Karsten Krogh-Jespersen

List of Publications by Year
in descending order

44 papers	1,379 citations	430874 18 h-index	330143 37 g-index
45 all docs	45 docs citations	45 times ranked	1472 citing authors

#	Article	IF	Citations
1	Origin of Regioselectivity in the Dehydrogenation of Alkanes by Pincerâ€“Iridium Complexes: A Combined Experimental and Computational Study. ACS Catalysis, 2021, 11, 12038-12051.	11.2	7
2	Alkane Dehydrogenation Catalyzed by a Fluorinated Phebox Iridium Complex. ACS Catalysis, 2021, 11, 14194-14209.	11.2	8
3	Formation of Enamines via Catalytic Dehydrogenation by Pincer-Iridium Complexes. Journal of Organic Chemistry, 2020, 85, 3020-3028.	3.2	12
4	Catalytic Alkane Transfer Dehydrogenation by PSP-Pincer-Ligated Ruthenium. Deactivation of an Extremely Reactive Fragment by Formation of Allyl Hydride Complexes. ACS Catalysis, 2019, 9, 4072-4083.	11.2	29
5	Polar molecules catalyze CO insertion into metal-alkyl bonds through the displacement of an agostic C-H bond. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 3419-3424.	7.1	5
6	Selective Dehydrogenative Coupling of Ethylene to Butadiene via an Iridacyclopentane Complex. Journal of the American Chemical Society, 2018, 140, 2260-2264.	13.7	16
7	Extremely reactive carbenes: electrophiles and nucleophiles. Journal of Physical Organic Chemistry, 2017, 30, e3555.	1.9	10
8	Complexes and Negative Activation Energies in Arylhalocarbene/Alkene Additions: Activation Parameter Dependence on Alkane Solvent Chain Length. Journal of Organic Chemistry, 2017, 82, 4216-4225.	3.2	4
9	Î²-Hydride Elimination and Câ€“H Activation by an Iridium Acetate Complex, Catalyzed by Lewis Acids. Alkane Dehydrogenation Cocatalyzed by Lewis Acids and [2,6-Bis(4,4-dimethyloxazolinyl)-3,5-dimethylphenyl]iridium. Journal of the American Chemical Society, 2017, 139, 6338-6350.	13.7	38
10	Catalytic Dehydrogenative Câ€“C Coupling by a Pincer-Ligated Iridium Complex. Journal of the American Chemical Society, 2017, 139, 8977-8989.	13.7	35
11	Single and Double Câ€“H Activation of Biphenyl or Phenanthrene. An Example of Câ€“H Addition to Ir(III) More Facile than Addition to Ir(I). Organometallics, 2016, 35, 1613-1623.	2.3	16
12	Two Equilibria of (N-Methyl-3-pyridinium)chlorocarbene, a Cationic Carbene. Journal of Physical Chemistry A, 2016, 120, 699-708.	2.5	1
13	Evaluating the Thermodynamics of Electrocatalytic N₂ Reduction in Acetonitrile. ACS Energy Letters, 2016, 1, 698-704.	17.4	115
14	Assessment of the Electronic Factors Determining the Thermodynamics of â€œOxidative Additionâ€•of Câ€“H and Nâ€“H Bonds to Ir(I) Complexes. Journal of the American Chemical Society, 2016, 138, 149-163.	13.7	52
15	Experimental and computational study of alkane dehydrogenation catalyzed by a carbazolide-based rhodium PNP pincer complex. Chemical Science, 2016, 7, 2579-2586.	7.4	31
16	Dehydrogenation of n-Alkanes by Solid-Phase Molecular Pincer-Iridium Catalysts. High Yields of Î±-Olefin Product. Journal of the American Chemical Society, 2015, 137, 9894-9911.	13.7	74
17	Activation Parameters for Additions to Alkenes of Arylchlorocarbenes with Enhanced Electrophilicity. Journal of Organic Chemistry, 2015, 80, 7590-7593.	3.2	10
18	Copper, Indium, Tin, and Lead Complexes with Fluorinated Selenolate Ligands: Precursors to MSex. Inorganic Chemistry, 2015, 54, 8896-8904.	4.0	19

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19	Non-covalent interactions of nitrous oxide with aromatic compounds: Spectroscopic and computational evidence for the formation of 1:1 complexes. Journal of Chemical Physics, 2014, 140, 144304.	3.0	10
20	(POP)Rh pincer hydride complexes: unusual reactivity and selectivity in oxidative addition and olefin insertion reactions. Chemical Science, 2013, 4, 3683.	7.4	52
21	Covalent Bonding and the Trans Influence in Lanthanide Compounds. Inorganic Chemistry, 2010, 49, 552-560.	4.0	55
22	Conformational Dependence of Electronic Coupling Across Peptide Bonds: A Ramachandran Map. Journal of Physical Chemistry C, 2010, 114, 20809-20812.	3.1	16
23	Solid-State Changes in Ligand-to-Metal Charge-Transfer Spectra of (NH₃)₅Ru^{III}(2,4-dihydroxybenzoate) and (NH₃)₅Ru^{III}(xanthine) Chromophores. Inorganic Chemistry, 2008, 47, 9813-9827.	4.0	6
24	New mechanisms centered on reactive intermediates: Examples from diazirine and carbene chemistry. Pure and Applied Chemistry, 2007, 79, 993-1001.	1.9	16
25	DFT Calculations on the Mechanism of (PCP)Ir-Catalyzed Acceptorless Dehydrogenation of Alkanes. ACS Symposium Series, 2004, , 216-233.	0.5	4
26	On the Mechanism of (PCP)Ir-Catalyzed Acceptorless Dehydrogenation of Alkanes:â€‰ A Combined Computational and Experimental Study. Journal of the American Chemical Society, 2002, 124, 11404-11416.	13.7	115
27	Combined Computational and Experimental Study of Substituent Effects on the Thermodynamics of H2, CO, Arene, and Alkane Addition to Iridium. Journal of the American Chemical Society, 2002, 124, 10797-10809.	13.7	128
28	Alternating Planarity/Nonplanarity in n-Doped Odd-Membered, All- Trans Polyenes: Molecular Structures of NaC n H n+2 (n = 3, 5, 7, and 9). Journal of Molecular Modeling, 2000, 6, 248-256.	1.8	1
29	Addition of Câ^'H Bonds to the Catalytically Active Complex (PCP)Ir (PCP = Î·3-2,6-(tBu2PCH2)2C6H3). Journal of the American Chemical Society, 2000, 122, 11017-11018.	13.7	135
30	Transition States for Oxidative Addition to Three-Coordinate Ir(I): H-H, C-H, C-C, and C-F Bond Activation Processes. ACS Symposium Series, 1999, , 151-162.	0.5	10
31	Modulation of Carbenic Reactivity by Ï€-Complexation to Aromatics. Journal of the American Chemical Society, 1998, 120, 1088-1089.	13.7	44
32	Phosphate cleavage by organoiodinane oxyanion analogues ofo-iodosobenzoate: experimental and computational studies. Journal of Physical Organic Chemistry, 1997, 10, 27-32.	1.9	12
33	The 1:1 glycine zwitterion-water complex: Anab initio electronic structure study. Journal of Computational Chemistry, 1996, 17, 338-349.	3.3	93
34	Evaluating polarizable potentials on distributed memory parallel computers: Program development and applications. Journal of Computational Chemistry, 1995, 16, 1141-1152.	3.3	10
35	Cyclopropylmethoxycarbene: A kinetic limit on the 1,2-carbon migration. Journal of Physical Organic Chemistry, 1992, 5, 104-107.	1.9	12
36	The Isomers of the Acetylene Derivatives C2Li4: Transferable Structural Units in Hyperlithiated Compounds. Angewandte Chemie International Edition in English, 1992, 31, 1602-1603.	4.4	10

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37	Molecular electrostatic potentials and partial atomic charges from correlated wave functions: Applications to the electronic ground and excited states of 3-methylindole. Journal of Computational Chemistry, 1992, 13, 979-989.	3.3	17
38	Die Isomere des Acetylenderivats C₂Li₄: Ã¼bertragbare Struktureinheiten in hyperlithiierten Spezies. Angewandte Chemie, 1992, 104, 1678-1680.	2.0	5
39	The nonplanarity ofn-doped polyenes and of carbanions with alkali metal counterions. International Journal of Quantum Chemistry, 1988, 34, 51-57.	2.0	4
40	Ab initio all-electron and effective core potential calculations on CuCl2?4. International Journal of Quantum Chemistry, 1988, 34, 245-255.	2.0	4
41	An Extraordinary Structure and Topomerization Mechanism forâ€œDiboramethylenecyclopropaneâ€: Angewandte Chemie International Edition in English, 1984, 23, 825-826.	4.4	56
42	Diboramethylencyclopropan, theoretische Studien zur Struktur und zum Mechanismus der Topomerisierung. Angewandte Chemie, 1984, 96, 809-811.	2.0	39
43	Electronic states and barriers to internal rotation in silaallenes. Journal of Computational Chemistry, 1982, 3, 571-579.	3.3	15
44	Carbodications. I. The structures and energies of C4H42+ isomers. Journal of Computational Chemistry, 1981, 2, 356-360.	3.3	27