Kendall N Houk

List of Publications by Citations

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	Kemp elimination catalysts by computational enzyme design. *Nature*, **2008**, 453, 190-5	50.4	977
108	De novo computational design of retro-aldol enzymes. *Science*, **2008**, 319, 1387-91	33.3	892
107	Computational design of an enzyme catalyst for a stereoselective bimolecular Diels-Alder reaction. *Science*, **2010**, 329, 309-13	33.3	652
106	Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. *Angewandte Chemie - International Edition*, **2017**, 56, 10070-10086	16.4	649
105	Frontier molecular orbital theory of cycloaddition reactions. *Accounts of Chemical Research*, **1975**, 8, 361-369	24.3	619
104	Pericyclic Reaction Transition States: Passions and Punctilios, 1935-1995. *Accounts of Chemical Research*, **1995**, 28, 81-90	24.3	558
103	Transition Structures of Hydrocarbon Pericyclic Reactions. *Angewandte Chemie International Edition in English*, **1992**, 31, 682-708		512
102	Constructive molecular configurations for surface-defect passivation of perovskite photovoltaics. *Science*, **2019**, 366, 1509-1513	33.3	434
101	A hierarchy of homodesmotic reactions for thermochemistry. *Journal of the American Chemical Society*, **2009**, 131, 2547-60	16.4	418
100	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, 10958-63	11.5	287
99	Bifurcations on potential energy surfaces of organic reactions. *Angewandte Chemie - International Edition*, **2008**, 47, 7592-601	16.4	262
98	Iterative approach to computational enzyme design. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 3790-5	11.5	245
97	Theozymes and compuzymes: theoretical models for biological catalysis. *Current Opinion in Chemical Biology*, **1998**, 2, 743-50	9.7	196
96	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, 10358-63	11.5	174
95	The concept of protobranching and its many paradigm shifting implications for energy evaluations. *Chemistry - A European Journal*, **2007**, 13, 7731-44	4.8	173
94	Palladium-Catalyzed Suzuki-Miyaura Coupling of Aryl Esters. *Journal of the American Chemical Society*, **2017**, 139, 1311-1318	16.4	165
93	Sources of error in DFT computations of C-C bond formation thermochemistries: pi-->sigma transformations and error cancellation by DFT methods. *Angewandte Chemie - International Edition*, **2008**, 47, 7746-9	16.4	148

92	Dynamics, transition states, and timing of bond formation in Diels-Alder reactions. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 12860-5	11.5	144
91	From Porphyrin Isomers to Octapyrrolic Figure Eight Macrocycles. *Angewandte Chemie International Edition in English*, **1995**, 34, 2511-2514		143
90	Das Distortion/Interaction-Activation-Strain-Modell zur Analyse von Reaktionsgeschwindigkeiten. *Angewandte Chemie*, **2017**, 129, 10204-10221	3.6	136
89	An antibody exo Diels-Alderase inhibitor complex at 1.95 angstrom resolution. *Science*, **1998**, 279, 1934-40	33.3	127
88	Nickel-Catalyzed Activation of Acyl C-O Bonds of Methyl Esters. *Angewandte Chemie - International Edition*, **2016**, 55, 2810-4	16.4	115
87	Brønsted acid catalyzed asymmetric propargylation of aldehydes. *Angewandte Chemie - International Edition*, **2012**, 51, 1391-4	16.4	108
86	Evolution of shape complementarity and catalytic efficiency from a primordial antibody template. *Science*, **1999**, 286, 2345-8	33.3	106
85	Enzymatic catalysis of anti-Baldwin ring closure in polyether biosynthesis. *Nature*, **2012**, 483, 355-8	50.4	96
84	Metal-free directed sp-C-H borylation. *Nature*, **2019**, 575, 336-340	50.4	93
83	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. *Chemistry - A European Journal*, **2009**, 15, 13219-31	4.8	91
82	Übergangsstrukturen in pericyclischen Reaktionen von Kohlenwasserstoffen. *Angewandte Chemie*, **1992**, 104, 711-739	3.6	85
81	The origin of the halogen effect on reactivity and reversibility of Diels-Alder cycloadditions involving furan. *Angewandte Chemie - International Edition*, **2006**, 45, 1442-5	16.4	84
80	High-yield sorting of small-diameter carbon nanotubes for solar cells and transistors. *ACS Nano*, **2014**, 8, 2609-17	16.7	82
79	The chemistry and biology of nitroxyl (HNO): a chemically unique species with novel and important biological activity. *ChemBioChem*, **2005**, 6, 612-9	3.8	81
78	Scalable and selective dispersion of semiconducting arc-discharged carbon nanotubes by dithiafulvalene/thiophene copolymers for thin film transistors. *ACS Nano*, **2013**, 7, 2659-68	16.7	79
77	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. *Nature Communications*, **2018**, 9, 2487	17.4	77
76	Origins of stereoselectivity in evolved ketoreductases. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E7065-72	11.5	76
75	Transition structures for the allylboration reactions of formaldehyde by allylborane and allylboronic acid. *Journal of the American Chemical Society*, **1989**, 111, 1236-1240	16.4	72

74	Bindungsaffinitäten von Wirt-Gast-, Protein-Ligand- und Protein-Übergangszustands-Komplexen. *Angewandte Chemie*, **2003**, 115, 5020-5046	3.6	71
73	Theoretical reduction potentials for nitrogen oxides from CBS-QB3 energetics and (C)PCM solvation calculations. *Inorganic Chemistry*, **2005**, 44, 4024-8	5.1	67
72	Involvement of Lipocalin-like CghA in Decalin-Forming Stereoselective Intramolecular [4+2] Cycloaddition. *ChemBioChem*, **2015**, 16, 2294-8	3.8	64
71	Solvent effects on polymer sorting of carbon nanotubes with applications in printed electronics. *Small*, **2015**, 11, 126-33	11	57
70	Structural basis for antibody catalysis of a disfavored ring closure reaction. *Biochemistry*, **1999**, 38, 7062-74	3.4	55
69	Enzyme-catalysed [6+4] cycloadditions in the biosynthesis of natural products. *Nature*, **2019**, 568, 122-126	50.4	53
68	Thermodynamics of the Conversion of Chorismate to Prephenate: Experimental Results and Theoretical Predictions. *Journal of Physical Chemistry B*, **1997**, 101, 10976-10982	3.4	53
67	Engineering synthetic recursive pathways to generate non-natural small molecules. *Nature Chemical Biology*, **2012**, 8, 518-26	11.7	46
66	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	11.5	45
65	Fluorine-directed diastereoselective iodocyclizations. *Angewandte Chemie - International Edition*, **2008**, 47, 357-60	16.4	42
64	Polyether Catalysis of Ester Aminolysis—A Computational and Experimental Study. *Liebigs Annalen*, **1996**, 1996, 1511-1522		42
63	Nitrone Ionization Potentials and Cycloaddition Regioselectivities. *Heterocycles*, **1977**, 7, 293	0.8	40
62	Unexpected regioselectivity in the reductive cleavage of epoxides: a theoretical rationalization. *Journal of the American Chemical Society*, **1989**, 111, 8976-8978	16.4	39
61	Theoretical and experimental insights into cycloaddition reactions **1979**, 1-40		39
60	Brønsted Acid Catalyzed Asymmetric Propargylation of Aldehydes. *Angewandte Chemie*, **2012**, 124, 1420-1423	3.6	38
59	Pericyclic cascade with chirality transfer: reaction pathway and origin of enantioselectivity of the hetero-Claisen approach to oxindoles. *Angewandte Chemie - International Edition*, **2011**, 50, 11478-82	16.4	37
58	Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies. *Chemistry - A European Journal*, **2019**, 25, 6342-6348	4.8	34
57	Mild Ring-Opening 1,3-Hydroborations of Non-Activated Cyclopropanes. *Angewandte Chemie - International Edition*, **2018**, 57, 16861-16865	16.4	34

56	Synthesis of [F]Fluoroarenes by Nucleophilic Radiofluorination of N-Arylsydnones. *Angewandte Chemie - International Edition*, **2017**, 56, 13006-13010	16.4	32
55	Structures and stabilities of diacetylene-expanded polyhedranes by quantum mechanics and molecular mechanics. *Journal of Organic Chemistry*, **2005**, 70, 1671-8	4.2	31
54	Photochemical intermolecular dearomative cycloaddition of bicyclic azaarenes with alkenes. *Science*, **2021**, 371, 1338-1345	33.3	29
53	Axial preferences in allylations via the Zimmerman-Traxler transition state. *Chemistry - A European Journal*, **2011**, 17, 8000-4	4.8	28
52	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. *Angewandte Chemie - International Edition*, **1999**, 38, 2728-2730	16.4	28
51	Chiral Phosphoric Acid Dual-Function Catalysis: Asymmetric Allylation with Vinyl Allylboron Reagents. *Angewandte Chemie - International Edition*, **2020**, 59, 10540-10548	16.4	27
50	N-Type Conjugated Polymer-Enabled Selective Dispersion of Semiconducting Carbon Nanotubes for Flexible CMOS-Like Circuits. *Advanced Functional Materials*, **2015**, 25, 1837-1844	15.6	27
49	The influence of constitutional isomerism and change on molecular recognition processes. *Chemistry - A European Journal*, **2004**, 10, 5406-21	4.8	27
48	Orbital Interactions in MBius-Type Molecules as Studied by Photoelectron Spectroscopy. *Helvetica Chimica Acta*, **1982**, 65, 1743-1751	2	27
47	Evolution of the Diels-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	16.4	27
46	Competition between concerted and stepwise dynamics in the triplet di- methane rearrangement. *Angewandte Chemie - International Edition*, **2014**, 53, 8664-7	16.4	23
45	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	11.5	22
44	Synthetic, Mechanistic, and Biological Interrogation of Chemical Space En Route to (-)-Bilobalide. *Journal of the American Chemical Society*, **2020**, 142, 18599-18618	16.4	20
43	Reactivity of Single-Walled Carbon Nanotubes in the Diels-Alder Cycloaddition Reaction: Distortion-Interaction Analysis along the Reaction Pathway. *Chemistry - A European Journal*, **2016**, 22, 12819-24	4.8	20
42	Enantioselective homocrotylboration of aliphatic aldehydes. *Journal of the American Chemical Society*, **2013**, 135, 82-5	16.4	19
41	Thermodynamic and Quantum Chemical Study of the Conversion of Chorismate to (Pyruvate + 4-Hydroxybenzoate). *Journal of Physical Chemistry B*, **1998**, 102, 8634-8639	3.4	19
40	Investigation of Trimethyllysine Binding by the HP1 Chromodomain via Unnatural Amino Acid Mutagenesis. *Journal of the American Chemical Society*, **2017**, 139, 17253-17256	16.4	18
39	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, 9581-6	16.4	17

38	Catalytic mechanism and endo-to-exo selectivity reversion of an octalin-forming natural Diels–Alderase. *Nature Catalysis*, **2021**, 4, 223-232	36.5	17
37	Aromatic Claisen Rearrangements of O-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	3.2	16
36	The Origin of the Halogen Effect on Reactivity and Reversibility of Diels–Alder Cycloadditions Involving Furan. *Angewandte Chemie*, **2006**, 118, 1470-1473	3.6	16
35	Palladiumkomplexe der neuen Porphyrinisomere (Z)- und (E)-Isoporphycen – PdII-induzierte Cyclisierungen von Tetrapyrrolaldehyden. *Angewandte Chemie*, **1997**, 109, 363-367	3.6	14
34	autoDIAS: a python tool for an automated distortion/interaction activation strain analysis. *Journal of Computational Chemistry*, **2019**, 40, 2509-2515	3.5	13
33	Metal-Free Directed C-H Borylation of Pyrroles. *Angewandte Chemie - International Edition*, **2021**, 60, 8500-8504	16.4	12
32	H12461. Fluorine as a Regiocontrol Element in the Ring Openings of Bicyclic Aziridiniums. *Helvetica Chimica Acta*, **2012**, 95, 2265-2277	2	11
31	Transition Structures of the Electrocyclic Reactions of cis,cis,cis-1,3,5-Cyclooctatriene. *Israel Journal of Chemistry*, **1993**, 33, 287-293	3.4	11
30	Mild Ring-Opening 1,3-Hydroborations of Non-Activated Cyclopropanes. *Angewandte Chemie*, **2018**, 130, 17103-17107	3.6	11
29	Chiral Phosphoric Acid Dual-Function Catalysis: Asymmetric Allylation with β-Vinyl Allylboron Reagents. *Angewandte Chemie*, **2020**, 132, 10627-10635	3.6	9
28	Synthesis of [18F]Fluoroarenes by Nucleophilic Radiofluorination of N-Arylsydnones. *Angewandte Chemie*, **2017**, 129, 13186-13190	3.6	9
27	Performance-limiting formation dynamics in mixed-halide perovskites. *Science Advances*, **2021**, 7, eabj1799	14.3	9
26	Origins of Endo Selectivity in Diels-Alder Reactions of Cyclic Allene Dienophiles. *Angewandte Chemie - International Edition*, **2021**, 60, 14989-14997	16.4	8
25	Computational Protocol to Understand P450 Mechanisms and Design of Efficient and Selective Biocatalysts. *Frontiers in Chemistry*, **2018**, 6, 663	5	8
24	Direct Synthesis of Ketones from Methyl Esters by Nickel-Catalyzed Suzuki-Miyaura Coupling. *Angewandte Chemie - International Edition*, **2021**, 60, 13476-13483	16.4	6
23	Understand the Specific Regio- and Enantioselectivity of Fluostatin Conjugation in the Post-Biosynthesis. *Biomolecules*, **2020**, 10,	5.9	5
22	Theoretical enzyme design using the Kepler scientific workflows on the Grid. *Procedia Computer Science*, **2010**, 1, 1175-1184	1.6	5
21	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. *Angewandte Chemie - International Edition*, **2021**, 60, 24096-24106	16.4	5

20	How the Lewis Base F Catalyzes the 1,3-Dipolar Cycloaddition between Carbon Dioxide and Nitrilimines. *Journal of Organic Chemistry*, **2021**, 86, 4320-4325	4.2	5
19	Computational Exploration of Ambiphilic Reactivity of Azides and Sustmann's Paradigmatic Parabola. *Journal of Organic Chemistry*, **2021**, 86, 5792-5804	4.2	4
18	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. *Angewandte Chemie*, **2021**, 133, 12768-12790	3.6	4
17	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. *Angewandte Chemie - International Edition*, **2021**,	16.4	3
16	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. *Angewandte Chemie*, **2021**, 133, 24298-24308	3.6	3
15	Direct Synthesis of Ketones from Methyl Esters by Nickel-Catalyzed Suzuki–Miyaura Coupling. *Angewandte Chemie*, **2021**, 133, 13588-13595	3.6	3
14	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	3.7	3
13	Metal-Free Directed C–H Borylation of Pyrroles. *Angewandte Chemie*, **2021**, 133, 8581-8585	3.6	3
12	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. *Angewandte Chemie - International Edition*, **2021**, 60, 18201-18208	16.4	3
11	Rolf Huisgen's Classic Studies of Cyclic Triene Diels-Alder Reactions Elaborated by Modern Computational Analysis. *Angewandte Chemie - International Edition*, **2020**, 59, 12506-12519	16.4	2
10	Facilitating e-Science Discovery Using Scientific Workflows on the Grid. *Computer Communications and Networks*, **2011**, 353-382	0.5	2
9	Facile access to fused 2D/3D rings via intermolecular cascade dearomative [2 + 2] cycloaddition/rearrangement reactions of quinolines with alkenes. *Nature Catalysis*, **2022**, 5, 405-413	36.5	2
8	Rolf Huisgen's Classic Studies of Cyclic Triene Diels–Alder Reactions Elaborated by Modern Computational Analysis. *Angewandte Chemie*, **2020**, 132, 12606-12619	3.6	1
7	Competition Between Concerted and Stepwise Dynamics in the Triplet Di-π-Methane Rearrangement. *Angewandte Chemie*, **2014**, 126, 8808-8811	3.6	1
6	Control of Hetero-Diels-Alder Stereoselectivity through Solvent Polarity and Brønsted or Lewis Acid Catalysis; Theory and Experiment. *Synlett*, **2013**, 24, 2446-2450	2.2	1
5	Pericyclic Cascade with Chirality Transfer: Reaction Pathway and Origin of Enantioselectivity of the Hetero-Claisen Approach to Oxindoles. *Angewandte Chemie*, **2011**, 123, 11680-11684	3.6	1
4	Origins of Endo Selectivity in Diels–Alder Reactions of Cyclic Allene Dienophiles. *Angewandte Chemie*, **2021**, 133, 15116-15124	3.6	1
3	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. *Angewandte Chemie*, **2021**, 133, 18349-18356	3.6	1

2	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	2.1
1	Stereodivergent Attached-Ring Synthesis via Non-Covalent Interactions: A Short Formal Synthesis of Merrilactone A. *Angewandte Chemie*, **2022**, 134, e202114514	3.6