Hubert Joe Isaac

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

209 papers	5,227 citations	36 h-index	64 g-index
232 ext. papers	5,770 ext. citations	3 avg, IF	5.81 L-index

#	Paper	IF	Citations
209	Spectroscopic and quantum chemical computation on molecular structure, AIM, ELF, RDG, NCI, and NLO activity of 4-VINYL benzoic acid: A DFT approach. *Journal of Molecular Structure*, **2022**, 1253, 132273	3.4	1
208	Experimental and theoretical approach on third-order optical nonlinearity of a highly efficient anthracene-based chalcone derivative for optical power limiting. *Journal of Molecular Structure*, **2022**, 1250, 131704	3.4	0
207	Spectroscopic, quantum chemical and molecular docking studies on friedelin, the major triterpenoid isolated from Garcinia imberti. *Journal of Molecular Structure*, **2022**, 1263, 133152	3.4	1
206	Molecular docking, photocatalytic activity and biomedical investigations of some metal complexes. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 5600-5612	3.6	2
205	Spectroscopic, electron localization function, chemical reactivity and antihypertensive activity study on hordenine alkaloid by density functional theory approach. *Journal of Molecular Structure*, **2021**, 1229, 129823	3.4	
204	Emergence of fifth-order optical nonlinearity in 2-(2-Quinolyl)-1,3-indandione with strong third-order nonlinear effect under low power CW laser excitation. *Chemical Physics Letters*, **2021**, 769, 138434	2.5	1
203	Quantum chemical computation and spectroscopic investigation on antiviral drug Acyclovir:-In-silico and in-vitro analysis. *Journal of Molecular Structure*, **2021**, 1233, 130033	3.4	1
202	Ultrafast nonlinear optical properties of cyclohexenone carboxylate derivatives and their application as organic saturable absorbers. *Optics and Laser Technology*, **2021**, 139, 106902	4.2	2
201	NLOphoric imidazole-fused fluorescent anthraquinone dyes. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 246, 119017	4.4	2
200	Spectroscopic, quantum chemical, hydrogen bonding, reduced density gradient analysis and anti-inflammatory activity study on piper amide alkaloid piperine and wisanine. *Journal of Molecular Structure*, **2021**, 1225, 129146	3.4	5
199	Spectroscopic, charge transfer interaction and docking studies of gardona insecticide. *Journal of Molecular Structure*, **2021**, 1227, 129557	3.4	1
198	Positional isomers of heterocyclic azo dyes: Investigation of NLO properties by Z-scan and correlative DFT studies. *Journal of the Indian Chemical Society*, **2021**, 98, 100091		0
197	Third-order NLO studies of 2, 4-Bis (4-fluorophenyl)-2, 3-dihydro-1H-1, 5-benzodiazepine using Z-scan technique and DFT method. *Journal of Molecular Structure*, **2021**, 1246, 131169	3.4	0
196	A combined experimental and quantum chemical study on molecular structure, spectroscopic properties and biological activity of anti-inflammatory Glucocorticosteroid drug, Dexamethasone. *Journal of Molecular Structure*, **2021**, 1245, 130999	3.4	3
195	Self-focusing behaviour of dichlorobis(sarcosinato)zinc(II) complex investigated by DFT computations, fluorescence, laser damaged threshold and Z-scan technique. *Chemical Physics Letters*, **2020**, 754, 137648	2.5	1
194	Spectroscopic, quantum mechanical and docking studies on organochlorine insecticides by density functional theory. *Journal of Molecular Structure*, **2020**, 1208, 127904	3.4	6
193	Experimental and theoretical investigation of linear and nonlinear optical properties of ethyl-3-hydroxy-2-napthoate azo dyes by solvatochromic, computational aspects, and Z-scan technique. *Journal of Physical Organic Chemistry*, **2020**, 33, e4050	2.1	5

192	Red Emitting Hydroxybenzazole (HBX) Based Azo Dyes: Linear and Non Linear Optical Properties, Optical Limiting, Z Scan Analysis with DFT Assessments. *Journal of Fluorescence*, **2020**, 30, 335-346	2.4	4
191	Experimental and theoretical spectroscopic analysis, hydrogen bonding, reduced density gradient and antibacterial activity study on 2-Phenyl quinoline alkaloid. *Chemical Physics*, **2020**, 536, 110827	2.3	8
190	Structural analysis, NLO activity and Hirshfeld surfaces of DL-cysteinium semioxalate crystal. *Journal of Molecular Structure*, **2020**, 1216, 128278	3.4	4
189	Experimental and computational approach on p-toluenesulfonamide and its derivatives. *Journal of Molecular Structure*, **2020**, 1218, 128503	3.4	2
188	Spectroscopic, quantum chemical, QTAIM analysis, molecular dynamics simulation, docking studies and solvent effect of pyridin-2-yl oxyacetic acid herbicide and its derivatives. *Journal of Molecular Structure*, **2020**, 1206, 127677	3.4	6
187	Spectroscopic, DFT and Z-scan approach to study linear and nonlinear optical properties of Disperse Red 277. *Optical Materials*, **2020**, 99, 109536	3.3	7
186	Benzothiazole pyrazole containing emissive azo dyes decorated with ESIPT core: Linear and non linear optical properties, Z scan, optical limiting, laser damage threshold with comparative DFT studies. *Journal of Molecular Structure*, **2020**, 1203, 127401	3.4	22
185	Molecular structure, vibrational spectra and density functional theory of the spiro-conjugated anticancer active molecule rubrocurcumin. *Spectroscopy Letters*, **2020**, 53, 12-31	1.1	1
184	Z-scan and DFT approach for investigating the NLO properties of imidazole fused anthraquinone dyes. *Journal of Photochemistry and Photobiology A: Chemistry*, **2020**, 390, 112327	4.7	9
183	Structural, spectroscopic and O□H?O hydrogen bonding interaction on monomer and dimer form of hydroxy phenoxy acetic acid derivatives by experimental and computational techniques. *Journal of Molecular Structure*, **2020**, 1204, 127471	3.4	2
182	Spectroscopic and molecular structure investigation of Propachlor herbicide: A combined experimental and theoretical study. *Journal of Molecular Structure*, **2020**, 1221, 128866	3.4	0
181	Linear and NLO Properties of Functional Group and Position Isomers of Azo and Azomethine: Comparative Photophysical-Electrochemical Properties, Z-Scan and DFT Studies. *ChemistrySelect*, **2020**, 5, 10743-10753	1.8	3
180	Vibrational spectra, hydrogen bonding analysis and herbicidal activity study of mefenacet: A DFT approach. *Journal of Molecular Structure*, **2020**, 1201, 127203	3.4	4
179	Effect of solvents on the nonlinear optical behavior and spectral findings of bis [4-(dimethylamino) phenyl] methaniminium chloride. *Chemical Physics Letters*, **2020**, 738, 136833	2.5	4
178	Density functional theory, spectroscopic and hydrogen bonding analysis of fenoxycarb□water complexes. *Journal of Molecular Structure*, **2020**, 1201, 127201	3.4	6
177	NLO characteristics of D-□A coumarin-thiophene bridged azo dyes by Z-scan and DFT methods. *Molecular Physics*, **2020**, 118, e1662127	1.7	8
176	Third-order nonlinear optical studies of two novel chalcone derivatives using Z-scan technique and DFT method. *Optics and Laser Technology*, **2019**, 120, 105697	4.2	24
175	Influence of acceptors in NLOphoric aacenaphthene and morpholine-thiourea hybrid dyes: Photophysical, viscosity, DFT and Z-Scan study. *Optical Materials*, **2019**, 89, 178-190	3.3	5

174	Spectroscopic investigation and non linear optical activity study on 7,7,8,8-tetra cyano quino dimethane. *Chemical Data Collections*, **2019**, 21, 100220	2.1	1
173	Structural activity (monomer and dimer), spectroscopic analysis, chemical reactivity, fungicidal activity and molecular dynamics simulation of phenyl benzamide fungicides: A combined experimental and theoretical approach. *Journal of Molecular Structure*, **2019**, 1193, 24-44	3.4	6
172	Structural studies of 3-[(E)-[(2E)-2-methyl-3-phenylprop-2-en-1-ylidene] amino]-1-phenylthiourea: Combined experimental and computational studies. *Journal of Molecular Structure*, **2019**, 1191, 206-217	3.4	3
171	NLO-Phoric Emissive Quinoxaline Analog of Quinoline Yellow 54 and Z-Scan Studies. *ChemistrySelect*, **2019**, 4, 3752-3761	1.8	4
170	Pyrene Based NLOphoric D-π-A-π-D Coumarin-Chalcone and Their Red Emitting OBO Difluoride Complex: Synthesis, Solvatochromism, Z-scan, and Detailed TD-DFT Studies. *ChemistrySelect*, **2019**, 4, 10385-10400	1.8	4
169	Non-Linear Optical Properties of Disperse Blue 354 and Disperse Blue183 by DFT and Z-Scan Technique. *Polycyclic Aromatic Compounds*, **2019**, 1-18	1.3	3
168	NLO Properties of 2-Napthol Monoazo Disperse Dyes by DFT and Z-Scan Technique □A Detailed Study. *ChemistrySelect*, **2019**, 4, 13846-13855	1.8	1
167	Spectroscopic investigation, fungicidal activity and molecular dynamics simulation on benzimidazol-2-yl carbamate derivatives. *Journal of Molecular Structure*, **2019**, 1176, 226-237	3.4	11
166	Structural activity, fungicidal activity and molecular dynamics simulation of certain triphenyl methyl imidazole derivatives by experimental and computational spectroscopic techniques. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 212, 105-120	4.4	8
165	Viscosity induced emission of red-emitting NLOphoric coumarin morpholine-thiazole hybrid styryl dyes as FMRs: Consolidated experimental and theoretical approach. *Optical Materials*, **2018**, 79, 90-107	3.3	14
164	(2 E)-2-[1-(1,3-Benzodioxol-5-yl)-3-(1 H -imidazol-1-yl)propylidene]- N -(4-methoxyphenyl)hydrazinecarboxamide: Synthesis, crystal structure, vibrational analysis, DFT computations, molecular docking and antifungal activity. *Journal of Molecular Structure*, **2018**, 1166, 121-130	3.4	9
163	Influence of stereoelectronic effects on the non-opioid analgesics gaboxadol and gaboxadol hydrochloride: Spectral and DFT study. *Journal of Physics and Chemistry of Solids*, **2018**, 116, 194-202	3.9	3
162	In-silico analysis of substituent effect on the static first order hyperpolarizability of electron donating mono substituted Chalcone derivatives. *Journal of Molecular Modeling*, **2018**, 24, 126	2	1
161	Experimental and theoretical investigation of third-order nonlinear optical properties of azo dye 1-(2, 5-Dimethoxy-phenylazo)-naphthalen-2-ol by Z-scan technique and quantum chemical computations. *Dyes and Pigments*, **2018**, 157, 163-178	4.6	36
160	Investigation of structural, optical and electrical properties of ZnS thin films prepared by nebulized spray pyrolysis for solar cell applications. *Optical and Quantum Electronics*, **2018**, 50, 1	2.4	12
159	Synthesis, spectroscopic investigations, DFT studies, molecular docking and antimicrobial potential of certain new indole-isatin molecular hybrids: Experimental and theoretical approaches. *Journal of Molecular Structure*, **2018**, 1153, 333-345	3.4	33
158	Triphenylamine derived coumarin chalcones and their red emitting OBO difluoride complexes: Synthesis, photophysical and NLO property study. *Dyes and Pigments*, **2018**, 148, 474-491	4.6	35
157	Synthesis and electronic structure studies of a novel nonlinear optical crystal L-leucinium squarate monohydrate: A spectroscopic view. *Journal of Physics and Chemistry of Solids*, **2018**, 122, 143-153	3.9	6

156	Density functional theory calculations, vibration spectral analysis and molecular docking of the antimicrobial agent 6-(1,3-benzodioxol-5-ylmethyl)-5-ethyl-2-{[2-(morpholin-4-yl)ethyl] sulfanyl}pyrimidin-4(3H)-one. *Open Chemistry*, **2018**, 16, 653-666	1.6	4
155	Synthesis, Spectroscopic Identification and Molecular Docking of Certain -(2-{[2-(1-Indol-2-ylcarbonyl) Hydrazinyl](oxo)Acetylphenyl)Acetamides and -[2-(2-{[2-(Acetylamino)Phenyl](oxo)Acetylhydrazinyl)-2-Oxoethyl]-1-Indole-2-Carboxamides: New Antimicrobial Agents. *Molecules*, **2018**, 23.	4.8	3
154	Third-order optical nonlinearities of 1,5-Diaminoanthraquinone for optical limiting application. *Optics and Laser Technology*, **2018**, 108, 218-234	4.2	33
153	Excitation energy transfer processes in BODIPY based donor-acceptor system - Synthesis, photophysics, NLO and DFT study. *Optical Materials*, **2018**, 84, 795-806	3.3	14
152	Triphenylamine Derived 3-Acetyl and 3-Benzothiazolyl Bis and Tris Coumarins: Synthesis, Photophysical and DFT Assisted Hyperpolarizability Study. *Journal of Electronic Materials*, **2018**, 47, 1431-1446	1.9	2
151	Cu:ZnS and Al:ZnS thin films prepared on FTO substrate by nebulized spray pyrolysis technique. *Journal of Materials Science: Materials in Electronics*, **2018**, 29, 4612-4623	2.1	13
150	Synthesis, Hirshfeld surface analysis, laser damage threshold, third-order nonlinear optical property and DFT computation studies of Dichlorobis(DL-valine)zinc(II): A spectroscopic approach. *Optical Materials*, **2018**, 75, 285-296	3.3	15
149	Synthesis, crystal structure, vibrational profiling, DFT studies and molecular docking of N-(4-chloro-2-{[2-(1H-indol-2-ylcarbonyl) hydrazinyl](oxo)acetyl}phenyl)acetamide.DMSO: A new antiproliferative agent. *Journal of Molecular Structure*, **2018**, 1155, 457-468	3.4	8
148	Coherent source interaction, third-order nonlinear response of synthesized PEG coated magnetite nanoparticles in polyethylene glycol and its application. *Optics and Laser Technology*, **2018**, 98, 84-91	4.2	7
147	Experimental and theoretical spectroscopic analysis, chemical reactivity and fungicidal activity study on benalaxyl along with quantum chemical computation on metalaxyl and furalaxyl. *Chemical Data Collections*, **2018**, 17-18, 370-393	2.1	3
146	Enhancement of NLO Properties in OBO Fluorophores Derived from Carbazole–Coumarin Chalcones Containing Carboxylic Acid at the N-Alykl Terminal End. *Journal of Physical Chemistry C*, **2018**, 122, 14313-14325	3.8	31
145	Non-linear optical study of BODIPY-benzimidazole conjugate by solvatochromic, Z-scan and theoretical methods. *Optical Materials*, **2017**, 64, 453-460	3.3	29
144	Spectroscopic, DFT and Z-scan supported investigation of dicyanoisophorone based push-pull NLOphoric styryl dyes. *Optical Materials*, **2017**, 66, 494-511	3.3	33
143	Non-opioid analgesic drug flupirtine: Spectral analysis, DFT computations, in vitro bioactivity and molecular docking study. *Chemical Physics Letters*, **2017**, 677, 41-49	2.5	4
142	Bio-activity of superparamagnetic maghemite nanorods capped with dl-alanine. *Journal of Molecular Liquids*, **2017**, 234, 382-390	6	1
141	NLOphoric multichromophoric auxiliary methoxy aided triphenylamine D-π-A chromophores – Spectroscopic and computational studies. *Optical Materials*, **2017**, 73, 602-616	3.3	22
140	Synthesis, characterization, crystal structure and theoretical studies of 4-[(E)-(3-chloro-4-hydroxyphenyl) diazenyl]-1, 5-dimethyl-2-phenyl-1, 2-dihydro-3H-pyrazol-3-one. *Journal of Molecular Structure*, **2017**, 1148, 185-195	3.4	3
139	Structure activity relationship, vibrational spectral investigation and molecular docking analysis of anti-neuronal drug 4-(2-Aminoethyl) morpholine. *Journal of Molecular Structure*, **2017**, 1148, 459-470	3.4	4

138	Z-scan measurements of the third-order optical nonlinearities and vibrational spectral studies by DFT computations on azo dye 1-(2-Methylphenylazo)-2-napthol. *Optics and Laser Technology*, **2017**, 97, 390-399	4.2	19
137	NLO properties of 1, 4-naphthoquinone, Juglone and Lawsone by DFT and Z-scan technique □A detailed study. *Optical Materials*, **2017**, 72, 549-558	3.3	25
136	Molecular docking and structural analysis of non-opioid analgesic drug acemetacin with halogen substitution: A DFT approach. *Journal of Molecular Structure*, **2016**, 1123, 180-190	3.4	12
135	Biological applications and spectroscopic investigations of 4-nitrophenol-urea dimer: A DFT approach. *Chemical Physics Letters*, **2016**, 645, 59-70	2.5	10
134	Structure and Nonlinear Optical Properties Study of 2-Amino-5-Chlorobenzophenone: (A Spectroscopic Approach). *Oriental Journal of Chemistry*, **2016**, 32, 637-649	0.8	3
133	Spectroscopic Investigations, DFT Calculations, and Molecular Docking Studies of the Anticonvulsant (2E)-2-[3-(1H-Imidazol-1-yl)-1-phenylpropylidene]-N-(4-methylphenyl)hydrazinecarboxamide. *Journal of Spectroscopy*, **2016**, 2016, 1-10	1.5	4
132	Normal coordinate analysis and fungicidal activity study on anilazine and its related compound using spectroscopic techniques. *Chemical Physics Letters*, **2016**, 654, 125-134	2.5	4
131	Vibrational and electronic profiles, molecular docking and biological prediction of 5-methoxy-1-[(5-methoxy- 1H-indol-2-yl)methyl]-1H-indole: Experimental and theoretical investigations. *Journal of Theoretical and Computational Chemistry*, **2016**, 15, 1650046	1.8	
130	Spectral investigations, DFT computations and molecular docking studies of the antimicrobial 5-nitroisatin dimer. *Chemical Physics Letters*, **2015**, 624, 93-101	2.5	42
129	FT-IR and Raman spectroscopic and DFT studies of anti-cancer active molecule N-{(meta-ferrocenyl) Benzoyl} - l-alanine - glycine ethyl ester. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 145, 523-530	4.4	8
128	Synthesis and Characterization of PMMA Adherent ZnS thin Films by Spin Coating Method. *Materials Today: Proceedings*, **2015**, 2, 1046-1050	1.4	2
127	Natural Bond Orbital Analysis and DFT Calculation of Non-opiod Analgesic Drug Lidocaine. *Materials Today: Proceedings*, **2015**, 2, 969-972	1.4	1
126	Design, Synthesis and Vibrational Spectroscopic Studies of the Nonlinear Optical Crystal l-histidine Potassium Chloride. *Materials Today: Proceedings*, **2015**, 2, 987-991	1.4	
125	Quantum chemical computations, vibrational spectroscopic analysis and antimicrobial studies of 2,3-Pyrazinedicarboxylic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 138, 723-35	4.4	18
124	FT-IR and FT-Raman spectra, MEP and HOMO-LUMO of 2,5-dichlorobenzonitrile: DFT study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 136 Pt B, 464-72	4.4	17
123	Spectroscopic analysis and charge transfer interaction studies of 4-benzyloxy-2-nitroaniline insecticide: a density functional theoretical approach. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 135, 583-96	4.4	22
122	Synthesis and Characterization of Iron Oxide Nanoparticles using DMSO as a Stabilizer. *Materials Today: Proceedings*, **2015**, 2, 1051-1055	1.4	8
121	DFT and Vibrational Spectroscopic Study on 3-alkyl-4-amino-6-aryl-1, 2, 4-triazin-5-one Herbicide. *Materials Today: Proceedings*, **2015**, 2, 894-898	1.4	

120	Chemical Computations and Vibrational Spectral Studies of 2,3-Pyrazinedicarboxylic Acid. *Materials Today: Proceedings*, **2015**, 2, 977-981	1.4	1
119	Structure and nonlinear optical property analysis of L-Methioninium oxalate: a DFT approach. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 143, 40-8	4.4	9
118	FT-IR spectroscopy as a sentinel technology in earthworm toxicology. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 120, 534-41	4.4	5
117	FT-IR, FT-Raman spectra and other molecular properties of 2,4- dichlorobenzonitrile: a interpretation by a DFT study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 123, 89-97	4.4	7
116	Molecular structure, vibrational spectral investigation and the confirmation analysis of 4-Methylesculetin molecule. *Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)*, **2014**, 116, 348-359	0.7	5
115	Studies on molecular structure, vibrational spectra and molecular docking analysis of 3-Methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl 4-aminobenzoate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 130, 591-603	4.4	8
114	Twist Sensitivity of Cladding-Mode Resonances and Its Cross-Sensitivity to Strain and Temperature in a Mechanically Induced Long-Period Fiber Grating. *Fiber and Integrated Optics*, **2014**, 33, 347-359	0.8	4
113	Vibrational spectroscopic studies and DFT computation of the nonlinear optical molecule L-Valinium formate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 126, 170-7	4.4	13
112	Feasibility of using near infrared spectroscopy to detect and quantify an adulterant in high quality sandalwood oil. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 568-73	4.4	17
111	Vibrational spectral investigation and natural bond orbital analysis of pharmaceutical compound 7-Amino-2,4-dimethylquinolinium formate - DFT approach. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 595-602	4.4	44
110	The biomolecule of 5-bromocytosine: FT-IR and FT-Raman spectra and DFT calculations. Identification of the tautomers in the isolated state and simulation the spectra in the solid state. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 111, 104-22	4.4	12
109	FT-IR, FT-Raman, NMR spectra and DFT simulations of 4-(4-fluoro-phenyl)-1H-imidazole. *Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)*, **2013**, 114, 525-536	0.7	16
108	Molecular structure and vibrational spectral investigation of charge transfer NLO crystal naphthalene picrate for THz application. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 108, 256-67	4.4	16
107	Simulation of a tetramer form of 5-chlorouracil: the vibrational spectra and molecular structure in the isolated and in the solid state by using DFT calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 110, 404-18	4.4	12
106	Structural conformations and density functional study on the intramolecular charge transfer based on vibrational spectra of 2,4-dihydroxy-NS(4-methoxybenzylidene)benzohydrazide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 110, 157-68	4.4	6
105	DFT computation and experimental analysis of vibrational and electronic spectra of phenoxy acetic acid herbicides. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 108, 89-99	4.4	22
104	FT-IR, FT-Raman spectra and other molecular properties of 3,5-dichlorobenzonitrile: a DFT study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 116, 509-17	4.4	10
103	Vibrational spectral investigations and density functional theory study of 4-Formylbenzoic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 114, 502-8	4.4	6

102	Vibrational spectral analysis of anti-neurodegenerative drug Levodopa: A DFT study. *Journal of Molecular Structure*, **2013**, 1034, 119-127	3.4	19
101	FT-Raman, FT-IR and UV-visible spectral investigations and ab initio computations of anti-epileptic drug: vigabatrin. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 114, 633-41	4.4	2
100	Growth and vibrational spectral investigation of nonlinear optical crystal L-Argininum Perchlorate-DFT study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 109, 173-8	4.4	17
99	Normal coordinate analysis and Nonlinear Optical Response of cross-conjugated system 4,4-Dimethyl Benzophenone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 116, 574-83	4.4	12
98	Electronic absorption and vibrational spectra and nonlinear optical properties of L-valinium succinate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 85, 66-73	4.4	8
97	Analysis of vibrational spectra and nonlinear optical properties of organic molecule L-alaninium formate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 86, 174-80	4.4	12
96	Vibrational spectra and natural bond orbital analysis of organic crystal L-prolinium picrate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 96, 10-7	4.4	16
95	Spectroscopic investigation and hydrogen-bonding analysis of triazinones. *Journal of Molecular Modeling*, **2012**, 18, 3587-608	2	13
94	Vibrational spectra and density functional theoretical calculations on the anti-neurodegenerative drug: Orphenadrine hydrochloride. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 97, 838-46	4.4	6
93	Qualitative and quantitative analysis in sandalwood oils using near infrared spectroscopy combined with chemometric techniques. *Food Chemistry*, **2012**, 135, 213-218	8.5	18
92	Vibrational spectral investigation and Natural Bond Orbital analysis of anti-rheumatoid drug ethyl 4-nitrophenylacetate--DFT approach. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 98, 413-22	4.4	4
91	Intramolecular charge transfer and Z-scan studies of a semiorganic nonlinear optical material sodium acid phthalate hemihydrate: a vibrational spectroscopic study. *Journal of Physical Chemistry A*, **2011**, 115, 8216-26	2.8	52
90	The effect of electron charge transfer in biological activity and vibrational wavenumbers of 2?-Deoxyuridine and 5-Fluoro-2?-Deoxyuridine: DFT approach. *Solid State Sciences*, **2011**, 13, 1906-1915	3.4	3
89	Density functional theory studies on molecular structure and vibrational spectra of NLO crystal l-phenylalanine phenylalanium nitrate for THz application. *Journal of Molecular Structure*, **2011**, 1006, 513-526	3.4	23
88	Vibrational spectra and first order hyperpolarizability studies of dimethyl amino pyridinium 4-nitrophenolate 4-nitrophenol. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 81, 151-61	4.4	25
87	DFT-based molecular modeling, NBO analysis and vibrational spectroscopic study of 3-(bromoacetyl)coumarin. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 82, 118-25	4.4	45
86	Vibrational spectra and DFT study of anticancer active molecule 2-(4-Bromophenyl)-1H-benzimidazole by normal coordinate analysis. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 78, 319-26	4.4	43
85	Surface-enhanced Raman scattering and DFT theoretical studies on the adsorption behavior of plumbagin on silver nanoparticles. *Indian Journal of Physics*, **2011**, 85, 477-484	1.4	9

84	Vibrational spectra and structural studies of nonlinear optical crystal ammonium D, L-tartrate: a density functional theoretical approach. *Journal of Raman Spectroscopy*, **2011**, 42, 676-684	2.3	48
83	Structural and nonlinear optical properties of cross-conjugated system benzophenone thiosemicarbazone: a vibrational spectroscopic study. *Journal of Raman Spectroscopy*, **2011**, 42, 815-824	2.3	15
82	Electronic and structural effects on the nonlinear optical behavior in π-conjugated structure bis(4-nitrophenyl) carbonate: a vibrational spectroscopic approach. *Journal of Raman Spectroscopy*, **2011**, 42, 1193-1201	2.3	5
81	Charge transfer interaction and nonlinear optical properties of barium chloride and thiourea complexes: a vibrational spectroscopic study. *Journal of Raman Spectroscopy*, **2011**, 42, 1462-1469	2.3	14
80	Molecular structure, vibrational spectra and nonlinear optical properties of l-Valine Hydrobromide: DFT study. *Journal of Molecular Structure*, **2011**, 985, 48-56	3.4	29
79	Molecular structure and vibrational spectra of 2,6-bis(benzylidene)cyclohexanone: a density functional theoretical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 78, 113-21	4.4	35
78	Intramolecular charge delocalization and nonlinear optical properties of push-pull chromophore 1-(4-N,N-dimethylaminopyridinium) acetic acid bromide monohydrate from vibrational spectra. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 78, 264-72	4.4	11
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76	FT-IR, Raman and DFT study of 2-amino-5-fluorobenzoic acid and its biological activity with other halogen (Cl, Br) substitution. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 79, 332-7	4.4	23
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