Velu Arjunan

List of Publications by Year in Descending Order

92 papers	1,393 citations	21 h-index	32 g-index
93 ext. papers	1,491 ext. citations	3.7 avg, IF	4.6 L-index

#	Paper	IF	Citations
92	Structure, conformations, vibrations and quantum chemical investigations of 2-(1H-Indol-3-yl)-2-oxoacetic acid. *Journal of Molecular Structure*, **2022**, 1256, 132570	3.4	0
91	FT-IR, FT-Raman, NMR Spectroscopic and DFT Quantum Chemical Investigations of 6-Methylcoumarin. *Asian Journal of Chemistry*, **2021**, 33, 2715-2722	0.4	
90	Energy profile, structure, spectroscopic and quantum chemical investigations of trans-3,4-(methylenedioxy)cinnamic acid. *Chemical Data Collections*, **2021**, 31, 100644	2.1	1
89	An insight into the structure and vibrations of 4-nitroindole and 7-nitroindole by spectroscopic and DFT methods. *Journal of Molecular Structure*, **2021**, 1238, 130420	3.4	0
88	An experimental and theoretical investigation on the structure, vibrations and reactivity properties of pharmacologically active compounds 3-acetylindole and indole-3-acetamide. *Journal of Molecular Structure*, **2020**, 1210, 128012	3.4	3
87	Conformations, structure, vibrations, chemical shift and reactivity properties of isoquinoline-1-carboxylic acid and isoquinoline-3-carboxylic acid - Comparative investigations by experimental and theoretical techniques. *Journal of Molecular Structure*, **2020**, 1207, 127841	3.4	1
86	Structure, Vibrations, Molecular Orbitals, Reactivity Properties of 3-Trifluoromethylphenylchloroformate by FT-IR, FT-Raman, FT-NMR and DFT Studies. *Asian Journal of Chemistry*, **2019**, 31, 1737-1747	0.4	1
85	Conformational analysis, spectroscopic, structure-activity relations and quantum chemical simulation studies of 4-(trifluoromethyl)benzylamine. *Journal of Molecular Structure*, **2018**, 1159, 103-117	3.4	2
84	Structure, electronic, spectroscopic and reactivity investigations of pharmacologically active compound 1-acetyl-3-indolecarboxaldehyde - An experimental and theoretical approach. *Journal of Molecular Structure*, **2018**, 1164, 57-69	3.4	5
83	Energy profile analysis, spectroscopic investigations (FT-IR, FT-Raman and FT-NMR), electronic properties, structure-activity aspects and DFT studies of (1,3-benzodioxol-5-yl)acetic acid. *Chemical Data Collections*, **2018**, 17-18, 75-94	2.1	4
82	Experimental, quantum chemical, natural bond orbitals and reactivity investigations of 4-hydroxy-6-(trifluoromethyl)pyrimidine. *Chemical Data Collections*, **2018**, 17-18, 143-158	2.1	3
81	Energy profile, spectroscopic (FT-IR, FT-Raman and FT-NMR) and DFT studies of 4-bromoisophthalic acid. *Journal of Molecular Structure*, **2018**, 1157, 132-148	3.4	6
80	Conformational Analysis, Structural and Vibrational Investigations of trans-2-Chlorocinnamic Acid and trans-4-Chlorocinnamic Acid. *Springer Proceedings in Physics*, **2017**, 563-598	0.2	
79	Crystal structure, vibrational spectra and DFT studies of hydrogen bonded 1,2,4-triazolium hydrogenselenate. *Journal of Molecular Structure*, **2017**, 1145, 211-221	3.4	4
78	An insight into the structure, vibrations, electronic and reactivity properties of the tautomers 1-(diaminomethylene)thiourea and 2-imino-4-thiobiuret. *Journal of Molecular Structure*, **2017**, 1133, 187-198	3.4	9
77	Structure, vibrations and quantum chemical investigations of hydrogen bonded complex of bis(1-hydroxy-2-methylpropan-2-aminium)selenate. *Journal of Molecular Structure*, **2017**, 1134, 6-16	3.4	7
76	Simulations on the structure, vibrations and electronic properties of 1,2-epoxy-3-phenoxy propane and 1,2-epoxy-3-(p-tolyloxy)propane by FT-IR, FT-Raman, FT-NMR and DFT methods. *Chemical Data Collections*, **2017**, 11-12, 139-167	2.1	1

75	Characterisation of 1,3-diammonium propylselenate monohydrate by XRD, FT-IR, FT-Raman, DSC and DFT studies. *Journal of Molecular Structure*, **2016**, 1107, 220-230	3.4	9
74	Potential energy profile, structural, vibrational and reactivity descriptors of trans-2-methoxycinnamic acid by FTIR, FT-Raman and quantum chemical studies. *Journal of Molecular Structure*, **2016**, 1113, 42-54	3.4	14
73	Substituent influence on the structural, vibrational and electronic properties of 2,5-dihydrothiophene-1,1-dioxide by experimental and DFT methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 150, 641-51	4.4	5
72	Structure activity studies of an analgesic drug tapentadol hydrochloride by spectroscopic and quantum chemical methods. *Journal of Molecular Structure*, **2015**, 1100, 188-202	3.4	1
71	Comprehensive quantum chemical and spectroscopic (FTIR, FT-Raman, (1)H, (13)C NMR) investigations of (1,2-epoxyethyl)benzene and (1,2-epoxy-2-phenyl)propane. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 135, 120-36	4.4	11
70	Structural and vibrational spectral investigations of melaminium glutarate monohydrate by FTIR, FT-Raman and DFT methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 135, 540-50	4.4	12
69	Conformational, structural, vibrational, electronic and quantum chemical investigations of cis-2-methoxycinnamic acid. *Journal of Molecular Structure*, **2015**, 1080, 122-136	3.4	6
68	DFT simulation, quantum chemical electronic structure, spectroscopic and structure-activity investigations of 2-benzothiazole acetonitrile. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 128, 22-36	4.4	9
67	Exploring the structure-activity relations of N-carbethoxyphthalimide by combining FTIR, FT-Raman and NMR spectroscopy with DFT electronic structure method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 120, 473-88	4.4	18
66	Comprehensive quantum chemical and spectroscopic (FTIR, FT-Raman, 1H, 13C NMR) investigations of O-desmethyltramadol hydrochloride an active metabolite in tramadol--an analgesic drug. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 122, 315-30	4.4	7
65	Structure-activity relations of 2-(methylthio)benzimidazole by FTIR, FT-Raman, NMR, DFT and conceptual DFT methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 118, 951-65	4.4	22
64	A new look into the quantum chemical and spectroscopic investigations of 5-chloro-1-methyl-4-nitroimidazole. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 125, 160-74	4.4	4
63	Synthesis, vibrational, NMR, quantum chemical and structure-activity relation studies of 2-hydroxy-4-methoxyacetophenone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 130, 164-77	4.4	55
62	Spectroscopic and structural investigations of 4-bromomethyl-5-methyl-1,3-dioxol-2-one and 4,5-bis(bromomethyl)-1,3-dioxol-2-one by quantum chemical simulations - A comparative study. *Journal of Molecular Structure*, **2014**, 1056-1057, 38-51	3.4	5
61	Spectroscopic and density functional theory studies of trans-3-(trans-4-imidazolyl)acrylic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 129, 466-77	4.4	5
60	Synthesis, FTIR and FT-Raman spectral analysis and structure-activity relations of N-(4-bromophenyl)-2,2-dichloroacetamide by DFT studies. *Journal of Molecular Structure*, **2014**, 1064, 15-26	3.4	6
59	Vibrational, NMR and quantum chemical investigations of acetoacetanilde, 2-chloroacetoacetanilide and 2-methylacetoacetanilide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 154-74	4.4	21
58	Primidone--an antiepileptic drug--characterisation by quantum chemical and spectroscopic (FTIR, FT-Raman, 1H, 13C NMR and UV-Visible) investigations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 109, 282-97	4.4	3

57	Structural and vibrational spectral investigations of melaminium maleate monohydrate by FTIR, FT-Raman and quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 107, 90-101	4.4	15
56	Electronic structure simulations of 2,6-dimethyl-2,5-heptadien-4-one by FTIR, FT-Raman, NMR, UV□is, NBO and density functional theory. *Molecular Simulation*, **2013**, 39, 185-198	2	1
55	Conformational analysis, spectroscopic and quantum chemical investigations of 2-bromo-3-nitroacetophenone. *Journal of Molecular Structure*, **2013**, 1037, 73-84	3.4	6
54	Structural, vibrational, electronic investigations and quantum chemical studies of 2-amino-4-methoxybenzothiazole. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 102, 327-40	4.4	8
53	Crystal structure, vibrational and DFT simulation studies of melaminium dihydrogen phosphite monohydrate. *Journal of Molecular Structure*, **2013**, 1045, 160-170	3.4	21
52	Structural, vibrational and nuclear magnetic resonance investigations of 4-bromoisoquinoline by experimental and theoretical DFT methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 107, 62-71	4.4	10
51	Conformational, structural, vibrational and quantum chemical analysis on 4-aminobenzohydrazide and 4-hydroxybenzohydrazide--a comparative study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 108, 100-14	4.4	8
50	A new look into conformational, vibrational and electronic structure analysis of 3,4-dimethoxybenzonitrile. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 113, 302-13	4.4	4
49	Conformational, vibrational, NMR and DFT studies of N-methylacetanilide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 104, 182-96	4.4	15
48	Vibrational, electronic and quantum chemical studies of 5-benzimidazole carboxylic acid. *Journal of Molecular Structure*, **2013**, 1036, 326-340	3.4	18
47	Vibrational, electronic and quantum chemical studies of 1,2,4-benzenetricarboxylic-1,2-anhydride. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 110, 141-50	4.4	15
46	FTIR, FT-Raman, FT-NMR and quantum chemical investigations of 3-acetylcoumarin. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 109, 79-89	4.4	26
45	Synthesis and characterization of an anticoagulant 4-hydroxy-1-thiocoumarin by FTIR, FT-Raman, NMR, DFT, NBO and HOMO□UMO analysis. *Journal of Molecular Structure*, **2013**, 1037, 305-316	3.4	30
44	Experimental, quantum chemical and natural bond orbital investigations of N-(2,4-dimethylphenyl)-2,2-dichloroacetamide and N-(3,5-dimethylphenyl)-2,2-dichloroacetamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 88, 192-209	4.4	5
43	FTIR, FT-Raman, FT-NMR, UV-visible and quantum chemical investigations of 2-amino-4-methylbenzothiazole. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 88, 220-31	4.4	31
42	Vibrational, conformational and electronic structure investigations of □dibromo-o-xylene, □dibromo-m-xylene and □dibromo-p-xylene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 91, 166-77	4.4	4
41	A comparative study on vibrational, conformational and electronic structure of □diol-o-xylene, □diol-m-xylene and □diol-p-xylene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 92, 1-15	4.4	0
40	A comparative study on vibrational, conformational and electronic structure of 2-chloro-4-methyl-3-nitropyridine and 2-chloro-6-methylpyridine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 92, 305-17	4.4	8

39	Structural characteristics and harmonic vibrational analysis of the stable conformer of 2,3-epoxypropanol by quantum chemical methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 96, 24-34	4.4	5
38	Experimental and theoretical quantum chemical investigations of 8-hydroxy-5-nitroquinoline. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 96, 506-16	4.4	28
37	A comparative spectroscopic, electronic structure and chemical shift investigations of o-Chloronitrobenzene, p-Chloronitrobenzene and m-Chloronitrobenzene. *Journal of Molecular Structure*, **2012**, 1007, 122-135	3.4	9
36	Combined spectroscopic and DFT studies on 2-chloro-4-nitrotoluene and 4-chloro-2-nitrotoluene. *Journal of Molecular Structure*, **2012**, 1016, 82-96	3.4	5
35	A comparative study on vibrational, conformational and electronic structure of 1,2-dimethyl-5-nitroimidazole and 2-methyl-5-nitroimidazole. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 97, 176-88	4.4	11
34	X-ray diffraction, vibrational and quantum chemical investigations of 2-methyl-4-nitroanilinium trichloroacetate trichloroacetic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 97, 625-38	4.4	14
33	Synthesis, vibrational and quantum chemical investigations of hydrogen bonded complex betaine dihydrogen selenite. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 96, 744-58	4.4	17
32	A comparative study on vibrational, conformational and electronic structure of 2-(hydroxymethyl)pyridine and 3-(hydroxymethyl)pyridine. *Journal of Molecular Structure*, **2012**, 1018, 156-170	3.4	17
31	Electronic structure investigations of 4-methyl-3-penten-2-one by UV–Visible and NMR spectral studies and natural bond orbital analysis by DFT calculations. *Journal of Molecular Structure*, **2012**, 1022, 37-48	3.4	4
30	FTIR, FT-Raman and quantum chemical investigations of 4,5-dimethyl-1,3-dioxol-2-one. *Journal of Molecular Structure*, **2012**, 1024, 54-64	3.4	4
29	Quantum chemical studies and vibrational analysis of 4-acetyl benzonitrile, 4-formyl benzonitrile and 4-hydroxy benzonitrile--a comparative study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 98, 156-69	4.4	14
28	Experimental spectroscopic (FTIR, FT-Raman, FT-NMR, UV–Visible) and DFT studies of 2-amino-5-chlorobenzoxazole. *Journal of Molecular Structure*, **2011**, 1003, 92-102	3.4	15
27	Vibrational, nuclear magnetic resonance and electronic spectra, quantum chemical investigations of 2-amino-6-fluorobenzothiazole. *Journal of Molecular Structure*, **2011**, 1006, 247-258	3.4	21
26	Vibrational spectroscopic, electronic and quantum chemical investigations on 2,3-hexadiene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 81, 620-30	4.4	18
25	Vibrational and electronic investigations, thermodynamic parameters, HOMO and LUMO analysis on crotonaldehyde by ab initio and DFT methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 83, 411-9	4.4	31
24	Spectroscopic, electronic structure and natural bond orbital analysis of o-fluoronitrobenzene and p-fluoronitrobenzene: a comparative study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 84, 196-209	4.4	16
23	Spectroscopic and quantum chemical electronic structure investigations of 2-(trifluoromethyl)aniline and 3-(trifluoromethyl)aniline. *Journal of Molecular Structure*, **2011**, 994, 179-193	3.4	18
22	Density functional theory studies on vibrational and electronic spectra of 2-chloro-6-methoxypyridine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 78, 1625-32	4.4	21

21	Experimental and theoretical investigations of benzamide oxime. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 79, 245-53	4.4	22
20	FTIR, FT-Raman, FT-NMR, ab initio and DFT electronic structure investigation on 8-chloroquinoline and 8-nitroquinoline. *Journal of Molecular Structure*, **2011**, 988, 91-101	3.4	63
19	DFT and ab initio quantum chemical studies on p-cyanobenzoic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 78, 1449-54	4.4	9
18	Synthesis, FTIR, FT-Raman, UV-visible, ab initio and DFT studies on benzohydrazide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 79, 486-96	4.4	37
17	Spectroscopic and quantum chemical studies on 4-acryloyl morpholine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 79, 1386-94	4.4	3
16	A combined experimental and theoretical quantum chemical studies on 4-morpholinecarboxaldehyde. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 79, 1395-401	4.4	3
15	Structural, vibrational and quantum chemical investigations on 5-chloro-2-hydroxybenzamide and 5-chloro-2-hydroxybenzoic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 79, 1886-95	4.4	12
14	Synthesis, FT-IR, FT-Raman and quantum chemical investigations of N-(3-methylphenyl)-2,2-dichloroacetamide. *European Journal of Chemistry*, **2011**, 2, 70-76	0.6	12
13	FTIR, FT-Raman, ab initio and density functional studies on 4-methyl-1,3-dioxolan-2-one and 4,5-dichloro-1,3-dioxolan-2-one. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2010**, 77, 28-35	4.4	9
12	Fourier transform infrared and FT-Raman spectra, assignment, ab initio, DFT and normal co-ordinate analysis of 2-chloro-4-methylaniline and 2-chloro-6-methylaniline. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 72, 436-44	4.4	91
11	Vibrational spectroscopic investigations, ab initio and DFT studies on 7-bromo-5-chloro-8-hydroxyquinoline. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 72, 783-8	4.4	25
10	Ab initio, density functional theory and structural studies of 4-amino-2-methylquinoline. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 74, 375-84	4.4	27
9	Synthesis, structural, vibrational and quantum chemical investigations of N-(2-methylphenyl)-2,2-dichloroacetamide and N-(4-methylphenyl)-2,2-dichloroacetamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 74, 607-16	4.4	14
8	Structural, vibrational and DFT studies on 2-chloro-1H-isoindole-1,3(2H)-dione and 2-methyl-1H-isoindole-1,3(2H)-dione. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 74, 642-9	4.4	39
7	Investigation of the structural and harmonic vibrational properties of 2-nitro-, 4-nitro- and 5-nitro-m-xylene by ab initio and density functional theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 74, 798-807	4.4	22
6	Quantum chemical and spectroscopic investigations of 5-aminoquinoline. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 74, 1215-23	4.4	19
5	Fourier transform infrared and FT-Raman spectral analysis and ab initio calculations for 4-chloro-2-methylaniline and 4-chloro-3-methylaniline. *Journal of Molecular Structure*, **2008**, 892, 289-299	3.4	65
4	Fourier transform infrared and Raman spectral assignments and analysis of 7-amino-4-trifluoromethylcoumarin. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2007**, 67, 1290-6	4.4	11

3	Fourier transform infrared and Raman spectral investigations of 5-aminoindole. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2006**, 64, 233-9	4.4	52
2	FTIR and FTR spectral studies of 2-amino-6-bromo-3-formylchromone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2004**, 60, 995-1000	4.4	36
1	Synthesis, Fourier transform infrared and Raman spectra, assignments and analysis of N-(phenyl)- and N-(chloro substituted phenyl)-2,2-dichloroacetamides. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2004**, 60, 1141-59	4.4	69