Friedrich Matthias Bickelhaupt

List of Publications by Year
in descending order

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393 papers	31,730 citations	9234 74 h-index	5227 165 g-index
436 all docs	436 docs citations	436 times ranked	18678 citing authors

#	Article	IF	Citations
1	Chemistry with ADF. Journal of Computational Chemistry, 2001, 22, 931-967.	1.5	8,854
2	Analyzing Reaction Rates with the Distortion/Interactionâ€Activation Strain Model. Angewandte Chemie - International Edition, 2017, 56, 10070-10086.	7.2	1,060
3	Voronoi deformation density (VDD) charges: Assessment of the Mulliken, Bader, Hirshfeld, Weinhold, and VDD methods for charge analysis. Journal of Computational Chemistry, 2004, 25, 189-210.	1.5	956
4	Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry. Reviews in Computational Chemistry, 2007, , 1-86.	1.5	775
5	The activation strain model and molecular orbital theory: understanding and designing chemical reactions. Chemical Society Reviews, 2014, 43, 4953-4967.	18.7	604
6	The activation strain model of chemical reactivity. Organic and Biomolecular Chemistry, 2010, 8, 3118.	1.5	599
7	Understanding reactivity with Kohn-Sham molecular orbital theory: E2-SN2 mechanistic spectrum and other concepts. Journal of Computational Chemistry, 1999, 20, 114-128.	1.5	515
8	Hydrogen Bonding in DNA Base Pairs:â€‰ Reconciliation of Theory and Experiment. Journal of the American Chemical Society, 2000, 122, 4117-4128.	6.6	418
9	Charge transport in columnar stacked triphenylenes: Effects of conformational fluctuations on charge transfer integrals and site energies. Journal of Chemical Physics, 2003, 119, 9809-9817.	1.2	395
10	The Nature of the Hydrogen Bond in DNA Base Pairs: The Role of Charge Transfer and Resonance Assistance. Chemistry - A European Journal, 1999, 5, 3581-3594.	1.7	340
11	Absolute Rates of Hole Transfer in DNA. Journal of the American Chemical Society, 2005, 127, 14894-14903.	6.6	325
12	Hydrogenâ€“Hydrogen Bonding in Planar Biphenyl, Predicted by Atoms-In-Molecules Theory, Does Not Exist. Chemistry - A European Journal, 2006, 12, 2889-2895.	1.7	314
13	Orbital Overlap and Chemical Bonding. Chemistry - A European Journal, 2006, 12, 9196-9216.	1.7	292
14	The Carbonâ^'Lithium Electron Pair Bond in (CH3Li)n(n= 1, 2, 4). Organometallics, 1996, 15, 2923-2931.	1.1	286
15	The activation strain model and molecular orbital theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 324-343.	6.2	280
16	The Nature of the Transition Metalâ^'Carbonyl Bond and the Question about the Valence Orbitals of Transition Metals. A Bond-Energy Decomposition Analysis of TM(CO)6q(TMq= Hf2-, Ta-, W, Re+, Os2+,) Tj ETQq0 0 0 rgBT /Overlock 10	6.6	280
17	The Case for Steric Repulsion Causing the Staggered Conformation of Ethane. Angewandte Chemie - International Edition, 2003, 42, 4183-4188.	7.2	225
18	A Model of the Chemical Bond Must Be Rooted in Quantum Mechanics, Provide Insight, and Possess Predictive Power. Chemistry - A European Journal, 2006, 12, 2902-2905.	1.7	216

#	Article	IF	Citations
19	Das Distortion/Interactionâ€Activationâ€Strainâ€Modell zur Analyse von Reaktionsgeschwindigkeiten. Angewandte Chemie, 2017, 129, 10204-10221.	1.6	209
20	Polycyclic Benzenoids:Â Why Kinked is More Stable than Straight. Journal of Organic Chemistry, 2007, 72, 1134-1142.	1.7	197
21	Nucleophilicity and Leaving-Group Ability in Frontside and Backside S_N2 Reactions. Journal of Organic Chemistry, 2008, 73, 7290-7299.	1.7	191
22	Central bond in the three CN.cntdot.dimers NC-CN, CN-CN and CN-NC: electron pair bonding and Pauli repulsion effects. The Journal of Physical Chemistry, 1992, 96, 4864-4873.	2.9	190
23	The many faces of halogen bonding: a review of theoretical models and methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 523-540.	6.2	188
24	Understanding chemical reactivity using the activation strain model. Nature Protocols, 2020, 15, 649-667.	5.5	188
25	Halogen Bonding versus Hydrogen Bonding: A Molecular Orbital Perspective. ChemistryOpen, 2012, 1, 96-105.	0.9	185
26	Alternatives to the CO Ligand: Coordination of the Isolobal Analogues BF, BNH2, BN(CH3)2, and BOâ‹® in Mono- and Binuclear First-Row Transition Metal Complexes. Chemistry - A European Journal, 1998, 4, 210-221.	1.7	172
27	Transition-State Energy and Position along the Reaction Coordinate in an Extended Activation Strain Model. ChemPhysChem, 2007, 8, 1170-1181.	1.0	171
28	Is CO a Special Ligand in Organometallic Chemistry? Theoretical Investigation of AB, Fe(CO)4AB, and Fe(AB)5(AB = N2, CO, BF, SiO). Inorganic Chemistry, 1998, 37, 1080-1090.	1.9	162
29	Nucleophilic Substitution at Silicon (SN2@Si) via a Central Reaction Barrier. Journal of Organic Chemistry, 2007, 72, 2201-2207.	1.7	154
30	Multicomponent Synthesis of 2-Imidazolines. Journal of Organic Chemistry, 2005, 70, 3542-3553.	1.7	152
31	Performance of various density functionals for the hydrogen bonds in DNA base pairs. Chemical Physics Letters, 2006, 426, 415-421.	1.2	149
32	Highly accelerated inverse electron-demand cycloaddition of electron-deficient azides with aliphatic cyclooctynes. Nature Communications, 2014, 5, 5378.	5.8	145
33	Activation of Hâ‹®H, Câ‹®H, Câ‹®C and Câ‹®Cl Bonds by Pd and PdCl-. Understanding Anion Assistance in Câ‹®X Bond Activation. Journal of Chemical Theory and Computation, 2005, 1, 286-298.	2.3	143
34	Nucleophilic Substitution at Phosphorus (SN2@P):Â Disappearance and Reappearance of Reaction Barriers. Journal of the American Chemical Society, 2006, 128, 10738-10744.	6.6	142
35	Nucleophilic Substitution (S_N2): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent. ChemPhysChem, 2018, 19, 1315-1330.	1.0	138
36	Oxidative addition of Pd to Câ€“H, Câ€“C and Câ€“Cl bonds: Importance of relativistic effects in DFT calculations. Journal of Chemical Physics, 2001, 115, 4030-4040.	1.2	136

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37	QUILD: QUantumâ€regions interconnected by local descriptions. Journal of Computational Chemistry, 2008, 29, 724-734.	1.5	135
38	Ab initio and DFT benchmark study for nucleophilic substitution at carbon (SN2@C) and silicon (SN2@Si). Journal of Computational Chemistry, 2005, 26, 1497-1504.	1.5	133
39	Telomere Structure and Stability: Covalency in Hydrogen Bonds, Not Resonance Assistance, Causes Cooperativity in Guanine Quartets. Chemistry - A European Journal, 2011, 17, 12612-12622.	1.7	130
40	Bonding capabilities of imidazol-2-ylidene ligands in group-10 transition-metal chemistry. Coordination Chemistry Reviews, 2009, 253, 678-686.	9.5	127
41	Ï€-Ï€ stacking tackled with density functional theory. Journal of Molecular Modeling, 2007, 13, 1245-1257.	0.8	126
42	Adenine versus guanine quartets in aqueous solution: dispersion-corrected DFT study on the differences in Ï€-stacking and hydrogen-bonding behavior. Theoretical Chemistry Accounts, 2010, 125, 245-252.	0.5	123
43	Activation of Hâˆ’H, Câˆ’H, Câˆ’C, and Câˆ’Cl Bonds by Pd(0). Insight from the Activation Strain Model. Journal of Physical Chemistry A, 2004, 108, 8460-8466.	1.1	117
44	Adenine Tautomers:â€‰ Relative Stabilities, Ionization Energies, and Mismatch with Cytosine. Journal of Physical Chemistry A, 2006, 110, 4012-4020.	1.1	115
45	Charge Transfer and Environment Effects Responsible for Characteristics of DNA Base Pairing. Angewandte Chemie - International Edition, 1999, 38, 2942-2945.	7.2	114
46	A new all-round density functional based on spin states and S[sub N]2 barriers. Journal of Chemical Physics, 2009, 131, 094103.	1.2	113
47	How Lewis Acids Catalyze Dielsâ€“Alder Reactions. Angewandte Chemie - International Edition, 2020, 59, 6201-6206.	7.2	113
48	Normal-to-Abnormal Rearrangement and NHC Activation in Three-Coordinate Iron(II) Carbene Complexes. Journal of the American Chemical Society, 2013, 135, 13338-13341.	6.6	110
49	Catalytic Carbonâˆ’Halogen Bond Activation:â€‰ Trends in Reactivity, Selectivity, and Solvation. Journal of Chemical Theory and Computation, 2007, 3, 514-529.	2.3	108
50	Contiguous Metalâ€Mediated Base Pairs Comprising Two Ag^I Ions. Chemistry - A European Journal, 2011, 17, 6533-6544.	1.7	108
51	para-Selective Câ€“H Olefination of Aniline Derivatives via Pd/S,O-Ligand Catalysis. Journal of the American Chemical Society, 2019, 141, 6719-6725.	6.6	108
52	Oxidative Insertion as Frontside SN2 Substitution: A Theoretical Study of the Model Reaction System Pd + CH3Cl. Organometallics, 1995, 14, 2288-2296.	1.1	102
53	Nature of the Three-Electron Bond in H2Sâˆ´SH2+Ââ€. Journal of Physical Chemistry A, 1998, 102, 9549-9553.	1.1	102
54	Optimization of strong and weak coordinates. International Journal of Quantum Chemistry, 2006, 106, 2536-2544.	1.0	101

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55	Why Do Cycloaddition Reactions Involving C₆₀ Prefer [6,6] over [5,6] Bonds?. Chemistry - A European Journal, 2013, 19, 7416-7422.	1.7	100
56	Mapping the Sites for Selective Oxidation of Guanines in DNA. Journal of the American Chemical Society, 2003, 125, 13658-13659.	6.6	97
57	DFT benchmark study for the oxidative addition of CH4 to Pd. Performance of various density functionals. Chemical Physics, 2005, 313, 261-270.	0.9	94
58	Alderâ€ene reaction: Aromaticity and activationâ€strain analysis. Journal of Computational Chemistry, 2012, 33, 509-516.	1.5	93
59	Proton Affinities in Water of Maingroup-Element Hydrides â€“ Effects of Hydration and Methyl Substitution. European Journal of Inorganic Chemistry, 2007, 2007, 3646-3654.	1.0	90
60	Hypervalent Silicon versus Carbon: Ballâ€inâ€aâ€Box Model. Chemistry - A European Journal, 2008, 14, 819-828.	1.7	90
61	How Dihalogens Catalyze Michael Addition Reactions. Angewandte Chemie - International Edition, 2019, 58, 8922-8926.	7.2	90
62	Energy landscapes of nucleophilic substitution reactions: A comparison of density functional theory and coupled cluster methods. Journal of Computational Chemistry, 2007, 28, 1551-1560.	1.5	89
63	Theoretical investigation on base-induced 1,2-eliminations in the model system fluoride ion + fluoroethane. The role of the base as a catalyst. Journal of the American Chemical Society, 1993, 115, 9160-9173.	6.6	87
64	Hydrogen Bonds of RNA Are Stronger than Those of DNA, but NMR Monitors Only Presence of Methyl Substituent in Uracil/Thymine. Journal of the American Chemical Society, 2004, 126, 16718-16719.	6.6	87
65	E2 and S_N2 Reactions of X^{â^'} + CH₃CH₂X (X = F, Cl); an ab Initio and DFT Benchmark Study. Journal of Chemical Theory and Computation, 2008, 4, 929-940.	2.3	86
66	Aromaticity and Activation Strain Analysis of [3 + 2] Cycloaddition Reactions between Group 14 Heteroallenes and Triple Bonds. Journal of Organic Chemistry, 2011, 76, 2310-2314.	1.7	86
67	Aromaticity: Molecular-Orbital Picture of an Intuitive Concept. Chemistry - A European Journal, 2007, 13, 6321-6328.	1.7	84
68	The Effect of Microsolvation on E2 and S_N2 Reactions: Theoretical Study of the Model System F^{â^'} + C₂H₅F + nHF. Chemistry - A European Journal, 1996, 2, 196-207.	1.7	83
69	Orbital Interactions in Strong and Weak Hydrogen Bonds are Essential for DNA Replication We thank the National Research School Combinationâ€"Catalysis (NRSCC) for a postdoctoral fellowship for C.F.G. and the National Computer Facilities (NCF) foundation of the Netherlands Organization for Scientific Research (NWO) for financial support.. Angewandte Chemie - International Edition, 2002, 41, 2092.	7.2	82
70	Oxidative Addition of the Chloromethane Câ^'Cl Bond to Pd, an ab Initio Benchmark and DFT Validation Study. Journal of Chemical Theory and Computation, 2006, 2, 322-335.	2.3	81
71	Theoretical study of structure, pKa, lipophilicity, solubility, absorption, and polar surface area of some centrally acting antihypertensives. Bioorganic and Medicinal Chemistry, 2006, 14, 1715-1728.	1.4	80
72	Typeâ€I Dyotropic Reactions: Understanding Trends in Barriers. Chemistry - A European Journal, 2012, 18, 12395-12403.	1.7	79

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73	Double Group Transfer Reactions: Role of Activation Strain and Aromaticity in Reaction Barriers. Chemistry - A European Journal, 2009, 15, 13022-13032.	1.7	76
74	Origin of the â€œendo ruleâ€•in Diels-Alder reactions. Journal of Computational Chemistry, 2014, 35, 371-376.	1.5	75
75	The Pauli Repulsion-Lowering Concept in Catalysis. Accounts of Chemical Research, 2021, 54, 1972-1981.	7.6	75
76	Catalyst selection based on intermediate stability measured by mass spectrometry. Nature Chemistry, 2010, 2, 417-421.	6.6	74
77	CH3â€¢Is Planar Due to Hâ‹¯H Steric Repulsion. Theoretical Study of MH3â€¢and MH3Cl (M = C, Si, Ge, Sn). Organometallics, 1996, 15, 1477-1487.	1.1	73
78	Ab initio benchmark study for the oxidative addition of CH4 to Pd: Importance of basis-set flexibility and polarization. Journal of Chemical Physics, 2004, 121, 9982-9992.	1.2	73
79	Chemical basis for the recognition of trimethyllysine by epigenetic reader proteins. Nature Communications, 2015, 6, 8911.	5.8	72
80	Cyclotrimerization Reactions Catalyzed by Rhodium(I) Half-Sandwich Complexes:â€‰ A Mechanistic Density Functional Study. Organometallics, 2007, 26, 3816-3830.	1.1	70
81	A Ditopic Ionâ€Pair Receptor Based on Stacked Nucleobase Quartets. Angewandte Chemie - International Edition, 2009, 48, 3285-3287.	7.2	70
82	Oxidative addition of the ethane Cï£¿C bond to Pd. Anab initiobenchmark and DFT validation study. Journal of Computational Chemistry, 2005, 26, 1006-1020.	1.5	69
83	The Donorâ€Stabilized Silylene Bis[N,Nâ€²â€diisopropylbenzamidinato(â‹¯)]silicon(II): Synthesis, Electronic Structure, and Reactivity. Chemistry - A European Journal, 2014, 20, 9319-9329.	1.7	69
84	Chemical reactivity from an activation strain perspective. Chemical Communications, 2021, 57, 5880-5896.	2.2	69
85	Double CH Activation of a Masked Cationic Bismuth Amide. Angewandte Chemie - International Edition, 2018, 57, 3825-3829.	7.2	66
86	Nucleophilic Substitution at C, Si and P: How Solvation Affects the Shape of Reaction Profiles. European Journal of Organic Chemistry, 2008, 2008, 649-654.	1.2	65
87	Controlling the oxidative addition of aryl halides to Au(I). Journal of Computational Chemistry, 2014, 35, 2140-2145.	1.5	65
88	B-DNA structure and stability: the role of hydrogen bonding, Ï€â€“Ï€ stacking interactions, twist-angle, and solvation. Organic and Biomolecular Chemistry, 2014, 12, 4691-4700.	1.5	64
89	Nucleophilic Substitution at Phosphorus Centers (S_N2@P). ChemPhysChem, 2007, 8, 2452-2463.	1.0	63
90	Might BF and BNR2 be alternatives to CO? A theoretical quest for new ligands in organometallic chemistry. New Journal of Chemistry, 1998, 22, 1-3.	1.4	61

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91	Oxidative Addition of the Fluoromethane Câ^'F Bond to Pd. An ab Initio Benchmark and DFT Validation Study. Journal of Physical Chemistry A, 2005, 109, 9685-9699.	1.1	61
92	The Steric Nature of the Bite Angle. Chemistry - A European Journal, 2009, 15, 6112-6115.	1.7	61
93	Silver(I)-mediated Hoogsteen-type base pairs. Journal of Inorganic Biochemistry, 2011, 105, 1398-1404.	1.5	59
94	Role of Orbital Interactions and Activation Strain (Distortion Energies) on Reactivities in the Normal and Inverse Electron-Demand Cycloadditions of Strained and Unstrained Cycloalkenes. Journal of Organic Chemistry, 2017, 82, 8668-8675.	1.7	59
95	Carbon monoxide insertion at a heavy p-block element: unprecedented formation of a cationic bismuth carbamoyl. Chemical Science, 2019, 10, 4169-4176.	3.7	59
96	Bonding of Imidazol-2-ylidene Ligands in Nickel Complexes. Organometallics, 2008, 27, 3410-3414.	1.1	58
97	On the origin of the steric effect. Physical Chemistry Chemical Physics, 2012, 14, 9846.	1.3	58
98	Role of Steric Attraction and Bite-Angle Flexibility in Metal-Mediated Câ€“H Bond Activation. ACS Catalysis, 2015, 5, 5766-5775.	5.5	58
99	PyFrag 2019â€”Automating the exploration and analysis of reaction mechanisms. Journal of Computational Chemistry, 2019, 40, 2227-2233.	1.5	57
100	Eneâ€eneâ€yne Reactions: Activation Strain Analysis and the Role of Aromaticity. Chemistry - A European Journal, 2014, 20, 10791-10801.	1.7	56
101	Proton Affinities of Anionic Bases:â€‰ Trends Across the Periodic Table, Structural Effects, and DFT Validation. Journal of Chemical Theory and Computation, 2006, 2, 281-287.	2.3	55
102	Origin of rate enhancement and asynchronicity in iminium catalyzed Dielsâ€“Alder reactions. Chemical Science, 2020, 11, 8105-8112.	3.7	55
103	The Short Nâ^'F Bond in N2F+and How Pauli Repulsion Influences Bond Lengths. Theoretical Study of N2X+, NF3X+, and NH3X+(X = F, H). Journal of the American Chemical Society, 2002, 124, 1500-1505.	6.6	54
104	Frontside versus Backside S_N2 Substitution at Groupâ€…14 Atoms: Origin of Reaction Barriers and Reasons for Their Absence. Chemistry - an Asian Journal, 2008, 3, 1783-1792.	1.7	54
105	Chemical Shifts in Nucleic Acids Studied by Density Functional Theory Calculations and Comparison with Experiment. Chemistry - A European Journal, 2012, 18, 12372-12387.	1.7	54
106	Unusual reactivity of small cyclophanes: nucleophilic attack on 11-chloro- and 8,11-dichloro[5]metacyclophane. Journal of the American Chemical Society, 1990, 112, 6638-6646.	6.6	53
107	Nucleophilic Substitution in Solution: Activation Strain Analysis of Weak and Strong Solvent Effects. Chemistry - A European Journal, 2018, 24, 5927-5938.	1.7	53
108	Theoretical investigation of the relative stabilities ofXSSXandX2SS isomers (X= F, Cl, H, and CH3). Journal of Computational Chemistry, 1995, 16, 465-477.	1.5	52

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109	Selectivity in DNA replication. Interplay of steric shape, hydrogen bonds, Ï€-stacking and solvent effects. Chemical Communications, 2011, 47, 7326.	2.2	52
110	Nonlinear d¹⁰â€“ML₂ Transitionâ€“Metal Complexes. ChemistryOpen, 2013, 2, 106-114.	0.9	52
111	Orbital Interactions in Hydrogen Bonds Important for Cohesion in Molecular Crystals and Mismatched Pairs of DNA Bases. Crystal Growth and Design, 2002, 2, 239-245.	1.4	50
112	Hypervalent Carbon Atom: â€œFreezingâ€•the S_N2 Transition State. Angewandte Chemie - International Edition, 2009, 48, 6469-6471.	7.2	49
113	Stepwise walden inversion in nucleophilic substitution at phosphorus. Physical Chemistry Chemical Physics, 2009, 11, 259-267.	1.3	49
114	Steric nature of the bite angle. A closer and a broader look. Dalton Transactions, 2011, 40, 3028.	1.6	49
115	Reactivity of the Donorâ€“Stabilized Silylenes [iPrNC(Ph)NiPr]₂Si and [iPrNC(NiPr₂)NiPr]₂Si: Activation of CO₂ and CS₂. Chemistry - A European Journal, 2015, 21, 16665-16672.	1.7	49
116	Activation-Strain Analysis Reveals Unexpected Origin of Fast Reactivity in Heteroaromatic Azadiene Inverse-Electron-Demand Dielsâ€“Alder Cycloadditions. Journal of Organic Chemistry, 2015, 80, 548-558.	1.7	49
117	Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies. Chemistry - A European Journal, 2019, 25, 6342-6348.	1.7	49
118	8 Energy decomposition analysis in the context of quantitative molecular orbital theory. , 2021, , 199-212.		49
119	Covalency in Highly Polar Bonds. Structure and Bonding of Methylalkalimetal Oligomers (CH3M)n (M) Tj ETQq1 1 0.784314 rgBT /Ov	2.3	48
120	Stereodivergent S_N2@P Reactions of Borane Oxazaphospholidines: Experimental and Theoretical Studies. Journal of the American Chemical Society, 2013, 135, 4483-4491.	6.6	48
121	Supramolecular Switches Based on the Guanineâ€“Cytosine (GC) Watsonâ€“Crick Pair: Effect of Neutral and Ionic Substituents. Chemistry - A European Journal, 2006, 12, 3032-3042.	1.7	47
122	Intercalation of Daunomycin into Stacked DNA Base Pairs. DFT Study of an Anticancer Drug. Journal of Biomolecular Structure and Dynamics, 2008, 26, 115-129.	2.0	47
123	Deeper Insight into the Dielsâ€“Alder Reaction through the Activation Strain Model. Chemistry - an Asian Journal, 2016, 11, 3297-3304.	1.7	47
124	Origin of the Î±â€Effect in S_N2 Reactions. Angewandte Chemie - International Edition, 2021, 60, 20840-20848.	7.2	47
125	Role of the Chalcogen (S, Se, Te) in the Oxidation Mechanism of the Glutathione Peroxidase Active Site. ChemPhysChem, 2017, 18, 2990-2998.	1.0	46
126	Understanding the Reactivity of Endohedral Metallofullerenes: C₇₈ versus Sc₃N@C₇₈. Chemistry - A European Journal, 2015, 21, 5760-5768.	1.7	45

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127	Î±-Stabilization of Carbanions: Fluorine Is More Effective than the Heavier Halogens. Angewandte Chemie - International Edition, 2006, 45, 823-826.	7.2	44
128	PyFragâ€"Streamlining your reaction path analysis. Journal of Computational Chemistry, 2008, 29, 312-315.	1.5	44
129	Reaction Coordinates and the Transition-Vector Approximation to the IRC. Journal of Chemical Theory and Computation, 2008, 4, 920-928.	2.3	43
130	Chemoselectivity of Tertiary Azides in Strainâ€Promoted Alkyneâ€Azide Cycloadditions. Chemistry - A European Journal, 2019, 25, 754-758.	1.7	43
131	Proton affinities of maingroup-element hydrides and noble gases: Trends across the periodic table, structural effects, and DFT validation. Journal of Computational Chemistry, 2006, 27, 1486-1493.	1.5	42
132	How Lewis Acids Catalyze Dielsâ€"Alder Reactions. Angewandte Chemie, 2020, 132, 6260-6265.	1.6	42
133	Hydrogen Bonding in Mimics of Watsonâ€"Crick Base Pairs Involving Cï£¿H Proton Donor and F Proton Acceptor Groups: A Theoretical Study. ChemPhysChem, 2004, 5, 481-487.	1.0	41
134	Oxidative addition to main group versus transition metals: Insights from the Activation Strain model. Journal of Organometallic Chemistry, 2006, 691, 4341-4349.	0.8	41
135	Theoretical and Experimental Study of Charge Transfer through DNA: Impact of Mercury Mediated T-Hg-T Base Pair. Journal of Physical Chemistry B, 2014, 118, 5374-5381.	1.2	41
136	Radon hydrides: structure and bonding. Physical Chemistry Chemical Physics, 2011, 13, 2222-2227.	1.3	40
137	Understanding E2 versus S_N2 Competition under Acidic and Basic Conditions. ChemistryOpen, 2014, 3, 29-36.	0.9	40
138	Regioselectivity of Epoxide Ringâ€Openings via S_N2 Reactions Under Basic and Acidic Conditions. European Journal of Organic Chemistry, 2020, 2020, 3822-3828.	1.2	40
139	Structure and Bonding of Transition Metalâ^'Boryl Compounds. Theoretical Study of [(PH3)2(CO)ClOsâ^'BR2] and [(PH3)2(CO)2ClOsâ^'BR2] (BR2= BH2, BF2, B(OH)2, B(OCHCHO), Bcat)â€. Inorganic Chemistry, 2000, 39, 4776-4785.	1.9	39
140	Bonding in Methylalkalimetals (CH3M)n(M = Li, Na, K;n= 1, 4). Agreement and Divergences between AIM and ELF Analysesâ€. Journal of Physical Chemistry B, 2006, 110, 7189-7198.	1.2	39
141	Didehydrophenanthrenes:â€‰ Structure, Singletâ^'Triplet Splitting, and Aromaticity. Journal of Physical Chemistry A, 2007, 111, 5063-5070.	1.1	39
142	Aromaticity and Antiaromaticity in 4-, 6-, 8-, and 10-Membered Conjugated Hydrocarbon Rings. Journal of Physical Chemistry A, 2008, 112, 12816-12822.	1.1	39
143	Bonding of Xenon Hydrides. Journal of Physical Chemistry A, 2009, 113, 9700-9706.	1.1	39
144	Neutral Six-Coordinate and Cationic Five-Coordinate Silicon(IV) Complexes with Two Bidentate Monoanionic N,S-Pyridine-2-thiolato(â^) Ligands. Inorganic Chemistry, 2013, 52, 10664-10676.	1.9	39

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145	Computationally Guided Molecular Design to Minimize the LE/CT Gap in Dâ€Ïâ€A Fluorinated Triarylboranes for Efficient TADF via D and Ïâ€Bridge Tuning. Advanced Functional Materials, 2020, 30, 2002064.	7.8	39
146	The pnictogen bond: a quantitative molecular orbital picture. Physical Chemistry Chemical Physics, 2021, 23, 13842-13852.	1.3	39
147	Orbital interactions and charge redistribution in weak hydrogen bonds: The Watsonâ€“Crick AT mimic adenine-2,4-difluorotoluene. Journal of Chemical Physics, 2003, 119, 4262-4273.	1.2	38
148	Oxidative Addition versus Dehydrogenation of Methane, Silane, and Heavier AH4Congeners Reacting with Palladium. Organometallics, 2006, 25, 4260-4268.	1.1	38
149	Origins of the Endo and Exo Selectivities in Cyclopropenone, Iminocyclopropene, and Triafulvene Dielsâ€“Alder Cycloadditions. Journal of Organic Chemistry, 2018, 83, 3164-3170.	1.7	38
150	A Unified Framework for Understanding Nucleophilicity and Protophilicity in the S_N2/E2 Competition. Chemistry - A European Journal, 2020, 26, 15538-15548.	1.7	38
151	Hypervalent versus Nonhypervalent Carbon in Nobleâ€Gas Complexes. Chemistry - A European Journal, 2008, 14, 6901-6911.	1.7	37
152	Additionâ€“Elimination or Nucleophilic Substitution? Understanding the Energy Profiles for the Reaction of Chalcogenolates with Dichalcogenides. Journal of Chemical Theory and Computation, 2016, 12, 2752-2761.	2.3	37
153	Elucidating the Trends in Reactivity of Azaâ€1,3â€Dipolar Cycloadditions. European Journal of Organic Chemistry, 2019, 2019, 378-386.	1.2	37
154	Bifunctional Hydrogen Bond Donorâ€Catalyzed Dielsâ€“Alder Reactions: Origin of Stereoselectivity and Rate Enhancement. Chemistry - A European Journal, 2021, 27, 5180-5190.	1.7	37
155	How Oriented External Electric Fields Modulate Reactivity. Chemistry - A European Journal, 2021, 27, 5683-5693.	1.7	37
156	3-Substituted xanthines as promising candidates for quadruplex formation: computational, synthetic and analytical studies. New Journal of Chemistry, 2011, 35, 476-482.	1.4	36
157	New Concepts for Designing d¹⁰â€M(L)_n Catalysts: d Regime, s Regime and Intrinsic Biteâ€Angle Flexibility. Chemistry - A European Journal, 2014, 20, 11370-11381.	1.7	36
158	Factors Controlling Î²â€Elimination Reactions in Groupâ€...10 Metal Complexes. Chemistry - A European Journal, 2015, 21, 14362-14369.	1.7	36
159	Direct detection of the mercuryâ€“nitrogen bond in the thymineâ€“Hg^{II}â€“thymine base-pair with ¹⁹⁹Hg NMR spectroscopy. Chemical Communications, 2015, 51, 8488-8491.	2.2	36
160	Highly Stable and Selective Tetrazines for the Coordination-Assisted Bioorthogonal Ligation with Vinylboronic Acids. Bioconjugate Chemistry, 2018, 29, 3054-3059.	1.8	36
161	Bismuth Amides Mediate Facile and Highly Selective Pnâ€“Pn Radicalâ€Coupling Reactions (Pn=N, P, As). Angewandte Chemie - International Edition, 2021, 60, 6441-6445.	7.2	36
162	Koordinationseigenschaften der isolobalen Phosphaniminatound Cyclopentadienyl-Liganden in TiCl3(NPH3), TiCl3Cp, ReO3(NPH3) und ReO3Cp. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 1999, 625, 892-900.	0.6	35

#	Article	IF	Citations
163	Fragment-oriented design of catalysts based on the activation strain model. Molecular Physics, 2005, 103, 995-998.	0.8	35
164	Mechanism of Thioredoxin-Catalyzed Disulfide Reduction. Activation of the Buried Thiol and Role of the Variable Active-Site Residues. Journal of Physical Chemistry B, 2008, 112, 2511-2523.	1.2	35
165	Reactivity in Nucleophilic Vinylic Substitution (SNV):SNVÏ€ versus SNVÏƒ Mechanistic Dichotomy. Journal of Organic Chemistry, 2013, 78, 8574-8584.	1.7	35
166	Interâ€•and intramolecular dispersion interactions. Journal of Computational Chemistry, 2011, 32, 1117-1127.	1.5	34
167	Origin of Reactivity Trends of Noble Gas Endohedral Fullerenes Ng₂@C₆₀ (Ng) Tj ETQq1 1 0.784314 rgBT /	2.3	34
168	(4 + 2) and (2 + 2) Cycloadditions of Benzyne to C₆₀ and Zig-Zag Single-Walled Carbon Nanotubes: The Effect of the Curvature. Journal of Physical Chemistry C, 2016, 120, 1716-1726.	1.5	34
169	Base-induced 1,4-elimination:Insights from theory and mass spectrometry. Mass Spectrometry Reviews, 2001, 20, 347-361.	2.8	33
170	Density Functional Calculations of E2 and S_N2 Reactions: Effects of the Choice of Method, Algorithm, and Numerical Accuracy. Journal of Chemical Theory and Computation, 2010, 6, 3145-3152.	2.3	33
171	Synthesis and structural characterisation of neutral pentacoordinate silicon(iv) complexes with a tridentate dianionic N,N,S chelate ligand. Dalton Transactions, 2012, 41, 2148-2162.	1.6	33
172	Understanding the Reactivity of Ionâ€Encapsulated Fullerenes. Chemistry - A European Journal, 2017, 23, 11030-11036.	1.7	33
173	Dihydrogen Bonding: Donorâ€“Acceptor Bonding (AHâ‹…â‹…â‹…HX) versus the H₂ Molecule (Aï£¿H₂ï£¿X). Chemistry - A European Journal, 2009, 15, 5814-5822.	1.7	32
174	Solvent effects on hydrogen bonds in Watsonâ€“Crick, mismatched, and modified DNA base pairs. Computational and Theoretical Chemistry, 2012, 998, 57-63.	1.1	32
175	Bâ€ÐNA Structure and Stability as Function of Nucleic Acid Composition: Dispersionâ€Corrected DFT Study of Dinucleoside Monophosphate Single and Double Strands. ChemistryOpen, 2013, 2, 186-193.	0.9	32
176	Indenyl Effect Due to Metal Slippage? Computational Exploration of Rhodiumâ€Catalyzed Acetylene [2+2+2] Cyclotrimerization. ChemPhysChem, 2014, 15, 219-228.	1.0	32
177	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. ChemistryOpen, 2021, 10, 391-401.	0.9	32
178	Thermodynamics of the Cu^{II} Î¼-Thiolate and Cu^I Disulfide Equilibrium: A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2014, 53, 8494-8504.	1.9	31
179	Reactivity and Selectivity of Bowlâ€Shaped Polycyclic Aromatic Hydrocarbons: Relationship to C₆₀. Chemistry - A European Journal, 2016, 22, 1368-1378.	1.7	31
180	Substituent Effects on Hydrogen Bonding in Watsonâ€“Crick Base Pairs. A Theoretical Study. Structural Chemistry, 2005, 16, 211-221.	1.0	30

#	Article	IF	Citations
181	Rare Tautomers of 1â€Methyluracil and 1â€Methylthymine: Tuning Relative Stabilities through Coordination to Pt^{II} Complexes. Chemistry - A European Journal, 2009, 15, 209-218.	1.7	30
182	Ionâ€Pair S_N2 Substitution: Activation Strain Analyses of Counterâ€Ion and Solvent Effects. Chemistry - A European Journal, 2016, 22, 4431-4439.	1.7	30
183	Chimeric GNA/DNA metal-mediated base pairs. Chemical Communications, 2011, 47, 11041.	2.2	29
184	Rationalizing the Structural Variability of the Exocyclic Amino Groups in Nucleobases and Their Metal Complexes: Cytosine and Adenine. Chemistry - A European Journal, 2014, 20, 9494-9499.	1.7	29
185	Stable Fourâ€Coordinate Guanidinatosilicon(IV) Complexes with SiN 3 El Skeletons (El=S, Se, Te) and Sïï£¾El Double Bonds. Chemistry - A European Journal, 2015, 21, 14011-14021.	1.7	29
186	Activation Strain Analysis of S_N2 Reactions at C, N, O, and F Centers. Journal of Physical Chemistry A, 2017, 121, 885-891.	1.1	29
187	How the electron-deficient cavity of heterocalixarenes recognizes anions: insights from computation. Physical Chemistry Chemical Physics, 2017, 19, 24696-24705.	1.3	29
188	1,4-Diphosphabutadiyne: A Realistic Target for Synthesis? A Theoretical Investigation of C2P2, C2N2, [Cr(CO)5PCCP], and [(CO)5Cr(PCCP)Cr(CO)5]. Chemistry - A European Journal, 1999, 5, 162-174.	1.7	28
189	Scope and Limitations of an Efficient Four-Component Reaction for Dihydropyridin-2-ones. Journal of Organic Chemistry, 2010, 75, 1723-1732.	1.7	28
190	Theoretical Study of the Structure and Bonding in ThC₂ and UC₂. Journal of Physical Chemistry A, 2012, 116, 747-755.	1.1	28
191	Silicon Î±-Effect: A Systematic Experimental and Computational Study of the Hydrolysis of C_{Î±}- and C_{Î³}-Functionalized Alkoxytriorganylsilanes of the Formula Type ROSiMe₂(CH₂)_nX (R = Me, Et; n = 1, 3; X = Functional) Tj ETQq1 1 0.784314 rg	1.1	28
192	Bis[N,Nâ€²â€diisopropylbenzamidinato(â^')]silicon(<scp>II</scp>): Lewis Acid/Base Reactions with Triorganylboranes. Chemistry - A European Journal, 2014, 20, 12411-12415.	1.7	28
193	Aromaticity in Heterocyclic and Inorganic Benzene Analogues. Australian Journal of Chemistry, 2008, 61, 209.	0.5	27
194	Methyl Cation Affinities of Neutral and Anionic Maingroup-Element Hydrides: Trends Across the Periodic Table and Correlation with Proton Affinities. Journal of Physical Chemistry A, 2010, 114, 7604-7608.	1.1	27
195	In Silico Design of Heteroaromatic Halfâ€Sandwich Rh^I Catalysts for Acetylene [2+2+2] Cyclotrimerization: Evidence of a Reverse Indenylâ€‰Effect. Chemistry - A European Journal, 2013, 19, 13337-13347.	1.7	27
196	Bite-angle bending as a key for understanding group-10 metal reactivity of d¹⁰-[M(NHC)₂] complexes with sterically modest NHC ligands. Chemical Science, 2015, 6, 1426-1432.	3.7	27
197	Oxidation of organic diselenides and ditellurides by H₂O₂for bioinspired catalyst design. Physical Chemistry Chemical Physics, 2018, 20, 20874-20885.	1.3	27
198	Nâ€‹Heterocyclic Silylenes as Ligands in Transition Metal Carbonyl Chemistry: Nature of Their Bonding and Supposed Innocence. Chemistry - A European Journal, 2020, 26, 11276-11292.	1.7	27

#	Article	IF	Citations
199	Halogen Bonds in Ligandâ€“Protein Systems: Molecular Orbital Theory for Drug Design. Journal of Chemical Information and Modeling, 2020, 60, 1317-1328.	2.5	27
200	Gas-Phase Base-Induced 1,4-Eliminations: Occurrence of Single-, Double-, and Triple-Well E1cb Mechanisms. Journal of the American Chemical Society, 1995, 117, 9889-9899.	6.6	26
201	Rational design of nearâ€infrared absorbing organic dyes: Controlling the HOMOâ€“LUMO gap using quantitative molecular orbital theory. Journal of Computational Chemistry, 2018, 39, 2690-2696.	1.5	26
202	Anion Recognition by Organometallic Calixarenes: Analysis from Relativistic DFT Calculations. Organometallics, 2018, 37, 2167-2176.	1.1	26
203	Arylic Câ€“X Bond Activation by Palladium Catalysts: Activation Strain Analyses of Reactivity Trends. Scientific Reports, 2018, 8, 10729.	1.6	26
204	Lewis Acidâ€Catalyzed Dielsâ€Alder Reactions: Reactivity Trends across the Periodic Table. Chemistry - A European Journal, 2021, 27, 10610-10620.	1.7	26
205	The Chemical Bond: When Atom Size Instead of Electronegativity Difference Determines Trend in Bond Strength. Chemistry - A European Journal, 2021, 27, 15616-15622.	1.7	26
206	How Solvation Influences the S_N2 versus E2 Competition. Journal of Organic Chemistry, 2022, 87, 1805-1813.	1.7	26
207	Structure and Stability of the Li2CN Molecule. An Experimental and ab Initio Study. The Journal of Physical Chemistry, 1995, 99, 6477-6482.	2.9	25
208	Understanding the Oxidative Addition of Ïƒâ€Bonds to Groupâ€…13 Compounds. Chemistry - A European Journal, 2016, 22, 13669-13676.	1.7	25
209	B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication. Physical Chemistry Chemical Physics, 2017, 19, 16969-16978.	1.3	25
210	Deracemization of a Racemic Allylic Sulfoxide Using Viedma Ripening. Crystal Growth and Design, 2017, 17, 4454-4457.	1.4	25
211	Doppelte CHâ€Aktivierung eines maskierten Bismutamidâ€Kations. Angewandte Chemie, 2018, 130, 3887-3891.	1.6	25
212	Clarifying notes on the bonding analysis adopted by the energy decomposition analysis. Physical Chemistry Chemical Physics, 2022, 24, 15726-15735.	1.3	25
213	Activation of Câ€“H, Câ€“C and Câ€“I bonds by Pd and cis-Pd(CO)2I2. Catalystâ€“substrate adaptation. Journal of Organometallic Chemistry, 2005, 690, 2191-2199.	0.8	24
214	Hypervalence and the delocalizing versus localizing propensities of H 3 â€“ , Li 3 â€“ , CH 5 â€“ and SiH 5 â€“. Structural Chemistry, 2007, 18, 813-819.	1.0	24
215	Linkage Isomerism of Nitriles in Rhodium Half-Sandwich Metallacycles. Organometallics, 2008, 27, 4028-4030.	1.1	24
216	Role of sâ^'p Orbital Mixing in the Bonding and Properties of Second-Period Diatomic Molecules. Journal of Physical Chemistry A, 2008, 112, 2437-2446.	1.1	24

#	Article	IF	Citations
217	Remote Communication in a DNAâ€Based Nanoswitch. Chemistry - A European Journal, 2011, 17, 8816-8818.	1.7	24
218	Not Carbon sâ€“p Hybridization, but Coordination Number Determines Câ^'H and Câ^'C Bond Length. Chemistry - A European Journal, 2021, 27, 7074-7079.	1.7	24
219	Reaction Mechanism and Regioselectivity of the Bingelâ€“Hirsch Addition of Dimethyl Bromomalonate to La@C_{2v}â€C₈₂. Chemistry - A European Journal, 2016, 22, 5953-5962.	1.7	23
220	Nature and strength of chalcogenâ€“Ï€ bonds. Physical Chemistry Chemical Physics, 2018, 20, 27592-27599.	1.3	23
221	Ambident Nucleophilic Substitution: Understanding Nonâ€HSAB Behavior through Activation Strain and Conceptual DFT Analyses. Chemistry - A European Journal, 2020, 26, 3884-3893.	1.7	23
222	Origin of asynchronicity in Dielsâ€“Alder reactions. Physical Chemistry Chemical Physics, 2021, 23, 20095-20106.	1.3	23
223	A Helicoid Ferrocene. Inorganic Chemistry, 2009, 48, 2714-2716.	1.9	22
224	Tuning Heterocalixarenes to Improve Their Anion Recognition: A Computational Approach. Journal of Physical Chemistry A, 2018, 122, 3328-3336.	1.1	22
225	Factors Controlling the Dielsâ€“Alder Reactivity of Heteroâ€1,3â€Butadienes. ChemistryOpen, 2018, 7, 995-1004.	0.9	22
226	S_N2 versus E2 Competition of F^{â€“}and PH₂^{â€“}Revisited. Journal of Organic Chemistry, 2020, 85, 14087-14093.	1.7	22
227	Switching between OPTX and PBE exchange functionals. Journal of Computational Methods in Sciences and Engineering, 2009, 9, 69-77.	0.1	21
228	Comment on â€œThe Interplay between Steric and Electronic Effects in SN2 Reactionsâ€. Chemistry - A European Journal, 2010, 16, 5538-5541.	1.7	21
229	Neutral Pentacoordinate Halogeno- and Pseudohalogenosilicon(IV) Complexes with a Tridentate Dianionic O,N,O or N,N,O Ligand: Synthesis and Structural Characterization in the Solid State and in Solution. European Journal of Inorganic Chemistry, 2012, 2012, 3216-3228.	1.0	21
230	Performance of TDDFT Vertical Excitation Energies of Coreâ€Substituted Naphthalene Diimides. Journal of Computational Chemistry, 2020, 41, 1448-1455.	1.5	21
231	Chalcogen bonds: Hierarchical ab initio benchmark and density functional theory performance study. Journal of Computational Chemistry, 2021, 42, 688-698.	1.5	21
232	Orbitalwechselwirkungen in starken und schwachen WasserstoffbrÃ¼cken sind essentiell fÃ¼r die DNA-Replikation Wir danken der Stiftung Nationale Computerfaciliteiten (NCF) der Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO) fÃ¼r finanzielle UnterstÃ¼tzung. C.F.G. dankt der National Research School Combination-Catalysis (NRSCC) fÃ¼r ein Stipendium.. Angewandte Chemie, 2002, 114, 2194.	1.6	20
233	Stereoselective Synthesis of 1-Tuberculosinyl Adenosine; a Virulence Factor of Mycobacterium tuberculosis. Journal of Organic Chemistry, 2016, 81, 6686-6696.	1.7	20
234	Wie Dihalogene Michaelâ€Additionsreaktionen katalysieren. Angewandte Chemie, 2019, 131, 9015-9020.	1.6	20

#	Article	IF	Citations
235	Understanding the 1,3â€Dipolar Cycloadditions of Allenes. Chemistry - A European Journal, 2020, 26, 11529-11539.	1.7	20
236	Highly polar bonds and the meaning of covalency and ionicityâ€"structure and bonding of alkali metal hydride oligomers. Faraday Discussions, 2007, 135, 451-468.	1.6	19
237	Halogen versus halide electronic structure. Science China Chemistry, 2010, 53, 210-215.	4.2	19
238	Symmetrical P4 cleavage at cobalt half sandwich complexes [(Î·5-C5H5)Co(L)] (L = CO, NHC) â€" a computational case study on the mechanism of symmetrical P4 degradation to P2 ligands. Dalton Transactions, 2013, 42, 7468.	1.6	19
239	How Alkali Cations Catalyze Aromatic Dielsâ€Alder Reactions. Chemistry - an Asian Journal, 2020, 15, 1167-1174.	1.7	19
240	Base-induced imine-forming 1,2-elimination reactions in the gas phase. Journal of Organic Chemistry, 1993, 58, 2436-2441.	1.7	18
241	Nanoswitches Based on DNA Base Pairs: Why Adenineâ€"Thymine is Less Suitable than Guanineâ€"Cytosine. ChemPhysChem, 2006, 7, 1971-1979.	1.0	18
242	Covalentversus ionic bonding in alkalimetal fluoride oligomers. Journal of Computational Chemistry, 2007, 28, 238-250.	1.5	18
243	Differential stabilization of adenine quartets by anions and cations. Journal of Biological Inorganic Chemistry, 2010, 15, 387-397.	1.1	18
244	Neutral and positively charged new purine tetramer structures: a computational study of xanthine and uric acid derivatives. New Journal of Chemistry, 2011, 35, 119-126.	1.4	18
245	Regioselectivity in Electrophilic Aromatic Substitution: Insights from Interaction Energy Decomposition Potentials. European Journal of Organic Chemistry, 2011, 2011, 2958-2968.	1.2	18
246	Stabilisation of 2,6â€Diarylpyridinium Cation by Throughâ€Space Polarâ€"Ï€ Interactions. Chemistry - A European Journal, 2014, 20, 6268-6271.	1.7	18
247	Reactions of the Donor-Stabilized Silylene Bis[N,Nâ€²-diisopropyl-benzamidinato(â^')]silicon(II) with BrÃ¸nsted Acids. Chemistry - A European Journal, 2014, 20, 16462-16466.	1.7	18
248	Stabilization of 2,6-Diarylanilinum Cation by Through-Space Cationâ^'Ï€ Interactions. Journal of Organic Chemistry, 2017, 82, 9418-9424.	1.7	18
249	Trifluoromethyl Vinyl Sulfide: A Building Block for the Synthesis of CF₃S-Containing Isoxazolidines. Journal of Organic Chemistry, 2018, 83, 1779-1789.	1.7	18
250	A methodology for the photocatalyzed radical trifluoromethylation of indoles: A combined experimental and computational study. Journal of Fluorine Chemistry, 2018, 214, 94-100.	0.9	18
251	Multi-step processes in gas-phase reactions of halomethyl anions XCH2? (X = Cl,Br) with CH3X and NH3. Journal of Physical Organic Chemistry, 1992, 5, 179-190.	0.9	17
252	Table Salt and Other Alkali Metal Chloride Oligomers:â€‰ Structure, Stability, and Bonding. Inorganic Chemistry, 2007, 46, 5411-5418.	1.9	17

#	Article	IF	Citations
253	Trends and anomalies in Hâ€“AHn and CH3â€“AHn bond strengths (AHn = CH3, NH2, OH, F). Physical Chemistry Chemical Physics, 2009, 11, 10317.	1.3	17
254	Aggregation and Cooperative Effects in the Aldol Reactions of Lithium Enolates. Chemistry - A European Journal, 2013, 19, 13761-13773.	1.7	17
255	Supramolecular H-bonded porous networks at surfaces: exploiting primary and secondary interactions in a bi-component melamineâ€“xanthine system. Physical Chemistry Chemical Physics, 2013, 15, 12442.	1.3	17
256	The substituent effect on benzene dications. Physical Chemistry Chemical Physics, 2014, 16, 4752-4763.	1.3	17
257	Eight-coordinate fluoride in a silicate double-four-ring. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 828-833.	3.3	17
258	Cesium's Offâ€theâ€Map Valence Orbital. Angewandte Chemie - International Edition, 2017, 56, 9772-9776.	7.2	17
259	Enhanced Ï€â€Backâ€Donation as a Way to Higher Coordination Numbers in d¹⁰ [M(NHC)_n] Complexes: A DFT Study. Chemistry - A European Journal, 2017, 23, 614-622.	1.7	17
260	How metallylenes activate small molecules. Chemical Science, 2021, 12, 4526-4535.	3.7	17
261	The Gauche Effect in XCH₂CH₂X Revisited. ChemPhysChem, 2021, 22, 641-648.	1.0	17
262	â€œForbiddenâ€•Four-Center Reactions:Â Molecular Orbital Considerations for N2+ N2and N2+ N2+. Journal of Physical Chemistry A, 1997, 101, 8255-8263.	1.1	16
263	X₂Y₂ Isomers: Tuning Structure and Relative Stability through Electronegativity Differences (X = H, Li, Na, F, Cl, Br, I; Y = O, S, Se, Te). Inorganic Chemistry, 2013, 52, 2458-2465.	1.9	16
264	Source of Cooperativity in Halogenâ€Bonded Haloamine Tetramers. ChemPhysChem, 2016, 17, 474-480.	1.0	16
265	Asymmetric identity SN2 transition states: Nucleophilic substitution at Î±-substituted carbon and silicon centers. International Journal of Mass Spectrometry, 2017, 413, 85-91.	0.7	16
266	How Mg²⁺ ions lower the S_N2@P barrier in enzymatic triphosphate hydrolysis. Chemical Communications, 2018, 54, 3448-3451.	2.2	16
267	Dual Activation of Aromatic Dielsâ€“Alder Reactions. Chemistry - A European Journal, 2019, 25, 9902-9912.	1.7	16
268	Ligandâ€Mediated Regioselective Rhodiumâ€Catalyzed Benzotriazoleâ€“Allene Coupling: Mechanistic Exploration and Quantum Chemical Analysis. Chemistry - A European Journal, 2020, 26, 2342-2348.	1.7	16
269	Origin of the Î±â€Effect in S_N2 Reactions. Angewandte Chemie, 2021, 133, 21008-21016.	1.6	16
270	(Ph4P)S6â€”A Compound Containing the Cyclic Radical Anion S6.â¯. Angewandte Chemie - International Edition, 2000, 39, 4580-4582.	7.2	15

#	Article	IF	Citations
271	Alkali Metal Complexes of Silyl-Substitutedansa-(Tris)allyl Ligands: Metal-, Co-Ligand- and Substituent-Dependent Stereochemistry. European Journal of Inorganic Chemistry, 2009, 2009, 4157-4167.	1.0	15
272	Structural Interpretation of J Coupling Constants in Guanosine and Deoxyguanosine: Modeling the Effects of Sugar Pucker, Backbone Conformation, and Base Pairing. Journal of Physical Chemistry A, 2009, 113, 8379-8386.	1.1	15
273	Steric effects on alkyl cation affinities of maingroupâ€element hydrides. Journal of Computational Chemistry, 2011, 32, 681-688.	1.5	15
274	Self-Assembly of N³-Substituted Xanthines in the Solid State and at the Solidâ€“Liquid Interface. Langmuir, 2013, 29, 7283-7290.	1.6	15
275	Computational (DFT) and Experimental (EXAFS) Study of the Interaction of [Ir(IMes)(H)₂(L)₃] with Substrates and Coâ€substrates Relevant for SABRE in Dilute Systems. Chemistry - A European Journal, 2015, 21, 10482-10489.	1.7	15
276	How the disulfide conformation determines the disulfide/thiol redox potential. Journal of Biomolecular Structure and Dynamics, 2015, 33, 93-103.	2.0	15
277	Recognition of shorter and longer trimethyllysine analogues by epigenetic reader proteins. Chemical Communications, 2018, 54, 2409-2412.	2.2	15
278	Tricarbonylchromium complexes of [5]- and [6]metacyclophane: an experimental and theoretical study. Tetrahedron, 2008, 64, 11641-11646.	1.0	14
279	Homolytic versus Heterolytic Dissociation of Alkalimetal Halides: The Effect of Microsolvation. ChemPhysChem, 2009, 10, 2955-2965.	1.0	14
280	A donor-functionalized, silyl-substituted pentadienyllithium: structural insight from experiment and theory. Chemical Communications, 2011, 47, 6162.	2.2	14
281	All-metal aromatic clusters M42â^' (M = B, Al, and Ga). Are Ï€-electrons distortive or not?. Physical Chemistry Chemical Physics, 2011, 13, 20673.	1.3	14
282	Formation of a Trifluorophosphane Platinum(II) Complex by Pâ^'F Bond Activation of Phosphorus Pentafluoride with a Pt⁰ Complex. Chemistry - A European Journal, 2017, 23, 5948-5952.	1.7	14
283	Ionâ€Pair S_N2 Reaction of OH^{â^'} and CH₃Cl: Activation Strain Analyses of Counterion and Solvent Effects. Chemistry - an Asian Journal, 2018, 13, 1138-1147.	1.7	14
284	Steric Effects Dictate the Formation of Terminal Arylborylene Complexes of Ruthenium from Dihydroboranes. Chemistry - A European Journal, 2019, 25, 13566-13571.	1.7	14
285	The Nature of Nonclassical Carbonyl Ligands Explained byâ€‰Kohnâ€“Sham Molecular Orbital Theory. Chemistry - A European Journal, 2020, 26, 15690-15699.	1.7	14
286	Proton Transfer and S N 2 Reactions as Steps of Fast Selenol and Thiol Oxidation in Proteins: A Model Molecular Study Based on GPx. ChemPlusChem, 2021, 86, 525-532.	1.3	14
287	On the Origin of Regioselectivity in Palladiumâ€Catalyzed Oxidation of Glucosides. European Journal of Organic Chemistry, 2021, 2021, 632-636.	1.2	14
288	Isolated excited electronic states in the unimolecular gas-phase ion dissociation processes of the radical cations of isocyanogen and cyanogen. International Journal of Mass Spectrometry and Ion Processes, 1991, 103, 157-168.	1.9	13

#	Article	IF	Citations
289	Hydrogen bonding of 3- and 5-methyl-6-aminouracil with natural DNA bases. New Journal of Chemistry, 2008, 32, 1981.	1.4	13
290	Multiscale modelling. Physical Chemistry Chemical Physics, 2011, 13, 10399.	1.3	13
291	tert-Butyl Cation Affinities of Maingroup-Element Hydrides: Effect of Methyl Substituents at the Protophilic Center. Journal of Physical Chemistry A, 2011, 115, 8310-8315.	1.1	13
292	Organomagnesium clusters: Structure, stability, and bonding in archetypal models. Journal of Organometallic Chemistry, 2011, 696, 4104-4111.	0.8	13
293	Selective Cå^'H and Cå^'C Bond Activation: Electronic Regimes as a Tool for Designing d¹⁰ ML_n Catalysts. Chemistry - an Asian Journal, 2015, 10, 2272-2282.	1.7	13
294	Group 9 Metallacyclopentadienes as Key Intermediates in [2+2+2] Alkyne Cyclotrimerizations. Insight from Activation Strain Analyses. ChemPhysChem, 2018, 19, 1766-1773.	1.0	13
295	Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. Communications Chemistry, 2020, 3, .	2.0	13
296	Diastereoselective Synthesis of Î²-Lactams by Ligand-Controlled Stereodivergent Intramolecular Tsujiâ€"Trost Allylation. Journal of Organic Chemistry, 2020, 85, 9566-9584.	1.7	13
297	Conformational Behavior of Basic Monomeric Building Units of Glycosaminoglycans:Â Isolated Systems and Solvent Effect. Journal of Physical Chemistry B, 2007, 111, 2313-2321.	1.2	12
298	The Role of Protein Plasticity in Computational Rationalization Studies on Regioselectivity in Testosterone Hydroxylation by Cytochrome P450 BM3 Mutants. Current Drug Metabolism, 2012, 13, 155-166.	0.7	12
299	Substituent effects on the optical properties of naphthalenediimides: A frontier orbital analysis across the periodic table. Journal of Computational Chemistry, 2016, 37, 304-313.	1.5	12
300	Alkali Metal Cation Affinities of Anionic Main Groupâ€Element Hydrides Across the Periodic Table. Chemistry - an Asian Journal, 2017, 12, 2604-2611.	1.7	12
301	Understanding the differences between iron and palladium in cross-coupling reactions. Physical Chemistry Chemical Physics, 2019, 21, 9651-9664.	1.3	12
302	Distortionâ€Controlled Redshift of Organic Dye Molecules. Chemistry - A European Journal, 2020, 26, 2080-2093.	1.7	12
303	How Lewis Acids Catalyze Ene Reactions. European Journal of Organic Chemistry, 2021, 2021, 5275-5283.	1.2	12
304	Structure and bonding of methyl alkali metal molecules. Journal of Molecular Modeling, 2006, 12, 563-568.	0.8	11
305	Role of the variable active site residues in the function of thioredoxin family oxidoreductases. Journal of Computational Chemistry, 2009, 30, 710-724.	1.5	11
306	Sixâ€Coordinate Groupâ€...13 Complexes: The Role of dâ€...Orbitals and Electronâ€Rich Multiâ€Center Bonding. Angewandte Chemie - International Edition, 2015, 54, 12034-12038.	7.2	11

#	Article	IF	Citations
307	Nature of the Ruâ^'NO Coordination Bond: Kohnâ€"Sham Molecular Orbital and Energy Decomposition Analysis. ChemistryOpen, 2017, 6, 410-416.	0.9	11
308	Regioselectivity of the Pausonâ€"Khand reaction in single-walled carbon nanotubes. Nanoscale, 2018, 10, 15078-15089.	2.8	11
309	Diels-Alder reactivities of cycloalkenediones with tetrazine. Journal of Molecular Modeling, 2019, 25, 33.	0.8	11
310	Probing Through-Space Polarâ^'Ï€ Interactions in 2,6-Diarylphenols. Journal of Organic Chemistry, 2019, 84, 3632-3637.	1.7	11
311	Probing Halogenâ^'Ï€ versus CHâ^'Ï€ Interactions in Molecular Balance. Organic Letters, 2020, 22, 7870-7873.	2.4	11
312	Câ^'X Bond Activation by Palladium: Steric Shielding versus Steric Attraction. Chemistry - A European Journal, 2022, 28, .	1.7	11
313	Oxidative Addition of Hydrogen Halides and Dihalogens to Pd. Trends in Reactivity and Relativistic Effects. Journal of Physical Chemistry A, 2006, 110, 7943-7951.	1.1	10
314	New Insights into the Reactivity of Cisplatin with Free and Restrained Nucleophiles: Microsolvation Effects and Base Selectivity in Cisplatinâ€"DNA Interactions. ChemPhysChem, 2016, 17, 3932-3947.	1.0	10
315	Watson-crick base pairs with thiocarbonyl groups: How sulfur changes the hydrogen bonds in DNA. Open Chemistry, 2008, 6, 15-21.	1.0	9
316	Toward Transitionâ€Metalâ€Templated Construction of Arylated B 4 Chains by Dihydroborane Dehydrocoupling. Chemistry - A European Journal, 2019, 25, 16544-16549.	1.7	9
317	Halfâ€Sandwich Metalâ€Catalyzed Alkyne [2+2+2] Cycloadditions and the Slippage Span Model. ChemistryOpen, 2019, 8, 143-154.	0.9	9
318	Throughâ€Space Polarâ€Ï€ Interactions in 2,6â€Diarylthiophenols. ChemPhysChem, 2020, 21, 1092-1100.	1.0	9
319	Radical Scavenging Potential of the Phenothiazine Scaffold: A Computational Analysis. ChemMedChem, 2021, 16, 3763-3771.	1.6	9
320	Bâ€DNA Structure and Stability: The Role of Nucleotide Composition and Order. ChemistryOpen, 2022, 11, e202100231.	0.9	9
321	S_N2 versus S_N2â€² Competition. Journal of Organic Chemistry, 2022, 87, 8892-8901.	1.7	9
322	High-resolution infrared spectroscopy of the charge-transfer complex [Arâ€"N2]+â^™: A combined experimental/theoretical study. Journal of Chemical Physics, 2005, 123, 144305.	1.2	8
323	Orbital interactions and charge redistribution in weak hydrogen bonds: Watson-Crick GC mimic involving Cï£¿H proton donor and F proton acceptor groups. International Journal of Quantum Chemistry, 2006, 106, 2428-2443.	1.0	8
324	Alkali-Metal-Supported Bismuth Polyhedraâ€"Principles and Theoretical Studies. Inorganic Chemistry, 2011, 50, 5755-5762.	1.9	8

#	Article	IF	Citations
325	Complexes of 4â€substituted phenolates with HF and HCN: Energy decomposition and electronic structure analyses of hydrogen bonding. Journal of Computational Chemistry, 2013, 34, 696-705.	1.5	8
326	Comparison of Molecular Recognition of Trimethyllysine and Trimethylthialysine by Epigenetic Reader Proteins. Molecules, 2020, 25, 1918.	1.7	8
327	Designing Rh(I)-Half-Sandwich Catalysts for Alkyne [2+2+2] Cycloadditions. Synlett, 2021, 32, 561-572.	1.0	8
328	Charge Transfer and Environment Effects Responsible for Characteristics of DNA Base Pairing. Angewandte Chemie - International Edition, 1999, 38, 2942-2945.	7.2	8
329	Probing the Lewis Acidity of Boronic Acids through Interactions with Arene Substituents. Chemistry - A European Journal, 2022, 28, .	1.7	8
330	Orbital interactions in strong and weak hydrogen bonds are essential for DNA replication. Angewandte Chemie - International Edition, 2002, 41, 2092-5.	7.2	8
331	Tandem mass spectrometry of silverâ€adducted ferrocenyl catalyst complexes. Journal of Mass Spectrometry, 2010, 45, 1332-1343.	0.7	7
332	Diastereoselective One-Pot Synthesis of Tetrafunctionalized 2-Imidazolines. Journal of Organic Chemistry, 2014, 79, 5219-5226.	1.7	7
333	Silyleneâ€induced Reduction of [Mn₂(CO)₁₀]: Formation of a Fiveâ€Coordinate Silicon(IV) Complex with an Oâ€Bound [(OC)₄Mn=Mn(CO)₄]^{2â€“} Ligand. European Journal of Inorganic Chemistry, 2017, 2017, 186-191.	1.0	7
334	Bismutamide als einfache Vermittler hochselektiver Pnâ¯Pnâ€Radikalâ€Kupplungsreaktionen (Pn=N, P, As). Angewandte Chemie, 2021, 133, 6513-6518.	1.6	7
335	Do Sulfonamides Interact with Aromatic Rings?. Chemistry - A European Journal, 2021, 27, 5721-5729.	1.7	7
336	C(spⁿ)â¯X (n=1â€“3) Bond Activation by Palladium. Chemistry - A European Journal, 2022, 28, .	1.7	7
337	Rational design of iron catalysts for C â€“ X bond activation. Journal of Computational Chemistry, 2022, , .	1.5	7
338	C(CN)5â€“: transition state or intermediate?. Mendeleev Communications, 2010, 20, 72-73.	0.6	6
339	A computational study on the reactivity enhancement in the free radical polymerization of alkyl Î±â€hydroxymethacrylate and acrylate derivatives. Journal of Polymer Science Part A, 2013, 51, 880-889.	2.5	6
340	Glucoseâ€“Nucleobase Pseudo Base Pairs: Biomolecular Interactions within DNA. Angewandte Chemie - International Edition, 2016, 55, 8643-8647.	7.2	6
341	Switch From Pauliâ€Lowering to LUMOâ€Lowering Catalysis in BrÃ¸nsted Acidâ€Catalyzed Azaâ€Dielsâ€Alder Reactions. ChemistryOpen, 2021, 10, 784-789.	0.9	6
342	Ï€â€Electronic communication through mono and multinuclear gold(I) complexes. International Journal of Quantum Chemistry, 2009, 109, 2507-2519.	1.0	5

#	Article	IF	Citations
343	Effects of the protonation state in the interaction of an HIV-1 reverse transcriptase (RT) amino acid, Lys101, and a non nucleoside RT inhibitor, GW420867X. Journal of Molecular Modeling, 2014, 20, 2332.	0.8	5
344	Is There a Need to Discuss Atomic Orbital Overlap When Teaching Hydrogenâ€“Halide Bond Strength and Acidity Trends in Organic Chemistry?. Journal of Chemical Education, 2015, 92, 286-290.	1.1	5
345	Regioâ€•and Stereoselectivity in 1,3â€Dipolar Cycloadditions: Activation Strain Analyses for Reactions of Hydrazoic Acid with Substituted Alkenes. European Journal of Organic Chemistry, 2017, 2017, 4313-4318.	1.2	5
346	Cesium's Offâ€theâ€Map Valence Orbital. Angewandte Chemie, 2017, 129, 9904-9908.	1.6	5
347	Macrocycles All Aflutter: Substitution at an Allylic Center Reveals the Conformational Dynamics of [13]â€Macrodilactones. Chemistry - an Asian Journal, 2017, 12, 2623-2633.	1.7	5
348	Hydride affinities of cationic maingroup-element hydrides across the periodic table. Results in Chemistry, 2019, 1, 100007.	0.9	5
349	Racemization and Deracemization through Intermolecular Redox Behaviour. Chemistry - A European Journal, 2019, 25, 9639-9642.	1.7	5
350	The Hydrogenation Problem in Cobaltâ€based Catalytic Hydroaminomethylation. ChemistrySelect, 2020, 5, 13981-13994.	0.7	5
351	Polycyclic Aromatic Hydrocarbons (PAHs) in Interstellar Ices: A Computational Study into How the Ice Matrix Influences the Ionic State of PAH Photoproducts. ACS Earth and Space Chemistry, 2022, 6, 766-774.	1.2	5
352	Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins. Communications Chemistry, 2022, 5, .	2.0	5
353	How Ionization Catalyzes Dielsâ€Alder Reactions. Chemistry - A European Journal, 2022, 28, .	1.7	5
354	The rotation barrier in ethane. Nachrichten Aus Der Chemie, 2004, 52, 581-581.	0.0	4
355	Alkali Metal Cation versus Proton and Methyl Cation Affinities: Structure and Bonding Mechanism. ChemistryOpen, 2016, 5, 247-253.	0.9	4
356	Alkali Metal Cation Affinities of Neutral Maingroup-Element Hydrides across the Periodic Table. Journal of Physical Chemistry A, 2019, 123, 9137-9148.	1.1	4
357	Nucleophilic substitution at di- and triphosphates: leaving group ability of phosphate versus diphosphate. Electronic Structure, 2019, 1, 024001.	1.0	4
358	Activation Strain Analyses of Counterion and Solvent Effects on the Ionâ€Pair S N 2 Reaction of and CH 3 Cl. Journal of Computational Chemistry, 2020, 41, 317-327.	1.5	4
359	Dipolar repulsion in Î±-halocarbonyl compounds revisited. Physical Chemistry Chemical Physics, 2021, 23, 20883-20891.	1.3	4
360	Palladiumâ€Catalyzed Activation of Carbonâ€“Halogen Bonds: Electrostaticsâ€Controlled Reactivity. European Journal of Organic Chemistry, 0, , .	1.2	4

#	Article	IF	Citations
361	Gas-Phase Base-Induced 1,4-Eliminations:â€‰ Occurrence of Single-, Double-, and Triple-Well E1cb Mechanisms J. Am. Chem. Soc. 1995, 117, 9889â˜9899. Journal of the American Chemical Society, 1996, 118, 1579-1579.	6.6	3
362	Supramolecular Ring Structures of 7-Methylguanine: A Computational Study of Its Self-assembly and Anion Binding. Molecules, 2013, 18, 225-235.	1.7	3
363	Synthesis and Hydrolysis of Alkoxy(aminoalkyl)diorganylsilanes of the Formula Type R2(RO)Si(CH2)nNH2(R = Alkyl,n= 1-3): A Systematic Experimental and Computational Study. European Journal of Inorganic Chemistry, 2016, 2016, 1641-1659.	1.0	3
364	Nucleophilic Substitution (S_N2): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent. ChemPhysChem, 2018, 19, 1248-1248.	1.0	3
365	Special Collection: Computational Chemistry. ChemistryOpen, 2019, 8, 814-816.	0.9	3
366	Proton Transfer and S N 2 Reactions as Steps of Fast Selenol and Thiol Oxidation in Proteins: A Model Molecular Study Based on GPx. ChemPlusChem, 2021, 86, 524-524.	1.3	3
367	Nature of Alkaliâ€•and Coinageâ€Metal Bonds versus Hydrogen Bonds. Chemistry - an Asian Journal, 2021, 16, 315-321.	1.7	3
368	Watsonâ€“Crick hydrogen bonds: nature and role in DNA replication. , 2006, , 79-97.		2
369	Outer valence orbital response to proton positions in prototropic tautomers of adenine. Journal of Computational Methods in Sciences and Engineering, 2007, 6, 251-267.	0.1	2
370	Aromaticity: Molecular-Orbital Picture of an Intuitive Concept. Chemistry - A European Journal, 2007, 13, 8371-8371.	1.7	2
371	Attractive and Convincing. Angewandte Chemie - International Edition, 2008, 47, 7172-7172.	7.2	2
372	Benchmark Study on the Smallest Bimolecular Nucleophilic Substitution Reaction: Hâ˜+CH4 â†'CH4+Hâ˜. Molecules, 2013, 18, 7726-7738.	1.7	2
373	Glucoseâ€“Nucleobase Pseudo Base Pairs: Biomolecular Interactions within DNA. Angewandte Chemie, 2016, 128, 8785-8789.	1.6	2
374	Glucose-nucleobase pairs within DNA: impact of hydrophobicity, alternative linking unit and DNA polymerase nucleotide insertion studies. Chemical Science, 2018, 9, 3544-3554.	3.7	2
375	Integrative Theory/Experimentâ€Driven Exploration of a Multicomponent Reaction towards Imidazolineâ€2â€(thi)ones. European Journal of Organic Chemistry, 2018, 2018, 104-112.	1.2	2
376	Probing Noncovalent Interactions in [3,3]Metaparacyclophanes. Journal of Organic Chemistry, 2022, 87, 6087-6096.	1.7	2
377	Through-Space Stabilization of an Imidazolium Cation by Aromatic Rings. Journal of Organic Chemistry, 2022, 87, 7875-7883.	1.7	2
378	Stacked DNA-base quartets: Structure, chemistry and computational intricacies. Procedia Computer Science, 2010, 1, 1147-1148.	1.2	1

#	Article	IF	Citations
379	d10-ML2 Complexes: Structure, Bonding, and Catalytic Activity. Structure and Bonding, 2014, , 139-161.	1.0	1
380	4th International Conference on Chemical Bonding. Journal of Physical Chemistry A, 2016, 120, 9353-9356.	1.1	1
381	Role of the Chalcogen (S, Se, Te) in the Oxidation Mechanism of the Glutathione Peroxidase Active Site. ChemPhysChem, 2017, 18, 2950-2950.	1.0	1
382	Cation affinities throughout the periodic table. Advances in Inorganic Chemistry, 2019, 73, 123-158.	0.4	1
383	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. ChemistryOpen, 2021, 10, 390-390.	0.9	1
384	A new DFT functional based on spin-states and SN2 barriers. , 2012, , .		0
385	Guanine, Xanthine and Uric Acid Assemblies: Comparative Theoretical and Experimental Studies. , 2012, , 179-193.		0
386	Editorial for PCCP themed issue â€œDevelopments in Density Functional Theoryâ€• Physical Chemistry Chemical Physics, 2016, 18, 20864-20867.	1.3	0
387	Innentitelbild: Das Distortion/Interactionâ€Activationâ€Strainâ€Modell zur Analyse von Reaktionsgeschwindigkeiten (Angew. Chem. 34/2017). Angewandte Chemie, 2017, 129, 10134-10134.	1.6	0
388	In My Element: Carbon. Chemistry - A European Journal, 2019, 25, 19-19.	1.7	0
389	Throughâ€Space Polarâ€Ï€ Interactions in 2,6â€Diarylthiophenols. ChemPhysChem, 2020, 21, 1080-1080.	1.0	0
390	InnenrÃ¼cktitelbild: Origin of the Î±â€Effect in S_N2 Reactions (Angew. Chem. 38/2021). Angewandte Chemie, 2021, 133, 21239-21239.	1.6	0
391	Bâ€DNA Structure and Stability: The Role of Nucleotide Composition and Order. ChemistryOpen, 2022, 11, e202200013.	0.9	0
392	How Ionization Catalyzes Dielsâ€“Alder Reactions. Chemistry - A European Journal, 0, , .	1.7	0
393	Front Cover: How Ionization Catalyzes Dielsâ€Alder Reactions (Chem. Eur. J. 40/2022). Chemistry - A European Journal, 2022, 28, .	1.7	0