Christopher Cramer

List of Publications by Year
in descending order

529 papers	61,142 citations	2318 98 h-index	1253 226 g-index
585 all docs	585 docs citations	585 times ranked	42308 citing authors

#	Article	IF	Citations
1	Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. Journal of Physical Chemistry B, 2009, 113, 6378-6396.	1.2	12,475
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Implicit Solvation Models:â€‰ Equilibria, Structure, Spectra, and Dynamics. Chemical Reviews, 1999, 99, 2161-2200.	23.0	2,123
4	Density functional theory for transition metals and transition metal chemistry. Physical Chemistry Chemical Physics, 2009, 11, 10757.	1.3	1,431
5	Consistent van der Waals Radii for the Whole Main Group. Journal of Physical Chemistry A, 2009, 113, 5806-5812.	1.1	1,325
6	Aqueous Solvation Free Energies of Ions and Ionâ^'Water Clusters Based on an Accurate Value for the Absolute Aqueous Solvation Free Energy of the Proton. Journal of Physical Chemistry B, 2006, 110, 16066-16081.	1.2	856
7	Parametrized Models of Aqueous Free Energies of Solvation Based on Pairwise Descreening of Solute Atomic Charges from a Dielectric Medium. The Journal of Physical Chemistry, 1996, 100, 19824-19839.	2.9	828
8	Use of Solution-Phase Vibrational Frequencies in Continuum Models for the Free Energy of Solvation. Journal of Physical Chemistry B, 2011, 115, 14556-14562.	1.2	828
9	Destruction of chemical warfare agents using metalâ€“organic frameworks. Nature Materials, 2015, 14, 512-516.	13.3	790
10	Charge Model 5: An Extension of Hirshfeld Population Analysis for the Accurate Description of Molecular Interactions in Gaseous and Condensed Phases. Journal of Chemical Theory and Computation, 2012, 8, 527-541.	2.3	661
11	Pairwise solute descreening of solute charges from a dielectric medium. Chemical Physics Letters, 1995, 246, 122-129.	1.2	648
12	Mechanically Activated, Catalyst-Free Polyhydroxyurethane Vitrimers. Journal of the American Chemical Society, 2015, 137, 14019-14022.	6.6	593
13	A Universal Approach to Solvation Modeling. Accounts of Chemical Research, 2008, 41, 760-768.	7.6	536
14	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
15	A Hafnium-Based Metalâ€“Organic Framework as an Efficient and Multifunctional Catalyst for Facile CO₂ Fixation and Regioselective and Enantioretentive Epoxide Activation. Journal of the American Chemical Society, 2014, 136, 15861-15864.	6.6	470
16	General parameterized SCF model for free energies of solvation in aqueous solution. Journal of the American Chemical Society, 1991, 113, 8305-8311.	6.6	457
17	Single-Ion Solvation Free Energies and the Normal Hydrogen Electrode Potential in Methanol, Acetonitrile, and Dimethyl Sulfoxide. Journal of Physical Chemistry B, 2007, 111, 408-422.	1.2	452
18	An SCF Solvation Model for the Hydrophobic Effect and Absolute Free Energies of Aqueous Solvation. Science, 1992, 256, 213-217.	6.0	439

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19	The restricted active space followed by second-order perturbation theory method: Theory and application to the study of CuO2 and Cu2O2 systems. Journal of Chemical Physics, 2008, 128, 204109.	1.2	430
20	Self-Consistent Reaction Field Model for Aqueous and Nonaqueous Solutions Based on Accurate Polarized Partial Charges. Journal of Chemical Theory and Computation, 2007, 3, 2011-2033.	2.3	426
21	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
22	Performance of SM6, SM8, and SMD on the SAMPL1 Test Set for the Prediction of Small-Molecule Solvation Free Energies. Journal of Physical Chemistry B, 2009, 113, 4538-4543.	1.2	418
23	SM6:Â A Density Functional Theory Continuum Solvation Model for Calculating Aqueous Solvation Free Energies of Neutrals, Ions, and Soluteâ^'Water Clusters. Journal of Chemical Theory and Computation, 2005, 1, 1133-1152.	2.3	414
24	Computational electrochemistry: prediction of liquid-phase reduction potentials. Physical Chemistry Chemical Physics, 2014, 16, 15068-15106.	1.3	407
25	Adding Explicit Solvent Molecules to Continuum Solvent Calculations for the Calculation of Aqueous Acid Dissociation Constants. Journal of Physical Chemistry A, 2006, 110, 2493-2499.	1.1	405
26	Divergence between Organometallic and Single-Electron-Transfer Mechanisms in Copper(II)-Mediated Aerobic Câ€“H Oxidation. Journal of the American Chemical Society, 2013, 135, 9797-9804.	6.6	396
27	Model for Aqueous Solvation Based on Class IV Atomic Charges and First Solvation Shell Effects. The Journal of Physical Chemistry, 1996, 100, 16385-16398.	2.9	358
28	Mononuclear Cuâ€“O2 Complexes: Geometries, Spectroscopic Properties, Electronic Structures, and Reactivity. Accounts of Chemical Research, 2007, 40, 601-608.	7.6	337
29	AM1-SM2 and PM3-SM3 parameterized SCF solvation models for free energies in aqueous solution. Journal of Computer-Aided Molecular Design, 1992, 6, 629-666.	1.3	316
30	Variable character of O–O and M–O bonding in side-on (Â2) 1:1 metal complexes of O2. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 3635-3640.	3.3	315
31	Class IV charge models: A new semiempirical approach in quantum chemistry. Journal of Computer-Aided Molecular Design, 1995, 9, 87-110.	1.3	309
32	The MIDI! basis set for quantum mechanical calculations of molecular geometries and partial charges. Theoretica Chimica Acta, 1996, 93, 281-301.	0.9	298
33	Methane Oxidation to Methanol Catalyzed by Cu-Oxo Clusters Stabilized in NU-1000 Metalâ€“Organic Framework. Journal of the American Chemical Society, 2017, 139, 10294-10301.	6.6	282
34	Sintering-Resistant Single-Site Nickel Catalyst Supported by Metalâ€“Organic Framework. Journal of the American Chemical Society, 2016, 138, 1977-1982.	6.6	273
35	New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. Journal of Physical Chemistry A, 1998, 102, 1820-1831.	1.1	259
36	Structural, Spectroscopic, and Theoretical Characterization of Bis(Î¼-oxo)dicopper Complexes, Novel Intermediates in Copper-Mediated Dioxygen Activation. Journal of the American Chemical Society, 1996, 118, 11555-11574.	6.6	255

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37	The Ruâ”Hbpp Water Oxidation Catalyst. Journal of the American Chemical Society, 2009, 131, 15176-15187.	6.6	253
38	Structures of Nonheme Oxoiron(IV) Complexes from X-ray Crystallography, NMR Spectroscopy, and DFT Calculations. Angewandte Chemie - International Edition, 2005, 44, 3690-3694.	7.2	247
39	Quantum-Chemical Characterization of the Properties and Reactivities of Metalâ€“Organic Frameworks. Chemical Reviews, 2015, 115, 6051-6111.	23.0	241
40	Equilibrium Mercury Isotope Fractionation between Dissolved Hg(II) Species and Thiol-Bound Hg. Environmental Science & Technology, 2010, 44, 4191-4197.	4.6	230
41	A Carbon-Free Sandwich Complex [(P5)2Ti]2-. Science, 2002, 295, 832-834.	6.0	229
42	Defining the Proton Topology of the Zr₆-Based Metalâ€“Organic Framework NU-1000. Journal of Physical Chemistry Letters, 2014, 5, 3716-3723.	2.1	228
43	Metalâ€“Organic Framework Nodes as Nearly Ideal Supports for Molecular Catalysts: NU-1000- and UiO-66-Supported Iridium Complexes. Journal of the American Chemical Society, 2015, 137, 7391-7396.	6.6	228
44	Quantum Mechanical Continuum Solvation Models for Ionic Liquids. Journal of Physical Chemistry B, 2012, 116, 9122-9129.	1.2	225
45	Metalâ€“Organic Framework Supported Cobalt Catalysts for the Oxidative Dehydrogenation of Propane at Low Temperature. ACS Central Science, 2017, 3, 31-38.	5.3	222
46	An Exceptionally Stable Metalâ€“Organic Framework Supported Molybdenum(VI) Oxide Catalyst for Cyclohexene Epoxidation. Journal of the American Chemical Society, 2016, 138, 14720-14726.	6.6	211
47	Computation of equilibrium oxidation and reduction potentials for reversible and dissociative electron-transfer reactions in solution. Theoretical Chemistry Accounts, 2004, 112, 217.	0.5	206
48	Practical computation of electronic excitation in solution: vertical excitation model. Chemical Science, 2011, 2, 2143.	3.7	202
49	Extension of the platform of applicability of the SM5.42R universal solvation model. Theoretical Chemistry Accounts, 1999, 103, 9-63.	0.5	197
50	Computational electrochemistry: aqueous one-electron oxidation potentials for substituted anilines. Physical Chemistry Chemical Physics, 2000, 2, 1231-1239.	1.3	194
51	Rapid Câ€“H Bond Activation by a Monocopper(III)â€“Hydroxide Complex. Journal of the American Chemical Society, 2011, 133, 17602-17605.	6.6	191
52	Quantum chemical conformational analysis of glucose in aqueous solution. Journal of the American Chemical Society, 1993, 115, 5745-5753.	6.6	185
53	Bergman, Aza-Bergman, and Protonated Aza-Bergman Cyclizations and Intermediate 2,5-Arynes:Â Chemistry and Challenges to Computation. Journal of the American Chemical Society, 1998, 120, 6261-6269.	6.6	185
54	Relative stability of alternative chair forms and hydroxymethyl conformations of Î²-d-glucopyranose. Carbohydrate Research, 1995, 276, 219-251.	1.1	184

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55	Dioxygen Activation at a Single Copper Site:Â Structure, Bonding, and Mechanism of Formation of 1:1 Cuâ"O2Adducts. Journal of the American Chemical Society, 2004, 126, 16896-16911.	6.6	184
56	Snapshots of Dioxygen Activation by Copper:â€‰ The Structure of a 1:1 Cu/O2 Adduct and Its Use in Syntheses of Asymmetric Bis(Î¼-oxo) Complexes. Journal of the American Chemical Society, 2002, 124, 10660-10661.	6.6	181
57	Theoretical Models on the Cu2O2 Torture Track:â€‰ Mechanistic Implications for Oxytyrosinase and Small-Molecule Analogues. Journal of Physical Chemistry A, 2006, 110, 1991-2004.	1.1	179
58	Synthesis and structural and spectroscopic characterization of mononuclear copper nitrosyl complexes: models for nitric oxide adducts of copper proteins and copper-exchanged zeolites. Journal of the American Chemical Society, 1993, 115, 11285-11298.	6.6	172
59	Generalized Born Solvation Model SM12. Journal of Chemical Theory and Computation, 2013, 9, 609-620.	2.3	170
60	Quantum Chemical Conformational Analysis of 1,2-Ethanediol: Correlation and Solvation Effects on the Tendency To Form Internal Hydrogen Bonds in the Gas Phase and in Aqueous Solution. Journal of the American Chemical Society, 1994, 116, 3892-3900.	6.6	168
61	PM3-SM3: A general parameterization for including aqueous solvation effects in the PM3 molecular orbital model. Journal of Computational Chemistry, 1992, 13, 1089-1097.	1.5	166
62	Universal Quantum Mechanical Model for Solvation Free Energies Based on Gas-Phase Geometries. Journal of Physical Chemistry B, 1998, 102, 3257-3271.	1.2	166
63	Combining Wave Function Methods with Density Functional Theory for Excited States. Chemical Reviews, 2018, 118, 7249-7292.	23.0	166
64	A reinvestigation of singlet benzyne thermochemistry predicted by CASPT2, coupled-cluster and density functional calculations. Chemical Physics Letters, 1997, 277, 311-320.	1.2	165
65	A porous, electrically conductive hexa-zirconium(<scp>iv</scp>) metalâ€"organic framework. Chemical Science, 2018, 9, 4477-4482.	3.7	158
66	Design of a Metalâ€"Organic Framework with Enhanced Back Bonding for Separation of N₂ and CH₄. Journal of the American Chemical Society, 2014, 136, 698-704.	6.6	157
67	Tuning the Surface Chemistry of Metal Organic Framework Nodes: Proton Topology of the Metal-Oxide-Like Zr₆ Nodes of UiO-66 and NU-1000. Journal of the American Chemical Society, 2016, 138, 15189-15196.	6.6	155
68	Hybrid Density Functional Methods Empirically Optimized for the Computation of 13C and 1H Chemical Shifts in Chloroform Solution. Journal of Chemical Theory and Computation, 2006, 2, 1085-1092.	2.3	151
69	Molecular Modeling of Environmentally Important Processes: Reduction Potentials. Journal of Chemical Education, 2004, 81, 596.	1.1	150
70	Tuning Zr₆ Metalâ€"Organic Framework (MOF) Nodes as Catalyst Supports: Site Densities and Electron-Donor Properties Influence Molecular Iridium Complexes as Ethylene Conversion Catalysts. ACS Catalysis, 2016, 6, 235-247.	5.5	150
71	Structure and Dynamics of Zr₆O₈ Metalâ€"Organic Framework Node Surfaces Probed with Ethanol Dehydration as a Catalytic Test Reaction. Journal of the American Chemical Society, 2018, 140, 3751-3759.	6.6	150
72	Computational Design of Functionalized Metalâ€"Organic Framework Nodes for Catalysis. ACS Central Science, 2018, 4, 5-19.	5.3	148

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73	A Hafnium-Based Metalâ€“Organic Framework as a Nature-Inspired Tandem Reaction Catalyst. Journal of the American Chemical Society, 2015, 137, 13624-13631.	6.6	137
74	Selective Methane Oxidation to Methanol on Cu-Oxo Dimers Stabilized by Zirconia Nodes of an NU-1000 Metalâ€“Organic Framework. Journal of the American Chemical Society, 2019, 141, 9292-9304.	6.6	131
75	A New Intermediate in Copper Dioxygen Chemistry: Breaking the O-O Bond To Form a {Cu2(.mu.-O)2}2+ Core. Journal of the American Chemical Society, 1995, 117, 8865-8866.	6.6	126
76	Computational Electrochemistry: The Aqueous Ru3+ | Ru2+Reduction Potential. Journal of Physical Chemistry C, 2007, 111, 5783-5799.	1.5	126
77	Mechanistic Insights into the Alternating Copolymerization of Epoxides and Cyclic Anhydrides Using a (Salph)AlCl and Iminium Salt Catalytic System. Journal of the American Chemical Society, 2017, 139, 15222-15231.	6.6	125
78	Ab Initio Characterization of Phenylnitrenium and Phenylcarbene: Remarkably Different Properties for Isoelectronic Species. Journal of the American Chemical Society, 1994, 116, 9787-9788.	6.6	123
79	Factors controlling relative stability of anomers and hydroxymethyl conformers of glucopyranose. Journal of Computational Chemistry, 1998, 19, 1111-1129.	1.5	122
80	Quantum chemical characterization of the mechanism of an iron-based water oxidation catalyst. Chemical Science, 2012, 3, 1293.	3.7	122
81	Presence versus Proximity: The Role of Pendant Amines in the Catalytic Hydrolysis of a Nerve Agent Simulant. Angewandte Chemie - International Edition, 2018, 57, 1949-1953.	7.2	121
82	Density functional solvation model based on CM2 atomic charges. Journal of Chemical Physics, 1998, 109, 9117-9133.	1.2	120
83	Universal Solvation Model Based on the Generalized Born Approximation with Asymmetric Descreening. Journal of Chemical Theory and Computation, 2009, 5, 2447-2464.	2.3	120
84	Improved methods for semiempirical solvation models. Journal of Computational Chemistry, 1995, 16, 422-440.	1.5	119
85	Targeted Single-Site MOF Node Modification: Trivalent Metal Loading via Atomic Layer Deposition. Chemistry of Materials, 2015, 27, 4772-4778.	3.2	116
86	Isotopic Probing of Molecular Oxygen Activation at Copper(I) Sites. Journal of the American Chemical Society, 2007, 129, 14697-14709.	6.6	114
87	Self-Sorting Chiral Subcomponent Rearrangement During Crystallization. Journal of the American Chemical Society, 2007, 129, 8774-8780.	6.6	114
88	Trimethylenemethane. Comparison of Multiconfiguration Self-Consistent Field and Density Functional Methods for a Non-KekulÃ© Hydrocarbon. The Journal of Physical Chemistry, 1996, 100, 9664-9670.	2.9	113
89	On the Nature of Actinideâ€“ and Lanthanideâ€“Metal Bonds in Heterobimetallic Compounds. Chemistry - A European Journal, 2011, 17, 8424-8433.	1.7	112
90	Site-Selective Copper-Catalyzed Azidation of Benzylic Câ€“H Bonds. Journal of the American Chemical Society, 2020, 142, 11388-11393.	6.6	112

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91	Effects of Thioether Substituents on the O2Reactivity of Î²-Diketiminateâ^'Cu(I) Complexes:Â Probing the Role of the Methionine Ligand in Copper Monooxygenases. Journal of the American Chemical Society, 2006, 128, 3445-3458.	6.6	111
92	Structural Transitions of the Metal-Oxide Nodes within Metalâ€"Organic Frameworks: On the Local Structures of NU-1000 and UiO-66. Journal of the American Chemical Society, 2016, 138, 4178-4185.	6.6	108
93	Copper-catalysed benzylic Câ€"H coupling with alcohols via radical relay enabled by redox buffering. Nature Catalysis, 2020, 3, 358-367.	16.1	108
94	Parameterization of charge model 3 for AM1, PM3, BLYP, and B3LYP. Journal of Computational Chemistry, 2003, 24, 1291-1304.	1.5	107
95	The cisâ€[Ru^{II}(bpy)₂(H₂O)₂]²⁺ Waterâ€Oxidation Catalyst Revisited. Angewandte Chemie - International Edition, 2010, 49, 7745-7747.	7.2	107
96	Direct Dynamics for Free Radical Kinetics in Solution:Â Solvent Effect on the Rate Constant for the Reaction of Methanol with Atomic Hydrogen. Journal of Physical Chemistry A, 1999, 103, 4893-4909.	1.1	103
97	Single-Site Organozirconium Catalyst Embedded in a Metalâ€"Organic Framework. Journal of the American Chemical Society, 2015, 137, 15680-15683.	6.6	103
98	New Universal Solvation Model and Comparison of the Accuracy of the SM5.42R, SM5.43R, C-PCM, D-PCM, and IEF-PCM Continuum Solvation Models for Aqueous and Organic Solvation Free Energies and for Vapor Pressures. Journal of Physical Chemistry A, 2004, 108, 6532-6542.	1.1	100
99	An Anionic, Tetragonal Copper(II) Superoxide Complex. Journal of the American Chemical Society, 2010, 132, 15869-15871.	6.6	100
100	Perturbing the Copper(III)â€"Hydroxide Unit through Ligand Structural Variation. Journal of the American Chemical Society, 2016, 138, 356-368.	6.6	100
101	Assessment of electronic structure methods for the determination of the ground spin states of Fe(<scp>ii</scp>), Fe(<scp>iii</scp>) and Fe(<scp>iv</scp>) complexes. Physical Chemistry Chemical Physics, 2017, 19, 13049-13069.	1.3	100
102	General Semiempirical Quantum Mechanical Solvation Model for Nonpolar Solvation Free Energies. n-Hexadecane. Journal of the American Chemical Society, 1995, 117, 1057-1068.	6.6	99
103	Ab Initio Characterization of the Isomerism between the Î¼-Î·2:Î·2-Peroxo- and Bis(Î¼-oxo)dicopper Cores. Journal of the American Chemical Society, 1996, 118, 11283-11287.	6.6	99
104	A universal model for the quantum mechanical calculation of free energies of solvation in non-aqueous solvents. Theoretical Chemistry Accounts, 1997, 98, 85-109.	0.5	99
105	Defining the Macromolecules of Tomorrow through Synergistic Sustainable Polymer Research. Chemical Reviews, 2022, 122, 6322-6373.	23.0	99
106	Molecular orbital theory calculations of aqueous solvation effects on chemical equilibria. Journal of the American Chemical Society, 1991, 113, 8552-8554.	6.6	98
107	Pyrene-Edged Fe^{II}₄L₆ Cages Adaptively Reconfigure During Guest Binding. Journal of the American Chemical Society, 2014, 136, 15615-15624.	6.6	98
108	Comparison of Real-Time and Linear-Response Time-Dependent Density Functional Theories for Molecular Chromophores Ranging from Sparse to High Densities of States. Journal of Chemical Theory and Computation, 2015, 11, 1102-1109.	2.3	98

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109	A Universal Organic Solvation Model. Journal of Organic Chemistry, 1996, 61, 8720-8721.	1.7	97
110	Predicting aqueous solubilities from aqueous free energies of solvation and experimental or calculated vapor pressures of pure substances. Journal of Chemical Physics, 2003, 119, 1661-1670.	1.2	97
111	Tuning the Properties of Zr₆O₈ Nodes in the Metal Organic Framework UiO-66 by Selection of Node-Bound Ligands and Linkers. Chemistry of Materials, 2019, 31, 1655-1663.	3.2	97
112	Full valence complete active space SCF, multireference CI, and density functional calculations of 1A1â€”3B1 singletâ€”triplet gaps for the valence-isoelectronic series BH-2, CH2, NH+2, AlH-2, SiH2, PH+2, GaH-2, GeH2, and AsH+2. Chemical Physics Letters, 1994, 218, 387-394.	1.2	96
113	Experimental and quantum chemical characterization of the water oxidation cycle catalysed by [RuII(damp)(bpy)(H2O)]2+. Chemical Science, 2012, 3, 2576.	3.7	96
114	Exo-anomeric effects on energies and geometries of different conformations of glucose and related systems in the gas phase and aqueous solution. Carbohydrate Research, 1997, 298, 1-14.	1.1	94
115	Prediction of SAMPL2 aqueous solvation free energies and tautomeric ratios using the SM8, SM8AD, and SMD solvation models. Journal of Computer-Aided Molecular Design, 2010, 24, 317-333.	1.3	94
116	Beyond the Active Site: Tuning the Activity and Selectivity of a Metalâ€“Organic Framework-Supported Ni Catalyst for Ethylene Dimerization. Journal of the American Chemical Society, 2018, 140, 11174-11178.	6.6	94
117	Universal reaction field model based on ab initio Hartreeâ€“Fock theory. Chemical Physics Letters, 1998, 288, 293-298.	1.2	93
118	Copper(I)â^'Î±-Ketocarboxylate Complexes:â€‰ Characterization and O₂ Reactions That Yield Copperâ^'Oxygen Intermediates Capable of Hydroxylating Arenes. Journal of the American Chemical Society, 2007, 129, 14190-14192.	6.6	93
119	Resonance Raman Spectroscopy as a Probe of the Bis(Î¼-oxo)dicopper Core. Journal of the American Chemical Society, 2000, 122, 792-802.	6.6	91
120	Theoretical Investigation of Enolborane Addition to Î±-Heteroatom-Substituted Aldehydes. Relevance of the Cornforth and Polar Felkinâ^'Anh Models for Asymmetric Induction. Journal of the American Chemical Society, 2006, 128, 2920-2930.	6.6	91
121	Experimental and Theoretical Investigations into the Unusual Regioselectivity of 4,5-, 5,6-, and 6,7-Indole Aryne Cycloadditions. Organic Letters, 2010, 12, 96-99.	2.4	91
122	Density functional calculations of the influence of substitution on singletâ€“triplet gaps in carbenes and vinylidenes. Journal of Physical Organic Chemistry, 1997, 10, 755-767.	0.9	90
123	Crystal Engineering Using the Unconventional Hydrogen Bond. Synthesis, Structure, and Theoretical Investigation of Cyclotrigallazane. Journal of the American Chemical Society, 1998, 120, 521-531.	6.6	90
124	Characterization of a 1:1 Cuâ^'O2Adduct Supported by an Anilido Imine Ligand. Inorganic Chemistry, 2005, 44, 6989-6997.	1.9	90
125	Quantum chemical studies of molecules incorporating a Cu2O22+ core. Coordination Chemistry Reviews, 2009, 253, 723-753.	9.5	90
126	Free Radical Mechanisms for the Treatment of Methyl tert-Butyl Ether (MTBE) via Advanced Oxidation/Reductive Processes in Aqueous Solutions. Chemical Reviews, 2009, 109, 1302-1345.	23.0	90

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127	Anomeric and reverse anomeric effects in the gas phase and aqueous solution. Journal of Organic Chemistry, 1992, 57, 7034-7043.	1.7	89
128	Use of calculated quantum chemical properties as surrogates for solvatochromic parameters in structure-activity relationships. Accounts of Chemical Research, 1993, 26, 599-605.	7.6	89
129	Density functional theory: excited states and spin annihilation. Chemical Physics Letters, 1995, 245, 165-170.	1.2	89
130	What causes aqueous acceleration of the Claisen rearrangement?. Journal of the American Chemical Society, 1992, 114, 8794-8799.	6.6	88
131	Reductive Dechlorination of Hexachloroethane in the Environment: Mechanistic Studies via Computational Electrochemistry. Journal of the American Chemical Society, 2001, 123, 2025-2031.	6.6	88
132	Sinterâ€Resistant Platinum Catalyst Supported by Metalâ€“Organic Framework. Angewandte Chemie - International Edition, 2018, 57, 909-913.	7.2	88
133	Electrostatic component of solvation: Comparison of SCRF continuum models. Journal of Computational Chemistry, 2003, 24, 284-297.	1.5	86
134	Copper-zirconia interfaces in UiO-66 enable selective catalytic hydrogenation of CO2 to methanol. Nature Communications, 2020, 11, 5849.	5.8	86
135	A Semiempirical Quantum Mechanical Solvation Model for Solvation Free Energies in All Alkane Solvents. The Journal of Physical Chemistry, 1995, 99, 7137-7146.	2.9	85
136	Ab Initio Characterization of [H3NÂ·BH3]2, [H3NÂ·AlH3]2, and [H3NÂ·GaH3]2. Inorganic Chemistry, 1997, 36, 5358-5362.	1.9	85
137	Electronic Interactions in Aryne Biradicals. Ab Initio Calculations of the Structures, Thermochemical Properties, and Singletâ^'Triplet Splittings of the Didehydronaphthalenes. Journal of Physical Chemistry A, 1998, 102, 9072-9081.	1.1	82
138	meta andpara substitution effects on the electronic state energies and ring-expansion reactivities of phenylnitrenes. International Journal of Quantum Chemistry, 2001, 85, 492-508.	1.0	82
139	A Selfâ€Improved Waterâ€Oxidation Catalyst: Is One Site Really Enough?. Angewandte Chemie - International Edition, 2014, 53, 205-209.	7.2	82
140	Quantum Chemical Characterization of Structural Single Fe(II) Sites in MIL-Type Metalâ€“Organic Frameworks for the Oxidation of Methane to Methanol and Ethane to Ethanol. ACS Catalysis, 2019, 9, 2870-2879.	5.5	82
141	Factors Controlling Regioselectivity in the Reduction of Polynitroaromatics in Aqueous Solution. Environmental Science & Technology, 1996, 30, 3028-3038.	4.6	80
142	Theoretical Characterization of End-On and Side-On Peroxide Coordination in Ligated Cu2O2 Models. Journal of Physical Chemistry A, 2006, 110, 11557-11568.	1.1	80
143	From Transition Metals to Lanthanides to Actinides: Metal-Mediated Tuning of Electronic Properties of Isostructural Metalâ€“Organic Frameworks. Inorganic Chemistry, 2018, 57, 13246-13251.	1.9	80
144	Structure, Dynamics, and Reactivity for Light Alkane Oxidation of Fe(II) Sites Situated in the Nodes of a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2019, 141, 18142-18151.	6.6	80

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145	Correlation and solvation effects on heterocyclic equilibria in aqueous solution. Journal of the American Chemical Society, 1993, 115, 8810-8817.	6.6	79
146	Understanding and Estimating Membrane/Water Partition Coefficients:Â Approaches To Derive Quantitative Structure Property Relationships. Chemical Research in Toxicology, 1998, 11, 847-854.	1.7	79
147	Reductive Dechlorination of 1,1,2,2-Tetrachloroethane. Environmental Science & Technology, 2002, 36, 3536-3541.	4.6	79
148	Thermochemistry of Simple Enols and Enol Cation Radicals Revisited. A G2(MP2) ab Initio Study. Journal of the American Chemical Society, 1995, 117, 12243-12253.	6.6	78
149	Two-response-time model based on CM2/INDO/S2 electrostatic potentials for the dielectric polarization component of solvatochromic shifts on vertical excitation energies. International Journal of Quantum Chemistry, 2000, 77, 264-280.	1.0	78
150	HF/6-31G* energy surfaces for disaccharide analogs. Journal of Computational Chemistry, 2001, 22, 65-78.	1.5	78
151	Computationally Guided Discovery of a Catalytic Cobalt-Decorated Metalâ€“Organic Framework for Ethylene Dimerization. Journal of Physical Chemistry C, 2016, 120, 23576-23583.	1.5	78
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