

Johannes E M N Klein

List of Publications by Citations

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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	Electron flow in reaction mechanisms--revealed from first principles. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 5518-22	16.4	191
37	The Stabilizing Effects in Gold Carbene Complexes. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 10336-40	16.4	85
36	Assessment of electronic structure methods for the determination of the ground spin states of Fe(ii), Fe(iii) and Fe(iv) complexes. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 13049-13069	3.6	72
35	The electronic ground state of [Fe(CO) ₃ (NO)](-): a spectroscopic and theoretical study. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 1790-4	16.4	59
34	Gold(I) Vinylidene Complexes as Reactive Intermediates and Their Tendency to β -Backbond. <i>Chemistry - A European Journal</i> , 2016 , 22, 2892-5	4.8	57
33	Elektronenfluss in Reaktionsmechanismen β -enth β lt aus quantenmechanischen Grundprinzipien. <i>Angewandte Chemie</i> , 2015 , 127, 5609-5613	3.6	53
32	Light-Induced Mechanistic Divergence in Gold(I) Catalysis: Revisiting the Reactivity of Diazonium Salts. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 16988-16993	16.4	43
31	cPCET versus HAT: A Direct Theoretical Method for Distinguishing X-H Bond-Activation Mechanisms. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 11913-11917	16.4	37
30	Zu den stabilisierenden Effekten in Carbengoldkomplexen. <i>Angewandte Chemie</i> , 2015 , 127, 10477-10483	3.6	36
29	Fe or Fe-NO catalysis? A quantum chemical investigation of the [Fe(CO) ₃ (NO)](-)-catalyzed Cloke-Wilson rearrangement. <i>Chemistry - A European Journal</i> , 2014 , 20, 7254-7	4.8	36
28	On the Accessible Reaction Channels of Vinyl Gold(I) Species: β and β Pathways. <i>Chemistry - A European Journal</i> , 2017 , 23, 10901-10905	4.8	34
27	Der elektronische Grundzustand von [Fe(CO) ₃ (NO)] β eine spektroskopische und theoretische Studie. <i>Angewandte Chemie</i> , 2014 , 126, 1820-1824	3.6	32
26	C(sp ⁻)-H Bond Activation by Vinylidene Gold(I) Complexes: A Concerted Asynchronous or Stepwise Process?. <i>Chemistry - A European Journal</i> , 2017 , 23, 16097-16103	4.8	25
25	Facile and Reversible Formation of Iron(III)-Oxo-Cerium(IV) Adducts from Nonheme Oxoiron(IV) Complexes and Cerium(III). <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 9091-9095	16.4	24
24	Characterization of the Fleeting Hydroxoiron(III) Complex of the Pentadentate TMC-py Ligand. <i>Inorganic Chemistry</i> , 2017 , 56, 11129-11140	5.1	24
23	Oxoiron(IV) Tetramethylcyclam Complexes with Axial Carboxylate Ligands: Effect of Tethering the Carboxylate on Reactivity. <i>Inorganic Chemistry</i> , 2017 , 56, 3287-3301	5.1	22
22	The Pentagonal-Pyramidal Hexamethylbenzene Dication: Many Shades of Coordination Chemistry at Carbon. <i>Chemistry - A European Journal</i> , 2018 , 24, 12340-12345	4.8	21

21	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	16.4	20
20	Why metal-oxos react with dihydroanthracene and cyclohexadiene at comparable rates, despite having different C-H bond strengths. A computational study. <i>Chemical Communications</i> , 2016 , 52, 10509-10512	5.8	20
19	Light-Induced Mechanistic Divergence in Gold(I) Catalysis: Revisiting the Reactivity of Diazonium Salts. <i>Angewandte Chemie</i> , 2019 , 131, 17144-17149	3.6	19
18	Noninnocence: Masked Phenyl-Cation Transfer at Formal Ni. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 13133-13139	16.4	14
17	cPCET versus HAT: A Direct Theoretical Method for Distinguishing X-H Bond-Activation Mechanisms. <i>Angewandte Chemie</i> , 2018 , 130, 12089-12093	3.6	14
16	The Two Faces of Tetramethylcyclam in Iron Chemistry: Distinct Fe-O-M Complexes Derived from [Fe(O)(TMC)] Isomers. <i>Inorganic Chemistry</i> , 2017 , 56, 518-527	5.1	11
15	Cationic Gold(I) Diarylallenylidene Complexes: Bonding Features and Ligand Effects. <i>ChemPhysChem</i> , 2019 , 20, 1671-1679	3.2	9
14	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	3.6	8
13	On the Lewis Acidity of the Oxoiron(IV) Unit in a Tetramethylcyclam Complex. <i>Chemistry - A European Journal</i> , 2018 , 24, 5373-5378	4.8	6
12	Noninnocence: Masked Phenyl-Cation Transfer at Formal NiIV. <i>Angewandte Chemie</i> , 2019 , 131, 13267-13273	3.2	4
11	Facile Conversion of syn-[Fe(O)(TMC)] into the anti Isomer via Meunier's Oxo-Hydroxo Tautomerism Mechanism. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 1995-1999	16.4	4
10	The electronic structure of carbones revealed: insights from valence bond theory. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 3327-3334	3.6	4
9	Epoxidation of Alkenes by Peracids: From Textbook Mechanisms to a Quantum Mechanically Derived Curly-Arrow Depiction. <i>ChemistryOpen</i> , 2019 , 8, 1244-1250	2.3	3
8	Facile Conversion of syn-[FeIV(O)(TMC)] ²⁺ into the anti Isomer via Meunier's Oxo-Hydroxo Tautomerism Mechanism. <i>Angewandte Chemie</i> , 2019 , 131, 2017-2021	3.6	2
7	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	5.8	1
6	Efficient Computation of Geometries for Gold Complexes. <i>ChemPhysChem</i> , 2021 , 22, 1262-1268	3.2	1
5	Gold-Alumanyl and Gold-Diarylboryl Complexes: Bonding and Reactivity with Carbon Dioxide.. <i>Inorganic Chemistry</i> , 2022 , 61, 7327-7337	5.1	1
4	Gold-Catalyzed Direct C(sp ³) β Acetoxylation of Saturated Hydrocarbons. <i>ChemCatChem</i> , 2021 , 13, 4087-4092	5.2	0

- 3 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} ○
- 2 Synthesis of a Sterically Encumbered Pincer Au(III)DH Complex. *European Journal of Inorganic Chemistry*, **2021**, 2021, 3561-3564 2.3 ○
- 1 Hydrogen-Atom Transfer Oxidation with HO Catalyzed by [FeII(1,2-bis(2,2'-bipyridyl-6-yl)ethane(HO))]: Likely Involvement of a (μ-Hydroxo)(μ,2-peroxo)diiron(III) Intermediate. *Israel Journal of Chemistry*, **2017**, 57, 990-998 3.4