Ponnambalam Venuvanalingam

List of Publications by Year
in descending order

134 papers	2,710 citations	185998 28 h-index	243296 44 g-index
136 all docs	136 docs citations	136 times ranked	3138 citing authors

#	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. Journal of Physical Chemistry A, 2012, 116, 4667-4677.	1.1	164
2	Interaction of anthraquinone dyes with lysozyme: Evidences from spectroscopic and docking studies. Journal of Hazardous Materials, 2010, 175, 985-991.	6.5	130
3	Hydrogenolysis of sorbitol over Ni and Pt loaded on NaY. Catalysis Communications, 2011, 12, 673-677.	1.6	90
4	Water-Soluble Mono- and Binuclear Ru(Î·⁶-p-cymene) Complexes Containing Indole Thiosemicarbazones: Synthesis, DFT Modeling, Biomolecular Interactions, and In Vitro Anticancer Activity through Apoptosis. Organometallics, 2018, 37, 1242-1257.	1.1	77
5	Biomolecular Interaction, Anti-Cancer and Anti-Angiogenic Properties of Cobalt(III) Schiff Base Complexes. Scientific Reports, 2019, 9, 2721.	1.6	65
6	Enhanced photocatalytic degradation of azo dyes using nano Fe3O4. Journal of the Iranian Chemical Society, 2012, 9, 101-109.	1.2	63
7	Ï€-systems as lithium/hydrogen bond acceptors: Some theoretical observations. Journal of Chemical Physics, 1998, 109, 9820-9830.	1.2	62
8	A DFT/TDDFT modelling of bithiophene azo chromophores for optoelectronic applications. Dyes and Pigments, 2014, 100, 261-268.	2.0	59
9	Surfactantâ€“copper(II) Schiff base complexes: synthesis, structural investigation, DNA interaction, docking studies, and cytotoxic activity. Journal of Biomolecular Structure and Dynamics, 2015, 33, 877-891.	2.0	58
10	Topological resonance energy predictions of the stability of fullerene clusters. Chemical Physics Letters, 1994, 222, 95-100.	1.2	47
11	Origin and Nature of Lithium and Hydrogen Bonds to Oxygen, Sulfur, and Selenium. Journal of Physical Chemistry A, 2000, 104, 10859-10867.	1.1	47
12	Single and double chain surfactantâ€“cobalt(<scp>iii</scp>) complexes: the impact of hydrophobicity on the interaction with calf thymus DNA, and their biological activities. RSC Advances, 2015, 5, 31746-31758.	1.7	46
13	Highly Emissive Luminogens Based on Imidazo[1,2â€a]pyridine for Electroluminescent Applications. Chemistry - an Asian Journal, 2014, 9, 294-304.	1.7	44
14	Designing benzosiloles for better optoelectronic properties using DFT & TDDFT approaches. Physical Chemistry Chemical Physics, 2012, 14, 14229.	1.3	43
15	Sorbitol Hydrogenolysis Over Ni, Pt and Ru Supported on NaY. Topics in Catalysis, 2012, 55, 897-907.	1.3	42
16	Are Re(<scp>i</scp>) phenanthroline complexes suitable candidates for OLEDs? Answers from DFT and TD-DFT investigations. Physical Chemistry Chemical Physics, 2014, 16, 21157-21171.	1.3	42
17	Ab initio study of tautomerism and hydrogen bonding of Î²-carbonylamine in the gas phase and in water solution. Theoretical Chemistry Accounts, 2000, 104, 226-234.	0.5	41
18	Influence of self-assembly on intercalative DNA binding interaction of double-chain surfactant Co(<scp>iii</scp>) complexes containing imidazo[4,5-f][1,10]phenanthroline and dipyrido[3,2-d:2â€²-3â€²-f]quinoxaline ligands: experimental and theoretical study. Dalton Transactions, 2014, 43, 18074-18086.	1.6	41

#	Article	IF	Citations
19	The role of cumulenic strain on the kinetic and thermodynamic control of the Dielsâ€“Alder reactions involving allenes as dienes. Journal of the Chemical Society Perkin Transactions II, 1997, , 1799-1804.	0.9	40
20	Novel uranyl(<scp>vi</scp>) complexes incorporating propylene-bridged salen-type N₂O₂-ligands: a structural and computational approach. Dalton Transactions, 2015, 44, 568-577.	1.6	40
21	AM1 and PM3 transition structures for the epoxidation of alkenes and allene by methylated dioxiranes. Computational and Theoretical Chemistry, 1997, 394, 41-47.	1.5	37
22	A combined experimental and computational study on the sulfoxidation by high-valent iron bispidine complexes. Dalton Transactions, 2011, 40, 11276.	1.6	36
23	Luminescent Re(<scp>i</scp>) terpyridine complexes for OLEDs: what does the DFT/TD-DFT probe reveal?. Dalton Transactions, 2015, 44, 8529-8542.	1.6	34
24	Synthesis, DNA binding and docking studies of copper(II) complexes containing modified phenanthroline ligands. Journal of Coordination Chemistry, 2015, 68, 1374-1386.	0.8	33
25	Lithium bonding interaction in H2CYâ‹¯LiF (Y=O,S) complexes: A theoretical probe. Journal of Chemical Physics, 1997, 107, 4329-4336.	1.2	31
26	1,3-Dipolar Reactions Involving Corannulene:â€‰ How Does Its Rim and Spoke Addition Vary?. Journal of Organic Chemistry, 2005, 70, 2528-2536.	1.7	31
27	Surfactantâ€“cobalt(III) complexes: The impact of hydrophobicity on interaction with HSA and DNA â€“ insights from experimental and theoretical approach. Colloids and Surfaces B: Biointerfaces, 2017, 153, 85-94.	2.5	30
28	Synthesis, DNA and BSA binding, in vitro anti-proliferative and in vivo anti-angiogenic properties of some cobalt(<scp>iii</scp>) Schiff base complexes. New Journal of Chemistry, 2019, 43, 11391-11407.	1.4	30
29	Evaluation of the Leaf Essential Oil from Artemisia vulgaris and Its Larvicidal and Repellent Activity against Dengue Fever Vector Aedes aegyptiâ€”An Experimental and Molecular Docking Investigation. ACS Omega, 2018, 3, 15657-15665.	1.6	29
30	Half-sandwich Ru(Î·6-p-cymene) complexes featuring pyrazole appended ligands: Synthesis, DNA binding and in vitro cytotoxicity. Journal of Inorganic Biochemistry, 2019, 194, 74-84.	1.5	29
31	Kinetics of polymerization of N,N-methylenebisacrylamide initiated by KMnO4-H2C2O4 redox system. European Polymer Journal, 1982, 18, 531-534.	2.6	28
32	Structure of the BenzeneÂ·Â·Â·ICl Complex:Â A UVPES and ab Initio Molecular Orbital Studyâ€. Journal of Physical Chemistry A, 1998, 102, 532-536.	1.1	28
33	Ab initio study of formazan and 3-nitroformazan. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3313-3319.	1.7	28
34	1,3-Dipolar additions involving allenes: A density functional study of concerted and stepwise mechanismsElectronic 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. Perkin Transactions II RSC, 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. RSC Advances, 2011, 1, 1333.	1.7	27
36	On the Nature of Hypercoordination in Dihalogenated Perhalocyclohexasilanes. Journal of Physical Chemistry A, 2013, 117, 3529-3538.	1.1	27

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37	Ab initio and DFT investigations of lithium/hydrogen bonded complexes of trimethylamine, dimethyl ether and dimethyl sulfide. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2669-2674.	1.7	26
38	Low-lying stepwise paths for ethylene 1,3-dipolar cycloadditions: A DFT study. International Journal of Quantum Chemistry, 2005, 104, 64-78.	1.0	25
39	Synthesis, characterisation and electroluminescence behaviour of Ï€-conjugated imidazoleâ€“isoquinoline derivatives. Dyes and Pigments, 2014, 102, 180-188.	2.0	25
40	A multispectroscopic and molecular docking investigation of the binding interaction between serum albumins and acid orange dye. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 192, 34-40.	2.0	25
41	Water-soluble Cobalt(II) & Cobalt(III) complexes supported by new triazine Schiff base ligands: Synthesis, structure and biological evaluation. Journal of Photochemistry and Photobiology B: Biology, 2018, 189, 152-164.	1.7	24
42	Allene and fluoroallenes as dienophiles in Dielsâ€“Alder reactions: an AM1 and PM3 study. Journal of the Chemical Society Perkin Transactions II, 1996, , 1423-1427.	0.9	23
43	A DFT/TDDFT mission to probe pushâ€“pull vinyl coupled thiophene oligomers for optoelectronic applications. RSC Advances, 2015, 5, 50353-50364.	1.7	22
44	Gain or loss of aromaticity in Dielsâ€“Alder transition states and adducts: a theoretical investigation. Journal of Physical Organic Chemistry, 1998, 11, 133-140.	0.9	21
45	Electron donor-acceptor complexes of I2 with diethyl ether and diethyl sulphide. An ab initio MO study. Chemical Physics Letters, 1996, 248, 153-157.	1.2	20
46	Open versus Closed 1,3-Dipolar Additions of C60: A Theoretical Investigation on Their Mechanism and Regioselectivity. Journal of Organic Chemistry, 2005, 70, 5426-5435.	1.7	20
47	Harmonic analysis of vibrations of morpholine-4-ylmethylthiourea: A DFT, midinfrared and Raman spectral study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 996-1002.	2.0	20
48	Investigations on the fluorescence quenching of 2,3-diazabicyclo[2.2.2]oct-2-ene by certain flavonoids. Journal of Photochemistry and Photobiology B: Biology, 2008, 91, 143-150.	1.7	20
49	Conjugated polymer based on oligobenzo[c]thiophene with low-lying HOMO energy level as potential donor for bulk heterojunction solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 262, 34-44.	2.0	20
50	Tunable single and dual emission behavior of imidazole fluorophores based on D-Ï€-A architecture. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 284, 36-48.	2.0	20
51	Interaction between toxic azo dye C.I. Acid Red 88 and serum albumins. Journal of Luminescence, 2013, 143, 715-722.	1.5	19
52	Computational evaluation of optoelectronic and photophysical properties of unsymmetrical distyrylbiphenyls. RSC Advances, 2014, 4, 53060-53071.	1.7	19
53	Câ€“H functionalisation through carbene and fluorocarbene insertionâ€”ab initio and DFT investigations. Computational and Theoretical Chemistry, 2005, 755, 169-178.	1.5	17
54	A new turn in codonâ€“anticodon selection through halogen bonds. Physical Chemistry Chemical Physics, 2014, 16, 7430.	1.3	17

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55	Antitumor activity of bent metallocenes: electronic structure analysis using DFT computations. Journal of Molecular Modeling, 2011, 17, 465-475.	0.8	16
56	Encapsulation of a hexaaza macrocyclic nickel(<scp>ii</scp>) complex in zeolite Y: an experimental and theoretical investigation. New Journal of Chemistry, 2017, 41, 9505-9512.	1.4	16
57	Tuning the Photophysical Properties of 2â€Quinolinoneâ€Based Donorâ€“Acceptor Molecules through Nâ€versus Oâ€Alkylation: Insights from Experimental and Theoretical Investigations. European Journal of Organic Chemistry, 2014, 2014, 753-766.	1.2	15
58	A combined experimental and theoretical investigation of imidazoleâ€“carbazole fluorophores. Journal of Luminescence, 2014, 147, 111-120.	1.5	15
59	The nature of Pdâ€“carbene and Pdâ€“halogen bonds in (bisNHC)PdX₂ type catalysts: insights from density functional theory. RSC Advances, 2015, 5, 80661-80667.	1.7	15
60	Rational design of cyclopenta[b]naphthalenes for better optoelectronic applications and their photophysical properties using DFT/TD-DFT methods. RSC Advances, 2016, 6, 44569-44577.	1.7	15
61	Structural elucidation and physicochemical properties of mononuclear Uranyl(VI) complexes incorporating dianionic units. Scientific Reports, 2016, 6, 32898.	1.6	15
62	Electronic structure and conformation of glyphosate: an ab initio MO study. Computational and Theoretical Chemistry, 2002, 618, 117-125.	1.5	14
63	Synthesis of conjugated perylene diimide-based copolymer with 5,5â€²-bis(4-aminophenyl)-2-2â€²-bifuryl moiety as an active material for organic photovoltaics. Journal of Photochemistry and Photobiology A: Chemistry, 2012, 247, 52-62.	2.0	14
64	Phenylacetylene dimer: Ab initio and DFT study. Chemical Physics, 2013, 415, 150-155.	0.9	14
65	The nature of hydrogen bonding inR²₂(8) crystal motifs â€“ a computational exploration. Molecular Physics, 2014, 112, 3195-3205.	0.8	14
66	Elucidating the structures and cooperative binding mechanism of cesium salts to the multitopic ion-pair receptor through density functional theory calculations. Dalton Transactions, 2015, 44, 15450-15462.	1.6	14
67	Cyclopolymerization Initiated by Peroxydisulfate Ion and Metal Ion Catalysis. Journal of Macromolecular Science Part A, Chemistry, 1986, 23, 117-128.	0.4	13
68	Transition states and charge analyses along the IRC for the singlet chlorocarbenes insertions into Câ€“H bond of alkanes. Chemical Physics Letters, 2006, 430, 414-419.	1.2	13
69	Green light-emitting 2-(1H-indol-3-yl)acetonitrile-based Dâ€“A fluorophores â€“ a combined theoretical and experimental study. Materials Chemistry Frontiers, 2017, 1, 1373-1383.	3.2	13
70	Structure and Reactivity of Pd Complexes in Various Oxidation States in Identical Ligand Environments with Reference to Câ€“C and Câ€“Cl Coupling Reactions: Insights from Density Functional Theory. Inorganic Chemistry, 2018, 57, 6833-6846.	1.9	13
71	Theoretical study on the mechanism and reactivity of fluorocumulenes in [42] cycloadditions. Journal of Fluorine Chemistry, 1995, 73, 171-174.	0.9	12
72	UVPES and ab Initio Molecular Orbital Studies on the Electron Donorâ”Acceptor Complexes of Bromine with Methylamines. Journal of Physical Chemistry A, 1997, 101, 1155-1159.	1.1	12

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73	Oxaphosphetane versus betaine formation in epoxide ring opening by PPh3: a mechanistic probe by ab initio and DFT modeling. Tetrahedron Letters, 2005, 46, 4087-4090.	0.7	12
74	Spectroscopic Studies on TiO2 Enhanced Binding of Hypocrellin B with DNA. Journal of Fluorescence, 2011, 21, 1887-1895.	1.3	12
75	Understanding the stability, electronic and molecular structure of some copper(III) complexes containing alkyl and non alkyl ligands: Insights from DFT calculations. Journal of Organometallic Chemistry, 2011, 696, 2627-2634.	0.8	12
76	Are cucurbiturils better drug carriers for bent metallocenes? Insights from theory. Journal of Biological Inorganic Chemistry, 2018, 23, 413-423.	1.1	12
77	Effect of increasing methoxyphenyl substitution on pyrene pyrazoline enduring green light emitting materials. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 377, 247-259.	2.0	11
78	A bowl-shaped phenoxido-bridged binuclear zinc complex: Experimental and theoretical studies. Inorganica Chimica Acta, 2022, 534, 120807.	1.2	11
79	Is corannulene a better diene or dienophile? A DFT analysis. Journal of Physical Organic Chemistry, 2008, 21, 146-154.	0.9	10
80	Application of activation hardness in perturbed pericyclic reactions: a case study involving electrocyclic ring opening reactions of heterocyclobutenes. Journal of Physical Organic Chemistry, 2011, 24, 460-465.	0.9	10
81	Semi-empirical MO-calculations on the electronic spectra of benzoquinonechlorimides. Spectrochimica Acta Part A: Molecular Spectroscopy, 1980, 36, 103-107.	0.1	9
82	A proton and carbon NMR spectroscopic study of 5-substituted acenaphthenes. Magnetic Resonance in Chemistry, 1998, 36, 943-946.	1.1	9
83	Theoretical investigation on the reactivity of sulfur-centered heterocumulenes as dienophiles in Diels-Alder reactions and endo-lone-pair effect. International Journal of Quantum Chemistry, 1998, 66, 309-322.	1.0	9
84	Quantitative property-property relationship (QPPR) approach in predicting flotation efficiency of chelating agents as mineral collectors. SAR and QSAR in Environmental Research, 2002, 13, 499-508.	1.0	9
85	Ab initio and DFT studies on conformations, hydrogen bonding and electronic structures of glyoxalmonoxime and its methyl derivatives. Computational and Theoretical Chemistry, 2004, 712, 175-185.	1.5	9
86	Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride. International Journal of Quantum Chemistry, 2005, 102, 139-146.	1.0	9
87	Ring Cleavage of Aziridines by Difluoroamine:Â Mechanistic Insights from ab Initio and DFT Study. Journal of Physical Chemistry A, 2005, 109, 4829-4835.	1.1	9
88	Molecular complexes of p-benzoquinonechlorimides with aromatic Ï€-donors. Spectrochimica Acta Part A: Molecular Spectroscopy, 1981, 37, 505-510.	0.1	8
89	Ultraviolet photoelectron spectroscopy of complexes of bromine with n-donors in the vapor phase. Chemical Physics Letters, 1994, 228, 431-435.	1.2	8
90	Diels-Alder addition of butadiene to various thiocarbonyl(R2C?SOn,n=0-2) heterodienophiles andendo-lone pair effect in heterocumulene. Journal of Physical Organic Chemistry, 1997, 10, 768-776.	0.9	8

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91	Ab initio Computational Modeling of Glyphosate Analogs: Conformational Perspective. Structural Chemistry, 2005, 16, 491-506.	1.0	8
92	Fluorine effect on pericyclic and pseudopericyclic processes: Evidences and ab initio theory. Journal of Chemical Sciences, 2009, 121, 859-866.	0.7	8
93	Spectroscopic and Molecular Docking Investigations on the Interaction of Rutin with Bovine Serum Albumin. Zeitschrift Fur Physikalische Chemie, 2011, 225, 441-454.	1.4	8
94	Studies on the inclusion behavior of 9-Aminoacridine into cyclodextrins: Spectroscopic and theoretical evidences. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 103, 18-24.	2.0	8
95	Effect on shifting of phenyl ring in pyrazoline pyrene luminophore and their photophysical and electrochemical investigation. Optical Materials, 2019, 94, 403-414.	1.7	8
96	Solid state light emitting polyaromatic luminogens containing pyrazoline chromophore. Journal of Luminescence, 2019, 214, 116547.	1.5	8
97	Charge transfer spectra of complexes with benzoquinonechlorimides as electron acceptors. Spectrochimica Acta Part A: Molecular Spectroscopy, 1981, 37, 1-3.	0.1	7
98	An artificial intelligence approach for the generation and enumeration of perfect matchings on graphs. Computers and Mathematics With Applications, 1995, 29, 115-121.	1.4	7
99	Biocatalysis of azidolysis of epoxides: Computational evidences on the role of halohydrin dehalogenase (HheC). Journal of Chemical Sciences, 2011, 123, 279-290.	0.7	7
100	The metal delivery mechanism of transferrin and the role of bent metallocene metals towards anticancer activity â€“ a theoretical exploration. RSC Advances, 2014, 4, 9556.	1.7	7
101	General Method for the Computation of Matching Polynomials of Graphs. Journal of Chemical Information and Computer Sciences, 1994, 34, 1122-1126.	2.8	5
102	Ab initiocomputational studies on molecular conformation of N-methyl-glyphosate. Molecular Physics, 2003, 101, 3073-3083.	0.8	5
103	Conformation and function of N-hydroxy-glyphosate and N-amino-glyphosate: a comparative study using ab initio MO theory. Computational and Theoretical Chemistry, 2005, 714, 99-108.	1.5	5
104	Electrostatic control on endo/exo selectivity in ionic cycloaddition. Chemical Physics Letters, 2005, 416, 354-357.	1.2	5
105	Ring opening of boriranes vis-Ã-vis aziridines: An ab initio and DFT probe on the mechanisms. International Journal of Quantum Chemistry, 2007, 107, 1590-1597.	1.0	5
106	Regio and stereoselectivity in ionic cycloadditions. Journal of Chemical Sciences, 2008, 120, 225-236.	0.7	5
107	Computational Insights into the Roles of Steric and Electrostatic Interactions in Arsenic Ylide Mediated Aziridination Reactions. European Journal of Organic Chemistry, 2011, 2011, 3458-3466.	1.2	5
108	Mechanism and diastereoselectivity of arsenic ylide mediated cyclopropanation: a theoretical study. RSC Advances, 2013, 3, 17793.	1.7	5

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109	Algorithms for the computation of molecular distance matrix and distance polynomial of chemical graphs on parallel computers. Journal of Chemical Information and Computer Sciences, 1993, 33, 412-414.	2.8	4
110	Ab initio and DFT investigations on the stereochemistry of ring opening of episulfides. Computational and Theoretical Chemistry, 2006, 763, 1-5.	1.5	4
111	Atomic partitioning of Mâ€“H2 bonds in [NiFe] hydrogenase â€“ a test case of concurrent binding. Physical Chemistry Chemical Physics, 2014, 16, 10698.	1.3	4
112	A Spectroscopic Approach with Theoretical Studies to Study the Interaction of 9-aminoacridine with Certain Phenols. Zeitschrift Fur Physikalische Chemie, 2017, 231, 939-956.	1.4	4
113	Impact of tunable 2-(1H-indol-3-yl)acetonitrile based fluorophores towards optical, thermal and electroluminescence properties. RSC Advances, 2019, 9, 14544-14557.	1.7	4
114	Heuristic enhancements of the search for the generation of all perfect matchings. Applied Mathematics Letters, 1996, 9, 49-53.	1.5	3
115	Hydrogen bond stabilization in Dielsâ€“Alder transition states: The cycloaddition of hydroxy-ortho-quinodimethane with fumaric acid and dimethylfumarate. Chemical Physics Letters, 2005, 406, 355-359.	1.2	3
116	Evidence for the powerful catalytic ability of imidozirconocene complex from its epoxide ring cleavage reactions â€“ A DFT mechanistic view#. Journal of Chemical Sciences, 2012, 124, 167-176.	0.7	3
117	Resemblances of experiment and theory on aryl substituted luminogenic polypyrazolines. New Journal of Chemistry, 2019, 43, 9439-9452.	1.4	3
118	Computer generation of Pauling bond orders using heuristic search. Journal of Chemical Information and Computer Sciences, 1995, 35, 717-722.	2.8	2
119	A semantic tree algorithm for the generation of sextet polynomials of hexagonal systems. Computers and Mathematics With Applications, 1999, 37, 97-104.	1.4	2
120	COMPUTATIONAL INSIGHTS ON THE LONE PAIR INDUCED BARRIER MODULATION IN THE THERMAL REARRANGEMENT OF 6-HALO-2-PYRONES. Journal of Theoretical and Computational Chemistry, 2007, 06, 233-243.	1.8	2
121	SINGLET METHYLENE AND HALOCARBENES INSERTIONS INTO POLAR Nâ€“H BONDS OF AMINES. Journal of Theoretical and Computational Chemistry, 2009, 08, 1143-1153.	1.8	2
122	Imidozirconoceneâ€Mediated Ring Cleavage of Epoxides â€“ Evidence for Bifunctional Reactivity from DFT. European Journal of Inorganic Chemistry, 2011, 2011, 2842-2855.	1.0	2
123	Insights from the computational studies on the oxidized as-isolated state of [NiFeSe] hydrogenase from D. vulgaris Hildenborough. Physical Chemistry Chemical Physics, 2015, 17, 20677-20686.	1.3	2
124	Parallel algorithm for the computation of characteristic polynomials of chemical graphs. Journal of Computational Chemistry, 1991, 12, 779-783.	1.5	1
125	Learning Approach for the Computation of Generalized Wheland Polynomials of Chemical Graphs. Journal of Chemical Information and Computer Sciences, 1994, 34, 1113-1117.	2.8	1
126	A fast graph traversal algorithm for the computer enumeration of P-V paths of benzenoid graphs. Computers & Chemistry, 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.	0.7	1
129	Singlet methylene insertion into polar Oï£¿H and Nï£¿H bonds of water and ammoniaâ€"Ab initio and DFT study. International Journal of Quantum Chemistry, 2010, 110, 1310-1316.	1.0	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.	1.0	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.	0.8	1
132	Noncovalent interactions between the second coordination sphere and the active site of [NiFeSe] hydrogenase. RSC Advances, 2016, 6, 81636-81646.	1.7	1
133	C-H Functionalisation Through Singlet Chlorocarbenes Insertions â€“ MP2 and DFT Investigations. Lecture Notes in Computer Science, 2006, , 143-152.	1.0	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.	1.0	0