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	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
2	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
3	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
4	Evaluating the Thermodynamics of Electrocatalytic N₂ Reduction in Acetonitrile. ACS Energy Letters, 2016, 1, 698-704.	17.4	115
5	The 1:1 glycine zwitterion-water complex: Anab initio electronic structure study. Journal of Computational Chemistry, 1996, 17, 338-349.	3.3	93
6	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
7	An Extraordinary Structure and Topomerization Mechanism forâ€œDiboramethylenecyclopropaneâ€• Angewandte Chemie International Edition in English, 1984, 23, 825-826.	4.4	56
8	Covalent Bonding and the Trans Influence in Lanthanide Compounds. Inorganic Chemistry, 2010, 49, 552-560.	4.0	55
9	(POP)Rh pincer hydride complexes: unusual reactivity and selectivity in oxidative addition and olefin insertion reactions. Chemical Science, 2013, 4, 3683.	7.4	52
10	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
11	Modulation of Carbenic Reactivity by Ï€-Complexation to Aromatics. Journal of the American Chemical Society, 1998, 120, 1088-1089.	13.7	44
12	Diboramethylencyclopropan, theoretische Studien zur Struktur und zum Mechanismus der Topomerisierung. Angewandte Chemie, 1984, 96, 809-811.	2.0	39
13	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
14	Catalytic Dehydrogenative Câ€“C Coupling by a Pincer-Ligated Iridium Complex. Journal of the American Chemical Society, 2017, 139, 8977-8989.	13.7	35
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	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
17	Carbodications. I. The structures and energies of C4H42+ isomers. Journal of Computational Chemistry, 1981, 2, 356-360.	3.3	27
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	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
20	New mechanisms centered on reactive intermediates: Examples from diazirine and carbene chemistry. Pure and Applied Chemistry, 2007, 79, 993-1001.	1.9	16
21	Conformational Dependence of Electronic Coupling Across Peptide Bonds: A Ramachandran Map. Journal of Physical Chemistry C, 2010, 114, 20809-20812.	3.1	16
22	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
23	Selective Dehydrogenative Coupling of Ethylene to Butadiene via an Iridacyclopentane Complex. Journal of the American Chemical Society, 2018, 140, 2260-2264.	13.7	16
24	Electronic states and barriers to internal rotation in silaallenes. Journal of Computational Chemistry, 1982, 3, 571-579.	3.3	15
25	Cyclopropylmethoxycarbene: A kinetic limit on the 1,2-carbon migration. Journal of Physical Organic Chemistry, 1992, 5, 104-107.	1.9	12
26	Phosphate cleavage by organoiodinane oxyanion analogues ofo-iodosobenzoate: experimental and computational studies. Journal of Physical Organic Chemistry, 1997, 10, 27-32.	1.9	12
27	Formation of Enamines via Catalytic Dehydrogenation by Pincer-Iridium Complexes. Journal of Organic Chemistry, 2020, 85, 3020-3028.	3.2	12
28	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
29	Evaluating polarizable potentials on distributed memory parallel computers: Program development and applications. Journal of Computational Chemistry, 1995, 16, 1141-1152.	3.3	10
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	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
32	Activation Parameters for Additions to Alkenes of Arylchlorocarbenes with Enhanced Electrophilicity. Journal of Organic Chemistry, 2015, 80, 7590-7593.	3.2	10
33	Extremely reactive carbenes: electrophiles and nucleophiles. Journal of Physical Organic Chemistry, 2017, 30, e3555.	1.9	10
34	Alkane Dehydrogenation Catalyzed by a Fluorinated Phebox Iridium Complex. ACS Catalysis, 2021, 11, 14194-14209.	11.2	8
35	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
36	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

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37	Die Isomere des Acetylenderivats C₂Li₄: Ã¼bertragbare Struktureinheiten in hyperlithiierten Spezies. Angewandte Chemie, 1992, 104, 1678-1680.	2.0	5
38	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
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	DFT Calculations on the Mechanism of (PCP)Ir-Catalyzed Acceptorless Dehydrogenation of Alkanes. ACS Symposium Series, 2004, , 216-233.	0.5	4
42	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
43	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
44	Two Equilibria of (N-Methyl-3-pyridinium)chlorocarbene, a Cationic Carbene. Journal of Physical Chemistry A, 2016, 120, 699-708.	2.5	1