Mehmet Karabacak

List of Publications by Year
in descending order

122	4,467	71102	133252
papers	citations	41 h-index	59 g-index

124	124	124	2918
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	3.9	139
2	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, 444-455.	3.9	116
3	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, 1162-1170.	3.9	116
4	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.	3.6	109
5	The spectroscopic (FT-Raman, FT-IR, UV and NMR), molecular electrostatic potential, polarizability and hyperpolarizability, NBO and HOMOâ€“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.	3.9	106
6	FT-IR, FT-Raman, NMR and UVâ€“vis spectra, vibrational assignments and DFT calculations of 4-butyl benzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 85, 179-189.	3.9	105
7	An experimental and theoretical study of molecular structure and vibrational spectra of 2-chloronicotinic acid by density functional theory and ab initio Hartreeâ€“Fock calculations. Journal of Molecular Structure, 2008, 885, 28-35.	3.6	90
8	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, 590-599.	3.9	89
9	Spectroscopic properties, NLO, HOMOâ€“LUMO and NBO analysis of 2,5-Lutidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 421-435.	3.9	86
10	FT-IR, FT-Raman, NMR spectra and DFT calculations on 4-chloro-N-methylaniline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 1523-1529.	3.9	83
11	Spectroscopic (FT-IR, FT-Raman, UV and NMR) investigation and NLO, HOMOâ€“LUMO, NBO analysis of organic 2,4,5-trichloroaniline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 231-245.	3.9	83
12	The spectroscopic (FT-IR and FT-Raman) and theoretical studies of 5-bromo-salicylic acid. Journal of Molecular Structure, 2009, 919, 215-222.	3.6	82
13	Experimental (UV, NMR, IR and Raman) and theoretical spectroscopic properties of 2-chloro-6-methylaniline. Molecular Physics, 2009, 107, 253-264.	1.7	77
14	FTâ€Raman, FTâ€IR spectra and DFT calculations on monomeric and dimeric structures of 5â€fluoroâ€and 5â€chloroâ€salicylic acid. Journal of Raman Spectroscopy, 2010, 41, 1085-1097.	2.5	77
15	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, 207-220.	3.9	76
16	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, 876-883.	3.9	74
17	Molecular structure, vibrational spectroscopic, first-order hyperpolarizability and HOMO, LUMO studies of 2-aminobenzimidazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 84, 184-195.	3.9	74
18	FT-IR, FT-Raman, ab initio, HF and DFT studies, NBO, HOMOâ€“LUMO and electronic structure calculations on 4-chloro-3-nitrotoluene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 89, 137-148.	3.9	73

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19	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.	3.6	69
20	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.	3.6	67
21	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.	3.6	63
22	Experimental and theoretical FTâ€IR and FTâ€Raman spectroscopic analysis of N1â€methylâ€2â€chloroaniline. Journal of Physical Organic Chemistry, 2009, 22, 321-330.	1.9	63
23	FT-IR, UVâ€“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, 561-569.	3.9	62
24	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.	3.6	62
25	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.	3.6	59
26	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, 556-567.	3.9	59
27	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.	3.6	57
28	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.	3.6	57
29	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, 145-154.	3.9	56
30	Experimental vibrational spectra (Raman, infrared) and DFT calculations on monomeric and dimeric structures of 2â€and 6â€bromonicotinic acid. Journal of Raman Spectroscopy, 2010, 41, 98-105.	2.5	54
31	Experimental (FT-IR and FT-Raman), electronic structure and DFT studies on 1-methoxynaphthalene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 646-653.	3.9	54
32	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, 283-295.	3.9	54
33	Molecular structure and vibrational assignments of hippuric acid: A detailed density functional theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 1197-1203.	3.9	51
34	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, 540-552.	3.9	51
35	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, 186-196.	3.9	51
36	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.	3.9	50

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37	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.	3.6	49
38	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, 1005-1013.	3.9	48
39	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.	3.9	48
40	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.	3.6	48
41	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.	2.0	44
42	Infrared and Raman spectrum, molecular structure and theoretical calculation of 3,4-dichlorophenylboronic acid. Journal of Molecular Structure, 2009, 921, 178-187.	3.6	43
43	The spectroscopic (FTIR, FT-Raman, NMR and UV), first-order hyperpolarizability and HOMOâ€“LUMO analysis of methylboronic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 92, 67-77.	3.9	43
44	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, 1076-1083.	3.9	42
45	Molecular structure (monomeric and dimeric structure) and HOMOâ€“LUMO analysis of 2-aminonicotinic acid: A comparison of calculated spectroscopic properties with FT-IR and UVâ€“vis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 91, 83-96.	3.9	42
46	The spectroscopic (FTIR, FT-Raman, UV and NMR), first-order hyperpolarizability and HOMOâ€“LUMO analysis of 4-amino-5-chloro-2-methoxybenzoic acid. Journal of Molecular Structure, 2012, 1024, 1-12.	3.6	41
47	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 Spectroscopy, 2012, 85, 43-52.	3.9	38
48	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.	3.9	38
49	FT-IR, FT-Raman, ab initio and DFT structural, vibrational frequency and HOMOâ€“LUMO analysis of 1-naphthaleneacetic acid methyl ester. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 82, 169-180.	3.9	36
50	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, 1511-1519.	3.9	33
51	DFT calculations and experimental FT-IR, FT-Raman, NMR, UVâ€“Vis spectral studies of 3-fluorophenylboronic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 306-320.	3.9	33
52	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, 250-258.	3.9	32
53	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, 251-260.	3.9	32
54	Vibrational frequencies, structural confirmation stability and HOMOâ€“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.	3.6	32

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55	Molecular structure, spectroscopic (FT-IR, FT-Raman, 13C and 1H NMR, UV), polarizability and first-order hyperpolarizability, HOMO and LUMO analysis of 4â€²-methylbiphenyl-2-carbonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 87, 273-285.	3.9	30
56	Experimental and theoretical FTIR and FT-Raman spectroscopic analysis of 1-pyrenecarboxylic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 114, 509-519.	3.9	29
57	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, 435-448.	3.9	28
58	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, 352-362.	3.9	28
59	Molecular structure, spectroscopic characterization, HOMO and LUMO analysis of 3,3â€²-diaminobenzidine with DFT quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 83-93.	3.9	28
60	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, 753-766.	3.9	27
61	Structures and energetics Of Pdn (n=2â€“20) clusters using an embedded-atom model potential. Surface Science, 2002, 507-510, 636-642.	1.9	26
62	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, 365-376.	3.9	26
63	Vibrational spectroscopic studies, NLO, HOMOâ€“LUMO and electronic structure calculations of Î±,Î±,Î±-trichlorotoluene using HF and DFT. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 94, 53-64.	3.9	26
64	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, 1205-1215.	3.9	25
65	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, 261-270.	3.9	24
66	Spectroscopic (FT-IR, FT-Raman and UVâ€“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, 139-151.	3.9	24
67	A comparative study of selected disperse azo dye derivatives based on spectroscopic (FT-IR, NMR and) Tj ETQq1 1 0.784314 rgBT /Ov Spectroscopy, 2014, 122, 682-689.	3.9	24
68	FT-IR, FT-Raman, NMR and UVâ€“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, 1315-1333.	3.9	24
69	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, 337-351.	3.9	22
70	Vibrational (FT-IR and FT-Raman), electronic (UVâ€“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, 516-525.	3.9	22
71	Synthesis, crystal structure and ab initio/DFT calculations of a derivative of dithiophosphonates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 582-590.	3.9	21
72	Experimental (FT-IR, FT-Raman, UVâ€“Vis, 1H and 13CNMR) and computational (density functional theory) studies on 3-bromophenylboronic acid. Journal of Molecular Structure, 2014, 1076, 358-372.	3.6	21

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73	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, 295-305.	3.9	21
74	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.	3.6	21
75	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, 622-634.	3.9	20
76	Ultrafast optical nonlinearity, electronic absorption, vibrational spectra and solvent effect studies of ninhydrin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 109, 331-343.	3.9	20
77	Spectroscopic (FT-IR, FT-Raman and NMR) and computational studies on 3-methoxyaniline. Journal of Molecular Structure, 2014, 1056-1057, 176-188.	3.6	20
78	FT-IR and FT-Raman, UV spectroscopic investigation of 1-bromo-3-fluorobenzene using DFT (B3LYP,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Spectroscopy, 2011, 82, 481-492.	3.9	19
79	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, 144-150.	3.9	19
80	The spectroscopic (FT-IR, FT-Raman, UV and NMR) first order hyperpolarizability and HOMOâ€“LUMO analysis of dansyl chloride. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 234-244.	3.9	18
81	Vibrational and UV spectra, first order hyperpolarizability, NBO and HOMOâ€“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.	3.9	18
82	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, 607-617.	3.9	18
83	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, 670-676.	3.9	18
84	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, 504-518.	3.9	17
85	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, 575-586.	3.9	17
86	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, 165-177.	3.9	17
87	Spectroscopic investigation, natural bond orbital analysis, HOMOâ€“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, 451-463.	3.9	16
88	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, 709-718.	3.9	15
89	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, 80-87.	3.9	15
90	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.	3.9	15

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91	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, 314-324.	3.9	14
92	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, 126-136.	3.9	14
93	A structural and spectroscopic study on para-aminohippuric acid with experimental and theoretical approaches. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 85, 241-250.	3.9	13
94	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.	3.9	13
95	Multi-photon absorption effect and intra-molecular charge transfer of donor-Ï€-acceptor chromophore ethyl p-amino benzoate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 108, 197-210.	3.9	12
96	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, 428-436.	3.9	12
97	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.	3.9	12
98	Spectral investigations of 2,5-difluoroaniline by using mass, electronic absorption, NMR, and vibrational spectra. Journal of Molecular Structure, 2016, 1123, 284-299.	3.6	12
99	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.	3.9	12
100	Structures and energetics of Pd21â€“Pd55 clusters. Surface Science, 2003, 532-535, 306-311.	1.9	11
101	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, 270-282.	3.9	11
102	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, 754-770.	3.9	11
103	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.	3.6	11
104	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.	3.6	10
105	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.	3.6	10
106	The spectroscopic and quantum chemical studies of 3,4-difluoroaniline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 143, 265-280.	3.9	10
107	Vibrational spectra, UV and NMR, first order hyperpolarizability and HOMOâ€“LUMO analysis of 2-amino-4-chloro-6-methylpyrimidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 811-824.	3.9	9
108	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, 451-459.	3.9	9

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109	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.	3.9	7
110	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.	3.9	7
111	Synthesis, single crystal structure, spectroscopic characterization andÂmolecular properties of (2E)-3-(2,6-dichlorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one. Journal of Molecular Structure, 2016, 1116, 135-145.	3.6	7
112	Chemistry, 2001, 40, 317-321.	1.6	6
113	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.	3.9	6
114	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, 126-133.	3.9	6
115	Synthesis and investigation of the properties of novel azocalix[4]arenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 146, 151-162.	3.9	6
116	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, 318-330.	3.9	5
117	Spectral investigation and theoretical study of zwitterionic and neutral forms of quinolinic acid. Journal of Molecular Structure, 2015, 1095, 100-111.	3.6	5
118	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.	3.6	3
119	Conformational and spectroscopic behaviors of 2,4-xylyl isothiocyanate. Journal of Molecular Structure, 2015, 1087, 113-120.	3.6	3
120	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, 644-656.	3.9	2
121	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.	3.9	1
122	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.	3.9	1