Mehmet Karabacak

List of Publications by Year
in descending order

122 papers	4,467 citations	81434 41 h-index	150775 59 g-index
124 all docs	124 docs citations	124 times ranked	3223 citing authors

#	Article	IF	Citations
1	Spectral investigations of 2,5-difluoroaniline by using mass, electronic absorption, NMR, and vibrational spectra. Journal of Molecular Structure, 2016, 1123, 284-299.	1.8	12
2	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.	1.8	7
3	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.	2.0	11
4	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.	1.8	11
5	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.	2.0	12
6	Synthesis and investigation of the properties of novel azocalix[4]arenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 146, 151-162.	2.0	6
7	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.	2.0	7
8	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.	2.0	28
9	The spectroscopic and quantum chemical studies of 3,4-difluoroaniline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 143, 265-280.	2.0	10
10	Conformational and spectroscopic behaviors of 2,4-xylyl isothiocyanate. Journal of Molecular Structure, 2015, 1087, 113-120.	1.8	3
11	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.	2.0	12
12	Spectral investigation and theoretical study of zwitterionic and neutral forms of quinolinic acid. Journal of Molecular Structure, 2015, 1095, 100-111.	1.8	5
13	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.	2.0	15
14	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.	2.0	21
15	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.	2.0	18
16	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.	2.0	33
17	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.	2.0	16
18	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.	1.8	21

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19	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.	1.8	62
20	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.	2.0	24
21	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.	2.0	18
22	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.	2.0	54
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, 270-282.	2.0	11
24	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.	2.0	25
25	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.	2.0	18
26	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.	2.0	21
27	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.	2.0	22
28	A comparative study of selected disperse azo dye derivatives based on spectroscopic (FT-IR, NMR and) Tj ETQq0 0 0 rgBT /Overlock 10 T Spectroscopy, 2014, 122, 682-689.	2.0	24
29	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.	2.0	18
30	Spectroscopic (FT-IR, FT-Raman and NMR) and computational studies on 3-methoxyaniline. Journal of Molecular Structure, 2014, 1056-1057, 176-188.	1.8	20
31	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.	2.0	14
32	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.	1.8	48
33	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.	1.8	21
34	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.	1.8	10
35	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.	2.0	19
36	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.	2.0	28

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37	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.	2.0	17
38	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.	2.0	29
39	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.	2.0	27
40	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.	2.0	15
41	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.	2.0	12
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, 622-634.	2.0	20
43	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.	2.0	12
44	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.	2.0	1
45	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.	2.0	9
46	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.	2.0	7
47	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.	2.0	38
48	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.	2.0	15
49	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.	1.8	10
50	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.	2.0	20
51	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.	2.0	51
52	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.	2.0	14
53	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.	2.0	22
54	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.	2.0	59

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55	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.	2.0	83
56	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.	2.0	28
57	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.	2.0	2
58	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.	2.0	9
59	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.	2.0	48
60	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.	1.8	41
61	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.	1.8	57
62	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.	2.0	38
63	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.	2.0	56
64	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.	2.0	105
65	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.	2.0	13
66	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.	2.0	32
67	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.	2.0	24
68	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.	2.0	24
69	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.	2.0	89
70	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.	2.0	30
71	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.	2.0	50
72	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.	2.0	73

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73	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.	2.0	1
74	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.	2.0	42
75	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.	2.0	43
76	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.	2.0	26
77	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.	2.0	106
78	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.	2.0	5
79	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.	2.0	13
80	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.	2.0	6
81	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.	2.0	26
82	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.	2.0	76
83	Spectroscopic properties, NLO, HOMOâ€“LUMO and NBO analysis of 2,5-Lutidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 421-435.	2.0	86
84	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.	1.8	32
85	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.	1.8	3
86	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.	2.0	139
87	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.	2.0	17
88	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.	2.0	6
89	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.	2.0	36
90	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.	2.0	116

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91	FT-IR and FT-Raman, UV spectroscopic investigation of 1-bromo-3-fluorobenzene using DFT (B3LYP,) Tj ETQq1 1 0.784314 rgBT /Overlo Spectroscopy, 2011, 82, 481-492.	2.0	19
92	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.	2.0	32
93	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.	2.0	51
94	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.	2.0	62
95	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.	2.0	17
96	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.	2.0	74
97	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.	1.0	44
98	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.	2.0	116
99	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.	1.8	69
100	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.	2.0	54
101	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.	2.0	33
102	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.	2.0	48
103	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.	1.2	54
104	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.	1.2	77
105	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.	2.0	83
106	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.	1.8	57
107	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.	1.8	109
108	Experimental (UV, NMR, IR and Raman) and theoretical spectroscopic properties of 2-chloro-6-methylaniline. Molecular Physics, 2009, 107, 253-264.	0.8	77

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109	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.	1.8	49
110	The spectroscopic (FT-IR and FT-Raman) and theoretical studies of 5-bromo-salicylic acid. Journal of Molecular Structure, 2009, 919, 215-222.	1.8	82
111	Experimental and theoretical FTâ€IR and FTâ€Raman spectroscopic analysis of N1â€methylâ€2â€chloroaniline. Journal of Physical Organic Chemistry, 2009, 22, 321-330.	0.9	63
112	Infrared and Raman spectrum, molecular structure and theoretical calculation of 3,4-dichlorophenylboronic acid. Journal of Molecular Structure, 2009, 921, 178-187.	1.8	43
113	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.	2.0	42
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