

Kendall N Houk

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

109 papers	10,682 citations	44 h-index	103 g-index
124 ext. papers	12,290 ext. citations	12.4 avg, IF	6.39 L-index

#	Paper	IF	Citations
109	Stereodivergent Attached-Ring Synthesis via Non-Covalent Interactions: A Short Formal Synthesis of Merrilactone A. <i>Angewandte Chemie</i> , 2022 , 134, e202114514	3.6	
108	Facile access to fused 2D/3D rings via intermolecular cascade dearomative [2 + 2] cycloaddition/rearrangement reactions of quinolines with alkenes. <i>Nature Catalysis</i> , 2022 , 5, 405-413	36.5	2
107	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. <i>Angewandte Chemie - International Edition</i> , 2021 ,	16.4	3
106	Performance-limiting formation dynamics in mixed-halide perovskites. <i>Science Advances</i> , 2021 , 7, eabj1792	17.3	9
105	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. <i>Angewandte Chemie</i> , 2021 , 133, 24298-24308	3.6	3
104	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 24096-24106	16.4	5
103	Computational Exploration of Ambiphilic Reactivity of Azides and Sustmann's Paradigmatic Parabola. <i>Journal of Organic Chemistry</i> , 2021 , 86, 5792-5804	4.2	4
102	Metal-Free Directed C-H Borylation of Pyrroles. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 8500-8504	16.4	12
101	Photochemical intermolecular dearomative cycloaddition of bicyclic azaarenes with alkenes. <i>Science</i> , 2021 , 371, 1338-1345	33.3	29
100	Catalytic mechanism and endo-to-exo selectivity reversion of an octalin-forming natural Diels-Alderase. <i>Nature Catalysis</i> , 2021 , 4, 223-232	36.5	17
99	Direct Synthesis of Ketones from Methyl Esters by Nickel-Catalyzed Suzuki-Miyaura Coupling. <i>Angewandte Chemie</i> , 2021 , 133, 13588-13595	3.6	3
98	Direct Synthesis of Ketones from Methyl Esters by Nickel-Catalyzed Suzuki-Miyaura Coupling. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 13476-13483	16.4	6
97	Origins of Endo Selectivity in Diels-Alder Reactions of Cyclic Allene Dienophiles. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 14989-14997	16.4	8
96	Origins of Endo Selectivity in Diels-Alder Reactions of Cyclic Allene Dienophiles. <i>Angewandte Chemie</i> , 2021 , 133, 15116-15124	3.6	1
95	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. <i>Angewandte Chemie</i> , 2021 , 133, 18349-18356	3.6	1
94	Die Evolution des Diels-Alder-Reaktionsmechanismus seit den 1930er Jahren: Woodward, Houk zusammen mit Woodward und der Einfluss der Computerchemie auf das Verständnis von Cycloadditionen. <i>Angewandte Chemie</i> , 2021 , 133, 12768-12790	3.6	4
93	Evolution of the Diels-Alder Reaction Mechanism since the 1930s: Woodward, Houk with Woodward, and the Influence of Computational Chemistry on Understanding Cycloadditions. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 12660-12681	16.4	27

92	How the Lewis Base F Catalyzes the 1,3-Dipolar Cycloaddition between Carbon Dioxide and Nitrilimines. <i>Journal of Organic Chemistry</i> , 2021 , 86, 4320-4325	4.2	5
91	Metal-Free Directed C-H Borylation of Pyrroles. <i>Angewandte Chemie</i> , 2021 , 133, 8581-8585	3.6	3
90	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 18201-18208	16.4	3
89	Rolf Huisgen's Classic Studies of Cyclic Triene Diels-Alder Reactions Elaborated by Modern Computational Analysis. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 12506-12519	16.4	2
88	Rolf Huisgen's Classic Studies of Cyclic Triene Diels-Alder Reactions Elaborated by Modern Computational Analysis. <i>Angewandte Chemie</i> , 2020 , 132, 12606-12619	3.6	1
87	Understand the Specific Regio- and Enantioselectivity of Fluostatin Conjugation in the Post-Biosynthesis. <i>Biomolecules</i> , 2020 , 10,	5.9	5
86	Chiral Phosphoric Acid Dual-Function Catalysis: Asymmetric Allylation with β -Vinyl Allylboron Reagents. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 10540-10548	16.4	27
85	Chiral Phosphoric Acid Dual-Function Catalysis: Asymmetric Allylation with β -Vinyl Allylboron Reagents. <i>Angewandte Chemie</i> , 2020 , 132, 10627-10635	3.6	9
84	Synthetic, Mechanistic, and Biological Interrogation of Chemical Space En Route to (-)-Bilobalide. <i>Journal of the American Chemical Society</i> , 2020 , 142, 18599-18618	16.4	20
83	Enabling microbial syringol conversion through structure-guided protein engineering. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 13970-13976	11.5	22
82	Enzyme-catalysed [6+4] cycloadditions in the biosynthesis of natural products. <i>Nature</i> , 2019 , 568, 122-126	16.4	53
81	Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies. <i>Chemistry - A European Journal</i> , 2019 , 25, 6342-6348	4.8	34
80	autoDIAS: a python tool for an automated distortion/interaction activation strain analysis. <i>Journal of Computational Chemistry</i> , 2019 , 40, 2509-2515	3.5	13
79	Constructive molecular configurations for surface-defect passivation of perovskite photovoltaics. <i>Science</i> , 2019 , 366, 1509-1513	33.3	434
78	Metal-free directed sp-C-H borylation. <i>Nature</i> , 2019 , 575, 336-340	50.4	93
77	Understanding the R882H mutation effects of DNA methyltransferase DNMT3A: a combination of molecular dynamics simulations and QM/MM calculations.. <i>RSC Advances</i> , 2019 , 9, 31425-31434	3.7	3
76	John D. Roberts, his beginnings at UCLA, his transformation of physical organic chemistry, and his impact on science. <i>Journal of Physical Organic Chemistry</i> , 2018 , 31, e3810	2.1	
75	Influence of water and enzyme SpnF on the dynamics and energetics of the ambimodal [6+4]/[4+2] cycloaddition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E848-E855	11.5	45

74	Computational Protocol to Understand P450 Mechanisms and Design of Efficient and Selective Biocatalysts. <i>Frontiers in Chemistry</i> , 2018 , 6, 663	5	8
73	Mild Ring-Opening 1,3-Hydroborations of Non-Activated Cyclopropanes. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 16861-16865	16.4	34
72	Mild Ring-Opening 1,3-Hydroborations of Non-Activated Cyclopropanes. <i>Angewandte Chemie</i> , 2018 , 130, 17103-17107	3.6	11
71	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. <i>Nature Communications</i> , 2018 , 9, 2487	17.4	77
70	Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 10070-10086	16.4	649
69	Das Distortion/Interaction-Activation-Strain-Modell zur Analyse von Reaktionsgeschwindigkeiten. <i>Angewandte Chemie</i> , 2017 , 129, 10204-10221	3.6	136
68	Palladium-Catalyzed Suzuki-Miyaura Coupling of Aryl Esters. <i>Journal of the American Chemical Society</i> , 2017 , 139, 1311-1318	16.4	165
67	Synthesis of [¹⁸ F]Fluoroarenes by Nucleophilic Radiofluorination of N-Arylsydnone. <i>Angewandte Chemie</i> , 2017 , 129, 13186-13190	3.6	9
66	Synthesis of [F]Fluoroarenes by Nucleophilic Radiofluorination of N-Arylsydnone. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 13006-13010	16.4	32
65	Investigation of Trimethyllysine Binding by the HP1 Chromodomain via Unnatural Amino Acid Mutagenesis. <i>Journal of the American Chemical Society</i> , 2017 , 139, 17253-17256	16.4	18
64	Nickel-Catalyzed Activation of Acyl C-O Bonds of Methyl Esters. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 2810-4	16.4	115
63	Reactivity of Single-Walled Carbon Nanotubes in the Diels-Alder Cycloaddition Reaction: Distortion-Interaction Analysis along the Reaction Pathway. <i>Chemistry - A European Journal</i> , 2016 , 22, 12819-24	4.8	20
62	Solvent effects on polymer sorting of carbon nanotubes with applications in printed electronics. <i>Small</i> , 2015 , 11, 126-33	11	57
61	Involvement of Lipocalin-like CghA in Decalin-Forming Stereoselective Intramolecular [4+2] Cycloaddition. <i>ChemBioChem</i> , 2015 , 16, 2294-8	3.8	64
60	Origins of stereoselectivity in evolved ketoreductases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, E7065-72	11.5	76
59	N-Type Conjugated Polymer-Enabled Selective Dispersion of Semiconducting Carbon Nanotubes for Flexible CMOS-Like Circuits. <i>Advanced Functional Materials</i> , 2015 , 25, 1837-1844	15.6	27
58	High-yield sorting of small-diameter carbon nanotubes for solar cells and transistors. <i>ACS Nano</i> , 2014 , 8, 2609-17	16.7	82
57	Competition between concerted and stepwise dynamics in the triplet di- π -methane rearrangement. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 8664-7	16.4	23

56	Competition Between Concerted and Stepwise Dynamics in the Triplet Di- π -Methane Rearrangement. <i>Angewandte Chemie</i> , 2014 , 126, 8808-8811	3.6	1
55	Scalable and selective dispersion of semiconducting arc-discharged carbon nanotubes by dithiafulvalene/thiophene copolymers for thin film transistors. <i>ACS Nano</i> , 2013 , 7, 2659-68	16.7	79
54	Aromatic Claisen Rearrangements of O-prenylated tyrosine and model prenyl aryl ethers: Computational study of the role of water on acceleration of Claisen rearrangements. <i>European Journal of Organic Chemistry</i> , 2013 , 2013, 2823	3.2	16
53	Enantioselective homocrotlylboration of aliphatic aldehydes. <i>Journal of the American Chemical Society</i> , 2013 , 135, 82-5	16.4	19
52	Control of Hetero-Diels-Alder Stereoselectivity through Solvent Polarity and Brønsted or Lewis Acid Catalysis; Theory and Experiment. <i>Synlett</i> , 2013 , 24, 2446-2450	2.2	1
51	Brønsted acid catalyzed asymmetric propargylation of aldehydes. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 1391-4	16.4	108
50	Enzymatic catalysis of anti-Baldwin ring closure in polyether biosynthesis. <i>Nature</i> , 2012 , 483, 355-8	50.4	96
49	H12461. Fluorine as a Regiocontrol Element in the Ring Openings of Bicyclic Aziridiniums. <i>Helvetica Chimica Acta</i> , 2012 , 95, 2265-2277	2	11
48	Iterative approach to computational enzyme design. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 3790-5	11.5	245
47	Dynamics, transition states, and timing of bond formation in Diels-Alder reactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 12860-5	11.5	144
46	Forming tertiary organolithiums and organocuprates from nitrile precursors and their bimolecular reactions with carbon electrophiles to form quaternary carbon stereocenters. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 9581-6	16.4	17
45	Engineering synthetic recursive pathways to generate non-natural small molecules. <i>Nature Chemical Biology</i> , 2012 , 8, 518-26	11.7	46
44	Bridging the gaps in design methodologies by evolutionary optimization of the stability and proficiency of designed Kemp eliminase KE59. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 10358-63	11.5	174
43	Brønsted Acid Catalyzed Asymmetric Propargylation of Aldehydes. <i>Angewandte Chemie</i> , 2012 , 124, 1420-1423	3.2	38
42	Pericyclic Cascade with Chirality Transfer: Reaction Pathway and Origin of Enantioselectivity of the Hetero-Claisen Approach to Oxindoles. <i>Angewandte Chemie</i> , 2011 , 123, 11680-11684	3.6	1
41	Pericyclic cascade with chirality transfer: reaction pathway and origin of enantioselectivity of the hetero-Claisen approach to oxindoles. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 11478-82	16.4	37
40	Axial preferences in allylations via the Zimmerman-Traxler transition state. <i>Chemistry - A European Journal</i> , 2011 , 17, 8000-4	4.8	28
39	Facilitating e-Science Discovery Using Scientific Workflows on the Grid. <i>Computer Communications and Networks</i> , 2011 , 353-382	0.5	2

38	Computational design of an enzyme catalyst for a stereoselective bimolecular Diels-Alder reaction. <i>Science</i> , 2010 , 329, 309-13	33.3	652
37	Theoretical enzyme design using the Kepler scientific workflows on the Grid. <i>Procedia Computer Science</i> , 2010 , 1, 1175-1184	1.6	5
36	Cycloaddition reactions of butadiene and 1,3-dipoles to curved arenes, fullerenes, and nanotubes: theoretical evaluation of the role of distortion energies on activation barriers. <i>Chemistry - A European Journal</i> , 2009 , 15, 13219-31	4.8	91
35	A hierarchy of homodesmotic reactions for thermochemistry. <i>Journal of the American Chemical Society</i> , 2009 , 131, 2547-60	16.4	418
34	Kemp elimination catalysts by computational enzyme design. <i>Nature</i> , 2008 , 453, 190-5	50.4	977
33	De novo computational design of retro-aldol enzymes. <i>Science</i> , 2008 , 319, 1387-91	33.3	892
32	Fluorine-directed diastereoselective iodocyclizations. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 357-60	16.4	42
31	Bifurcations on potential energy surfaces of organic reactions. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 7592-601	16.4	262
30	Sources of error in DFT computations of C-C bond formation thermochemistries: pi->sigma transformations and error cancellation by DFT methods. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 7746-9	16.4	148
29	The concept of protobranching and its many paradigm shifting implications for energy evaluations. <i>Chemistry - A European Journal</i> , 2007 , 13, 7731-44	4.8	173
28	The origin of the halogen effect on reactivity and reversibility of Diels-Alder cycloadditions involving furan. <i>Angewandte Chemie - International Edition</i> , 2006 , 45, 1442-5	16.4	84
27	The Origin of the Halogen Effect on Reactivity and Reversibility of Diels-Alder Cycloadditions Involving Furan. <i>Angewandte Chemie</i> , 2006 , 118, 1470-1473	3.6	16
26	Structures and stabilities of diacetylene-expanded polyhedranes by quantum mechanics and molecular mechanics. <i>Journal of Organic Chemistry</i> , 2005 , 70, 1671-8	4.2	31
25	Theoretical reduction potentials for nitrogen oxides from CBS-QB3 energetics and (C)PCM solvation calculations. <i>Inorganic Chemistry</i> , 2005 , 44, 4024-8	5.1	67
24	The chemistry and biology of nitroxyl (HNO): a chemically unique species with novel and important biological activity. <i>ChemBioChem</i> , 2005 , 6, 612-9	3.8	81
23	The influence of constitutional isomerism and change on molecular recognition processes. <i>Chemistry - A European Journal</i> , 2004 , 10, 5406-21	4.8	27
22	Bindungsaffinitäten von Wirt-Gast-, Protein-Ligand- und Protein-Übergangszustands-Komplexen. <i>Angewandte Chemie</i> , 2003 , 115, 5020-5046	3.6	71
21	The reduction potential of nitric oxide (NO) and its importance to NO biochemistry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 10958-63	11.5	287

20	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. <i>Angewandte Chemie - International Edition</i> , 1999 , 38, 2728-2730	16.4	28
19	Structural basis for antibody catalysis of a disfavored ring closure reaction. <i>Biochemistry</i> , 1999 , 38, 7062-7064	3.4	55
18	Evolution of shape complementarity and catalytic efficiency from a primordial antibody template. <i>Science</i> , 1999 , 286, 2345-8	33.3	106
17	Theozymes and compuzymes: theoretical models for biological catalysis. <i>Current Opinion in Chemical Biology</i> , 1998 , 2, 743-50	9.7	196
16	Thermodynamic and Quantum Chemical Study of the Conversion of Chorismate to (Pyruvate + 4-Hydroxybenzoate). <i>Journal of Physical Chemistry B</i> , 1998 , 102, 8634-8639	3.4	19
15	An antibody exo Diels-Alderase inhibitor complex at 1.95 angstrom resolution. <i>Science</i> , 1998 , 279, 1934-1937	49.3	127
14	Thermodynamics of the Conversion of Chorismate to Prephenate: Experimental Results and Theoretical Predictions. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 10976-10982	3.4	53
13	Palladiumkomplexe der neuen Porphyrinisomere (Z)- und (E)-Isoporphycen [PdII-induzierte Cyclisierungen von Tetrapyrrolaldehyden. <i>Angewandte Chemie</i> , 1997 , 109, 363-367	3.6	14
12	Polyether Catalysis of Ester Aminolysis [A Computational and Experimental Study. <i>Liebigs Annalen</i> , 1996 , 1996, 1511-1522		42
11	Pericyclic Reaction Transition States: Passions and Punctilios, 1935-1995. <i>Accounts of Chemical Research</i> , 1995 , 28, 81-90	24.3	558
10	From Porphyrin Isomers to Octapyrrolic Figure Eight [Macrocycles. <i>Angewandte Chemie International Edition in English</i> , 1995 , 34, 2511-2514		143
9	Transition Structures of the Electrocyclic Reactions of cis,cis,cis-1,3,5-Cyclooctatriene. <i>Israel Journal of Chemistry</i> , 1993 , 33, 287-293	3.4	11
8	Transition Structures of Hydrocarbon Pericyclic Reactions. <i>Angewandte Chemie International Edition in English</i> , 1992 , 31, 682-708		512
7	Bergangsstrukturen in pericyclischen Reaktionen von Kohlenwasserstoffen. <i>Angewandte Chemie</i> , 1992 , 104, 711-739	3.6	85
6	Unexpected regioselectivity in the reductive cleavage of epoxides: a theoretical rationalization. <i>Journal of the American Chemical Society</i> , 1989 , 111, 8976-8978	16.4	39
5	Transition structures for the allylboration reactions of formaldehyde by allylborane and allylboronic acid. <i>Journal of the American Chemical Society</i> , 1989 , 111, 1236-1240	16.4	72
4	[Orbital Interactions in M[bius-Type Molecules as Studied by Photoelectron Spectroscopy. <i>Helvetica Chimica Acta</i> , 1982 , 65, 1743-1751	2	27
3	Theoretical and experimental insights into cycloaddition reactions 1979 , 1-40		39

- 2 Nitrene Ionization Potentials and Cycloaddition Regioselectivities. *Heterocycles*, **1977**, 7, 293 0.8 40
- 1 Frontier molecular orbital theory of cycloaddition reactions. *Accounts of Chemical Research*, **1975**, 8, 361-369 619