

List of Publications by Year in descending order

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323
papers

11,345
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23500

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358
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358
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times ranked

5881
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#	ARTICLE	IF	CITATIONS
1	Cholesky Decomposition-Based Multiconfiguration Second-Order Perturbation Theory (CD-CASPT2): Application to the Spin-State Energetics of Co ^{III} (diiminato)(NPh). <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 694-702.	2.3	336
2	Electronic Structure of Corrole Derivatives: Insights from Molecular Structures, Spectroscopy, Electrochemistry, and Quantum Chemical Calculations. <i>Chemical Reviews</i> , 2017, 117, 3798-3881.	23.0	273
3	Electronic Absorption, Resonance Raman, and Electrochemical Studies of Planar and Saddled Copper(III) meso-Triarylcorroles. Highly Substituent-Sensitive Soret Bands as a Distinctive Feature of High-Valent Transition Metal Corroles. <i>Journal of the American Chemical Society</i> , 2002, 124, 8104-8116.	6.6	232
4	Catalytic generation of N ₂ O ₃ by the concerted nitrite reductase and anhydrase activity of hemoglobin. <i>Nature Chemical Biology</i> , 2007, 3, 785-794.	3.9	206
5	High-level ab initio calculations on the energetics of low-lying spin states of biologically relevant transition metal complexes: a first progress report. <i>Current Opinion in Chemical Biology</i> , 2003, 7, 113-124.	2.8	191
6	Electronic Structure of Gallium, Copper, and Nickel Complexes of Corrole. High-Valent Transition Metal Centers versus Noninnocent Ligands. <i>Journal of the American Chemical Society</i> , 2000, 122, 5100-5104.	6.6	183
7	DFT Calculations on the Spin-Crossover Complex Fe(salen)(NO): A Quest for the Best Functional. <i>Journal of Physical Chemistry B</i> , 2007, 111, 12621-12624.	1.2	183
8	Transition metal spin state energetics and noninnocent systems: challenges for DFT in the bioinorganic arena. <i>Journal of Biological Inorganic Chemistry</i> , 2006, 11, 712-724.	1.1	181
9	First-Principles Quantum Chemical Studies of Porphyrins. <i>Accounts of Chemical Research</i> , 1998, 31, 189-198.	7.6	176
10	The Structural Chemistry of Metalloporroles: Combined X-ray Crystallography and Quantum Chemistry Studies Afford Unique Insights. <i>Accounts of Chemical Research</i> , 2012, 45, 1203-1214.	7.6	155
11	A Perspective of One-Pot Pyrrole-Aldehyde Condensations as Versatile Self-Assembly Processes. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 1918-1931.	7.2	152
12	Electron correlation in tetrapyrroles: ab initio calculations on porphyrin and the tautomers of chlorin. <i>The Journal of Physical Chemistry</i> , 1993, 97, 10964-10970.	2.9	142
13	Do Nonplanar Porphyrins Have Red-Shifted Electronic Spectra? A DFT/SCI Study and Reinvestigation of a Recent Proposal. <i>Journal of the American Chemical Society</i> , 2000, 122, 6371-6374.	6.6	141
14	Electrochemical and Electronic Absorption Spectroscopic Studies of Substituent Effects in Iron(IV) and Manganese(IV) Corroles. Do the Compounds Feature High-Valent Metal Centers or Noninnocent Corrole Ligands? Implications for Peroxidase Compound I and II Intermediates. <i>Journal of Physical Chemistry B</i> , 2001, 105, 11406-11413.	1.2	139
15	Do Nonplanar Distortions of Porphyrins Bring about Strongly Red-Shifted Electronic Spectra? Controversy, Consensus, New Developments, and Relevance to Chelatases. <i>Journal of the American Chemical Society</i> , 2002, 124, 8099-8103.	6.6	133
16	Carbonyl Tilting and Bending Potential Energy Surface of Carbon Monoxyhememes. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6363-6367.	2.9	123
17	Substituent Effects on Valence Ionization Potentials of Free Base Porphyrins: A Local Density Functional Study. <i>Journal of the American Chemical Society</i> , 1995, 117, 4691-4699.	6.6	122
18	Electronic effects of peripheral substituents in porphyrins: x-ray photoelectron spectroscopy and ab initio self-consistent field calculations. <i>Journal of the American Chemical Society</i> , 1992, 114, 9990-10000.	6.6	119

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19	\hat{I}^2 -Octafluorocorroles. <i>Journal of the American Chemical Society</i> , 2003, 125, 16300-16309.	6.6	119
20	Electronic Structure of Trigonal-Planar Transition-Metal \hat{I}^2 Imido Complexes: Spin-State Energetics, Spin-Density Profiles, and the Remarkable Performance of the OLYP Functional. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 689-702.	2.3	110
21	Substituent Effects in Porphyrines and Phthalocyanines. <i>Journal of the American Chemical Society</i> , 1994, 116, 1932-1940.	6.6	105
22	Synthesis and Molecular Structure of Gold Triarylcorroles. <i>Inorganic Chemistry</i> , 2011, 50, 12844-12851.	1.9	105
23	Copper Corroles Are Inherently Saddled. <i>Inorganic Chemistry</i> , 2009, 48, 7794-7799.	1.9	103
24	Metalloporphyrin \hat{I}^2 NO Bonding: Building Bridges with Organometallic Chemistry. <i>Accounts of Chemical Research</i> , 2005, 38, 943-954.	7.6	102
25	Characterizing foreground for redshifted 21 \hat{I}^2 cm radiation: 150 \hat{I}^2 MHz Giant Metrewave Radio Telescope observations. <i>Monthly Notices of the Royal Astronomical Society</i> , 2012, 426, 3295-3314.	1.6	100
26	Synthesis, Structure, Electronic Spectroscopy, Photophysics, Electrochemistry, and X-ray Photoelectron Spectroscopy of Highly-Electron-Deficient [5,10,15,20-Tetrakis(perfluoroalkyl)porphinato]zinc(II) Complexes and Their Free Base Derivatives. <i>Journal of the American Chemical Society</i> , 1996, 118, 8344-8354.	6.6	92
27	Ligand Noninnocence in Coinage Metal Corroles: A Silver Knife \hat{I}^2 Edge. <i>Chemistry - A European Journal</i> , 2015, 21, 16839-16847.	1.7	92
28	Electrochemistry of Nickel and Copper \hat{I}^2 -Octahalogeno-meso-tetraarylporphyrins. Evidence for Important Role Played by Saddling-Induced Metal(dx \hat{I}^2 -y \hat{I}^2) \hat{I}^2 Porphyrin(\hat{I}^2 Orbital Interactions. <i>Journal of Physical Chemistry B</i> , 2001, 105, 8120-8124.	1.2	90
29	High-valent transition metal centers and noninnocent ligands in metalloporphyrins and related molecules: a broad overview based on quantum chemical calculations. <i>Journal of Biological Inorganic Chemistry</i> , 2001, 6, 739-752.	1.1	90
30	High-valent transition metal centers versus noninnocent ligands in metalloporroles: insights from electrochemistry and implications for high-valent heme protein intermediates. <i>Journal of Inorganic Biochemistry</i> , 2002, 91, 423-436.	1.5	89
31	Not Innocent: Verdict from Ab Initio Multiconfigurational Second-Order Perturbation Theory on the Electronic Structure of Chloroiron Corrole. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14099-14102.	1.2	87
32	Gold Tris(carboxyphenyl)corroles as Multifunctional Materials: Room Temperature Near-IR Phosphorescence and Applications to Photodynamic Therapy and Dye-Sensitized Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 18935-18942.	4.0	86
33	Copper \hat{I}^2 -Octakis(trifluoromethyl)corroles: New Paradigms for Ligand Substituent Effects in Transition Metal Complexes. <i>Inorganic Chemistry</i> , 2008, 47, 10469-10478.	1.9	82
34	Molecular structures and electron distributions of higher-valent iron and manganese porphyrins: Density functional theory calculations and some preliminary open-shell coupled-cluster results. <i>Journal of Porphyrins and Phthalocyanines</i> , 2001, 05, 345-356.	0.4	80
35	Molecular Structures, Tautomerism, and Carbon Nucleophilicity of Free-Base Inverted Porphyrins and Carbaporphyrins: A Density Functional Theoretical Study. <i>Journal of Physical Chemistry B</i> , 1998, 102, 10459-10467.	1.2	76
36	Nonplanar, Noninnocent, and Chiral: A Strongly Saddled Metalloporrole. <i>Inorganic Chemistry</i> , 2010, 49, 7608-7610.	1.9	76

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37	A First-Principles Quantum Chemical Analysis of the Factors Controlling Ruffling Deformations of Porphyrins: Insights from the Molecular Structures and Potential Energy Surfaces of Silicon, Phosphorus, Germanium, and Arsenic Porphyrins and of a Peroxidase Compound I Model. <i>Journal of the American Chemical Society</i> , 1999, 121, 12154-12160.	6.6	75
38	Gold corroles. <i>Journal of Porphyrins and Phthalocyanines</i> , 2011, 15, 106-110.	0.4	75
39	Robust estimation for independent non-homogeneous observations using density power divergence with applications to linear regression. <i>Electronic Journal of Statistics</i> , 2013, 7, .	0.4	75
40	Electronic Structure and FeNO Conformation of Nonheme Iron ^{II} Thiolate ⁺ NO Complexes: An Experimental and DFT Study. <i>Journal of the American Chemical Society</i> , 2007, 129, 10446-10456.	6.6	71
41	Seven Clues to Ligand Noninnocence: The Metallocorrole Paradigm. <i>Accounts of Chemical Research</i> , 2019, 52, 2003-2014.	7.6	71
42	Calibration of DFT Functionals for the Prediction of ⁵⁷ Fe Mössbauer Spectral Parameters in Iron ^{II} Nitrosyl and Iron ^{II} Sulfur Complexes: Accurate Geometries Prove Essential. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3232-3247.	2.3	70
43	Density Functional Theoretical Study of Oxo(porphyrinato)iron(IV) Complexes, Models of Peroxidase Compounds I and II. <i>The Journal of Physical Chemistry</i> , 1994, 98, 5576-5579.	2.9	67
44	Structure and Stability of cis-Porphyrin. <i>The Journal of Physical Chemistry</i> , 1995, 99, 1073-1075.	2.9	67
45	Determinants of the Vinyl Stretching Frequency in Protoporphyrins. Implications for Cofactor-Protein Interactions in Heme Proteins. <i>Journal of the American Chemical Society</i> , 1995, 117, 10959-10968.	6.6	67
46	Symmetry-Breaking Phenomena in Metalloporphyrin ⁺ Cation Radicals. <i>Journal of the American Chemical Society</i> , 2002, 124, 8122-8130.	6.6	65
47	Ab initio multiconfiguration reference perturbation theory calculations on the energetics of low-energy spin states of iron(III) porphyrins. <i>Journal of Biological Inorganic Chemistry</i> , 2003, 8, 507-511.	1.1	64
48	Oxidative Metalation as a Route to Size-Mismatched Macrocyclic Complexes: Osmium Corroles. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 14411-14414.	7.2	64
49	N-Confused Porphyrins and Singlet Carbenes: Is There a Connection?. <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 1028-1030.	4.4	63
50	Mechanism of Cobalt-Porphyrin ⁺ Catalyzed Aziridination. <i>ACS Catalysis</i> , 2011, 1, 597-600.	5.5	62
51	Platinum corroles. <i>Chemical Communications</i> , 2014, 50, 11093-11096.	2.2	62
52	Metal ⁺ Ligand Misfits: Facile Access to Rhenium ⁺ Oxo Corroles by Oxidative Metalation. <i>Chemistry - A European Journal</i> , 2016, 22, 517-520.	1.7	62
53	Improved foreground removal in GMRT 610 MHz observations towards redshifted 21-cm tomography. <i>Monthly Notices of the Royal Astronomical Society</i> , 2011, 418, 2584-2589.	1.6	61
54	Electronic Distinction between Porphyrins and Tetraazaporphyrins. Insights from X-Ray Photoelectron Spectra of Free Base Porphyrin, Porphyrzine, and Phthalocyanine Ligands. <i>Inorganic Chemistry</i> , 1994, 33, 6057-6060.	1.9	60

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55	Theoretical Studies of Low-Spin Six-Coordinate Iron(III) Porphyrins Relevant to Cytochromes b: Variable Electronic Configurations, Ligand Noninnocence, and Macrocycle Ruffling. <i>Journal of Physical Chemistry B</i> , 1999, 103, 1363-1367.	1.2	60
56	Density Functional Theory Based Configuration Interaction Calculations on the Electronic Spectra of Free-Base Porphyrin, Chlorin, Bacteriochlorin, and cis- and trans-Isobacteriochlorin. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2504-2507.	1.1	60
57	Iron(V) and Iron(VI) Porphyrins: A First Theoretical Exploration. <i>Journal of the American Chemical Society</i> , 2002, 124, 3206-3207.	6.6	60
58	Density Functional Theory Calculations on Mössbauer Parameters of Nonheme Iron Nitrosyls. <i>Inorganic Chemistry</i> , 2009, 48, 9155-9165.	1.9	60
59	A Theoretical Study of Axial Tilting and Equatorial Asymmetry in Metalloporphyrin Nitrosyl Complexes. <i>Journal of the American Chemical Society</i> , 2000, 122, 8101-8102.	6.6	59
60	Electronic Absorption and Resonance Raman Signatures of Hyperporphyrins and Nonplanar Porphyrins. <i>Journal of Physical Chemistry B</i> , 2003, 107, 3613-3623.	1.2	59
61	Spectroelectrochemical and ESR studies of highly substituted copper corroles. <i>Journal of Porphyrins and Phthalocyanines</i> , 2004, 08, 1236-1247.	0.4	58
62	A First TDDFT Study of Metalloporphyrin Electronic Spectra: Copper meso-Triarylcorroles Exhibit Hyper Spectra. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 1857-1864.	1.0	58
63	A thermally stable {FeNO} ₈ complex: properties and biological reactivity of reduced MNO systems. <i>Chemical Science</i> , 2012, 3, 364-369.	3.7	58
64	Theoretical Evidence Favoring True Iron(V)-Oxo Corrole and Corrolazine Intermediates. <i>Inorganic Chemistry</i> , 2006, 45, 4910-4913.	1.9	57
65	Constraining the epoch of reionization with the variance statistic: simulations of the LOFAR case. <i>Monthly Notices of the Royal Astronomical Society</i> , 2014, 443, 1113-1124.	1.6	54
66	A Quantum Chemical Survey of Metalloporphyrin Nitrosyl Linkage Isomers: Insights into the Observation of Multiple FeNO Conformations in a Recent Crystallographic Determination of Nitrophorin 4. <i>Journal of the American Chemical Society</i> , 2001, 123, 5680-5683.	6.6	53
67	Valence ionization potentials and cation radicals of prototype porphyrins. The remarkable performance of nonlocal density functional theory. <i>Theoretical Chemistry Accounts</i> , 1997, 97, 143-149.	0.5	52
68	Undecaphenylcorroles. <i>Inorganic Chemistry</i> , 2012, 51, 9911-9916.	1.9	52
69	Osmium-nitrido corroles as NIR indicators for oxygen sensors and triplet sensitizers for organic upconversion and singlet oxygen generation. <i>Journal of Materials Chemistry C</i> , 2016, 4, 5822-5828.	2.7	52
70	Electronic Structure of High-Spin Iron(IV) Complexes. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 4555-4560.	1.0	51
71	Spin-State Energetics and Spin-Crossover Behavior of Pseudotetrahedral Cobalt(III) Imido Complexes. The Role of the Tripodal Supporting Ligand. <i>Inorganic Chemistry</i> , 2007, 46, 7890-7898.	1.9	51
72	Corrole as a Binucleating Ligand: Preparation, Molecular Structure and Density Functional Theory Study of Diboron Corroles. <i>Journal of the American Chemical Society</i> , 2008, 130, 2888-2889.	6.6	51

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73	The ultraviolet photoelectron spectrum of free-base porphyrin revisited. The performance of local density functional theory. <i>Chemical Physics Letters</i> , 1993, 213, 519-521.	1.2	50
74	Theoretical Comparative Study of Free Base Porphyrin, Chlorin, Bacteriochlorin, and Isobacteriochlorin: Evaluation of the Potential Roles of <i>ab Initio</i> Hartree-Fock and Density Functional Theories in Hydroporphyrin Chemistry. <i>Journal of Physical Chemistry B</i> , 1997, 101, 3290-3297.	1.2	50
75	A Metalloporphyrin with Orthogonal Pyrrole Rings. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 1865-1870.	1.0	50
76	Molecular Structures and Energetics of Porphyrin Isomers: A Comprehensive Local Density Functional Theoretical Study. <i>Chemistry - A European Journal</i> , 1997, 3, 823-833.	1.7	49
77	Cobalt- and Rhodium-Porphyrin-Triphenylphosphine Complexes Revisited: The Question of a Noninnocent Porphyrin. <i>Inorganic Chemistry</i> , 2017, 56, 14788-14800.	1.9	49
78	Robust estimation in generalized linear models: the density power divergence approach. <i>Test</i> , 2016, 25, 269-290.	0.7	47
79	Molecular structure of a gold Au^{I} -octakis(trifluoromethyl)-meso-triarylporphyrin: an 85° difference in saddling dihedral relative to copper. <i>Molecular Physics</i> , 2012, 110, 2439-2444.	0.8	46
80	X-ray Absorption Spectroscopy as a Probe of Ligand Noninnocence in Metalloporphyrins: The Case of Copper Porphyrins. <i>Inorganic Chemistry</i> , 2019, 58, 6722-6730.	1.9	46
81	Theoretical Modeling of Putative Ni(III) F_4O Intermediates of Methylcoenzyme M Reductase. <i>Journal of the American Chemical Society</i> , 2001, 123, 1543-1544.	6.6	44
82	Just how good is DFT?. <i>Journal of Biological Inorganic Chemistry</i> , 2006, 11, 671-673.	1.1	44
83	Broken-Symmetry DFT Spin Densities of Iron Nitrosyls, Including Roussin's Red and Black Salts: Striking Differences between Pure and Hybrid Functionals. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10540-10547.	1.2	44
84	Visibility-based angular power spectrum estimation in low-frequency radio interferometric observations. <i>Monthly Notices of the Royal Astronomical Society</i> , 2014, 445, 4351-4365.	1.6	44
85	GMRT observation towards detecting the post-reionization 21-cm signal. <i>Monthly Notices of the Royal Astronomical Society</i> , 2011, 411, 2426-2438.	1.6	42
86	Resonance Raman spectroscopy and density functional theoretical calculations of manganese porphyrins. <i>Journal of Inorganic Biochemistry</i> , 2002, 88, 113-118.	1.5	41
87	Ligand Noninnocence in Iron Porphyrins: Insights from Optical and X-ray Absorption Spectroscopies and Electrochemical Redox Potentials. <i>Chemistry - A European Journal</i> , 2017, 23, 15098-15106.	1.7	41
88	Iron(IV) Porphyrin Difluoride Does Not Exist: Implications for DFT Calculations on Heme Protein Reaction Pathways. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 597-600.	2.3	40
89	Hemoglobin as a Nitrite Anhydrase: Modeling Methemoglobin-Mediated N_2O_3 Formation. <i>Chemistry - A European Journal</i> , 2011, 17, 6348-6358.	1.7	40
90	Capturing the spin state diversity of iron(III)-aryl porphyrins: OLYP is better than TPSSh. <i>Journal of Inorganic Biochemistry</i> , 2011, 105, 84-91.	1.5	40

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91	Electronic Structure of Cobaltâ€“Corroleâ€“Pyridine Complexes: Noninnocent Five-Coordinate Co(II) Corroleâ€“Radical States. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9589-9598.	1.1	40
92	Deconstructing F430: quantum chemical perspectives of biological methanogenesis. <i>Current Opinion in Chemical Biology</i> , 2001, 5, 744-750.	2.8	39
93	Cryptic noninnocence: FeNO corroles in a new light. <i>Dalton Transactions</i> , 2015, 44, 10146-10151.	1.6	39
94	Direct Porphyrinâˆ“Aryl Orbital Overlaps in Somemeso-Tetraarylporphyrins. <i>Journal of the American Chemical Society</i> , 1998, 120, 6227-6230.	6.6	38
95	Theoretical studies on high-valent manganese porphyrins: Toward a deeper understanding of the energetics, electron distributions, and structural features of the reactive intermediates of enzymatic and synthetic manganese-catalyzed oxidative processes. <i>Israel Journal of Chemistry</i> , 2000, 40, 1-8.	1.0	38
96	Substituent effects on metallocorrole spectra: insights from chromium-oxo and molybdenum-oxo triarylcorroles. <i>Journal of Porphyrins and Phthalocyanines</i> , 2011, 15, 1335-1344.	0.4	38
97	The visibility-based tapered gridded estimator (TGE) for the redshifted 21-cm power spectrum. <i>Monthly Notices of the Royal Astronomical Society</i> , 2016, 463, 4093-4107.	1.6	38
98	A First-Principles Quantum Chemical Study of Coenzyme F430:Â Interplay of Skeletal Stereoisomerism and Conformation in the Stabilization of Nickel(I). <i>Journal of the American Chemical Society</i> , 2000, 122, 6375-6381.	6.6	37
99	Norcorrole and Dihydronorcorrole: A Predictive Quantum Chemical Study. <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 4479-4485.	1.0	37
100	Reductive demetalation of copper corroles: first simple route to free-base \hat{I}^2 -octabromocorroles. <i>Journal of Porphyrins and Phthalocyanines</i> , 2008, 12, 964-967.	0.4	37
101	Low-Energy States of Manganeseâ€“Oxo Corrole and Corrolazine: Multiconfiguration Reference ab Initio Calculations. <i>Inorganic Chemistry</i> , 2012, 51, 4002-4006.	1.9	37
102	Robust estimation for non-homogeneous data and the selection of the optimal tuning parameter: the density power divergence approach. <i>Journal of Applied Statistics</i> , 2015, 42, 2056-2072.	0.6	37
103	Relativity or aromaticity? A first-principles perspective of chemical shifts in osmabenzene and osmapentalene derivatives. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10863-10869.	1.3	37
104	Iron(III)âˆ“Nitro Porphyrins:Â Theoretical Exploration of a Unique Class of Reactive Molecules. <i>Inorganic Chemistry</i> , 2006, 45, 4902-4909.	1.9	36
105	Bonding in Low-Coordinate Environments:â€“ Electronic Structure of Pseudotetrahedral Ironâˆ“Imido Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 448-457.	2.3	36
106	Ab Initio Hartree-Fock and Local Density Functional Calculations on Prototype Halogenated Porphyrins. Do Electrochemically Measured Substituent Effects Reflect Gas-Phase Trends?. <i>The Journal of Physical Chemistry</i> , 1994, 98, 11004-11006.	2.9	34
107	Stable Eight-Coordinate Iron(III/II) Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 2032-2034.	1.9	34
108	Corroles Cannot Ruffle. <i>Inorganic Chemistry</i> , 2011, 50, 3247-3251.	1.9	34

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109	Molecular Structures of Free-Base Corroles: Nonplanarity, Chirality, and Enantiomerization. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3452-3457.	1.1	34
110	Mono- and Diboron Corroles: Factors Controlling Stoichiometry and Hydrolytic Reactivity. <i>Inorganic Chemistry</i> , 2014, 53, 5486-5493.	1.9	33
111	Spin Coupling in Roussin's Red and Black Salts. <i>Chemistry - A European Journal</i> , 2010, 16, 10397-10408.	1.7	32
112	Understanding the Unusually Straight: A Search For MO Insights into Linear {FeNO}7 Units. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8517-8524.	1.2	32
113	Robust Bayes estimation using the density power divergence. <i>Annals of the Institute of Statistical Mathematics</i> , 2016, 68, 413-437.	0.5	32
114	Ligand noninnocence in FeNO corroles: insights from μ^2 -octabromocorrole complexes. <i>Dalton Transactions</i> , 2016, 45, 681-689.	1.6	32
115	A Wald-type test statistic for testing linear hypothesis in logistic regression models based on minimum density power divergence estimator. <i>Electronic Journal of Statistics</i> , 2017, 11, .	0.4	32
116	Electronic Structure of High-Valent Transition Metal Corrolazine Complexes. The Young and Innocent?. <i>Journal of the American Chemical Society</i> , 2002, 124, 8117-8121.	6.6	31
117	Synthesis and Reactivity Studies of a Tin(II) Corrole Complex. <i>Inorganic Chemistry</i> , 2014, 53, 7047-7054.	1.9	31
118	Influence analysis of robust Wald-type tests. <i>Journal of Multivariate Analysis</i> , 2016, 147, 102-126.	0.5	31
119	Toward Modeling H-NOX Domains: A DFT Study of Heme-NO Complexes as Hydrogen Bond Acceptors. <i>Inorganic Chemistry</i> , 2005, 44, 7802-7805.	1.9	30
120	Electronic Structure of Non-Heme High-Valent Oxoiron Complexes with the Unprecedented $[\text{Fe}_2(\mu_4\text{O})_2]^{3+}$ Core. <i>Angewandte Chemie International Edition in English</i> , 1996, 35, 770-772.	4.4	29
121	Models of High-Valent Heme Protein Intermediates: A Quantum Chemical Study of Iron(IV) Porphyrins with Two Univalent Axial σ -Bonding Ligands. <i>Journal of Physical Chemistry B</i> , 2004, 108, 452-456.	1.2	29
122	Synthesis and Molecular Structure of ^{99}Tc Corroles. <i>Chemistry - A European Journal</i> , 2016, 22, 18747-18751.	1.7	29
123	Stepwise Deoxygenation of Nitrite as a Route to Two Families of Ruthenium Corroles: Group 8 Periodic Trends and Relativistic Effects. <i>Inorganic Chemistry</i> , 2017, 56, 5285-5294.	1.9	29
124	The Story of 5d Metallocorroles: From Metal-Ligand Misfits to New Building Blocks for Cancer Phototherapeutics. <i>Accounts of Chemical Research</i> , 2021, 54, 3095-3107.	7.6	29
125	Valence tautomerism and macrocycle ruffling in nickel(III) porphyrins. <i>Journal of Inorganic Biochemistry</i> , 2000, 78, 79-82.	1.5	28
126	Stable Platinum(IV) Corroles: Synthesis, Molecular Structure, and Room-Temperature Near-IR Phosphorescence. <i>ACS Omega</i> , 2018, 3, 9360-9368.	1.6	28

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127	Molecular Structure and Conformation of Dinitrosylheme. <i>Journal of the American Chemical Society</i> , 2003, 125, 4968-4969.	6.6	27
128	Modeling Side-On NO Coordination to Type 2 Copper in Nitrite Reductase: Structures, Energetics, and Bonding. <i>Journal of the American Chemical Society</i> , 2005, 127, 15384-15385.	6.6	27
129	Predictions for the 21 cm-galaxy cross-power spectrum observable with LOFAR and Subaru. <i>Monthly Notices of the Royal Astronomical Society</i> , 2016, 457, 666-675.	1.6	27
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