# 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 | A bowl-shaped phenoxido-bridged binuclear zinc complex: Experimental and theoretical studies. Inorganica Chimica Acta, 2022, 534, 120807. | 1.2 | 11 |
| 2 | 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 |
| 3 | Solid state light emitting polyaromatic luminogens containing pyrazoline chromophore. Journal of Luminescence, 2019, 214, 116547. | 1.5 | 8 |
| 4 | 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 |
| 5 | 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 |
| 6 | Resemblances of experiment and theory on aryl substituted luminogenic polypyrazolines. New Journal of Chemistry, 2019, 43, 9439-9452. | 1.4 | 3 |
| 7 | 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 |
| 8 | 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 |
| 9 | Biomolecular Interaction, Anti-Cancer and Anti-Angiogenic Properties of Cobalt(III) Schiff Base Complexes. Scientific Reports, 2019, 9, 2721. | 1.6 | 65 |
| 10 | Are cucurbiturils better drug carriers for bent metallocenes? Insights from theory. Journal of Biological Inorganic Chemistry, 2018, 23, 413-423. | 1.1 | 12 |
| 11 | Water-Soluble Mono- and Binuclear Ru(Î·<sup>6</sup>-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 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | 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 |
| 16 | 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 |
| 17 | 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 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | Noncovalent interactions between the second coordination sphere and the active site of [NiFeSe] hydrogenase. RSC Advances, 2016, 6, 81636-81646. | 1.7 | 1 |
| 22 | Structural elucidation and physicochemical properties of mononuclear Uranyl(VI) complexes incorporating dianionic units. Scientific Reports, 2016, 6, 32898. | 1.6 | 15 |
| 23 | A DFT/TDDFT mission to probe pushâ€“pull vinyl coupled thiophene oligomers for optoelectronic applications. RSC Advances, 2015, 5, 50353-50364. | 1.7 | 22 |
| 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 | 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 |
| 26 | 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 |
| 27 | 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 |
| 28 | The nature of Pdâ€“carbene and Pdâ€“halogen bonds in (bisNHC)PdX<sub>2</sub> type catalysts: insights from density functional theory. RSC Advances, 2015, 5, 80661-80667. | 1.7 | 15 |
| 29 | 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 |
| 30 | Novel uranyl(<scp>vi</scp>) complexes incorporating propylene-bridged salen-type N<sub>2</sub>O<sub>2</sub>-ligands: a structural and computational approach. Dalton Transactions, 2015, 44, 568-577. | 1.6 | 40 |
| 31 | 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 |
| 32 | Highly Emissive Luminogens Based on Imidazo[1,2â€a]pyridine for Electroluminescent Applications. Chemistry - an Asian Journal, 2014, 9, 294-304. | 1.7 | 44 |
| 33 | 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 |
| 34 | A combined experimental and theoretical investigation of imidazoleâ€“carbazole fluorophores. Journal of Luminescence, 2014, 147, 111-120. | 1.5 | 15 |
| 35 | 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 |
| 36 | A DFT/TDDFT modelling of bithiophene azo chromophores for optoelectronic applications. Dyes and Pigments, 2014, 100, 261-268. | 2.0 | 59 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Synthesis, characterisation and electroluminescence behaviour of Ï€-conjugated imidazoleâ€“isoquinoline derivatives. Dyes and Pigments, 2014, 102, 180-188. | 2.0 | 25 |
| 38 | 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 |
| 39 | Computational evaluation of optoelectronic and photophysical properties of unsymmetrical distyrylbiphenyls. RSC Advances, 2014, 4, 53060-53071. | 1.7 | 19 |
| 40 | 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 |
| 41 | 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 |
| 42 | The nature of hydrogen bonding inR<sup>2</sup><sub>2</sub>(8) crystal motifs â€“ a computational exploration. Molecular Physics, 2014, 112, 3195-3205. | 0.8 | 14 |
| 43 | 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 |
| 44 | A new turn in codonâ€“anticodon selection through halogen bonds. Physical Chemistry Chemical Physics, 2014, 16, 7430. | 1.3 | 17 |
| 45 | 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 |
| 46 | Interaction between toxic azo dye C.I. Acid Red 88 and serum albumins. Journal of Luminescence, 2013, 143, 715-722. | 1.5 | 19 |
| 47 | Mechanism and diastereoselectivity of arsenic ylide mediated cyclopropanation: a theoretical study. RSC Advances, 2013, 3, 17793. | 1.7 | 5 |
| 48 | On the Nature of Hypercoordination in Dihalogenated Perhalocyclohexasilanes. Journal of Physical Chemistry A, 2013, 117, 3529-3538. | 1.1 | 27 |
| 49 | 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 |
| 50 | 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 |
| 51 | Phenylacetylene dimer: Ab initio and DFT study. Chemical Physics, 2013, 415, 150-155. | 0.9 | 14 |
| 52 | 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 |
| 53 | Sorbitol Hydrogenolysis Over Ni, Pt and Ru Supported on NaY. Topics in Catalysis, 2012, 55, 897-907. | 1.3 | 42 |
| 54 | Designing benzosiloles for better optoelectronic properties using DFT & TDDFT approaches. Physical Chemistry Chemical Physics, 2012, 14, 14229. | 1.3 | 43 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | 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 |
| 56 | Enhanced photocatalytic degradation of azo dyes using nano Fe3O4. Journal of the Iranian Chemical Society, 2012, 9, 101-109. | 1.2 | 63 |
| 57 | 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 |
| 58 | 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 |
| 59 | A combined experimental and computational study on the sulfoxidation by high-valent iron bispidine complexes. Dalton Transactions, 2011, 40, 11276. | 1.6 | 36 |
| 60 | Hydrogenolysis of sorbitol over Ni and Pt loaded on NaY. Catalysis Communications, 2011, 12, 673-677. | 1.6 | 90 |
| 61 | Spectroscopic Studies on TiO2 Enhanced Binding of Hypocrellin B with DNA. Journal of Fluorescence, 2011, 21, 1887-1895. | 1.3 | 12 |
| 62 | Antitumor activity of bent metallocenes: electronic structure analysis using DFT computations. Journal of Molecular Modeling, 2011, 17, 465-475. | 0.8 | 16 |
| 63 | 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 |
| 64 | 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 |
| 65 | 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 |
| 66 | 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 |
| 67 | 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 |
| 68 | 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 |
| 69 | 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 |
| 70 | Interaction of anthraquinone dyes with lysozyme: Evidences from spectroscopic and docking studies. Journal of Hazardous Materials, 2010, 175, 985-991. | 6.5 | 130 |
| 71 | 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 |
| 72 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Fluorine effect on pericyclic and pseudopericyclic processes: Evidences and ab initio theory. Journal of Chemical Sciences, 2009, 121, 859-866. | 0.7 | 8 |
| 74 | Regio and stereoselectivity in ionic cycloadditions. Journal of Chemical Sciences, 2008, 120, 225-236. | 0.7 | 5 |
| 75 | Is corannulene a better diene or dienophile? A DFT analysis. Journal of Physical Organic Chemistry, 2008, 21, 146-154. | 0.9 | 10 |
| 76 | 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 |
| 77 | 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 |
| 78 | 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 |
| 79 | 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 |
| 80 | 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 |
| 81 | 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 |
| 82 | 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 |
| 83 | Ab initio and DFT investigations on the stereochemistry of ring opening of episulfides. Computational and Theoretical Chemistry, 2006, 763, 1-5. | 1.5 | 4 |
| 84 | C-H Functionalisation Through Singlet Chlorocarbenes Insertions â€“ MP2 and DFT Investigations. Lecture Notes in Computer Science, 2006, , 143-152. | 1.0 | 1 |
| 85 | 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 |
| 86 | 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 |
| 87 | An ab initio and DFT study on the hydrolysis of carbonyl dichloride. Computational and Theoretical Chemistry, 2005, 730, 155-160. | 1.5 | 1 |
| 88 | Câ€“H functionalisation through carbene and fluorocarbene insertionâ€”ab initio and DFT investigations. Computational and Theoretical Chemistry, 2005, 755, 169-178. | 1.5 | 17 |
| 89 | 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 |
| 90 | Electrostatic control on endo/exo selectivity in ionic cycloaddition. Chemical Physics Letters, 2005, 416, 354-357. | 1.2 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Ab initio Computational Modeling of Glyphosate Analogs: Conformational Perspective. Structural Chemistry, 2005, 16, 491-506. | 1.0 | 8 |
| 92 | 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 |
| 93 | 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 |
| 94 | 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 |
| 95 | 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 |
| 96 | 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 |
| 97 | 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 |
| 98 | Ab initiocomputational studies on molecular conformation of N-methyl-glyphosate. Molecular Physics, 2003, 101, 3073-3083. | 0.8 | 5 |
| 99 | 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 |
| 100 | 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 |
| 101 | Electronic structure and conformation of glyphosate: an ab initio MO study. Computational and Theoretical Chemistry, 2002, 618, 117-125. | 1.5 | 14 |
| 102 | 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 |
| 103 | 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 |
| 104 | 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 |
| 105 | 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 |
| 106 | A proton and carbon NMR spectroscopic study of 5-substituted acenaphthenes. Magnetic Resonance in Chemistry, 1998, 36, 943-946. | 1.1 | 9 |
| 107 | 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 |
| 108 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Ab initio study of formazan and 3-nitroformazan. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3313-3319. | 1.7 | 28 |
| 110 | Ï€-systems as lithium/hydrogen bond acceptors: Some theoretical observations. Journal of Chemical Physics, 1998, 109, 9820-9830. | 1.2 | 62 |
| 111 | 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 |
| 112 | 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 |
| 113 | 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 |
| 114 | Lithium bonding interaction in H2CYâ‹¯LiF (Y=O,S) complexes: A theoretical probe. Journal of Chemical Physics, 1997, 107, 4329-4336. | 1.2 | 31 |
| 115 | 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 |
| 116 | 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 |
| 117 | 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 |
| 118 | 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 |
| 119 | Heuristic enhancements of the search for the generation of all perfect matchings. Applied Mathematics Letters, 1996, 9, 49-53. | 1.5 | 3 |
| 120 | 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 |
| 121 | Theoretical study on the mechanism and reactivity of fluorocumulenes in [42] cycloadditions. Journal of Fluorine Chemistry, 1995, 73, 171-174. | 0.9 | 12 |
| 122 | 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 |
| 123 | Computer generation of Pauling bond orders using heuristic search. Journal of Chemical Information and Computer Sciences, 1995, 35, 717-722. | 2.8 | 2 |
| 124 | Topological resonance energy predictions of the stability of fullerene clusters. Chemical Physics Letters, 1994, 222, 95-100. | 1.2 | 47 |
| 125 | Ultraviolet photoelectron spectroscopy of complexes of bromine with n-donors in the vapor phase. Chemical Physics Letters, 1994, 228, 431-435. | 1.2 | 8 |
| 126 | General Method for the Computation of Matching Polynomials of Graphs. Journal of Chemical Information and Computer Sciences, 1994, 34, 1122-1126. | 2.8 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | 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 |
| 128 | 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 |
| 129 | Parallel algorithm for the computation of characteristic polynomials of chemical graphs. Journal of Computational Chemistry, 1991, 12, 779-783. | 1.5 | 1 |
| 130 | Cyclopolymerization Initiated by Peroxydisulfate Ion and Metal Ion Catalysis. Journal of Macromolecular Science Part A, Chemistry, 1986, 23, 117-128. | 0.4 | 13 |
| 131 | Kinetics of polymerization of N,N-methylenebisacrylamide initiated by KMnO4-H2C2O4 redox system. European Polymer Journal, 1982, 18, 531-534. | 2.6 | 28 |
| 132 | Charge transfer spectra of complexes with benzoquinonechlorimides as electron acceptors. Spectrochimica Acta Part A: Molecular Spectroscopy, 1981, 37, 1-3. | 0.1 | 7 |
| 133 | Molecular complexes of p-benzoquinonechlorimides with aromatic Ï€-donors. Spectrochimica Acta Part A: Molecular Spectroscopy, 1981, 37, 505-510. | 0.1 | 8 |
| 134 | Semi-empirical MO-calculations on the electronic spectra of benzoquinonechlorimides. Spectrochimica Acta Part A: Molecular Spectroscopy, 1980, 36, 103-107. | 0.1 | 9 |