

# Luke A Burke

## List of Publications by Year in descending order

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34  
papers

1,016  
citations

471509

17  
h-index

414414

32  
g-index

36  
all docs

36  
docs citations

36  
times ranked

733  
citing authors

| #  | ARTICLE  | IF   | CITATIONS |
|----|--|------|-----------|
| 1  | 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        |
| 2  | 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-( <i>p</i> -methoxyphenyl) pyrazoles, a 2-( <i>p</i> -methoxyphenyl) tetrazole and application of the methodology to 1-( <i>p</i> -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> . <i>Chemical Communications</i> , 2003, , 1016-1017. | 4.1  | 91        |
| 3  | Theoretical study of the azido-tetrazole isomerization. <i>Journal of the American Chemical Society</i> , 1976, 98, 1685-1690.   | 13.7 | 85        |
| 4  | 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        |
| 5  | Theoretical study of the Diels-Alder reaction. <i>Theoretica Chimica Acta</i> , 1975, 40, 313-321.   | 0.8  | 65        |
| 6  | Theoretical study of water clusters. I. Pentamer. <i>Chemical Physics Letters</i> , 1993, 206, 293-296.  | 2.6  | 59        |
| 7  | 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        |
| 8  | Theoretical study of water clusters: octamer. <i>Chemical Physics Letters</i> , 1995, 246, 13-19.  | 2.6  | 52        |
| 9  | Theoretical study of the vinyl azide-ε-triazole isomerization. <i>Journal of the American Chemical Society</i> , 1978, 100, 3668-3674.   | 13.7 | 50        |
| 10 | Theoretical study of water clusters. II. Hexamer. <i>Chemical Physics Letters</i> , 1994, 217, 311-318.  | 2.6  | 42        |
| 11 | Pentazole chemistry: the mechanism of the reaction of aryl diazonium chlorides with azide ion at 80°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        |
| 12 | Theoretical study of water clusters: Heptamers. <i>Chemical Physics Letters</i> , 1995, 241, 253-260.  | 2.6  | 39        |
| 13 | 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</i> , 2002, , 1897-1915.  | 1.1  | 38        |
| 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 study of water clusters: nonamers. <i>Chemical Physics Letters</i> , 1996, 260, 499-506.   | 2.6  | 24        |
| 16 | Ion pair formation in water clusters: a theoretical study. <i>Chemical Physics Letters</i> , 1997, 276, 145-151.   | 2.6  | 20        |
| 17 | The kinetic profile of phthalazinium-2-dicyanomethanide 1,3-dipole with ε-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        |
| 18 | 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) <sub>4</sub> ClN <sub>5</sub> , and Fe(NH <sub>3</sub> ) <sub>4</sub> ClN <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        |

| #  | ARTICLE   | IF  | CITATIONS |
|----|---|-----|-----------|
| 19 | 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        |
| 20 | Synchronism in the Diels-Alder reaction. <i>International Journal of Quantum Chemistry</i> , 1986, 29, 511-518.   | 2.0 | 10        |
| 21 | The theoretical study of (2 + 2) cycloadditions of the concerted ethylene dimerizations reaction. <i>Bulletin Des Sociétés Chimiques Belges</i> , 1979, 88, 379-393.  | 0.0 | 10        |
| 22 | Selective Activation of C=C Bond in Sustainable Phenolic Compounds from Lignin via Photooxidation: Experiment and Density Functional Theory Calculations. <i>Photochemistry and Photobiology</i> , 2015, 91, 1332-1339.   | 2.5 | 10        |
| 23 | 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         |
| 24 | The reactions of 1,2,3-triazolium-1-imides with dipolarophiles: kinetics and mechanism. Azolium 1,3-dipoles. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1992, , 1103.  | 0.9 | 9         |
| 25 | Theoretical study of the possible isomers and high-energy intermediates of HCN-H <sub>2</sub> O complexes. <i>Computational and Theoretical Chemistry</i> , 1998, 427, 199-209.   | 1.5 | 9         |
| 26 | Uncharacteristic thione behavior in a Huisgen cycloaddition reaction: a kinetic and theoretical study. <i>Tetrahedron Letters</i> , 2007, 48, 6684-6687.  | 1.4 | 9         |
| 27 | 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         |
| 28 | 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         |
| 29 | 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         |
| 30 | An unusual substituent effect in a cycloaddition of an azolium ylide 1,3-dipole: An inverted Hammett plot. <i>Journal of Heterocyclic Chemistry</i> , 1997, 34, 1825-1827.  | 2.6 | 3         |
| 31 | 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         |
| 32 | A self-assembled, metallo-organic supramolecular frequency doubler. <i>Chemical Communications</i> , 2012, 48, 1000-1002.   | 4.1 | 3         |
| 33 | 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         |
| 34 | Spectroscopic and photophysical properties of dicopper(I) metallocyclophanes. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 3061-3071.   | 2.0 | 1         |