Hubert Joe Isaac

List of Publications by Citations

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	Structural conformation and vibrational spectroscopic studies of 2,6-bis(p-N,N-dimethyl benzylidene)cyclohexanone using density functional theory. *Journal of Raman Spectroscopy*, **2006**, 37, 1381-1392	2.3	388
208	Structural and electronic contributions to hyperpolarizability in methyl p-hydroxy benzoate. *Journal of Molecular Structure*, **2006**, 785, 43-53	3.4	351
207	Charge transfer interactions and nonlinear optical properties of push–pull chromophore benzaldehyde phenylhydrazone: A vibrational approach. *Chemical Physics Letters*, **2008**, 460, 552-558	2.5	345
206	Spectroscopic analysis and DFT calculations of a food additive carmoisine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 72, 654-62	4.4	255
205	Density functional study on the structural conformations and intramolecular charge transfer from the vibrational spectra of the anticancer drug combretastatin-A2. *Journal of Raman Spectroscopy*, **2009**, 40, 419-428	2.3	208
204	NIR-FT Raman and infrared spectra and ab initio computations of glycinium oxalate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2004**, 60, 173-80	4.4	173
203	Efficient □-electrons delocalization in prospective push–pull non-linear optical chromophore 4-[N,N-dimethylamino]-4?-nitro stilbene (DANS): A vibrational spectroscopic study. *Chemical Physics* , **2008**, 343, 83-99	2.3	167
202	Efficient □-electron conjugated push–pull nonlinear optical chromophore 1-(4-methoxyphenyl)-3-(3,4-dimethoxyphenyl)-2-propen-1-one: A vibrational spectral study. *Journal of Molecular Structure*, **2009**, 917, 27-36	3.4	94
201	NIR-FT Raman, FT-IR and surface-enhanced Raman scattering spectra of organic nonlinear optic material: p-hydroxy acetophenone. *Journal of Raman Spectroscopy*, **2006**, 37, 508-519	2.3	90
200	Vibrational spectral studies of methyl 3-(4-methoxyphenyl)prop-2-enoate, a new organic non-linear optic crystal. *Journal of Raman Spectroscopy*, **2005**, 36, 221-236	2.3	75
199	Theoretical and vibrational spectral investigation of sodium salt of acenocoumarol. *Journal of Raman Spectroscopy*, **2009**, 40, 1033-1038	2.3	71
198	NIR-FT Raman and FT-IR spectral studies and ab initio calculations of the anti-cancer drug combretastatin-A4. *Journal of Raman Spectroscopy*, **2004**, 35, 939-946	2.3	70
197	Vibrational spectroscopic studies on the natural product, columbianadin. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2003**, 59, 193-9	4.4	70
196	Near-infrared Fourier transform Raman, surface-enhanced Raman scattering and Fourier transform infrared spectra and ab initio calculations of the natural product nodakenetin angelate. *Journal of Raman Spectroscopy*, **2005**, 36, 63-72	2.3	70
195	DFT computations and spectroscopic analysis of a pesticide: chlorothalonil. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2010**, 77, 36-44	4.4	54
194	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
193	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

192	Electronic absorption and vibrational spectra and nonlinear optical properties of 4-methoxy-2-nitroaniline. *Physical Chemistry Chemical Physics*, **2010**, 12, 9452-60	3.6	48
191	FT-Raman, IR and UV-visible spectral investigations and ab initio computations of a nonlinear food dye amaranth. *Journal of Raman Spectroscopy*, **2008**, 39, 928-936	2.3	48
190	Density functional theory calculations and vibrational spectral analysis of 3,5-(dinitrobenzoic acid). *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 78, 1437-44	4.4	47
189	Vibrational analysis and Y-aromaticity in bis (N,N?-diphenyl guanidinium) oxalate crystal: A DFT study. *Journal of Molecular Structure*, **2006**, 784, 32-46	3.4	47
188	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
187	NBO analysis and vibrational spectra of 2,6-bis(p-methyl benzylidene cyclohexanone) using density functional theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 74, 349-56	4.4	45
186	Vibrational contributions to the second-order nonlinear optical properties of □conjugated structure acetoacetanilide. *Chemical Physics*, **2010**, 369, 1-7	2.3	45
185	FTIR as a Tool to Study High-Temperature Phase Formation in Sol□el Aluminium Titanate. *Journal of Solid State Chemistry*, **1997**, 131, 181-184	3.3	45
184	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
183	FT-Raman and FTIR spectra, normal coordinate analysis and ab initio computations of (2-methylphenoxy)acetic acid dimer. *Vibrational Spectroscopy*, **2008**, 47, 10-20	2.1	44
182	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
181	Spectral investigations, DFT computations and molecular docking studies of the antimicrobial 5-nitroisatin dimer. *Chemical Physics Letters*, **2015**, 624, 93-101	2.5	42
180	Intramolecular charge transfer and hydrogen bonding interactions of nonlinear optical material N-benzoyl glycine: Vibrational spectral study. *Vibrational Spectroscopy*, **2010**, 54, 72-80	2.1	42
179	Electron□phonon coupling and vibrational modes contributing to linear electro-optic effect of the efficient NLO chromophore 4-(N,N-dimethylamino)-N-methyl-4?-toluene sulfonate (DAST) from their vibrational spectra. *Journal of Raman Spectroscopy*, **2009**, 40, 52-63	2.3	41
178	Infrared and Raman spectra, vibrational assignment, NBO analysis and DFT calculations of 6-aminoflavone. *Journal of Molecular Structure*, **2010**, 980, 24-30	3.4	41
177	NIR-FT Raman and FT-IR spectral investigations of the nonlinear optical chromophore p-bromoacetanilide. *Journal of Raman Spectroscopy*, **2007**, 38, 1148-1158	2.3	41
176	Vibrational spectra and density functional theoretical calculations on the antitumor drug, plumbagin. *Journal of Raman Spectroscopy*, **2005**, 36, 1001-1011	2.3	40
175	Vibrational spectra and ab initio molecular orbital calculations of the novel anti-cancer drug combretastatin A-4 prodrug. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 70, 1208-16	4.4	37

174	Molecular structure, spectroscopic studies and first-order molecular hyperpolarizabilities of p-amino acetanilide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 71, 355-67	4.4	37
173	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
172	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
171	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
170	Vibrational spectra and scaled quantum chemical studies of the structure of Martius yellow sodium salt monohydrate. *Journal of Raman Spectroscopy*, **2009**, 40, 1121-1126	2.3	34
169	Spectroscopic, DFT and Z-scan supported investigation of dicyanoisophorone based push-pull NLOphoric styryl dyes. *Optical Materials*, **2017**, 66, 494-511	3.3	33
168	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
167	Third-order optical nonlinearities of 1,5-Diaminoanthraquinone for optical limiting application. *Optics and Laser Technology*, **2018**, 108, 218-234	4.2	33
166	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
165	Changes in the vibrational spectral modes by the nonbonded interactions in the NLO crystal vanillin. *Journal of Raman Spectroscopy*, **2005**, 36, 1091-1100	2.3	30
164	Non-linear optical study of BODIPY-benzimidazole conjugate by solvatochromic, Z-scan and theoretical methods. *Optical Materials*, **2017**, 64, 453-460	3.3	29
163	Vibrational spectra and potential energy distributions for 1-benzyl-1H-imidazole by normal coordinate analysis. *Journal of Raman Spectroscopy*, **2009**, 40, 537-545	2.3	29
162	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
161	Non-bonded interactions and its contribution to the NLO activity of Glycine Sodium Nitrate – A vibrational approach. *Journal of Molecular Structure*, **2008**, 877, 20-35	3.4	28
160	Vibrational spectra and phase transition in triglycine sulpho-phosphate. *Crystal Research and Technology*, **1994**, 29, 685-692	1.3	28
159	NIR-FT Raman, FT-IR and surface-enhanced Raman scattering spectra, with theoretical simulations on chloramphenicol. *Journal of Raman Spectroscopy*, **2008**, 39, 1772-1783	2.3	27
158	Detection and quantification of adulteration in sandalwood oil through near infrared spectroscopy. *Analyst, The*, **2010**, 135, 2676-81	5	26
157	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

156	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
155	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
154	Vibrational spectral studies and the non-linear optical properties of a novel NLO material L-prolinium tartrate. *Journal of Raman Spectroscopy*, **2006**, 37, 1427-1441	2.3	24
153	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
152	Charge transfer interaction and terahertz studies of a nonlinear optical material L-glutamine picrate: A DFT study. *Journal of Physical Chemistry A*, **2010**, 114, 13055-64	2.8	23
151	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
150	Vibrational spectra and normal coordinate analysis of plant growth regulator 1-naphthalene acetamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2010**, 75, 859-66	4.4	23
149	NLOphoric multichromophoric auxiliary methoxy aided triphenylamine D-A chromophores Spectroscopic and computational studies. *Optical Materials*, **2017**, 73, 602-616	3.3	22
148	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
147	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
146	Density functional theory calculation and vibrational spectral analysis of 4-hydroxy-3-(3-oxo-1-phenylbutyl)-2H-1-benzopyran-2-one. *Journal of Raman Spectroscopy*, **2010**, 41, 1076-1084	2.3	22
145	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
144	Natural bond orbital analysis and vibrational spectroscopic studies of H-bonded N,N?-diphenylguanidinium nitrate. *Journal of Molecular Structure*, **2007**, 830, 156-166	3.4	21
143	Quantum chemical computations and Fourier transform infrared spectral studies of a nonlinear food dye E110. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 69, 82-90	4.4	20
142	Vibrational spectral analysis of anti-neurodegenerative drug Levodopa: A DFT study. *Journal of Molecular Structure*, **2013**, 1034, 119-127	3.4	19
141	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
140	Raman and IR spectra of alanine and sarcosine monophosphates. *Journal of Raman Spectroscopy*, **1991**, 22, 423-425	2.3	19
139	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

138	Qualitative and quantitative analysis in sandalwood oils using near infrared spectroscopy combined with chemometric techniques. *Food Chemistry*, **2012**, 135, 213-218	8.5	18
137	Spectroscopic investigations and ab initio computations of the dye Chromotrope 2R. *Solid State Sciences*, **2009**, 11, 1275-1282	3.4	18
136	NIR-FT Raman, FT-IR and surface-enhanced Raman scattering and DFT based theoretical studies on the adsorption behaviour of (S)-phenylsuccinic acid on silver nanoparticles. *Journal of Chemical Sciences*, **2010**, 122, 511-519	1.8	18
135	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
134	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
133	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
132	Nonplanar property study of antifungal agent tolnaftate-spectroscopic approach. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 79, 993-1003	4.4	17
131	Vibrational spectra and first-order molecular hyperpolarizabilities of p-hydroxybenzaldehyde dimer. *Journal of Molecular Structure*, **2010**, 983, 12-21	3.4	17
130	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
129	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
128	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
127	Vibrational spectral studies on charge transfer and ionic hydrogen-bonding interactions of nonlinear optical material L-arginine nitrate hemihydrate. *Journal of Raman Spectroscopy*, **2009**, 40, 18-30	2.3	16
126	Azure A chloride: computational and spectroscopic study. *Journal of Raman Spectroscopy*, **2009**, 40, 176-182	2.3	16
125	DFT based relaxed PES scan studies and SERS of anti cancer drug, Combretastatin A-4. *Laser Physics Letters*, **2005**, 2, 544-550	1.5	16
124	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
123	Analysis of vibrational spectra of L-alanylglycine based on density functional theory calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 71, 252-62	4.4	15
122	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
121	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

120	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
119	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
118	First order molecular hyperpolarizabilities and intramolecular charge transfer from the vibrational spectra of NLO material: ethyl-3-(3, 4-dihydroxyphenyl)-2-propenoate. *Journal of Raman Spectroscopy*, **2009**, 40, 1822-1830	2.3	14
117	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
116	Spectroscopic investigation and hydrogen-bonding analysis of triazinones. *Journal of Molecular Modeling*, **2012**, 18, 3587-608	2	13
115	Vibrational spectra of CaNa2P2O7 4H2O, CaNH4NaP2O7 3H2O and CdNH4NaP2O7 3H2O. *Journal of Raman Spectroscopy*, **1991**, 22, 537-539	2.3	13
114	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
113	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
112	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
111	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
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	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
108	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
107	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
106	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
105	Biological applications and spectroscopic investigations of 4-nitrophenol-urea dimer: A DFT approach. *Chemical Physics Letters*, **2016**, 645, 59-70	2.5	10
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	Influence of intermolecular amide hydrogen bonding on the geometry, atomic charges, and spectral modes of acetanilide: An ab initio study. *Laser Physics*, **2006**, 16, 1253-1263	1.2	10

102	(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
101	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
100	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
99	Structural conformations and electronic interactions of the natural product, oroxylin: a vibrational spectroscopic study. *Journal of Raman Spectroscopy*, **2008**, 39, 1821-1831	2.3	9
98	Vibrational Spectra and Density functional calculation of Organic Nonlinear Optic Crystal p-Amino Acetanilide. *Journal of Physics: Conference Series*, **2006**, 28, 123-126	0.3	9
97	Vibrational spectra and ab initio computations of sarcosinium oxalate monohydrate. *Laser Physics*, **2006**, 16, 1242-1252	1.2	9
96	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
95	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
94	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
93	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
92	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
91	Synthesis and Characterization of Iron Oxide Nanoparticles using DMSO as a Stabilizer. *Materials Today: Proceedings*, **2015**, 2, 1051-1055	1.4	8
90	Molecular structure, vibrational spectra and first-order molecular hyperpolarizabilities of potential anti-cancer drug, combretastatin-A1. *Journal of Molecular Structure*, **2008**, 889, 129-143	3.4	8
89	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
88	NLO characteristics of D-π-A coumarin-thiophene bridged azo dyes by Z-scan and DFT methods. *Molecular Physics*, **2020**, 118, e1662127	1.7	8
87	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
86	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
85	Molecular first order hyperpolarizability and vibrational spectral investigation of Warfarin sodium. *Chemical Physics*, **2010**, 378, 88-102	2.3	7

84	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
83	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
82	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
81	Spectroscopic, quantum mechanical and docking studies on organochlorine insecticides by density functional theory. *Journal of Molecular Structure*, **2020**, 1208, 127904	3.4	6
80	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
79	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
78	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
77	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
76	Vibrational Spectra of □Aminobutyric Acid **2008**,		6
75	Vibrational spectra of tris(methylammonium) cyclotriphosphate. *Journal of Raman Spectroscopy*, **1992**, 23, 417-419	2.3	6
74	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
73	Density functional theory, spectroscopic and hydrogen bonding analysis of fenoxycarb□water complexes. *Journal of Molecular Structure*, **2020**, 1201, 127201	3.4	6
72	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
71	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
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