

# Johannes E M N Klein

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3013187/publications.pdf>

Version: 2024-02-01

37  
papers

1,418  
citations

361413

20  
h-index

330143

37  
g-index

46  
all docs

46  
docs citations

46  
times ranked

1453  
citing authors

#	ARTICLE	IF	CITATIONS
1	Electron Flow in Reaction Mechanismsâ€”Revealed from First Principles. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 5518-5522.	13.8	293
2	The Stabilizing Effects in Gold Carbene Complexes. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 10336-10340.	13.8	103
3	Assessment of electronic structure methods for the determination of the ground spin states of Fe( $\text{II}$ ), Fe( $\text{III}$ ) and Fe( $\text{IV}$ ) complexes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13049-13069.	2.8	100
4	cPCET versus HAT: A Direct Theoretical Method for Distinguishing Xâ€”H Bondâ€”Activation Mechanisms. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 11913-11917.	13.8	77
5	The Electronic Ground State of $[\text{Fe}(\text{CO})_3(\text{NO})]^+$ : A Spectroscopic and Theoretical Study. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 1790-1794.	13.8	71
6	Gold(I) Vinylidene Complexes as Reactive Intermediates and Their Tendency to Î€”Backbond. <i>Chemistry - A European Journal</i> , 2016, 22, 2892-2895.	3.3	65
7	Lightâ€”Induced Mechanistic Divergence in Gold(I) Catalysis: Revisiting the Reactivity of Diazonium Salts. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 16988-16993.	13.8	62
8	On the Accessible Reaction Channels of Vinyl Gold(I) Species: Î€”and Îƒ”Pathways. <i>Chemistry - A European Journal</i> , 2017, 23, 10901-10905.	3.3	44
9	Fe or FeÎƒ;NO Catalysis? A Quantum Chemical Investigation of the $[\text{Fe}(\text{CO})_3(\text{NO})]^+$ â€”Catalyzed Clokeâ€”Wilson Rearrangement. <i>Chemistry - A European Journal</i> , 2014, 20, 7254-7257.	3.3	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. <i>Journal of the American Chemical Society</i> , 2017, 139, 18705-18713.	13.7	33
11	C( $\text{sp}^3$ )â€”H Bond Activation by Vinylidene Gold(I) Complexes: Aâ€”Concerted Asynchronous or Stepwise Process?. <i>Chemistry - A European Journal</i> , 2017, 23, 16097-16103.	3.3	32
12	Why metalâ€”oxos react with dihydroanthracene and cyclohexadiene at comparable rates, despite having different Câ€”H bond strengths. A computational study. <i>Chemical Communications</i> , 2016, 52, 10509-10512.	4.1	28
13	Facile and Reversible Formation of Iron(III)â€”Oxoâ€”Cerium(IV) Adducts from Nonheme Oxoiron(IV) Complexes and Cerium(III). <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9091-9095.	13.8	28
14	Îƒ”Noninnocence: Masked Phenylâ€”Cation Transfer at Formal Ni $\text{IV}$ . <i>Angewandte Chemie - International Edition</i> , 2019, 58, 13133-13139.	13.8	27
15	Characterization of the Fleeting Hydroxoiron(III) Complex of the Pentadentate TMC-py Ligand. <i>Inorganic Chemistry</i> , 2017, 56, 11129-11140.	4.0	25
16	Oxoiron(IV) Tetramethylcyclam Complexes with Axial Carboxylate Ligands: Effect of Tethering the Carboxylate on Reactivity. <i>Inorganic Chemistry</i> , 2017, 56, 3287-3301.	4.0	24
17	The Pentagonalâ€”Pyramidal Hexamethylbenzene Dication: Many Shades of Coordination Chemistry at Carbon. <i>Chemistry - A European Journal</i> , 2018, 24, 12340-12345.	3.3	24
18	cPCET versus HAT: A Direct Theoretical Method for Distinguishing Xâ€”H Bondâ€”Activation Mechanisms. <i>Angewandte Chemie</i> , 2018, 130, 12089-12093.	2.0	20

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19	Light-Induced Mechanistic Divergence in Gold(I) Catalysis: Revisiting the Reactivity of Diazonium Salts. <i>Angewandte Chemie</i> , 2019, 131, 17144-17149.	2.0	20
20	Cationic Gold(I) Diarylallenylidene Complexes: Bonding Features and Ligand Effects. <i>ChemPhysChem</i> , 2019, 20, 1671-1679.	2.1	18
21	The Two Faces of Tetramethylcyclam in Iron Chemistry: Distinct Fe <sup>IV</sup> (O) Complexes Derived from [Fe <sup>IV</sup> (O)(anti-syn)(TMC)] <sup>2+</sup> Isomers. <i>Inorganic Chemistry</i> , 2017, 56, 518-527.	4.0	14
22	On the Lewis Acidity of the Oxoiron(IV) Unit in a Tetramethylcyclam Complex. <i>Chemistry - A European Journal</i> , 2018, 24, 5373-5378.	3.3	11
23	Epoxidation of Alkenes by Peracids: From Textbook Mechanisms to a Quantum Mechanically Derived Curly-Arrow Depiction. <i>ChemistryOpen</i> , 2019, 8, 1244-1250.	1.9	11
24	Gold-Alumanyl and Gold-Diarylboryl Complexes: Bonding and Reactivity with Carbon Dioxide. <i>Inorganic Chemistry</i> , 2022, 61, 7327-7337.	4.0	10
25	Facile Conversion of syn-[Fe <sup>IV</sup> (O)(TMC)] <sup>2+</sup> into the anti Isomer via Meunier's Oxo-Hydroxo Tautomerism Mechanism. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1995-1999.	13.8	9
26	Facile and Reversible Formation of Iron(III)-Oxo-Cerium(IV) Adducts from Nonheme Oxoiron(IV) Complexes and Cerium(III). <i>Angewandte Chemie</i> , 2017, 129, 9219-9223.	2.0	8
27	Iron-Noninnocence: Masked Phenyl-Cation Transfer at Formal Ni <sup>IV</sup> . <i>Angewandte Chemie</i> , 2019, 131, 13267-13273.	2.0	8
28	Homolytic X-H Bond Cleavage at a Gold(III) Hydroxide: Insights into One-Electron Events at Gold. <i>Chemistry - A European Journal</i> , 2022, 28, .	3.3	8
29	Toward Environmentally Benign Electrophilic Chlorinations: From Chloroperoxidase to Bioinspired Isoporphyrins. <i>Inorganic Chemistry</i> , 2022, 61, 8105-8111.	4.0	7
30	Spin-resolved charge displacement analysis as an intuitive tool for the evaluation of cPCET and HAT scenarios. <i>Chemical Communications</i> , 2020, 56, 12146-12149.	4.1	6
31	The electronic structure of carbones revealed: insights from valence bond theory. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 3327-3334.	2.8	6
32	Gold-Catalyzed Direct C(sp <sup>3</sup> )-H Acetoxylation of Saturated Hydrocarbons. <i>ChemCatChem</i> , 2021, 13, 4087-4091.	3.7	6
33	Synthesis of a Sterically Encumbered Pincer Au(III)-OH Complex. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3561-3564.	2.0	6
34	Combining Structural with Functional Model Properties in Iron Synthetic Analogue Complexes for the Active Site in Rabbit Lipoxygenase. <i>Journal of the American Chemical Society</i> , 2021, 143, 13145-13155.	13.7	5
35	Facile Conversion of syn-[Fe <sup>IV</sup> (O)(TMC)] <sup>2+</sup> into the anti Isomer via Meunier's Oxo-Hydroxo Tautomerism Mechanism. <i>Angewandte Chemie</i> , 2019, 131, 2017-2021.	2.0	4
36	Efficient Computation of Geometries for Gold Complexes. <i>ChemPhysChem</i> , 2021, 22, 1262-1268.	2.1	4

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37	Hydrogen-Atom Transfer Oxidation with H <sub>2</sub> O <sub>2</sub> Catalyzed by		