

# Luke A Burke

## List of Publications by Year in descending order

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citations

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733

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#	ARTICLE	IF	CITATIONS
1	Selective Activation of C=C Bond in Sustainable Phenolic Compounds from Lignin <i>via</i> Photooxidation: Experiment and Density Functional Theory Calculations. <i>Photochemistry and Photobiology</i> , 2015, 91, 1332-1339.	2.5	10
2	A self-assembled, metallo-organic supramolecular frequency doubler. <i>Chemical Communications</i> , 2012, 48, 1000-1002.	4.1	3
3	Spectroscopic and photophysical properties of dicopper(I) metallocyclophanes. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 3061-3071.	2.0	1
4	Correlation analysis of the interconversion and nitrogen loss reactions of aryl pentazenes and pentazoles derived from aryl diazonium and azide ions. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3613-3618.	2.0	11
5	Computational Investigation of Rearrangements in Huisgen Cycloadducts of Azolium N-Dicyanomethanide 1,3-Dipoles with Alkynes: A Mechanistic Panoply. <i>Journal of Organic Chemistry</i> , 2009, 74, 5199-5210.	3.2	5
6	A Ceric Ammonium Nitrate N-Dearylation of <i>N</i>-<i>p</i>-Anisylazoles Applied to Pyrazole, Triazole, Tetrazole, and Pentazole Rings: Release of Parent Azoles. Generation of Unstable Pentazole, HN<sub>5</sub>/N<sub>5</sub><sup>-</sup>, in Solution. <i>Journal of Organic Chemistry</i> , 2008, 73, 1354-1364.	3.2	96
7	Uncharacteristic thione behavior in a Huisgen cycloaddition reaction: a kinetic and theoretical study. <i>Tetrahedron Letters</i> , 2007, 48, 6684-6687.	1.4	9
8	Spirally twisted imidazolium iminyl ylide structures from 1,2-rearrangements in reactions of imidazolium dicyanomethanide 1,3-dipoles with maleic anhydride: new perspectives on the Boekelheide-Fedoruk ring expansions. <i>Tetrahedron Letters</i> , 2006, 47, 6107-6111.	1.4	3
9	Consideration of spin states in determining the structure and decomposition of the transition metal pentazoles FeClN <sub>5</sub> , Fe(N <sub>5</sub> ) <sub>2</sub> , Fe(H <sub>2</sub> O)4ClN <sub>5</sub> , and Fe(NH <sub>3</sub> )4ClN <sub>5</sub> . Electronic supplementary information (ESI) available: energies for all structures with the various basis sets. See <a href="http://www.rsc.org/suppdata/cc/b3/b315812h/">http://www.rsc.org/suppdata/cc/b3/b315812h/</a> . <i>Chemical Communications</i> , 2004, , 1082.	4.1	12
10	The Influence of Water on the Rates of 1,3-Dipolar Cycloaddition Reactions: Trigger Points for Exponential Rate Increases in Water-Organic Solvent Mixtures. Water-Super versus Water-Normal Dipolarophiles. <i>Journal of the American Chemical Society</i> , 2004, 126, 11923-11929.	13.7	77
11	First generation of pentazole (HN <sub>5</sub> , pentazolic acid), the final azole, and a zinc pentazolate salt in solution: A new N-dearylation of 1-(p-methoxyphenyl) pyrazoles, a 2-(p-methoxyphenyl) tetrazole and application of the methodology to 1-(p-methoxyphenyl) pentazole. Electronic supplementary information (ESI) available: experimental details. See <a href="http://www.rsc.org/suppdata/cc/b3/b301491f/">http://www.rsc.org/suppdata/cc/b3/b301491f/</a> .	4.1	91
12	Kinetic and synthetic influences of water and solvent-free conditions on 1,3-dipolar cycloaddition reactions: the phthalazinium and pyridazinium dicyanomethanide 1,3-dipoles: surprisingly successful synthetic methods. Electronic supplementary information (ESI) available: sample kinetic graphs and optimised transition state structures. See <a href="http://www.rsc.org/suppdata/p2/b2/b206028k/">http://www.rsc.org/suppdata/p2/b2/b206028k/</a> . <i>Perkin Transactions II RSC</i> , 2002, , 1807-1815.	1.1	38
13	The kinetic profile of phthalazinium-2-dicyanomethanide 1,3-dipole with 2 <i>π</i> -dipolarophiles: U-shaped dipolarophilic activity and classic type II dipole behaviour. Reaction rates and DFT calculations. <i>Perkin Transactions II RSC</i> , 2001, , 1781-1784.	1.1	17
14	Regioselectivity and endo/exo selectivity in the cycloadditions of the phthalazinium dicyanomethanide 1,3-dipole with unsymmetrical alkene and alkyne dipolarophiles. Unexpected reversals of regiochemistry: a combined experimental and DFT theoretical study. <i>Journal of the Chemical Society, Perkin Transactions 1</i> , 2001, , 1391-1397.	1.3	27
15	Theoretical characterization of pentazole anion with metal counter ions. Calculated and experimental <sup>15</sup> N shifts of aryl diazonium, -azide and -pentazole systems. <i>Perkin Transactions II RSC</i> , 2001, , 1679-1684.	1.1	53
16	Alternating Planarity/Nonplanarity in n-Doped Odd-Membered, All-Trans Polyenes: Molecular Structures of NaC <sub>n</sub> H <sub>n+2</sub> (n = 3, 5, 7, and 9). <i>Journal of Molecular Modeling</i> , 2000, 6, 248-256.	1.8	1
17	Theoretical study of the possible isomers and high-energy intermediates of HCN <sup>+</sup> -H <sub>2</sub> O complexes. <i>Computational and Theoretical Chemistry</i> , 1998, 427, 199-209.	1.5	9
18	Pentazole chemistry: the mechanism of the reaction of aryl diazonium chlorides with azide ion at $\sim 80^\circ\text{C}$ : concerted versus stepwise formation of aryl pentazoles, detection of a pentazene intermediate, a combined <sup>1</sup> H and <sup>15</sup> N NMR experimental and ab initio theoretical study. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1998, , 2243-2248.	0.9	40

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19	An unusual substituent effect in a cycloaddition of an azonium ylide 1,3-dipole: An inverted V-shaped hammett plot. <i>Journal of Heterocyclic Chemistry</i> , 1997, 34, 1825-1827.	2.6	3
20	Ion pair formation in water clusters: a theoretical study. <i>Chemical Physics Letters</i> , 1997, 276, 145-151.	2.6	20
21	Theoretical study of water clusters: nonamers. <i>Chemical Physics Letters</i> , 1996, 260, 499-506.	2.6	24
22	Theoretical study of possible products of the combination of H <sub>2</sub> O and HCN. <i>Computational and Theoretical Chemistry</i> , 1996, 370, 245-252.	1.5	6
23	Theoretical study of water clusters: Heptamers. <i>Chemical Physics Letters</i> , 1995, 241, 253-260.	2.6	39
24	Theoretical study of water clusters: octamer. <i>Chemical Physics Letters</i> , 1995, 246, 13-19.	2.6	52
25	Theoretical study of water clusters. II. Hexamer. <i>Chemical Physics Letters</i> , 1994, 217, 311-318.	2.6	42
26	Theoretical study of water clusters. I. Pentamer. <i>Chemical Physics Letters</i> , 1993, 206, 293-296.	2.6	59
27	The reactions of 1,2,3-triazolium-1-imides with dipolarophiles: kinetics and mechanism. Azonium 1,3-dipoles. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1992, , 1103.	0.9	9
28	The nonplanarity of n-doped polyenes and of carbanions with alkali metal counterions. <i>International Journal of Quantum Chemistry</i> , 1988, 34, 51-57.	2.0	4
29	Synchronism in the Diels-Alder reaction. <i>International Journal of Quantum Chemistry</i> , 1986, 29, 511-518.	2.0	10
30	The influence of the cyclic product's structure on the Diels-Alder transition state. <i>Theoretica Chimica Acta</i> , 1985, 68, 101-105.	0.8	9
31	The theoretical study of (2 + 2) cycloadditions —the concerted ethylene dimerizations reaction. <i>Bulletin Des Sociétés Chimiques Belges</i> , 1979, 88, 379-393.	0.0	10
32	Theoretical study of the vinyl azide- $\text{\textmu}$ -triazole isomerization. <i>Journal of the American Chemical Society</i> , 1978, 100, 3668-3674.	13.7	50
33	Theoretical study of the azido-tetrazole isomerization. <i>Journal of the American Chemical Society</i> , 1976, 98, 1685-1690.	13.7	85
34	Theoretical study of the Diels-Alder reaction. <i>Theoretica Chimica Acta</i> , 1975, 40, 313-321.	0.8	65