

Trevor A Hamlin

List of Publications by Year in descending order

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102
papers

2,820
citations

172207

29
h-index

243296

44
g-index

133
all docs

133
docs citations

133
times ranked

1897
citing authors

#	ARTICLE	IF	CITATIONS
1	Understanding chemical reactivity using the activation strain model. <i>Nature Protocols</i> , 2020, 15, 649-667.	5.5	188
2	Nucleophilic Substitution (S_N2): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent. <i>ChemPhysChem</i> , 2018, 19, 1315-1330.	1.0	138
3	How Lewis Acids Catalyze Diels-Alder Reactions. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 6201-6206.	7.2	113
4	How Dihalogens Catalyze Michael Addition Reactions. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 8922-8926.	7.2	90
5	The Pauli Repulsion-Lowering Concept in Catalysis. <i>Accounts of Chemical Research</i> , 2021, 54, 1972-1981.	7.6	75
6	Oxoammonium Salt Oxidations of Alcohols in the Presence of Pyridine Bases. <i>Journal of Organic Chemistry</i> , 2014, 79, 1055-1067.	1.7	69
7	Chemical reactivity from an activation strain perspective. <i>Chemical Communications</i> , 2021, 57, 5880-5896.	2.2	69
8	Oxidation of β -Trifluoromethyl Alcohols Using a Recyclable Oxoammonium Salt. <i>Journal of Organic Chemistry</i> , 2012, 77, 8131-8141.	1.7	66
9	Role of Orbital Interactions and Activation Strain (Distortion Energies) on Reactivities in the Normal and Inverse Electron-Demand Cycloadditions of Strained and Unstrained Cycloalkenes. <i>Journal of Organic Chemistry</i> , 2017, 82, 8668-8675.	1.7	59
10	PyFrag 2019: Automating the exploration and analysis of reaction mechanisms. <i>Journal of Computational Chemistry</i> , 2019, 40, 2227-2233.	1.5	57
11	Toward a Unified Mechanism for Oxoammonium Salt-Mediated Oxidation Reactions: A Theoretical and Experimental Study Using a Hydride Transfer Model. <i>Journal of Organic Chemistry</i> , 2015, 80, 8150-8167.	1.7	55
12	Origin of rate enhancement and asynchronicity in iminium catalyzed Diels-Alder reactions. <i>Chemical Science</i> , 2020, 11, 8105-8112.	3.7	55
13	Nucleophilic Substitution in Solution: Activation Strain Analysis of Weak and Strong Solvent Effects. <i>Chemistry - A European Journal</i> , 2018, 24, 5927-5938.	1.7	53
14	Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies. <i>Chemistry - A European Journal</i> , 2019, 25, 6342-6348.	1.7	49
15	8 Energy decomposition analysis in the context of quantitative molecular orbital theory. , 2021, , 199-212.		49
16	Origin of the β -Effect in S_N2 Reactions. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20840-20848.	7.2	47
17	Chemoselectivity of Tertiary Azides in Strain-Promoted Alkyne-Azide Cycloadditions. <i>Chemistry - A European Journal</i> , 2019, 25, 754-758.	1.7	43
18	Methylenation of Perfluoroalkyl Ketones using a Peterson Olefination Approach. <i>Journal of Organic Chemistry</i> , 2014, 79, 1145-1155.	1.7	42

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19	How Lewis Acids Catalyze Diels–Alder Reactions. <i>Angewandte Chemie</i> , 2020, 132, 6260-6265.	1.6	42
20	Regioselectivity of Epoxide Ring–Openings via S_N2 Reactions Under Basic and Acidic Conditions. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 3822-3828.	1.2	40
21	The pnictogen bond: a quantitative molecular orbital picture. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13842-13852.	1.3	39
22	Origins of the <i>Endo</i> and <i>Exo</i> Selectivities in Cyclopropanone, Iminocyclopropene, and Triafulvene Diels–Alder Cycloadditions. <i>Journal of Organic Chemistry</i> , 2018, 83, 3164-3170.	1.7	38
23	A Unified Framework for Understanding Nucleophilicity and Protophilicity in the $S_N2/E2$ Competition. <i>Chemistry - A European Journal</i> , 2020, 26, 15538-15548.	1.7	38
24	A Continuous-Flow Approach to 3,3,3-Trifluoromethylpropenes: Bringing Together Grignard Addition, Peterson Elimination, Inline Extraction, and Solvent Switching. <i>Organic Process Research and Development</i> , 2014, 18, 1253-1258.	1.3	37
25	Elucidating the Trends in Reactivity of Aza $\pi,3\pi$ Dipolar Cycloadditions. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 378-386.	1.2	37
26	Bifunctional Hydrogen Bond Donor–Catalyzed Diels–Alder Reactions: Origin of Stereoselectivity and Rate Enhancement. <i>Chemistry - A European Journal</i> , 2021, 27, 5180-5190.	1.7	37
27	How Oriented External Electric Fields Modulate Reactivity. <i>Chemistry - A European Journal</i> , 2021, 27, 5683-5693.	1.7	37
28	Palladium–Catalyzed Cascade to Benzoxepins by Using Vinyl–Substituted Donor–Acceptor Cyclopropanes. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 14410-14414.	7.2	36
29	One-Step Assembly of Functionalized Morpholinones and 1,4-Oxazepane-3-ones via [3 + 3]- and [3 + 4]-Annulation of Aza-Oxyallyl Cation and Amphoteric Compounds. <i>Journal of Organic Chemistry</i> , 2019, 84, 15255-15266.	1.7	33
30	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. <i>ChemistryOpen</i> , 2021, 10, 391-401.	0.9	32
31	Raman spectroscopy as a tool for monitoring mesoscale continuous-flow organic synthesis: Equipment interface and assessment in four medically-relevant reactions. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 1843-1852.	1.3	30
32	1,1,4,4-Tetracyanobutadiene-Functionalized Anthracenes: Regioselectivity of Cycloadditions in the Synthesis of Small Near-IR Dyes. <i>Organic Letters</i> , 2021, 23, 2007-2012.	2.4	30
33	Nature and Strength of Lewis Acid/Base Interaction in Boron and Nitrogen Trihalides. <i>Chemistry - an Asian Journal</i> , 2020, 15, 4043-4054.	1.7	28
34	How Lewis Acids Catalyze Ring-Openings of Cyclohexene Oxide. <i>Journal of Organic Chemistry</i> , 2021, 86, 3565-3573.	1.7	28
35	Dehydrogenation of Perfluoroalkyl Ketones by Using a Recyclable Oxoammonium Salt. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 3658-3661.	1.2	27
36	General Pyrrolidine Synthesis via Iridium-Catalyzed Reductive Azomethine Ylide Generation from Tertiary Amides and Lactams. <i>ACS Catalysis</i> , 2021, 11, 7489-7497.	5.5	27

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37	Lewis acid catalyzed annulation of spirocyclic donor-acceptor cyclopropanes with <i>exo</i> -heterocyclic olefins: access to highly functionalized bis-spirocyclopentane oxindole frameworks. <i>Chemical Communications</i> , 2019, 55, 7069-7072.	2.2	26
38	Lewis Acid-Catalyzed Diels-Alder Reactions: Reactivity Trends across the Periodic Table. <i>Chemistry - A European Journal</i> , 2021, 27, 10610-10620.	1.7	26
39	The Chemical Bond: When Atom Size Instead of Electronegativity Difference Determines Trend in Bond Strength. <i>Chemistry - A European Journal</i> , 2021, 27, 15616-15622.	1.7	26
40	How Solvation Influences the S_N2 versus E2 Competition. <i>Journal of Organic Chemistry</i> , 2022, 87, 1805-1813.	1.7	26
41	B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16969-16978.	1.3	25
42	Not Carbon sp Hybridization, but Coordination Number Determines $C-H$ and $C-C$ Bond Length. <i>Chemistry - A European Journal</i> , 2021, 27, 7074-7079.	1.7	24
43	Bifunctional Iminophosphorane-Catalyzed Enantioselective Sulfa-Michael Addition to Unactivated α,β -Unsaturated Amides. <i>Journal of the American Chemical Society</i> , 2022, 144, 1006-1015.	6.6	24
44	Nature and strength of chalcogen- π bonds. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27592-27599.	1.3	23
45	Ambident Nucleophilic Substitution: Understanding Non-HSAB Behavior through Activation Strain and Conceptual DFT Analyses. <i>Chemistry - A European Journal</i> , 2020, 26, 3884-3893.	1.7	23
46	Switchable, Reagent-Controlled Diastereodivergent Photocatalytic Carbocyclisation of Imine-Derived α -Amino Radicals. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24116-24123.	7.2	23
47	Origin of asynchronicity in Diels-Alder reactions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20095-20106.	1.3	23
48	Factors Controlling the Diels-Alder Reactivity of Hetero-1,3-Butadienes. <i>ChemistryOpen</i> , 2018, 7, 995-1004.	0.9	22
49	S_N2 versus E2 Competition of F^+ and PH_2^+ Revisited. <i>Journal of Organic Chemistry</i> , 2020, 85, 14087-14093.	1.7	22
50	Performance of TDDFT Vertical Excitation Energies of Core-Substituted Naphthalene Diimides. <i>Journal of Computational Chemistry</i> , 2020, 41, 1448-1455.	1.5	21
51	A bifunctional iminophosphorane squaramide catalyzed enantioselective synthesis of hydroquinazolines via intramolecular aza-Michael reaction to α,β -unsaturated esters. <i>Chemical Science</i> , 2021, 12, 6064-6072.	3.7	21
52	Chalcogen bonds: Hierarchical <i>ab initio</i> benchmark and density functional theory performance study. <i>Journal of Computational Chemistry</i> , 2021, 42, 688-698.	1.5	21
53	1,3-Silyl-elimination in electron-deficient cationic systems. <i>Chemical Science</i> , 2014, 5, 3983.	3.7	20
54	Wie Dihalogene Michael-Additionsreaktionen katalysieren. <i>Angewandte Chemie</i> , 2019, 131, 9015-9020.	1.6	20

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55	Understanding the 1,3-Dipolar Cycloadditions of Allenes. <i>Chemistry - A European Journal</i> , 2020, 26, 11529-11539.	1.7	20
56	How Alkali Cations Catalyze Aromatic Diels-Alder Reactions. <i>Chemistry - an Asian Journal</i> , 2020, 15, 1167-1174.	1.7	19
57	Trifluoromethyl Vinyl Sulfide: A Building Block for the Synthesis of CF ₃ -S-Containing Isoxazolidines. <i>Journal of Organic Chemistry</i> , 2018, 83, 1779-1789.	1.7	18
58	A methodology for the photocatalyzed radical trifluoromethylation of indoles: A combined experimental and computational study. <i>Journal of Fluorine Chemistry</i> , 2018, 214, 94-100.	0.9	18
59	How metallylenes activate small molecules. <i>Chemical Science</i> , 2021, 12, 4526-4535.	3.7	17
60	The <i>Gauche</i> Effect in XCH ₂ CH ₂ X Revisited. <i>ChemPhysChem</i> , 2021, 22, 641-648.	1.0	17
61	How the Lewis Base F ⁻ Catalyzes the 1,3-Dipolar Cycloaddition between Carbon Dioxide and Nitrilimines. <i>Journal of Organic Chemistry</i> , 2021, 86, 4320-4325.	1.7	17
62	A combined computational and experimental investigation of the oxidative ring-opening of cyclic ethers by oxoammonium cations. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 3883-3888.	1.5	16
63	How Mg ²⁺ ions lower the S _N 2@P barrier in enzymatic triphosphate hydrolysis. <i>Chemical Communications</i> , 2018, 54, 3448-3451.	2.2	16
64	Dual Activation of Aromatic Diels-Alder Reactions. <i>Chemistry - A European Journal</i> , 2019, 25, 9902-9912.	1.7	16
65	Ligand-Mediated Regioselective Rhodium-Catalyzed Benzotriazole-Allene Coupling: Mechanistic Exploration and Quantum Chemical Analysis. <i>Chemistry - A European Journal</i> , 2020, 26, 2342-2348.	1.7	16
66	Origin of the $\hat{\sigma}$ -Effect in S _N 2 Reactions. <i>Angewandte Chemie</i> , 2021, 133, 21008-21016.	1.6	16
67	Computational and NMR Studies on the Complexation of Lithium Ion to 8-Crown-4. <i>ChemPhysChem</i> , 2019, 20, 2103-2109.	1.0	15
68	A New Organocatalytic Desymmetrization Reaction Enables the Enantioselective Total Synthesis of Madangamine E. <i>Journal of the American Chemical Society</i> , 2022, 144, 1407-1415.	6.6	15
69	Delocalization of Charge and Electron Density in the Humulyl Cation—Implications for Terpene Biosynthesis. <i>Journal of Organic Chemistry</i> , 2015, 80, 4046-4053.	1.7	14
70	On the Origin of Regioselectivity in Palladium-Catalyzed Oxidation of Glucosides. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 632-636.	1.2	14
71	Diastereoselective Synthesis of $\hat{\sigma}$ -Lactams by Ligand-Controlled Stereodivergent Intramolecular Tsuji-Trost Allylation. <i>Journal of Organic Chemistry</i> , 2020, 85, 9566-9584.	1.7	13
72	How Divalent Cations Interact with the Internal Channel Site of Guanine Quadruplexes. <i>ChemPhysChem</i> , 2021, 22, 2286-2296.	1.0	13

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73	Understanding the differences between iron and palladium in cross-coupling reactions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9651-9664.	1.3	12
74	Distortionâ€Controlled Redshift of Organic Dye Molecules. <i>Chemistry - A European Journal</i> , 2020, 26, 2080-2093.	1.7	12
75	How Lewis Acids Catalyze Ene Reactions. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 5275-5283.	1.2	12
76	Diels-Alder reactivities of cycloalkenediones with tetrazine. <i>Journal of Molecular Modeling</i> , 2019, 25, 33.	0.8	11
77	Dual catalytic enantioselective desymmetrization of allene-tethered cyclohexanones. <i>Chemical Science</i> , 2020, 11, 7444-7450.	3.7	11
78	C ⁿ X Bond Activation by Palladium: Steric Shielding versus Steric Attraction. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	11
79	Rules of Macrocycle Topology: A [13]â€Macrolactone Case Study. <i>Chemistry - A European Journal</i> , 2016, 22, 6001-6011.	1.7	9
80	Radical Scavenging Potential of the Phenothiazine Scaffold: A Computational Analysis. <i>ChemMedChem</i> , 2021, 16, 3763-3771.	1.6	9
81	Bâ€DNA Structure and Stability: The Role of Nucleotide Composition and Order. <i>ChemistryOpen</i> , 2022, 11, e202100231.	0.9	9
82	S_N2 versus S_N2â€2 Competition. <i>Journal of Organic Chemistry</i> , 2022, 87, 8892-8901.	1.7	9
83	CⁿX (n=1â€3) Bond Activation by Palladium. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	7
84	Rational design of iron catalysts for C â€ X bond activation. <i>Journal of Computational Chemistry</i> , 2022, , .	1.5	7
85	Palladiumâ€Catalyzed Cascade to Benzoxepins by Using Vinylâ€Substituted Donorâ€Acceptor Cyclopropanes. <i>Angewandte Chemie</i> , 2021, 133, 14531-14535.	1.6	6
86	Switchable, Reagentâ€Controlled Diastereodivergent Photocatalytic Carbocyclisation of Imineâ€Derived Iâ€Amino Radicals. <i>Angewandte Chemie</i> , 2021, 133, 24318.	1.6	6
87	Switch From Pauliâ€Lowering to LUMOâ€Lowering Catalysis in Brønsted Acidâ€Catalyzed Azaâ€Dielsâ€Alder Reactions. <i>ChemistryOpen</i> , 2021, 10, 784-789.	0.9	6
88	Macrocycles All Aflutter: Substitution at an Allylic Center Reveals the Conformational Dynamics of [13]â€Macrolactones. <i>Chemistry - an Asian Journal</i> , 2017, 12, 2623-2633.	1.7	5
89	How Divalent Cations Interact with the Internal Channel Site of Guanine Quadruplexes. <i>ChemPhysChem</i> , 2021, 22, 2265-2265.	1.0	5
90	How Ionization Catalyzes Dielsâ€Alder Reactions. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	5

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91	Nucleophilic substitution at di- and triphosphates: leaving group ability of phosphate versus diphosphate. <i>Electronic Structure</i> , 2019, 1, 024001.	1.0	4
92	Dipolar repulsion in $\hat{\pm}$ -halocarbonyl compounds revisited. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20883-20891.	1.3	4
93	Boron Tunneling in the $\hat{\pm}$ Weak $\hat{\pm}$ Bond $\hat{\pm}$ Stretch Isomerization of $N\hat{\pm}B$ Lewis Adducts. <i>ChemPhysChem</i> , 2021, 22, 1857-1862.	1.0	4
94	Palladium $\hat{\pm}$ Catalyzed Activation of Carbon $\hat{\pm}$ Halogen Bonds: Electrostatics $\hat{\pm}$ Controlled Reactivity. <i>European Journal of Organic Chemistry</i> , 0, , .	1.2	4
95	Nucleophilic Substitution ($S_{\text{N}}2$): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent. <i>ChemPhysChem</i> , 2018, 19, 1248-1248.	1.0	3
96	Real-time Monitoring of Reactions Performed Using Continuous-flow Processing: The Preparation of 3-Acetylcoumarin as an Example. <i>Journal of Visualized Experiments</i> , 2015, , .	0.2	2
97	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. <i>ChemistryOpen</i> , 2021, 10, 390-390.	0.9	1
98	9. Incorporation of continuous-flow processing into the undergraduate teaching laboratory: key concepts and two case studies. , 2014, , 259-276.		0
99	Innen $\hat{\pm}$ cktitelbild: Origin of the $\hat{\pm}$ Effect in $S_{\text{N}}2$ Reactions (<i>Angew. Chem.</i> 38/2021). <i>Angewandte Chemie</i> , 2021, 133, 21239-21239.	1.6	0
100	B $\hat{\pm}$ DNA Structure and Stability: The Role of Nucleotide Composition and Order. <i>ChemistryOpen</i> , 2022, 11, e202200013.	0.9	0
101	How Ionization Catalyzes Diels $\hat{\pm}$ Alder Reactions. <i>Chemistry - A European Journal</i> , 0, , .	1.7	0
102	Front Cover: How Ionization Catalyzes Diels $\hat{\pm}$ Alder Reactions (<i>Chem. Eur. J.</i> 40/2022). <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	0