. Journal of the American Chemical Society, 2008, 130, 16890-16897.	6.6	70
32	Assembling an alkyl rotor to access abrupt and reversible crystalline deformation of a cobalt(II) complex. Nature Communications, 2015, 6, 8810.	5.8	69
33	A Cocatalyst that Stabilizes a Hydride Intermediate during Photocatalytic Hydrogen Evolution over a Rhodiumâ€Doped TiO₂ Nanosheet. Angewandte Chemie - International Edition, 2018, 57, 9073-9077.	7.2	62
34	Nickel(II), Palladium(II), and Platinum(II) Î·3-Allyl Complexes Bearing a Bidentate Titanium(IV) Phosphinoamide Ligand: A Tiâ†’M2 Dative Bond Enhances the Electrophilicity of the Ï€-Allyl Moiety. Organometallics, 2009, 28, 1988-1991.	1.1	61
35	Role of Tyrosine Residue in Methane Activation at the Dicopper Site of Particulate Methane Monooxygenase: A Density Functional Theory Study. Inorganic Chemistry, 2013, 52, 7907-7917.	1.9	58
36	Superior thermoelasticity and shape-memory nanopores in a porous supramolecular organic framework. Nature Communications, 2016, 7, 11564.	5.8	58

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37	Formation of an Iron-Oxo Species upon Decomposition of Dinitrogen Oxide on a Model of Fe-ZSM-5 Zeolite. Bulletin of the Chemical Society of Japan, 2000, 73, 29-36.	2.0	56
38	A Theoretical Study of Alcohol Oxidation by Ferrate. Journal of Organic Chemistry, 2001, 66, 4122-4131.	1.7	56
39	Multiply-fused porphyrinsâ€"effects of extended Ï€-conjugation on the optical and electrochemical properties. Chemical Communications, 2013, 49, 5939.	2.2	56
40	Conversion of Methane to Methanol on Diiron and Dicopper Enzyme Models of Methane Monooxygenase: A Theoretical Study on a Concerted Reaction Pathway. Bulletin of the Chemical Society of Japan, 2000, 73, 815-827.	2.0	54
41	Kinetic Isotope Effects in a Câˆ'H Bond Dissociation by the Iron-Oxo Species of Cytochrome P450. Journal of Physical Chemistry B, 2000, 104, 12365-12370.	1.2	49
42	Theoretical Study of the Mechanism of Valence Tautomerism in Cobalt Complexes. Journal of Physical Chemistry A, 2010, 114, 12928-12935.	1.1	49
43	Mechanistic Insights into Homogeneous Electrocatalytic and Photocatalytic Hydrogen Evolution Catalyzed by High-Spin Ni(II) Complexes with S₂N₂-Type Tetradentate Ligands. Inorganic Chemistry, 2018, 57, 7180-7190.	1.9	47
44	Directional Electron Transfer in Crystals of [CrCo] Dinuclear Complexes Achieved by Chirality-Assisted Preparative Method. Journal of the American Chemical Society, 2016, 138, 14170-14173.	6.6	46
45	An Azuleneâ€Fused Tetracene Diimide with a Small HOMOâ€"LUMO Gap. ChemPlusChem, 2017, 82, 1010-1014.	1.3	45
46	Ground-State Copper(III) Stabilized by N-Confused/N-Linked Corroles: Synthesis, Characterization, and Redox Reactivity. Journal of the American Chemical Society, 2018, 140, 6883-6892.	6.6	45
47	Macroscopic Polarization Change via Electron Transfer in a Valence Tautomeric Cobalt Complex. Nature Communications, 2020, 11, 1992.	5.8	41
48	Femtosecond Dynamics of the Methaneâˆ'Methanol and Benzeneâˆ'Phenol Conversions by an Ironâˆ'Oxo Species. Journal of Physical Chemistry A, 2000, 104, 2552-2561.	1.1	40
49	DFT study of the mechanism for methane hydroxylation by soluble methane monooxygenase (sMMO): effects of oxidation state, spin state, and coordination number. Dalton Transactions, 2013, 42, 1011-1023.	1.6	40
50	A New Family of Anionic Fe^{III} Spin Crossover Complexes Featuring a Weakâ€Field N₂O₄ Coordination Octahedron. Chemistry - A European Journal, 2016, 22, 1253-1257.	1.7	39
51	Giant anisotropic thermal expansion actuated by thermodynamically assisted reorientation of imidazoliums in a single crystal. Nature Communications, 2019, 10, 4805.	5.8	39
52	Disilaruthena- and Ferracyclic Complexes Containing Isocyanide Ligands as Effective Catalysts for Hydrogenation of Unfunctionalized Sterically Hindered Alkenes. Journal of the American Chemical Society, 2018, 140, 4119-4134.	6.6	38
53	Mechanistic Proposals for Direct Benzene Hydroxylation over Feâˆ'ZSM-5 Zeolite. Journal of Physical Chemistry B, 2003, 107, 11404-11410.	1.2	37
54	Formation and characterization of a reactive chromium(<scp>v</scp>)â€"oxo complex: mechanistic insight into hydrogen-atom transfer reactions. Chemical Science, 2015, 6, 945-955.	3.7	37

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55	Photocatalytic alkene reduction by a B₁₂â€“TiO₂ hybrid catalyst coupled with Câ€“F bond cleavage for gem-difluoroolefin synthesis. Chemical Communications, 2017, 53, 9478-9481.	2.2	37
56	Dioxygen Activation on Cu-MOR Zeolite: Theoretical Insights into the Formation of Cu₂O and Cu₃O₃ Active Species. Inorganic Chemistry, 2018, 57, 10146-10152.	1.9	37
57	QM/MM Study on the Catalytic Mechanism of Benzene Hydroxylation over Feâˆ'ZSM-5. Organometallics, 2006, 25, 3118-3123.	1.1	34
58	Theoretical Study of Thermal Spin Transition between the Singlet State and the Quintet State in the [Fe(2-picolylamine)3]2+Spin Crossover System. Journal of Physical Chemistry A, 2010, 114, 5862-5869.	1.1	34
59	A Ruthenium(III)â€“Oxyl Complex Bearing Strong Radical Character. Angewandte Chemie - International Edition, 2016, 55, 14041-14045.	7.2	34
60	Heterometallic Fe^{III}/K Coordination Polymer with a Wide Thermal Hysteretic Spin Transition at Room Temperature. Chemistry - A European Journal, 2016, 22, 532-538.	1.7	34
61	A Theoretical Study of Reactivity and Regioselectivity in the Hydroxylation of Adamantane by Ferrate(VI). Journal of Organic Chemistry, 2003, 68, 3958-3965.	1.7	33
62	Mechanism for the Direct Oxidation of Benzene to Phenol by FeO+. Organometallics, 2005, 24, 3532-3538.	1.1	33
63	Role of Acidic Proton in the Decomposition of NO over Dimeric Cu(I) Active Sites in Cu-ZSM-5 Catalyst: A QM/MM Study. ACS Catalysis, 2014, 4, 2075-2085.	5.5	33
64	Hydrogen atom abstraction reactions independent of Câ€“H bond dissociation energies of organic substrates in water: significance of oxidantâ€“substrate adduct formation. Chemical Science, 2014, 5, 1429-1436.	3.7	33
65	Visible light-driven cross-coupling reactions of alkyl halides with phenylacetylene derivatives for C(sp³)â€“C(sp) bond formation catalyzed by a B₁₂ complex. Chemical Communications, 2019, 55, 13070-13073.	2.2	33
66	Catalytic Câ€“H amination driven by intramolecular ligand-to-nitrene one-electron transfer through a rhodium(<scp>iii</scp>) centre. Chemical Communications, 2017, 53, 4849-4852.	2.2	32
67	Theoretical Investigation of Methane Hydroxylation over Isoelectronic [FeO]²⁺- and [MnO]⁺-Exchanged Zeolites Activated by N₂O. Inorganic Chemistry, 2017, 56, 10370-10380.	1.9	32
68	Anisotropic Change in the Magnetic Susceptibility of a Dynamic Single Crystal of a Cobalt(II) Complex. Angewandte Chemie - International Edition, 2017, 56, 717-721.	7.2	30
69	Mechanistic Insight into Concerted Protonâ€“Electron Transfer of a Ru(IV)-Oxo Complex: A Possible Oxidative Asynchronicity. Journal of the American Chemical Society, 2020, 142, 16982-16989.	6.6	30
70	DFT Study on N2 Activation by a Hydride-Bridged Diniobium Complex. Nâ‰¡N Bond Cleavage Accompanied by H2 Evolution. Inorganic Chemistry, 2009, 48, 3875-3881.	1.9	29
71	Thiophene-Fused Bisdehydro[12]annulene That Undergoes Transannular Alkyne Cycloaddition by Either Light or Heat. Journal of the American Chemical Society, 2013, 135, 1731-1734.	6.6	29
72	Novel Aspects of the [1,3] Sigmatropic Silyl Shift in Allylsilane. Journal of the American Chemical Society, 1997, 119, 807-815.	6.6	28

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73	Energetics for the Oxygen Rebound Mechanism of Alkane Hydroxylation by the Iron-Oxo Species of Cytochrome P450. Bulletin of the Chemical Society of Japan, 2000, 73, 2669-2673.	2.0	28
74	Possible Peroxo State of the Dicopper Site of Particulate Methane Monooxygenase from Combined Quantum Mechanics and Molecular Mechanics Calculations. Inorganic Chemistry, 2016, 55, 2771-2775.	1.9	28
75	Quenching and Restoration of Orbital Angular Momentum through a Dynamic Bond in a Cobalt(II) Complex. Journal of the American Chemical Society, 2020, 142, 11434-11441.	6.6	28
76	Role of molecular distortions in the spinâ€“orbit coupling between the singlet and triplet states of the 4Ï€ electron systems C4H4, C5H5+, and C3H3âˆ’. Journal of Chemical Physics, 2001, 115, 9243-9254.	1.2	26
77	Synthesis and Characterization of Novel Ferrocene-Containing Pyridylamine Ligands and Their Ruthenium(II) Complexes:â€‰ Electronic Communication through Hydrogen-Bonded Amide Linkage. Inorganic Chemistry, 2008, 47, 886-895.	1.9	25
78	Thermally Induced Intraâ€‘Carboxyl Proton Shuttle in a Molecular Rackâ€‘andâ€‘Pinion Cascade Achieving Macroscopic Crystal Deformation. Angewandte Chemie - International Edition, 2016, 55, 14628-14632.	7.2	25
79	Observation of Proton Transfer Coupled Spin Transition and Trapping of Photoinduced Metastable Proton Transfer State in an Fe(II) Complex. Journal of the American Chemical Society, 2019, 141, 14384-14393.	6.6	23
80	Siliconâˆ’Carbon Unsaturated Compounds. 69. Reactions of Silenes Produced Thermally from Pivaloyl- and Adamantoyltris(trimethylsilyl)silane with Silyl-Substituted Butadiynes and Enynes. Organometallics, 2004, 23, 4277-4287.	1.1	22
81	Mechanistic Insights into Câ€“H Oxidations by Ruthenium(III)-Pterin Complexes: Impact of Basicity of the Pterin Ligand and Electron Acceptability of the Metal Center on the Transition States. Journal of the American Chemical Society, 2016, 138, 9508-9520.	6.6	22
82	Synergy of Electrostatic and van der Waals Interactions in the Adhesion of Epoxy Resin with Carbon-Fiber and Glass Surfaces. Bulletin of the Chemical Society of Japan, 2017, 90, 500-505.	2.0	22
83	Formation and High Reactivity of the <i>anti</i>â€‘Dioxo Form of Highâ€‘Spin Î¼â€‘Oxodioxodiiron(IV) as the Active Species That Cleaves Strong Câˆ’H Bonds. Chemistry - A European Journal, 2016, 22, 5924-5936.	1.7	21
84	Photochemical Intramolecular Câˆ’H Addition of Dimesityl(hetero)arylboranes through a [1,6]â€‘Sigmatropic Rearrangement. Angewandte Chemie - International Edition, 2017, 56, 12210-12214.	7.2	21
85	An Azulene-Based Chiral Helicene and Its Air-Stable Cation Radical. Bulletin of the Chemical Society of Japan, 2019, 92, 1867-1873.	2.0	21
86	Room-Temperature Activation of Methane and Direct Formations of Acetic Acid and Methanol on Zn-ZSM-5 Zeolite: A Mechanistic DFT Study. Bulletin of the Chemical Society of Japan, 2020, 93, 345-354.	2.0	21
87	Manipulating electron redistribution to achieve electronic pyroelectricity in molecular [FeCo] crystals. Nature Communications, 2021, 12, 4836.	5.8	21
88	Proton-Coupled Electron Shuttling in a Covalently Linked Rutheniumâ€“Copper Heterodinuclear Complex. Journal of the American Chemical Society, 2011, 133, 18570-18573.	6.6	20
89	Catalytic Performance of a Dicopperâ€“Oxo Complex for Methane Hydroxylation. Inorganic Chemistry, 2018, 57, 8-11.	1.9	20
90	One-Pot Synthesis of Tertiary Amides from Organic Trichlorides through Oxygen Atom Incorporation from Air by Convergent Paired Electrolysis. Journal of Organic Chemistry, 2021, 86, 5983-5990.	1.7	20

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91	Density Functional Study on Possible Peroxo Form of Non-heme Diiron Enzyme Model. Chemistry Letters, 1997, 26, 587-588.	0.7	19
92	Roles of carboxylate donors in Oâ€“O bond scission of peroxodi-iron(<scp>iii</scp>) to high-spin oxodi-iron(<scp>iv</scp>) with a new carboxylate-containing dinucleating ligand. Chemical Science, 2014, 5, 2282-2292.	3.7	19
93	Proton-Assisted Mechanism of NO Reduction on a Dinuclear Ruthenium Complex. Inorganic Chemistry, 2015, 54, 7181-7191.	1.9	19
94	Cupric-superoxide complex that induces a catalytic aldol reaction-type Câ€“C bond formation. Communications Chemistry, 2019, 2, .	2.0	19
95	Theoretical Study of the Catalytic Hydrogenation of Alkenes by a Disilaferracyclic Complex: Can the Feâ€“Si Ïƒ-Bond-Assisted Activation of Hâ€“H Bonds Allow Development of a Catalysis of Iron?. Journal of Organic Chemistry, 2016, 81, 10900-10911.	1.7	18
96	Cobaltâ€“Carbon Bond Formation Reaction via Ligand Reduction of Porphyceneâ€“Cobalt(II) Complex and Its Noninnocent Reactivity. ACS Omega, 2018, 3, 4027-4034.	1.6	17
97	Contribution of Coulomb Interactions to a Two-Step Crystal Structure Phase Transformation Coupled with a Significant Change in Spin Crossover Behavior for a Series of Charged Fe^{II} Complexes from 2,6-Bis(2-methylthiazol-4-yl)pyridine. Inorganic Chemistry, 2018, 57, 1277-1287.	1.9	17
98	Theoretical Study of the Direct Conversion of Methane to Methanol Using H₂O₂ as an Oxidant on Pd and Au/Pd Surfaces. Journal of Physical Chemistry C, 2020, 124, 13231-13239.	1.5	17
99	Redox-Noninnocent Behavior of Tris(2-pyridylmethyl)amine Bound to a Lewis Acidic Rh(III) Ion Induced by Câ€“H Deprotonation. Journal of the American Chemical Society, 2015, 137, 11222-11225.	6.6	16
100	Persistent four-coordinate iron-centered radical stabilized by Ï€-donation. Chemical Science, 2016, 7, 191-198.	3.7	16
101	Theoretical Study of Thermal Isomerization of Silacyclobutene to Cyclopropene. Organometallics, 2004, 23, 4744-4749.	1.1	15
102	The Role of Coulomb Interactions for Spin Crossover Behaviors and Crystal Structural Transformation in Novel Anionic Fe(III) Complexes from a Ï€-Extended ONO Ligand. Crystals, 2016, 6, 49.	1.0	15
103	A Ruthenium(III)â€“Oxyl Complex Bearing Strong Radical Character. Angewandte Chemie, 2016, 128, 14247-14251.	1.6	15
104	Threeâ€Step Spin State Transition and Hysteretic Proton Transfer in the Crystal of an Iron(II) Hydrazone Complex. Angewandte Chemie - International Edition, 2020, 59, 14781-14787.	7.2	15
105	QM/MM Study of the Mononuclear Non-Heme Iron Active Site of Phenylalanine Hydroxylase. Journal of Physical Chemistry B, 2004, 108, 17226-17237.	1.2	14
106	A Cocatalyst that Stabilizes a Hydride Intermediate during Photocatalytic Hydrogen Evolution over a Rhodiumâ€Doped TiO₂ Nanosheet. Angewandte Chemie, 2018, 130, 9211-9215.	1.6	14
107	Real-space observation of far- and near-field-induced photolysis of molecular oxygen on an Ag(110) surface by visible light. Journal of Chemical Physics, 2019, 151, 144705.	1.2	14
108	Cleavage of Câ€“H Bond of Methane on Intermediate Q of Methane Monooxygenase. Chemistry Letters, 1997, 26, 1213-1214.	0.7	13

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109	Synthesis and Characterization of Ruthenium(II)â€“Nitrile Complexes with Bisamide-tpa Ligands (tpa =) Tj ETQq1 1 0.784314 rgBT /Ov	2.0	13
110	Synthesis and Characterization of Ruthenium(II)â[^]'Pyridylamine Complexes with Catechol Pendants as Metal Binding Sites. Inorganic Chemistry, 2010, 49, 3737-3745.	1.9	13
111	<i>cis</i>-1,2-Aminohydroxylation of Alkenes Involving a Catalytic Cycle of Osmium(III) and Osmium(V) Centers: Os^V(O)(NHTs) Active Oxidant with a Macrocyclic Tetradentate Ligand. Inorganic Chemistry, 2015, 54, 7073-7082.	1.9	13
112	Thermodynamics and Photodynamics of a Monoprotonated Porphyrin Directly Stabilized by Hydrogen Bonding with Polar Protic Solvents. Chemistry - A European Journal, 2017, 23, 4669-4679.	1.7	13
113	Acidâ€“Base Properties of a Freebase Form of a Quadruply Ring-Fused Porphyrinâ€"Stepwise Protonation Induced by Rigid Ring-Fused Structure. Journal of Organic Chemistry, 2017, 82, 322-330.	1.7	13
114	Intermediate-Spin Iron(III) Complexes Having a Redox-Noninnocent Macrocyclic Tetraamido Ligand. Inorganic Chemistry, 2018, 57, 9683-9695.	1.9	13
115	Possible Nitrogen Fixation by Disilabutadiene. Organometallics, 1997, 16, 5058-5063.	1.1	12
116	Mechanistic Insights into Photochromic Behavior of a Ruthenium(II)â€“Pterin Complex. Chemistry - A European Journal, 2011, 17, 6652-6662.	1.7	12
117	Fundamental electron-transfer and proton-coupled electron-transfer properties of Ru(iv)-oxo complexes. Dalton Transactions, 2019, 48, 13154-13161.	1.6	12
118	Temperature dependence of spherical electron transfer in a nanosized [Fe14] complex. Nature Communications, 2019, 10, 5510.	5.8	12
119	Specific Enhancement of Catalytic Activity by a Dicopper Core: Selective Hydroxylation of Benzene to Phenol with Hydrogen Peroxide. Angewandte Chemie, 2017, 129, 7887-7890.	1.6	11
120	High-Temperature Cooperative Spin Crossover Transitions and Single-Crystal Reflection Spectra of [FeIII(qsal)2](CH3OSO3) and Related Compounds. Crystals, 2019, 9, 81.	1.0	11
121	Photocatalytic hydrogen evolution using a Ru(ii)-bound heteroaromatic ligand as a reactive site. Dalton Transactions, 2020, 49, 17230-17242.	1.6	11
122	Local Structures and Dynamics of Imidazole Molecules in Poly(vinylphosphonic acid)â€“Imidazole Composite Investigated by Molecular Dynamics. ACS Applied Polymer Materials, 2020, 2, 1561-1568.	2.0	11
123	Mechanistic Study for the Reaction of B₁₂ Complexes with <i>m</i>-Chloroperbenzoic Acid in Catalytic Alkane Oxidations. Inorganic Chemistry, 2022, 61, 9710-9724.	1.9	11
124	Theoretical Study of Oxidation of Cyclohexane Diol to Adipic Anhydride by [RuIV(O)(tpa)(H2O)]2+Complex (tpa â•Tris(2-pyridylmethyl)amine). Inorganic Chemistry, 2011, 50, 6200-6209.	1.9	10
125	Theoretical Study on the Formation of Silacyclopropene from Acylsilane and Acetylene via Silene-to-Silylene Rearrangement. Organometallics, 2011, 30, 3160-3167.	1.1	10
126	Controlling the redox properties of a pyrroloquinolinequinone (PQQ) derivative in a ruthenium(<scp>ii</scp>) coordination sphere. Dalton Transactions, 2015, 44, 3151-3158.	1.6	10

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127	Formation and Isolation of a Fourâ€Electronâ€Reduced Porphyrin Derivative by Reduction of a Stable 20Ï€ Isophlorin. Angewandte Chemie - International Edition, 2018, 57, 1973-1977.	7.2	10
128	Anthranoxides as Highly Reactive Arynophiles for the Synthesis of Triptycenes. Chemistry - A European Journal, 2020, 26, 8506-8510.	1.7	10
129	<i>Ïƒ</i>-CAM Mechanisms for the Hydrogenation of Alkenes by <i>cis</i>- and <i>trans</i>-Disilametallacyclic Carbonyl Complexes (M = Fe, Ru, Os): Experimental and Theoretical Studies. Bulletin of the Chemical Society of Japan, 2017, 90, 613-626.	2.0	9
130	Pushâ€“pull fluorenones and benzazulenequinones: regioselective [4+2] and [2+2] cycloadditions of benzopentalenequinone derivative and alkynes bearing an aniline moiety. Tetrahedron Letters, 2016, 57, 4604-4607.	0.7	8
131	Trithiazolyl-1,3,5-triazines bearing decyloxybenzene moieties: synthesis, photophysical and electrochemical properties, and self-assembly behavior. Organic and Biomolecular Chemistry, 2018, 16, 3584-3595.	1.5	8
132	Importance of the Reactant-State Potentials of Chromium(V)â€“Oxo Complexes to Determine the Reactivity in Hydrogen-Atom Transfer Reactions. Inorganic Chemistry, 2018, 57, 13929-13936.	1.9	8
133	Role of Amino Acid Residues for Dioxygen Activation in the Second Coordination Sphere of the Dicopper Site of pMMO. Inorganic Chemistry, 2019, 58, 12280-12288.	1.9	8
134	Formation of a Ruthenium(V)â€"Imido Complex and the Reactivity in Substrate Oxidation in Water through the Nitrogen Non-Rebound Mechanism. Inorganic Chemistry, 2019, 58, 12815-12824.	1.9	8
135	Selective catalytic 2e^{âˆ’}-oxidation of organic substrates by an Fe^{II} complex having an N-heterocyclic carbene ligand in water. Chemical Communications, 2020, 56, 9783-9786.	2.2	8
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