Johannes E M N Klein

List of Publications by Year
in descending order

37	1,418	361045	329751
papers	citations	20 h-index	37 g-index

46	46	46	1453
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electron Flow in Reaction Mechanismsâ€"Revealed from First Principles. Angewandte Chemie - International Edition, 2015, 54, 5518-5522.	7.2	293
2	The Stabilizing Effects in Gold Carbene Complexes. Angewandte Chemie - International Edition, 2015, 54, 10336-10340.	7.2	103
3	Assessment of electronic structure methods for the determination of the ground spin states of Fe(<scp>ii</scp>), Fe(<scp>iii</scp>) and Fe(<scp>iv</scp>) complexes. Physical Chemistry Chemical Physics, 2017, 19, 13049-13069.	1.3	100
4	cPCET versus HAT: A Direct Theoretical Method for Distinguishing Xâ€"H Bondâ€Activation Mechanisms. Angewandte Chemie - International Edition, 2018, 57, 11913-11917.	7.2	77
5	The Electronic Ground State of [Fe(CO)₃(NO)]^{â^'}: A Spectroscopic and Theoretical Study. Angewandte Chemie - International Edition, 2014, 53, 1790-1794.	7.2	71
6	Gold(I) Vinylidene Complexes as Reactive Intermediates and Their Tendency to Ï€â€Backbond. Chemistry - A European Journal, 2016, 22, 2892-2895.	1.7	65
7	Lightâ€Induced Mechanistic Divergence in Gold(I) Catalysis: Revisiting the Reactivity of Diazonium Salts. Angewandte Chemie - International Edition, 2019, 58, 16988-16993.	7.2	62
8	On the Accessible Reaction Channels of Vinyl Gold(I) Species: Ï€â€•and Ïƒâ€Pathways. Chemistry - A European Journal, 2017, 23, 10901-10905.	1.7	44
9	Fe or Feï£¿NO Catalysis? A Quantum Chemical Investigation of the [Fe(CO)₃(NO)]^{â^'}â€Catalyzed Clokeâ€"Wilson Rearrangement. Chemistry - A European Journal, 2014, 20, 7254-7257.	1.7	41
10	Privileged Role of Thiolate as the Axial Ligand in Hydrogen Atom Transfer Reactions by Oxoiron(IV) Complexes in Shaping the Potential Energy Surface and Inducing Significant H-Atom Tunneling. Journal of the American Chemical Society, 2017, 139, 18705-18713.	6.6	33
11	C(sp³)â^'H Bond Activation by Vinylidene Gold(I) Complexes: Aâ€‰Concerted Asynchronous or Stepwise Process?. Chemistry - A European Journal, 2017, 23, 16097-16103.	1.7	32
12	Why metalâ€"oxos react with dihydroanthracene and cyclohexadiene at comparable rates, despite having different Câ€"H bond strengths. A computational study. Chemical Communications, 2016, 52, 10509-10512.	2.2	28
13	Facile and Reversible Formation of Iron(III)â€"Oxoâ€"Cerium(IV) Adducts from Nonheme Oxoiron(IV) Complexes and Cerium(III). Angewandte Chemie - International Edition, 2017, 56, 9091-9095.	7.2	28
14	Ïƒâ€Noninnocence: Masked Phenylâ€Cation Transfer at Formal Ni^{IV}. Angewandte Chemie - International Edition, 2019, 58, 13133-13139.	7.2	27
15	Characterization of the Fleeting Hydroxoiron(III) Complex of the Pentadentate TMC-py Ligand. Inorganic Chemistry, 2017, 56, 11129-11140.	1.9	25
16	Oxoiron(IV) Tetramethylcyclam Complexes with Axial Carboxylate Ligands: Effect of Tethering the Carboxylate on Reactivity. Inorganic Chemistry, 2017, 56, 3287-3301.	1.9	24
17	The Pentagonalâ€Pyramidal Hexamethylbenzene Dication: Many Shades of Coordination Chemistry at Carbon. Chemistry - A European Journal, 2018, 24, 12340-12345.	1.7	24
18	cPCET versus HAT: A Direct Theoretical Method for Distinguishing Xâ€"H Bondâ€Activation Mechanisms. Angewandte Chemie, 2018, 130, 12089-12093.	1.6	20

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19	Lightâ€Induced Mechanistic Divergence in Gold(I) Catalysis: Revisiting the Reactivity of Diazonium Salts. Angewandte Chemie, 2019, 131, 17144-17149.	1.6	20
20	Cationic Gold(I) Diarylallenylidene Complexes: Bonding Features and Ligand Effects. ChemPhysChem, 2019, 20, 1671-1679.	1.0	18
21	The Two Faces of Tetramethylcyclam in Iron Chemistry: Distinct Feâ€“Oâ€“M Complexes Derived from [Fe^{IV}(O_{anti/syn})(TMC)]²⁺ Isomers. Inorganic Chemistry, 2017, 56, 518-527.	1.9	14
22	On the Lewis Acidity of the Oxoiron(IV) Unit in a Tetramethylcyclam Complex. Chemistry - A European Journal, 2018, 24, 5373-5378.	1.7	11
23	Epoxidation of Alkenes by Peracids: From Textbook Mechanisms to a Quantum Mechanically Derived Curlyâ€Arrow Depiction. ChemistryOpen, 2019, 8, 1244-1250.	0.9	11
24	Gold-Aluminyl and Gold-Diarylboryl Complexes: Bonding and Reactivity with Carbon Dioxide. Inorganic Chemistry, 2022, 61, 7327-7337.	1.9	10
25	Facile Conversion of syn â€[Fe IV (O)(TMC)] 2+ into the anti Isomer via Meunier's Oxoâ€“Hydroxo Tautomerism Mechanism. Angewandte Chemie - International Edition, 2019, 58, 1995-1999.	7.2	9
26	Facile and Reversible Formation of Iron(III)â€“Oxoâ€“Cerium(IV) Adducts from Nonheme Oxoiron(IV) Complexes and Cerium(III). Angewandte Chemie, 2017, 129, 9219-9223.	1.6	8
27	Ïƒâ€Noninnocence: Masked Phenylâ€Cation Transfer at Formal Ni^{IV}. Angewandte Chemie, 2019, 131, 13267-13273.	1.6	8
28	Homolytic Xâ€H Bond Cleavage at a Gold(III) Hydroxide: Insights into Oneâ€Electron Events at Gold. Chemistry - A European Journal, 2022, 28, .	1.7	8
29	Toward Environmentally Benign Electrophilic Chlorinations: From Chloroperoxidase to Bioinspired Isoporphyrins. Inorganic Chemistry, 2022, 61, 8105-8111.	1.9	7
30	Spin-resolved charge displacement analysis as an intuitive tool for the evaluation of cPCET and HAT scenarios. Chemical Communications, 2020, 56, 12146-12149.	2.2	6
31	The electronic structure of carbones revealed: insights from valence bond theory. Physical Chemistry Chemical Physics, 2021, 23, 3327-3334.	1.3	6
32	Goldâ€Catalyzed Direct C(sp³)â^'H Acetoxylation of Saturated Hydrocarbons. ChemCatChem, 2021, 13, 4087-4091.	1.8	6
33	Synthesis of a Sterically Encumbered Pincer Au(III)â^'OH Complex. European Journal of Inorganic Chemistry, 2021, 2021, 3561-3564.	1.0	6
34	Combining Structural with Functional Model Properties in Iron Synthetic Analogue Complexes for the Active Site in Rabbit Lipoxygenase. Journal of the American Chemical Society, 2021, 143, 13145-13155.	6.6	5
35	Facile Conversion of syn â€[Fe IV (O)(TMC)] 2+ into the anti Isomer via Meunier's Oxoâ€“Hydroxo Tautomerism Mechanism. Angewandte Chemie, 2019, 131, 2017-2021.	1.6	4
36	Efficient Computation of Geometries for Gold Complexes. ChemPhysChem, 2021, 22, 1262-1268.	1.0	4

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37	Hydrogenâ€Atom Transfer Oxidation with H₂O₂ Catalyzed by		