Johannes E M N Klein

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

38 papers	1,072 citations	20 h-index	32 g-index
46 ext. papers	1,314 ext. citations	7.1 avg, IF	5.03 L-index

#	Paper	IF	Citations
38	Gold-Aluminyl and Gold-Diarylboryl Complexes: Bonding and Reactivity with Carbon Dioxide.. *Inorganic Chemistry*, **2022**, 61, 7327-7337	5.1	1
37	Efficient Computation of Geometries for Gold Complexes. *ChemPhysChem*, **2021**, 22, 1262-1268	3.2	1
36	The electronic structure of carbones revealed: insights from valence bond theory. *Physical Chemistry Chemical Physics*, **2021**, 23, 3327-3334	3.6	4
35	Gold-Catalyzed Direct C(sp3)–H Acetoxylation of Saturated Hydrocarbons. *ChemCatChem*, **2021**, 13, 4087	5.2	0
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	16.4	0
33	Synthesis of a Sterically Encumbered Pincer Au(III)–OH Complex. *European Journal of Inorganic Chemistry*, **2021**, 2021, 3561-3564	2.3	0
32	Spin-resolved charge displacement analysis as an intuitive tool for the evaluation of cPCET and HAT scenarios. *Chemical Communications*, **2020**, 56, 12146-12149	5.8	1
31	Noninnocence: Masked Phenyl-Cation Transfer at Formal Ni. *Angewandte Chemie - International Edition*, **2019**, 58, 13133-13139	16.4	14
30	Cationic Gold(I) Diarylallenylidene Complexes: Bonding Features and Ligand Effects. *ChemPhysChem*, **2019**, 20, 1671-1679	3.2	9
29	Facile Conversion of syn-[FeIV(O)(TMC)]2+ into the anti Isomer via Meunier's Oxo–Hydroxo Tautomerism Mechanism. *Angewandte Chemie*, **2019**, 131, 2017-2021	3.6	2
28	Light-Induced Mechanistic Divergence in Gold(I) Catalysis: Revisiting the Reactivity of Diazonium Salts. *Angewandte Chemie - International Edition*, **2019**, 58, 16988-16993	16.4	43
27	Noninnocence: Masked Phenyl-Cation Transfer at Formal NiIV. *Angewandte Chemie*, **2019**, 131, 13267-13273	3.6	4
26	Epoxidation of Alkenes by Peracids: From Textbook Mechanisms to a Quantum Mechanically Derived Curly-Arrow Depiction. *ChemistryOpen*, **2019**, 8, 1244-1250	2.3	3
25	Light-Induced Mechanistic Divergence in Gold(I) Catalysis: Revisiting the Reactivity of Diazonium Salts. *Angewandte Chemie*, **2019**, 131, 17144-17149	3.6	19
24	Facile Conversion of syn-[Fe (O)(TMC)] into the anti Isomer via Meunier's Oxo-Hydroxo Tautomerism Mechanism. *Angewandte Chemie - International Edition*, **2019**, 58, 1995-1999	16.4	4
23	The Pentagonal-Pyramidal Hexamethylbenzene Dication: Many Shades of Coordination Chemistry at Carbon. *Chemistry - A European Journal*, **2018**, 24, 12340-12345	4.8	21
22	cPCET versus HAT: A Direct Theoretical Method for Distinguishing X–H Bond-Activation Mechanisms. *Angewandte Chemie*, **2018**, 130, 12089-12093	3.6	14

21	cPCET versus HAT: A Direct Theoretical Method for Distinguishing X-H Bond-Activation Mechanisms. *Angewandte Chemie - International Edition*, **2018**, 57, 11913-11917	16.4	37
20	On the Lewis Acidity of the Oxoiron(IV) Unit in a Tetramethylcyclam Complex. *Chemistry - A European Journal*, **2018**, 24, 5373-5378	4.8	6
19	Oxoiron(IV) Tetramethylcyclam Complexes with Axial Carboxylate Ligands: Effect of Tethering the Carboxylate on Reactivity. *Inorganic Chemistry*, **2017**, 56, 3287-3301	5.1	22
18	Assessment of electronic structure methods for the determination of the ground spin states of Fe(ii), Fe(iii) and Fe(iv) complexes. *Physical Chemistry Chemical Physics*, **2017**, 19, 13049-13069	3.6	72
17	Facile and Reversible Formation of Iron(III)-Oxo-Cerium(IV) Adducts from Nonheme Oxoiron(IV) Complexes and Cerium(III). *Angewandte Chemie - International Edition*, **2017**, 56, 9091-9095	16.4	24
16	On the Accessible Reaction Channels of Vinyl Gold(I) Species: □and □Pathways. *Chemistry - A European Journal*, **2017**, 23, 10901-10905	4.8	34
15	The Two Faces of Tetramethylcyclam in Iron Chemistry: Distinct Fe-O-M Complexes Derived from [Fe(O)(TMC)] Isomers. *Inorganic Chemistry*, **2017**, 56, 518-527	5.1	11
14	Characterization of the Fleeting Hydroxoiron(III) Complex of the Pentadentate TMC-py Ligand. *Inorganic Chemistry*, **2017**, 56, 11129-11140	5.1	24
13	Hydrogen-Atom Transfer Oxidation with HO Catalyzed by [FeII(1,2-bis(2,2□bipyridyl-6-yl)ethane(HO)]: Likely Involvement of a (□Hydroxo)(□1,2-peroxo)diiron(III) Intermediate. *Israel Journal of Chemistry*, **2017**, 57, 990-998	3.4	
12	C(sp)-H Bond Activation by Vinylidene Gold(I) Complexes: A Concerted Asynchronous or Stepwise Process?. *Chemistry - A European Journal*, **2017**, 23, 16097-16103	4.8	25
11	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	16.4	20
10	Facile and Reversible Formation of Iron(III)□Oxo□Cerium(IV) Adducts from Nonheme Oxoiron(IV) Complexes and Cerium(III). *Angewandte Chemie*, **2017**, 129, 9219-9223	3.6	8
9	Gold(I) Vinylidene Complexes as Reactive Intermediates and Their Tendency to □Backbond. *Chemistry - A European Journal*, **2016**, 22, 2892-5	4.8	57
8	Why metal-oxos react with dihydroanthracene and cyclohexadiene at comparable rates, despite having different C-H bond strengths. A computational study. *Chemical Communications*, **2016**, 52, 10509-12	5.8	20
7	Electron flow in reaction mechanisms--revealed from first principles. *Angewandte Chemie - International Edition*, **2015**, 54, 5518-22	16.4	191
6	The Stabilizing Effects in Gold Carbene Complexes. *Angewandte Chemie - International Edition*, **2015**, 54, 10336-40	16.4	85
5	Zu den stabilisierenden Effekten in Carbengoldkomplexen. *Angewandte Chemie*, **2015**, 127, 10477-10481	3.6	36
4	Elektronenfluss in Reaktionsmechanismen □enth□t aus quantenmechanischen Grundprinzipien. *Angewandte Chemie*, **2015**, 127, 5609-5613	3.6	53

3	The electronic ground state of [Fe(CO)3 (NO)](-) : a spectroscopic and theoretical study. *Angewandte Chemie - International Edition*, **2014**, 53, 1790-4	16.4	59
2	Fe or Fe-NO catalysis? A quantum chemical investigation of the [Fe(CO)3(NO)](-)-catalyzed Cloke-Wilson rearrangement. *Chemistry - A European Journal*, **2014**, 20, 7254-7	4.8	36
1	Der elektronische Grundzustand von [Fe(CO)3(NO)]□eine spektroskopische und theoretische Studie. *Angewandte Chemie*, **2014**, 126, 1820-1824	3.6	32