Kendall N Houk

List of Publications by Year
in descending order

108 papers	13,859 citations	47006 47 h-index	24258 110 g-index
124 all docs	124 docs citations	124 times ranked	11639 citing authors

#	Article	IF	Citations
1	Stereodivergent Attachedâ€Ring Synthesis via Nonâ€Covalent Interactions: A Short Formal Synthesis of Merrilactone A. Angewandte Chemie - International Edition, 2022, 61, .	13.8	8
2	Stereodivergent Attachedâ€Ring Synthesis via Nonâ€Covalent Interactions: A Short Formal Synthesis of Merrilactone A. Angewandte Chemie, 2022, 134, e202114514.	2.0	0
3	Systematic Variation of Both the Aromatic Cage and Dialkyllysine via GCE-SAR Reveal Mechanistic Insights in CBX5 Reader Protein Binding. Journal of Medicinal Chemistry, 2022, 65, 2646-2655.	6.4	13
4	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. Angewandte Chemie - International Edition, 2022, 61, .	13.8	19
5	Computationally designed ligands enable tunable borylation of remote Câ€“H bonds in arenes. CheM, 2022, 8, 1775-1788.	11.7	14
6	Facile access to fused 2D/3D rings via intermolecular cascade dearomative [2â€‰+â€‰2] cycloaddition/rearrangement reactions of quinolines with alkenes. Nature Catalysis, 2022, 5, 405-413.	34.4	42
7	Organic Chemistry and Synthesis Rely More and More upon Catalysts. Catalysts, 2022, 12, 758.	3.5	2
8	Die Evolution des Dielsâ€Alderâ€Reaktionsmechanismus seit den 1930er Jahren: Woodward, Houk zusammen mit Woodward und der Einfluss der Computerchemie auf das VerstÄndnis von Cycloadditionen. Angewandte Chemie, 2021, 133, 12768-12790.	2.0	15
9	Evolution of the Dielsâ€“Alder Reaction Mechanism since the 1930s: Woodward, Houk with Woodward, and the Influence of Computational Chemistry on Understanding Cycloadditions. Angewandte Chemie - International Edition, 2021, 60, 12660-12681.	13.8	85
10	How the Lewis Base F^{â€“}Catalyzes the 1,3-Dipolar Cycloaddition between Carbon Dioxide and Nitrilimines. Journal of Organic Chemistry, 2021, 86, 4320-4325.	3.2	17
11	Metalâ€Free Directed Câ^'H Borylation of Pyrroles. Angewandte Chemie, 2021, 133, 8581-8585.	2.0	12
12	Computational Exploration of Ambiphilic Reactivity of Azides and Sustmannâ€™s Paradigmatic Parabola. Journal of Organic Chemistry, 2021, 86, 5792-5804.	3.2	11
13	Metalâ€Free Directed Câ^'H Borylation of Pyrroles. Angewandte Chemie - International Edition, 2021, 60, 8500-8504.	13.8	40
14	Photochemical intermolecular dearomative cycloaddition of bicyclic azaarenes with alkenes. Science, 2021, 371, 1338-1345.	12.6	119
15	Catalytic mechanism and endo-to-exo selectivity reversion of an octalin-forming natural Dielsâ€“Alderase. Nature Catalysis, 2021, 4, 223-232.	34.4	35
16	Direct Synthesis of Ketones from Methyl Esters by Nickelâ€Catalyzed Suzukiâ€“Miyaura Coupling. Angewandte Chemie, 2021, 133, 13588-13595.	2.0	7
17	Direct Synthesis of Ketones from Methyl Esters by Nickelâ€Catalyzed Suzukiâ€“Miyaura Coupling. Angewandte Chemie - International Edition, 2021, 60, 13476-13483.	13.8	22
18	Origins of Endo Selectivity in Dielsâ€“Alder Reactions of Cyclic Allene Dienophiles. Angewandte Chemie - International Edition, 2021, 60, 14989-14997.	13.8	24

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19	Origins of Endo Selectivity in Dielsâ€“Alder Reactions of Cyclic Allene Dienophiles. Angewandte Chemie, 2021, 133, 15116-15124.	2.0	3
20	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. Angewandte Chemie, 2021, 133, 18349-18356.	2.0	4
21	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. Angewandte Chemie - International Edition, 2021, 60, 18201-18208.	13.8	15
22	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. Angewandte Chemie, 2021, 133, 24298-24308.	2.0	8
23	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. Angewandte Chemie - International Edition, 2021, 60, 24096-24106.	13.8	28
24	Performance-limiting formation dynamics in mixed-halide perovskites. Science Advances, 2021, 7, eabj1799.	10.3	54
25	Synthetic, Mechanistic, and Biological Interrogation of Ginkgo biloba Chemical Space En Route to (â^')-Bilobalide. Journal of the American Chemical Society, 2020, 142, 18599-18618.	13.7	40
26	Rolf Huisgen's Classic Studies of Cyclic Triene Dielsâ€“Alder Reactions Elaborated by Modern Computational Analysis. Angewandte Chemie - International Edition, 2020, 59, 12506-12519.	13.8	13
27	Rolf Huisgen's Classic Studies of Cyclic Triene Dielsâ€“Alder Reactions Elaborated by Modern Computational Analysis. Angewandte Chemie, 2020, 132, 12606-12619.	2.0	1
28	Understand the Specific Regio- and Enantioselectivity of Fluostatin Conjugation in the Post-Biosynthesis. Biomolecules, 2020, 10, 815.	4.0	15
29	Chiral Phosphoric Acid Dualâ€Function Catalysis: Asymmetric Allylation with Î±â€Vinyl Allylboron Reagents. Angewandte Chemie - International Edition, 2020, 59, 10540-10548.	13.8	42
30	Chiral Phosphoric Acid Dualâ€Function Catalysis: Asymmetric Allylation with Î±â€Vinyl Allylboron Reagents. Angewandte Chemie, 2020, 132, 10627-10635.	2.0	10
31	autoDIAS: a python tool for an automated distortion/interaction activation strain analysis. Journal of Computational Chemistry, 2019, 40, 2509-2515.	3.3	28
32	Enabling microbial syringol conversion through structure-guided protein engineering. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 13970-13976.	7.1	41
33	Enzyme-catalysed [6+4] cycloadditions in the biosynthesis of natural products. Nature, 2019, 568, 122-126.	27.8	83
34	Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies. Chemistry - A European Journal, 2019, 25, 6342-6348.	3.3	49
35	Constructive molecular configurations for surface-defect passivation of perovskite photovoltaics. Science, 2019, 366, 1509-1513.	12.6	846
36	Metal-free directed sp2-Câ€“H borylation. Nature, 2019, 575, 336-340.	27.8	175

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37	Understanding the R882H mutation effects of DNA methyltransferase DNMT3A: a combination of molecular dynamics simulations and QM/MM calculations. RSC Advances, 2019, 9, 31425-31434.	3.6	7
38	John D. Roberts, his beginnings at UCLA, his transformation of physical organic chemistry, and his impact on science. Journal of Physical Organic Chemistry, 2018, 31, e3810.	1.9	0
39	Influence of water and enzyme SpnF on the dynamics and energetics of the ambimodal [6+4]/[4+2] cycloaddition. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E848-E855.	7.1	57
40	Mild Ringâ€Opening 1,3â€Hydroborations of Nonâ€Activated Cyclopropanes. Angewandte Chemie - International Edition, 2018, 57, 16861-16865.	13.8	52
41	Mild Ringâ€Opening 1,3â€Hydroborations of Nonâ€Activated Cyclopropanes. Angewandte Chemie, 2018, 130, 17103-17107.	2.0	33
42	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. Nature Communications, 2018, 9, 2487.	12.8	135
43	Computational Protocol to Understand P450 Mechanisms and Design of Efficient and Selective Biocatalysts. Frontiers in Chemistry, 2018, 6, 663.	3.6	12
44	Analyzing Reaction Rates with the Distortion/Interactionâ€Activation Strain Model. Angewandte Chemie - International Edition, 2017, 56, 10070-10086.	13.8	1,060
45	Das Distortion/Interactionâ€Activationâ€Strainâ€Modell zur Analyse von Reaktionsgeschwindigkeiten. Angewandte Chemie, 2017, 129, 10204-10221.	2.0	209
46	Palladium-Catalyzed Suzukiâ€“Miyaura Coupling of Aryl Esters. Journal of the American Chemical Society, 2017, 139, 1311-1318.	13.7	212
47	Synthesis of [¹⁸F]Fluoroarenes by Nucleophilic Radiofluorination of Nâ€Arylsydnones. Angewandte Chemie, 2017, 129, 13186-13190.	2.0	10
48	Synthesis of [¹⁸F]Fluoroarenes by Nucleophilic Radiofluorination of Nâ€Arylsydnones. Angewandte Chemie - International Edition, 2017, 56, 13006-13010.	13.8	39
49	Investigation of Trimethyllysine Binding by the HP1 Chromodomain via Unnatural Amino Acid Mutagenesis. Journal of the American Chemical Society, 2017, 139, 17253-17256.	13.7	27
50	Nickelâ€Catalyzed Activation of Acyl Cî’O Bonds of Methyl Esters. Angewandte Chemie - International Edition, 2016, 55, 2810-2814.	13.8	142
51	Reactivity of Singleâ€Walled Carbon Nanotubes in the Dielsâ€“Alder Cycloaddition Reaction: Distortionâ€“Interaction Analysis along the Reaction Pathway. Chemistry - A European Journal, 2016, 22, 12819-12824.	3.3	21
52	Involvement of Lipocalinâ€like CghA in Decalinâ€Forming Stereoselective Intramolecular [4+2] Cycloaddition. ChemBioChem, 2015, 16, 2294-2298.	2.6	80
53	Origins of stereoselectivity in evolved ketoreductases. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E7065-72.	7.1	104
54	Nâ€Type Conjugated Polymerâ€Enabled Selective Dispersion of Semiconducting Carbon Nanotubes for Flexible CMOSâ€Like Circuits. Advanced Functional Materials, 2015, 25, 1837-1844.	14.9	32

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55	Solvent Effects on Polymer Sorting of Carbon Nanotubes with Applications in Printed Electronics. Small, 2015, 11, 126-133.	10.0	69
56	High-Yield Sorting of Small-Diameter Carbon Nanotubes for Solar Cells and Transistors. ACS Nano, 2014, 8, 2609-2617.	14.6	91
57	Competition Between Concerted and Stepwise Dynamics in the Triplet Diâ€Ïâ€Methane Rearrangement. Angewandte Chemie - International Edition, 2014, 53, 8664-8667.	13.8	28
58	Scalable and Selective Dispersion of Semiconducting Arc-Discharged Carbon Nanotubes by Dithiafulvalene/Thiophene Copolymers for Thin Film Transistors. ACS Nano, 2013, 7, 2659-2668.	14.6	88
59	Aromatic Claisen Rearrangements of Oâ€Prenylated Tyrosine and Model Prenyl Aryl Ethers: Computational Study of the Role of Water on Acceleration of Claisen Rearrangements. European Journal of Organic Chemistry, 2013, 2013, 2823-2831.	2.4	18
60	Enantioselective Homocrotylboration of Aliphatic Aldehydes. Journal of the American Chemical Society, 2013, 135, 82-85.	13.7	26
61	Control of Hetero-Diels-Alder Stereoselectivity through Solvent Polarity and BrÃ¸nsted or Lewis Acid Catalysis; Theory and Experiment. Synlett, 2013, 24, 2446-2450.	1.8	2
62	Enzymatic catalysis of anti-Baldwin ring closure in polyether biosynthesis. Nature, 2012, 483, 355-358.	27.8	117
63	Fluorine as a Regiocontrol Element in the Ring Opening of Bicyclic Aziridiniums. Helvetica Chimica Acta, 2012, 95, 2265-2277.	1.6	13
64	Iterative approach to computational enzyme design. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 3790-3795.	7.1	291
65	Dynamics, transition states, and timing of bond formation in Dielsâ€“Alder reactions. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 12860-12865.	7.1	166
66	Forming Tertiary Organolithiums and Organocuprates from Nitrile Precursors and their Bimolecular Reactions with Carbon Electrophiles to Form Quaternary Carbon Stereocenters. Angewandte Chemie - International Edition, 2012, 51, 9581-9586.	13.8	26
67	Engineering synthetic recursive pathways to generate non-natural small molecules. Nature Chemical Biology, 2012, 8, 518-526.	8.0	51
68	Bridging the gaps in design methodologies by evolutionary optimization of the stability and proficiency of designed Kemp eliminase KE59. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 10358-10363.	7.1	205
69	BrÃ¸nsted Acid Catalyzed Asymmetric Propargylation of Aldehydes. Angewandte Chemie - International Edition, 2012, 51, 1391-1394.	13.8	124
70	Pericyclic Cascade with Chirality Transfer: Reaction Pathway and Origin of Enantioselectivity of the Heteroâ€Claisen Approach to Oxindoles. Angewandte Chemie - International Edition, 2011, 50, 11478-11482.	13.8	45
71	Axial Preferences in Allylations via the Zimmermanâ€“Traxler Transition State. Chemistry - A European Journal, 2011, 17, 8000-8004.	3.3	33
72	Facilitating e-Science Discovery Using Scientific Workflows on the Grid. Computer Communications and Networks, 2011, , 353-382.	0.8	5

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73	Theoretical enzyme design using the Kepler scientific workflows on the Grid. Procedia Computer Science, 2010, 1, 1175-1184.	2.0	7
74	Computational Design of an Enzyme Catalyst for a Stereoselective Bimolecular Diels-Alder Reaction. Science, 2010, 329, 309-313.	12.6	776
75	Cycloaddition Reactions of Butadiene and 1,3â€Dipoles to Curved Arenes, Fullerenes, and Nanotubes: Theoretical Evaluation of the Role of Distortion Energies on Activation Barriers. Chemistry - A European Journal, 2009, 15, 13219-13231.	3.3	92
76	A Hierarchy of Homodesmotic Reactions for Thermochemistry. Journal of the American Chemical Society, 2009, 131, 2547-2560.	13.7	508
77	Fluorineâ€Directed Diastereoselective Iodocyclizations. Angewandte Chemie - International Edition, 2008, 47, 357-360.	13.8	45
78	Bifurcations on Potential Energy Surfaces of Organic Reactions. Angewandte Chemie - International Edition, 2008, 47, 7592-7601.	13.8	316
79	Sources of Error in DFT Computations of Cï¿C Bond Formation Thermochemistries: Ï€â†'Ïƒ Transformations and Error Cancellation by DFT Methods. Angewandte Chemie - International Edition, 2008, 47, 7746-7749.	13.8	162
80	Kemp elimination catalysts by computational enzyme design. Nature, 2008, 453, 190-195.	27.8	1,130
81	De Novo Computational Design of Retro-Aldol Enzymes. Science, 2008, 319, 1387-1391.	12.6	1,031
82	The Concept of Protobranching and Its Many Paradigm Shifting Implications for Energy Evaluations. Chemistry - A European Journal, 2007, 13, 7731-7744.	3.3	185
83	The Origin of the Halogen Effect on Reactivity and Reversibility of Dielsâ€"Alder Cycloadditions Involving Furan. Angewandte Chemie - International Edition, 2006, 45, 1442-1445.	13.8	97
84	The Chemistry and Biology of Nitroxyl (HNO): A Chemically Unique Species with Novel and Important Biological Activity. ChemBioChem, 2005, 6, 612-619.	2.6	95
85	Structures and Stabilities of Diacetylene-Expanded Polyhedranes by Quantum Mechanics and Molecular Mechanics. Journal of Organic Chemistry, 2005, 70, 1671-1678.	3.2	33
86	Theoretical Reduction Potentials for Nitrogen Oxides from CBS-QB3 Energetics and (C)PCM Solvation Calculations. Inorganic Chemistry, 2005, 44, 4024-4028.	4.0	82
87	The Influence of Constitutional Isomerism and Change on Molecular Recognition Processes. Chemistry - A European Journal, 2004, 10, 5406-5421.	3.3	28
88	The reduction potential of nitric oxide (NO) and its importance to NO biochemistry. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 10958-10963.	7.1	339
89	A Convergent Strategy for the Asymmetric Synthesis of Enantiomerically Pure Bicyclic Compounds by Using a Silicon-Directed Cycloaddition Reaction: The Synthesis of Enantiomerically Pure Bicyclo[3.2.0]hept-2-en-6-one. Angewandte Chemie - International Edition, 1999, 38, 2728-2730.	13.8	36
90	Structural Basis for Antibody Catalysis of a Disfavored Ring Closure Reaction,. Biochemistry, 1999, 38, 7062-7074.	2.5	69

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91	Evolution of Shape Complementarity and Catalytic Efficiency from a Primordial Antibody Template. Science, 1999, 286, 2345-2348.	12.6	116
92	Theozymes and compuzymes: theoretical models for biological catalysis. Current Opinion in Chemical Biology, 1998, 2, 743-750.	6.1	223
93	Thermodynamic and Quantum Chemical Study of the Conversion of Chorismate to (Pyruvate +) Tj ETQq1 1 0.784314 rgBT /Overlock 10	2.6	19
94	An Antibody exo Diels-Alderase Inhibitor Complex at 1.95 Angstrom Resolution. Science, 1998, 279, 1934-1940.	12.6	141
95	Thermodynamics of the Conversion of Chorismate to Prephenate:â€‰ Experimental Results and Theoretical Predictions. Journal of Physical Chemistry B, 1997, 101, 10976-10982.	2.6	58
96	Palladiumkomplexe der neuen Porphyrinisomere (Z)â€•und (E)â€•isoporphycen â€“ Pd^{<scp>II</scp>}â€•induzierte Cyclisierungen von Tetrapyrrolaldehyden. Angewandte Chemie, 1997, 109, 363-367.	2.0	16
97	Polyether Catalysis of Ester Aminolysis â€“ A Computational and Experimental Study. Liebigs Annalen, 1996, 1996, 1511-1522.	0.8	44
98	From Porphyrin Isomers to Octapyrrolicâ€œFigure Eightâ€•Macrocycles. Angewandte Chemie International Edition in English, 1995, 34, 2511-2514.	4.4	168
99	Pericyclic Reaction Transition States: Passions and Punctilios, 1935-1995. Accounts of Chemical Research, 1995, 28, 81-90.	15.6	626
100	Transition Structures of the Electrocyclic Reactions of cis,cis,cisâ€•1,3,5â€Cyclooctatriene. Israel Journal of Chemistry, 1993, 33, 287-293.	2.3	15
101	Transition Structures of Hydrocarbon Pericyclic Reactions. Angewandte Chemie International Edition in English, 1992, 31, 682-708.	4.4	586
102	Ãœbergangsstrukturen in pericyclischen Reaktionen von Kohlenwasserstoffen. Angewandte Chemie, 1992, 104, 711-739.	2.0	111
103	Unexpected regioselectivity in the reductive cleavage of epoxides: a theoretical rationalization. Journal of the American Chemical Society, 1989, 111, 8976-8978.	13.7	51
104	Transition structures for the allylboration reactions of formaldehyde by allylborane and allylboronic acid. Journal of the American Chemical Society, 1989, 111, 1236-1240.	13.7	83
105	Theoretical and experimental insights into cycloaddition reactions. , 1979, , 1-40.		42
106	Nitrone Ionization Potentials and Cycloaddition Regioselectivities. Heterocycles, 1977, 7, 293.	0.7	48
107	Frontier molecular orbital theory of cycloaddition reactions. Accounts of Chemical Research, 1975, 8, 361-369.	15.6	733
108	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. Angewandte Chemie, 0, , .	2.0	6