

Abdulaziz A Al-Saadi

List of Publications by Year in descending order

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138
papers

3,984
citations

125106

35
h-index

169272

56
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138
all docs

138
docs citations

138
times ranked

4098
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.	1.7	7
2	Structural and energetic effect of the intramolecular hydrogen bonding in 4,6-dihaloresorcinols: ab initio calculation, vibrational spectroscopy, and molecular docking studies. <i>Structural Chemistry</i> , 2022, 33, 57-69.	1.0	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.	1.8	5
4	Surface-enhanced Raman scattering (SERS) spectroscopy for prostate cancer diagnosis: A review. <i>Photodiagnosis and Photodynamic Therapy</i> , 2022, 37, 102690.	1.3	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, .	0.9	28
6	A First-Principles Study on the Multilayer Graphene Nanosheets Anode Performance for Boron-Ion Battery. <i>Nanomaterials</i> , 2022, 12, 1280.	1.9	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.	2.3	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.	2.0	7
9	Spectroanalytical SERS-based detection of trace-level procainamide using green-synthesized gold nanoparticles. <i>Surfaces and Interfaces</i> , 2022, 31, 102059.	1.5	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.	1.7	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.	2.0	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.	0.8	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.	1.7	8
14	Porous Fluorocarbon from Rice Husk for the Efficient Separation of Gases. <i>Global Challenges</i> , 2021, 5, 2000124.	1.8	1
15	Electrochemically modulated SERS detection of procaine using FTO electrodes modified with silver-decorated carbon nanosphere. <i>Electrochimica Acta</i> , 2021, 387, 138463.	2.6	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.	2.0	5
17	Fast and sensitive detection of Procainamide: Combined SERS and DFT modeling studies. <i>Journal of Molecular Liquids</i> , 2021, 343, 117633.	2.3	23
18	Blue- and white-light-emitting 2D-coordination polymers and their solid-state photodimerization reaction. <i>CrystEngComm</i> , 2021, 23, 7663-7670.	1.3	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.	1.4	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.	1.7	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.	4.0	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.	0.7	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.	0.8	13
24	Spectral characterization, thermochemical studies, periodic SAPT calculations and detailed quantum mechanical profiling various physico-chemical properties of 3,4-dichlorodiuron. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117580.	2.0	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.	0.8	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.	1.6	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.	0.3	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.	1.1	8
29	SERS-based trace-level quantification of sulindac: Spectroscopic and molecular modeling evaluation. <i>Journal of Molecular Liquids</i> , 2020, 312, 113402.	2.3	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.	1.2	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.	1.8	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.	1.2	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.	1.4	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.	1.8	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.	2.7	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.	2.0	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.	2.2	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.	1.2	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.	1.2	125
40	Characterization of valeric acid using substrate of silver nanoparticles with SERS. <i>Journal of Molecular Liquids</i> , 2019, 273, 536-542.	2.3	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.	3.1	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.	1.2	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.	1.0	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.	1.2	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.	1.5	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.	4.0	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.	1.7	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.	2.3	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.	1.2	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.	2.0	59
51	Synthesis and characterization of functionalized polythiophene for polymer-sensitized solar cell. <i>Dyes and Pigments</i> , 2017, 141, 406-412.	2.0	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.	0.8	12
53	Silver nanoparticles for detection of methimazole by surface-enhanced Raman spectroscopy. <i>Materials Research Bulletin</i> , 2017, 91, 173-178.	2.7	65
54	Ultra-trace detection of methimazole by surface-enhanced Raman spectroscopy using gold substrate. <i>Vibrational Spectroscopy</i> , 2017, 90, 96-103.	1.2	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.	3.8	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.	0.8	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.	1.8	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.	1.8	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.	1.8	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.	1.2	7
61	Silver colloid and film substrates in surface-enhanced Raman scattering for 2-thiouracil detection. <i>RSC Advances</i> , 2016, 6, 75282-75292.	1.7	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.	1.7	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.	1.6	181
64	Dimethylphosphinate bridged binuclear Rh(i) catalysts for the alkoxy-carbonylation of aromatic C-H bonds. <i>Dalton Transactions</i> , 2016, 45, 16955-16965.	1.6	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.	1.8	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.	6.6	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- α -derivatized and trimethylsilyl- α -derivatized estradiols: similarities in fragmentation patterns. <i>Journal of Mass Spectrometry</i> , 2015, 50, 308-315.	0.7	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.	1.3	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.	2.0	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.	2.0	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.	1.2	9

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73	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMOâ€“LUMO analysis and molecular docking study of 1-hydroxy-4,5,8-tris(4-methoxyphenyl) anthraquinone. <i>Journal of Physics and Chemistry of Solids</i> , 2015, 87, 110-121.	1.9	20
74	Iridium complexes as catalysts in the hydrogen transfer of isopropanol to acetophenone: Ligand effects and DFT studies. <i>Inorganica Chimica Acta</i> , 2015, 436, 146-151.	1.2	14
75	FT-IR, HOMOâ€“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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 198-207.	2.0	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 350-359.	2.0	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 335-349.	2.0	15
78	Vibrational spectra, HOMO, LUMO, NBO, MEP analysis and molecular docking study of 2,2-diphenyl-4-(piperidin-1-yl)butanamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 543-556.	2.0	59
79	Spectroscopic investigations, NBO, HOMOâ€“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. <i>Journal of Molecular Structure</i> , 2015, 1096, 1-14.	1.8	50
80	1-Alkyl-1-methylpiperazine-1,4-dium salts: Synthetic, acidâ€“base, XRD-analytical, FT-IR, FT-Raman spectral and quantum chemical study. <i>Journal of Molecular Structure</i> , 2015, 1094, 210-236.	1.8	15
81	Spectroscopic investigation (FTIR spectrum), NBO, HOMOâ€“LUMO energies, NLO and thermodynamic properties of 8-Methyl-N-vanillyl-6-nonenamide by DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 146, 177-186.	2.0	52
82	Surface characterization and sorption efficacy of tireâ€“obtained carbon: experimental and semiempirical study of rhodamine B adsorption. <i>Surface and Interface Analysis</i> , 2015, 47, 785-792.	0.8	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. <i>BioMetals</i> , 2015, 28, 827-844.	1.8	16
84	Normal co-ordinate analysis, molecular structural, non-linear optical, second order perturbation studies of Tizanidine by density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 189-199.	2.0	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 138, 529-538.	2.0	36
86	Spectroscopic investigation (FT-IR, FT-Raman), HOMOâ€“LUMO, NBO analysis and molecular docking study of a potential chemotherapeutic agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 520-533.	2.0	8
87	Molecular structure, FT-IR, vibrational assignments, HOMOâ€“LUMO, MEP, NBO analysis and molecular docking study of ethyl-6-(4-chlorophenyl)-4-(4-fluorophenyl)-2-oxocyclohex-3-ene-1-carboxylate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 138, 73-84.	2.0	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 135, 973-983.	2.0	37
92	Vibrational spectroscopic studies and molecular docking of 10,10-Dimethylanthrone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 135, 652-661.	2.0	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 134, 63-72.	2.0	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. <i>Research on Chemical Intermediates</i> , 2015, 41, 2753-2766.	1.3	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 135, 608-616.	2.0	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 483-493.	2.0	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 473-482.	2.0	67
98	Vibrational spectroscopic and molecular docking study of 2-Benzylsulfanyl-4-[(4-methylphenyl)-sulfanyl]-6-pentylpyrimidine-5-carbonitrile, a potential chemotherapeutic agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 569-580.	2.0	21
99	Spectroscopic investigation (FT-IR, FT-Raman and SERS), vibrational assignments, HOMOâ€“LUMO analysis and molecular docking study of Opipramol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 547-559.	2.0	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. <i>BioMetals</i> , 2014, 27, 1115-1136.	1.8	20
101	Synthesis of g-C ₃ N ₄ /BiOClxBr ⁿ hybrid photocatalysts and the photoactivity enhancement driven by visible light. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2014, 461, 202-211.	2.3	50
102	Vibrational spectra of 3,5-diamino-6-chloro-N-(diaminomethylene) pyrazine-2-carboxamide: Combined experimental and theoretical studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 127, 157-167.	2.0	15
103	Carbonaceous adsorbent prepared from waste tires: Experimental and computational evaluations of organic dye methyl orange. <i>Journal of Molecular Liquids</i> , 2014, 191, 85-91.	2.3	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 129, 438-450.	2.0	15
105	The vibrational assignments of the infrared and Raman spectra of the symmetrically substituted 2,3-diphenylquinoxaline and its N,Nâ€“dioxide: Experimental and computational study. <i>Journal of Molecular Structure</i> , 2014, 1058, 284-290.	1.8	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. <i>Journal of Colloid and Interface Science</i> , 2014, 416, 212-219.	5.0	113
107	Intermolecular hydroamination versus stereoregular polymerization of phenylacetylene by rhodium catalysts based on Nâ€“O bidentate ligands. <i>Inorganic Chemistry Communication</i> , 2014, 40, 78-81.	1.8	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 133, 639-650.	2.0	26

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109	Theoretical Studies on the Mechanism of Iridium-Catalyzed Alkene Hydrogenation by the Cationic Complex [IrH ₂ (NCMe) ₃ (P ⁱ) ₃] ⁺ . <i>Organometallics</i> , 2014, 33, 5156-5163.	1.1	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.	2.0	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.	2.0	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.	2.0	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.	5.0	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.	2.3	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.	1.2	10
116	Conformational analysis and vibrational assignments of benzohydroxamic acid and benzohydrazide. <i>Journal of Molecular Structure</i> , 2012, 1023, 115-122.	1.8	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.	0.9	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.	5.0	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.	1.8	2
120	Conformational profile and vibrational assignments of hippuric and 4-aminohippuric acids. <i>Journal of Molecular Structure</i> , 2011, 990, 176-182.	1.8	3
121	Structural stability and analysis of vibrational spectra of 1,2,4,5-tetroxane and 3,6-diphenyl-1,2,4,5-tetroxane. <i>Journal of Molecular Structure</i> , 2010, 969, 197-203.	1.8	4
122	Intramolecular π -Type Hydrogen Bonding and Conformations of 3-Cyclopenten-1-ol. 1. Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7453-7456.	1.1	15
123	Intramolecular π -Type Hydrogen Bonding and Conformations of 3-Cyclopenten-1-ol. 2. Infrared and Raman Spectral Studies at High Temperatures. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7457-7461.	1.1	17
124	Structural stability, NH ₂ inversion and vibrational assignments of 2,4,6-trichloroaniline and 2,3,5,6-tetrachloroaniline. <i>Journal of Molecular Structure</i> , 2009, 938, 41-47.	1.8	13
125	Raman and infrared spectra, ab initio and DFT calculations, and vibrational assignments for 2,3-cyclopentenopyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 326-331.	2.0	6
126	Structure, Vibrational Spectra, and DFT and Ab Initio Calculations of Silacyclobutanes. <i>Organometallics</i> , 2008, 27, 3435-3443.	1.1	23

#	ARTICLE	IF	CITATIONS
127	Vibrational Spectra, Ab Initio Calculations, and Ring-Puckering Potential Energy Function for β -Crotonolactone. Journal of Physical Chemistry A, 2007, 111, 3302-3305.	1.1	14
128	Ab initio and DFT calculations for the structure and vibrational spectra of cyclopentene and its isotopomers. Journal of Molecular Structure, 2007, 830, 46-57.	1.8	44
129	The ring-puckering potential energy function and theoretical calculations for silacyclopent-2-ene-d0 and 1,1-d2 and the difluoro and dichloro derivatives. Journal of Molecular Spectroscopy, 2007, 242, 17-24.	0.4	6
130	Spectroscopic and Computational Studies of the Intramolecular Hydrogen Bonding of 2-Indanol. Journal of Physical Chemistry A, 2006, 110, 12292-12297.	1.1	24
131	Conformational stability and normal coordinate analyses of imidoylketene $\text{OCCH}=\text{CHNH}$. Journal of Molecular Structure, 2006, 784, 259-264.	1.8	0
132	Theoretical vibrational spectra and analyses of isocyanatoketene $\text{O}=\text{C}=\text{N}=\text{C}=\text{O}$. Computational and Theoretical Chemistry, 2004, 676, 35-40.	1.5	1
133	DFT-B3LYP versus MP2, MP3 and MP4 calculations of the structural stability of azidoketene $\text{O}=\text{C}=\text{CH}=\text{N}=\text{N}$. Computational and Theoretical Chemistry, 2004, 712, 131-138.	1.5	5
134	Theoretical potential functions of halocarbonyl ketenes and halocarbonyl isocyanates and vibrational spectra of the bromides. Computational and Theoretical Chemistry, 2002, 582, 11-26.	1.5	7
135	Vibrational assignments and derived potential energy distributions for tri- and difluoromethyl ketene by density functional calculations. Journal of Molecular Modeling, 2001, 7, 343-353.	0.8	11
136	Density functional calculations of vibrational wavenumbers and derived potential energy distributions for fluoro- and chlorocarbonyl ketenes. Journal of Molecular Structure, 2001, 561, 103-119.	1.8	5
137	$\text{C}=\text{C}$ and $\text{C}=\text{N}$ rotational barriers in vinyl ketene and vinyl isocyanate. Computational and Theoretical Chemistry, 2001, 535, 183-197.	1.5	21
138	An investigation of structural stability and analysis of vibrational spectra of formyl ketene based on ab initio calculations. Computational and Theoretical Chemistry, 2000, 505, 19-30.	1.5	14