Abdulaziz A Al-Saadi

List of Publications by Year
in descending order

138 papers	3,984 citations	109264 35 h-index	149623 56 g-index
138 all docs	138 docs citations	138 times ranked	3659 citing authors

#	Article	IF	Citations
1	First Theoretical Framework of Triphenylamineâ€“Dicyanovinylene-Based Nonlinear Optical Dyes: Structural Modification of Ï€-Linkers. Journal of Physical Chemistry C, 2018, 122, 4009-4018.	1.5	193
2	Graphene Dendrimer-stabilized silver nanoparticles for detection of methimazole using Surface-enhanced Raman scattering with computational assignment. Scientific Reports, 2016, 6, 32185.	1.6	181
3	Photodegradation of Rhodamine B over unexcited semiconductor compounds of BiOCl and BiOBr. Journal of Colloid and Interface Science, 2012, 377, 291-298.	5.0	172
4	First theoretical probe for efficient enhancement of nonlinear optical properties of quinacridone based compounds through various modifications. Chemical Physics Letters, 2019, 715, 222-230.	1.2	125
5	Facile preparation of g-C3N4 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.	5.0	113
6	Carbonaceous adsorbent prepared from waste tires: Experimental and computational evaluations of organic dye methyl orange. Journal of Molecular Liquids, 2014, 191, 85-91.	2.3	108
7	Quantum chemical designing of indolo[3,2,1-jk]carbazole-based dyes for highly efficient nonlinear optical properties. Chemical Physics Letters, 2019, 719, 59-66.	1.2	108
8	Adsorption of lead ions from aqueous solution using porous carbon derived from rubber tires: Experimental and computational study. Journal of Colloid and Interface Science, 2013, 396, 264-269.	5.0	107
9	In Silico Modeling of New â€œY-Seriesâ€•Based Near-Infrared Sensitive Non-Fullerene Acceptors for Efficient Organic Solar Cells. ACS Omega, 2020, 5, 24125-24137.	1.6	103
10	Silver loaded graphene as a substrate for sensing 2-thiouracil using surface-enhanced Raman scattering. Sensors and Actuators B: Chemical, 2018, 254, 1110-1117.	4.0	100
11	Silver colloid and film substrates in surface-enhanced Raman scattering for 2-thiouracil detection. RSC Advances, 2016, 6, 75282-75292.	1.7	77
12	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.	2.0	67
13	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.	2.0	65
14	Silver nanoparticles for detection of methimazole by surface-enhanced Raman spectroscopy. Materials Research Bulletin, 2017, 91, 173-178.	2.7	65
15	Hydroxylamine reduced silver colloid for naphthalene and phenanthrene detection using surface-enhanced Raman spectroscopy. Chemical Engineering Journal, 2016, 304, 141-148.	6.6	60
16	Spectroscopic and computational evaluation of cadmium adsorption using activated carbon produced from rubber tires. Journal of Molecular Liquids, 2013, 188, 136-142.	2.3	59
17	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.	2.0	59
18	Silver-loaded graphene as an effective SERS substrate for clotrimazole detection: DFT and spectroscopic studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 201, 354-361.	2.0	59

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19	Surface characterization and sorption efficacy of tireâ€obtained carbon: experimental and semiempirical study of rhodamine B adsorption. Surface and Interface Analysis, 2015, 47, 785-792.	0.8	58
20	Characterization of valeric acid using substrate of silver nanoparticles with SERS. Journal of Molecular Liquids, 2019, 273, 536-542.	2.3	57
21	Impact of electron-withdrawing and electron-donating substituents on the corrosion inhibitive properties of benzimidazole derivatives: A quantum chemical study. Journal of Molecular Structure, 2019, 1196, 348-355.	1.8	55
22	Spectroscopic investigation (FTIR spectrum), NBO, HOMOâ€"LUMO energies, NLO and thermodynamic properties of 8-Methyl-N-vanillyl-6-nonenamideby DFT methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 146, 177-186.	2.0	52
23	Mechanistic studies of the influence of halogen substituents on the corrosion inhibitive efficiency of selected imidazole molecules: A synergistic computational and experimental approach. Applied Surface Science, 2019, 471, 494-505.	3.1	51
24	Synthesis of g-C3N4/BiOClxBr1â^'x hybrid photocatalysts and the photoactivity enhancement driven by visible light. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2014, 461, 202-211.	2.3	50
25	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. Journal of Molecular Structure, 2015, 1096, 1-14.	1.8	50
26	Spherical silver nanoparticles as substrates in surface-enhanced Raman spectroscopy for enhanced characterization of ketoconazole. Materials Science and Engineering C, 2017, 76, 356-364.	3.8	50
27	Conformational profile, vibrational assignments, NLO properties and molecular docking of biologically active herbicide1,1-dimethyl-3-phenylurea. Heliyon, 2019, 5, e01987.	1.4	46
28	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
29	Sensitive SERS detection and characterization of procaine in aqueous media by reduced gold nanoparticles. Sensors and Actuators B: Chemical, 2020, 304, 127057.	4.0	44
30	Theoretical investigations on the molecular structure, vibrational spectral, HOMOâ€"LUMO and NBO analysis of 9-[3-(Dimethylamino)propyl]-2-trifluoro-methyl-9H-thioxanthen-9-ol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 491-501.	2.0	42
31	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. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 151, 198-207.	2.0	41
32	Ultra-trace detection of methimazole by surface-enhanced Raman spectroscopy using gold substrate. Vibrational Spectroscopy, 2017, 90, 96-103.	1.2	40
33	Molecular conformational analysis, vibrational spectra, NBO, NLO, HOMOâ€"LUMO and molecular docking studies of ethyl 3-(E)-(anthracen-9-yl)prop-2-enoate based on density functional theory calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 533-542.	2.0	39
34	Structural properties, vibrational spectra and surface-enhanced Raman scattering of 2,4,6-trichloro- and tribromoanilines: A comparative study. Journal of Molecular Structure, 2016, 1121, 7-15.	1.8	38
35	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.	2.0	37
36	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.	2.0	36

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37	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.	2.0	36
38	Principal components analysis of Raman spectral data for screening of Hepatitis C infection. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 221, 117173.	2.0	36
39	Electrochemically modulated SERS detection of procaine using FTO electrodes modified with silver-decorated carbon nanosphere. Electrochimica Acta, 2021, 387, 138463.	2.6	33
40	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. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 131, 471-483.	2.0	32
41	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.	2.0	32
42	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.	2.0	30
43	Insights into endâ€capped modifications effect on the photovoltaic and optoelectronic properties of Sâ€shaped fullereneâ€free acceptor molecules: A density functional theory computational study for organic solar cells. Journal of Physical Organic Chemistry, 2022, 35, .	0.9	28
44	Molecular conformational analysis, vibrational spectra, NBO analysis and first hyperpolarizability of (2E)-3-phenylprop-2-enoic anhydride based on density functional theory calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 638-646.	2.0	27
45	Vibrational spectroscopic studies, normal co-ordinate analysis, first order hyperpolarizability, HOMOâ€“LUMO of midodrine by using density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 134, 127-142.	2.0	27
46	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.	2.0	26
47	A selective detection approach for copper(<scp>ii</scp>) ions using a hydrazone-based colorimetric sensor: spectroscopic and DFT study. RSC Advances, 2018, 8, 39983-39991.	1.7	26
48	Spectral characterization, thermochemical studies, periodic SAPT calculations and detailed quantum mechanical profiling various physico-chemical properties of 3,4-dichlorodiuron. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117580.	2.0	26
49	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. Journal of Organometallic Chemistry, 2017, 848, 175-183.	0.8	25
50	Spectroscopic and Computational Studies of the Intramolecular Hydrogen Bonding of 2-Indanol. Journal of Physical Chemistry A, 2006, 110, 12292-12297.	1.1	24
51	Spectroscopic, DFT and trace detection study of procaine using surface-enhanced Raman scattering technique. Chemical Physics Letters, 2019, 730, 617-622.	1.2	24
52	Structure, Vibrational Spectra, and DFT and ab Initio Calculations of Silacyclobutanes. Organometallics, 2008, 27, 3435-3443.	1.1	23
53	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[5.2.1.02,6]dec-8-ene-3,5-dione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 129, 438-450.	2.0	23
54	Theoretical Studies on the Mechanism of Iridium-Catalyzed Alkene Hydrogenation by the Cationic Complex [IrH₂(NCMe)₃(PⁱPr₃)]⁺. Organometallics, 2014, 33, 5156-5163.	1.1	23

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55	Fast and sensitive detection of Procainamide: Combined SERS and DFT modeling studies. Journal of Molecular Liquids, 2021, 343, 117633.	2.3	23
56	Surface-enhanced Raman scattering (SERS) spectroscopy for prostate cancer diagnosis: A review. Photodiagnosis and Photodynamic Therapy, 2022, 37, 102690.	1.3	23
57	FT-IR, molecular structure, first order hyperpolarizability, NBO analysis, HOMO and LUMO and MEP analysis of 1-(10H-phenothiazin-2-yl)ethanone by HF and density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 162-171.	2.0	22
58	Câ€“C and Câ€“N rotational barriers in vinyl ketene and vinyl isocyanate. Computational and Theoretical Chemistry, 2001, 535, 183-197.	1.5	21
59	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.	2.0	21
60	SERS-based trace-level quantification of sulindac: Spectroscopic and molecular modeling evaluation. Journal of Molecular Liquids, 2020, 312, 113402.	2.3	21
61	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.	1.8	20
62	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. Journal of Physics and Chemistry of Solids, 2015, 87, 110-121.	1.9	20
63	Conformational, NBO, NLO, HOMO-LUMO, NMR, electronic spectral study and molecular docking study of N,N-Dimethyl-3-(10H-phenothiazin-10-yl)-1-propanamine. Journal of Molecular Structure, 2016, 1122, 268-279.	1.8	19
64	Intramolecular Ï€-Type Hydrogen Bonding and Conformations of 3-Cyclopenten-1-ol. 2. Infrared and Raman Spectral Studies at High Temperatures. Journal of Physical Chemistry A, 2010, 114, 7457-7461.	1.1	17
65	Conformational analysis and vibrational assignments of benzohydroxamic acid and benzohydrazide. Journal of Molecular Structure, 2012, 1023, 115-122.	1.8	17
66	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMOâ€“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. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 139, 413-424.	2.0	17
67	Synthesis and characterization of functionalized polythiophene for polymer-sensitized solar cell. Dyes and Pigments, 2017, 141, 406-412.	2.0	17
68	Preparation and Characterization of Biomass Carbonâ€“Based Solid Acid Catalysts for the Esterification of Marine Algae for Biodiesel Production. Bioenergy Research, 2019, 12, 433-442.	2.2	17
69	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.	1.8	16
70	Synthesis, conformational, characterization and reactivity study of 1,7-bis(4-bromophenyl)heptane-1,7-dione. Journal of Molecular Structure, 2019, 1175, 269-279.	1.8	16
71	Intramolecular Ï€-Type Hydrogen Bonding and Conformations of 3-Cyclopenten-1-ol. 1. Theoretical Calculations. Journal of Physical Chemistry A, 2010, 114, 7453-7456.	1.1	15
72	BiOCl-assisted photodegradation of Rhodamine B under white light and monochromatic green pulsed laser irradiation. Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering, 2012, 47, 1192-1200.	0.9	15

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73	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.	2.0	15
74	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.	2.0	15
75	1-Alkyl-1-methylpiperazine-1,4-diium salts: Synthetic, acidâ€“base, XRD-analytical, FT-IR, FT-Raman spectral and quantum chemical study. Journal of Molecular Structure, 2015, 1094, 210-236.	1.8	15
76	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. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 138, 73-84.	2.0	15
77	Synthesis, X-ray structure and cytotoxicity evaluation of carbene-based gold(I) complexes of selenones. Inorganica Chimica Acta, 2018, 476, 46-53.	1.2	15
78	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
79	Vibrational Spectra, Ab Initio Calculations, and Ring-Puckering Potential Energy Function for Î³-Crotonolactone. Journal of Physical Chemistry A, 2007, 111, 3302-3305.	1.1	14
80	Iridium complexes as catalysts in the hydrogen transfer of isopropanol to acetophenone: Ligand effects and DFT studies. Inorganica Chimica Acta, 2015, 436, 146-151.	1.2	14
81	Molecular conformational analysis, vibrational spectra, NBO, NLO analysis and molecular docking study of bis[(E)-anthranyl-9-acrylic]anhydride based on density functional theory calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 151, 350-359.	2.0	14
82	Impact of Degree of Hydrophilicity of Pyridinium Bromide Derivatives on HCl Pickling of X-60 Mild Steel: Experimental and Theoretical Evaluations. Coatings, 2020, 10, 185.	1.2	14
83	Structural stability, NH2 inversion and vibrational assignments of 2,4,6-trichloroaniline and 2,3,5,6-tetrachloroaniline. Journal of Molecular Structure, 2009, 938, 41-47.	1.8	13
84	Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and LUMO		

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91	Structural, spectroscopic and docking properties of resorcinol, its -OD isotopomer and dianion derivative: a comparative study. Structural Chemistry, 2018, 29, 403-414.	1.0	11
92	A First-Principles Study on the Multilayer Graphene Nanosheets Anode Performance for Boron-Ion Battery. Nanomaterials, 2022, 12, 1280.	1.9	11
93	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. Vibrational Spectroscopy, 2012, 62, 188-199.	1.2	10
94	Intermolecular hydroamination versus stereoregular polymerization of phenylacetylene by rhodium catalysts based on Nâ€“O bidentate ligands. Inorganic Chemistry Communication, 2014, 40, 78-81.	1.8	9
95	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. Applied Sciences (Switzerland), 2015, 5, 955-972.	1.3	9
96	First principle calculations of the chemisorption of SO on doped carbon nanotubes and graphene. Chemical Physics Letters, 2015, 621, 65-70.	1.2	9
97	Vibrational spectroscopic studies and molecular docking of 10,10-Dimethylanthrone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 652-661.	2.0	9
98	Droplet flow-assisted heterogeneous electro-Fenton reactor for degradation of beta-blockers: response surface optimization, and mechanism elucidation. Environmental Science and Pollution Research, 2019, 26, 14313-14327.	2.7	9
99	Spectroscopic investigation (FT-IR, FT-Raman), HOMOâ€“LUMO, NBO analysis and molecular docking study of a potential chemotherapeutic agent. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 520-533.	2.0	8
100	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.	1.3	8
101	DFT evaluation of the effects of OH, NH₂ and Br substituents on the properties of 2,2â€²-bipyridine derivatives. Journal of Taibah University for Science, 2020, 14, 1527-1537.	1.1	8
102	Comparative Exposure Assessment of Potential Health Risks through the Consumption of Vegetables Irrigated by Freshwater/Wastewater: Gujranwala, Pakistan. Chemical Research in Toxicology, 2021, 34, 1417-1429.	1.7	8
103	NMR evidence for hydrogen bonding stabilized anti conformation of 1-methoxy-1-methyl-3-phenylurea and the concentration detection by SERS. Journal of Molecular Liquids, 2022, 357, 119096.	2.3	8
104	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
105	Spectroscopic and theoretical evaluation of the metal-olefin interaction in di-Î¼-chlorobis (1,5-cyclooctadiene) complexes of Ir and Rh. Vibrational Spectroscopy, 2016, 86, 109-123.	1.2	7
106	Selective colorimetric sensing of nickel (II) ions using 2-hydroxy-5-nitrobenzaldehyde-4-hydroxybenzoylhydrazone ligand: Spectroscopic and DFT insights. Journal of Molecular Liquids, 2018, 264, 58-65.	2.3	7
107	Nitrogen-Enhanced Charge Transfer Efficacy on the Carbon Sheet: A Theoretical Insight Into the Adsorption of Anionic Dyes. Arabian Journal for Science and Engineering, 2022, 47, 419-427.	1.7	7
108	SERS and EC-SERS detection of local anesthetic procaine using Pd loaded highly reduced graphene oxide nanocomposite substrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 278, 121381.	2.0	7

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109	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
110	Raman and infrared spectra, ab initio and DFT calculations, and vibrational assignments for 2,3-cyclopentenopyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 326-331.	2.0	6
111	Density functional theory study of the substituent effect on the structure, conformation and vibrational spectra in halosubstituted anilines. RSC Advances, 2016, 6, 67794-67804.	1.7	6
112	Dimethylphosphinate bridged binuclear Rh(i) catalysts for the alkoxycarbonylation of aromatic Câ€“H bonds. Dalton Transactions, 2016, 45, 16955-16965.	1.6	6
113	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
114	DFT-B3LYP versus MP2, MP3 and MP4 calculations of the structural stability of azidoketene O=C=CHâ€“NNN. Computational and Theoretical Chemistry, 2004, 712, 131-138.	1.5	5
115	Spectroscopic and DFT assessment of bridging ligand effect on the structural and electronic properties of dinuclear iridium- and rhodium-based complexes. Inorganica Chimica Acta, 2018, 482, 299-306.	1.2	5
116	Synthesis, spectroscopic characterization and in vitro cytotoxic as well as docking studies of cis-diammine platinum(II) complexes of thiones. Inorganica Chimica Acta, 2019, 484, 347-351.	1.2	5
117	Understanding the Influence of Electron-Donating and Electron-Withdrawing Substituents on the Anticorrosive Properties of Imidazole: A Quantum-Chemical Approach. Arabian Journal for Science and Engineering, 2020, 45, 153-166.	1.7	5
118	Conformational analysis and concentration detection of linuron: Spectroscopic NMR and SERS study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 263, 120223.	2.0	5
119	Evaluation of the inhibition performance of piperazine-based polyurea towards mild steel corrosion: The role of keto-enol tautomerization. Journal of Molecular Structure, 2022, 1248, 131485.	1.8	5
120	Spectroanalytical SERS-based detection of trace-level procainamide using green-synthesized gold nanoparticles. Surfaces and Interfaces, 2022, 31, 102059.	1.5	5
121	Structural stability and analysis of vibrational spectra of 1,2,4,5-tetroxane and 3,6-diphenyl-1,2,4,5-tetroxane. Journal of Molecular Structure, 2010, 969, 197-203.	1.8	4
122	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. Chromatographia, 2020, 83, 95-105.	0.7	4
123	Molecular docking, spectroscopic, and quantum chemical studies on aromatic heterocycle tetrakis(4-pyridyl)cyclobutane regioisomers: potential membrane-permeable inhibitors. Journal of Molecular Modeling, 2021, 27, 94.	0.8	4
124	Conformational profile and vibrational assignments of hippuric and 4-aminohippuric acids. Journal of Molecular Structure, 2011, 990, 176-182.	1.8	3
125	Spectroscopic (FT-IR, FT-Raman, UV, 1H and 13C NMR) profiling and theoretical calculations of (2E)-2-[3-(1H-imidazol-1-yl)-1-phenylpropylidene]hydrazinecarboxamide: An anticonvulsant agent. Journal of Molecular Structure, 2016, 1118, 219-232.	1.8	3
126	Structural and energetic effect of the intramolecular hydrogen bonding in 4,6-dihaloresorcinols: ab initio calculation, vibrational spectroscopy, and molecular docking studies. Structural Chemistry, 2022, 33, 57-69.	1.0	3

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127	UV-absorbing benzamide-based dendrimer precursors: synthesis, theoretical calculation, and spectroscopic characterization. New Journal of Chemistry, 2021, 46, 75-85.	1.4	3
128	Structural properties and vibrational spectra of 2-formyloxazole and its 2-thioformyl and 2-selenoformyl derivatives. Journal of Molecular Structure, 2011, 1006, 655-664.	1.8	2
129	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.	2.0	2
130	Computational study of SERS effects in some aliphatic and cyclic carboxylic acids with silver nanomaterials. Journal of Physics: Conference Series, 2020, 1564, 012008.	0.3	2
131	SERS-Based Ultralow Concentration Detection of Anticancer Gemcitabine Using Size-Controlled Silver Nanoparticles. Arabian Journal for Science and Engineering, 2022, 47, 7197-7205.	1.7	2
132	Theoretical vibrational spectra and analyses of isocyanatoketene Oĩ...Cĩ...CHâ€“Nĩ...Cĩ...O. Computational and Theoretical Chemistry, 2004, 676, 35-40.	1.5	1
133	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.	1.8	1
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