

Avat Arman Taherpour

List of Publications by Year in descending order

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146
papers

1,905
citations

331259

21
h-index

344852

36
g-index

149
all docs

149
docs citations

149
times ranked

1974
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanical buckling of nanocomposite rectangular plate reinforced by aligned and straight single-walled carbon nanotubes. <i>Composites Part B: Engineering</i> , 2012, 43, 2031-2040.	5.9	145
2	Resolving the Multiple Emission Centers in Carbon Dots: From Fluorophore Molecular States to Aromatic Domain States and Carbon-Core States. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4189-4198.	2.1	142
3	Experimental and theoretical studies of the nanostructured $\{Fe_3O_4@SiO_2@CH_2\}_3C(CN)_3$ catalyst for 2-amino-3-cyanopyridine preparation via an anomeric based oxidation. <i>RSC Advances</i> , 2016, 6, 50100-50111.	1.7	92
4	Structural relationships and theoretical study of the free energies of electron transfer, electrochemical properties, and electron transfer kinetic of cephalosporin antibiotics derivatives with fullerenes in nanostructure of $[R]_nC_n$ ($R=$ cefadroxil, cefepime, cephalexin, cefotaxime.) <i>Tj ETQqO O 0 rgBT #Overlock 10 Tf 50 6</i>	1.0	70
5	Determination of Hg^{2+} and Cu^{2+} ions by dual-emissive Ag/Au nanocluster/carbon dots nano hybrids: Switching the selectivity by pH adjustment. <i>Journal of Hazardous Materials</i> , 2019, 367, 437-446.	6.5	70
6	Ionically Tagged Magnetic Nanoparticles with Urea Linkers: Application for Preparation of 2-Aryl-quinoline-4-carboxylic Acids via an Anomeric-Based Oxidation Mechanism. <i>ACS Omega</i> , 2020, 5, 3207-3217.	1.6	48
7	Hydrophobic amino acids grafted onto chitosan: a novel amphiphilic chitosan nanocarrier for hydrophobic drugs. <i>Drug Development and Industrial Pharmacy</i> , 2017, 43, 1-11.	0.9	43
8	Aptamer-Based Fluorescent Biosensing of Adenosine Triphosphate and Cytochrome c via Aggregation-Induced Emission Enhancement on Novel Label-Free DNA-Capped Silver Nanoclusters/Graphene Oxide Nano hybrids. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 46077-46089.	4.0	40
9	Chemical composition analysis of the essential oil of <i>Mentha piperita</i> L. from Kermanshah, Iran by hydrodistillation and HS/SPME methods. <i>Journal of Analytical Science and Technology</i> , 2017, 8, .	1.0	38
10	The structural relationship between $Rand\ddot{A}$ indices, adjacency matrixes, distance matrixes and maximum wave length of linear simple conjugated polyene compounds. <i>Computational and Theoretical Chemistry</i> , 2005, 726, 183-188.	1.5	37
11	Structural Relationship Between Degree of Unsaturation with Polarizability of (5,5) Armchair Single-Wall Carbon Nanotubes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2007, 15, 279-289.	1.0	30
12	The first computational study for the oxidative aromatization of pyrazolines and 1,4-dihydropyridines using 1,2,4-triazolinediones: an anomeric-based oxidation. <i>RSC Advances</i> , 2016, 6, 102280-102291.	1.7	30
13	A convenient method for preparation of 2-amino-4,6-diphenylnicotinonitrile using HBF_4 as an efficient catalyst via an anomeric based oxidation: A joint experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2017, 1137, 674-680.	1.8	29
14	Formation and HERON Reactivity of Cyclic N,N-Dialkoxyamides. <i>Australian Journal of Chemistry</i> , 2014, 67, 507.	0.5	27
15	DFT and TD-DFT theoretical studies on photo-induced electron transfer process on [Cefamandole]. C_{60} nano-complex. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 42-48.	1.3	27
16	In Situ Chromophore Doping: A New Mechanism for the Long-Wavelength Emission of Carbon Dots. <i>Journal of Physical Chemistry C</i> , 2020, 124, 10638-10646.	1.5	27
17	Racemic R,S-venlafaxine hydrochloride-DNA interaction: Experimental and computational evidence. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 145, 540-552.	2.0	26
18	Synthesis, Characterization, and DNA Binding Studies of a New Pt(II) Complex Containing the Drug Levetiracetam: Combining Experimental and Computational Methods. <i>Applied Biochemistry and Biotechnology</i> , 2014, 172, 2436-2454.	1.4	25

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19	Application of novel nanostructured dinitropyrazine molten salt catalyst for the synthesis of sulfanylpyridines via anomeric based oxidation. <i>Journal of the Iranian Chemical Society</i> , 2017, 14, 1839-1852.	1.2	23
20	A rhodium-decorated carbon nanotube cathode material in the dye-sensitized solar cell: Conversion efficiency reached to 11%. <i>Electrochimica Acta</i> , 2019, 308, 373-383.	2.6	23
21	Chemical composition analysis of the essential oil of <i>Melissa officinalis</i> L. from Kurdistan, Iran by HS/SPME method and calculation of the biophysicochemical coefficients of the components. <i>Natural Product Research</i> , 2012, 26, 152-160.	1.0	22
22	Development of a novel PVC-membrane fluorescent sensor based on N,N'-bis(dansylamidoethyl)-N,N'-bis(2-pyridylmethyl)propylene-diamine as a new fluoroionophore for highly sensitive and selective monitoring of trace amounts of La ³⁺ ions in aqueous solutions. <i>Sensors and Actuators B: Chemical</i> , 2014, 192, 378-385.	4.0	22
23	Sub-femtomolar detection of HIV-1 gene using DNA immobilized on composite platform reinforced by a conductive polymer sandwiched between two nanostructured layers: A solid signal-amplification strategy. <i>Analytica Chimica Acta</i> , 2019, 1055, 7-16.	2.6	22
24	Carboxyketenes from 4-Hydroxy-1,3-oxazin-6-ones and Meldrum's Acid Derivatives. <i>Journal of Organic Chemistry</i> , 2007, 72, 1399-1404.	1.7	21
25	Quantitative Relationship Study of Mechanical Structure Properties of Empty Fullerenes, Fullerenes Nanotubes and Carbon Nanostructures, 2008, 16, 196-205.	1.0	21
26	First principles studies of electronic and optical properties of helium adsorption on Sc-doped BN monolayer. <i>Journal of the Iranian Chemical Society</i> , 2015, 12, 1983-1990.	1.2	21
27	Quantitative Structural Relationship Study of Cis-Unsaturated Thiocrown Ethers and Their Supramolecular [X@C ₆₀] and [X@La@C ₈₂] Complexes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2007, 15, 405-415.	1.0	20
28	Quantitative structural relationship and theoretical study of electrochemical properties of C ₆₀ @[SWCN(5,5)-Armchair-C _n H ₂₀] complexes. <i>Chemical Physics Letters</i> , 2009, 469, 135-139.	1.2	20
29	Theoretical and Quantitative Structural Relationship Study of the Electrochemical Properties of [M ₂ @C _x]@[SWCNT(5,5)-Armchair-C _n H ₂₀] (M = Er and Sc, x = 82 and 84, and n = 20~300) Complexes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 5402-5408.	1.5	20
30	Recognition of switching on or off fluorescence emission spectrum on the Schiff-bases as a Mg ²⁺ chemosensor: A first principle DFT and TD-DFT study. <i>Journal of Molecular Structure</i> , 2017, 1147, 815-820.	1.8	20
31	Comprehensive insights into the structure and coordination behavior of thiosemicarbazone ligands: a computational assessment of the E-Z interconversion mechanism during coordination. <i>New Journal of Chemistry</i> , 2015, 39, 9313-9324.	1.4	19
32	Structural Relationship Between Degree of Unsaturation with Fermi Energy, Chemical Hardness, and The HOMO-LUMO Gap of (5,5) Armchair Single-Walled Carbon Nanotubes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2009, 17, 26-37.	1.0	18
33	One-pot microwave-assisted solvent free synthesis of simple alkyl 1,2,3-triazole-4-carboxylates by using trimethylsilyl azide. <i>Journal of Heterocyclic Chemistry</i> , 2009, 46, 131-133.	1.4	18
34	Interrupting the flux of delocalized electrons on a dibenzo-18-crown-6-embedded graphite sheet and its relative counteraction in the presence of potassium ions. <i>Analyst</i> , 2016, 141, 4227-4234.	1.7	18
35	Manganese mediated oxidation of progesterone in alkaline medium: Mechanism study and quantitative determination. <i>Electrochimica Acta</i> , 2017, 225, 292-302.	2.6	18
36	Synthesis and characterization of glucose-capped CdSe quantum dots. Electrochemical and computational studies of corresponding carbon-ionic liquid electrode for quantitative determination of minoxidil. <i>Journal of Electroanalytical Chemistry</i> , 2016, 778, 116-125.	1.9	16

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37	Novel donor-acceptor non-fullerene metal-organic solar cells: A first DFT and TD-DFT study. <i>Physica B: Condensed Matter</i> , 2018, 542, 37-43.	1.3	15
38	Synthesis, structural determination and HSA interaction studies of a new water-soluble Cu(II) complex derived from 1,10-phenanthroline and ranitidine drug. <i>Journal of Coordination Chemistry</i> , 2017, 70, 3186-3198.	0.8	13
39	Adsorption, intercalation and sensing of helium on yttrium functionalized open edge boron nitride: A first principle DFT and TDDFT study. <i>Chemical Physics Letters</i> , 2018, 691, 231-237.	1.2	13
40	Theoretical and quantitative structural relationships of the electrochemical and electron transfer properties of [Mx@C82]@[SWCNT(5,5)-armchair-CnH20] (x=0, 1; for x=1: M=Ce & Gd and n=20-300) nanostructure complexes. <i>Chemical Physics Letters</i> , 2009, 483, 233-240.	1.2	12
41	Theoretical and Quantitative Structural Relationship Studies of Electrochemical Properties of the Nanostructures of Cis-Unsaturated Thiocrown Ethers and Their Supramolecular Complexes [X-UT-Y][M@C ₈₂] (M=Ce, Gd). <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2010, 185, 422-432.	0.8	12
42	Chemical composition of the essential oil of <i>Valeriana alliariifolia</i> Adams of Iran. <i>Natural Product Research</i> , 2010, 24, 973-978.	1.0	12
43	The simulation of UV spectroscopy and electronic analysis of temozolomide and dacarbazine chemical decomposition to their metabolites. <i>Journal of Molecular Modeling</i> , 2016, 22, 270.	0.8	12
44	Electrochemical sensing of trifluralin in water by fluconazole-immobilized Fe ₃ O ₄ /SiO ₂ nanomagnetic core-shell linked to carbon nanotube modified glassy carbon electrode; an experimental and theoretical modeling. <i>Journal of the Iranian Chemical Society</i> , 2018, 15, 719-732.	1.2	12
45	A carbon nanotube-iron (III) oxide nanocomposite as a cathode in dye-sensitized solar cells: Computational modeling and electrochemical investigations. <i>Electrochimica Acta</i> , 2019, 318, 617-624.	2.6	12
46	Harnessing the enantiomeric recognition ability of hydrophobic polymers of intrinsic microporosity (PIM-1) toward amino acids by converting them into hydrophilic polymer dots. <i>Journal of Materials Chemistry C</i> , 2020, 8, 13827-13835.	2.7	12
47	Chemical composition of the essential oil of <i>Pelargonium quercetorum</i> Agnew. of Iran. <i>Natural Product Research</i> , 2007, 21, 24-27.	1.0	11
48	Topological Relationship Between Wiener, Padmakar-Ivan, and Szeged Indices and Energy and Electric Moments in Armchair Polyhex Nanotubes with the Same Circumference and Varying Lengths. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2010, 18, 72-86.	1.0	11
49	Mechanistic study of the hydrolytic degradation and protonation of temozolomide. <i>RSC Advances</i> , 2015, 5, 41112-41119.	1.7	11
50	Human serum albumin binding studies of a new platinum(IV) complex containing the drug pregabalin: experimental and computational methods. <i>Journal of Coordination Chemistry</i> , 2019, 72, 600-618.	0.8	11
51	Mechanism-Based Inactivation of Cytochrome P450 Enzymes: Computational Insights. <i>Chemical Research in Toxicology</i> , 2021, 34, 959-987.	1.7	11
52	Computational note on ab initio studies of 1,3-dipolar cycloaddition reactions between 7-10 membered simple cycloalkynes and nitriloxide. <i>Computational and Theoretical Chemistry</i> , 2008, 849, 23-24.	1.5	10
53	Free Energies of Electron Transfer, Electron Transfer Kinetic Theoretical and Quantitative Structural Relationships and Electrochemical Properties Studies of Gadolinium Nitride Cluster Fullerenes Gd ₃ N@C _n [X-UT-Y][Gd ₃ N@C _n] (n = 80, 82, 84, 86 and 88) Supramolecular Complexes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2013, 21, 485-502.	1.0	10
54	Photoinduced electron transfer process on emission spectrum of N,N'-bis(salicylidene)-1,2-phenylenediamine as a Mg ²⁺ cation chemosensor: A first principle DFT and TDDFT study. <i>Journal of Molecular Structure</i> , 2018, 1161, 339-344.	1.8	10

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55	A low-overpotential nature-inspired molecular chromium water oxidation catalyst. <i>Electrochimica Acta</i> , 2018, 265, 316-325.	2.6	10
56	Regioselective Ortho- C-H sulfonylation of free phenols catalyzed by Co(II)-immobilized on silica-coated magnetic nanoparticles. <i>Molecular Catalysis</i> , 2020, 484, 110772.	1.0	10
57	When a "Dimroth Rearrangement" Is Not a Dimroth Rearrangement. <i>Journal of Organic Chemistry</i> , 2021, 86, 8286-8294.	1.7	10
58	N-doped graphene quantum dots from graphene oxide and dendrimer and application in photothermal therapy: An experimental and theoretical study. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 636, 128066.	2.3	10
59	Quantitative Structural Relationship Study of Electrochemical Properties on the Nano Structures of Cis- π -Unsaturated Thiocrown Ethers and Their Supramolecular Complexes [X@C84] and [X@C82]. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2008, 16, 142-153.	1.0	9
60	A study of the effects of solvent on structural and conformational properties of ranitidine tautomer forms by DFT method. <i>Structural Chemistry</i> , 2015, 26, 517-529.	1.0	9
61	Introduction of a carbon paste electrode based on nickel carbide for investigation of interaction between warfarin and vitamin K1. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2017, 139, 156-164.	1.4	9
62	Synthesis, characterization and <i>in vitro</i> DNA binding studies of a new copper(II) complex containing antioxidant ferulic acid. <i>Journal of Coordination Chemistry</i> , 2017, 70, 2589-2605.	0.8	9
63	Synthesis, characterization, HSA interaction, and antibacterial activity of a new water-soluble Pt(II) complex containing the drug cephalexin. <i>Journal of Coordination Chemistry</i> , 2018, 71, 3708-3730.	0.8	9
64	Electrochemical sensing of 2-methyl-4, 6-dinitrophenol by nanomagnetic core shell linked to carbon nanotube modified glassy carbon electrode. <i>Materials Science and Engineering C</i> , 2019, 99, 211-221.	3.8	9
65	Theoretical Study of Structural Relationships and Electrochemical Properties of Supramolecular [14-MR Macrolides]@C _n Complexes. <i>Analytical Letters</i> , 2010, 43, 658-673.	1.0	8
66	Highly selective and sensitive fluorescence optode membrane for uranyl ion based on 5-(9-anthracenylmethyl)-5-aza-2,8-dithia[9],(2,9)-1,10-phenanthroline. <i>RSC Advances</i> , 2015, 5, 92061-92070.	1.7	8
67	Mechanistic study of allopurinol oxidation using aldehyde oxidase, xanthine oxidase and cytochrome P450 enzymes. <i>RSC Advances</i> , 2016, 6, 109672-109680.	1.7	8
68	Synthesis, characterization and <i>in vitro</i> DNA binding studies of a new copper(II) complex containing an antiviral drug, valganciclovir. <i>Journal of Coordination Chemistry</i> , 2017, 70, 201-222.	0.8	8
69	Chemical composition analysis of the essential oil of <i>Solanum nigrum</i> L. by HS/SPME method and calculation of the biochemical coefficients of the components. <i>Arabian Journal of Chemistry</i> , 2017, 10, S2372-S2375.	2.3	8
70	Comprehensive facilitating of water oxidation reaction by ultrasonic attenuation of hydrogen-bonded structure of water. <i>Ultrasonics Sonochemistry</i> , 2018, 42, 381-389.	3.8	8
71	Efficient ethanol oxidation by hemoglobin-capped gold nanoclusters: The critical role of Fe in the heme group as an oxophilic metal active site. <i>Electrochemistry Communications</i> , 2019, 103, 42-47.	2.3	8
72	Structural Relationship Study of Electrochemical Properties of the Nano Structures of Cis- π -Unsaturated Thiocrown Ethers and Their Supramolecular Complexes [X@C84][La@C ₇₂ (C ₆ H ₃ Cl ₂)] Non-IPR Carbon Cage. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2009, 17, 171-186.	1.0	7

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73	Theoretical and Quantitative Structural Relationships of the Electron Transfer and Electrochemical Properties of <i>Cis</i> -Unsaturated Thiocrown Ethers and Supramolecular Complexes [X-UT-Y]@[La ₂ @C ₇₂ (Adamantylidene Mono-Adducts) _n] (n=0,1), Fullerenes Nanotubes and Carbon Nanostructures, 2011, 19, 166-181.	1.0	7
74	Theoretical studies on the rotamers and dynamic behaviors of ethyl-5-acetyl-4-(3,4-dimethoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3-carboxylate. Structural Chemistry, 2013, 24, 191-200.	1.0	7
75	9-Azidoacridine and 9-Azocridinyl nitrene. Journal of Physical Organic Chemistry, 2010, 23, 382-389.	0.9	6
76	Structural Relationships and Theoretical Study of Electron Transfer Properties of 1,3,2-Dithiazolyl Radicals with Fullerenes in Nanostructure [1,3,2-DTA(s)]@C _n Supramolecular Complexes. Phosphorus, Sulfur and Silicon and the Related Elements, 2010, 185, 1604-1614.	0.8	6
77	Theoretical study of 1,3-dipolar cycloaddition reactions between 7-10-membered simple cycloalkynes and triazoles R ⁻ N ₃ (R=H, CH ₃ , Ph). Structural Chemistry, 2013, 24, 523-534.	1.0	6
78	The first principle computational study for the competitive mechanisms of oxidative aromatization of 2-substituted imidazolines using KMnO ₄ /SiO ₂ . Journal of the Iranian Chemical Society, 2017, 14, 2485-2493.	1.2	6
79	Reply to the "Comments on "Experimental and theoretical studies of the nanostructured {Fe ₃ O ₄ @SiO ₂ }(CH ₂) ₃ Im}C(CN) ₃ catalyst for 2-amino-3-cyanopyridine preparation via an anomeric based oxidation", RSC Adv., 2016, 6, 50100-50111, and "The first computational study for the oxidative aromatization of pyrazolines and 1,4-dihydropyridines using 1,2,4-triazolinediones: an anomeric-based oxidation", RSC Adv., 2016, 6, 102, RSC Advances, 2017, 7, 53617-53621.	1.7	6
80	A DFT study of both the hydrolytic degradation and protonation of semustine in variation conditions of pH and interaction of drug with DNA nucleobases. Structural Chemistry, 2018, 29, 1465-1474.	1.0	6
81	A DFT Study of Electronic Structures and Relative Stabilities of Isomeric <i>n,m</i> -Diazaphenanthrenes. Polycyclic Aromatic Compounds, 2019, 39, 462-469.	1.4	6
82	Chemical composition of the essential oil of <i>Thalectrum minus</i> L. of Iran. Natural Product Research, 2008, 22, 97-100.	1.0	5
83	Theoretical Study of Structural Relationships and Electrochemical Properties of Supramolecular [Tetracyclines].CnComplexes. Fullerenes Nanotubes and Carbon Nanostructures, 2009, 17, 636-651.	1.0	5
84	Theoretical Study and Structural Relationships of Free Energies of Electron Transfer, Electrochemical Properties and Electron Transfer Kinetics of Ferrocene Derivatives with Fullerenes in Nanostructures of [(R)2Cp2-Fe].CnSupramolecular Complexes. Fullerenes Nanotubes and Carbon Nanostructures, 2013, 21, 653-680.	1.0	5
85	Transduction of interaction between trace tryptophan and surface-confined chromium salen using impedance spectroscopy. A sensing device that works based on highly selective inhibition of mediator's Faradaic process. Analytica Chimica Acta, 2018, 1030, 70-76.	2.6	5
86	Proton shuttle efficiency of bicarbonate: A theoretical study on tautomerization and CO ₂ hydration. Tetrahedron, 2019, 75, 130693.	1.0	5
87	Structural Assessment of Hydrogen Bonds on Methylpentynol Azide Clusters To Achieve Regiochemical Outcome of 1,3-Dipolar Cycloaddition Reactions Using Density Functional Theory. ACS Omega, 2020, 5, 5964-5975.	1.6	5
88	Feasibility of using two benzo-substituted pyrilium-based compounds in dye-sensitized solar cells. Materials Science in Semiconductor Processing, 2021, 123, 105468.	1.9	5
89	Thermal Rearrangement of Azulenes to Naphthalenes: A Deeper Insight into the Mechanisms. Journal of Organic Chemistry, 2022, 87, 3296-3310.	1.7	5
90	Conformational properties of simple monocyclic conjugated enediynes. Computational and Theoretical Chemistry, 1998, 422, 213-218.	1.5	4

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91	AM1 study of conformational properties of cyclohexaketene and expanded cyclohexaketenes. Computational and Theoretical Chemistry, 1999, 488, 141-149.	1.5	4
92	One-pot Microwave-Assisted Synthesis of 1H-Phenanthro[9,10- d][1,2,3]triazole. MolBank, 2008, 2008, M577.	0.2	4
93	Relationship study of octanol-water partitioning coefficients and total biodegradation of linear simple conjugated polyene and carotene compounds by use of the Randić index and maximum UV wavelength. Physics and Chemistry of Liquids, 2009, 47, 349-359.	0.4	4
94	Theoretical and Quantitative Structural Relationships of the Electrochemical Properties of [M@C ₈₂][SWCNT(5,5)-armchair-C _n H ₂₀] (M = La, Y and n =) Tj ETQq0 0 0 rgBT /Overlock 10 T Chemistry, 2010, 1, P97-P109.	1.5	4
95	Efficient synthesis of 2-hydroxyalkyl alkanedithioates from 1,3-diketones, CS ₂ , and epoxides. Journal of Sulfur Chemistry, 2012, 33, 385-390.	1.0	4
96	One-pot microwave-assisted solvent-free synthesis, theoretical and experimental studies on barrier rotation of C-N bond of N-alkenyl-1,2,3-triazoles. Structural Chemistry, 2014, 25, 1483-1493.	1.0	4
97	Theoretical study of electron transfer process between fullerenes and neurotransmitters; acetylcholine, dopamine, serotonin and epinephrine in nanostructures [neurotransmitters].C n complexes. Journal of Chemical Biology, 2016, 9, 19-29.	2.2	4
98	Theoretical and Instrumental Studies of the Competitive Interaction Between Aromatic β -Aminobisphosphonates with DNA Using Binding Probes. Applied Biochemistry and Biotechnology, 2017, 182, 925-943.	1.4	4
99	N 2 elimination thermolysis reactions of 9-(4- and 5-substituted-1,2,3-triazol-1-yl)acridines to produce 1 H -pyrido-[4,3,2- kl] derivatives - A theoretical study. Chemical Physics Letters, 2017, 676, 154-168.	1.2	4
100	Theoretical studies of the free energies of electron transfer and electron transfer kinetics in nanostructure supramolecular complexes of cis -unsaturated thiocrown ethers and Ce and Gd endohedral metallofullerenes [X -UT- Y][M@C 82] (M = Ce, Gd). Arabian Journal of Chemistry, 2017, 10, S609-S616.	2.3	4
101	Tautomeric preferences of the cis and trans isomers of axitinib. Chemical Physics, 2018, 507, 10-18.	0.9	4
102	Fabrication of Template-Less Self-Propelled Micromotors Based on A Metal-Sandwiched Polytryptophan Body: An Experimental and DFT Study. ChemPlusChem, 2020, 85, 1129-1136.	1.3	4
103	Unveiling the mechanistic implications of water oxidation reactions boosted by guanidine proton relays: a chemical-electrochemical-chemical pathway and a non-concerted proton-electron transfer. Journal of Materials Chemistry A, 2021, 9, 2937-2947.	5.2	4
104	Novel donor-acceptor non-fullerene metal-organic solar cells based on open edge Sc@BN: a DFT and TD-DFT study. Journal of the Iranian Chemical Society, 2021, 18, 2271-2282.	1.2	4
105	Catalytic application of sulfamic acid-functionalized magnetic Fe ₃ O ₄ nanoparticles (SA-MNPs) for protection of aromatic carbonyl compounds and alcohols: experimental and theoretical studies. RSC Advances, 2020, 10, 44946-44957.	1.7	4
106	AM1 study of the equilibrium geometries and racemization mechanisms in open-chain carbodiimides. Conformational and configurational energy surface of 1,3,4,6-tetraazacyclonona-1,2,4,5-tetraene. Computational and Theoretical Chemistry, 1998, 427, 185-190.	1.5	3
107	Theoretical free energies of electron transfer, electrochemical properties, electron transfer kinetic and quantitative structural relationships studies of alkynyl-dihydrofullerene in [X-UT-Y][R-C60-M+] supramolecular complexes. European Journal of Chemistry, 2012, 3, 340-347.	0.3	3
108	Synthesis of alkyl bis(dimethylamino)methylenecarbamodithioates from 1,1,3,3-tetramethylguanidine, CS ₂ and oxiranes. Chinese Chemical Letters, 2012, 23, 699-702.	4.8	3

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109	Spectrophotometric study of formation, structure, stability and kinetics of charge-transfer complexation of iodine with 1,4,7,10,13,16-hexamethyl-1,4,7,10,13,16-hexaazacyclooctadecane in chloroform solution. Application of hard-modeling approaches and theoretical calculations. <i>Journal of Molecular Structure</i> , 2013, 1047, 179-185.	1.8	3
110	One-pot Solvent-free Catalytic Dimerization Reaction of Phenylacetylene to 1-Phenylnaphthalene. <i>Journal of Chemical Sciences</i> , 2015, 127, 1523-1530.	0.7	3
111	Theoretical Calculation of Thermodynamic and Kinetic Quantities for 1,3 Dipolar Cycloaddition Reactions Between Nitrile Sulfides R ⁿ CNS (R ⁿ =H, CH ₃ , Ph and Ph(CH ₃) ₃) with 7-10 Membered Simple Cycloalkynes. <i>Iranian Journal of Science and Technology, Transaction A: Science</i> , 2017, 41, 1139-1148.	0.7	3
112	Molecular interactions between PAMAM dendrimer and some medicines that suppress the growth of hepatitis virus (Adefovir, Entecavir, Telbivudine, Lamivudine, Tenofovir): a theoretical study. <i>International Nano Letters</i> , 2019, 9, 231-244.	2.3	3
113	Structural distortions of fullerene C ₆₀ n (n=0 to 6) by first principle density functional theory. <i>Journal of Molecular Structure</i> , 2019, 1184, 546-556.	1.8	3
114	Chemical compositions of the essential oil and calculation the biophysicochemical coefficients of the components of <i>Hymenocrater longiflorus</i> Benth. of Iran. <i>Natural Science</i> , 2011, 03, 104-108.	0.2	3
115	Structural relationship between photophysical data of 1,3,5-trisubstituted oligoaryleneethynylene benzene star-shaped molecules and number of carbon atoms. <i>Physics and Chemistry of Liquids</i> , 2010, 48, 289-297.	0.4	2
116	Conductometric and ¹ H NMR studies of thermodynamics of complexation of Zn ²⁺ , Cd ²⁺ and Pb ²⁺ ions with tetrathia-12-crown-4 in dimethylsulfoxide-nitrobenzene mixtures. <i>Journal of Inclusion Phenomena and Macroscopic Chemistry</i> , 2014, 78, 429-436.	0.9	2
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