Mehmet Karabacak

List of Publications by Citations

122 papers	3,657 citations	38 h-index	52 g-index
124 ext. papers	4,006 ext. citations	3.9 avg, IF	5.53 L-index

#	Paper	IF	Citations
122	Natural bond orbital analysis, electronic structure, non-linear properties and vibrational spectral analysis of L-histidinium bromide monohydrate: a density functional theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 81, 85-98	4.4	98
121	FT-IR, UV spectroscopic and DFT quantum chemical study on the molecular conformation, vibrational and electronic transitions of 2-aminoterephthalic acid. *Journal of Molecular Structure*, **2010**, 982, 22-27	3.4	91
120	Synthesis, molecular conformation, vibrational and electronic transition, isometric chemical shift, polarizability and hyperpolarizability analysis of 3-(4-methoxy-phenyl)-2-(4-nitro-phenyl)-acrylonitrile: a combined experimental and theoretical analysis. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 82, 444-55	4.4	89
119	Molecular structure, vibrational, UV and NBO analysis of 4-chloro-7-nitrobenzofurazan by DFT calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 79, 1162-70	4.4	86
118	FT-IR, FT-Raman, NMR and UV-vis spectra, vibrational assignments and DFT calculations of 4-butyl benzoic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 85, 179-89	4.4	85
117	The spectroscopic (FT-Raman, FT-IR, UV and NMR), molecular electrostatic potential, polarizability and hyperpolarizability, NBO and HOMO-LUMO analysis of monomeric and dimeric structures of 4-chloro-3,5-dinitrobenzoic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 93, 33-46	4.4	83
116	An experimental and theoretical study of molecular structure and vibrational spectra of 2-chloronicotinic acid by density functional theory and ab initio Hartree–Fock calculations. *Journal of Molecular Structure*, **2008**, 885, 28-35	3.4	82
115	FT-IR, FT-Raman, UV spectra and DFT calculations on monomeric and dimeric structure of 2-amino-5-bromobenzoic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 86, 590-9	4.4	78
114	FT-Raman, FT-IR spectra and DFT calculations on monomeric and dimeric structures of 5-fluoro- and 5-chloro-salicylic acid. *Journal of Raman Spectroscopy*, **2010**, 41, 1085-1097	2.3	71
113	The spectroscopic (FT-IR and FT-Raman) and theoretical studies of 5-bromo-salicylic acid. *Journal of Molecular Structure*, **2009**, 919, 215-222	3.4	70
112	Experimental (UV, NMR, IR and Raman) and theoretical spectroscopic properties of 2-chloro-6-methylaniline. *Molecular Physics*, **2009**, 107, 253-264	1.7	67
111	FT-IR, FT-Raman, NMR spectra and DFT calculations on 4-chloro-N-methylaniline. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2010**, 75, 1523-9	4.4	67
110	Comparison of experimental and density functional study on the molecular structure, infrared and Raman spectra and vibrational assignments of 6-chloronicotinic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 71, 876-83	4.4	67
109	Spectroscopic properties, NLO, HOMO-LUMO and NBO analysis of 2,5-Lutidine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 96, 421-35	4.4	66
108	X-ray, FT-Raman, FT-IR spectra and ab initio HF, DFT calculations of 2-[(5-methylisoxazol-3-yl)amino]-2-oxo-ethyl methacrylate. *Journal of Molecular Structure*, **2008**, 886, 148-157	3.4	63
107	Molecular structure, vibrational spectroscopic, first-order hyperpolarizability and HOMO, LUMO studies of 2-aminobenzimidazole. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 84, 184-95	4.4	60
106	FT-IR, FT-Raman, ab initio, HF and DFT studies, NBO, HOMO-LUMO and electronic structure calculations on 4-chloro-3-nitrotoluene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 89, 137-48	4.4	58

105	Spectroscopic (infrared, Raman, UV and NMR) analysis, Gaussian hybrid computational investigation (MEP maps/HOMO and LUMO) on cyclohexanone oxime. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 96, 207-20	4.4	58
104	Spectroscopic (FT-IR, FT-Raman, UV and NMR) investigation and NLO, HOMO-LUMO, NBO analysis of organic 2,4,5-trichloroaniline. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 97, 231-45	4.4	56
103	Experimental and theoretical FT-IR and FT-Raman spectroscopic analysis of N1-methyl-2-chloroaniline. *Journal of Physical Organic Chemistry*, **2009**, 22, 321-330	2.1	56
102	FT-IR and FT-Raman spectra, vibrational assignments, NBO analysis and DFT calculations of 2-amino-4-chlorobenzonitrile. *Journal of Molecular Structure*, **2011**, 985, 148-156	3.4	56
101	FT-IR, FT-Raman, NMR spectra, and molecular structure investigation of 2,3-dibromo-N-methylmaleimide: A combined experimental and theoretical study. *Journal of Molecular Structure*, **2008**, 892, 125-131	3.4	55
100	Experimental (FT-IR and FT-Raman spectra) and theoretical (ab initio HF, DFT) study of 2-chloro-5-methylaniline. *Journal of Molecular Structure*, **2008**, 892, 25-31	3.4	54
99	FT-IR, UV-vis, 1H and 13C NMR spectra and the equilibrium structure of organic dye molecule disperse red 1 acrylate: a combined experimental and theoretical analysis. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 83, 561-9	4.4	53
98	DFT based computational study on the molecular conformation, NMR chemical shifts and vibrational transitions for N-(2-methylphenyl) methanesulfonamide and N-(3-methylphenyl) methanesulfonamide. *Journal of Molecular Structure*, **2010**, 968, 108-114	3.4	52
97	FT-Raman, FT-IR, UV spectra and DFT and ab initio calculations on monomeric and dimeric structures of 3,5-pyridinedicarboxylic acid. *Journal of Molecular Structure*, **2012**, 1027, 1-14	3.4	50
96	Synthesis, analysis of spectroscopic and nonlinear optical properties of the novel compound: (S)-N-benzyl-1-phenyl-5-(thiophen-3-yl)-4-pentyn-2-amine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 97, 556-67	4.4	49
95	Experimental vibrational spectra (Raman, infrared) and DFT calculations on monomeric and dimeric structures of 2- and 6-bromonicotinic acid. *Journal of Raman Spectroscopy*, **2010**, 41, 98-105	2.3	49
94	Molecular structure and vibrational assignments of hippuric acid: a detailed density functional theoretical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 74, 1197-203	4.4	46
93	Experimental (FT-IR and FT-Raman), electronic structure and DFT studies on 1-methoxynaphthalene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 79, 646-53	4.4	46
92	NMR, UV, FT-IR, FT-Raman spectra and molecular structure (monomeric and dimeric structures) investigation of nicotinic acid N-oxide: A combined experimental and theoretical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 85, 145-54	4.4	44
91	Theoretical investigation on the molecular structure, Infrared, Raman and NMR spectra of para-halogen benzenesulfonamides, 4-X-C6H4SO2NH2 (X = Cl, Br or F). *Journal of Molecular Structure*, **2009**, 919, 26-33	3.4	44
90	Monomeric and dimeric structures analysis and spectroscopic characterization of 3,5-difluorophenylboronic acid with experimental (FT-IR, FT-Raman, 1H and 13C NMR, UV) techniques and quantum chemical calculations. *Journal of Molecular Structure*, **2014**, 1058, 79-96	3.4	43
89	Experimental (FT-IR, FT-Raman, UV and NMR) and quantum chemical studies on molecular structure, spectroscopic analysis, NLO, NBO and reactivity descriptors of 3,5-Difluoroaniline. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 135, 283-95	4.4	41
88	Molecular structure investigation and spectroscopic studies on 2,3-difluorophenylboronic acid: a combined experimental and theoretical analysis. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 97, 892-908	4.4	41

87	Synthesis, molecular conformation, vibrational, electronic transition, and chemical shift assignments of 4-(thiophene-3-ylmethoxy)phthalonitrile: a combined experimental and theoretical analysis. *Structural Chemistry*, **2011**, 22, 45-56	1.8	41
86	Vibrational spectroscopic analysis of 2-chlorotoluene and 2-bromotoluene: a combined experimental and theoretical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2010**, 77, 1005-13	4.4	40
85	Infrared and Raman spectrum, molecular structure and theoretical calculation of 3,4-dichlorophenylboronic acid. *Journal of Molecular Structure*, **2009**, 921, 178-187	3.4	39
84	Molecular structure (monomeric and dimeric structure) and HOMO-LUMO analysis of 2-aminonicotinic acid: a comparison of calculated spectroscopic properties with FT-IR and UV-vis. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 91, 83-96	4.4	37
83	Electronic absorption, vibrational spectra, nonlinear optical properties, NBO analysis and thermodynamic properties of N-(4-nitro-2-phenoxyphenyl) methanesulfonamide molecule by ab initio HF and density functional methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 108, 186-96	4.4	37
82	Vibrational spectroscopy (FT-IR and FT-Raman) investigation, and hybrid computational (HF and DFT) analysis on the structure of 2,3-naphthalenediol. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 83, 540-52	4.4	37
81	FT-IR, FT-Raman vibrational spectra and molecular structure investigation of 2-chloro-4-methylaniline: a combined experimental and theoretical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 72, 1076-83	4.4	37
80	Molecular structure, polarizability, hyperpolarizability analysis and spectroscopic characterization of 1-(chloromethyl)-2-methylnaphthalene with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular*	4.4	36
79	FT-IR, FT-Raman and UV spectral investigation: computed frequency estimation analysis and electronic structure calculations on chlorobenzene using HF and DFT. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 88, 37-48	4.4	36
78	Synthesis, structure, spectroscopic studies (FT-IR, FT-Raman and UV), normal coordinate, NBO and NLO analysis of salicylaldehyde p-chlorophenylthiosemicarbazone. *Journal of Molecular Structure*, **2015**, 1081, 400-412	3.4	33
77	The spectroscopic (FTIR, FT-Raman, UV and NMR), first-order hyperpolarizability and HOMO–LUMO analysis of 4-amino-5-chloro-2-methoxybenzoic acid. *Journal of Molecular Structure*, **2012**, 1024, 1-12	3.4	32
76	The spectroscopic (FTIR, FT-Raman, NMR and UV), first-order hyperpolarizability and HOMO-LUMO analysis of methylboronic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 92, 67-77	4.4	30
75	Molecular structure, electronic properties, NLO, NBO analysis and spectroscopic characterization of Gabapentin with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 109, 298-307	4.4	30
74	FT-IR, FT-Raman, ab initio and DFT structural, vibrational frequency and HOMO-LUMO analysis of 1-naphthaleneacetic acid methyl ester. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 82, 169-80	4.4	30
73	Structural and spectroscopic characterization of 2,3-difluorobenzoic acid and 2,4-difluorobenzoic acid with experimental techniques and quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 79, 1511-9	4.4	30
72	FT-IR, FT-Raman and UV spectral investigation; computed frequency estimation analysis and electronic structure calculations on 1-nitronaphthalene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 85, 251-60	4.4	28
71	Vibrational frequencies, structural confirmation stability and HOMO–LUMO analysis of nicotinic acid ethyl ester with experimental (FT-IR and FT-Raman) techniques and quantum mechanical calculations. *Journal of Molecular Structure*, **2012**, 1017, 1-13	3.4	28
70	Molecular structure, spectroscopic (FT-IR, FT-Raman, 13C and 1H NMR, UV), polarizability and first-order hyperpolarizability, HOMO and LUMO analysis of 4Smethylbiphenyl-2-carbonitrile. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 87, 273-85	4.4	26

69	Spectroscopic (NMR, UV, FT-IR and FT-Raman) analysis and theoretical investigation of nicotinamide N-oxide with density functional theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 83, 250-8	4.4	26
68	The spectroscopic (FT-IR, FT-Raman, UV) and first order hyperpolarizability, HOMO and LUMO analysis of 3-aminobenzophenone by density functional method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 92, 365-76	4.4	25
67	Experimental and theoretical FTIR and FT-Raman spectroscopic analysis of 1-pyrenecarboxylic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 114, 509-19	4.4	25
66	Synthesis, spectroscopic characterization and quantum chemical computational studies of (S)-N-benzyl-1-phenyl-5-(pyridin-2-yl)-pent-4-yn-2-amine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 97, 435-48	4.4	25
65	DFT calculations and experimental FT-IR, FT-Raman, NMR, UV-Vis spectral studies of 3-fluorophenylboronic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 136 Pt B, 306-20	4.4	24
64	Structures and energetics Of Pdn (n=2□0) clusters using an embedded-atom model potential. *Surface Science*, **2002**, 507-510, 636-642	1.8	24
63	Spectroscopic (FT-IR, FT-Raman and UV-vis) investigation and frontier molecular orbitals analysis on 3-methyl-2-nitrophenol using hybrid computational calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 86, 139-51	4.4	23
62	An experimental and theoretical investigation of Acenaphthene-5-boronic acid: conformational study, NBO and NLO analysis, molecular structure and FT-IR, FT-Raman, NMR and UV spectra. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 753-66	4.4	23
61	FT-IR, FT-Raman, NMR, UV and quantum chemical studies on monomeric and dimeric conformations of 3,5-dimethyl-4-methoxybenzoic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 123, 352-62	4.4	22
60	Vibrational spectroscopic studies, NLO, HOMO-LUMO and electronic structure calculations of □trichlorotoluene using HF and DFT. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 94, 53-64	4.4	20
59	Spectroscopic (FT-IR/FT-Raman) and computational (HF/DFT) investigation and HOMO/LUMO/MEP analysis on 2-amino-4-chlorophenol. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 104, 337-51	4.4	20
58	FT-IR, FT-Raman, NMR and UV-Vis spectra and DFT calculations of 5-bromo-2-ethoxyphenylboronic acid (monomer and dimer structures). *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 137, 1315-33	4.4	19
57	Determination of structural and vibrational spectroscopic properties of 2-, 3-, 4-nitrobenzenesulfonamide using FT-IR and FT-Raman experimental techniques and DFT quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 85, 261-70	4.4	19
56	Molecular structure, spectroscopic characterization, HOMO and LUMO analysis of 3,3Sdiaminobenzidine with DFT quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 150, 83-93	4.4	19
55	Synthesis, crystal structure and ab initio/DFT calculations of a derivative of dithiophosphonates. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 122, 582-90	4.4	17
54	A comparative study of selected disperse azo dye derivatives based on spectroscopic (FT-IR, NMR and UV-Vis) and nonlinear optical behaviors. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 122, 682-9	4.4	17
53	Experimental (FT-IR, FT-Raman) and theoretical (HF and DFT) investigation and HOMO and LUMO analysis on the structure of p-fluoronitrobenzene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 83, 575-86	4.4	17
52	Synthesis and DFT calculation of a novel 5,17-di(2-antracenylazo)-25,27-di(ethoxycarbonylmethoxy)-26,28-dihydroxycalix[4]arene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 136 Pt B, 607-17	4.4	16

51	Spectroscopic (FT-IR, FT-Raman and NMR) and computational studies on 3-methoxyaniline. *Journal of Molecular Structure*, **2014**, 1056-1057, 176-188	3.4	16
50	FT-IR, FT-Raman and UV spectroscopic investigation, electronic properties, electric moments, and NBO analysis of anethole using quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 133, 165-77	4.4	16
49	FT-IR and FT-Raman vibrational analysis, ab initio HF and DFT simulations of isocyanic acid 1-naphthyl ester. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 81, 504-18	4.4	16
48	FT-IR and FT-Raman, UV spectroscopic investigation of 1-bromo-3-fluorobenzene using DFT (B3LYP, B3PW91 and MPW91PW91) calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 82, 481-92	4.4	16
47	Spectral features, electric properties, NBO analysis and reactivity descriptors of 2-(2-Benzothiazolylthio)-Ethanol: Combined experimental and DFT studies. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 136 Pt C, 1205-15	4.4	15
46	Vibrational (FT-IR and FT-Raman), electronic (UV-Vis), NMR (1H and 13C) spectra and reactivity analyses of 4,5-dimethyl-o-phenylenediamine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 130, 516-25	4.4	15
45	Vibrational and UV spectra, first order hyperpolarizability, NBO and HOMO-LUMO analysis of 4-chloro-N-(2-methyl-2,3-dihydroindol-1-yl)-3-sulfamoyl-benzamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 122, 1-14	4.4	15
44	Experimental (FT-IR, FT-Raman, UV–Vis, 1H and 13CNMR) and computational (density functional theory) studies on 3-bromophenylboronic acid. *Journal of Molecular Structure*, **2014**, 1076, 358-372	3.4	15
43	Identification of structural and spectral features of synthesized cyano-stilbene dye derivatives: a comparative experimental and DFT study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 120, 144-50	4.4	15
42	FT-IR and FT-Raman, NMR and UV spectroscopic investigation and hybrid computational (HF and DFT) analysis on the molecular structure of mesitylene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 116, 622-34	4.4	15
41	FT-IR, FT-Raman, dispersive Raman, NMR spectroscopic studies and NBO analysis of 2-Bromo-1H-Benzimidazol by density functional method. *Journal of Molecular Structure*, **2015**, 1081, 506-518	3.4	14
40	Ultrafast optical nonlinearity, electronic absorption, vibrational spectra and solvent effect studies of ninhydrin. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 109, 331-43	4.4	14
39	Conformational analysis, spectroscopic study (FT-IR, FT-Raman, UV, 1H and 13C NMR), molecular orbital energy and NLO properties of 5-iodosalicylic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 136 Pt B, 295-305	4.4	13
38	Spectroscopic investigation, natural bond orbital analysis, HOMO-LUMO and thermodynamic functions of 2-tert-butyl-5-methyl anisole using DFT (B3LYP) calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 136 Pt B, 451-63	4.4	13
37	An experimental and density functional study on conformational and spectroscopic analysis of 5-methoxyindole-2-carboxylic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 137, 670-6	4.4	13
36	Analysis of vibrational spectra (FT-IR and FT-Raman) and nonlinear optical properties of organic 2-chloro-p-xylene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 94, 36-47	4.4	13
35	Molecular structure, spectroscopic characterization (FT-IR, FT-Raman, UV and NMR), HOMO and LUMO analysis of 3-ethynylthiophene with DFT quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 709-18	4.4	13
34	Quantum-chemical (DFT, MP2) and spectroscopic studies (FT-IR and UV) of monomeric and dimeric structures of 2(3H)-Benzothiazolone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 120, 126-36	4.4	12

33	Multi-photon absorption effect and intra-molecular charge transfer of donor-acceptor chromophore ethyl p-amino benzoate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 108, 197-210	4.4	12
32	Determination of conformational and spectroscopic features of ethyl trans-alfa-cyano-3-indole-acrylate compound: an experimental and quantum chemical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 104, 428-36	4.4	12
31	A structural and spectroscopic study on para-aminohippuric acid with experimental and theoretical approaches. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 85, 241-50	4.4	11
30	Determination of structural, spectrometric and nonlinear optical features of 2-(4-hydroxyphenylazo)benzoic acid by experimental techniques and quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 105, 80-7	4.4	11
29	Quantum chemical calculation (electronic and topologic) and experimental (FT-IR, FT-Raman and UV) analysis of isonicotinic acid N-oxide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 140, 85-95	4.4	11
28	The spectroscopic (FT-IR, FT-Raman, UV and NMR) first order hyperpolarizability and HOMO-LUMO analysis of dansyl chloride. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 117, 234-44	4.4	11
27	Spectral investigations of 2,5-difluoroaniline by using mass, electronic absorption, NMR, and vibrational spectra. *Journal of Molecular Structure*, **2016**, 1123, 284-299	3.4	11
26	Synthesis, molecular structure, spectral investigation on (E)-1-(4-bromophenyl)-3-(4-(dimethylamino)phenyl)prop-2-en-1-one. *Journal of Molecular Structure*, **2016**, 1103, 145-155	3.4	10
25	Synthesis and spectroscopic characterization on 4-(2,5-di-2-thienyl-1H-pyrrol-1-yl) benzoic acid: A DFT approach. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2016**, 152, 8-17	4.4	10
24	Theoretical study on molecular structure and vibrational analysis included FT-IR, FT-Raman and UV techniques of 2,4,5-trimethylbenzoic acid (monomer and dimer structures). *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 134, 598-607	4.4	10
23	Molecular structure investigation of neutral, dimer and anion forms of 3,4-pyridinedicarboxylic acid: a combined experimental and theoretical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 135, 270-82	4.4	10
22	FT-IR, FT-Raman and UV spectral investigation: computed frequency estimation analysis and electronic structure calculations on 1-bromo-2-methylnaphthalene. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 101, 314-24	4.4	10
21	Structures and energetics of Pd21-Pd55 clusters. *Surface Science*, **2003**, 532-535, 306-311	1.8	10
20	Vibrational spectra, UV and NMR, first order hyperpolarizability and HOMO-LUMO analysis of 2-amino-4-chloro-6-methylpyrimidine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 97, 811-24	4.4	9
19	The spectroscopic (FT-IR, FT-Raman, dispersive Raman and NMR) study of ethyl-6-chloronicotinate molecule by combined density functional theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2016**, 153, 754-70	4.4	8
18	The infrared, Raman, NMR and UV spectra, ab initio calculations and spectral assignments of 2-amino-4-chloro-6-methoxypyrimidine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 116, 451-9	4.4	8
17	The spectroscopic and quantum chemical studies of 3,4-difluoroaniline. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 143, 265-80	4.4	8
16	A combined experimental and theoretical investigation of 2-Thienylboronic acid: Conformational search, molecular structure, NBO, NLO and FT-IR, FT-Raman, NMR and UV spectral analysis. *Journal of Molecular Structure*, **2014**, 1076, 639-650	3.4	7

15	FT-IR, FT-Raman and UV spectral investigation; computed frequency estimation analysis and electronic structure calculations on 4-hydroxypteridine. *Journal of Molecular Structure*, **2013**, 1038, 114-125	3.4	7
14	Synthesis, FT-IR, FT-Raman, dispersive Raman and NMR spectroscopic study of a host molecule which potential applications in sensor devices. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 94, 126-33	4.4	6
13	Determination of structural and vibrational spectroscopic features of neutral and anion forms of dinicotinic acid by using NMR, infrared and Raman experimental methods combined with DFT and HF. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 114, 38-45	4.4	6
12	Vibrational investigation on FT-IR and FT-Raman spectra, IR intensity, Raman activity, peak resemblance, ideal estimation, standard deviation of computed frequencies analyses and electronic structure on 3-methyl-1,2-butadiene using HF and DFT (LSDA/B3LYP/B3PW91) calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 82, 79-90	4.4	6
11	Cyclohexylamine) 2 M(CN) 4 ?2C 6 H 6 (M = Cd or Hg). *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **2001**, 40, 317-321		5
10	Synthesis and investigation of the properties of novel azocalix[4]arenes. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 146, 151-62	4.4	4
9	Molecular structure, vibrational, electronic and thermal properties of 4-vinylcyclohexene by quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 145, 340-352	4.4	4
8	Synthesis, single crystal structure, spectroscopic characterization and molecular properties of (2E)-3-(2,6-dichlorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one. *Journal of Molecular Structure*, **2016**, 1116, 135-145	3.4	4
7	Spectral investigation and theoretical study of zwitterionic and neutral forms of quinolinic acid. *Journal of Molecular Structure*, **2015**, 1095, 100-111	3.4	3
6	Spectroscopic analysis (FT-IR/FT-Raman) and molecular structure investigation on m-fluoronitrobenzene using hybrid computational calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 94, 318-30	4.4	3
5	Conformational and spectroscopic behaviors of 2,4-xylyl isothiocyanate. *Journal of Molecular Structure*, **2015**, 1087, 113-120	3.4	3
4	A comparative experimental and quantum chemical study on monomeric and dimeric structures of 3,5-dibromoanthranilic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 96, 644-56	4.4	2
3	Neural network consistent empirical physical formula construction for DFT based nonlinear vibrational spectra intensities of N-(2-methylphenyl) and N-(3-methylphenyl) methanesulfonamides. *Journal of Molecular Structure*, **2011**, 1006, 642-649	3.4	2
2	Synthesis, conformational and spectroscopic characterization of monomeric styrene derivatives having pendant p-substituted benzylic ether groups. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 111, 97-103	4.4	1
1	Neural network consistent empirical physical formula construction for density functional theory based nonlinear vibrational absorbance and intensity of 6-choloronicotinic acid molecule. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 90, 55-62	4.4	0