Bernd Engels

List of Publications by Year
in descending order

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264	8,568	50170	71532
papers	citations	46 h-index	76 g-index

267	267	267	7884
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Nitrogen fixation and reduction at boron. Science, 2018, 359, 896-900.	6.0	948
2	Exciton Trapping in Ï€-Conjugated Materials: A Quantum-Chemistry-Based Protocol Applied to Perylene Bisimide Dye Aggregates. Journal of the American Chemical Society, 2008, 130, 12858-12859.	6.6	290
3	New algorithms for an individually selecting MR-CI program. Chemical Physics, 1997, 225, 197-202.	0.9	154
4	Electron Delocalization in Reduced Forms of 2-(BMes₂)pyrene and 2,7-Bis(BMes₂)pyrene. Journal of the American Chemical Society, 2015, 137, 6750-6753.	6.6	134
5	Ultrafast Exciton Self-Trapping upon Geometry Deformation in Perylene-Based Molecular Aggregates. Journal of Physical Chemistry Letters, 2013, 4, 792-796.	2.1	123
6	Siâ‹¯E (E = N, O, F) Bonding in a Hexacoordinated Silicon Complex:Â New Facts from Experimental and Theoretical Charge Density Studies. Journal of the American Chemical Society, 2004, 126, 5563-5568.	6.6	119
7	First-principles calculations of anisotropic charge-carrier mobilities in organic semiconductor crystals. Physical Review B, 2011, 83, .	1.1	117
8	Temporary anions - calculation of energy and lifetime by absorbing potentials: the resonance. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 4107-4122.	0.6	114
9	SN versus S+N-:Â An Experimental and Theoretical Charge Density Study. Journal of the American Chemical Society, 2004, 126, 1781-1793.	6.6	109
10	Novel Dengue Virus NS2B/NS3 Protease Inhibitors. Antimicrobial Agents and Chemotherapy, 2015, 59, 1100-1109.	1.4	108
11	Understanding Ground- and Excited-State Properties of Perylene Tetracarboxylic Acid Bisimide Crystals by Means of Quantum Chemical Computations. Journal of the American Chemical Society, 2009, 131, 15660-15668.	6.6	104
12	Structureâ€“property relationships for 1,7-diphenoxy-perylene bisimides in solution and in the solid state. Chemical Science, 2014, 5, 608-619.	3.7	94
13	A Clear Correlation between the Diradical Character of 1,3-Dipoles and Their Reactivity toward Ethylene or Acetylene. Journal of the American Chemical Society, 2010, 132, 7631-7637.	6.6	93
14	The Pentaphenylboroleâ€“2,6â€Lutidine Adduct: A System with Unusual Thermochromic and Photochromic Properties. Angewandte Chemie - International Edition, 2011, 50, 2833-2836.	7.2	90
15	What Controls the Reactivity of 1,3â€Dipolar Cycloadditions?. Angewandte Chemie - International Edition, 2009, 48, 7968-7970.	7.2	86
16	On the Accuracy of Theoretically and Experimentally Determined Electron Densities of Polar Bonds. Journal of Physical Chemistry A, 2004, 108, 9442-9452.	1.1	84
17	Recent Developments in Configuration Interaction and Density Functional Theory Calculations of Radical Hyperfine Structure.. Advances in Quantum Chemistry, 1996, 27, 297-369.	0.4	83
18	A Theoretical Comparison of Two Competing Diradical Cyclizations in Enyne-Allenes:Â The Myersâ‹¯Saito and the Novel C2â‹¯C6Cyclization. Journal of the American Chemical Society, 1998, 120, 6356-6361.	6.6	79

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19	Contribution of Surface Resonances to Scanning Tunneling Microscopy Images: (110) Surfaces of III-V Semiconductors. Physical Review Letters, 1996, 77, 2997-3000.	2.9	78
20	Comparison betweenab initiotheory and scanning tunneling microscopy for (110) surfaces of III-V semiconductors. Physical Review B, 1998, 58, 7799-7815.	1.1	71
21	Assessment of quantum chemical methods and basis sets for excitation energy transfer. Chemical Physics, 2008, 346, 275-285.	0.9	71
22	Assessment of TDâ€ÐFTâ€•and TDâ€HFâ€bbased approaches for the prediction of exciton coupling parameters, potential energy curves, and electronic characters of electronically excited aggregates. Journal of Computational Chemistry, 2011, 32, 1971-1981.	1.5	70
23	Quantum Chemical-Based Protocol for the Rational Design of Covalent Inhibitors. Journal of the American Chemical Society, 2016, 138, 8332-8335.	6.6	69
24	â€œKnock-Outâ€•Analogues as a Tool to Quantify Supramolecular Processes:Â A Theoretical Study of Molecular Interactions in Guanidiniocarbonyl Pyrrole Carboxylate Dimers. Journal of the American Chemical Society, 2005, 127, 11115-11124.	6.6	67
25	A comparative ab initio study of the Si2C4, Si3C3, and Si4C2 clusters. Journal of Chemical Physics, 1994, 101, 6790-6799.	1.2	64
26	Two Novel Thermal Biradical Cyclizations of Enyne-Ketenimines: Theory, Experiment, and Synthetic Potential. Angewandte Chemie - International Edition, 1998, 37, 1562-1564.	7.2	63
27	Two Novel Thermal Biradical Cyclizations in Theory and Experiment: New Synthetic Routes to 6H-Indolo[2,3-b]quinolines and 2-Aminoquinolines from Enyne-Carbodiimides. Angewandte Chemie - International Edition, 1998, 37, 2371-2373.	7.2	63
28	Computational Assessment of the Electronic Structures of Cyclohexa-1,2,4-triene, 1-Oxacyclohexa-2,3,5-triene (3Î´2-Pyran), Their Benzo Derivatives, and Cyclohexa-1,2-diene. An Experimental Approach to 3Î´2-Pyran. Journal of the American Chemical Society, 2002, 124, 287-297.	6.6	62
29	Multiple Reduction of 2,5â€Bis(borolyl)thiophene: Isolation of a Negative Bipolaron by Comproportionation. Angewandte Chemie - International Edition, 2013, 52, 12852-12855.	7.2	62
30	Isolation of diborenes and their 90Â°-twisted diradical congeners. Nature Communications, 2018, 9, 1197.	5.8	62
31	The Importance of the Ene Reaction for the C2â^'C6Cyclization of Enyneâ^'Allenes. Journal of the American Chemical Society, 2001, 123, 5557-5562.	6.6	61
32	Accurate Intermolecular Potentials with Physically Grounded Electrostatics. Journal of Chemical Theory and Computation, 2011, 7, 1791-1803.	2.3	60
33	Calculation of hyperfine coupling constants. Molecular Physics, 1987, 62, 109-127.	0.8	58
34	On the Origin of the Stabilization of the Zwitterionic Resting State of Cysteine Proteases: A Theoretical Study. Journal of the American Chemical Society, 2008, 130, 8696-8705.	6.6	58
35	Theoretical Studies about the Influence of Different Ring Substituents on the Nucleophilic Ring Opening of Three-Membered Heterocycles and Possible Implications for the Mechanisms of Cysteine Protease Inhibitors. Journal of Organic Chemistry, 2005, 70, 233-237.	1.7	57
36	Stable Fiveâ€Memberedâ€Ring Allenes with Secondâ€Row Elements Only: Not Allenes, But Zwitterions. Angewandte Chemie - International Edition, 2009, 48, 1538-1539.	7.2	57

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37	Aziridide-Based Inhibitors of Cathepsinâ€…L: Synthesis, Inhibition Activity, and Docking Studies. ChemMedChem, 2006, 1, 1126-1141.	1.6	56
38	Singlet Exciton Diffusion in Organic Crystals Based on Marcus Transfer Rates. Journal of Chemical Theory and Computation, 2014, 10, 1242-1255.	2.3	56
39	Identification of Ultrafast Relaxation Processes As a Major Reason for Inefficient Exciton Diffusion in Perylene-Based Organic Semiconductors. Journal of the American Chemical Society, 2014, 136, 9327-9337.	6.6	56
40	The dimer-approach to characterize opto-electronic properties of and exciton trapping and diffusion in organic semiconductor aggregates and crystals. Physical Chemistry Chemical Physics, 2017, 19, 12604-12619.	1.3	56
41	Comparison of the electronic structure of different peryleneâ€based dyeâ€aggregates. Journal of Computational Chemistry, 2012, 33, 1544-1553.	1.5	55
42	cAACâ€Stabilized 9,10â€diboraanthracenesâ€”Acenes with Openâ€Shell Singlet Biradical Ground States. Angewandte Chemie - International Edition, 2020, 59, 19338-19343.	7.2	54
43	Model Calculations about the Influence of Protic Environments on the Alkylation Step of Epoxide, Aziridine, and Thiirane Based Cysteine Protease Inhibitors. Journal of Physical Chemistry A, 2004, 108, 7691-7701.	1.1	53
44	Multidimensional spectroscopy of photoreactivity. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 4764-4769.	3.3	53
45	Ab initio study of the energy difference between the cyclic and linear forms of the C6 molecule. Journal of Chemical Physics, 1994, 101, 4042-4048.	1.2	51
46	Structural and chemical insights into the covalent-allosteric inhibition of the protein kinase Akt. Chemical Science, 2019, 10, 3573-3585.	3.7	49
47	The hyperfine coupling constants of theX3â^'-states of NH. Molecular Physics, 1989, 67, 583-600.	0.8	48
48	Ab initio investigation of the vibronic structure of the C2H spectrum: Computation of the vibronically averaged values for the hyperfine coupling constants. Journal of Molecular Spectroscopy, 1991, 150, 70-85.	0.4	47
49	Study of influences of various excitation classes onab initio calculated isotropic hyperfine coupling constants. Theoretica Chimica Acta, 1993, 86, 429-437.	0.9	47
50	Study of the hyperfine coupling constants of the molecules NH2, NHD and ND2. Chemical Physics Letters, 1990, 172, 180-186.	1.2	46
51	Methylbismuth: an organometallic bismuthinidene biradical. Chemical Science, 2020, 11, 7562-7568.	3.7	46
52	A multireference configuration interaction study of the hyperfine structure of the molecules CCO, CNN, and NCN in their triplet ground states. Journal of Chemical Physics, 1994, 101, 7686-7691.	1.2	45
53	An Experimental and Computational Study on the Reactivity and Regioselectivity for the Nitrosoarene Ene Reaction:Â Comparison with Triazolinedione and Singlet Oxygen. Journal of the American Chemical Society, 2001, 123, 5542-5548.	6.6	45
54	Lewis-Base Stabilization of the Parent Al(I) Hydride under Ambient Conditions. Journal of the American Chemical Society, 2019, 141, 16954-16960.	6.6	45

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55	Benchmarking singlet and triplet excitation energies of molecular semiconductors for singlet fission: Tuning the amount of HF exchange and adjusting local correlation to obtain accurate functionals for singletâ€“triplet gaps. Chemical Physics, 2017, 482, 319-338.	0.9	44
56	Atomistic Insights into the Inhibition of Cysteine Proteases: First QM/MM Calculations Clarifying the Stereoselectivity of Epoxide-Based Inhibitors. Journal of Physical Chemistry B, 2008, 112, 11798-11808.	1.2	43
57	Atomistic Insights into the Inhibition of Cysteine Proteases:â€‰ First QM/MM Calculations Clarifying the Regiospecificity and the Inhibition Potency of Epoxide- and Aziridine-Based Inhibitors. Journal of Physical Chemistry B, 2008, 112, 5458-5469.	1.2	43
58	A detailed study of the configuration selected multireference configuration interaction method combined with perturbation theory to correct the wave function. Journal of Chemical Physics, 1994, 100, 1380-1386.	1.2	42
59	Interaction of (benzylidene-hydrazono)-1,4-dihydropyridines with Î²-amyloid, acetylcholine, and butyrylcholine esterases. Bioorganic and Medicinal Chemistry, 2010, 18, 2049-2059.	1.4	42
60	Dipeptidyl Nitroalkenes as Potent Reversible Inhibitors of Cysteine Proteases Rhodesain and Cruzain. ACS Medicinal Chemistry Letters, 2016, 7, 1073-1076.	1.3	42
61	Estimation of the influence of the configurations neglected within truncated multi-reference CI wavefunctions on molecular properties. Chemical Physics Letters, 1991, 179, 398-404.	1.2	41
62	Benchmark Study for the Cysteineâ€“Histidine Proton Transfer Reaction in a Protein Environment: Gas Phase, COSMO, QM/MM Approaches. Journal of Chemical Theory and Computation, 2013, 9, 1765-1777.	2.3	41
63	Comparison of different rate constant expressions for the prediction of charge and energy transport in oligoacenes. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 694-720.	6.2	41
64	An MRD-CI study of low-lying electronic states in CaF. Chemical Physics Letters, 1991, 176, 407-412.	1.2	40
65	Theoretical study of electron spin resonance parameters: H2CN and H2CO+. Journal of Chemical Physics, 1994, 100, 2936-2942.	1.2	40
66	Difficulties in the calculation of electron spin resonance parameters using density functional methods. Chemical Physics Letters, 1994, 230, 398-404.	1.2	40
67	New Dyes Based on Amino-Substituted Acridizinium Salts-Synthesis and Exceptional Photochemical Properties. Chemistry - A European Journal, 2000, 6, 2854-2864.	1.7	40
68	On the Regioselectivity of the Cyclization of Enyneâ^'Ketenes:â€‰ A Computational Investigation and Comparison with the Myers-Saito and Schmittel Reaction. Journal of the American Chemical Society, 2002, 124, 1823-1828.	6.6	39
69	Ab initio configuration interaction description of excitation energy transfer between closely packed molecules. Chemical Physics, 2008, 343, 353-361.	0.9	39
70	Phenylene Ethynyleneâ€Tethered Perylene Bisimide Foldaâ€Dimer and Foldaâ€Trimer: Investigations on Folding Features in Ground and Excited States. Chemistry - A European Journal, 2015, 21, 615-630.	1.7	39
71	Environmental Effects on Charge Densities of Biologically Active Molecules: Do Molecule Crystal Environments Indeed Approximate Protein Surroundings?. Journal of Physical Chemistry B, 2009, 113, 5072-5082.	1.2	38
72	The Importance of the Active Site Histidine for the Activity of Epoxide- or Aziridine-Based Inhibitors of Cysteine Proteases. ChemMedChem, 2007, 2, 120-128.	1.6	37

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73	Structureâ€“Property Relationship of Perylene Bisimide Macrocycles Probed by Atomic Force Microscopy and Single-Molecule Fluorescence Spectroscopy. ACS Nano, 2013, 7, 5064-5076.	7.3	36
74	Theoretical Analysis of the Relaxation Dynamics in Perylene Bisimide Dimers Excited by Femtosecond Laser Pulses. Journal of Physical Chemistry A, 2014, 118, 1403-1412.	1.1	36
75	Ab initio investigation of the vibronic structure of the C2H spectrum: Calculation of the hyperfine coupling constants for the three lowest-lying electronic states. Journal of Molecular Spectroscopy, 1991, 150, 56-69.	0.4	35
76	Ring size effects in the C2â€“C6 biradical cyclisation of enyneâ€“allenes and the relevance for neocarzinostatin. Perkin Transactions II RSC, 2001, , 1331-1339.	1.1	35
77	A Combined Computational and Experimental Study of the Hydrogen-Bonded Dimers of Xanthine and Hypoxanthine. Journal of Physical Chemistry A, 2005, 109, 1703-1712.	1.1	35
78	Anisotropy of singlet exciton diffusion in organic semiconductor crystals from ab initio approaches. Journal of Chemical Physics, 2014, 140, 024503.	1.2	35
79	Photoisomerization among ring-open merocyanines. I. Reaction dynamics and wave-packet oscillations induced by tunable femtosecond pulses. Journal of Chemical Physics, 2014, 140, 224310.	1.2	35
80	Unravelling the Dramatic Electrostructural Differences Between N-Heterocyclic Carbene- and Cyclic (Alkyl)(amino)carbene-Stabilized Low-Valent Main Group Species. Journal of the American Chemical Society, 2018, 140, 12580-12591.	6.6	35
81	The structure of 5-cyanoindole in the ground and the lowest electronically excited singlet states, deduced from rotationally resolved electronic spectroscopy and ab initio theory. Physical Chemistry Chemical Physics, 2012, 14, 10266.	1.3	34
82	Cationâˆ'Ï€ Interactions: Accurate Intermolecular Potential from Symmetry-Adapted Perturbation Theory. Journal of Physical Chemistry B, 2013, 117, 10093-10102.	1.2	34
83	Theoretical study of the potential energy surface governing the stereochemistry in chloroethyl radical reactions. The Journal of Physical Chemistry, 1990, 94, 1267-1275.	2.9	33
84	Geometry and Cooperativity Effects in Adenosineâˆ'Carboxylic Acid Complexes. Journal of the American Chemical Society, 2005, 127, 16151-16158.	6.6	33
85	Theoretical study of weak CC double bond coordination in a gold (I) catalyst precursor. Computational and Theoretical Chemistry, 2010, 957, 21-25.	1.5	33
86	Oligo(borolyl)benzenesâ€”Synthesis and Properties. Chemistry - A European Journal, 2012, 18, 14292-14304.	1.7	33
87	Conformational analysis of arginine in gas phaseâ€”A strategy for scanning the potential energy surface effectively. Journal of Computational Chemistry, 2008, 29, 407-415.	1.5	32
88	Mechanistic Study of the Reaction of Thiolâ€Containing Enzymes with Î±,Î²â€Unsaturated Carbonyl Substrates by Computation and Chemoassays. ChemMedChem, 2010, 5, 869-880.	1.6	32
89	Theoretical study of FC2H4. The Journal of Physical Chemistry, 1989, 93, 4462-4470.	2.9	31
90	Anionic Boron- and Carbon-Based Hetero-Diradicaloids Spanned by a p-Phenylene Bridge. Journal of the American Chemical Society, 2021, 143, 3687-3692.	6.6	31

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91	Origin of the Reactivity Differences of Substituted Aziridines: CN vs CC Bond Breakages. Journal of Organic Chemistry, 2009, 74, 5244-5249.	1.7	30
92	A general ansatz for constructing quasi-diabatic states in electronically excited aggregated systems. Journal of Chemical Physics, 2015, 143, 084106.	1.2	30
93	On a theoretical model for the Rennerâ€“Teller effect in tetraâ€atomic molecules. Journal of Chemical Physics, 1996, 105, 8569-8585.	1.2	29
94	Theoretical study of the reaction of alkynes with furan catalyzed by AuCl3 and AuCl. International Journal of Quantum Chemistry, 2007, 107, 359-365.	1.0	29
95	On the applicability of timeâ€dependent density functional theory (TDDFT) and semiempirical methods to the computation of excitedâ€state potential energy surfaces of peryleneâ€based dyeâ€aggregates. International Journal of Quantum Chemistry, 2017, 117, e25337.	1.0	29
96	Study of the hyperfine coupling constants (14N and 1H) of the NH2 molecules in the Xâ€‰2B1 ground state and the Aâ€‰2A1 excited state. Journal of Chemical Physics, 1992, 96, 4526-4535.	1.2	28
97	The Stereochemical Course of the Generation and Interception of aSix-Membered Cyclic Allene: 3Î´2-1H-Naphthalene (2,3-Didehydro-1,2-dihydronaphthalene). European Journal of Organic Chemistry, 2006, 2006, 5045-5058.	1.2	28
98	Structureâ€“Property Relationships from Atomistic Multiscale Simulations of the Relevant Processes in Organic Solar Cells. I. Thermodynamic Aspects. Journal of Physical Chemistry C, 2017, 121, 4-25.	1.5	28
99	Advantages and limitations of Kohnâ€“Sham orbitals as single electron basis for multireference configuration interaction and multireference perturbation theory. Journal of Chemical Physics, 2003, 119, 11591-11601.	1.2	27
100	Paracyclophanes as model compounds for strongly interacting Ï€-systems. Part 1. Pseudo-ortho-dihydroxy[2.2]paracyclophane. Physical Chemistry Chemical Physics, 2010, 12, 9339.	1.3	26
101	Structureâ€“Property Relationships for Exciton and Charge Reorganization Energies of Dipolar Organic Semiconductors: A Combined Valence Bond Self-Consistent Field and Time-Dependent Hartree-Fock and DFT Study of Merocyanine Dyes. Journal of Physical Chemistry C, 2015, 119, 17602-17611.	1.5	26
102	A theoretical description of charge reorganization energies in molecular organic Pâ€type semiconductors. Journal of Computational Chemistry, 2016, 37, 1335-1344.	1.5	26
103	Benchmarking Ground-State Geometries and Vertical Excitation Energies of a Selection of P-Type Semiconducting Molecules with Different Polarity. Journal of Physical Chemistry A, 2015, 119, 12876-12891.	1.1	25
104	The electronic character of PTCDA thin films in comparison to other perylene-based organic semi-conductors: ab initio-, TD-DFT and semi-empirical computations of the opto-electronic properties of large aggregates. Physical Chemistry Chemical Physics, 2017, 19, 2434-2448.	1.3	25
105	A New Class of Neutral Boronâ€Based Diradicals Spanned by a Twoâ€Carbonâ€Atom Bridge. Angewandte Chemie - International Edition, 2019, 58, 1842-1846.	7.2	25
106	Reexchange Controlled Diffusion in Surfactant-Mediated Epitaxial Growth: Si on As-Terminated Si(111). Physical Review Letters, 1998, 80, 2873-2876.	2.9	24
107	Femtosecond Dynamics of the tert-Butyl Radical, t-C4H9. Journal of Physical Chemistry A, 2007, 111, 1771-1779.	1.1	24
108	Isolation and Reactivity of an Antiaromatic sâ€Block Metal Compound. Angewandte Chemie - International Edition, 2021, 60, 3812-3819.	7.2	24

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109	Specific Purine-Purine Base Pairing in Linear Alanyl-Peptide Nucleic Acids. Helvetica Chimica Acta, 2000, 83, 2580-2593.	1.0	23
110	Individually selecting multi-reference CI and its application to biradicalic cyclizations. Computers & Chemistry, 2001, 25, 15-38.	1.2	23
111	Theoretical study of the bridging in Î²-halo ethyl. Computational and Theoretical Chemistry, 1986, 138, 59-68.	1.5	22
112	Analysis and Deperturbation of the C2Î and D2Î£+ States of CaF. Journal of Molecular Spectroscopy, 1993, 161, 303-311.	0.4	22
113	Ab initio treatment of the Renner-Teller effect in tetra-atomic molecules undergoing large amplitude bending vibrations. Chemical Physics, 1997, 225, 63-76.	0.9	22
114	Predicting the tautomeric equilibrium of acetylacetone in solution. I. The right answer for the wrong reason?. Journal of Computational Chemistry, 2010, 31, 665-670.	1.5	22
115	Efficiency of tabuâ€searchâ€based conformational search algorithms. Journal of Computational Chemistry, 2011, 32, 2245-2253.	1.5	22
116	How Important Is Molecular Rigidity for the Complex Stability of Artificial Hostâ€“Guest Systems? A Theoretical Study on Self-Assembly of Gas-Phase Arginine. Chemistry - A European Journal, 2007, 13, 6644-6653.	1.7	21
117	Rational Design of Improved Aziridine-Based Inhibitors of Cysteine Proteases. Journal of Physical Chemistry B, 2009, 113, 5282-5289.	1.2	21
118	Paracyclophanes as model compounds for strongly interacting Ï€-systems. Part 2: mono-hydroxy[2.2]paracyclophane. Physical Chemistry Chemical Physics, 2011, 13, 11076.	1.3	21
119	Protocol for Rational Design of Covalently Interacting Inhibitors. ChemPhysChem, 2014, 15, 3226-3235.	1.0	21
120	Nonthermally activated exciton transport in crystalline organic semiconductor thin films. Physical Review B, 2014, 89, .	1.1	21
121	Inhibitorâ€induced Dimerization of an Essential Oxidoreductase from African Trypanosomes. Angewandte Chemie - International Edition, 2019, 58, 3640-3644.	7.2	21
122	Diborane(4) Azides: Surprisingly Stable Sources of Transient Iminoboranes. Angewandte Chemie - International Edition, 2020, 59, 15480-15486.	7.2	21
123	Ab Initio Study of the Renner-Teller Effect in the X2Îu Electronic State of B2H+2. Journal of Molecular Spectroscopy, 1995, 171, 494-503.	0.4	20
124	Orbitals from a self-interaction free Kohnâ€“Sham potential as a single electron basis for ab initio methods. Chemical Physics Letters, 2002, 360, 175-181.	1.2	20
125	Gradient tabu search. Journal of Computational Chemistry, 2007, 28, 601-611.	1.5	20
126	Solvent Controlled Energy Transfer Processes in Triarylamine-Triazole Based Dendrimers. Journal of Physical Chemistry C, 2013, 117, 19816-19831.	1.5	20

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127	The electronic structure of pyracene: a spectroscopic and computational study. Physical Chemistry Chemical Physics, 2013, 15, 8151.	1.3	20
128	Experimental and theoretical investigations into the stability of cyclic aminals. Beilstein Journal of Organic Chemistry, 2016, 12, 2280-2292.	1.3	20
129	Reduction and Rearrangement of a Boron(I) Carbonyl Complex. Angewandte Chemie - International Edition, 2021, 60, 2963-2968.	7.2	20
130	Fluorovinylsulfones and -Sulfonates as Potent Covalent Reversible Inhibitors of the Trypanosomal Cysteine Protease Rhodesain: Structureâ€“Activity Relationship, Inhibition Mechanism, Metabolism, and In Vivo Studies. Journal of Medicinal Chemistry, 2021, 64, 12322-12358.	2.9	20
131	Naphthoquinones as Covalent Reversible Inhibitors of Cysteine Proteasesâ€”Studies on Inhibition Mechanism and Kinetics. Molecules, 2020, 25, 2064.	1.7	20
132	Study of the 1s and 2s shell contributions to the isotropic hyperfine coupling constant in nitrogen. Journal of Physics B: Atomic, Molecular and Optical Physics, 1988, 21, 3459-3471.	0.6	19
133	New Tabu Search based global optimization methods outline of algorithms and study of efficiency. Journal of Computational Chemistry, 2008, 29, 768-780.	1.5	19
134	Tabu Search Based Strategies for Conformational Search. Journal of Physical Chemistry A, 2009, 113, 11699-11705.	1.1	19
135	Photoisomerization among ring-open merocyanines. II. A computational study. Journal of Chemical Physics, 2014, 140, 224311.	1.2	19
136	Vinyl sulfone building blocks in covalently reversible reactions with thiols. New Journal of Chemistry, 2015, 39, 5841-5853.	1.4	19
137	Product-oriented chemical surface modification of a levansucrase (SacB) via an ene-type reaction. Chemical Science, 2018, 9, 5312-5321.	3.7	19
138	The Dimethylbismuth Cation: Entry Into Dative Biâ¯Bi Bonding and Unconventional Methyl Exchange. Angewandte Chemie - International Edition, 2021, 60, 24388-24394.	7.2	19
139	The hyperfine coupling constants of the five lowest states of CH: An ab initio MRDCI study. Chemical Physics Letters, 1988, 152, 397-401.	1.2	18
140	Ab Initio Investigation of the Vibronic and Magnetic Hyperfine Effects in theX2ÎuState of[formula]. Journal of Molecular Spectroscopy, 1995, 174, 334-352.	0.4	18
141	Structure and dynamics of the silacyclobutane radical cation, studied by ab initio and density functional theory and electron spin resonance spectroscopy. Journal of Chemical Physics, 1997, 107, 297-306.	1.2	18
142	Ab initio investigation of the vibronic spectrum involving the two lowest-lying electronic states of HCCO. Journal of Chemical Physics, 1999, 110, 7802-7810.	1.2	18
143	1â€Phenylâ€1,2â€cyclohexadiene: Astoundingly High Enantioselectivities on Generation in a Doeringâ€“Mooreâ€“SkattebÃl Reaction and Interception by Activated Olefins. Chemistry - A European Journal, 2009, 15, 11266-11272.	1.7	18
144	Excited-State Dynamics in Perylene-Based Organic Semiconductor Thin Films: Theory Meets Experiment. Journal of Physical Chemistry C, 2019, 123, 27561-27572.	1.5	18

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145	Pentadiynylidene and Its Methyl-Substituted Derivates: Threshold Photoelectron Spectroscopy of R₁-C₅-R₂ Triplet Carbon Chains. Journal of Physical Chemistry A, 2019, 123, 2008-2017.	1.1	18
146	The hyperfine coupling constants of19F?2: An ab initioMRD-CI basis set study. International Journal of Quantum Chemistry, 1989, 36, 255-263.	1.0	17
147	Ab Initio Study of the Electronic Spectrum of B2H2. Journal of Molecular Spectroscopy, 1997, 182, 280-294.	0.4	17
148	Theoretical study of the ethylene radical cation: geometry and hyperfine structure. Chemical Physics, 1998, 236, 53-61.	0.9	17
149	Measurement and theoretical simulation of the HCCOâ^' anion photoelectron spectrum. Journal of Chemical Physics, 2001, 115, 1777-1788.	1.2	17
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