Shigeyoshi Sakaki Or S Sakaki

List of Publications by Year
in descending order

226 papers	10,324 citations	31976 53 h-index	49909 87 g-index
231 all docs	231 docs citations	231 times ranked	8380 citing authors

#	Article	IF	Citations
1	Bidirectional Chemoâ€Switching of Spin State in a Microporous Framework. Angewandte Chemie - International Edition, 2009, 48, 4767-4771.	13.8	474
2	Self-Accelerating CO Sorption in a Soft Nanoporous Crystal. Science, 2014, 343, 167-170.	12.6	434
3	Design and control of gas diffusion process in a nanoporous soft crystal. Science, 2019, 363, 387-391.	12.6	332
4	Iridium-Catalyzed Borylation of Benzene with Diboron. Theoretical Elucidation of Catalytic Cycle Including Unusual Iridium(V) Intermediate. Journal of the American Chemical Society, 2003, 125, 16114-16126.	13.7	266
5	Câˆ'H Bond Activation of Benzene and Methane by M(Î·2-O2CH)2 (M = Pd or Pt). A Theoretical Study. Organometallics, 2000, 19, 3895-3908.	2.3	205
6	Ruthenium(II)-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. Theoretical Study of Real Catalyst, Ligand Effects, and Solvation Effects. Journal of the American Chemical Society, 2005, 127, 4021-4032.	13.7	183
7	Discrete Sandwich Compounds of Monolayer Palladium Sheets. Science, 2006, 313, 1104-1107.	12.6	182
8	The Suzukiâ€"Miyaura Coupling of Nitroarenes. Journal of the American Chemical Society, 2017, 139, 9423-9426.	13.7	158
9	Theoretical Study of Platinum(0)-Catalyzed Hydrosilylation of Ethylene. Chalkâˆ'Harrod Mechanism or Modified Chalkâˆ'Harrod Mechanism. Organometallics, 1998, 17, 2510-2523.	2.3	157
10	Theoretical Study of Trans-metalation Process in Palladium-Catalyzed Borylation of Iodobenzene with Diboron. Journal of the American Chemical Society, 2004, 126, 10457-10471.	13.7	153
11	Efficient Catalyst for Acceptorless Alcohol Dehydrogenation: Interplay of Theoretical and Experimental Studies. ACS Catalysis, 2014, 4, 1010-1020.	11.2	151
12	para-Selective Alkylation of Benzamides and Aromatic Ketones by Cooperative Nickel/Aluminum Catalysis. Journal of the American Chemical Society, 2016, 138, 14699-14704.	13.7	149
13	Theoretical Study of Ruthenium-Catalyzed Hydrogenation of Carbon Dioxide into Formic Acid. Reaction Mechanism Involving a New Type of Ïƒ-Bond Metathesis. Journal of the American Chemical Society, 2000, 122, 3867-3877.	13.7	132
14	A Dualâ€Ligand Porous Coordination Polymer Chemiresistor with Modulated Conductivity and Porosity. Angewandte Chemie - International Edition, 2020, 59, 172-176.	13.8	124
15	Oxidative addition reactions of saturated Si-X bonds (X = H, F, C, or Si) to Pt(PH3)2. An ab initio MO/MP4 study. Journal of the American Chemical Society, 1993, 115, 2373-2381.	13.7	120
16	Density Gradation of Open Metal Sites in the Mesospace of Porous Coordination Polymers. Journal of the American Chemical Society, 2017, 139, 11576-11583.	13.7	118
17	Why Does the Rhodium-Catalyzed Hydrosilylation of Alkenes Take Place through a Modified Chalkâˆ'Harrod Mechanism? A Theoretical Study. Organometallics, 2002, 21, 3788-3802.	2.3	110
18	Synthesis of a new copper(i) complex, [Cu(tmdcbpy)2]+ (tmdcbpy =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 67 Td (4,4â€², 6,6â€²-tetram Transactions RSC, 2002, , 840.	2.3	105

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19	Theoretical Study of the Cp2Zr-Catalyzed Hydrosilylation of Ethylene. Reaction Mechanism Including New Ïƒ-Bond Activation. Journal of the American Chemical Society, 2004, 126, 3332-3348.	13.7	105
20	Theoretical Study of Rhodium(III)-Catalyzed Hydrogenation of Carbon Dioxide into Formic Acid. Significant Differences in Reactivity among Rhodium(III), Rhodium(I), and Ruthenium(II) Complexes. Journal of the American Chemical Society, 2002, 124, 7588-7603.	13.7	103
21	New generation of the reference interaction site model self-consistent field method: Introduction of spatial electron density distribution to the solvation theory. Journal of Chemical Physics, 2007, 126, 244504.	3.0	103
22	Structures and binding energies of benzeneâ€“methane and benzeneâ€“benzene complexes. An ab initio SCF/MP2 study. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 659-664.	1.7	96
23	Ruthenium(II)-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. Theoretical Study of Significant Acceleration by Water Molecules. Organometallics, 2006, 25, 3352-3363.	2.3	96
24	Nickel-Catalyzed Double Carboxylation of Alkynes Employing Carbon Dioxide. Organic Letters, 2014, 16, 4960-4963.	4.6	96
25	Rhodium Complexes Bearing PAlP Pincer Ligands. Journal of the American Chemical Society, 2018, 140, 7070-7073.	13.7	96
26	Theoretical Study on Ïƒ-Bond Activation of (HO)2Bâˆ’XH3by M(PH3)2(X = C, Si, Ge, or Sn; M = Pd or Pt). Noteworthy Contribution of the Boryl pÏ€Orbital to Mâˆ’Boryl Bonding and Activation of the Bâˆ’X Ïƒ-Bond. Organometallics, 1999, 18, 4825-4837.	2.3	93
27	Carbon dioxide capture and efficient fixation in a dynamic porous coordination polymer. Nature Communications, 2019, 10, 4362.	12.8	91
28	Why Does Fluoride Anion Accelerate Transmetalation between Vinylsilane and Palladium(II)âˆ’Vinyl Complex? Theoretical Study. Journal of the American Chemical Society, 2008, 130, 12975-12985.	13.7	88
29	Syntheses, Structures, and Coordination Chemistry of Phosphole-Containing Hybrid Calixphyrins:Â Promising Macrocyclic P,N2,X-Mixed Donor Ligands for Designing Reactive Transition-Metal Complexes. Journal of the American Chemical Society, 2008, 130, 990-1002.	13.7	85
30	Aromatic Câ€“H Ïƒ-Bond Activation by Ni⁰, Pd⁰, and Pt⁰ Alkene Complexes: Concerted Oxidative Addition to Metal vs Ligand-to-Ligand H Transfer Mechanism. Organometallics, 2017, 36, 2761-2771.	2.3	84
31	Structure and coordinate bonding nature of nickel(0) and copper(I) carbon dioxide complexes. An ab initio molecular orbital study. Inorganic Chemistry, 1982, 21, 760-765.	4.0	82
32	Is a Transition State Planar or Nonplanar in Oxidative Additions of Câˆ’H, Siâˆ’H, Câˆ’C, and Siâˆ’C Ïƒ-Bonds to Pt(PH3)2? A Theoretical Study. Journal of Physical Chemistry A, 1998, 102, 8027-8036.	2.5	78
33	Reaction of BX2âˆ’BX2(X = H or OH) with M(PH3)2(M = Pd or Pt). A Theoretical Study of the Characteristic Features. Inorganic Chemistry, 1997, 36, 226-229.	4.0	76
34	A Theoretical Investigation on CO Oxidation by Singleâ€Atom Catalysts M₁/Î³â€Al₂O₃ (M=Pd, Fe, Co, and Ni). ChemCatChem, 2017, 9, 1222-1229.	3.7	76
35	Levoglucosan Formation from Crystalline Cellulose: Importance of a Hydrogen Bonding Network in the Reaction. ChemSusChem, 2013, 6, 2356-2368.	6.8	74
36	Absorption of CO₂ and CS₂ into the Hofmann-Type Porous Coordination Polymer: Electrostatic versus Dispersion Interactions. Journal of the American Chemical Society, 2013, 135, 4840-4849.	13.7	72

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37	Cooperative Bond Scission in a Soft Porous Crystal Enables Discriminatory Gate Opening for Ethylene over Ethane. Journal of the American Chemical Society, 2017, 139, 18313-18321.	13.7	72
38	Phosphorus-Containing Hybrid Calixphyrins:Â Promising Mixed-Donor Ligands for Visible and Efficient Palladium Catalysts. Journal of the American Chemical Society, 2006, 128, 11760-11761.	13.7	71
39	C2H4 Insertion into PtII-SiH3 and PtII-H Bonds. An ab Initio MO/MP4 Study. Journal of the American Chemical Society, 1994, 116, 7258-7265.	13.7	67
40	Remarkably Wide Range of Bond Distance Adjustment of d9â^'d9Pdâ^'Pd Interactions to Change in Coordination Environment. Journal of the American Chemical Society, 1998, 120, 4536-4537.	13.7	65
41	Theoretical Study of Câ^'H and Nâ^'H Ïƒ-Bond Activation Reactions by Titinium(IV)-Imido Complex. Good Understanding Based on Orbital Interaction and Theoretical Proposal for Nâ^'H Ïƒ-Bond Activation of Ammonia. Journal of the American Chemical Society, 2007, 129, 8615-8624.	13.7	65
42	Thermal Degradation of Methyl Î²-<scp>d</scp>-Glucoside. A Theoretical Study of Plausible Reaction Mechanisms. Journal of Organic Chemistry, 2009, 74, 6891-6894.	3.2	65
43	Unexpected Electronic Process of H₂ Activation by a New Nickel Borane Complex: Comparison with the Usual Homolytic and Heterolytic Activations. Inorganic Chemistry, 2013, 52, 2844-2853.	4.0	64
44	The crucial role of a Ni(i) intermediate in Ni-catalyzed carboxylation of aryl chloride with CO2: a theoretical study. Chemical Communications, 2013, 49, 10715.	4.1	62
45	An ab initio MO/SD-CI study of model complexes of intermediates in electrochemical reduction of carbon dioxide catalyzed by NiCl2(cyclam). Journal of the American Chemical Society, 1992, 114, 2055-2062.	13.7	61
46	Pt-catalyzed hydrosilylation of ethylene. A theoretical study of the reaction mechanism. Coordination Chemistry Reviews, 1999, 190-192, 933-960.	18.8	60
47	A Theoretical Study of Nickel(0)-Catalyzed Phenylcyanation of Alkynes. Reaction Mechanism and Regioselectivity. Organometallics, 2009, 28, 2583-2594.	2.3	60
48	Ïƒ-Bond Activation of Small Molecules and Reactions Catalyzed by Transition-Metal Complexes: Theoretical Understanding of Electronic Processes. Inorganic Chemistry, 2014, 53, 6444-6457.	4.0	60
49	Magnesiation of Aryl Fluorides Catalyzed by a Rhodiumâ€“Aluminum Complex. Journal of the American Chemical Society, 2020, 142, 11647-11652.	13.7	59
50	A Theoretical Study of the Câ^'H Activation of Methane Derivatives. Significant Effects of Electron-Withdrawing Substituents. Organometallics, 1998, 17, 1278-1289.	2.3	58
51	Bonding in Ni(PH3)2(C2H4) and Ni(PH3)2(C2H2). Ab initio SCF-MO study. Inorganic Chemistry, 1981, 20, 2292-2297.	4.0	57
52	Catalytic Transfer Hydrogenation by a Trivalent Phosphorus Compound: Phosphorusâ€Ligand Cooperation Pathway or P^{III}/P^V Redox Pathway?. Angewandte Chemie - International Edition, 2014, 53, 4633-4637.	13.8	57
53	Theoretical Study of M(PH3)2Complexes of C60, Corannulene (C20H10), and Sumanene (C21H12) (M = Pd) Tj ETQq1 1 0.784314 rg 8055-8063.	2.5	56
54	Pd(ii)-promoted direct cross-coupling reaction of arenes via highly regioselective aromatic Câ€“H activation: a theoretical study. Dalton Transactions, 2010, 39, 3279.	3.3	55

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55	Reasons Two Nonstrained Câ€“C Ïƒ-Bonds Can Be Easily Cleaved in Decyanative [4 + 2] Cycloaddition Catalyzed by Nickel(0)/Lewis Acid Systems. Theoretical Insight. ACS Catalysis, 2015, 5, 1-10.	11.2	55
56	Comparison of Electronic Structure Theories for Solvated Molecules:â€‰ RISM-SCF versus PCM. Journal of Physical Chemistry A, 2004, 108, 1629-1634.	2.5	53
57	Ab initio MO study of carbon dioxide insertion into a copper(I)-hydrogen bond. Semiquantitative understanding of changes in geometry, bonding, and electron distribution during the reaction. Inorganic Chemistry, 1989, 28, 2583-2590.	4.0	51
58	Theoretical Study of Pyrazolate-Bridged Dinuclear Platinum(II) Complexes: Interesting Potential Energy Curve of the Lowest Energy Triplet Excited State and Phosphorescence Spectra. Inorganic Chemistry, 2008, 47, 4329-4337.	4.0	51
59	Successful photocatalytic reduction of methylviologen (MV2+) with [Cu(NN)(PPh3)2]+ (NN =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 and a novel solvent effect on its catalytic activity. Inorganic Chemistry, 1986, 25, 2330-2333.	4.0	50
60	Theoretical Study of the Structure, Bonding Nature, and Reductive Elimination Reaction of Pd(XH3)(Î·3-C3H5)(PH3) (X = C, Si, Ge, Sn). Hypervalent Behavior of Group 14 Elements. Organometallics, 1999, 18, 4015-4026.	2.3	50
61	New Insights into Structures, Stability, and Bonding of Î¼-Allyl Ligands Coordinated with Pdâ^'Pd and Pdâ^'Pt Fragments. Organometallics, 1996, 15, 2089-2097.	2.3	49
62	Heteropolynuclear Complexes of 3,5-Dimethylpyrazolate [Pt₂M₄(Me₂pz)₈] (M = Ag, Cu). Highly Luminescent Character of the Triplet Excited State Based on Mixed-Metal Cores. Inorganic Chemistry, 2008, 47, 5033-5035.	4.0	49
63	A palladium-catalyzed reaction of a .pi.-allyl ligand with a nucleophile. An MO study about a feature of the reaction and a ligand effect on the reactivity. Journal of the American Chemical Society, 1980, 102, 4062-4069.	13.7	48
64	Reaction paths of carbonyl insertion into the platinum(II)-methyl bond. An MO study. Journal of the American Chemical Society, 1983, 105, 2280-2286.	13.7	48
65	Theoretical Insight into Gate-Opening Adsorption Mechanism and Sigmoidal Adsorption Isotherm into Porous Coordination Polymer. Journal of the American Chemical Society, 2018, 140, 13958-13969.	13.7	48
66	A Theoretical Analysis of a Dielsâ^'Alder Reaction in Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 8227-8230.	2.6	47
67	Factors Controlling the Reactivity of Heteroarenes in Direct Arylation with Arylpalladium Acetate Complexes. Organometallics, 2013, 32, 4423-4430.	2.3	47
68	The crucial roles of MgCl₂ as a non-innocent additive in the Ni-catalyzed carboxylation of benzyl halide with CO₂. Chemical Communications, 2014, 50, 13026-13029.	4.1	47
69	Can carbon dioxide coordinate to a nickel(I) complex? An ab initio MO/SD-CI study. Journal of the American Chemical Society, 1990, 112, 7813-7814.	13.7	46
70	Evaluation of the Ïƒ-Donation from Group 11 Metals (Cu, Ag, Au) to Silane, Germane, and Stannane Based on the Experimental/Theoretical Systematic Approach. Organometallics, 2015, 34, 1440-1448.	2.3	46
71	Bonding nature and reaction behavior of inter-element linkages with transition metal complexes. A theoretical study. Journal of Organometallic Chemistry, 2000, 611, 288-298.	1.8	45
72	Ab Initio MO Study of the CO2 Insertion into the Cu(I)-R Bond (R = H, CH3, or OH). Comparison between the CO2 Insertion and the C2H4 Insertion. Inorganic Chemistry, 1995, 34, 1914-1923.	4.0	44

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73	Theory of emission state of tris(8-quinolinolato)aluminum and its related compounds. Journal of Applied Physics, 2001, 90, 6092-6097.	2.5	44
74	sp³ Câ€“H Borylation Catalyzed by Iridium(III) Triboryl Complex: Comprehensive Theoretical Study of Reactivity, Regioselectivity, and Prediction of Excellent Ligand. Journal of the American Chemical Society, 2019, 141, 9854-9866.	13.7	44
75	Geometries, Bonding Nature, and Relative Stabilities of Dinuclear Palladium(I) Ï€-Allyl and Mononuclear Palladium(II) Ï€-Allyl Complexes. A Theoretical Study. Organometallics, 1997, 16, 2995-3003.	2.3	43
76	Generation of Dihydrogen Molecule and Hydrosilylation of Carbon Dioxide Catalyzed by Zinc Hydride Complex: Theoretical Understanding and Prediction. Inorganic Chemistry, 2014, 53, 8485-8493.	4.0	43
77	Theoretical Study of Rhenium Dinuclear Complexes:Â Reâ‹¯Re Bonding Nature and Electronic Structure. Journal of Physical Chemistry A, 2006, 110, 9710-9717.	2.5	42
78	Binding Energy of Transition-Metal Complexes with Large Ï€-Conjugate Systems. Density Functional Theory vs Post-Hartreeâ‹¯Fock Methods. Journal of Physical Chemistry A, 2007, 111, 7124-7132.	2.5	42
79	Cooperative Catalysis of Combined Systems of Transitionâ€Metal Complexes with Lewis Acids: Theoretical Understanding. Chemical Record, 2016, 16, 2405-2425.	5.8	42
80	Theoretical Study of Reactivity of Ge(II)-hydride Compound: Comparison with Rh(I)-Hydride Complex and Prediction of Full Catalytic Cycle by Ge(II)-hydride. Journal of the American Chemical Society, 2013, 135, 8955-8965.	13.7	41
81	Catalytic Hydrogenation of Carbon Dioxide with Ammoniaâ€“Borane by Pincer-Type Phosphorus Compounds: Theoretical Prediction. Journal of the American Chemical Society, 2016, 138, 13481-13484.	13.7	41
82	Pd/NHC-catalyzed cross-coupling reactions of nitroarenes. Chemical Communications, 2019, 55, 9291-9294.	4.1	41
83	Oxidative addition of silane to Pt(PH3)2. An ab initio MO/MP4 study. Journal of the American Chemical Society, 1991, 113, 5063-5065.	13.7	40
84	Analytical energy gradient for reference interaction site model self-consistent field explicitly including spatial electron density distribution. Journal of Chemical Physics, 2009, 131, 214504.	3.0	40
85	Geometry, electronic structure, and coordination ability of (diiminoethane)bis(phosphine)copper(1+) at the lowest energy triplet metal-to-ligand charge-transfer excited state. A theoretical study. Inorganic Chemistry, 1992, 31, 4575-4581.	4.0	39
86	Ab Initio MO Study of the Geometry, Î·3â‡„ Î·1Conversion, and Reductive Elimination of a Palladium(II) Î·3-Allyl Hydride Complex and Its Platinum(II) Analogue. Organometallics, 1996, 15, 1713-1720.	2.3	38
87	Structuralâ€Deformationâ€Energyâ€Modulation Strategy in a Soft Porous Coordination Polymer with an Interpenetrated Framework. Angewandte Chemie - International Edition, 2020, 59, 15517-15521.	13.8	38
88	Ab initio MO study of palladium-assisted nucleophilic attack on a coordinated olefin: semiquantitative understanding of the reaction and the mechanism of palladium acceleration. Inorganic Chemistry, 1987, 26, 2499-2505.	4.0	37
89	Ab initio MO study of carbon dioxide insertion into a methyl-copper(I) bond. Critical difference from CO2 insertion into a hydrogen-copper(I) bond. Organometallics, 1989, 8, 2970-2973.	2.3	37
90	Oxygen Atom Transfer Reactions of Iridium and Osmium Complexes: Theoretical Study of Characteristic Features and Significantly Large Differences Between These Two Complexes. Inorganic Chemistry, 2009, 48, 8154-8163.	4.0	37

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91	Oxidative addition of a Câ€“H Ïƒ bond to M(PH3)2 (Mâ€…=â€…Pd or Pt). An ab initio molecular orbital study on the chelate phosphine effect. Journal of the Chemical Society Dalton Transactions, 1997, , 803-810.	1.1	35
92	The barrier origin on the reaction of CO2+OHâˆ’ in aqueous solution. Chemical Physics Letters, 2007, 443, 264-268.	2.6	35
93	Solvation effects in oxidative addition reaction of Methyliodide to Pt(II) complex: A theoretical study with RISMâ€“SCF method. Chemical Physics Letters, 2008, 458, 329-332.	2.6	35
94	Ab initio MO study of nickel(0) complexes: stereochemistry of Ni(PH3)2L (L = H2CO or (CO)2) and comparison of coordinate bonds of various ligands. Inorganic Chemistry, 1983, 22, 104-108.	4.0	34
95	Characteristic features of carbon dioxide insertion into a copper-hydrogen bond. An ab initio MO study. Inorganic Chemistry, 1988, 27, 2020-2021.	4.0	34
96	Formation of the Oxanickelacyclopentene Complex from Nickel(0), Carbon Dioxide, and Alkyne. Anab initioMO/SD-CI Study. Bulletin of the Chemical Society of Japan, 1993, 66, 3289-3299.	3.2	34
97	Chromatographic separation of geometrical isomers using highly oriented polymer-immobilized silica gels. Journal of Chromatography A, 1994, 672, 237-241.	3.7	34
98	Theoretical and Computational Study of a Complex System Consisting of Transition Metal Element(s): How to Understand and Predict Its Geometry, Bonding Nature, Molecular Property, and Reaction Behavior. Bulletin of the Chemical Society of Japan, 2015, 88, 889-938.	3.2	34
99	Transition-Metal-Mediated Germaniumâ€“Fluorine Activation: Inverse Electron Flow in Ïƒ-Bond Metathesis. Organometallics, 2016, 35, 713-719.	2.3	34
100	Theoretical Study of Nickel-Catalyzed Selective Alkenylation of Pyridine: Reaction Mechanism and Crucial Roles of Lewis Acid and Ligands in Determining the Selectivity. Journal of Organic Chemistry, 2017, 82, 289-301.	3.2	34
101	Ethylene, silene, and disilene coordinate bonds with platinum(0) and platinum(II). An ab initio MO/MP4 and SD-CI study. Inorganic Chemistry, 1991, 30, 4218-4224.	4.0	33
102	Reactivity of Pd(PH3)2 for Oxidative Additions of the Si-X .sigma.-Bonds (X = H, C, Si). An ab Initio MO/MP4 Study. Inorganic Chemistry, 1994, 33, 1660-1665.	4.0	33
103	Carbon dioxide capture at the molecular level. Physical Chemistry Chemical Physics, 2009, 11, 8556.	2.8	33
104	New Palladium(II) Complex of P,S-Containing Hybrid Calixphyrin. Theoretical Study of Electronic Structure and Reactivity for Oxidative Addition. Journal of the American Chemical Society, 2009, 131, 10955-10963.	13.7	32
105	Theoretical Study on the Transition-Metal Oxoboryl Complex: Mâ€“BO Bonding Nature, Mechanism of the Formation Reaction, and Prediction of a New Oxoboryl Complex. Inorganic Chemistry, 2012, 51, 4597-4605.	4.0	32
106	A Theoretical Study on the Oxidative Addition of an Si-X Bond (X = H or Si) to M(PH3)2 (M = Pd or Pt). A Comparison of the Reactivity between Pt(PH3)2 and Pd(PH3)2. The Journal of Physical Chemistry, 1995, 99, 9933-9939.	2.9	31
107	Photoinduced electron transfer between [Cu(dmphen)L2]+[dmphen = 2,9-dimethyl-1,10-phenanthroline, L = PPhn(C6H4OMe-p)3 â€“n(n= 0â€“3)] and methyl viologen. Journal of the Chemical Society Dalton Transactions, 1996, , 1909-1914.	1.1	31
108	Theoretical and computational studies of organometallic reactions: successful or not?. Chemical Record, 2010, 10, 29-45.	5.8	31

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109	Transitionâ€Metalâ€Mediated Cleavage of Fluoroâ€Silanes under Mild Conditions. Chemistry - A European Journal, 2016, 22, 2370-2375.	3.3	30
110	Noble Reaction Features of Bromoborane in Oxidative Addition of Bâ€“Br Ïƒ-Bond to [M(PMe₃)₂] (M = Pt or Pd): Theoretical Study. Inorganic Chemistry, 2011, 50, 5290-5297.	4.0	29
111	Syntheses and Luminescent Properties of 3,5-Diphenylpyrazolato-Bridged Heteropolynuclear Platinum Complexes. The Influence of Chloride Ligands on the Emission Energy Revealed by the Systematic Replacement of Chloride Ligands by 3,5-Dimethylpyrazolate. Inorganic Chemistry, 2012, 51, 7977-7992.	4.0	29
112	Electronic structure and enhanced reactivity of carbon dioxide coordinated with a rhodium(I) complex. An ab initio MO study. Inorganic Chemistry, 1989, 28, 103-109.	4.0	28
113	M2E2 four-member ring structure, M2(Î¼-EH2)2(P2)2 (M=Pd or Pt; E=Si or Ge; P2=(PH3)2 or) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 142 Td study. Journal of Organometallic Chemistry, 2001, 635, 173-186.	1.8	28
114	Distortion of Electronic Structure in Solvated Molecules:Â Tautomeric Equilibrium of 2-Pyridone and 2-Hydroxypridine in Water Studied by the RISM-SCF Method. Journal of Physical Chemistry A, 2004, 108, 2097-2102.	2.5	28
115	Luminescent Heteropolynuclear Complexes of 3,5â€Dimethylpyrazolate [Pt₂Au₂M₂(Me₂pz)₈] (M=Ag, Cu) Showing the Synergistic Effect of Three Transition Elements in the Excited State. Chemistry - A European Journal, 2009, 15, 4238-4242.	3.3	28
116	RISM-SCF-SEDD Study on the Symmetry Breaking of Carbonate and Nitrate Anions in Aqueous Solution. Journal of Physical Chemistry B, 2010, 114, 10513-10519.	2.6	28
117	Effects of PAr₃ Ligands on Direct Arylation of Heteroarenes with Isolated [Pd(2,6-Me₂C₆H₃)(Î¼-O₂CMe)(PAr₃)]₂ Complexes. Organometallics, 2014, 33, 6247-6252.	2.6	28
118	DRIFT and Theoretical Studies of Ethylene/Ethane Separation on Flexible and Microporous [Cu₂(2,3â€pyrazinedicarboxylate)₂(pyrazine)]_n. European Journal of Inorganic Chemistry, 2014, 2014, 2747-2752.	2.0	28
119	Electronic structures and stereochemistry of some side-on dioxygen complexes. Inorganic Chemistry, 1978, 17, 3183-3188.	4.0	27
120	Platinum-catalyzed hydrosilylation of ethylene. A theoretical study on the reaction mechanism involving cisâ€“trans isomerization of PtH(SiH3)(PH3)2. Computational and Theoretical Chemistry, 1999, 461-462, 533-546.	1.5	27
121	Modulating fluorescence of 8-quinolinolato compounds by functional groups: A theoretical study. Applied Physics Letters, 2001, 79, 2348-2350.	3.3	27
122	Theoretical Study of Oxidative Additions of H₂ and MeCN to a Nickel(0) Complex:â€‰ Significantly Large Correlation Effects and Characteristic Features of the Reaction. Journal of Physical Chemistry A, 2007, 111, 7915-7924.	2.5	27
123	Evaluation Procedure of Electrostatic Potential in 3D-RISM-SCF Method and Its Application to Hydrolyses of Cis- and Transplatin Complexes. Journal of Physical Chemistry B, 2012, 116, 13045-13062.	2.6	27
124	Characterization of Rhâ€“Al Bond in Rh(PAlP) (PAlP = Pincer-type Diphosphino-Aluminyl Ligand) in Comparison with Rh(L)(PMe₃)₂ (L = AlMe₂,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 142 Td (Al(NM	4.0	27
125	Theoretical Study of Hydrogenation Catalysis of Phosphorus Compound and Prediction of Catalyst with High Activity and Wide Application Scope. ACS Catalysis, 2016, 6, 4859-4870.	11.2	26
126	Formation of the Oxanickelacyclopentene Complex from Nickel(0), Carbon Dioxide, and Alkyne. Anab initioMO/SD-CI Study. Part II. Reactivity and Regioselectivity of Hydroxyacetylene. Bulletin of the Chemical Society of Japan, 1995, 68, 1873-1882.	3.2	25

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127	How to Stabilize Î·³-Silapropargyl/Alkynylsilyl Complex of [CpL₂M]⁺(L = CO, PMe₃, or PF₃ and M =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	2.3	24
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