

VÃ-ctor Polo

List of Publications by Year in descending order

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117
papers

4,120
citations

109321

35
h-index

133252

59
g-index

132
all docs

132
docs citations

132
times ranked

4105
citing authors

#	ARTICLE	IF	CITATIONS
1	Dehydrogenation of formic acid using iridium-NSi species as catalyst precursors. Dalton Transactions, 2022, 51, 4386-4393.	3.3	8
2	Rhodiumâ€NHCâ€Catalyzed <i>gem</i> -Specific <i>O</i> -Selective Hydropyridonation of Terminal Alkynes. Angewandte Chemie - International Edition, 2022, 61, .	13.8	8
3	Nucleophilic Reactivity at a α -CH Arm of a Lutidine-Based CNC/Rh System: Unusual Alkyne and CO ₂ Activation. Inorganic Chemistry, 2022, 61, 7120-7129.	4.0	4
4	Metalâ€Ligand Cooperative Proton Transfer as an Efficient Trigger for Rhodium-NHC-Pyridonato Catalyzed <i>gem</i> -Specific Alkyne Dimerization. ACS Catalysis, 2021, 11, 7553-7567.	11.2	14
5	Impact of Green Cosolvents on the Catalytic Dehydrogenation of Formic Acid: The Case of Iridium Catalysts Bearing NHC-phosphane Ligands. Inorganic Chemistry, 2021, 60, 15497-15508.	4.0	11
6	Spin polarisation in dual catalysts for the oxygen evolution and reduction reactions. Current Opinion in Electrochemistry, 2021, 30, 100798.	4.8	11
7	A Bond Charge Model Ansatz for Intrinsic Bond Energies: Application to Câ€C Bonds. Journal of Physical Chemistry A, 2020, 124, 176-184.	2.5	2
8	Tunable from Blue to Red Emissive Composites and Solids of Silver Diphosphane Systems with Higher Quantum Yields than the Diphosphane Ligands. Inorganic Chemistry, 2020, 59, 14447-14456.	4.0	9
9	2-Pyridone-stabilized iridium silylene/silyl complexes: structure and QTAIM analysis. Dalton Transactions, 2020, 49, 17665-17673.	3.3	7
10	Magnetism and Heterogeneous Catalysis: In Depth on the Quantum Spin-Exchange Interactions in Pt ₃ M (M = V, Cr, Mn, Fe, Co, Ni, and Y)(111) Alloys. ACS Applied Materials & Interfaces, 2020, 12, 50484-50494.	8.0	22
11	Human riboflavin kinase: Speciesâ€specific traits in the biosynthesis of the FMN cofactor. FASEB Journal, 2020, 34, 10871-10886.	0.5	10
12	Iridium catalysts featuring amine-containing ligands for the dehydrogenation of formic acid. Journal of Organometallic Chemistry, 2020, 916, 121259.	1.8	3
13	Carboxylate-Assisted \hat{I}^2 - <i>Z</i> Stereoselective Hydrosilylation of Terminal Alkynes Catalyzed by a Zwitterionic Bis-NHC Rhodium(III) Complex. ACS Catalysis, 2020, 10, 7367-7380.	11.2	24
14	Towards the competent conformation for catalysis in the ferredoxin-NADP+ reductase from the Brucella ovis pathogen. Biochimica Et Biophysica Acta - Bioenergetics, 2019, 1860, 148058.	1.0	5
15	Mechanistic Insights on the Functionalization of CO ₂ with Amines and Hydrosilanes Catalyzed by a Zwitterionic Iridium Carboxylateâ€Functionalized Bisâ€NHC Catalyst. ChemCatChem, 2019, 11, 5524-5535.	3.7	20
16	Hydrideâ€Rhodium(III)- <i>N</i> -Heterocyclic Carbene Catalyst for Tandem Alkylation/Alkenylation via Câ€H Activation. ACS Catalysis, 2019, 9, 9372-9386.	11.2	11
17	Localizing electron density errors in density functional theory. Physical Chemistry Chemical Physics, 2019, 21, 20927-20938.	2.8	9
18	Ir-catalyzed selective reduction of CO ₂ to the methoxy or formate level with HSiMe(OSiMe ₃) ₂ . Catalysis Science and Technology, 2019, 9, 2858-2867.	4.1	23

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19	Synthesis and reactivity at the Ir-MeTp ^m platform: from Ir ^I -N coordination to Ir ^{III} -N-based organometallic chemistry. Dalton Transactions, 2019, 48, 6455-6463.	3.3	2
20	A bonding evolution theory study on the catalytic Noyori hydrogenation reaction. Molecular Physics, 2019, 117, 1315-1324.	1.7	14
21	Understanding the reaction mechanism of the oxidative addition of ammonia by (PXP)Ir complexes: the role of the X group. Physical Chemistry Chemical Physics, 2018, 20, 1105-1113.	2.8	18
22	Orbital Physics of Perovskites for the Oxygen Evolution Reaction. Topics in Catalysis, 2018, 61, 267-275.	2.8	16
23	Synergistic catalysis: enantioselective cyclopropanation of alkylidene benzoxazoles by Pd and secondary amine catalysis. Scope, limitations and mechanistic insight. Organic Chemistry Frontiers, 2018, 5, 806-812.	4.5	18
24	A highly efficient Ir-catalyst for the solventless dehydrogenation of formic acid: the key role of an N-heterocyclic olefin. Green Chemistry, 2018, 20, 4875-4879.	9.0	29
25	Amido Complexes of Iridium with a PNP Pincer Ligand: Reactivity toward Alkynes and Hydroamination Catalysis. Organometallics, 2018, 37, 2618-2629.	2.3	13
26	Proteasome versus Thioredoxin Reductase Competition as Possible Biological Targets in Antitumor Mixed Thiolate-Dithiocarbamate Gold(III) Complexes. Inorganic Chemistry, 2018, 57, 10832-10845.	4.0	33
27	On the Role of Ferromagnetic Interactions in Highly Active Mo-Based Catalysts for Ammonia Synthesis. ChemPhysChem, 2018, 19, 2843-2847.	2.1	16
28	Iridium-catalyzed formation of silylphosphinecarboxylates from the reaction of CO ₂ with P(SiMe ₃) ₂ R ₂ (R = Ph, Cy). Catalysis Science and Technology, 2017, 7, 1372-1378.	4.1	6
29	Chiral supramolecular organization from a sheet-like achiral gel: a study of chiral photoinduction. Physical Chemistry Chemical Physics, 2017, 19, 13622-13628.	2.8	5
30	Analysis of the Magnetic Entropy in Oxygen Reduction Reactions Catalysed by Manganite Perovskites. ChemCatChem, 2017, 9, 3358-3363.	3.7	22
31	Mechanistic Insights on the Reduction of CO ₂ to Silylformates Catalyzed by Ir-NSiN Species. Chemistry - A European Journal, 2017, 23, 11898-11907.	3.3	30
32	Design of Highly Selective Alkyne Hydrothiolation Rh ^I -NHC Catalysts: Carbonyl-Triggered Nonoxidative Mechanism. Organometallics, 2017, 36, 2198-2207.	2.3	34
33	A well-defined NHC-Ir(III) catalyst for the silylation of aromatic C-H bonds: substrate survey and mechanistic insights. Chemical Science, 2017, 8, 4811-4822.	7.4	44
34	Efficient preparation of carbamates by Rh-catalysed oxidative carbonylation: unveiling the role of the oxidant. Chemical Communications, 2017, 53, 404-407.	4.1	15
35	Reactivity of the parent amido complexes of iridium with olefins: C-NH ₂ bond formation versus C-H activation. Dalton Transactions, 2017, 46, 11459-11468.	3.3	3
36	Molecular Rearrangement of an Aza-Scorpiand Macrocycle Induced by pH: A Computational Study. International Journal of Molecular Sciences, 2016, 17, 1131.	4.1	6

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37	2,5-Norbornadiene C=C Coupling Reactions Mediated by Iridium Complexes. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 3489-3499.	2.0	3
38	Oxidative Addition of the N-H Bond of Ammonia to Iridium Bis(phosphane) Complexes: A Combined Experimental and Theoretical Study. <i>Organometallics</i> , 2016, 35, 720-731.	2.3	16
39	Temperature Dual Enantioselective Control in a Rhodium-Catalyzed Michael-Type Friedel-Crafts Reaction: A Mechanistic Explanation. <i>Chemistry - A European Journal</i> , 2016, 22, 11064-11083.	3.3	22
40	C=N Bond Coupling Reactions of Ammonia with Acetone Promoted by Iridium and Rhodium Complexes: Experimental and DFT Studies. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5347-5355.	2.0	2
41	Rhodium-Catalyzed Dehydrogenative Silylation of Acetophenone Derivatives: Formation of Silyl Enol Ethers versus Silyl Ethers. <i>Chemistry - A European Journal</i> , 2016, 22, 14717-14729.	3.3	21
42	N-Heterocyclic olefins as ancillary ligands in catalysis: a study of their behaviour in transfer hydrogenation reactions. <i>Dalton Transactions</i> , 2016, 45, 12835-12845.	3.3	37
43	Mechanistic insight into the pyridine enhanced β -selectivity in alkyne hydrothiolation catalysed by quinolinolate-rhodium-N-heterocyclic carbene complexes. <i>Catalysis Science and Technology</i> , 2016, 6, 8548-8561.	4.1	24
44	A DFT study of the role of water in the rhodium-catalyzed hydrogenation of acetone. <i>Chemical Communications</i> , 2016, 52, 13881-13884.	4.1	17
45	Experimental and Computational Studies on the Reactivity and Binding Mode of Thiophene with N-Heterocyclic Carbene Iridium Complexes. <i>Organometallics</i> , 2016, 35, 569-578.	2.3	4
46	Alkoxy carbonylation of β , γ -unsaturated amides catalyzed by palladium complexes: a DFT study of the mechanism. <i>RSC Advances</i> , 2016, 6, 8440-8448.	3.6	6
47	Efficient Rhodium-Catalyzed Multicomponent Reaction for the Synthesis of Novel Propargylamines. <i>Chemistry - A European Journal</i> , 2015, 21, 17701-17707.	3.3	27
48	Solvent-Free Iridium-Catalyzed Reactivity of CO ₂ with Secondary Amines and Hydrosilanes. <i>ChemCatChem</i> , 2015, 7, 3895-3902.	3.7	40
49	An Insight into Transfer Hydrogenation Reactions Catalysed by Iridium(III) Bis-N-heterocyclic Carbenes. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 4388-4395.	2.0	17
50	Mechanism Switch in Mannich-Type Reactions: ELF and NCI Topological Analyses of the Reaction between Nitrones and Lithium Enolates. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 4143-4152.	2.4	16
51	Orthometallation of N-substituents at the NHC ligand of [Rh(Cl)(COD)(NHC)] complexes: its role in the catalytic hydrosilylation of ketones. <i>Catalysis Science and Technology</i> , 2015, 5, 1878-1887.	4.1	9
52	Catalytic Hydrodechlorination of Benzyl Chloride Promoted by Rh-N-heterocyclic Carbene Catalysts. <i>ChemSusChem</i> , 2015, 8, 495-503.	6.8	15
53	Iridium complexes as catalysts in the hydrogen transfer of isopropanol to acetophenone: Ligand effects and DFT studies. <i>Inorganica Chimica Acta</i> , 2015, 436, 146-151.	2.4	14
54	Tuning PCP-Ir complexes: the impact of an N-heterocyclic olefin. <i>Chemical Communications</i> , 2015, 51, 12431-12434.	4.1	37

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55	Understanding Bond Formation in Polar One-Step Reactions. Topological Analyses of the Reaction between Nitrones and Lithium Ynolates. <i>Journal of Organic Chemistry</i> , 2015, 80, 4076-4083.	3.2	32
56	A bimetallic iridium(ii) catalyst: $[\{\text{Ir}(\text{IDipp})(\text{H})\}_2][\text{BF}_4]_2$ (IDipp =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 702 Td (1,3-bis(2,6-diisopropylph	4.1	21
57	Nâ€H Activation of Ammonia by $[\text{M}(\text{I}^{\frac{1}{4}}\text{-OMe})(\text{cod})]_2$ (M = Ir, Rh) Complexes: A DFT Study. <i>Organometallics</i> , 2015, 34, 3959-3966.	2.3	20
58	Iridiumâ€Catalyzed Hydrogen Production from Hydrosilanes and Water. <i>ChemCatChem</i> , 2014, 6, 1691-1697.	3.7	41
59	Selective Cî¿H Bond Functionalization of 2â€(2â€Thienyl)pyridine by a Rhodium Nâ€Heterocyclic Carbene Catalyst. <i>ChemCatChem</i> , 2014, 6, 3192-3199.	3.7	28
60	Pâ€H activation of secondary phosphanes on a parent amido diiridium complex. <i>Dalton Transactions</i> , 2014, 43, 1609-1619.	3.3	18
61	New insights into the chemistry of di- and trimetallic iron dithiolene derivatives. Structural, MĂssbauer, magnetic, electrochemical and theoretical studies. <i>Dalton Transactions</i> , 2014, 43, 13187-13195.	3.3	7
62	Cî¿NH₂ Bond Formation Mediated by Iridium Complexes. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 9627-9631.	13.8	12
63	Theoretical Studies on the Mechanism of Iridium-Catalyzed Alkene Hydrogenation by the Cationic Complex $[\text{IrH}_2(\text{NCMe})_3(\text{P}^{\supset}(\text{Pr})_3)]^+$. <i>Organometallics</i> , 2014, 33, 5156-5163.	2.3	23
64	Hydroxoâ€Rhodiumâ€N-Heterocyclic Carbene Complexes as Efficient Catalyst Precursors for Alkyne Hydrothiolation. <i>ACS Catalysis</i> , 2013, 3, 2910-2919.	11.2	53
65	Halogen-Bonding Complexes Based on Bis(iodoethynyl)benzene Units: A New Versatile Route to Supramolecular Materials. <i>Chemistry of Materials</i> , 2013, 25, 4503-4510.	6.7	77
66	CO₂ Activation and Catalysis Driven by Iridium Complexes. <i>ChemCatChem</i> , 2013, 5, 3481-3494.	3.7	53
67	Heterolytic H2 activation on a carbene-ligated rhodathiaborane promoted by isonido-nido cage opening. <i>Chemical Communications</i> , 2013, 49, 9863.	4.1	11
68	Pyridineâ€Enhanced Headâ€Tail Dimerization of Terminal Alkynes by a Rhodiumâ€Nâ€Heterocyclicâ€Carbene Catalyst. <i>Chemistry - A European Journal</i> , 2013, 19, 15304-15314.	3.3	46
69	An Alternative Mechanistic Paradigm for the Î²â€Z</i> Hydrosilylation of Terminal Alkynes: The Role of Acetone as a Silane Shuttle. <i>Chemistry - A European Journal</i> , 2013, 19, 17559-17566.	3.3	81
70	Cubane-Type Mo₃FeS₄ ^{4+,5+} Complexes Containing Outer Diphosphane Ligands: Ligand Substitution Reactions, Spectroscopic Studies, and Electronic Structure. <i>Inorganic Chemistry</i> , 2012, 51, 10512-10521.	4.0	11
71	A synthon for a 14-electron Ir(iii) species: catalyst for highly selective Î²-(Z) hydrosilylation of terminal alkynes. <i>Chemical Communications</i> , 2012, 48, 9480.	4.1	60
72	Synthesis, molecular and electronic structure of an incomplete cuboidal Re3S4 cluster with an unusual quadruplet ground state. <i>Chemical Communications</i> , 2012, 48, 2713.	4.1	11

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73	Ligand-Controlled Regioselectivity in the Hydrothiolation of Alkynes by Rhodium N-Heterocyclic Carbene Catalysts. <i>Journal of the American Chemical Society</i> , 2012, 134, 8171-8183.	13.7	170
74	Effective Fixation of CO ₂ by Iridium-Catalyzed Hydrosilylation. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 12824-12827.	13.8	130
75	Non-adiabatic effects within a single thermally averaged potential energy surface: Thermal expansion and reaction rates of small molecules. <i>Journal of Chemical Physics</i> , 2012, 137, 22A533.	3.0	5
76	Synthesis and structure of a paramagnetic Mo ₃ S ₄ incomplete cuboidal cluster with seven cluster skeletal electrons. <i>Dalton Transactions</i> , 2012, 41, 14031.	3.3	16
77	The Dehydrogenation of Alcohols through a Concerted Bimetallic Mechanism Involving an Amido-Bridged Diiridium Complex. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 8259-8263.	13.8	33
78	Fluorescence Detection by Intensity Change Based Sensors: A Theoretical Model. <i>Journal of Fluorescence</i> , 2012, 22, 381-389.	2.5	2
79	Olefin Epoxidation by Molybdenum Peroxo Compound: Molecular Mechanism Characterized by the Electron Localization Function and Catastrophe Theory. <i>Journal of Physical Chemistry A</i> , 2011, 115, 514-522.	2.5	23
80	Mild and Selective H/D Exchange at the α -Position of Aromatic Olefins by N-Heterocyclic Carbene-Hydride-Rhodium Catalysts. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 3938-3942.	13.8	72
81	Direct Access to Parent Amido Complexes of Rhodium and Iridium through N ₂ H Activation of Ammonia. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11735-11738.	13.8	60
82	Hybrid Organic/Inorganic Complexes Based on Electroactive Tetrathiafulvalene-Functionalized Diphosphanes Tethered to C ₃ -Symmetrized Mo ₃ Q ₄ (Q = S, Se) Clusters. <i>Inorganic Chemistry</i> , 2010, 49, 1894-1904.	4.0	26
83	Sulfur-Based Redox Reactions in Mo ₃ S ₇ ⁴⁺ and Mo ₃ S ₄ ⁴⁺ Clusters Bearing Halide and 1,2-Dithiolene Ligands: a Mass Spectrometric and Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2010, 49, 8045-8055.	4.0	11
84	<i>Ab initio</i> molecular dynamics on the electronic Boltzmann equilibrium distribution. <i>New Journal of Physics</i> , 2010, 12, 083064.	2.9	11
85	Spin-Spin Interactions in Porphyrin-Based Monoverdazyl Radical Hybrid Spin Systems. <i>Inorganic Chemistry</i> , 2010, 49, 3516-3524.	4.0	38
86	The thiocyanate anion as a polydentate halogen bond acceptor. <i>CrystEngComm</i> , 2010, 12, 558-566.	2.6	67
87	A theoretical study on the thermal ring opening rearrangement of 1H-bicyclo[3.1.0]hexa-3,5-dien-2-one: a case of two state reactivity. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 7189.	2.8	11
88	A Density Functional Theory Study of the Magnetic Exchange Coupling in Dinuclear Manganese(II) Inverse Crown Structures. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14008-14013.	2.5	17
89	An electron localization function and catastrophe theory analysis on the molecular mechanism of gas-phase identity S _N 2 reactions. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 341-349.	1.4	41
90	Combined ¹³ C NMR and DFT/GIAO studies of the polyketides Aurasperone A and Fonsecinone A. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2408-2416.	2.0	3

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91	Halogen Bonding Interactions of <i>sym</i> -Triiodotrifluorobenzene with Halide Anions: A Combined Structural and Theoretical Study. <i>Crystal Growth and Design</i> , 2008, 8, 2241-2247.	3.0	74
92	Towards understanding of magnetic interactions within a series of tetrathiafulvalene-ferrocene conjugated-verdazyl diradical cation system: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 857-864.	2.8	60
93	Understanding Reaction Mechanisms in Organic Chemistry from Catastrophe Theory Applied to the Electron Localization Function Topology. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7128-7136.	2.5	165
94	Heterometallic Cuboidal Clusters $M_3M'Q_4$ (M = Mo, W; $M' =$ Sn, Pb, As, Sb; Q = S, Se): From Coordination Compounds to Supramolecular Adducts. <i>Inorganic Chemistry</i> , 2008, 47, 306-314.	4.0	22
95	Trinuclear Mo_3S_7 Clusters Coordinated to Dithiolate or Diselenolate Ligands and Their Use in the Preparation of Magnetic Single Component Molecular Conductors. <i>Inorganic Chemistry</i> , 2008, 47, 9400-9409.	4.0	48
96	Theoretical Study on the Reaction Mechanism of VO_2^+ with Propyne in Gas Phase. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1808-1816.	2.5	16
97	Synthesis and Molecular and Electronic Structures of a Series of Mo_3CoSe_4 Cluster Complexes with Three Different Metal Electron Populations. <i>Inorganic Chemistry</i> , 2008, 47, 3661-3668.	4.0	9
98	Synthesis and characterization of a TTF-ferrocene-verdazyl radical—a new building block for conducting and/or magnetic systems. <i>New Journal of Chemistry</i> , 2007, 31, 1973.	2.8	26
99	A Theoretical Study on the Electronic Structure of $Au^+XO(0,-1,+1)$ ($X =$ C, N, and O) Complexes: A Effect of an External Electric Field. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13255-13263.	2.5	27
100	Lewis Acid and Substituent Effects on the Molecular Mechanism for the Nazarov Reaction of Penta-1,4-dien-3-one and Derivatives. A Topological Analysis Based on the Combined Use of Electron Localization Function and Catastrophe Theory. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 816-823.	5.3	31
101	<i>sym</i> -Symmetric Trinuclear Molybdenum Cluster Sulfides: Configurational Stability, Supramolecular Stereocontrol, and Absolute Configuration Assignment. <i>Inorganic Chemistry</i> , 2007, 46, 10717-10723.	4.0	21
102	New insights on the bridge carbon-carbon bond in propellanes: A theoretical study based on the analysis of the electron localization function. <i>Journal of Computational Chemistry</i> , 2007, 28, 857-864.	3.3	47
103	Better Understanding of the Ring-Cleavage Process of Cyanocyclopropyl Anionic Derivatives. A Theoretical Study Based on the Electron Localization Function. <i>Journal of Organic Chemistry</i> , 2006, 71, 754-762.	3.2	24
104	Reply to "Comment on "About the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction error" [J. Chem. Phys. 123, 164110 (2005)]. <i>Journal of Chemical Physics</i> , 2006, 124, 107102.	3.0	47
105	An electron localization function study of the trimerization of acetylene: Reaction mechanism and development of aromaticity. <i>Chemical Physics Letters</i> , 2005, 406, 393-397.	2.6	54
106	About the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction error. <i>Journal of Chemical Physics</i> , 2005, 123, 164110.	3.0	318
107	A joint study based on the electron localization function and catastrophe theory of the chameleonic and centauric models for the Cope rearrangement of 1,5-hexadiene and its cyano derivatives. <i>Journal of Computational Chemistry</i> , 2005, 26, 1427-1437.	3.3	56
108	A Theoretical Study on the Reaction Mechanism for the Bergman Cyclization from the Perspective of the Electron Localization Function and Catastrophe Theory. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3687-3693.	2.5	57

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109	Toward an Understanding of the Catalytic Role of Hydrogen-Bond Donor Solvents in the Hetero-Diels-Alder Reaction between Acetone and Butadiene Derivative. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10438-10444.	2.5	43
110	Understanding the Molecular Mechanism of the 1,3-Dipolar Cycloaddition between Fulminic Acid and Acetylene in Terms of the Electron Localization Function and Catastrophe Theory. <i>Chemistry - A European Journal</i> , 2004, 10, 5165-5172.	3.3	95
111	Long-range and short-range Coulomb correlation effects as simulated by Hartree-Fock, local density approximation, and generalized gradient approximation exchange functionals. <i>Theoretical Chemistry Accounts</i> , 2003, 109, 22-35.	1.4	81
112	Electron correlation and the self-interaction error of density functional theory. <i>Molecular Physics</i> , 2002, 100, 1771-1790.	1.7	202
113	Implicit and Explicit Coverage of Multi-reference Effects by Density Functional Theory. <i>International Journal of Molecular Sciences</i> , 2002, 3, 604-638.	4.1	111
114	Some thoughts about the stability and reliability of commonly used exchange-correlation functionals: coverage of dynamic and nondynamic correlation effects. <i>Theoretical Chemistry Accounts</i> , 2002, 107, 291-303.	1.4	116
115	Influence of the self-interaction error on the structure of the DFT exchange hole. <i>Chemical Physics Letters</i> , 2002, 352, 469-478.	2.6	65
116	Rh Complexes with Pincer Carbene CNC Lutidine-Based Ligands: Reactivity Studies toward H ₂ Addition. <i>Organometallics</i> , 0, , .	2.3	7
117	Rhodium-NHC-Catalyzed <i>gem</i> -Specific <i>o</i> -Selective Hydroxyridination of Terminal Alkynes. <i>Angewandte Chemie</i> , 0, , .	2.0	0