

Abdulaziz A Al-Saadi

List of Publications by Year in descending order

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138
papers

3,984
citations

109321
35
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149698
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138
all docs

138
docs citations

138
times ranked

3659
citing authors

#	ARTICLE	IF	CITATIONS
1	Nitrogen-Enhanced Charge Transfer Efficacy on the Carbon Sheet: A Theoretical Insight Into the Adsorption of Anionic Dyes. <i>Arabian Journal for Science and Engineering</i> , 2022, 47, 419-427.	3.0	7
2	Structural and energetic effect of the intramolecular hydrogen bonding in 4,6-dihalo-resorcinols: ab initio calculation, vibrational spectroscopy, and molecular docking studies. <i>Structural Chemistry</i> , 2022, 33, 57-69.	2.0	3
3	Evaluation of the inhibition performance of piperazine-based polyurea towards mild steel corrosion: The role of keto-enol tautomerization. <i>Journal of Molecular Structure</i> , 2022, 1248, 131485.	3.6	5
4	Surface-enhanced Raman scattering (SERS) spectroscopy for prostate cancer diagnosis: A review. <i>Photodiagnosis and Photodynamic Therapy</i> , 2022, 37, 102690.	2.6	23
5	Insights into end-capped modifications effect on the photovoltaic and optoelectronic properties of S-shaped fullerene-free acceptor molecules: A density functional theory computational study for organic solar cells. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, .	1.9	28
6	A First-Principles Study on the Multilayer Graphene Nanosheets Anode Performance for Boron-Ion Battery. <i>Nanomaterials</i> , 2022, 12, 1280.	4.1	11
7	NMR evidence for hydrogen bonding stabilized anti conformation of 1-methoxy-1-methyl-3-phenylurea and the concentration detection by SERS. <i>Journal of Molecular Liquids</i> , 2022, 357, 119096.	4.9	8
8	SERS and EC-SERS detection of local anesthetic procaine using Pd loaded highly reduced graphene oxide nanocomposite substrate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 278, 121381.	3.9	7
9	Spectroanalytical SERS-based detection of trace-level procainamide using green-synthesized gold nanoparticles. <i>Surfaces and Interfaces</i> , 2022, 31, 102059.	3.0	5
10	SERS-Based Ultralow Concentration Detection of Anticancer Gemcitabine Using Size-Controlled Silver Nanoparticles. <i>Arabian Journal for Science and Engineering</i> , 2022, 47, 7197-7205.	3.0	2
11	Pilotyâ€™s acid and its hydrazide analogue: Insights from the density functional theory and vibrational spectroscopy on the conformational stability and chemical reactivity. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 249, 119317.	3.9	1
12	Molecular docking, spectroscopic, and quantum chemical studies on aromatic heterocycle tetrakis(4-pyridyl)cyclobutane regioisomers: potential membrane-permeable inhibitors. <i>Journal of Molecular Modeling</i> , 2021, 27, 94.	1.8	4
13	Comparative Exposure Assessment of Potential Health Risks through the Consumption of Vegetables Irrigated by Freshwater/Wastewater: Gujranwala, Pakistan. <i>Chemical Research in Toxicology</i> , 2021, 34, 1417-1429.	3.3	8
14	Porous Fluorocarbon from Rice Husk for the Efficient Separation of Gases. <i>Global Challenges</i> , 2021, 5, 2000124.	3.6	1
15	Electrochemically modulated SERS detection of procaine using FTO electrodes modified with silver-decorated carbon nanosphere. <i>Electrochimica Acta</i> , 2021, 387, 138463.	5.2	33
16	Conformational analysis and concentration detection of linuron: Spectroscopic NMR and SERS study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 263, 120223.	3.9	5
17	Fast and sensitive detection of Procainamide: Combined SERS and DFT modeling studies. <i>Journal of Molecular Liquids</i> , 2021, 343, 117633.	4.9	23
18	Blue- and white-light-emitting 2D-coordination polymers and their solid-state photodimerization reaction. <i>CrystEngComm</i> , 2021, 23, 7663-7670.	2.6	1

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19	UV-absorbing benzamide-based dendrimer precursors: synthesis, theoretical calculation, and spectroscopic characterization. <i>New Journal of Chemistry</i> , 2021, 46, 75-85.	2.8	3
20	Understanding the Influence of Electron-Donating and Electron-Withdrawing Substituents on the Anticorrosive Properties of Imidazole: A Quantum-Chemical Approach. <i>Arabian Journal for Science and Engineering</i> , 2020, 45, 153-166.	3.0	5
21	Sensitive SERS detection and characterization of procaine in aqueous media by reduced gold nanoparticles. <i>Sensors and Actuators B: Chemical</i> , 2020, 304, 127057.	7.8	44
22	Synthesis and Characterization of Fluorocarbon from Rice Husk and its Application as an Efficient Sorbent for Micro-Solid-Phase Extraction of N-Nitrosamines in Desalinated Water Samples. <i>Chromatographia</i> , 2020, 83, 95-105.	1.3	4
23	New imidazole-based dimers as potential inhibitors for mild steel corrosion in acidic media: Electrochemical and DFT evaluation. <i>Materials and Corrosion - Werkstoffe Und Korrosion</i> , 2020, 71, 292-299.	1.5	13
24	Spectral characterization, thermochemical studies, periodic SAPT calculations and detailed quantum mechanical profiling various physico-chemical properties of 3,4-dichlorodiuiron. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117580.	3.9	26
25	Inhibition of mild steel corrosion in CO ₂ and H ₂ S-saturated acidic media by a new polyurea-based material. <i>Materials and Corrosion - Werkstoffe Und Korrosion</i> , 2020, 71, 646-662.	1.5	13
26	In Silico Modeling of New α -Series-Based Near-Infrared Sensitive Non-Fullerene Acceptors for Efficient Organic Solar Cells. <i>ACS Omega</i> , 2020, 5, 24125-24137.	3.5	103
27	Computational study of SERS effects in some aliphatic and cyclic carboxylic acids with silver nanomaterials. <i>Journal of Physics: Conference Series</i> , 2020, 1564, 012008.	0.4	2
28	DFT evaluation of the effects of OH, NH ₂ and Br substituents on the properties of 2,2'-bipyridine derivatives. <i>Journal of Taibah University for Science</i> , 2020, 14, 1527-1537.	2.5	8
29	SERS-based trace-level quantification of sulindac: Spectroscopic and molecular modeling evaluation. <i>Journal of Molecular Liquids</i> , 2020, 312, 113402.	4.9	21
30	Impact of Degree of Hydrophilicity of Pyridinium Bromide Derivatives on HCl Pickling of X-60 Mild Steel: Experimental and Theoretical Evaluations. <i>Coatings</i> , 2020, 10, 185.	2.6	14
31	Synthesis, conformational, characterization and reactivity study of 1,7-bis(4-bromophenyl)heptane-1,7-dione. <i>Journal of Molecular Structure</i> , 2019, 1175, 269-279.	3.6	16
32	Spectroscopic, DFT and trace detection study of procaine using surface-enhanced Raman scattering technique. <i>Chemical Physics Letters</i> , 2019, 730, 617-622.	2.6	24
33	Conformational profile, vibrational assignments, NLO properties and molecular docking of biologically active herbicide 1,1-dimethyl-3-phenylurea. <i>Heliyon</i> , 2019, 5, e01987.	3.2	46
34	Impact of electron-withdrawing and electron-donating substituents on the corrosion inhibitive properties of benzimidazole derivatives: A quantum chemical study. <i>Journal of Molecular Structure</i> , 2019, 1196, 348-355.	3.6	55
35	Droplet flow-assisted heterogeneous electro-Fenton reactor for degradation of beta-blockers: response surface optimization, and mechanism elucidation. <i>Environmental Science and Pollution Research</i> , 2019, 26, 14313-14327.	5.3	9
36	Principal components analysis of Raman spectral data for screening of Hepatitis C infection. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 221, 117173.	3.9	36

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37	Preparation and Characterization of Biomass Carbon-Based Solid Acid Catalysts for the Esterification of Marine Algae for Biodiesel Production. <i>Bioenergy Research</i> , 2019, 12, 433-442.	3.9	17
38	Quantum chemical designing of indolo[3,2,1-jk]carbazole-based dyes for highly efficient nonlinear optical properties. <i>Chemical Physics Letters</i> , 2019, 719, 59-66.	2.6	108
39	First theoretical probe for efficient enhancement of nonlinear optical properties of quinacridone based compounds through various modifications. <i>Chemical Physics Letters</i> , 2019, 715, 222-230.	2.6	125
40	Characterization of valeric acid using substrate of silver nanoparticles with SERS. <i>Journal of Molecular Liquids</i> , 2019, 273, 536-542.	4.9	57
41	Mechanistic studies of the influence of halogen substituents on the corrosion inhibitive efficiency of selected imidazole molecules: A synergistic computational and experimental approach. <i>Applied Surface Science</i> , 2019, 471, 494-505.	6.1	51
42	Synthesis, spectroscopic characterization and in vitro cytotoxic as well as docking studies of cis-diammine platinum(II) complexes of thiones. <i>Inorganica Chimica Acta</i> , 2019, 484, 347-351.	2.4	5
43	Structural, spectroscopic and docking properties of resorcinol, its -OD isotopomer and dianion derivative: a comparative study. <i>Structural Chemistry</i> , 2018, 29, 403-414.	2.0	11
44	Synthesis, X-ray structure and cytotoxicity evaluation of carbene-based gold(I) complexes of selenones. <i>Inorganica Chimica Acta</i> , 2018, 476, 46-53.	2.4	15
45	First Theoretical Framework of Triphenylamine-Dicyanovinylene-Based Nonlinear Optical Dyes: Structural Modification of π -Linkers. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4009-4018.	3.1	193
46	Silver loaded graphene as a substrate for sensing 2-thiouracil using surface-enhanced Raman scattering. <i>Sensors and Actuators B: Chemical</i> , 2018, 254, 1110-1117.	7.8	100
47	A selective detection approach for copper(II) ions using a hydrazone-based colorimetric sensor: spectroscopic and DFT study. <i>RSC Advances</i> , 2018, 8, 39983-39991.	3.6	26
48	Selective colorimetric sensing of nickel (II) ions using 2-hydroxy-5-nitrobenzaldehyde-4-hydroxybenzoylhydrazone ligand: Spectroscopic and DFT insights. <i>Journal of Molecular Liquids</i> , 2018, 264, 58-65.	4.9	7
49	Spectroscopic and DFT assessment of bridging ligand effect on the structural and electronic properties of dinuclear iridium- and rhodium-based complexes. <i>Inorganica Chimica Acta</i> , 2018, 482, 299-306.	2.4	5
50	Silver-loaded graphene as an effective SERS substrate for clotrimazole detection: DFT and spectroscopic studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 201, 354-361.	3.9	59
51	Synthesis and characterization of functionalized polythiophene for polymer-sensitized solar cell. <i>Dyes and Pigments</i> , 2017, 141, 406-412.	3.7	17
52	Synthesis, characterization and in vitro cytotoxicity of platinum(II) complexes of selenones [Pt(selenone) ₂ Cl ₂]. <i>Journal of Coordination Chemistry</i> , 2017, 70, 1020-1031.	2.2	12
53	Silver nanoparticles for detection of methimazole by surface-enhanced Raman spectroscopy. <i>Materials Research Bulletin</i> , 2017, 91, 173-178.	5.2	65
54	Ultra-trace detection of methimazole by surface-enhanced Raman spectroscopy using gold substrate. <i>Vibrational Spectroscopy</i> , 2017, 90, 96-103.	2.2	40

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55	Spherical silver nanoparticles as substrates in surface-enhanced Raman spectroscopy for enhanced characterization of ketoconazole. <i>Materials Science and Engineering C</i> , 2017, 76, 356-364.	7.3	50
56	Synthesis, X-ray structures and anticancer activity of gold(I)-carbene complexes with selenones as co-ligands and their molecular docking studies with thioredoxin reductase. <i>Journal of Organometallic Chemistry</i> , 2017, 848, 175-183.	1.8	25
57	Conformational, vibrational and DFT studies of a newly synthesized arylpiperazine-based drug and evaluation of its reactivity towards the human GABA receptor. <i>Journal of Molecular Structure</i> , 2017, 1147, 266-280.	3.6	11
58	Structural properties, vibrational spectra and surface-enhanced Raman scattering of 2,4,6-trichloro- and tribromoanilines: A comparative study. <i>Journal of Molecular Structure</i> , 2016, 1121, 7-15.	3.6	38
59	Spectroscopic (FT-IR, FT-Raman, UV, ¹ H and ¹³ C NMR) profiling and theoretical calculations of (2E)-2-[3-(1H-imidazol-1-yl)-1-phenylpropylidene]hydrazinecarboxamide: An anticonvulsant agent. <i>Journal of Molecular Structure</i> , 2016, 1118, 219-232.	3.6	3
60	Spectroscopic and theoretical evaluation of the metal-olefin interaction in di- η^4 -chlorobis (1,5-cyclooctadiene) complexes of Ir and Rh. <i>Vibrational Spectroscopy</i> , 2016, 86, 109-123.	2.2	7
61	Silver colloid and film substrates in surface-enhanced Raman scattering for 2-thiouracil detection. <i>RSC Advances</i> , 2016, 6, 75282-75292.	3.6	77
62	Density functional theory study of the substituent effect on the structure, conformation and vibrational spectra in halosubstituted anilines. <i>RSC Advances</i> , 2016, 6, 67794-67804.	3.6	6
63	Graphene Dendrimer-stabilized silver nanoparticles for detection of methimazole using Surface-enhanced Raman scattering with computational assignment. <i>Scientific Reports</i> , 2016, 6, 32185.	3.3	181
64	Dimethylphosphinate bridged binuclear Rh(i) catalysts for the alkoxycarbonylation of aromatic C-H bonds. <i>Dalton Transactions</i> , 2016, 45, 16955-16965.	3.3	6
65	Conformational, NBO, NLO, HOMO-LUMO, NMR, electronic spectral study and molecular docking study of N,N-Dimethyl-3-(10H-phenothiazin-10-yl)-1-propanamine. <i>Journal of Molecular Structure</i> , 2016, 1122, 268-279.	3.6	19
66	Hydroxylamine reduced silver colloid for naphthalene and phenanthrene detection using surface-enhanced Raman spectroscopy. <i>Chemical Engineering Journal</i> , 2016, 304, 141-148.	12.7	60
67	Kinetic and computational evaluation of activated carbon produced from rubber tires toward the adsorption of nickel in aqueous solutions. <i>Desalination and Water Treatment</i> , 2016, 57, 17570-17578.	1.0	11
68	Collision induced dissociations of non-derivatized and trimethylsilyl-derivatized estradiols: similarities in fragmentation patterns. <i>Journal of Mass Spectrometry</i> , 2015, 50, 308-315.	1.6	0
69	Experimental and Theoretical Studies of the Vibrational and Electronic Properties of (2E)-2-[3-(1H-imidazol-1-yl)-1-phenyl-propylidene]-N-phenylhydrazinecarboxamide: An Anticonvulsant Agent. <i>Applied Sciences (Switzerland)</i> , 2015, 5, 955-972.	2.5	9
70	Molecular conformational analysis, vibrational spectra, NBO, NLO, HOMO-LUMO and molecular docking studies of ethyl 3-(E)-(anthracen-9-yl)prop-2-enoate based on density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 533-542.	3.9	39
71	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO, NBO, MEP analysis and molecular docking study of 2-[(4-chlorobenzyl)sulfanyl]-4-(2-methylpropyl)-6-(phenylsulfanyl)-pyrimidine-5-carbonitrile, a potential chemotherapeutic agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 413-424.	3.9	17
72	First principle calculations of the chemisorption of SO on doped carbon nanotubes and graphene. <i>Chemical Physics Letters</i> , 2015, 621, 65-70.	2.6	9

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73	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO–LUMO analysis and molecular docking study of 1-hydroxy-4,5,8-tris(4-methoxyphenyl) anthraquinone. Journal of Physics and Chemistry of Solids, 2015, 87, 110-121.	4.0	20
74	Iridium complexes as catalysts in the hydrogen transfer of isopropanol to acetophenone: Ligand effects and DFT studies. Inorganica Chimica Acta, 2015, 436, 146-151.	2.4	14
75	FT-IR, HOMO–LUMO, NBO, MEP analysis and molecular docking study of 3-Methyl-4-[(E)-[4-(methylsulfanyl)-benzylidene]amino}1H-1,2,4-triazole-5(4H)-thione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 151, 198-207.	3.9	41
76	Molecular conformational analysis, vibrational spectra, NBO, NLO analysis and molecular docking study of bis[(E)-anthranil-9-acrylic]anhydride based on density functional theory calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 151, 350-359.	3.9	14
77	Vibrational spectroscopic and molecular docking study of (2 E)- N -(4-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylprop-2-enamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 151, 335-349.	3.9	15
78	Vibrational spectra, HOMO, LUMO, NBO, MEP analysis and molecular docking study of 2,2-diphenyl-4-(piperidin-1-yl)butanamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 543-556.	3.9	59
79	Spectroscopic investigations, NBO, HOMO–LUMO, NLO analysis and molecular docking of 5-(adamantan-1-yl)-3-anilinomethyl-2,3-dihydro-1,3,4-oxadiazole-2-thione, a potential bioactive agent. Journal of Molecular Structure, 2015, 1096, 1-14.	3.6	50
80	1-Alkyl-1-methylpiperazine-1,4-dium salts: Synthetic, acid–base, XRD-analytical, FT-IR, FT-Raman spectral and quantum chemical study. Journal of Molecular Structure, 2015, 1094, 210-236.	3.6	15
81	Spectroscopic investigation (FTIR spectrum), NBO, HOMO–LUMO energies, NLO and thermodynamic properties of 8-Methyl-N-vanillyl-6-nonenamide by DFT methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 146, 177-186.	3.9	52
82	Surface characterization and sorption efficacy of tire–obtained carbon: experimental and semiempirical study of rhodamine B adsorption. Surface and Interface Analysis, 2015, 47, 785-792.	1.8	58
83	Synthesis, characterization and theoretical calculations of (1,2-diaminocyclohexane)(1,3-diaminopropane)gold(III) chloride complexes: in vitro cytotoxic evaluations against human cancer cell lines. BioMetals, 2015, 28, 827-844.	4.1	16
84	Normal co-ordinate analysis, molecular structural, non-linear optical, second order perturbation studies of Tizanidine by density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 139, 189-199.	3.9	2
85	Infrared spectrum, structural and optical properties and molecular docking study of 3-(4-fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 138, 529-538.	3.9	36
86	Spectroscopic investigation (FT-IR, FT-Raman), HOMO–LUMO, NBO analysis and molecular docking study of a potential chemotherapeutic agent. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 520-533.	3.9	8
87	Molecular structure, FT-IR, vibrational assignments, HOMO–LUMO, MEP, NBO analysis and molecular docking study of ethyl-6-(4-chlorophenyl)-4-(4-fluorophenyl)-2-oxocyclohex-3-ene-1-carboxylate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 138, 73-84.	3.9	15
88	Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and LUMO		

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91	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMOâ€“LUMO analysis and molecular docking study of 2-(Adamantan-1-yl)-5-(4-nitrophenyl)-1,3,4-oxadiazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 973-983.	3.9	37
92	Vibrational spectroscopic studies and molecular docking of 10,10-Dimethylanthrone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 652-661.	3.9	9
93	FT-IR, molecular structure, first order hyperpolarizability, MEP, HOMO and LUMO analysis and NBO analysis of 4-[(3-acetylphenyl)amino]-2-methylidene-4-oxobutanoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 134, 63-72.	3.9	36
94	Visible light-induced photodegradation of rhodamine dyes over BiOCl, and the vital importance of the frontier orbital energy of the dye molecules in the reaction kinetics. Research on Chemical Intermediates, 2015, 41, 2753-2766.	2.7	8
95	Synthesis, structural and vibrational investigation on 2-phenyl-N-(pyrazin-2-yl)acetamide combining XRD diffraction, FT-IR and NMR spectroscopies with DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 608-616.	3.9	30
96	FT-IR, NBO, HOMOâ€“LUMO, MEP analysis and molecular docking study of 1-[3-(4-Fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazol-1-yl]ethanone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 483-493.	3.9	65
97	Molecular structure, FT-IR, vibrational assignments, HOMOâ€“LUMO analysis and molecular docking study of 1-[5-(4-Bromophenyl)-3-(4-fluorophenyl)-4,5-dihydro-1H-pyrazol-1-yl]ethanone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 473-482.	3.9	67
98	Vibrational spectroscopic and molecular docking study of 2-Benzylsulfanyl-4-[(4-methylphenyl)-sulfanyl]-6-pentylpyrimidine-5-carbonitrile, a potential chemotherapeutic agent. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 569-580.	3.9	21
99	Spectroscopic investigation (FT-IR, FT-Raman and SERS), vibrational assignments, HOMOâ€“LUMO analysis and molecular docking study of Opipramol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 547-559.	3.9	32
100	Synthesis, spectroscopic characterization, electrochemical behavior and computational analysis of mixed diamine ligand gold(III) complexes: antiproliferative and in vitro cytotoxic evaluations against human cancer cell lines. BioMetals, 2014, 27, 1115-1136.	4.1	20
101	Synthesis of g-C ₃ N ₄ /BiOClxBr _{1-x} hybrid photocatalysts and the photoactivity enhancement driven by visible light. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2014, 461, 202-211.	4.7	50
102	Vibrational spectra of 3,5-diamino-6-chloro-N-(diaminomethylene) pyrazine-2-carboxamide: Combined experimental and theoretical studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 127, 157-167.	3.9	15
103	Carbonaceous adsorbent prepared from waste tires: Experimental and computational evaluations of organic dye methyl orange. Journal of Molecular Liquids, 2014, 191, 85-91.	4.9	108
104	Spectroscopic (FT-IR, FT-Raman) investigations and quantum chemical calculations of 1,7,8,9-tetrachloro-10,10-dimethoxy-4-{3-[4-(3-methoxyphenyl)piperazin-1-yl]propyl}-4-azatricyclo[5.2.1.0 ^{2,6}]dec-8-ene-3,5-dione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 129, 438-450.	3.9	15
105	The vibrational assignments of the infrared and Raman spectra of the symmetrically substituted 2,3-diphenylquinoxaline and its N,Nâ€“2-dioxide: Experimental and computational study. Journal of Molecular Structure, 2014, 1058, 284-290.	3.6	1
106	Facile preparation of g-C ₃ N ₄ modified BiOCl hybrid photocatalyst and vital role of frontier orbital energy levels of model compounds in photoactivity enhancement. Journal of Colloid and Interface Science, 2014, 416, 212-219.	9.4	113
107	Intermolecular hydroamination versus stereoregular polymerization of phenylacetylene by rhodium catalysts based on Nâ€“O bidentate ligands. Inorganic Chemistry Communication, 2014, 40, 78-81.	3.9	9
108	Theoretical investigations on the molecular structure, vibrational spectra, HOMOâ€“LUMO analyses and NBO study of 1-[(Cyclopropylmethoxy)methyl]-5-ethyl-6-(4-methylbenzyl)-1,2,3,4-tetrahydropyrimidine-2,4-dione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 639-650.	3.9	26

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109	Theoretical Studies on the Mechanism of Iridium-Catalyzed Alkene Hydrogenation by the Cationic Complex $[\text{IrH}(\text{NCMe})_3(\text{P}^i\text{Pr}_3)]^+$. <i>Organometallics</i> , 2014, 33, 5156-5163.	2.3	23
110	Molecular conformational analysis, vibrational spectra, NBO analysis and first hyperpolarizability of (2E)-3-(3-chlorophenyl)prop-2-enoic anhydride based on density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 131, 471-483.	3.9	32
111	Molecular conformational analysis, vibrational spectra, NBO analysis and first hyperpolarizability of (2E)-3-phenylprop-2-enoic anhydride based on density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 638-646.	3.9	27
112	Theoretical investigations on the molecular structure, vibrational spectral, HOMO-LUMO and NBO analysis of 9-[3-(Dimethylamino)propyl]-2-trifluoro-methyl-9H-thioxanthen-9-ol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 491-501.	3.9	42
113	Adsorption of lead ions from aqueous solution using porous carbon derived from rubber tires: Experimental and computational study. <i>Journal of Colloid and Interface Science</i> , 2013, 396, 264-269.	9.4	107
114	Spectroscopic and computational evaluation of cadmium adsorption using activated carbon produced from rubber tires. <i>Journal of Molecular Liquids</i> , 2013, 188, 136-142.	4.9	59
115	Further insights on the molecular structure, vibrational spectra and ring-puckering potentials of silacyclopent-3-ene and its 1,1-dihalo derivatives: Ab initio and DFT study. <i>Vibrational Spectroscopy</i> , 2012, 62, 188-199.	2.2	10
116	Conformational analysis and vibrational assignments of benzohydroxamic acid and benzohydrazide. <i>Journal of Molecular Structure</i> , 2012, 1023, 115-122.	3.6	17
117	BiOCl-assisted photodegradation of Rhodamine B under white light and monochromatic green pulsed laser irradiation. <i>Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering</i> , 2012, 47, 1192-1200.	1.7	15
118	Photodegradation of Rhodamine B over unexcited semiconductor compounds of BiOCl and BiOBr. <i>Journal of Colloid and Interface Science</i> , 2012, 377, 291-298.	9.4	172
119	Structural properties and vibrational spectra of 2-formyloxazole and its 2-thioformyl and 2-selenoformyl derivatives. <i>Journal of Molecular Structure</i> , 2011, 1006, 655-664.	3.6	2
120	Conformational profile and vibrational assignments of hippuric and 4-aminohippuric acids. <i>Journal of Molecular Structure</i> , 2011, 990, 176-182.	3.6	3
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