Maurice van Gastel

List of Publications by Year
in descending order

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89 papers	3,478 citations	147801 31 h-index	155660 55 g-index
89 all docs	89 docs citations	89 times ranked	3464 citing authors

#	Article	IF	Citations
1	A Combined Spectroscopic and Computational Study on the Mechanism of Iron-Catalyzed Aminofunctionalization of Olefins Using Hydroxylamine Derived Nâ€“O Reagent as the â€œAminoâ€•Source and â€œOxidantâ€• Journal of the American Chemical Society, 2022, 144, 2637-2656.	13.7	29
2	Metalloradical Cations and Dications Based on Divinyldiphosphene and Divinyldiarsene Ligands. Chemistry - A European Journal, 2021, 27, 5803-5809.	3.3	12
3	Productive Alkyne Metathesis with â€œCanopy Catalystsâ€•Mandates Pseudorotation. Journal of the American Chemical Society, 2021, 143, 5643-5648.	13.7	33
4	Converged Structural and Spectroscopic Properties for Refined QM/MM Models of Azurin. Inorganic Chemistry, 2021, 60, 7399-7412.	4.0	10
5	Spectroscopic and Theoretical Study on Siloxy-Based Molybdenum and Tungsten Alkylidyne Catalysts for Alkyne Metathesis. ACS Catalysis, 2021, 11, 9086-9101.	11.2	15
6	Sterically Stabilized End-On Superoxocopper(II) Complexes and Mechanistic Insights into Their Reactivity with Oâ€“H, Nâ€“H, and Câ€“H Substrates. Journal of the American Chemical Society, 2021, 143, 19731-19747.	13.7	12
7	Where Is the Fluoro Wall?: A Quantum Chemical Investigation. Inorganic Chemistry, 2020, 59, 1556-1565.	4.0	7
8	Isolation of singlet carbene derived 2-phospha-1,3-butadienes and their sequential one-electron oxidation to radical cations and dications. Chemical Science, 2020, 11, 1975-1984.	7.4	19
9	Isolation of a Homoleptic Non-oxo Mo(V) Alkoxide Complex: Synthesis, Structure, and Electronic Properties of Penta-tert-Butoxymolybdenum. Journal of the American Chemical Society, 2020, 142, 16392-16402.	13.7	11
10	A Manganese(IV)-Hydroperoxo Intermediate Generated by Protonation of the Corresponding Manganese(III)-Superoxo Complex. Journal of the American Chemical Society, 2020, 142, 10255-10260.	13.7	22
11	Isolation of singlet carbene derived 2-arsa-1,3-butadiene radical cations and dications. Chemical Communications, 2020, 56, 3575-3578.	4.1	14
12	Diphosphene radical cations and dications with a Ï€-conjugated C₂P₂C₂-framework. Chemical Communications, 2019, 55, 10408-10411.	4.1	36
13	Mononuclear Manganese(III) Superoxo Complexes: Synthesis, Characterization, and Reactivity. Inorganic Chemistry, 2019, 58, 9756-9765.	4.0	21
14	Crystalline Divinyldiarsene Radical Cations and Dications. Angewandte Chemie - International Edition, 2019, 58, 17599-17603.	13.8	31
15	Crystalline Divinyldiarsene Radical Cations and Dications. Angewandte Chemie, 2019, 131, 17763-17767.	2.0	6
16	Spectroscopic and Quantum Chemical Investigation of Benzene-1,2-dithiolate-Coordinated Diiron Complexes with Relevance to Dinitrogen Activation. Inorganic Chemistry, 2019, 58, 5111-5125.	4.0	9
17	Solvent-Controlled CO₂ Reduction by a Triphosâ€“Iron Hydride Complex. Organometallics, 2019, 38, 289-299.	2.3	17
18	Crystalline Radicals Derived from Classical Nâ€Heterocyclic Carbenes. Angewandte Chemie - International Edition, 2018, 57, 4765-4768.	13.8	57

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19	Palladium-catalysed electrophilic aromatic Câ€“H fluorination. Nature, 2018, 554, 511-514.	27.8	131
20	High surface area black TiO2 templated from ordered mesoporous carbon for solar driven hydrogen evolution. Microporous and Mesoporous Materials, 2018, 268, 162-169.	4.4	18
21	Nâ€Heterocyclic Carbene Analogues of Thiele and Chichibabin Hydrocarbons. Angewandte Chemie - International Edition, 2018, 57, 5838-5842.	13.8	55
22	Electronic Structure and Spin Multiplicity of Iron Tetraphenylporphyrins in Their Reduced States as Determined by a Combination of Resonance Raman Spectroscopy and Quantum Chemistry. Inorganic Chemistry, 2018, 57, 2141-2148.	4.0	48
23	Diradical Character Enhancement by Spacing: Nâ€Heterocyclic Carbene Analogues of MÃ¼ller's Hydrocarbon. Chemistry - A European Journal, 2018, 24, 16537-16542.	3.3	31
24	Sulfide Protects [FeFe] Hydrogenases From O₂. Journal of the American Chemical Society, 2018, 140, 9346-9350.	13.7	47
25	Electronic Structure of a Formal Iron(0) Porphyrin Complex Relevant to CO₂ Reduction. Inorganic Chemistry, 2017, 56, 4745-4750.	4.0	85
26	Spontaneous Siâ€“C bond cleavage in (Triphos^{Si})-nickel complexes. Dalton Transactions, 2017, 46, 907-917.	3.3	16
27	The active site for the water oxidising anodic iridium oxide probed through in situ Raman spectroscopy. Chemical Communications, 2017, 53, 12414-12417.	4.1	68
28	Reactive Electrophilic O^{Iâ€™} Species Evidenced in Highâ€Performance Iridium Oxohydroxide Water Oxidation Electrocatalysts. ChemSusChem, 2017, 10, 4786-4798.	6.8	49
29	Mechanistic Implications for the Ni(I)-Catalyzed Kumada Cross-Coupling Reaction. Inorganics, 2017, 5, 78.	2.7	25
30	Raman Spectroscopy as a Method to Investigate Catalytic Intermediates: CO₂ Reducing [Re(Cl)(bpy-R)(CO)₃] Catalyst. Journal of Physical Chemistry A, 2016, 120, 7465-7474.	2.5	9
31	Cobalt Phosphino-Î±-Iminopyridine-Catalyzed Hydrofunctionalization of Alkenes: Catalyst Development and Mechanistic Analysis. Organometallics, 2016, 35, 2900-2914.	2.3	31
32	Hydrogen evolution in [NiFe] hydrogenases and related biomimetic systems: similarities and differences. Physical Chemistry Chemical Physics, 2016, 18, 24681-24692.	2.8	15
33	Probing the Structure of a Water-Oxidizing Anodic Iridium Oxide Catalyst using Raman Spectroscopy. ACS Catalysis, 2016, 6, 8098-8105.	11.2	104
34	Combined Spectroscopic and Electrochemical Detection of a Ni^Iâ‹…â‹…â‹…Hï£¿N Bonding Interaction with Relevance to Electrocatalytic H₂ Production. Chemistry - A European Journal, 2015, 21, 10338-10347.	3.3	14
35	EPR and Quantum Chemical Investigation of a Bioinspired Hydrogenase Model with a Redox-Active Ligand in the First Coordination Sphere. Organometallics, 2015, 34, 995-1000.	2.3	13
36	Nickel(<scp>ii</scp>) radical complexes of thiosemicarbazone ligands appended by salicylidene, aminophenol and aminothiophenol moieties. Dalton Transactions, 2015, 44, 12743-12756.	3.3	24

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37	Structural differences between the active sites of the Ni-A and Ni-B states of the [NiFe] hydrogenase: an approach by quantum chemistry and single crystal ENDOR spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 16204-16212.	2.8	21
38	Hydride bridge in [NiFe]-hydrogenase observed by nuclear resonance vibrational spectroscopy. Nature Communications, 2015, 6, 7890.	12.8	96
39	Finding the Reactive Electron in Paramagnetic Systems: A Critical Evaluation of Accuracies for EPR Spectroscopy and Density Functional Theory Using 1,3,5-Triphenyl Verdazyl Radical as a Testcase. Applied Magnetic Resonance, 2015, 46, 117-139.	1.2	8
40	Copper(II)-Coordinated Î±-Azophenols: Effect of the Metal-Ion Geometry on Phenoxyl/Phenolate Oxidation Potential and Reactivity. European Journal of Inorganic Chemistry, 2014, 2014, 4263-4267.	2.0	12
41	A singlet ground state for a cobalt(<scp>ii</scp>)â€“anilinosalen radical complex. Chemical Communications, 2014, 50, 4924-4926.	4.1	17
42	Spectroscopic and Quantum Chemical Study of the Ni(PPh2NC6H4CH2P(O)(OEt)22)2 Electrocatalyst for Hydrogen Production with Emphasis on the NiI Oxidation State. Journal of Physical Chemistry C, 2014, 118, 2350-2360.	3.1	16
43	Characterization of one-electron oxidized copper(<scp>ii</scp>)-salophen-type complexes; effects of electronic and geometrical structures on reactivities. Dalton Transactions, 2014, 43, 2283-2293.	3.3	45
44	An Intermediate Cobalt(IV) Nitrido Complex and its N-Migratory Insertion Product. Journal of the American Chemical Society, 2014, 136, 15072-15078.	13.7	84
45	Comparative ENDOR study at 34ÂGHz of the triplet state of the primary donor in bacterial reaction centers of Rb. sphaeroides and Bl. viridis. Photosynthesis Research, 2014, 120, 99-111.	2.9	6
46	Synthesis, Reactivity, and Electronic Structure of a Bioinspired Heterobimetallic [Ni(Î¼-S₂)Fe] Complex with Disulfur Monoradical character. Organometallics, 2014, 33, 3154-3162.	2.3	3
47	Theoretical Spectroscopy of the Ni^{II} Intermediate States in the Catalytic Cycle and the Activation of [NiFe] Hydrogenases. ChemBioChem, 2013, 14, 1898-1905.	2.6	56
48	Structural and Spectroscopic Investigation of an Anilinosalen Cobalt Complex with Relevance to Hydrogen Production. Inorganic Chemistry, 2013, 52, 14428-14438.	4.0	22
49	A Metalâ€“Metal Bond in the Light-Induced State of [NiFe] Hydrogenases with Relevance to Hydrogen Evolution. Journal of the American Chemical Society, 2013, 135, 3915-3925.	13.7	95
50	Radical-Based Epoxide Opening by Titanocenes. Inorganic Chemistry, 2013, 52, 11859-11866.	4.0	20
51	A Functional [NiFe]-Hydrogenase Model Compound That Undergoes Biologically Relevant Reversible Thiolate Protonation. Journal of the American Chemical Society, 2012, 134, 20745-20755.	13.7	101
52	Reversed Freeze Quench Method near the Solvent Phase Transition. Journal of Physical Chemistry A, 2012, 116, 3899-3906.	2.5	3
53	Computational study of the electronic structure and magnetic properties of the Niâ€“C state in [NiFe] hydrogenases including the second coordination sphere. Journal of Biological Inorganic Chemistry, 2012, 17, 1269-1281.	2.6	46
54	Electronic Structure of the Lowest Triplet State of Flavin Mononucleotide. Journal of Physical Chemistry A, 2012, 116, 10090-10098.	2.5	12

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55	H₂O Activation for Hydrogenâ€Atom Transfer: Correct Structures and Revised Mechanisms. Angewandte Chemie - International Edition, 2012, 51, 3266-3270.	13.8	72
56	An Unusal Case of Facile Nonâ€Degenerate Pï£¿C Bond Making and Breaking. Chemistry - an Asian Journal, 2012, 7, 1708-1712.	3.3	16
57	Deoxygenation of Coordinated Oxaphosphiranes: A New Route to Pï£¾C Doubleâ€Bond Systems. Chemistry - A European Journal, 2012, 18, 9780-9783.	3.3	15
58	Radical 4â€exo Cyclizations via Template Catalysis. Chemistry - A European Journal, 2012, 18, 2591-2599.	3.3	25
59	Openâ€Shell Complexes Containing Metalâ€“Germanium Triple Bonds. Angewandte Chemie - International Edition, 2012, 51, 789-793.	13.8	44
60	EPR and ENDOR Study of the Frozen Ammoniated Electron at Low Alkali-Metal Concentrations. Journal of Physical Chemistry A, 2011, 115, 1939-1945.	2.5	11
61	Monomeric and Dimeric Conformation of the Vinculin Tail Five-Helix Bundle in Solution Studied by EPR Spectroscopy. Biophysical Journal, 2011, 101, 1772-1780.	0.5	12
62	Photoinduced Charge Separation in an Organic Donorâ€“Acceptor Hybrid Molecule. Journal of Physical Chemistry B, 2011, 115, 13526-13533.	2.6	11
63	Zinc-Bacteriochlorophyllide Dimers in de Novo Designed Four-Helix Bundle Proteins. A Model System for Natural Light Energy Harvesting and Dissipation. Journal of the American Chemical Society, 2011, 133, 9526-9535.	13.7	39
64	Structural Features of the Unready Ni-A State of [NiFe] Hydrogenase Revealed by X-Ray Crystallography and EPR Spectroscopy. Applied Magnetic Resonance, 2010, 37, 207-218.	1.2	8
65	Insights into the Chemistry of Transient Pâ€Chlorophosphanyl Complexes. Angewandte Chemie - International Edition, 2010, 49, 6894-6898.	13.8	33
66	Zero-Field Splitting of the Lowest Excited Triplet States of C₆₀ and C₇₀ and Benzene. Journal of Physical Chemistry A, 2010, 114, 10864-10870.	2.5	12
67	Pulsed EPR spectroscopy. Photosynthesis Research, 2009, 102, 367-373.	2.9	5
68	Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Investigation of the Diradical Bis(Î±-iminopyridinato)zinc Complex. Inorganic Chemistry, 2009, 48, 2626-2632.	4.0	29
69	Spin Density Distribution of the Excited Triplet State of Bacteriochlorophylls. Pulsed ENDOR and DFT Studies. Journal of Physical Chemistry B, 2009, 113, 6917-6927.	2.6	20
70	The effect of spin polarization on zero field splitting parameters in paramagnetic Ï€-electron molecules. Journal of Chemical Physics, 2009, 131, 124111.	3.0	13
71	EPR Investigation of [NiFe] Hydrogenases. Biological Magnetic Resonance, 2009, , 441-470.	0.4	7
72	Electronic Structure of a Binuclear Nickel Complex of Relevance to [NiFe] Hydrogenase. Inorganic Chemistry, 2008, 47, 11688-11697.	4.0	19

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73	Entropic Changes Control the Charge Separation Process in Triads Mimicking Photosynthetic Charge Separation. Journal of Physical Chemistry A, 2008, 112, 4215-4223.	2.5	52
74	Electronâ"Electron Double Resonance-Detected NMR to Measure Metal Hyperfine Interactions:â€‰⁶¹Ni in the Niâ"B State of the [NiFe] Hydrogenase ofDesulfovibrio vulgarisMiyazaki F. Journal of the American Chemical Society, 2008, 130, 2402-2403.	13.7	33
75	Triplet States in Photosynthetic Reaction Centers of Rb. sphaeroides. , 2008, , 133-136.		0
76	[NiFe] and [FeFe] Hydrogenases Studied by Advanced Magnetic Resonance Techniques. Chemical Reviews, 2007, 107, 4331-4365.	47.7	458
77	Spin-Density Distribution of the Carotenoid Triplet State in the Peridinin-Chlorophyll-Protein Antenna. A Q-Band Pulse Electron-Nuclear Double Resonance and Density Functional Theory Study. Journal of the American Chemical Society, 2007, 129, 15442-15443.	13.7	31
78	Low-Temperature Pulsed EPR Study at 34 GHz of the Triplet States of the Primary Electron Donor P₈₆₅ and the Carotenoid in Native and Mutant Bacterial Reaction Centers of Rhodobacter sphaeroides. Biochemistry, 2007, 46, 14782-14794.	2.5	18
79	Hydrogen Bonding Affects the [NiFe] Active Site of Desulfovibrio vulgaris Miyazaki F Hydrogenase:â€‰ A Hyperfine Sublevel Correlation Spectroscopy and Density Functional Theory Study. Journal of Physical Chemistry B, 2006, 110, 8142-8150.	2.6	28
80	A single-crystal ENDOR and density functional theory study of the oxidized states of the [NiFe] hydrogenase from Desulfovibrio vulgaris Miyazaki F. Journal of Biological Inorganic Chemistry, 2006, 11, 41-51.	2.6	103
81	An orientation-selected ENDOR and HYSCORE study of the Ni-C active state of Desulfovibrio vulgaris Miyazaki F hydrogenase. Journal of Biological Inorganic Chemistry, 2005, 10, 51-62.	2.6	110
82	What are the structural features of the active site that define binuclear copper proteins function?. Micron, 2004, 35, 143-145.	2.2	4
83	An EPR/ENDOR study of the asymmetric hydrogen bond between the quinone electron acceptor and the protein backbone in Photosystem I. Journal of Molecular Structure, 2004, 700, 233-241.	3.6	20
84	Electronic Structure of the Cysteine Thiyl Radical:â€‰ A DFT and Correlated ab Initio Study. Journal of the American Chemical Society, 2004, 126, 2237-2246.	13.7	47
85	EPR and ENDOR Studies of [NiFe] Hydrogenase: Contributions to Understanding the Mechanism of Biological Hydrogen Conversion. ACS Symposium Series, 2003, , 128-149.	0.5	10
86	Direct Detection of a Hydrogen Ligand in the [NiFe] Center of the Regulatory H2-Sensing Hydrogenase fromRalstoniaeutrophain Its Reduced State by HYSCORE and ENDOR Spectroscopy. Journal of the American Chemical Society, 2003, 125, 13075-13083.	13.7	259
87	Wavelength dependence of the photo-induced conversion of the Niâ€"C to the Niâ€"L redox state in the [NiFe] hydrogenase of Desulfovibrio vulgaris Miyazaki F. Physical Chemistry Chemical Physics, 2003, 5, 5507-5513.	2.8	33
88	Spectroscopic Characterization of the Electronic Changes in the Active Site of Streptomyces antibioticus Tyrosinase upon Binding of Transition State Analogue Inhibitors. Journal of Biological Chemistry, 2003, 278, 7381-7389.	3.4	34
89	EPR study of the dinuclear active copper site of tyrosinase from Streptomyces antibioticus. FEBS Letters, 2000, 474, 228-232.	2.8	40