Per-Ola Norrby

List of Publications by Year
in descending order

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211	10,061	23565	48312
papers	citations	58 h-index	88 g-index

245	245	245	7945
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Automated fitting of transition state force fields for biomolecular simulations. PLoS ONE, 2022, 17, e0264960.	2.5	5
2	Machine learning meets mechanistic modelling for accurate prediction of experimental activation energies. Chemical Science, 2021, 12, 1163-1175.	7.4	102
3	Enantioselective Synthesis of Atropisomeric Biaryls using Biaryl 2,5â€Diphenylphospholanes as Ligands for Palladiumâ€Catalysed Suzukiâ€Miyaura Reactions. Advanced Synthesis and Catalysis, 2021, 363, 259-267.	4.3	15
4	Microsecond timescale MD simulations at the transition state of PmHMGR predict remote allosteric residues. Chemical Science, 2021, 12, 6413-6418.	7.4	7
5	Stereoselectivity Predictions for the Pd-Catalyzed 1,4-Conjugate Addition Using Quantum-Guided Molecular Mechanics. Journal of Organic Chemistry, 2021, 86, 5660-5667.	3.2	6
6	Organic reactivity from mechanism to machine learning. Nature Reviews Chemistry, 2021, 5, 240-255.	30.2	88
7	Experimental and Computational Models for Side Chain Discrimination in Peptideâ€“Protein Interactions. Chemistry - A European Journal, 2021, 27, 10883-10897.	3.3	6
8	Proofreading experimentally assigned stereochemistry through Q2MM predictions in Pd-catalyzed allylic aminations. Nature Communications, 2021, 12, 6719.	12.8	5
9	Synthetic and mechanistic studies in enantioselective allylic substitutions catalysed by palladium complexes of a modular class of axially chiral quinazoline-containing ligands. Tetrahedron, 2020, 76, 130780.	1.9	8
10	From desktop to benchtop with automated computational workflows for computer-aided design in asymmetric catalysis. Nature Catalysis, 2020, 3, 574-584.	34.4	31
11	Applications of Quantum Chemistry in Pharmaceutical Process Development: Current State and Opportunities. Organic Process Research and Development, 2020, 24, 1496-1507.	2.7	25
12	Palladium Catalyzed Stereoselective Arylation of Biocatalytically Derived Cyclic 1,3-Dienes: Chirality Transfer via a Heck-Type Mechanism. Organic Letters, 2020, 22, 2464-2469.	4.6	4
13	Transition State Force Field for the Asymmetric Redox-Relay Heck Reaction. Journal of the American Chemical Society, 2020, 142, 9700-9707.	13.7	15
14	Degradation of Pharmaceuticals through Sequential Photon Absorption and Photoionization in Amiloride Derivatives. Cell Reports Physical Science, 2020, 1, 100274.	5.6	5
15	Holistic models of reaction selectivity. Nature, 2019, 571, 332-333.	27.8	3
16	Relative Strength of Common Directing Groups in Palladium-Catalyzed Aromatic Câ^'H Activation. IScience, 2019, 20, 373-391.	4.1	34
17	An Improved Class of Phosphite-Oxazoline Ligands for Pd-Catalyzed Allylic Substitution Reactions. ACS Catalysis, 2019, 9, 6033-6048.	11.2	18
18	Is Excitedâ€State Aromaticity a Driving Force for Planarization of Dibenzannelated 8Ïâ€Electron Heterocycles?. ChemPlusChem, 2019, 84, 712-721.	2.8	38

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19	A Predictive Tool for Electrophilic Aromatic Substitutions Using Machine Learning. Journal of Organic Chemistry, 2019, 84, 4695-4703.	3.2	70
20	Rapid virtual screening of enantioselective catalysts using CatVS. Nature Catalysis, 2019, 2, 41-45.	34.4	81
21	Nonclassical Mechanism in the Cyclodehydration of Diols Catalyzed by a Bifunctional Iridium Complex. Chemistry - A European Journal, 2019, 25, 2631-2636.	3.3	6
22	Computational prediction of chemical reactions: current status and outlook. Drug Discovery Today, 2018, 23, 1203-1218.	6.4	126
23	Revisiting the Stereodetermining Step in Enantioselective Iridium-Catalyzed Imine Hydrogenation. ACS Catalysis, 2018, 8, 615-623.	11.2	38
24	Designing flexible low-viscous sieving media for capillary electrophoresis analysis of ribonucleic acids. Journal of Chromatography A, 2018, 1562, 108-114.	3.7	17
25	Degradation caused by incompatibility between sodium stearyl fumarate (PRUV) and AZD7986 in the drug product. Journal of Pharmaceutical and Biomedical Analysis, 2018, 158, 82-87.	2.8	5
26	Enantioselective Synthesis of Sterically Hindered Tertiary Î±â€Aryl Oxindoles via Palladiumâ€Catalyzed Decarboxylative Protonation. An Experimental and Theoretical Mechanistic Investigation. Advanced Synthesis and Catalysis, 2018, 360, 3124-3137.	4.3	11
27	Application of Q2MM to predictions in stereoselective synthesis. Chemical Communications, 2018, 54, 8294-8311.	4.1	37
28	Manganeseâ€Catalyzed Crossâ€Coupling of Aryl Halides and Grignard Reagents by a Radical Mechanism. European Journal of Organic Chemistry, 2017, 2017, 4758-4764.	2.4	14
29	Competing Pathways in Oâ€Arylations with Diaryliodonium Salts: Mechanistic Insights. Chemistry - A European Journal, 2017, 23, 13249-13258.	3.3	56
30	The Manganeseâ€Catalyzed Crossâ€Coupling Reaction and the Influence of Trace Metals. European Journal of Organic Chemistry, 2017, 2017, 5269-5274.	2.4	13
31	Kinetic and Theoretical Investigation of Iron(III)â€Catalyzed Silane Chlorination. ChemCatChem, 2016, 8, 584-592.	3.7	3
32	Prediction of Stereochemistry using Q2MM. Accounts of Chemical Research, 2016, 49, 996-1005.	15.6	76
33	Anomeric Effects in Sulfamides. Journal of Physical Chemistry A, 2016, 120, 3677-3682.	2.5	9
34	Asymmetric Catalyzed Allylic Substitution Using a Pd/Pâ€“S Catalyst Library with Exceptional High Substrate and Nucleophile Versatility: DFT and Pd-Ï€-allyl Key Intermediates Studies. Organometallics, 2016, 35, 3323-3335.	2.3	21
35	Mechanistic Insights into the Iridiumâ€Catalyzed Hydrogenations of Î±,Î²â€Unsaturated Ketones. ChemCatChem, 2016, 8, 3099-3106.	3.7	14
36	Glycerol Upgrading via Hydrogen Borrowing: Direct Ruthenium-Catalyzed Amination of the Glycerol Derivative Solketal. ACS Sustainable Chemistry and Engineering, 2016, 4, 5730-5736.	6.7	18

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37	Stereoselectivity in (Acyloxy)borane-Catalyzed Mukaiyama Aldol Reactions. Journal of Organic Chemistry, 2016, 81, 5314-5321.	3.2	11
38	Conformational Preferences of a Tropos Biphenyl Phosphinooxazolineâ€“a Ligand with Wide Substrate Scope. ACS Catalysis, 2016, 6, 1701-1712.	11.2	30
39	Theoretical and Experimental Optimization of a New Amino Phosphite Ligand Library for Asymmetric Palladiumâ€Catalyzed Allylic Substitution. ChemCatChem, 2015, 7, 4091-4107.	3.7	21
40	Singleâ€Flask Multicomponent Palladiumâ€Catalyzed Î±,Î³â€Coupling of Ketone Enolates: Facile Preparation of Complex Carbon Scaffolds. Angewandte Chemie - International Edition, 2015, 54, 11822-11825.	13.8	20
41	Mechanistic Studies on the Alkylation of Amines with Alcohols Catalyzed by a Bifunctional Iridium Complex. ACS Catalysis, 2015, 5, 3704-3716.	11.2	72
42	Ni-Catalyzed Alkenylation of Ketone Enolates under Mild Conditions: Catalyst Identification and Optimization. Journal of the American Chemical Society, 2015, 137, 7019-7022.	13.7	53
43	New insights into the mechanism of iron-catalyzed cross-coupling reactions. Dalton Transactions, 2015, 44, 3959-3962.	3.3	30
44	On the Radical Nature of Ironâ€Catalyzed Crossâ€Coupling Reactions. Chemistry - A European Journal, 2015, 21, 5946-5953.	3.3	63
45	Pd-Î·³-C₆H₉ complexes of the Trost modular ligand: high nuclearity columnar aggregation controlled by concentration, solvent and counterion. Chemical Science, 2015, 6, 5793-5801.	7.4	12
46	Improving the <scp>Q2MM</scp> method for transition state force field modeling. Journal of Computational Chemistry, 2015, 36, 244-250.	3.3	9
47	Epoxyalcohols: Bioactivation and Conjugation Required for Skin Sensitization. Chemical Research in Toxicology, 2014, 27, 1860-1870.	3.3	10
48	Mechanistic Aspects of Submolâ€‰% Copperâ€Catalyzed Cï£¿N Crossâ€Coupling. ChemCatChem, 2014, 6, 1277-1282.	3.7	16
49	Breaking conjugation: unusual regioselectivity with 2-substituted allylic substrates in the Tsujiâ€“Trost reaction. Chemical Science, 2014, 5, 1241-1250.	7.4	9
50	Mechanistic Investigations of Palladium-Catalyzed Allylic Fluorination. Organometallics, 2014, 33, 2121-2133.	2.3	63
51	Role of the Base in Buchwaldâ€“Hartwig Amination. Journal of Organic Chemistry, 2014, 79, 11961-11969.	3.2	74
52	Investigating the Nature of Palladium Chain-Walking in the Enantioselective Redox-Relay Heck Reaction of Alkenyl Alcohols. Journal of Organic Chemistry, 2014, 79, 11841-11850.	3.2	95
53	Fast and reversible insertion of carbon dioxide into zirconoceneâ€“alkoxide bonds. A mechanistic study. Dalton Transactions, 2014, 43, 8894-8898.	3.3	4
54	Stereoselectivity in Asymmetric Catalysis: The Case of Ruthenium-Catalyzed Ketone Hydrogenation. Journal of Chemical Theory and Computation, 2014, 10, 2427-2435.	5.3	27

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55	Palladium-Catalyzed Alkenylation of Ketone Enolates under Mild Conditions. Organic Letters, 2014, 16, 3970-3973.	4.6	36
56	Mechanism, Reactivity, and Selectivity in Palladium-Catalyzed Redox-Relay Heck Arylations of Alkenyl Alcohols. Journal of the American Chemical Society, 2014, 136, 1960-1967.	13.7	187
57	On the oxidation state of iron in iron-mediated Câ€“C couplings. Journal of Organometallic Chemistry, 2013, 748, 51-55.	1.8	50
58	Chelation-Controlled Addition of Organozincs to Î±-Chloro Aldimines. Journal of the American Chemical Society, 2012, 134, 17599-17604.	13.7	30
59	Mechanistic Studies of the CuH-Catalyzed Synthesis of Î±-Hydroxyallenes. Organometallics, 2012, 31, 8024-8030.	2.3	11
60	A computational study of the enantioselective addition of n-BuLi to benzaldehyde in the presence of a chiral lithium N,P amide. Organic and Biomolecular Chemistry, 2012, 10, 2807.	2.8	12
61	Mild and Efficient Nickel-Catalyzed Heck Reactions with Electron-Rich Olefins. Journal of the American Chemical Society, 2012, 134, 443-452.	13.7	138
62	New efficient ligand for sub-mol % copper-catalyzed Câ€“N cross-coupling reactions running under air. Beilstein Journal of Organic Chemistry, 2012, 8, 1909-1915.	2.2	9
63	Transmetallation Versus Î²â€Hydride Elimination: The Role of 1,4â€Benzoquinone in Chelationâ€Controlled Arylation Reactions with Arylboronic Acids. Chemistry - A European Journal, 2012, 18, 4714-4722.	3.3	39
64	Aggregation and Solvation of Chiral N,Pâ€Amide Ligands in Coordinating Solvents: A Computational and NMR Spectroscopic Study. ChemPlusChem, 2012, 77, 799-806.	2.8	11
65	tBu or not tBu?. Chemistry - A European Journal, 2012, 18, 1640-1649.	3.3	35
66	Low Temperature Studies of Ironâ€Catalyzed Crossâ€Coupling of Alkyl Grignard Reagents with Aryl Electrophiles. Advanced Synthesis and Catalysis, 2012, 354, 448-456.	4.3	43
67	A highly selective agonist for the metabotropic glutamate receptor mGluR2. MedChemComm, 2011, 2, 1120.	3.4	9
68	Experimental and Theoretical Investigations of the Autoxidation of Geranial: A Dioxolane Hydroperoxide Identified as a Skin Sensitizer. Chemical Research in Toxicology, 2011, 24, 1507-1515.	3.3	19
69	Computational Insights into Palladium-Mediated Allylic Substitution Reactions. Topics in Organometallic Chemistry, 2011, , 65-93.	0.7	24
70	A DFT comparison of the neutral and cationic Heck pathways. Dalton Transactions, 2011, 40, 11308.	3.3	36
71	Sterically Governed Selectivity in Palladium-Assisted Allylic Alkylation. Organometallics, 2011, 30, 230-238.	2.3	15
72	Pyranoside Phosphiteâ€“Oxazoline Ligands for the Highly Versatile and Enantioselective Ir-Catalyzed Hydrogenation of Minimally Functionalized Olefins. A Combined Theoretical and Experimental Study. Journal of the American Chemical Society, 2011, 133, 13634-13645.	13.7	163

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73	Dispersion and Backâ€Donation Gives Tetracoordinate [Pd(PPh₃)₄]. Angewandte Chemie - International Edition, 2011, 50, 11794-11797.	13.8	77
74	Î³â€•and Î´â€Lactams through Palladiumâ€Catalyzed Intramolecular Allylic Alkylation: Enantioselective Synthesis, NMR Investigation, and DFT Rationalization. Chemistry - A European Journal, 2011, 17, 2885-2896.	3.3	36
75	Ironâ€Catalyzed Coupling of Aryl Grignard Reagents with Alkyl Halides: A Competitive Hammett Study. Chemistry - A European Journal, 2011, 17, 11991-11993.	3.3	48
76	Palladiumâ€Catalyzed Allylic Sulfinylation and the Mislowâ€“Bravermanâ€“Evans Rearrangement. Chemistry - A European Journal, 2011, 17, 13963-13965.	3.3	5
77	Application of Q2MM to Stereoselective Reactions. Current Organic Chemistry, 2010, 14, 1629-1645.	1.6	19
78	Î±â€Arylation by Rearrangement: On the Reaction of Enolates with Diaryliodonium Salts. Chemistry - A European Journal, 2010, 16, 8251-8254.	3.3	122
79	DFT Investigation of the Palladiumâ€Catalyzed Eneâ€“Yne Coupling. Chemistry - A European Journal, 2010, 16, 9494-9501.	3.3	15
80	Kinetic Investigation of a Ligandâ€Accelerated Subâ€molâ€‰% Copperâ€Catalyzed Cï£¿N Crossâ€Coupling Reaction. Chemistry - A European Journal, 2010, 16, 13613-13616.	3.3	40
81	On the mechanism of the rhodium catalyzed acrylamide hydrogenationâ˜†. Journal of Molecular Catalysis A, 2010, 324, 9-14.	4.8	11
82	Trans effects in the Heck reactionâ€”A model study. Journal of Molecular Catalysis A, 2010, 328, 108-113.	4.8	18
83	Memory and dynamics in Pd-catalyzed allylic alkylation with P,N-ligands. Tetrahedron: Asymmetry, 2010, 21, 1585-1592.	1.8	26
84	Copperâ€Catalyzed Crossâ€Couplings with Partâ€perâ€Million Catalyst Loadings. Angewandte Chemie - International Edition, 2009, 48, 5691-5693.	13.8	238
85	Mechanistic Investigation of Ironâ€Catalyzed Coupling Reactions. ChemCatChem, 2009, 1, 152-161.	3.7	119
86	DFT-Based Explanation of the Effect of Simple Anionic Ligands on the Regioselectivity of the Heck Arylation of Acrolein Acetals. Organometallics, 2009, 28, 6201-6205.	2.3	23
87	Structure-Based Rationale for Selectivity in the Asymmetric Allylic Alkylation of Cycloalkenyl Esters Employing the Trost â€˜Standard Ligandâ€™ (TSL): Isolation, Analysis and Alkylation of the Monomeric form of the Cationic Î·³-Cyclohexenyl Complex [(Î·³-c-C₆H₉)Pd(TSL)]⁺. Journal of the American Chemical Society, 2009, 131, 9945-9957.	13.7	166
88	Prediction of Enantioselectivity in Rhodium Catalyzed Hydrogenations. Journal of the American Chemical Society, 2009, 131, 410-411.	13.7	110
89	Acidâ€Catalyzed Nucleophilic Aromatic Substitution: Experimental and Theoretical Exploration of a Multistep Mechanism. Chemistry - A European Journal, 2008, 14, 3954-3960.	3.3	23
90	Mechanisms of Air Oxidation of Ethoxylated Surfactantsâ€”Computational Estimations of Energies and Reaction Behaviors. Chemistry - A European Journal, 2008, 14, 9549-9554.	3.3	8

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91	Asymmetric Synthesis of Iridoid Derivatives Using Resolved 2â€Phenylindoline as a Chiral Auxiliary. European Journal of Organic Chemistry, 2008, 2008, 5915-5921.	2.4	9
92	Mechanism of Air Oxidation of the Fragrance Terpene Geraniol. Journal of Chemical Theory and Computation, 2008, 4, 101-106.	5.3	34
93	Unusual Selectivity-Determining Factors in the Phosphine-Free Heck Arylation of Allyl Ethers. Organometallics, 2008, 27, 3187-3195.	2.3	28
94	Steric Influence on the Excited-State Lifetimes of Ruthenium Complexes with Bipyridylâ^'Alkanyleneâ^'Pyridyl Ligands. Inorganic Chemistry, 2008, 47, 3540-3548.	4.0	127
95	Transition-State Docking of Flunitrazepam and Progesterone in Cytochrome P450. Journal of Chemical Theory and Computation, 2008, 4, 673-681.	5.3	26
96	Combined Experimental and Theoretical Study of the Mechanism and Enantioselectivity of Palladium-Catalyzed Intermolecular Heck Coupling. Journal of the American Chemical Society, 2008, 130, 10414-10421.	13.7	97
97	Development of a Q2MM Force Field for the Asymmetric Rhodium Catalyzed Hydrogenation of Enamides. Journal of Chemical Theory and Computation, 2008, 4, 1313-1323.	5.3	63
98	On the Nature of the Intermediates and the Role of Chloride Ions in Pd-Catalyzed Allylic Alkylations: Added Insight from Density Functional Theory. Journal of Physical Chemistry A, 2008, 112, 12862-12867.	2.5	46
99	The Mechanism for the Rhodium-Catalyzed Decarbonylation of Aldehydes: A Combined Experimental and Theoretical Study. Journal of the American Chemical Society, 2008, 130, 5206-5215.	13.7	180
100	General Transition-State Force Field for Cytochrome P450 Hydroxylation. Journal of Chemical Theory and Computation, 2007, 3, 1765-1773.	5.3	54
101	Oxidative Addition of Aryl Chlorides to Monoligated Palladium(0):Â A DFT-SCRF Study. Organometallics, 2007, 26, 550-553.	2.3	190
102	Memory Effects in Palladiumâ€Catalyzed Allylic Alkylations of 2â€Cyclohexenâ€1â€yl Acetate. Advanced Synthesis and Catalysis, 2007, 349, 2631-2640.	4.3	27
103	The Mechanism of the Phosphine-Free Palladium-Catalyzed Hydroarylation of Alkynes. Journal of the American Chemical Society, 2006, 128, 12785-12793.	13.7	61
104	Regioselectivity in lithiation of 1-methylpyrazole: experimental, density functional theory and multinuclear NMR study. Organic and Biomolecular Chemistry, 2006, 4, 1261.	2.8	13
105	Modulation of the reactivity, stability and substrate- and enantioselectivity of an epoxidation catalyst by noncovalent dynamic attachment of a receptor functionalityâ€"aspects on the mechanism of the Jacobsenâ€"Katsuki epoxidation applied to a supramolecular system. Organic and Biomolecular Chemistry, 2006, 4, 1927-1948.	2.8	45
106	Divergence en Route to Nonclassical Annonaceous Acetogenins. Synthesis of Pyranicin and Pyragonicinâ€. Journal of Organic Chemistry, 2006, 71, 1879-1891.	3.2	37
107	Direct Determination of Absolute Configuration of Methyl-Substituted Phenyloxiranes:â€‰ Combined Experimental and Theoretical Approach. Journal of Physical Chemistry A, 2006, 110, 9123-9129.	2.5	9
108	On the Performance of Continuum Solvation Models for the Solvation Energy of Small Anions. Organometallics, 2006, 25, 45-47.	2.3	23

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109	Combining Q2MM modeling and kinetic studies for refinement of the osmium-catalyzed asymmetric dihydroxylation (AD) mnemonic. Journal of Organometallic Chemistry, 2006, 691, 2182-2198.	1.8	33
110	Theoretical Evidence for Low-Ligated Palladium(0):â€‰[Pdâ^'L] as the Active Species in Oxidative Addition Reactions. Organometallics, 2006, 25, 2066-2073.	2.3	174
111	Steric Effects in Release of Amides from Linkers in Solid-Phase Synthesis. Molecular Mechanics Modeling of Key Step in Peptide and Combinatorial Chemistry. International Journal of Peptide Research and Therapeutics, 2006, 12, 335-339.	1.9	3
112	An Experimental and Theoretical Study of the Mechanism of Stannylcupration of Î±,Î²-Acetylenic Ketones and Esters. Chemistry - A European Journal, 2006, 12, 2866-2873.	3.3	12
113	Deconvoluting the Memory Effect in Pd-Catalyzed Allylic Alkylation: Effect of Leaving Group and Added Chloride. Chemistry - A European Journal, 2006, 12, 5352-5360.	3.3	61
114	Heck Coupling with Nonactivated Alkenyl Tosylates and Phosphates: Examples of Effective 1,2-Migrations of the Alkenyl Palladium(II) Intermediates. Angewandte Chemie - International Edition, 2006, 45, 3349-3353.	13.8	196
115	An Intramolecular Heck Reaction that Prefers a 5-endo- to a 6-exo-trig Cyclization Pathway. Synlett, 2006, 2006, 3140-3144.	1.8	5
116	A Dynamic Supramolecular System Exhibiting Substrate Selectivity in the Catalytic Epoxidation of Olefins.. ChemInform, 2005, 36, no.	0.0	0
117	Surprisingly Mild â€œEnolate-Counterion-Freeâ€•Pd(0)-Catalyzed Intramolecular Allylic Alkylations.. ChemInform, 2005, 36, no.	0.0	0
118	ZnMe2-Mediated Addition of Acetylenes to Aldehydes and Ketones.. ChemInform, 2005, 36, no.	0.0	0
119	Design and Synthesis of a New Type of Ferrocene-Based Planar Chiral DMAP Analogues. A New Catalyst System for Asymmetric Nucleophilic Catalysisâ€. Journal of Organic Chemistry, 2005, 70, 8332-8337.	3.2	81
120	New Insights into the Stereoselectivity of the Aryl Zinc Addition to Aldehydes. Journal of the American Chemical Society, 2005, 127, 1548-1552.	13.7	79
121	A dynamic supramolecular system exhibiting substrate selectivity in the catalytic epoxidation of olefins. Chemical Communications, 2005, , 549-551.	4.1	39
122	Surprisingly Mild â€œEnolate-Counterion-Freeâ€•Pd(0)-Catalyzed Intramolecular Allylic Alkylations. Organic Letters, 2005, 7, 995-998.	4.6	48
123	Palladium(0) alkyne complexes as active species: a DFT investigation. Chemical Communications, 2005, , 4196.	4.1	24
124	A New Strategy for the Improvement of Photophysical Properties in Ruthenium(II) Polypyridyl Complexes. Synthesis and Photophysical and Electrochemical Characterization of Six Mononuclear Ruthenium(II) Bisterpyridine-Type Complexes. Inorganic Chemistry, 2005, 44, 3215-3225.	4.0	97
125	Me2Zn-Mediated Addition of Acetylenes to Aldehydes and Ketones. Journal of Organic Chemistry, 2005, 70, 5733-5736.	3.2	54
126	Nonradical Zincâ^'Barbier Reaction for Diastereoselective Synthesis of Vicinal Amino Alcohols. Journal of the American Chemical Society, 2005, 127, 15756-15761.	13.7	67

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127	Probing Competitive Enantioselective Approach Vectors Operating in the Jacobsenâ^'Katsuki Epoxidation:Â A Kinetic Study of Methyl-Substituted Styrenes. Journal of the American Chemical Society, 2005, 127, 13672-13679.	13.7	41
128	Chiral Diamineâ^'Silver(I)â^'Alkene Complexes:â€‰ A Quantum Chemical and NMR Study. Organometallics, 2005, 24, 3737-3745.	2.3	10
129	Structure Investigation of TiIV-BODOLates Involved in the Catalytic Asymmetric Reduction of Ketones Using Catecholborane. Chemistry - A European Journal, 2004, 10, 182-189.	3.3	11
130	Reactivity and Regioselectivity in the Heck Reaction:â€‰ Hammett Study of 4-Substituted Styrenes. Organometallics, 2004, 23, 6160-6165.	2.3	87
131	Transition states from empirical force fields. Theoretical Chemistry Accounts, 2003, 109, 1-7.	1.4	71
132	An Unprecedented [2+3] Cycloadditive Dimerization of a Transient Thiocarbonyl S-Ylide. European Journal of Organic Chemistry, 2003, 2003, 813-815.	2.4	15
133	Diastereoselective Addition of Î±-Metalated Sulfoxides to Imines Revisited: Mechanism, Computational Studies, and the Effect of External Chiral Ligands.. ChemInform, 2003, 34, no.	0.0	0
134	Updating the asymmetric osmium-catalyzed dihydroxylation (AD) mnemonic: Q2MM modeling and new kinetic measurements. Chirality, 2003, 15, 360-368.	2.6	44
135	Phenyl versus Ethyl Transfer in the Addition ofâ€‰Organozinc Reagents to Aldehydes: Aâ€‰Theoretical Study. Angewandte Chemie - International Edition, 2003, 42, 3002-3005.	13.8	62
136	A DFT exploration of the enantioselective rearrangement of cyclohexene oxide to cyclohexenol. Tetrahedron, 2003, 59, 9695-9700.	1.9	8
137	Modeling the Stereoselectivity of the Î²-Amino Alcohol-Promoted Addition of Dialkylzinc to Aldehydes. Journal of the American Chemical Society, 2003, 125, 5130-5138.	13.7	65
138	Rationalizing Ring-Size Selectivity in Intramolecular Pd-Catalyzed Allylations of Resonance-Stabilized Carbanions. Organometallics, 2003, 22, 1849-1855.	2.3	21
139	A DFT Study of Râ^'X Bond Dissociation Enthalpies of Relevance to the Initiation Process of Atom Transfer Radical Polymerization. Macromolecules, 2003, 36, 8551-8559.	4.8	161
140	Experimental and quantum-mechanical investigation of the vinylsilane-iminium ion cyclizationElectronic supplementary information (ESI) available: experimental procedures, spectroscopic data and copies of 13C NMR spectra for compounds 4â€“16. Selected bond lengths in geometry optimized structures of Î±-substituted (Z)-vinylsilanes. Cartesian coordinates, raw energies and lower frequencies of computationally characterized species 17Aâ€“32H. See http://www.rsc.org/suppdata/ob/b2/b212333a/. Organic and Biomolecular Chemistry, 2003, 1, 1041-1048.	2.8	13
141	Diastereoselective Addition of Î±-Metalated Sulfoxides to Imines Revisited: Mechanism, Computational Studies, and the Effect of External Chiral Ligands. Collection of Czechoslovak Chemical Communications, 2003, 68, 885-898.	1.0	9
142	Molecular Mechanics and Comparison of Force Fields. , 2003, , .		0
143	Quantum Chemical Calculations on the Peterson Olefination with Î±-Silyl Ester Enolates. Journal of Organic Chemistry, 2002, 67, 7378-7388.	3.2	24
144	S-Adenosylmethionine Conformations in Solution and in Protein Complexes:Â Conformational Influences of the Sulfonium Groupâ€. Biochemistry, 2002, 41, 7636-7646.	2.5	46

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145	On the Mechanism of the Copper-Catalyzed Cyclopropanation Reaction. Chemistry - A European Journal, 2002, 8, 177-184.	3.3	91
146	Experimental Evidence for Multiple Oxidation Pathways in the (salen)Mn-Catalyzed Epoxidation of Alkenes. Chemistry - A European Journal, 2002, 8, 2568.	3.3	49
147	Chromiumâ€"Salen-Mediated Alkene Epoxidation: A Theoretical and Experimental Study Indicates the Importance of Spin-Surface Crossing and the Presence of a Discrete Intermediate. Chemistry - A European Journal, 2002, 8, 4299-4307.	3.3	62
148	Computational Investigation of the Role of Fluoride in Tamao Oxidations. Chemistry - A European Journal, 2002, 8, 5043-5048.	3.3	10
149	Investigation of the metal binding site in methionine aminopeptidase by density functional theory. Journal of Computer-Aided Molecular Design, 2002, 16, 167-179.	2.9	12
150	Unprecedented Migration ofN-Alkoxycarbonyl Groups in Protected Pyroglutaminol. Organic Letters, 2001, 3, 433-435.	4.6	23
151	Enantioconvergent Synthesis by Sequential Asymmetric Hornerâ^'Wadsworthâ^'Emmons and Palladium-Catalyzed Allylic Substitution Reactions. Journal of the American Chemical Society, 2001, 123, 9738-9742.	13.7	56
152	Theoretical Investigation of Steric and Electronic Effects in Coenzyme B12Models. Organometallics, 2001, 20, 550-556.	2.3	58
153	Characterization of New Six-Membered Transition States of the Amino-Alcohol Promoted Addition of Dialkyl Zinc to Aldehydes. Journal of the American Chemical Society, 2001, 123, 2464-2465.	13.7	57
154	Quantum Chemical Investigation of Mechanisms of Silane Oxidation. Journal of the American Chemical Society, 2001, 123, 1970-1976.	13.7	22
155	An NMR and ab Initio Quantum Chemical Study of Acidâ^'Base Equilibria for Conformationally Constrained Acidic Î±-Amino Acids in Aqueous Solution. Journal of the American Chemical Society, 2001, 123, 2003-2006.	13.7	8
156	Conformational Analysis of Indole Alkaloids Corynantheine and Dihydrocorynantheine by Dynamic1H NMR Spectroscopy and Computational Methods:Â Steric Effects of Ethyl vs Vinyl Group. Journal of Organic Chemistry, 2001, 66, 2217-2221.	3.2	17
157	Molecular Modeling of Bifunctional Chelate Peptide Conjugates. 1. Copper and Indium Parameters for the AMBER Force Field. Inorganic Chemistry, 2001, 40, 5223-5230.	4.0	19
158	Deriving force field parameters for coordination complexes. Coordination Chemistry Reviews, 2001, 212, 79-109.	18.8	90
159	Racemic Compound FormationversusConglomerate Formation with [M(bpy)3](PF6)2 (M = Ni, Zn, Ru); Lattice Energy Minimisations and Implications for Structure Prediction. European Journal of Inorganic Chemistry, 2000, 2000, 2409-2419.	2.0	13
160	Selectivity in asymmetric synthesis from QM-guided molecular mechanics. Computational and Theoretical Chemistry, 2000, 506, 9-16.	1.5	44
161	Mechanistic Studies of Copper-Catalyzed Alkene Aziridination. Journal of the American Chemical Society, 2000, 122, 8013-8020.	13.7	212
162	Quantum Mechanical Conformational Analysis of Î²-Alanine Zwitterion in Aqueous Solution. Journal of the American Chemical Society, 2000, 122, 3151-3155.	13.7	39

#	Article	IF	Citations
163	Stabilization of the Ammonium-Carboxylate Ion-Pair by an Aromatic Ring. , 2000, , 367-368.		0
164	Molecular Mechanics as a Predictive Tool in Asymmetric Catalysis. ACS Symposium Series, 1999, , 163-172.	0.5	8
165	A Solvated Transition State for the Nucleophilic Attack on CationicÎ·3-Allylpalladium Complexes. Chemistry - A European Journal, 1999, 5, 902-909.	3.3	58
166	Rationalizing the Stereoselectivity of Osmium Tetroxide Asymmetric Dihydroxylations with Transition State Modeling Using Quantum Mechanics-Guided Molecular Mechanics. Journal of the American Chemical Society, 1999, 121, 10186-10192.	13.7	86
167	Timing Is Critical:â€‰ Effect of Spin Changes on the Diastereoselectivity in Mn(salen)-Catalyzed Epoxidation. Journal of the American Chemical Society, 1999, 121, 5083-5084.	13.7	119
168	New Molecular Mechanics (MM3*) Force Field Parameters for Calculations on (Î·3-Allyl)palladium Complexes with Nitrogen and Phosphorus Ligands. Organometallics, 1999, 18, 2884-2895.	2.3	38
169	Rationalization of Product Selectivities in Asymmetric Hornerâ^'Wadsworthâ^'Emmons Reactions by Use of a New Method for Transition-State Modeling. Journal of Organic Chemistry, 1999, 64, 5845-5852.	3.2	36
170	Molecular Mechanics (MM3*) Force Field Parameters for Calculations on Palladium Olefin Complexes with Phosphorus Ligands. Organometallics, 1999, 18, 4574-4583.	2.3	29
171	Asymmetric Horner-Wadsworth-Emmons Reactions with Meso-Dialdehydes: Scope, Mechanism, and Synthetic Applications. Phosphorus, Sulfur and Silicon and the Related Elements, 1999, 144, 169-172.	1.6	2
172	Strong Decrease of the Benzeneâ^'Ammonium Ion Interaction upon Complexation with a Carboxylate Anion. Journal of the American Chemical Society, 1999, 121, 2303-2306.	13.7	30
173	Selectivity and reactivity in asymmetric allylic alkylation. Pure and Applied Chemistry, 1999, 71, 1477-1483.	1.9	22
174	Asymmetric Horner-Wadsworth-Emmons Reactions with Meso-Dialdehydes: Scope, Mechanism, and Synthetic Applications. Phosphorus, Sulfur and Silicon and the Related Elements, 1999, 144, 169-172.	1.6	1
175	Conformational energy penalties of protein-bound ligands. Journal of Computer-Aided Molecular Design, 1998, 12, 383-383.	2.9	223
176	A bis(crown-ether) analogue of TrÃ¶ger's base: Recognition of achiral and chiral primary bisammonium salts. Tetrahedron Letters, 1998, 39, 4565-4568.	1.4	54
177	Automated molecular mechanics parameterization with simultaneous utilization of experimental and quantum mechanical data. Journal of Computational Chemistry, 1998, 19, 1146-1166.	3.3	99
178	Reagent Control of Geometric Selectivity and Enantiotopic Group Preference in Asymmetric Hornerâ^'Wadsworthâ^'Emmons Reactions withmeso-Dialdehydesâ€. Journal of Organic Chemistry, 1998, 63, 8284-8294.	3.2	27
179	Molecular Mechanics (MM3*) Parameters for Ruthenium(II)â^'Polypyridyl Complexes. Inorganic Chemistry, 1998, 37, 4120-4127.	4.0	67
180	A Quantum Chemical Exploration of the Hornerâ^'Wadsworthâ^'Emmons Reaction. Journal of Organic Chemistry, 1998, 63, 1280-1289.	3.2	43

#	Article	IF	Citations
181	The theoretical basis of the isoinversion principle. Journal of the Chemical Society Perkin Transactions II, 1997, , 939-944.	0.9	28
182	Steric Influences on the Selectivity in Palladium-Catalyzed Allylation. Organometallics, 1997, 16, 3015-3021.	2.3	96
183	Toward an Understanding of the High Enantioselectivity in the Osmium-Catalyzed Asymmetric Dihydroxylation. 4. Electronic Effects in Amine-Accelerated Osmylations. Journal of the American Chemical Society, 1997, 119, 1840-1858.	13.7	128
184	Molybdenum-Catalyzed Allylic Substitution. Influence of 1,10-Phenanthroline Ligands on Reactivity and Selectivity. Organometallics, 1997, 16, 942-950.	2.3	51
185	Anab InitioStudy of the Trimethylamineâ^'Formic Acid and the Trimethylammonium Ionâ^'Formate Anion Complexes, Their Monohydrates, and Continuum Solvation. Journal of the American Chemical Society, 1997, 119, 1052-1058.	13.7	49
186	Structural characteristics of isoxazol-3-ol and isothiazol-3-ol, carboxy group bioisosteres examined by X-ray crystallography and ab initio calculations. Journal of the Chemical Society Perkin Transactions II, 1997, , 1783-1792.	0.9	23
187	Is There a Radical Intermediate in the(salen)Mn-Catalyzed Epoxidation of Alkenes?. Angewandte Chemie International Edition in English, 1997, 36, 1723-1725.	4.4	77
188	Gibt es eine radikalische Zwischenstufe bei der Mangan(salen)â€katalysierten Epoxidierung von Alkenen?. Angewandte Chemie, 1997, 109, 1802-1803.	2.0	21
189	High Yield Preparation of 4'-(4-Bromophenyl)-2,2':6',2"-terpyridine by a Condensation Reaction. Determination of the Stereochemistry of Two Complex By-products by a Combination of Molecular Mechanics and NMR Spectroscopy.. Acta Chemica Scandinavica, 1997, 51, 760-766.	0.7	34
190	Molecular Mechanics Predictions and Experimental Testing of Asymmetric Palladium-Catalyzed Allylation Reactions Using New Chiral Phenanthroline Ligands. Journal of the American Chemical Society, 1996, 118, 4299-4313.	13.7	119
191	Toward an Understanding of the High Enantioselectivity in the Osmium-Catalyzed Asymmetric Dihydroxylation. 3. New Insights into Isomeric Forms of the Putative Osmaoxetane Intermediate. Journal of the American Chemical Society, 1996, 118, 35-42.	13.7	95
192	Kinetic constraints on possible reaction pathways for osmium-catalysed asymmetric dihydroxylation. Journal of the Chemical Society Perkin Transactions II, 1996, , 171.	0.9	13
193	A comparison of conformational energies calculated by several molecular mechanics methods. Journal of Computational Chemistry, 1996, 17, 429-449.	3.3	151
194	Conformational Preference of 2â€(Halomethyl)â€•and 2â€(Oxymethyl)Pyridines: Microwave Spectrum, Ab Initio, and MM3 Studies of 2â€(Fluoromethyl)Pyridine. Chemistry - A European Journal, 1996, 2, 516-522.	3.3	14
195	A comparison of conformational energies calculated by several molecular mechanics methods. Journal of Computational Chemistry, 1996, 17, 429-449.	3.3	1
196	Studies of Allylic Substitution Catalysed by a Palladium Complex of a C₂â€Symmetric Bis(aziridine): Preparation and NMR Spectroscopic Investigation of a Chiral Ï€â€Allyl Species. Chemistry - A European Journal, 1995, 1, 12-16.	3.3	75
197	Unusual conformational-determining interactions in oxymethylpyridines: Anab initiostudy and an improved method for refining molecular mechanics parameters. Journal of Computational Chemistry, 1995, 16, 620-627.	3.3	18
198	On the Chirality Transfer in the Epoxidation of Alkenes Catalyzed by Mn(salen) Complexes. Journal of the American Chemical Society, 1995, 117, 11035-11036.	13.7	72

#	Article	IF	Citations
199	Conformations of (.eta.3-Cyclohexenyl)palladium Systems. A Molecular Mechanics (MM2) Study. Organometallics, 1995, 14, 1688-1693.	2.3	18
200	A Detailed Study of (eta3-Cyclohexenyl)palladium Systems.. Acta Chemica Scandinavica, 1995, 49, 888-893.	0.7	10
201	Comparing two models for the selectivity in the asymmetric dihydroxylation reaction (AD). Tetrahedron Letters, 1994, 35, 7315-7318.	1.4	47
202	Toward an Understanding of the High Enantioselectivity in the Osmium-Catalyzed Asymmetric Dihydroxylation. 2. A Qualitative Molecular Mechanics Approach. Journal of the American Chemical Society, 1994, 116, 8470-8478.	13.7	115
203	Calculations on the reaction of ruthenium tetroxide with olefins using density functional theory (DFT). Implications for the possibility of intermediates in osmium-catalyzed asymmetric dihydroxylation. Organometallics, 1994, 13, 344-347.	2.3	75
204	Molecular mechanics (MM2) parameters for the (.eta.3-allyl)palladium moiety. Journal of the American Chemical Society, 1993, 115, 4859-4867.	13.7	59
205	Calculation of NMR observables from computed conformers as a tool of structure verification. Confirmation of the stereochemistry of trans-methyl 2,3-dimethyl-5-methoxy-2-cyclohexene-1-carboxylate. Journal of Organic Chemistry, 1993, 58, 1400-1406.	3.2	8
206	Effects of phenanthroline type ligands on the dynamic processes of (.eta.3-allyl)palladium complexes. Molecular structure of (2,9-dimethyl-1,10-phenanthroline)[(1,2,3-.eta.)-3-methyl-2-butenyl]chloropalladium. Organometallics, 1993, 12, 4940-4948.	2.3	121
207	Selective stabilization of the anti isomer of (.eta.3-allyl)palladium and -platinum complexes. Organometallics, 1992, 11, 3954-3964.	2.3	105
208	Alkylation with Oxalic Esters. Scope and mechanism. Tetrahedron, 1990, 46, 6113-6124.	1.9	30
209	Structure elucidation of some products obtained by acid-catalyzed condensation of indole with acetone. Tetrahedron, 1989, 45, 5549-5564.	1.9	36
210	Interrogation of a dynamic multi-catalyst ensemble in asymmetric catalysis. Faraday Discussions, 0, 145, 27-47.	3.2	8
211	Explaining Regioâ€Đivergent Vinylations with Vinylbenziodoxolones. Angewandte Chemie, 0, , .	2.0	0