Athanassios V Nicolaides

List of Publications by Year
in descending order

37	1,251	471509 17	361022 35
papers	citations	h-index	g-index

40	40	40	903
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Heats of Formation from G2, G2(MP2), and G2(MP2,SVP) Total Energies. The Journal of Physical Chemistry, 1996, 100, 17460-17464.	2.9	327
2	Phenyl Radical, Cation, and Anion. The Tripletâ^'Singlet Gap and Higher Excited States of the Phenyl Cation. Journal of the American Chemical Society, 1997, 119, 8083-8088.	13.7	103
3	Ring Opening of the Cyclopropylcarbinyl Radical and ItsN- andO-Substituted Analogues:Â A Theoretical Examination of Very Fast Unimolecular Reactions. Journal of the American Chemical Society, 1998, 120, 10223-10233.	13.7	96
4	CI calculations on didehydrobenzenes predict heats of formation for the meta and para isomers that are substantially higher than previous experimental values. Journal of the American Chemical Society, 1993, 115, 11951-11957.	13.7	83
5	An evaluation of the performance of G2, G2(MP2) and G2(MP2,SVP) theories for heats of formation and heats of reaction in the case of 'large' hydrocarbons. Molecular Physics, 1996, 88, 759-765.	1.7	66
6	Seven-Membered Ring or Phenyl-Substituted Cation? Relative Stabilities of the Tropylium and Benzyl Cations and Their Silicon Analogs. Journal of the American Chemical Society, 1994, 116, 9769-9770.	13.7	48
7	A Theoretical Study of Chlorine Atom and Methyl Radical Addition to Nitrogen Bases:Â Why Do Cl Atoms Form Two-Centerâ^'Three-Electron Bonds Whereas CH3Radicals Form Two-Centerâ^'Two-Electron Bonds?. Journal of the American Chemical Society, 1996, 118, 10571-10576.	13.7	46
8	Is the most stable gas-phase isomer of the benzenium cation a face-protonated Ï€-complex?. Journal of the Chemical Society Chemical Communications, 1995, .	2.0	45
9	Relative Stabilities and Hydride Affinities of Silatropylium and Silabenzyl Cations and Their Isomers. Comparison with the Carbon Analogues Tropylium and Benzyl Cations. Journal of the American Chemical Society, 1996, 118, 10561-10570.	13.7	38
10	Synthesis and Study of the (Ph3P)2Pt Complexes of Three Members of a Series of Highly Pyramidalized Alkenes. Organometallics, 1995, 14, 3475-3485.	2.3	34
11	Direct Observation and Characterization ofp-Phenylenebisnitrene. A Labile Quinoidal Diradical. Journal of the American Chemical Society, 1998, 120, 11530-11531.	13.7	33
12	A Simple Failing of G2 Theory: Heats of Combustion. The Journal of Physical Chemistry, 1994, 98, 3092-3093.	2.9	32
13	Of Ortho-Conjugatively Linked Reactive Intermediates:Â The Cases of Ortho-Phenylene-(Bis)Nitrene, -Carbenonitrene, and -(Bis)Carbene. Journal of the American Chemical Society, 1999, 121, 10563-10572.	13.7	30
14	p-Phenylenecarbenonitrene and Its Halogen Derivatives: How Does Resonance Interaction between a Nitrene and a Carbene Center Affect the Overall Electronic Configuration?. Journal of the American Chemical Society, 2001, 123, 2628-2636.	13.7	30
15	Surface mechanism of the boron adsorption on alumina in aqueous solutions. Desalination and Water Treatment, 2013, 51, 6130-6136.	1.0	25
16	The Elusive Benzocyclobutenylidene:Â A Combined Computational and Experimental Attempt. Journal of the American Chemical Society, 2001, 123, 2870-2876.	13.7	24
17	Classical and Nonclassical Isomers of Tropylium, Silatropylium, and Germatropylium Cations. Descending the Periodic Table Increases the Preference for Nonclassical Structures. Journal of the American Chemical Society, 1997, 119, 11933-11937.	13.7	23
18	Triggering selective uranium separation from aqueous solutions by using salophen-modified biochar fibers. Journal of Radioanalytical and Nuclear Chemistry, 2018, 318, 2199-2203.	1.5	17

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19	Effect of Angle Strain in Conjugated Cycloalkenylidenes. Singletâ^'Triplet Splitting of Cyclobutenylidene and Its Ground-State Intramolecular Rearrangements. Journal of Organic Chemistry, 1999, 64, 3299-3305.	3.2	16
20	Evidence for the Formation of the (Ph3P)2Pt Complex of 3,7-Dimethyltricyclo[3.3.0.03,7]oct-1(5)-ene, the Most Highly Pyramidalized Alkene in a Homologous Series. Isolation and X-ray Structure of the Product of the Ethanol Addition to the Complex. Organic Letters, 2006, 8, 3001-3004.	4.6	16
21	Halogen Derivatives ofm-Phenylene(carbeno)nitrene:Â A Switch in Ground-State Multiplicity. Journal of Organic Chemistry, 2002, 67, 5578-5587.	3.2	15
22	Photochemistry of an Azido-Functionalized Cryptand:Â Controlling the Reactivity of an Extremely Long-Lived Singlet Aryl Nitrene by Complexation to Alkali Cations. Journal of the American Chemical Society, 2005, 127, 6883-6892.	13.7	13
23	A computational study of the conformations of the boric acid (B(OH)3), its conjugate base ((HO)2BOâ^') and borate anion. Computational and Theoretical Chemistry, 2008, 853, 33-38.	1.5	13
24	An improved synthesis of diiodonoradamantane. Tetrahedron Letters, 2009, 50, 6938-6940.	1.4	10
25	Connectivity Effects in Isomeric Naphthalenedinitrenes. Organic Letters, 2001, 3, 357-360.	4.6	9
26	o-Phenylene Halocarbenonitrenes ando-Phenylene Chlorocarbenocarbene:Â A Combined Experimental and Computational Approach. Journal of Organic Chemistry, 2005, 70, 7744-7754.	3.2	9
27	Singlet Hydrocarbon Carbenes with High Barriers Toward Isomerization:â€‰ A Computational Investigation. Journal of the American Chemical Society, 2003, 125, 9070-9073.	13.7	7
28	Estimating the Ï€-bond energies and the stabilities of oxy-substituted carbocations. Computational and Theoretical Chemistry, 2007, 811, 355-359.	1.5	6
29	Synthesis of a novel diene from a cyclobutane precursor: an entry toÂ2,9-disubstituted [2]diadamantanes. Tetrahedron, 2013, 69, 8064-8068.	1.9	6
30	A computational study on the possible role of oxygen in the oxidation of methionine and dimethylsulfide initiated by OH radicals. Computational and Theoretical Chemistry, 2013, 1009, 24-29.	2.5	5
31	Geometrically Strained Carbenes: Interdependence among Geometry, Spin Multiplicity, and Reactivity.. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 2001, 59, 1070-1077.	0.1	4
32	Hula-twist photoisomerization of a styrene derivative examined by argon-matrix-infrared-spectroscopic method. Molecular Physics, 2006, 104, 1009-1015.	1.7	3
33	Lipidomics and Free Radical Modifications of Lipids. Chimia, 2008, 62, 713.	0.6	3
34	Electron affinities of a homologous series of tertiary alkyl radicals and their Câ€“H bond dissociation energies (BDEs). Tetrahedron, 2009, 65, 1655-1659.	1.9	2
35	Determination of the chirality of enantiomeric [16O, 17O, 18O] sulfate esters by IR spectroscopy: an ab initio evaluation. Journal of the Chemical Society Chemical Communications, 1995, , 701.	2.0	1
36	Tricyclo[3.3.1.03,7]nonane-3,7-diyl bis(methanesulfonate). Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o409-o409.	0.2	1

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37	Effect of halogen substitution onp-phenylenebiscarbene. International Journal of Quantum Chemistry, 2005, 104, 475-481.	2.0	0