

Ponnambalam Venuvanalingam

List of Publications by Year in descending order

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134
papers

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#	ARTICLE	IF	CITATIONS
1	Tuning Nonlinear Optical and Optoelectronic Properties of Vinyl Coupled Triazene Chromophores: A Density Functional Theory and Time-Dependent Density Functional Theory Investigation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4667-4677.	2.5	164
2	Interaction of anthraquinone dyes with lysozyme: Evidences from spectroscopic and docking studies. <i>Journal of Hazardous Materials</i> , 2010, 175, 985-991.	12.4	130
3	Hydrogenolysis of sorbitol over Ni and Pt loaded on NaY. <i>Catalysis Communications</i> , 2011, 12, 673-677.	3.3	90
4	Water-Soluble Mono- and Binuclear Ru(η^6 -cymene) Complexes Containing Indole Thiosemicarbazones: Synthesis, DFT Modeling, Biomolecular Interactions, and <i>In Vitro</i> Anticancer Activity through Apoptosis. <i>Organometallics</i> , 2018, 37, 1242-1257.	2.3	77
5	Biomolecular Interaction, Anti-Cancer and Anti-Angiogenic Properties of Cobalt(III) Schiff Base Complexes. <i>Scientific Reports</i> , 2019, 9, 2721.	3.3	65
6	Enhanced photocatalytic degradation of azo dyes using nano Fe ₃ O ₄ . <i>Journal of the Iranian Chemical Society</i> , 2012, 9, 101-109.	2.2	63
7	π -systems as lithium/hydrogen bond acceptors: Some theoretical observations. <i>Journal of Chemical Physics</i> , 1998, 109, 9820-9830.	3.0	62
8	A DFT/TDDFT modelling of bithiophene azo chromophores for optoelectronic applications. <i>Dyes and Pigments</i> , 2014, 100, 261-268.	3.7	59
9	Surfactant-copper(II) Schiff base complexes: synthesis, structural investigation, DNA interaction, docking studies, and cytotoxic activity. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 877-891.	3.5	58
10	Topological resonance energy predictions of the stability of fullerene clusters. <i>Chemical Physics Letters</i> , 1994, 222, 95-100.	2.6	47
11	Origin and Nature of Lithium and Hydrogen Bonds to Oxygen, Sulfur, and Selenium. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10859-10867.	2.5	47
12	Single and double chain surfactant-cobalt(III) complexes: the impact of hydrophobicity on the interaction with calf thymus DNA, and their biological activities. <i>RSC Advances</i> , 2015, 5, 31746-31758.	3.6	46
13	Highly Emissive Luminogens Based on Imidazo[1,2-a]pyridine for Electroluminescent Applications. <i>Chemistry - an Asian Journal</i> , 2014, 9, 294-304.	3.3	44
14	Designing benzosiloles for better optoelectronic properties using DFT & TDDFT approaches. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14229.	2.8	43
15	Sorbitol Hydrogenolysis Over Ni, Pt and Ru Supported on NaY. <i>Topics in Catalysis</i> , 2012, 55, 897-907.	2.8	42
16	Are Re(phenanthroline) complexes suitable candidates for OLEDs? Answers from DFT and TD-DFT investigations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21157-21171.	2.8	42
17	Ab initio study of tautomerism and hydrogen bonding of $\hat{1}^2$ -carbonylamine in the gas phase and in water solution. <i>Theoretical Chemistry Accounts</i> , 2000, 104, 226-234.	1.4	41
18	Influence of self-assembly on intercalative DNA binding interaction of double-chain surfactant Co(III) complexes containing imidazo[4,5-f][1,10]phenanthroline and dipyrido[3,2-d:2'-3'-f]quinoxaline ligands: experimental and theoretical study. <i>Dalton Transactions</i> , 2014, 43, 18074-18086.	3.3	41

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19	The role of cumulenic strain on the kinetic and thermodynamic control of the Diels-Alder reactions involving allenes as dienes. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 1799-1804.	0.9	40
20	Novel uranyl(ν) complexes incorporating propylene-bridged salen-type N_2O_2 -ligands: a structural and computational approach. <i>Dalton Transactions</i> , 2015, 44, 568-577.	3.3	40
21	AM1 and PM3 transition structures for the epoxidation of alkenes and allene by methylated dioxiranes. <i>Computational and Theoretical Chemistry</i> , 1997, 394, 41-47.	1.5	37
22	A combined experimental and computational study on the sulfoxidation by high-valent iron bispidine complexes. <i>Dalton Transactions</i> , 2011, 40, 11276.	3.3	36
23	Luminescent $Re(\nu)$ terpyridine complexes for OLEDs: what does the DFT/TD-DFT probe reveal?. <i>Dalton Transactions</i> , 2015, 44, 8529-8542.	3.3	34
24	Synthesis, DNA binding and docking studies of copper(II) complexes containing modified phenanthroline ligands. <i>Journal of Coordination Chemistry</i> , 2015, 68, 1374-1386.	2.2	33
25	Lithium bonding interaction in $H_2CY\hat{c}LiF$ ($Y=O,S$) complexes: A theoretical probe. <i>Journal of Chemical Physics</i> , 1997, 107, 4329-4336.	3.0	31
26	1,3-Dipolar Reactions Involving Corannulene: How Does Its Rim and Spoke Addition Vary?. <i>Journal of Organic Chemistry</i> , 2005, 70, 2528-2536.	3.2	31
27	Surfactant-cobalt(III) complexes: The impact of hydrophobicity on interaction with HSA and DNA insights from experimental and theoretical approach. <i>Colloids and Surfaces B: Biointerfaces</i> , 2017, 153, 85-94.	5.0	30
28	Synthesis, DNA and BSA binding, <i>in vitro</i> anti-proliferative and <i>in vivo</i> anti-angiogenic properties of some cobalt(ν) Schiff base complexes. <i>New Journal of Chemistry</i> , 2019, 43, 11391-11407.	2.8	30
29	Evaluation of the Leaf Essential Oil from <i>Artemisia vulgaris</i> and Its Larvicidal and Repellent Activity against Dengue Fever Vector <i>Aedes aegypti</i> An Experimental and Molecular Docking Investigation. <i>ACS Omega</i> , 2018, 3, 15657-15665.	3.5	29
30	Half-sandwich $Ru(\hat{c}6\text{-p-cymene})$ complexes featuring pyrazole appended ligands: Synthesis, DNA binding and <i>in vitro</i> cytotoxicity. <i>Journal of Inorganic Biochemistry</i> , 2019, 194, 74-84.	3.5	29
31	Kinetics of polymerization of N,N-methylenebisacrylamide initiated by $KMnO_4$ - $H_2C_2O_4$ redox system. <i>European Polymer Journal</i> , 1982, 18, 531-534.	5.4	28
32	Structure of the Benzene- $\hat{c}ICl$ Complex: A UVPES and <i>ab Initio</i> Molecular Orbital Study. <i>Journal of Physical Chemistry A</i> , 1998, 102, 532-536.	2.5	28
33	<i>Ab initio</i> study of formazan and 3-nitroformazan. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 3313-3319.	1.7	28
34	1,3-Dipolar additions involving allenes: A density functional study of concerted and stepwise mechanisms Electronic supplementary information (ESI) available: Cartesian co-ordinates of all the structures with their computed total energies. See http://www.rsc.org/suppdata/p2/b2/b206470g . <i>Perkin Transactions II RSC</i> , 2002, , 2130-2139.	1.1	28
35	Elucidating the structures and binding of halide ions bound to cucurbit[6]uril, hemi-cucurbit[6]uril and bambus[6]uril using DFT calculations. <i>RSC Advances</i> , 2011, 1, 1333.	3.6	27
36	On the Nature of Hypercoordination in Dihalogenated Perhalocyclohexasilanes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3529-3538.	2.5	27

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37	Ab initio and DFT investigations of lithium/hydrogen bonded complexes of trimethylamine, dimethyl ether and dimethyl sulfide. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 2669-2674.	1.7	26
38	Low-lying stepwise paths for ethylene 1,3-dipolar cycloadditions: A DFT study. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 64-78.	2.0	25
39	Synthesis, characterisation and electroluminescence behaviour of π -conjugated imidazole-isoquinoline derivatives. <i>Dyes and Pigments</i> , 2014, 102, 180-188.	3.7	25
40	A multispectroscopic and molecular docking investigation of the binding interaction between serum albumins and acid orange dye. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 192, 34-40.	3.9	25
41	Water-soluble Cobalt(II) & Cobalt(III) complexes supported by new triazine Schiff base ligands: Synthesis, structure and biological evaluation. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2018, 189, 152-164.	3.8	24
42	Allene and fluoroallenes as dienophiles in Diels-Alder reactions: an AM1 and PM3 study. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1996, , 1423-1427.	0.9	23
43	A DFT/TDDFT mission to probe push-pull vinyl coupled thiophene oligomers for optoelectronic applications. <i>RSC Advances</i> , 2015, 5, 50353-50364.	3.6	22
44	Gain or loss of aromaticity in Diels-Alder transition states and adducts: a theoretical investigation. <i>Journal of Physical Organic Chemistry</i> , 1998, 11, 133-140.	1.9	21
45	Electron donor-acceptor complexes of I ₂ with diethyl ether and diethyl sulphide. An ab initio MO study. <i>Chemical Physics Letters</i> , 1996, 248, 153-157.	2.6	20
46	Open versus Closed 1,3-Dipolar Additions of C ₆₀ : A Theoretical Investigation on Their Mechanism and Regioselectivity. <i>Journal of Organic Chemistry</i> , 2005, 70, 5426-5435.	3.2	20
47	Harmonic analysis of vibrations of morpholine-4-ylmethylthiourea: A DFT, midinfrared and Raman spectral study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 996-1002.	3.9	20
48	Investigations on the fluorescence quenching of 2,3-diazabicyclo[2.2.2]oct-2-ene by certain flavonoids. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2008, 91, 143-150.	3.8	20
49	Conjugated polymer based on oligobenzo[c]thiophene with low-lying HOMO energy level as potential donor for bulk heterojunction solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013, 262, 34-44.	3.9	20
50	Tunable single and dual emission behavior of imidazole fluorophores based on D-A architecture. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2014, 284, 36-48.	3.9	20
51	Interaction between toxic azo dye C.I. Acid Red 88 and serum albumins. <i>Journal of Luminescence</i> , 2013, 143, 715-722.	3.1	19
52	Computational evaluation of optoelectronic and photophysical properties of unsymmetrical distyrylbiphenyls. <i>RSC Advances</i> , 2014, 4, 53060-53071.	3.6	19
53	C-H functionalisation through carbene and fluorocarbene insertion ab initio and DFT investigations. <i>Computational and Theoretical Chemistry</i> , 2005, 755, 169-178.	1.5	17
54	A new turn in codon-anticodon selection through halogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7430.	2.8	17

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55	Antitumor activity of bent metallocenes: electronic structure analysis using DFT computations. <i>Journal of Molecular Modeling</i> , 2011, 17, 465-475.	1.8	16
56	Encapsulation of a hexaaza macrocyclic nickel(Ni^{II}) complex in zeolite Y: an experimental and theoretical investigation. <i>New Journal of Chemistry</i> , 2017, 41, 9505-9512.	2.8	16
57	Tuning the Photophysical Properties of 2-Quinolinone-Based Donor-Acceptor Molecules through N-versus O-Alkylation: Insights from Experimental and Theoretical Investigations. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 753-766.	2.4	15
58	A combined experimental and theoretical investigation of imidazole-carbazole fluorophores. <i>Journal of Luminescence</i> , 2014, 147, 111-120.	3.1	15
59	The nature of Pd-carbene and Pd-halogen bonds in $(\text{bisNHC})\text{PdX}_2$ type catalysts: insights from density functional theory. <i>RSC Advances</i> , 2015, 5, 80661-80667.	3.6	15
60	Rational design of cyclopenta[b]naphthalenes for better optoelectronic applications and their photophysical properties using DFT/TD-DFT methods. <i>RSC Advances</i> , 2016, 6, 44569-44577.	3.6	15
61	Structural elucidation and physicochemical properties of mononuclear Uranyl(VI) complexes incorporating dianionic units. <i>Scientific Reports</i> , 2016, 6, 32898.	3.3	15
62	Electronic structure and conformation of glyphosate: an ab initio MO study. <i>Computational and Theoretical Chemistry</i> , 2002, 618, 117-125.	1.5	14
63	Synthesis of conjugated perylene diimide-based copolymer with 5,5-bis(4-aminophenyl)-2-bifuryl moiety as an active material for organic photovoltaics. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2012, 247, 52-62.	3.9	14
64	Phenylacetylene dimer: Ab initio and DFT study. <i>Chemical Physics</i> , 2013, 415, 150-155.	1.9	14
65	The nature of hydrogen bonding in $\text{R}_2\text{X}_2(8)$ crystal motifs – a computational exploration. <i>Molecular Physics</i> , 2014, 112, 3195-3205.	1.7	14
66	Elucidating the structures and cooperative binding mechanism of cesium salts to the multitopic ion-pair receptor through density functional theory calculations. <i>Dalton Transactions</i> , 2015, 44, 15450-15462.	3.3	14
67	Cyclopolymerization Initiated by Peroxydisulfate Ion and Metal Ion Catalysis. <i>Journal of Macromolecular Science Part A, Chemistry</i> , 1986, 23, 117-128.	0.3	13
68	Transition states and charge analyses along the IRC for the singlet chlorocarbenes insertions into C-H bond of alkanes. <i>Chemical Physics Letters</i> , 2006, 430, 414-419.	2.6	13
69	Green light-emitting 2-(1H-indol-3-yl)acetonitrile-based D-A fluorophores – a combined theoretical and experimental study. <i>Materials Chemistry Frontiers</i> , 2017, 1, 1373-1383.	5.9	13
70	Structure and Reactivity of Pd Complexes in Various Oxidation States in Identical Ligand Environments with Reference to C and Cl Coupling Reactions: Insights from Density Functional Theory. <i>Inorganic Chemistry</i> , 2018, 57, 6833-6846.	4.0	13
71	Theoretical study on the mechanism and reactivity of fluorocumulenes in [4+2] cycloadditions. <i>Journal of Fluorine Chemistry</i> , 1995, 73, 171-174.	1.7	12
72	LVPES and ab Initio Molecular Orbital Studies on the Electron Donor-Acceptor Complexes of Bromine with Methylamines. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1155-1159.	2.5	12

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73	Oxaphosphetane versus betaine formation in epoxide ring opening by PPh ₃ : a mechanistic probe by ab initio and DFT modeling. <i>Tetrahedron Letters</i> , 2005, 46, 4087-4090.	1.4	12
74	Spectroscopic Studies on TiO ₂ Enhanced Binding of Hypocrellin B with DNA. <i>Journal of Fluorescence</i> , 2011, 21, 1887-1895.	2.5	12
75	Understanding the stability, electronic and molecular structure of some copper(III) complexes containing alkyl and non alkyl ligands: Insights from DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 2627-2634.	1.8	12
76	Are cucurbiturils better drug carriers for bent metallocenes? Insights from theory. <i>Journal of Biological Inorganic Chemistry</i> , 2018, 23, 413-423.	2.6	12
77	Effect of increasing methoxyphenyl substitution on pyrene pyrazoline enduring green light emitting materials. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 377, 247-259.	3.9	11
78	A bowl-shaped phenoxido-bridged binuclear zinc complex: Experimental and theoretical studies. <i>Inorganica Chimica Acta</i> , 2022, 534, 120807.	2.4	11
79	Is corannulene a better diene or dienophile? A DFT analysis. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 146-154.	1.9	10
80	Application of activation hardness in perturbed pericyclic reactions: a case study involving electrocyclic ring opening reactions of heterocyclobutenes. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 460-465.	1.9	10
81	Semi-empirical MO-calculations on the electronic spectra of benzoquinonechlorimides. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1980, 36, 103-107.	0.1	9
82	A proton and carbon NMR spectroscopic study of 5-substituted acenaphthenes. <i>Magnetic Resonance in Chemistry</i> , 1998, 36, 943-946.	1.9	9
83	Theoretical investigation on the reactivity of sulfur-centered heterocumulenes as dienophiles in Diels-Alder reactions and endo-lone-pair effect. <i>International Journal of Quantum Chemistry</i> , 1998, 66, 309-322.	2.0	9
84	Quantitative property-property relationship (QPPR) approach in predicting flotation efficiency of chelating agents as mineral collectors. <i>SAR and QSAR in Environmental Research</i> , 2002, 13, 499-508.	2.2	9
85	Ab initio and DFT studies on conformations, hydrogen bonding and electronic structures of glyoxalmonoxime and its methyl derivatives. <i>Computational and Theoretical Chemistry</i> , 2004, 712, 175-185.	1.5	9
86	Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 139-146.	2.0	9
87	Ring Cleavage of Aziridines by Difluoroamine: Mechanistic Insights from ab Initio and DFT Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4829-4835.	2.5	9
88	Molecular complexes of p-benzoquinonechlorimides with aromatic π -donors. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1981, 37, 505-510.	0.1	8
89	Ultraviolet photoelectron spectroscopy of complexes of bromine with n-donors in the vapor phase. <i>Chemical Physics Letters</i> , 1994, 228, 431-435.	2.6	8
90	Diels-Alder addition of butadiene to various thiocarbonyl(R ₂ C=SO _n , n=0-2) heterodienophiles and endo-lone pair effect in heterocumulene. <i>Journal of Physical Organic Chemistry</i> , 1997, 10, 768-776.	1.9	8

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91	Ab initio Computational Modeling of Glyphosate Analogs: Conformational Perspective. <i>Structural Chemistry</i> , 2005, 16, 491-506.	2.0	8
92	Fluorine effect on pericyclic and pseudopericyclic processes: Evidences and ab initio theory. <i>Journal of Chemical Sciences</i> , 2009, 121, 859-866.	1.5	8
93	Spectroscopic and Molecular Docking Investigations on the Interaction of Rutin with Bovine Serum Albumin. <i>Zeitschrift Fur Physikalische Chemie</i> , 2011, 225, 441-454.	2.8	8
94	Studies on the inclusion behavior of 9-Aminoacridine into cyclodextrins: Spectroscopic and theoretical evidences. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 103, 18-24.	3.9	8
95	Effect on shifting of phenyl ring in pyrazoline pyrene luminophore and their photophysical and electrochemical investigation. <i>Optical Materials</i> , 2019, 94, 403-414.	3.6	8
96	Solid state light emitting polyaromatic luminogens containing pyrazoline chromophore. <i>Journal of Luminescence</i> , 2019, 214, 116547.	3.1	8
97	Charge transfer spectra of complexes with benzoquinonechlorimides as electron acceptors. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1981, 37, 1-3.	0.1	7
98	An artificial intelligence approach for the generation and enumeration of perfect matchings on graphs. <i>Computers and Mathematics With Applications</i> , 1995, 29, 115-121.	2.7	7
99	Biocatalysis of azidolysis of epoxides: Computational evidences on the role of halohydrin dehalogenase (HheC). <i>Journal of Chemical Sciences</i> , 2011, 123, 279-290.	1.5	7
100	The metal delivery mechanism of transferrin and the role of bent metallocene metals towards anticancer activity – a theoretical exploration. <i>RSC Advances</i> , 2014, 4, 9556.	3.6	7
101	General Method for the Computation of Matching Polynomials of Graphs. <i>Journal of Chemical Information and Computer Sciences</i> , 1994, 34, 1122-1126.	2.8	5
102	Ab initio computational studies on molecular conformation of N-methyl-glyphosate. <i>Molecular Physics</i> , 2003, 101, 3073-3083.	1.7	5
103	Conformation and function of N-hydroxy-glyphosate and N-amino-glyphosate: a comparative study using ab initio MO theory. <i>Computational and Theoretical Chemistry</i> , 2005, 714, 99-108.	1.5	5
104	Electrostatic control on endo/exo selectivity in ionic cycloaddition. <i>Chemical Physics Letters</i> , 2005, 416, 354-357.	2.6	5
105	Ring opening of boriranes vis-à-vis aziridines: An ab initio and DFT probe on the mechanisms. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1590-1597.	2.0	5
106	Regio and stereoselectivity in ionic cycloadditions. <i>Journal of Chemical Sciences</i> , 2008, 120, 225-236.	1.5	5
107	Computational Insights into the Roles of Steric and Electrostatic Interactions in Arsenic Ylide Mediated Aziridination Reactions. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 3458-3466.	2.4	5
108	Mechanism and diastereoselectivity of arsenic ylide mediated cyclopropanation: a theoretical study. <i>RSC Advances</i> , 2013, 3, 17793.	3.6	5

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109	Algorithms for the computation of molecular distance matrix and distance polynomial of chemical graphs on parallel computers. <i>Journal of Chemical Information and Computer Sciences</i> , 1993, 33, 412-414.	2.8	4
110	Ab initio and DFT investigations on the stereochemistry of ring opening of episulfides. <i>Computational and Theoretical Chemistry</i> , 2006, 763, 1-5.	1.5	4
111	Atomic partitioning of H ₂ bonds in [NiFe] hydrogenase – a test case of concurrent binding. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10698.	2.8	4
112	A Spectroscopic Approach with Theoretical Studies to Study the Interaction of 9-aminoacridine with Certain Phenols. <i>Zeitschrift Fur Physikalische Chemie</i> , 2017, 231, 939-956.	2.8	4
113	Impact of tunable 2-(1 <i>H</i> -indol-3-yl)acetonitrile based fluorophores towards optical, thermal and electroluminescence properties. <i>RSC Advances</i> , 2019, 9, 14544-14557.	3.6	4
114	Heuristic enhancements of the search for the generation of all perfect matchings. <i>Applied Mathematics Letters</i> , 1996, 9, 49-53.	2.7	3
115	Hydrogen bond stabilization in Diels-Alder transition states: The cycloaddition of hydroxy-ortho-quinodimethane with fumaric acid and dimethylfumarate. <i>Chemical Physics Letters</i> , 2005, 406, 355-359.	2.6	3
116	Evidence for the powerful catalytic ability of imidozirconocene complex from its epoxide ring cleavage reactions – A DFT mechanistic view#. <i>Journal of Chemical Sciences</i> , 2012, 124, 167-176.	1.5	3
117	Resemblances of experiment and theory on aryl substituted luminogenic polypyrazolines. <i>New Journal of Chemistry</i> , 2019, 43, 9439-9452.	2.8	3
118	Computer generation of Pauling bond orders using heuristic search. <i>Journal of Chemical Information and Computer Sciences</i> , 1995, 35, 717-722.	2.8	2
119	A semantic tree algorithm for the generation of sextet polynomials of hexagonal systems. <i>Computers and Mathematics With Applications</i> , 1999, 37, 97-104.	2.7	2
120	COMPUTATIONAL INSIGHTS ON THE LONE PAIR INDUCED BARRIER MODULATION IN THE THERMAL REARRANGEMENT OF 6-HALO-2-PYRONES. <i>Journal of Theoretical and Computational Chemistry</i> , 2007, 06, 233-243.	1.8	2
121	SINGLET METHYLENE AND HALOCARBENES INSERTIONS INTO POLAR N-H BONDS OF AMINES. <i>Journal of Theoretical and Computational Chemistry</i> , 2009, 08, 1143-1153.	1.8	2
122	Imidozirconocene-Mediated Ring Cleavage of Epoxides – Evidence for Bifunctional Reactivity from DFT. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 2842-2855.	2.0	2
123	Insights from the computational studies on the oxidized as-isolated state of [NiFeSe] hydrogenase from <i>D. vulgaris</i> Hildenborough. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20677-20686.	2.8	2
124	Parallel algorithm for the computation of characteristic polynomials of chemical graphs. <i>Journal of Computational Chemistry</i> , 1991, 12, 779-783.	3.3	1
125	Learning Approach for the Computation of Generalized Wheland Polynomials of Chemical Graphs. <i>Journal of Chemical Information and Computer Sciences</i> , 1994, 34, 1113-1117.	2.8	1
126	A fast graph traversal algorithm for the computer enumeration of P-V paths of benzenoid graphs. <i>Computers & Chemistry</i> , 1995, 19, 101-106.	1.2	1

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127	An ab initio and DFT study on the hydrolysis of carbonyl dichloride. Computational and Theoretical Chemistry, 2005, 730, 155-160.	1.5	1
128	Insertion of singlet chlorocarbenes across C-H bonds in alkanes: Evidence for two phase mechanism. Journal of Chemical Sciences, 2007, 119, 467-473.	1.5	1
129	Singlet methylene insertion into polar O-H and N-H bonds of water and ammonia—Ab initio and DFT study. International Journal of Quantum Chemistry, 2010, 110, 1310-1316.	2.0	1
130	Half rotations leading to retention of stereochemistry in epoxide ring opening by selenocyanate ion: Insights from DFT modeling. International Journal of Quantum Chemistry, 2011, 111, 2317-2323.	2.0	1
131	Sequence selectivity of azinomycin B in DNA alkylation and cross-linking: a QM/MM study. Journal of Molecular Modeling, 2013, 19, 383-390.	1.8	1
132	Noncovalent interactions between the second coordination sphere and the active site of [NiFeSe] hydrogenase. RSC Advances, 2016, 6, 81636-81646.	3.6	1
133	C-H Functionalisation Through Singlet Chlorocarbenes Insertions — MP2 and DFT Investigations. Lecture Notes in Computer Science, 2006, , 143-152.	1.3	1
134	Ab Initio and DFT Investigations of the Mechanistic Pathway of Singlet Bromocarbenes Insertion into C-H Bonds of Methane and Ethane. Lecture Notes in Computer Science, 2007, , 288-295.	1.3	0