

Velu Arjunan

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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	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 72, 436-44	4.4	91
91	Synthesis, Fourier transform infrared and Raman spectra, assignments and analysis of N-(phenyl)- and N-(chloro substituted phenyl)-2,2-dichloroacetamides. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2004 , 60, 1141-59	4.4	69
90	Fourier transform infrared and FT-Raman spectral analysis and ab initio calculations for 4-chloro-2-methylaniline and 4-chloro-3-methylaniline. <i>Journal of Molecular Structure</i> , 2008 , 892, 289-299	3.4	65
89	FTIR, FT-Raman, FT-NMR, ab initio and DFT electronic structure investigation on 8-chloroquinoline and 8-nitroquinoline. <i>Journal of Molecular Structure</i> , 2011 , 988, 91-101	3.4	63
88	Synthesis, vibrational, NMR, quantum chemical and structure-activity relation studies of 2-hydroxy-4-methoxyacetophenone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 130, 164-77	4.4	55
87	Fourier transform infrared and Raman spectral investigations of 5-aminoindole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006 , 64, 233-9	4.4	52
86	Structural, vibrational and DFT studies on 2-chloro-1H-isoindole-1,3(2H)-dione and 2-methyl-1H-isoindole-1,3(2H)-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 74, 642-9	4.4	39
85	Synthesis, FTIR, FT-Raman, UV-visible, ab initio and DFT studies on benzohydrazide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 79, 486-96	4.4	37
84	FTIR and FTR spectral studies of 2-amino-6-bromo-3-formylchromone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2004 , 60, 995-1000	4.4	36
83	FTIR, FT-Raman, FT-NMR, UV-visible and quantum chemical investigations of 2-amino-4-methylbenzothiazole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 88, 220-31	4.4	31
82	Vibrational and electronic investigations, thermodynamic parameters, HOMO and LUMO analysis on crotonaldehyde by ab initio and DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 83, 411-9	4.4	31
81	Synthesis and characterization of an anticoagulant 4-hydroxy-1-thiocoumarin by FTIR, FT-Raman, NMR, DFT, NBO and HOMO/LUMO analysis. <i>Journal of Molecular Structure</i> , 2013 , 1037, 305-316	3.4	30
80	Experimental and theoretical quantum chemical investigations of 8-hydroxy-5-nitroquinoline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 96, 506-16	4.4	28
79	Ab initio, density functional theory and structural studies of 4-amino-2-methylquinoline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 74, 375-84	4.4	27
78	FTIR, FT-Raman, FT-NMR and quantum chemical investigations of 3-acetylcoumarin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 109, 79-89	4.4	26
77	Vibrational spectroscopic investigations, ab initio and DFT studies on 7-bromo-5-chloro-8-hydroxyquinoline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 72, 783-8	4.4	25
76	Structure-activity relations of 2-(methylthio)benzimidazole by FTIR, FT-Raman, NMR, DFT and conceptual DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 118, 951-65	4.4	22

75	Experimental and theoretical investigations of benzamide oxime. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 79, 245-53	4.4	22
74	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 74, 798-807	4.4	22
73	Vibrational, NMR and quantum chemical investigations of acetoacetanilide, 2-chloroacetoacetanilide and 2-methylacetoacetanilide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 115, 154-74	4.4	21
72	Crystal structure, vibrational and DFT simulation studies of melaminium dihydrogen phosphite monohydrate. <i>Journal of Molecular Structure</i> , 2013 , 1045, 160-170	3.4	21
71	Vibrational, nuclear magnetic resonance and electronic spectra, quantum chemical investigations of 2-amino-6-fluorobenzothiazole. <i>Journal of Molecular Structure</i> , 2011 , 1006, 247-258	3.4	21
70	Density functional theory studies on vibrational and electronic spectra of 2-chloro-6-methoxypyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 78, 1625-32	4.4	21
69	Quantum chemical and spectroscopic investigations of 5-aminoquinoline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 74, 1215-23	4.4	19
68	Exploring the structure-activity relations of N-carbethoxyphthalimide by combining FTIR, FT-Raman and NMR spectroscopy with DFT electronic structure method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 120, 473-88	4.4	18
67	Vibrational, electronic and quantum chemical studies of 5-benzimidazole carboxylic acid. <i>Journal of Molecular Structure</i> , 2013 , 1036, 326-340	3.4	18
66	Vibrational spectroscopic, electronic and quantum chemical investigations on 2,3-hexadiene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 81, 620-30	4.4	18
65	Spectroscopic and quantum chemical electronic structure investigations of 2-(trifluoromethyl)aniline and 3-(trifluoromethyl)aniline. <i>Journal of Molecular Structure</i> , 2011 , 994, 179-193	3.4	18
64	Synthesis, vibrational and quantum chemical investigations of hydrogen bonded complex betaine dihydrogen selenite. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 96, 744-58	4.4	17
63	A comparative study on vibrational, conformational and electronic structure of 2-(hydroxymethyl)pyridine and 3-(hydroxymethyl)pyridine. <i>Journal of Molecular Structure</i> , 2012 , 1018, 156-170	3.4	17
62	Spectroscopic, electronic structure and natural bond orbital analysis of o-fluoronitrobenzene and p-fluoronitrobenzene: a comparative study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 84, 196-209	4.4	16
61	Structural and vibrational spectral investigations of melaminium maleate monohydrate by FTIR, FT-Raman and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 107, 90-101	4.4	15
60	Conformational, vibrational, NMR and DFT studies of N-methylacetanilide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 104, 182-96	4.4	15
59	Vibrational, electronic and quantum chemical studies of 1,2,4-benzenetricarboxylic-1,2-anhydride. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 110, 141-50	4.4	15
58	Experimental spectroscopic (FTIR, FT-Raman, FT-NMR, UV-Visible) and DFT studies of 2-amino-5-chlorobenzoxazole. <i>Journal of Molecular Structure</i> , 2011 , 1003, 92-102	3.4	15

57	Potential energy profile, structural, vibrational and reactivity descriptors of trans- β -methoxycinnamic acid by FTIR, FT-Raman and quantum chemical studies. <i>Journal of Molecular Structure</i> , 2016 , 1113, 42-54	3-4	14
56	X-ray diffraction, vibrational and quantum chemical investigations of 2-methyl-4-nitroanilinium trichloroacetate trichloroacetic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 97, 625-38	4-4	14
55	Quantum chemical studies and vibrational analysis of 4-acetyl benzonitrile, 4-formyl benzonitrile and 4-hydroxy benzonitrile--a comparative study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 98, 156-69	4-4	14
54	Synthesis, structural, vibrational and quantum chemical investigations of N-(2-methylphenyl)-2,2-dichloroacetamide and N-(4-methylphenyl)-2,2-dichloroacetamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 74, 607-16	4-4	14
53	Structural and vibrational spectral investigations of melaminium glutarate monohydrate by FTIR, FT-Raman and DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 135, 540-50	4-4	12
52	Structural, vibrational and quantum chemical investigations on 5-chloro-2-hydroxybenzamide and 5-chloro-2-hydroxybenzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 79, 1886-95	4-4	12
51	Synthesis, FT-IR, FT-Raman and quantum chemical investigations of N-(3-methylphenyl)-2,2-dichloroacetamide. <i>European Journal of Chemistry</i> , 2011 , 2, 70-76	0.6	12
50	Comprehensive quantum chemical and spectroscopic (FTIR, FT-Raman, ^1H , ^{13}C NMR) investigations of (1,2-epoxyethyl)benzene and (1,2-epoxy-2-phenyl)propane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 135, 120-36	4-4	11
49	A comparative study on vibrational, conformational and electronic structure of 1,2-dimethyl-5-nitroimidazole and 2-methyl-5-nitroimidazole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 97, 176-88	4-4	11
48	Fourier transform infrared and Raman spectral assignments and analysis of 7-amino-4-trifluoromethylcoumarin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007 , 67, 1290-6	4-4	11
47	Structural, vibrational and nuclear magnetic resonance investigations of 4-bromoisoquinoline by experimental and theoretical DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 107, 62-71	4-4	10
46	An insight into the structure, vibrations, electronic and reactivity properties of the tautomers 1 β -(diaminomethylene)thiourea and 2 β -imino- β -thiobiuret. <i>Journal of Molecular Structure</i> , 2017 , 1133, 187-198	3-4	9
45	Characterisation of 1,3-diammonium propylselenate monohydrate by XRD, FT-IR, FT-Raman, DSC and DFT studies. <i>Journal of Molecular Structure</i> , 2016 , 1107, 220-230	3-4	9
44	DFT simulation, quantum chemical electronic structure, spectroscopic and structure-activity investigations of 2-benzothiazole acetonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 128, 22-36	4-4	9
43	A comparative spectroscopic, electronic structure and chemical shift investigations of o-Chloronitrobenzene, p-Chloronitrobenzene and m-Chloronitrobenzene. <i>Journal of Molecular Structure</i> , 2012 , 1007, 122-135	3-4	9
42	DFT and ab initio quantum chemical studies on p-cyanobenzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 78, 1449-54	4-4	9
41	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010 , 77, 28-35	4-4	9
40	A comparative study on vibrational, conformational and electronic structure of 2-chloro-4-methyl-3-nitropyridine and 2-chloro-6-methylpyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 92, 305-17	4-4	8

39	Structural, vibrational, electronic investigations and quantum chemical studies of 2-amino-4-methoxybenzothiazole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 102, 327-40	4.4	8
38	Conformational, structural, vibrational and quantum chemical analysis on 4-aminobenzohydrazide and 4-hydroxybenzohydrazide—a comparative study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 108, 100-14	4.4	8
37	Structure, vibrations and quantum chemical investigations of hydrogen bonded complex of bis(1-hydroxy-2-methylpropan-2-aminium)selenate. <i>Journal of Molecular Structure</i> , 2017 , 1134, 6-16	3.4	7
36	Comprehensive quantum chemical and spectroscopic (FTIR, FT-Raman, ¹ H, ¹³ C NMR) investigations of O-desmethyltramadol hydrochloride an active metabolite in tramadol—an analgesic drug. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 122, 315-30	4.4	7
35	Conformational, structural, vibrational, electronic and quantum chemical investigations of cis-2-methoxycinnamic acid. <i>Journal of Molecular Structure</i> , 2015 , 1080, 122-136	3.4	6
34	Synthesis, FTIR and FT-Raman spectral analysis and structure-activity relations of N-(4-bromophenyl)-2,2-dichloroacetamide by DFT studies. <i>Journal of Molecular Structure</i> , 2014 , 1064, 15-26	3.4	6
33	Conformational analysis, spectroscopic and quantum chemical investigations of 2-bromo-3-nitroacetophenone. <i>Journal of Molecular Structure</i> , 2013 , 1037, 73-84	3.4	6
32	Energy profile, spectroscopic (FTIR, FT-Raman and FT-NMR) and DFT studies of 4-bromoisophthalic acid. <i>Journal of Molecular Structure</i> , 2018 , 1157, 132-148	3.4	6
31	Substituent influence on the structural, vibrational and electronic properties of 2,5-dihydrothiophene-1,1-dioxide by experimental and DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 150, 641-51	4.4	5
30	Structure, electronic, spectroscopic and reactivity investigations of pharmacologically active compound 1-hexyl-2-hydroxycarboxaldehyde [An experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2018 , 1164, 57-69	3.4	5
29	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. <i>Journal of Molecular Structure</i> , 2014 , 1056-1057, 38-51	3.4	5
28	Spectroscopic and density functional theory studies of trans-3-(trans-4-imidazolyl)acrylic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 129, 466-77	4.4	5
27	Experimental, quantum chemical and natural bond orbital investigations of N-(2,4-dimethylphenyl)-2,2-dichloroacetamide and N-(3,5-dimethylphenyl)-2,2-dichloroacetamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 88, 192-209	4.4	5
26	Structural characteristics and harmonic vibrational analysis of the stable conformer of 2,3-epoxypropanol by quantum chemical methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 96, 24-34	4.4	5
25	Combined spectroscopic and DFT studies on 2-chloro-4-nitrotoluene and 4-chloro-2-nitrotoluene. <i>Journal of Molecular Structure</i> , 2012 , 1016, 82-96	3.4	5
24	Crystal structure, vibrational spectra and DFT studies of hydrogen bonded 1,2,4-triazolium hydrogenselenate. <i>Journal of Molecular Structure</i> , 2017 , 1145, 211-221	3.4	4
23	Energy profile analysis, spectroscopic investigations (FTIR, FT-Raman and FT-NMR), electronic properties, structure-activity aspects and DFT studies of (1,3-benzodioxol-5-yl)acetic acid. <i>Chemical Data Collections</i> , 2018 , 17-18, 75-94	2.1	4
22	A new look into the quantum chemical and spectroscopic investigations of 5-chloro-1-methyl-4-nitroimidazole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 125, 160-74	4.4	4

21	Vibrational, conformational and electronic structure investigations of 1,3-dibromo-o-xylene, 1,3-dibromo-m-xylene and 1,3-dibromo-p-xylene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 91, 166-77	4.4	4
20	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. <i>Journal of Molecular Structure</i> , 2012 , 1022, 37-48	3.4	4
19	FTIR, FT-Raman and quantum chemical investigations of 4,5-dimethyl-1,3-dioxol-2-one. <i>Journal of Molecular Structure</i> , 2012 , 1024, 54-64	3.4	4
18	A new look into conformational, vibrational and electronic structure analysis of 3,4-dimethoxybenzonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 113, 302-13	4.4	4
17	An experimental and theoretical investigation on the structure, vibrations and reactivity properties of pharmacologically active compounds 3-acetylindole and indole-3-acetamide. <i>Journal of Molecular Structure</i> , 2020 , 1210, 128012	3.4	3
16	Experimental, quantum chemical, natural bond orbitals and reactivity investigations of 4-hydroxy-2-(trifluoromethyl)pyrimidine. <i>Chemical Data Collections</i> , 2018 , 17-18, 143-158	2.1	3
15	Primidone--an antiepileptic drug--characterisation by quantum chemical and spectroscopic (FTIR, FT-Raman, ¹ H, ¹³ C NMR and UV-Visible) investigations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 109, 282-97	4.4	3
14	Spectroscopic and quantum chemical studies on 4-acryloyl morpholine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 79, 1386-94	4.4	3
13	A combined experimental and theoretical quantum chemical studies on 4-morpholinecarboxaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 79, 1395-401	4.4	3
12	Conformational analysis, spectroscopic, structure-activity relations and quantum chemical simulation studies of 4-(trifluoromethyl)benzylamine. <i>Journal of Molecular Structure</i> , 2018 , 1159, 103-117	3.4	2
11	Simulations on the structure, vibrations and electronic properties of 1,2-epoxy-3-phenoxypropane and 1,2-epoxy-3-(p-benzyloxy)propane by FTIR, FT-Raman, FT-NMR and DFT methods. <i>Chemical Data Collections</i> , 2017 , 11-12, 139-167	2.1	1
10	Structure activity studies of an analgesic drug tapentadol hydrochloride by spectroscopic and quantum chemical methods. <i>Journal of Molecular Structure</i> , 2015 , 1100, 188-202	3.4	1
9	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. <i>Journal of Molecular Structure</i> , 2020 , 1207, 127841	3.4	1
8	Structure, Vibrations, Molecular Orbitals, Reactivity Properties of 3-Trifluoromethylphenylchloroformate by FT-IR, FT-Raman, FT-NMR and DFT Studies. <i>Asian Journal of Chemistry</i> , 2019 , 31, 1737-1747	0.4	1
7	Electronic structure simulations of 2,6-dimethyl-2,5-heptadien-4-one by FTIR, FT-Raman, NMR, UV-Vis, NBO and density functional theory. <i>Molecular Simulation</i> , 2013 , 39, 185-198	2	1
6	Energy profile, structure, spectroscopic and quantum chemical investigations of trans-3,4-(methylenedioxy)cinnamic acid. <i>Chemical Data Collections</i> , 2021 , 31, 100644	2.1	1
5	A comparative study on vibrational, conformational and electronic structure of 1,3-diol-o-xylene, 1,3-diol-m-xylene and 1,3-diol-p-xylene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 92, 1-15	4.4	0
4	Structure, conformations, vibrations and quantum chemical investigations of 2-(1H-indol-3-yl)ethanoic acid. <i>Journal of Molecular Structure</i> , 2022 , 1256, 132570	3.4	0

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| 3 | An insight into the structure and vibrations of 4-Nitroindole and 7-Nitroindole by spectroscopic and DFT methods. <i>Journal of Molecular Structure</i> , 2021 , 1238, 130420 | 3.4 | o |
| 2 | Conformational Analysis, Structural and Vibrational Investigations of trans-2-Chlorocinnamic Acid and trans-4-Chlorocinnamic Acid. <i>Springer Proceedings in Physics</i> , 2017 , 563-598 | 0.2 | |
| 1 | FT-IR, FT-Raman, NMR Spectroscopic and DFT Quantum Chemical Investigations of 6-Methylcoumarin. <i>Asian Journal of Chemistry</i> , 2021 , 33, 2715-2722 | 0.4 | |