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	Bâ€ÐNA Structure and Stability: The Role of Nucleotide Composition and Order. ChemistryOpen, 2022, 11, e202100231.	0.9	9
2	C(spⁿ)â^'X (n=1â€“3) Bond Activation by Palladium. Chemistry - A European Journal, 2022, 28, .	1.7	7
3	Probing the Lewis Acidity of Boronic Acids through Interactions with Arene Substituents. Chemistry - A European Journal, 2022, 28, .	1.7	8
4	Bâ€ÐNA Structure and Stability: The Role of Nucleotide Composition and Order. ChemistryOpen, 2022, 11, e202200013.	0.9	0
5	Rational design of iron catalysts for C â€“ X bond activation. Journal of Computational Chemistry, 2022, , .	1.5	7
6	How Solvation Influences the S_N2 versus E2 Competition. Journal of Organic Chemistry, 2022, 87, 1805-1813.	1.7	26
7	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
8	Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins. Communications Chemistry, 2022, 5, .	2.0	5
9	How Ionization Catalyzes Dielsâ€Alder Reactions. Chemistry - A European Journal, 2022, 28, .	1.7	5
10	Câ^'X Bond Activation by Palladium: Steric Shielding versus Steric Attraction. Chemistry - A European Journal, 2022, 28, .	1.7	11
11	Probing Noncovalent Interactions in [3,3]Metaparacyclophanes. Journal of Organic Chemistry, 2022, 87, 6087-6096.	1.7	2
12	Clarifying notes on the bonding analysis adopted by the energy decomposition analysis. Physical Chemistry Chemical Physics, 2022, 24, 15726-15735.	1.3	25
13	Through-Space Stabilization of an Imidazolium Cation by Aromatic Rings. Journal of Organic Chemistry, 2022, 87, 7875-7883.	1.7	2
14	Front Cover: How Ionization Catalyzes Dielsâ€Alder Reactions (Chem. Eur. J. 40/2022). Chemistry - A European Journal, 2022, 28, .	1.7	0
15	S_N2 versus S_N2â€² Competition. Journal of Organic Chemistry, 2022, 87, 8892-8901.	1.7	9
16	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
17	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
18	Designing Rh(I)-Half-Sandwich Catalysts for Alkyne [2+2+2] Cycloadditions. Synlett, 2021, 32, 561-572.	1.0	8

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19	Bismutamide als einfache Vermittler hochselektiver Pnâ˜Pnâ€Radikalâ€Kupplungsreaktionen (Pn=N, P, As). Angewandte Chemie, 2021, 133, 6513-6518.	1.6	7
20	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
21	How Oriented External Electric Fields Modulate Reactivity. Chemistry - A European Journal, 2021, 27, 5683-5693.	1.7	37
22	On the Origin of Regioselectivity in Palladiumâ€Catalyzed Oxidation of Glucosides. European Journal of Organic Chemistry, 2021, 2021, 632-636.	1.2	14
23	Dipolar repulsion in Î±-halocarbonyl compounds revisited. Physical Chemistry Chemical Physics, 2021, 23, 20883-20891.	1.3	4
24	How metallylenes activate small molecules. Chemical Science, 2021, 12, 4526-4535.	3.7	17
25	The pnictogen bond: a quantitative molecular orbital picture. Physical Chemistry Chemical Physics, 2021, 23, 13842-13852.	1.3	39
26	Chemical reactivity from an activation strain perspective. Chemical Communications, 2021, 57, 5880-5896.	2.2	69
27	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
28	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. ChemistryOpen, 2021, 10, 391-401.	0.9	32
29	The Gauche Effect in XCH₂CH₂X Revisited. ChemPhysChem, 2021, 22, 641-648.	1.0	17
30	Chalcogen bonds: Hierarchical ab initio benchmark and density functional theory performance study. Journal of Computational Chemistry, 2021, 42, 688-698.	1.5	21
31	The Pauli Repulsion-Lowering Concept in Catalysis. Accounts of Chemical Research, 2021, 54, 1972-1981.	7.6	75
32	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
33	Do Sulfonamides Interact with Aromatic Rings?. Chemistry - A European Journal, 2021, 27, 5721-5729.	1.7	7
34	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. ChemistryOpen, 2021, 10, 390-390.	0.9	1
35	8 Energy decomposition analysis in the context of quantitative molecular orbital theory. , 2021, , 199-212.		49
36	Lewis Acidâ€Catalyzed Dielsâ€Alder Reactions: Reactivity Trends across the Periodic Table. Chemistry - A European Journal, 2021, 27, 10610-10620.	1.7	26

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37	Origin of the Î±â€Effect in S_N2 Reactions. Angewandte Chemie, 2021, 133, 21008-21016.	1.6	16
38	Origin of the Î±â€Effect in S_N2 Reactions. Angewandte Chemie - International Edition, 2021, 60, 20840-20848.	7.2	47
39	InnenrÃ¼cktitelbild: Origin of the Î±â€Effect in S_N2 Reactions (Angew. Chem. 38/2021). Angewandte Chemie, 2021, 133, 21239-21239.	1.6	0
40	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
41	How Lewis Acids Catalyze Ene Reactions. European Journal of Organic Chemistry, 2021, 2021, 5275-5283.	1.2	12
42	Radical Scavenging Potential of the Phenothiazine Scaffold: A Computational Analysis. ChemMedChem, 2021, 16, 3763-3771.	1.6	9
43	Origin of asynchronicity in Dielsâ€“Alder reactions. Physical Chemistry Chemical Physics, 2021, 23, 20095-20106.	1.3	23
44	Nature of Alkaliâ€•and Coinageâ€Metal Bonds versus Hydrogen Bonds. Chemistry - an Asian Journal, 2021, 16, 315-321.	1.7	3
45	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
46	Understanding chemical reactivity using the activation strain model. Nature Protocols, 2020, 15, 649-667.	5.5	188
47	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
48	Distortionâ€Controlled Redshift of Organic Dye Molecules. Chemistry - A European Journal, 2020, 26, 2080-2093.	1.7	12
49	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
50	Probing Halogenâ‹¯Ï€ versus CHâ‹¯Ï€ Interactions in Molecular Balance. Organic Letters, 2020, 22, 7870-7873.	2.4	11
51	S_N2 versus E2 Competition of F^{â€“}and PH₂^{â€“}Revisited. Journal of Organic Chemistry, 2020, 85, 14087-14093.	1.7	22
52	The Nature of Nonclassical Carbonyl Ligands Explained byâ€‰Kohnâ€“Sham Molecular Orbital Theory. Chemistry - A European Journal, 2020, 26, 15690-15699.	1.7	14
53	The Hydrogenation Problem in Cobaltâ€based Catalytic Hydroaminomethylation. ChemistrySelect, 2020, 5, 13981-13994.	0.7	5
54	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

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55	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
56	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
57	Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. Communications Chemistry, 2020, 3, .	2.0	13
58	Throughâ€Space Polarâ€Ï€ Interactions in 2,6â€Diarylthiophenols. ChemPhysChem, 2020, 21, 1080-1080.	1.0	0
59	Performance of TDDFT Vertical Excitation Energies of Coreâ€Substituted Naphthalene Diimides. Journal of Computational Chemistry, 2020, 41, 1448-1455.	1.5	21
60	Understanding the 1,3â€Dipolar Cycloadditions of Allenes. Chemistry - A European Journal, 2020, 26, 11529-11539.	1.7	20
61	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
62	Origin of rate enhancement and asynchronicity in iminium catalyzed Dielsâ€“Alder reactions. Chemical Science, 2020, 11, 8105-8112.	3.7	55
63	Diastereoselective Synthesis of Î²-Lactams by Ligand-Controlled Stereodivergent Intramolecular Tsujiâ€“Trost Allylation. Journal of Organic Chemistry, 2020, 85, 9566-9584.	1.7	13
64	How Alkali Cations Catalyze Aromatic Dielsâ€Alder Reactions. Chemistry - an Asian Journal, 2020, 15, 1167-1174.	1.7	19
65	How Lewis Acids Catalyze Dielsâ€“Alder Reactions. Angewandte Chemie, 2020, 132, 6260-6265.	1.6	42
66	How Lewis Acids Catalyze Dielsâ€“Alder Reactions. Angewandte Chemie - International Edition, 2020, 59, 6201-6206.	7.2	113
67	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
68	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
69	Throughâ€Space Polarâ€Ï€ Interactions in 2,6â€Diarylthiophenols. ChemPhysChem, 2020, 21, 1092-1100.	1.0	9
70	Comparison of Molecular Recognition of Trimethyllysine and Trimethylthialysine by Epigenetic Reader Proteins. Molecules, 2020, 25, 1918.	1.7	8
71	Elucidating the Trends in Reactivity of Azaâ€1,3â€Dipolar Cycloadditions. European Journal of Organic Chemistry, 2019, 2019, 378-386.	1.2	37
72	Steric Effects Dictate the Formation of Terminal Arylborylene Complexes of Ruthenium from Dihydroboranes. Chemistry - A European Journal, 2019, 25, 13566-13571.	1.7	14

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73	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
74	Special Collection: Computational Chemistry. ChemistryOpen, 2019, 8, 814-816.	0.9	3
75	Toward Transitionâ€Metalâ€Templated Construction of Arylated B 4 Chains by Dihydroborane Dehydrocoupling. Chemistry - A European Journal, 2019, 25, 16544-16549.	1.7	9
76	Diels-Alder reactivities of cycloalkenediones with tetrazine. Journal of Molecular Modeling, 2019, 25, 33.	0.8	11
77	Hydride affinities of cationic maingroup-element hydrides across the periodic table. Results in Chemistry, 2019, 1, 100007.	0.9	5
78	Cation affinities throughout the periodic table. Advances in Inorganic Chemistry, 2019, 73, 123-158.	0.4	1
79	Halfâ€Sandwich Metalâ€Catalyzed Alkyne [2+2+2] Cycloadditions and the Slippage Span Model. ChemistryOpen, 2019, 8, 143-154.	0.9	9
80	Racemization and Deracemization through Intermolecular Redox Behaviour. Chemistry - A European Journal, 2019, 25, 9639-9642.	1.7	5
81	PyFrag 2019â€"Automating the exploration and analysis of reaction mechanisms. Journal of Computational Chemistry, 2019, 40, 2227-2233.	1.5	57
82	Dual Activation of Aromatic Dielsâ€"Alder Reactions. Chemistry - A European Journal, 2019, 25, 9902-9912.	1.7	16
83	Nucleophilic substitution at di- and triphosphates: leaving group ability of phosphate versus diphosphate. Electronic Structure, 2019, 1, 024001.	1.0	4
84	Wie Dihalogene Michaelâ€Additionsreaktionen katalysieren. Angewandte Chemie, 2019, 131, 9015-9020.	1.6	20
85	How Dihalogens Catalyze Michael Addition Reactions. Angewandte Chemie - International Edition, 2019, 58, 8922-8926.	7.2	90
86	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
87	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
88	Probing Through-Space Polarâˆ'Ï€ Interactions in 2,6-Diarylphenols. Journal of Organic Chemistry, 2019, 84, 3632-3637.	1.7	11
89	Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies. Chemistry - A European Journal, 2019, 25, 6342-6348.	1.7	49
90	Understanding the differences between iron and palladium in cross-coupling reactions. Physical Chemistry Chemical Physics, 2019, 21, 9651-9664.	1.3	12

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91	In My Element: Carbon. Chemistry - A European Journal, 2019, 25, 19-19.	1.7	0
92	Chemoselectivity of Tertiary Azides in Strainâ€Promoted Alkyneâ€Azide Cycloadditions. Chemistry - A European Journal, 2019, 25, 754-758.	1.7	43
93	Nucleophilic Substitution in Solution: Activation Strain Analysis of Weak and Strong Solvent Effects. Chemistry - A European Journal, 2018, 24, 5927-5938.	1.7	53
94	Recognition of shorter and longer trimethyllysine analogues by epigenetic reader proteins. Chemical Communications, 2018, 54, 2409-2412.	2.2	15
95	How Mg²⁺ ions lower the S_N2@P barrier in enzymatic triphosphate hydrolysis. Chemical Communications, 2018, 54, 3448-3451.	2.2	16
96	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
97	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
98	Doppelte CHâ€Aktivierung eines maskierten Bismutamidâ€Kations. Angewandte Chemie, 2018, 130, 3887-3891.	1.6	25
99	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
100	Double CH Activation of a Masked Cationic Bismuth Amide. Angewandte Chemie - International Edition, 2018, 57, 3825-3829.	7.2	66
101	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
102	Trifluoromethyl Vinyl Sulfide: A Building Block for the Synthesis of CF₃S-Containing Isoxazolidines. Journal of Organic Chemistry, 2018, 83, 1779-1789.	1.7	18
103	Nucleophilic Substitution (S_N2): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent. ChemPhysChem, 2018, 19, 1248-1248.	1.0	3
104	Nucleophilic Substitution (S_N2): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent. ChemPhysChem, 2018, 19, 1315-1330.	1.0	138
105	Tuning Heterocalixarenes to Improve Their Anion Recognition: A Computational Approach. Journal of Physical Chemistry A, 2018, 122, 3328-3336.	1.1	22
106	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
107	Nature and strength of chalcogenâ€“Ï€ bonds. Physical Chemistry Chemical Physics, 2018, 20, 27592-27599.	1.3	23
108	Factors Controlling the Dielsâ€“Alder Reactivity of Heteroâ€1,3â€Butadienes. ChemistryOpen, 2018, 7, 995-1004.	0.9	22

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109	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
110	Anion Recognition by Organometallic Calixarenes: Analysis from Relativistic DFT Calculations. Organometallics, 2018, 37, 2167-2176.	1.1	26
111	Oxidation of organic diselenides and ditellurides by H₂O₂for bioinspired catalyst design. Physical Chemistry Chemical Physics, 2018, 20, 20874-20885.	1.3	27
112	Highly Stable and Selective Tetrazines for the Coordination-Assisted Bioorthogonal Ligation with Vinylboronic Acids. Bioconjugate Chemistry, 2018, 29, 3054-3059.	1.8	36
113	Regioselectivity of the Pausonâ€“Khand reaction in single-walled carbon nanotubes. Nanoscale, 2018, 10, 15078-15089.	2.8	11
114	Arylic Câ€“X Bond Activation by Palladium Catalysts: Activation Strain Analyses of Reactivity Trends. Scientific Reports, 2018, 8, 10729.	1.6	26
115	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
116	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
117	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
118	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
119	Understanding the Reactivity of Ionâ€Encapsulated Fullerenes. Chemistry - A European Journal, 2017, 23, 11030-11036.	1.7	33
120	Analyzing Reaction Rates with the Distortion/Interactionâ€Activation Strain Model. Angewandte Chemie - International Edition, 2017, 56, 10070-10086.	7.2	1,060
121	Cesium's Offâ€theâ€Map Valence Orbital. Angewandte Chemie - International Edition, 2017, 56, 9772-9776.	7.2	17
122	Das Distortion/Interactionâ€Activationâ€Strainâ€Modell zur Analyse von Reaktionsgeschwindigkeiten. Angewandte Chemie, 2017, 129, 10204-10221.	1.6	209
123	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
124	Nature of the Ruâ€NO Coordination Bond: Kohnâ€“Sham Molecular Orbital and Energy Decomposition Analysis. ChemistryOpen, 2017, 6, 410-416.	0.9	11
125	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
126	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

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127	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
128	Stabilization of 2,6-Diarylanilinum Cation by Through-Space Cationâˆ'Ï€ Interactions. Journal of Organic Chemistry, 2017, 82, 9418-9424.	1.7	18
129	Innentitelbild: Das Distortion/Interactionâ€Activationâ€Strainâ€Modell zur Analyse von Reaktionsgeschwindigkeiten (Angew. Chem. 34/2017). Angewandte Chemie, 2017, 129, 10134-10134.	1.6	0
130	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
131	Cesium's Offâ€theâ€Map Valence Orbital. Angewandte Chemie, 2017, 129, 9904-9908.	1.6	5
132	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
133	How the electron-deficient cavity of heterocalixarenes recognizes anions: insights from computation. Physical Chemistry Chemical Physics, 2017, 19, 24696-24705.	1.3	29
134	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
135	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
136	Deracemization of a Racemic Allylic Sulfoxide Using Viedma Ripening. Crystal Growth and Design, 2017, 17, 4454-4457.	1.4	25
137	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
138	Formation of a Trifluorophosphane Platinum(II) Complex by Pâˆ'F Bond Activation of Phosphorus Pentafluoride with a Pt⁰ Complex. Chemistry - A European Journal, 2017, 23, 5948-5952.	1.7	14
139	Glucoseâ€“Nucleobase Pseudo Base Pairs: Biomolecular Interactions within DNA. Angewandte Chemie, 2016, 128, 8785-8789.	1.6	2
140	Glucoseâ€“Nucleobase Pseudo Base Pairs: Biomolecular Interactions within DNA. Angewandte Chemie - International Edition, 2016, 55, 8643-8647.	7.2	6
141	Reactivity and Selectivity of Bowlâ€Shaped Polycyclic Aromatic Hydrocarbons: Relationship to C₆₀. Chemistry - A European Journal, 2016, 22, 1368-1378.	1.7	31
142	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
143	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
144	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

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145	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
146	Alkali Metal Cation versus Proton and Methyl Cation Affinities: Structure and Bonding Mechanism. ChemistryOpen, 2016, 5, 247-253.	0.9	4
147	Understanding the Oxidative Addition of Ïƒâ€Bonds to Groupâ€…13 Compounds. Chemistry - A European Journal, 2016, 22, 13669-13676.	1.7	25
148	Stereoselective Synthesis of 1-Tuberculosinyl Adenosine; a Virulence Factor of Mycobacterium tuberculosis. Journal of Organic Chemistry, 2016, 81, 6686-6696.	1.7	20
149	Editorial for PCCP themed issue â€œDevelopments in Density Functional Theoryâ€• Physical Chemistry Chemical Physics, 2016, 18, 20864-20867.	1.3	0
150	4th International Conference on Chemical Bonding. Journal of Physical Chemistry A, 2016, 120, 9353-9356.	1.1	1
151	Deeper Insight into the Dielsâ€“Alder Reaction through the Activation Strain Model. Chemistry - an Asian Journal, 2016, 11, 3297-3304.	1.7	47
152	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
153	Source of Cooperativity in Halogenâ€Bonded Haloamine Tetramers. ChemPhysChem, 2016, 17, 474-480.	1.0	16
154	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
155	(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
156	The activation strain model and molecular orbital theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 324-343.	6.2	280
157	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
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