H Bernhard Schlegel

List of Publications by Year
in descending order

222 papers	34,171 citations	22099 59 h-index	3563 181 g-index
227 all docs	227 docs citations	227 times ranked	18259 citing authors

#	Article	IF	Citations
1	An improved algorithm for reaction path following. Journal of Chemical Physics, 1989, 90, 2154-2161.	1.2	5,658
2	Reaction path following in mass-weighted internal coordinates. The Journal of Physical Chemistry, 1990, 94, 5523-5527.	2.9	5,548
3	Optimization of equilibrium geometries and transition structures. Journal of Computational Chemistry, 1982, 3, 214-218.	1.5	3,470
4	Using redundant internal coordinates to optimize equilibrium geometries and transition states. Journal of Computational Chemistry, 1996, 17, 49-56.	1.5	2,592
5	Combining Synchronous Transit and Quasiâ€Newton Methods to Find Transition States. Israel Journal of Chemistry, 1993, 33, 449-454.	1.0	1,830
6	Accurate reaction paths using a Hessian based predictorâ€“corrector integrator. Journal of Chemical Physics, 2004, 120, 9918-9924.	1.2	796
7	Improved algorithms for reaction path following: Higherâ€order implicit algorithms. Journal of Chemical Physics, 1991, 95, 5853-5860.	1.2	692
8	Potential energy curves using unrestricted Mo/llerâ€“Plesset perturbation theory with spin annihilation. Journal of Chemical Physics, 1986, 84, 4530-4534.	1.2	663
9	A direct method for the location of the lowest energy point on a potential surface crossing. Chemical Physics Letters, 1994, 223, 269-274.	1.2	639
10	Geometry optimization with QM/MM, ONIOM, and other combined methods. I. Microiterations and constraints. Journal of Computational Chemistry, 2003, 24, 760-769.	1.5	560
11	Ab initiomolecular dynamics: Propagating the density matrix with Gaussian orbitals. Journal of Chemical Physics, 2001, 114, 9758-9763.	1.2	522
12	Identification and treatment of internal rotation in normal mode vibrational analysis. Journal of Chemical Physics, 1998, 108, 2314-2325.	1.2	430
13	Harmonic frequency scaling factors for Hartree-Fock, S-VWN, B-LYP, B3-LYP, B3-PW91 and MP2 with the Sadlej pVTZ electric property basis set. Theoretical Chemistry Accounts, 2001, 105, 413-421.	0.5	411
14	Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals. II. Generalizations based on mass-weighting, idempotency, energy conservation and choice of initial conditions. Journal of Chemical Physics, 2001, 115, 10291.	1.2	375
15	Exploring potential energy surfaces for chemical reactions: An overview of some practical methods. Journal of Computational Chemistry, 2003, 24, 1514-1527.	1.5	311
16	A combined method for determining reaction paths, minima, and transition state geometries. Journal of Chemical Physics, 1997, 107, 375-384.	1.2	284
17	Ab initio classical trajectories on the Bornâ€“Oppenheimer surface: Hessian-based integrators using fifth-order polynomial and rational function fits. Journal of Chemical Physics, 1999, 111, 3800-3805.	1.2	276
18	Finding minima, transition states, and following reaction pathways on ab initio potential energy surfaces. , 2005, , 195-249.		266

#	Article	IF	Citations
19	Geometry optimization. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 790-809.	6.2	250
20	An efficient algorithm for calculating ab initio energy gradients using s, p Cartesian Gaussians. Journal of Chemical Physics, 1982, 77, 3676-3681.	1.2	239
21	Ascorbic acid: The chemistry underlying its antioxidant properties. Free Radical Biology and Medicine, 2020, 159, 37-43.	1.3	224
22	Molecular Orbital Study of the First Excited State of the OLED Material Tris(8-hydroxyquinoline)aluminum(III). Chemistry of Materials, 2001, 13, 2632-2640.	3.2	221
23	Some reasons not to use spin projected density functional theory. Journal of Chemical Physics, 1996, 105, 6574-6577.	1.2	188
24	Estimating the hessian for gradient-type geometry optimizations. Theoretica Chimica Acta, 1984, 66, 333-340.	0.9	181
25	Calculation of pK_a Values of Nucleobases and the Guanine Oxidation Products Guanidinohydantoin and Spiroiminodihydantoin using Density Functional Theory and a Polarizable Continuum Model. Journal of Physical Chemistry B, 2008, 112, 16860-16873.	1.2	179
26	Methods for optimizing large molecules. II. Quadratic search. Journal of Chemical Physics, 1999, 111, 10806-10814.	1.2	169
27	AMBER Force Field Parameters for the Naturally Occurring Modified Nucleosides in RNA. Journal of Chemical Theory and Computation, 2007, 3, 1464-1475.	2.3	168
28	Comparison of the performance of local, gradient-corrected, and hybrid density functional models in predicting infrared intensities. Journal of Chemical Physics, 1998, 109, 10587-10593.	1.2	163
29	GEOMETRY OPTIMIZATION ON POTENTIAL ENERGY SURFACES. Advanced Series in Physical Chemistry, 1995, , 459-500.	1.5	162
30	Evaluation ofS2for correlated wave functions and spin projection of unrestricted Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1994, 101, 5957-5968.	1.2	146
31	Density Functional Theory Calculation of pK_aâ€™s of Thiols in Aqueous Solution Using Explicit Water Molecules and the Polarizable Continuum Model. Journal of Physical Chemistry A, 2016, 120, 5726-5735.	1.1	146
32	Comparison study of the prediction of Raman intensities using electronic structure methods. Journal of Chemical Physics, 1999, 111, 8819-8824.	1.2	137
33	Ab initio classical trajectories on the Bornâ€“Oppenheimer surface: Updating methods for Hessian-based integrators. Journal of Chemical Physics, 1999, 111, 8773-8777.	1.2	134
34	Transformation between Cartesian and pure spherical harmonic Gaussians. International Journal of Quantum Chemistry, 1995, 54, 83-87.	1.0	133
35	Hybrid Ab-Initio/Empirical Molecular Dynamics:â€‰Combining the ONIOM Scheme with the Atom-Centered Density Matrix Propagation (ADMP) Approach. Journal of Physical Chemistry B, 2004, 108, 4210-4220.	1.2	131
36	Ab initio molecular dynamics studies of the photodissociation of formaldehyde, H2COâ†’H2+CO: Direct classical trajectory calculations by MP2 and density functional theory. Journal of Chemical Physics, 2000, 113, 10062-10067.	1.2	127

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37	Effects of the Protein Environment on the Structure and Energetics of Active Sites of Metalloenzymes. ONIOM Study of Methane Monooxygenase and Ribonucleotide Reductase. Journal of the American Chemical Society, 2002, 124, 192-193.	6.6	124
38	Optimization of Equilibrium Geometries and Transition Structures. Advances in Chemical Physics, 2007, , 249-286.	0.3	124
39	Ab initio calculations on the barrier height for the hydrogen addition to ethylene and formaldehyde. The importance of spin projection. International Journal of Quantum Chemistry, 1986, 29, 1001-1015.	1.0	120
40	Methods for optimizing large molecules. Part III. An improved algorithm for geometry optimization using direct inversion in the iterative subspace (GDIIS). Physical Chemistry Chemical Physics, 2002, 4, 11-15.	1.3	114
41	Surprising Titanium Complexes Bearing Î·2-Pyrazolato Ligands:â€‰ Synthesis, Structure, and Molecular Orbital Studies. Journal of the American Chemical Society, 1997, 119, 3387-3388.	6.6	112
42	Calculations of pK_aâ€™s and Redox Potentials of Nucleobases with Explicit Waters and Polarizable Continuum Solvation. Journal of Physical Chemistry A, 2015, 119, 5134-5144.	1.1	111
43	A theoretical study of ascorbic acid oxidation andHOOË™/O₂Ë™^{â¯}radical scavenging. Organic and Biomolecular Chemistry, 2017, 15, 4417-4431.	1.5	108
44	Combined Experimental and Computational Investigation of the Mechanism of Nickel-Catalyzed Three-Component Addition Processes. Organometallics, 2004, 23, 4636-4646.	1.1	106
45	NO Affinities ofS-Nitrosothiols:Â A Direct Experimental and Computational Investigation of RSâ¯NO Bond Dissociation Energies. Journal of the American Chemical Society, 2001, 123, 2903-2904.	6.6	103
46	Electronic optical response of molecules in intense fields: Comparison of TD-HF, TD-CIS, and TD-CIS(D) approaches. Journal of Chemical Physics, 2007, 126, 244110.	1.2	96
47	Ruthenium Complexes Bearing Î·5-Pyrazolato Ligands. Journal of the American Chemical Society, 1999, 121, 4536-4537.	6.6	95
48	Sequential nonadiabatic excitation of large molecules and ions driven by strong laser fields. Physical Review A, 2004, 69, .	1.0	92
49	Improved method for calculating projected frequencies along a reaction path. Journal of Chemical Physics, 1997, 107, 9413-9417.	1.2	91
50	Strong field ionization rates simulated with time-dependent configuration interaction and an absorbing potential. Journal of Chemical Physics, 2014, 140, 174113.	1.2	89
51	An Exploration of Mechanisms for the Transformation of 8-Oxoguanine to Guanidinohydantoin and Spiroiminodihydantoin by Density Functional Theory. Journal of the American Chemical Society, 2008, 130, 5245-5256.	6.6	85
52	A nonorthogonal CI treatment of symmetry breaking in sigma formyloxyl radical. Journal of Chemical Physics, 1998, 108, 7560-7567.	1.2	79
53	Improved pK_a Prediction of Substituted Alcohols, Phenols, and Hydroperoxides in Aqueous Medium Using Density Functional Theory and a Cluster-Continuum Solvation Model. Journal of Physical Chemistry A, 2017, 121, 4698-4706.	1.1	77
54	A Single Transition State Serves Two Mechanisms:ÂAn ab Initio Classical Trajectory Study of the Electron Transfer and Substitution Mechanisms in Reactions of Ketyl Radical Anions with Alkyl Halides. Journal of the American Chemical Society, 2001, 123, 130-134.	6.6	76

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55	Nonadiabatic dynamics of polyatomic molecules and ions in strong laser fields. Physical Review A, 2003, 68, .	1.0	74
56	Theoretical Determination of One-Electron Oxidation Potentials for Nucleic Acid Bases. Journal of Chemical Theory and Computation, 2012, 8, 5107-5123.	2.3	72
57	Ab initio molecular dynamics: Propagating the density matrix with gaussian orbitals. IV. Formal analysis of the deviations from born-oppenheimer dynamics. Israel Journal of Chemistry, 2002, 42, 191-202.	1.0	71
58	Methods for geometry optimization of large molecules. I. An O(N2) algorithm for solving systems of linear equations for the transformation of coordinates and forces. Journal of Chemical Physics, 1998, 109, 7100-7104.	1.2	65
59	A redundant internal coordinate algorithm for optimization of periodic systems. Journal of Chemical Physics, 2001, 114, 2919-2923.	1.2	64
60	Steepest descent reaction path integration using a first-order predictorâ€“corrector method. Journal of Chemical Physics, 2010, 133, 224101.	1.2	63
61	Empirical Valence-Bond Models for Reactive Potential Energy Surfaces Using Distributed Gaussians. Journal of Chemical Theory and Computation, 2006, 2, 905-911.	2.3	62
62	Matrix Metalloproteinase 2 Inhibition: Combined Quantum Mechanics and Molecular Mechanics Studies of the Inhibition Mechanism of (4-Phenoxyphenylsulfonyl)methylthiirane and Its Oxirane Analogue. Biochemistry, 2009, 48, 9839-9847.	1.2	62
63	TD-CI Simulation of the Electronic Optical Response of Molecules in Intense Fields: Comparison of RPA, CIS, CIS(D), and EOM-CCSD. Journal of Physical Chemistry A, 2011, 115, 4678-4690.	1.1	62
64	Ligand Transformations and Efficient Proton/Water Reduction with Cobalt Catalysts Based on Pentadentate Pyridineâ€Rich Environments. Angewandte Chemie - International Edition, 2015, 54, 2105-2110.	7.2	61
65	Thermochemistry of Iron Chlorides and Their Positive and Negative Ions. The Journal of Physical Chemistry, 1996, 100, 8770-8776.	2.9	56
66	Angle-Dependent Ionization of Small Molecules by Time-Dependent Configuration Interaction and an Absorbing Potential. Journal of Physical Chemistry Letters, 2015, 6, 2140-2146.	2.1	56
67	The structure of (H3O2)â˜. Journal of Chemical Physics, 1983, 78, 2498-2503.	1.2	55
68	Structural, spectroscopic, and electrochemical behavior of trans-phenolato cobalt(iii) complexes of asymmetric NNâ€²O ligands as archetypes for metallomesogens. Dalton Transactions, 2006, , 2517-2525.	1.6	55
69	Analytical gradients for unrestricted Hartreeâ€“Fock and second order Mo/llerâ€“Plesset perturbation theory with single spin annihilation. Journal of Chemical Physics, 1989, 90, 2363-2369.	1.2	52
70	Density matrix search using direct inversion in the iterative subspace as a linear scaling alternative to diagonalization in electronic structure calculations. Journal of Chemical Physics, 2003, 119, 7651-7658.	1.2	52
71	X-ray Crystal Structure of the Acylated Î²-Lactam Sensor Domain of BlaR1 fromStaphylococcus aureusand the Mechanism of Receptor Activation for Signal Transduction. Journal of the American Chemical Society, 2004, 126, 13945-13947.	6.6	51
72	A toolkit to assist ONIOM calculations. Journal of Computational Chemistry, 2010, 31, 2363-2369.	1.5	51

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73	Structures and Energetics of Some Siliconâ"Phosphorus Compounds:â€‰ SiHmPHn, SiHmPHnSiHo, and (SiH3)3P. An ab Initio Molecular Orbital Study. Journal of the American Chemical Society, 1996, 118, 8444-8451.	6.6	47
74	Exploration of Mechanisms for the Transformation of 8-Hydroxy Guanine Radical to FAPyG by Density Functional Theory. Chemical Research in Toxicology, 2007, 20, 432-444.	1.7	46
75	Following gradient extremal paths. Theoretica Chimica Acta, 1992, 83, 15-20.	0.9	45
76	Mechanism of Ascorbic Acid Oxidation by Cytochromeb561. Biochemistry, 2001, 40, 11905-11911.	1.2	45
77	Early Transition Metal Complexes Containing 1,2,4-Triazolato and Tetrazolato Ligands:â€‰ Synthesis, Structure, and Molecular Orbital Studies. Inorganic Chemistry, 2001, 40, 6451-6462.	1.9	45
78	Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology. Journal of Chemical Theory and Computation, 2010, 6, 2566-2580.	2.3	44
79	Computational Prediction of One-Electron Reduction Potentials and Acid Dissociation Constants for Guanine Oxidation Intermediates and Products. Journal of Physical Chemistry B, 2013, 117, 9518-9531.	1.2	43
80	TD-CI Simulation of the Electronic Optical Response of Molecules in Intense Fields II: Comparison of DFT Functionals and EOM-CCSD. Journal of Physical Chemistry A, 2011, 115, 11832-11840.	1.1	42
81	Lysine carboxylation in proteins: OXA-10 Î²-lactamase. Proteins: Structure, Function and Bioinformatics, 2005, 61, 246-257.	1.5	41
82	Optical Excitations in Carbon Architectures Based on Dodecadehydrotribenzo[18]annuleneâ€. Journal of Physical Chemistry A, 2006, 110, 1305-1318.	1.1	41
83	Selective Photodissociation of Acetonitrile Ligands in Ruthenium Polypyridyl Complexes Studied by Density Functional Theory. Inorganic Chemistry, 2015, 54, 8003-8011.	1.9	38
84	Theoretical Calculation of pK_aâ€™s of Selenols in Aqueous Solution Using an Implicit Solvation Model and Explicit Water Molecules. Journal of Physical Chemistry A, 2016, 120, 8916-8922.	1.1	38
85	Phenanthrolineâ€Catalyzed Stereoretentive Glycosylations. Angewandte Chemie - International Edition, 2019, 58, 6957-6961.	7.2	38
86	Strong-field ionization rates of linear polyenes simulated with time-dependent configuration interaction with an absorbing potential. Journal of Chemical Physics, 2014, 141, 174104.	1.2	37
87	Bond Dissociation Energy of Peroxides Revisited. Journal of Physical Chemistry A, 2020, 124, 4742-4751.	1.1	37
88	Ab InitioMolecular Orbital Calculations of Electronic Effects on the Kinetics of Cyclopropylcarbinyl Radical Ring Openings. Journal of Organic Chemistry, 1998, 63, 3618-3623.	1.7	36
89	Photophysical characterization of a highly luminescent divalent-europium-containing azacryptate. Chemical Communications, 2018, 54, 4545-4548.	2.2	36
90	Heats of formation of SiHmFn calculated by ab initio molecular orbital methods. Journal of Chemical Physics, 1990, 92, 5404-5416.	1.2	35

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91	Computational study on nature of transition structure for oxygen transfer from dioxirane and carbonyloxide. Journal of Computational Chemistry, 1998, 19, 1353-1369.	1.5	35
92	Evaluation of the coordination preferences and catalytic pathways of heteroaxial cobalt oximes towards hydrogen generation. Chemical Science, 2016, 7, 3264-3278.	3.7	35
93	DFT Investigation of Ligand Photodissociation in [Ru^{II}(tpy)(bpy)(py)]²⁺ and [Ru^{II}(tpy)(Me₂bpy)(py)]²⁺ Complexes. Inorganic Chemistry, 2018, 57, 231-240.	1.9	35
94	Are BrÃ¸nsted Acids the True Promoter of Metal-Triflate-Catalyzed Glycosylations? A Mechanistic Probe into 1,2-cis-Aminoglycoside Formation by Nickel Triflate. ACS Catalysis, 2019, 9, 2110-2123.	5.5	35
95	Glyoxal photodissociation. An ab initio direct classical trajectory study of C2H2O2â†'H2+2â€ŠCO. Journal of Chemical Physics, 2001, 114, 8897-8904.	1.2	34
96	Computational Study of Oxidation of Guanine by Singlet Oxygen (¹Î”_g) and Formation of Guanine:Lysine Crossâ€Links. Chemistry - A European Journal, 2017, 23, 5804-5813.	1.7	34
97	Attosecond Electron Correlation Dynamics in Double Ionization of Benzene Probed with Two-Electron Angular Streaking. Physical Review Letters, 2017, 119, 123201.	2.9	34
98	An ab initio quasi-classical direct dynamics investigation of the F+C2H4â†'C2H3F+H product energy distributions. Physical Chemistry Chemical Physics, 1999, 1, 999-1011.	1.3	32
99	Distributed Gaussian Valence Bond Surface Derived from Ab Initio Calculations. Journal of Chemical Theory and Computation, 2009, 5, 949-961.	2.3	32
100	Unusually Stable Pyrazolate-Bridged Dialuminum Complexes Containing Bridging Methyl Groups. Journal of the American Chemical Society, 2000, 122, 9338-9339.	6.6	31
101	Angle-Dependent Ionization of Hydrides AH_n Calculated by Time-Dependent Configuration Interaction with an Absorbing Potential. Journal of Physical Chemistry A, 2015, 119, 10212-10220.	1.1	30
102	Efficient electro/photocatalytic water reduction using a [Ni^{II}(N₂Py₃)]²⁺ complex. Chemical Communications, 2016, 52, 13357-13360.	2.2	30
103	Diastereoselective sp³ Câ€“O Bond Formation via Visible Light-Induced, Copper-Catalyzed Cross-Couplings of Glycosyl Bromides with Aliphatic Alcohols. ACS Catalysis, 2020, 10, 5990-6001.	5.5	30
104	The Bond Dissociation Energy of the Nâ€“O Bond. Journal of Physical Chemistry A, 2021, 125, 5014-5021.	1.1	30
105	Hydrogen and Dihydrogen Bonding as Important Features of the Reactivity of the Bridging Hydride in Pyrazolate-Bridged Dialuminum Complexes. Organometallics, 2001, 20, 4301-4303.	1.1	29
106	Single Transition State Serves Two Mechanisms. Ab Initio Classical Trajectory Calculations of the Substitutionâ˜Electron Transfer Branching Ratio in CH2Oâ€¢- + CH3Cl. Journal of Physical Chemistry A, 2004, 108, 8526-8532.	1.1	29
107	Selective Release of Aromatic Heterocycles from Ruthenium Tris(2-pyridylmethyl)amine with Visible Light. Inorganic Chemistry, 2016, 55, 10-12.	1.9	29
108	Mechanistic Aspects of the Formation of Guanidinohydantoin from Spiroiminodihydantoin under Acidic Conditions. Chemical Research in Toxicology, 2009, 22, 526-535.	1.7	27

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109	Insight into the Complex and Dynamic Process of Activation of Matrix Metalloproteinases. Journal of the American Chemical Society, 2001, 123, 3108-3113.	6.6	26
110	Angular Dependence of Strong Field Ionization of CH₃X (X = F, Cl, Br, or I) Using Time-Dependent Configuration Interaction with an Absorbing Potential. Journal of Physical Chemistry A, 2017, 121, 5940-5946.	1.1	26
111	Disentangling Strong-Field Multielectron Dynamics with Angular Streaking. Journal of Physical Chemistry Letters, 2018, 9, 2539-2545.	2.1	26
112	Luminescence differences between two complexes of divalent europium. Journal of Organometallic Chemistry, 2018, 857, 88-93.	0.8	25
113	A comparison of geometry optimization with internal, cartesian, and mixed coordinates. International Journal of Quantum Chemistry, 1992, 44, 243-252.	1.0	24
114	Potential Surfaces for Unimolecular and Bimolecular Gas Phase Reactions of BHmClnCalculated at the G2 Level of Theory. The Journal of Physical Chemistry, 1996, 100, 9774-9779.	2.9	24
115	Molecular Orbital Studies of Titanium Nitride Chemical Vapor Deposition:Â Gas Phase Complex Formation, Ligand Exchange, and Elimination Reactions. Chemistry of Materials, 2000, 12, 2466-2474.	3.2	24
116	Fluorophore-LabeledS-Nitrosothiols. Journal of Organic Chemistry, 2001, 66, 6064-6073.	1.7	24
117	Geometry optimization methods for modeling large molecules. Computational and Theoretical Chemistry, 2003, 666-667, 31-39.	1.5	24
118	A Reaction Accelerator: Mid-infrared Strong Field Dissociation Yields Mode-Selective Chemistry. Journal of Physical Chemistry Letters, 2012, 3, 2541-2547.	2.1	24
119	Effects of Methyl Substitution in Ruthenium Tris(2-pyridylmethyl)amine Photocaging Groups for Nitriles. Inorganic Chemistry, 2016, 55, 6968-6979.	1.9	24
120	A theoretical study of the infrared vibrational intensities of CH3F. Journal of Chemical Physics, 1987, 86, 6937-6945.	1.2	23
121	QM/MM Studies of the Matrix Metalloproteinase 2 (MMP2) Inhibition Mechanism of (S)-SB-3CT and its Oxirane Analogue. Journal of Chemical Theory and Computation, 2010, 6, 3580-3587.	2.3	23
122	Angular Dependence of Ionization by Circularly Polarized Light Calculated with Time-Dependent Configuration Interaction with an Absorbing Potential. Journal of Physical Chemistry A, 2017, 121, 1336-1343.	1.1	23
123	Structures, Energies, and Electrostatics for Methane Complexed with Alumina Clusters. Journal of Physical Chemistry A, 2000, 104, 4920-4927.	1.1	22
124	Synthesis, Structure, and Properties of Magnesocene Amine Adducts. Structural Distortions Arising from Nâ^'HÂ·Â·Â·C5H5-Hydrogen Bonding and Molecular Orbital Calculations Thereof. Organometallics, 2003, 22, 4060-4069.	1.1	22
125	Protonated acetylene revisited. Theoretical Chemistry Accounts, 2007, 118, 75-80.	0.5	22
126	Ab Initio Classical Trajectory Study of the Dissociation of Neutral and Positively Charged Methanimine (CH₂NHⁿ⁺ n = 0â^'2). Journal of Physical Chemistry A, 2009, 113, 9958-9964.	1.1	22

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127	The Mechanisms of Rectification in Au	Molecule	Au Devices Based on Langmuirâ€“Blodgett Monolayers of Iron(III) and Copper(II) Surfactants. Angewandte Chemie - International Edition, 2014, 53, 14462-14467.	7.2	22
128	An ab initio study of the vibrational frequencies and infrared intensities of CH2F2. Journal of Chemical Physics, 1990, 92, 4351-4356.	1.2	21
129	Dissociation of acetone radical cation (CH3COCH3+Ë™ â†' CH3CO++CH3Ë™): An ab initio direct classical trajectory study. Physical Chemistry Chemical Physics, 2004, 6, 5166-5171.	1.3	21
130	Distinct Proton and Water Reduction Behavior with a Cobalt(III) Electrocatalyst Based on Pentadentate Oximes. Angewandte Chemie - International Edition, 2015, 54, 7139-7143.	7.2	21
131	Bimetallic Cooperativity in Proton Reduction with an Amidoâ€Bridged Cobalt Catalyst. Chemistry - A European Journal, 2017, 23, 9272-9279.	1.7	21
132	A pentadentate nitrogen-rich copper electrocatalyst for water reduction with pH-dependent molecular mechanisms. Dalton Transactions, 2017, 46, 16812-16820.	1.6	21
133	A Single Transition State Serves Two Mechanisms. The Branching Ratio for CH2Oâ€¢-+ CH3Cl on Improved Potential Energy Surfaces. Journal of Physical Chemistry A, 2006, 110, 2801-2806.	1.1	20
134	Matrix Metalloproteinase 2 (MMP2) Inhibition: DFT and QM/MM Studies of the Deprotonation-Initialized Ring-Opening Reaction of the Sulfoxide Analogue of SB-3CT. Journal of Physical Chemistry B, 2010, 114, 1030-1037.	1.2	20
135	Can Metallapyrimidines Be Aromatic? A Computational Study into a New Class of Metallacycles. Journal of Chemical Theory and Computation, 2012, 8, 4950-4959.	2.3	20
136	Structures and Energetics of Some Potential Intermediates in Titanium Nitride Chemical Vapor Deposition:Â TiClm(NH2)n, TiClm(NH2)nNH, and TiClm(NH2)nN. An ab Initio Molecular Orbital Study. Journal of Physical Chemistry B, 1998, 102, 5152-5157.	1.2	19
137	Photodissociation of glyoxal: Resolution of a paradox. Journal of Chemical Physics, 2001, 114, 8.	1.2	19
138	Glyoxal photodissociation. II. An ab initio direct classical trajectory study of C2H2O2â†'CO+H2CO. Journal of Chemical Physics, 2001, 115, 6907-6912.	1.2	19
139	Unimolecular Dissociation of Formyl Halides HXCO â†' CO + HX (X= F, Cl):â€‰ An Ab Initio Direct Classical Trajectory Study. Journal of Physical Chemistry A, 2002, 106, 11623-11629.	1.1	19
140	Angular Dependence of Strong Field Ionization of Haloacetylenes HCCX (X = F, Cl, Br, I), Using Time-Dependent Configuration Interaction with an Absorbing Potential. Journal of Physical Chemistry C, 2018, 122, 13751-13757.	1.5	19
141	Metallapyrimidines and Metallapyrimidiniums from Oxidative Addition of Pyrazolate Nâ€“N Bonds to Niobium(III), Niobium(IV), and Tantalum(IV) Metal Centers and Assessment of Their Aromatic Character. Organometallics, 2012, 31, 5971-5974.	1.1	18
142	Immobilization of an Amphiphilic Molecular Cobalt Catalyst on Carbon Black for Ligand-Assisted Water Oxidation. Inorganic Chemistry, 2018, 57, 9748-9756.	1.9	18
143	Ab initio calculations on H + C2H2 ? C2H3 using unrestricted Mï¿½ller-Plesset perturbation theory with spin projection. International Journal of Quantum Chemistry, 1987, 32, 267-282.	1.0	17
144	Analytical second derivatives of two electron integrals over s and p Cartesian Gaussians. Journal of Chemical Physics, 1989, 90, 5630-5634.	1.2	17

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145	Fragmentation Pathways in a Series of CH3COX Molecules in the Strong Field Regimeâ€. Journal of Physical Chemistry A, 2004, 108, 3162-3165.	1.1	17
146	Molecular Orbital Studies of Zinc Oxide Chemical Vapor Deposition:â€‰ Gas-Phase Radical Reactions. Chemistry of Materials, 2006, 18, 1878-1884.	3.2	17
147	Energy Dependence of the Ruthenium(II)-Bipyridine Metal-to-Ligand-Charge-Transfer Excited State Radiative Lifetimes: Effects of Ï€Ï€*(bipyridine) Mixing. Journal of Physical Chemistry B, 2015, 119, 7393-7406.	1.2	17
148	Modulation of electronic and redox properties in phenolate-rich cobalt(iii) complexes and their implications for catalytic proton reduction. Dalton Transactions, 2015, 44, 3454-3466.	1.6	17
149	Using bonding to guide transition state optimization. Journal of Computational Chemistry, 2015, 36, 1157-1166.	1.5	17
150	Computational Study of the Radical Mediated Mechanism of the Formation of C8, C5, and C4 Guanine:Lysine Adducts in the Presence of the Benzophenone Photosensitizer. Chemical Research in Toxicology, 2016, 29, 1396-1409.	1.7	16
151	Calculations of pK_a Values for a Series of Naturally Occurring Modified Nucleobases. Journal of Physical Chemistry A, 2022, 126, 1518-1529.	1.1	16
152	Hartreeâ€“Fock energy derivatives with respect to basis set exponents. Integral derivatives using Rys polynomials. Journal of Chemical Physics, 1987, 87, 514-519.	1.2	15
153	Sequential Phenolate Oxidations in Octahedral Cobalt(III) Complexes with [N2O3] Ligands. European Journal of Inorganic Chemistry, 2012, 2012, 4622-4631.	1.0	15
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