

Mehmet Karabacak

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Synthesis, molecular structure, spectral investigation on (E)-1-(4-bromophenyl)-3-(4-(dimethylamino)phenyl)prop-2-en-1-one. <i>Journal of Molecular Structure</i> , 2016 , 1103, 145-155	3.4	10
121	Synthesis and spectroscopic characterization on 4-(2,5-di-2-thienyl-1H-pyrrol-1-yl) benzoic acid: A DFT approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016 , 152, 8-17	4.4	10
120	The spectroscopic (FT-IR, FT-Raman, dispersive Raman and NMR) study of ethyl-6-chloronicotinate molecule by combined density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016 , 153, 754-70	4.4	8
119	Spectral investigations of 2,5-difluoroaniline by using mass, electronic absorption, NMR, and vibrational spectra. <i>Journal of Molecular Structure</i> , 2016 , 1123, 284-299	3.4	11
118	Synthesis, single crystal structure, spectroscopic characterization and molecular properties of (2E)-3-(2,6-dichlorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one. <i>Journal of Molecular Structure</i> , 2016 , 1116, 135-145	3.4	4
117	Spectral investigation and theoretical study of zwitterionic and neutral forms of quinolinic acid. <i>Journal of Molecular Structure</i> , 2015 , 1095, 100-111	3.4	3
116	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). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 134, 598-607	4.4	10
115	Conformational analysis, spectroscopic study (FT-IR, FT-Raman, UV, ¹ H and ¹³ C NMR), molecular orbital energy and NLO properties of 5-iodosalicylic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 136 Pt B, 295-305	4.4	13
114	Synthesis and DFT calculation of a novel 5,17-di(2-antracenyloxy)-25,27-di(ethoxycarbonylmethoxy)-26,28-dihydroxycalix[4]arene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 136 Pt B, 607-17	4.4	16
113	DFT calculations and experimental FT-IR, FT-Raman, NMR, UV-Vis spectral studies of 3-fluorophenylboronic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 136 Pt B, 306-20	4.4	24
112	Spectroscopic investigation, natural bond orbital analysis, HOMO-LUMO and thermodynamic functions of 2-tert-butyl-5-methyl anisole using DFT (B3LYP) calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 136 Pt B, 451-63	4.4	13
111	FT-IR, FT-Raman, dispersive Raman, NMR spectroscopic studies and NBO analysis of 2-Bromo-1H-Benzimidazol by density functional method. <i>Journal of Molecular Structure</i> , 2015 , 1081, 506-518	3.4	14
110	Synthesis, structure, spectroscopic studies (FT-IR, FT-Raman and UV), normal coordinate, NBO and NLO analysis of salicylaldehyde p-chlorophenylthiosemicarbazone. <i>Journal of Molecular Structure</i> , 2015 , 1081, 400-412	3.4	33
109	FT-IR, FT-Raman, NMR and UV-Vis spectra and DFT calculations of 5-bromo-2-ethoxyphenylboronic acid (monomer and dimer structures). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 137, 1315-33	4.4	19
108	An experimental and density functional study on conformational and spectroscopic analysis of 5-methoxyindole-2-carboxylic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 137, 670-6	4.4	13
107	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 135, 283-95	4.4	41
106	Molecular structure investigation of neutral, dimer and anion forms of 3,4-pyridinedicarboxylic acid: a combined experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 135, 270-82	4.4	10

105	Spectral features, electric properties, NBO analysis and reactivity descriptors of 2-(2-Benzothiazolythio)-Ethanol: Combined experimental and DFT studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 136 Pt C, 1205-15	4.4	15
104	Synthesis and investigation of the properties of novel azocalix[4]arenes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 146, 151-62	4.4	4
103	Molecular structure, vibrational, electronic and thermal properties of 4-vinylcyclohexene by quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 145, 340-352	4.4	4
102	Molecular structure, spectroscopic characterization, HOMO and LUMO analysis of 3,3Sdiaminobenzidine with DFT quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 150, 83-93	4.4	19
101	The spectroscopic and quantum chemical studies of 3,4-difluoroaniline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 143, 265-80	4.4	8
100	Conformational and spectroscopic behaviors of 2,4-xylyl isothiocyanate. <i>Journal of Molecular Structure</i> , 2015 , 1087, 113-120	3.4	3
99	Quantum chemical calculation (electronic and topologic) and experimental (FT-IR, FT-Raman and UV) analysis of isonicotinic acid N-oxide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 140, 85-95	4.4	11
98	Synthesis, crystal structure and ab initio/DFT calculations of a derivative of dithiophosphonates. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 122, 582-90	4.4	17
97	Vibrational (FT-IR and FT-Raman), electronic (UV-Vis), NMR (1H and 13C) spectra and reactivity analyses of 4,5-dimethyl-o-phenylenediamine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 130, 516-25	4.4	15
96	A comparative study of selected disperse azo dye derivatives based on spectroscopic (FT-IR, NMR and UV-Vis) and nonlinear optical behaviors. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 122, 682-9	4.4	17
95	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 122, 1-14	4.4	15
94	Spectroscopic (FT-IR, FT-Raman and NMR) and computational studies on 3-methoxyaniline. <i>Journal of Molecular Structure</i> , 2014 , 1056-1057, 176-188	3.4	16
93	Quantum-chemical (DFT, MP2) and spectroscopic studies (FT-IR and UV) of monomeric and dimeric structures of 2(3H)-Benzothiazolone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 120, 126-36	4.4	12
92	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. <i>Journal of Molecular Structure</i> , 2014 , 1058, 79-96	3.4	43
91	Experimental (FT-IR, FT-Raman, UV-Vis, 1H and 13CNMR) and computational (density functional theory) studies on 3-bromophenylboronic acid. <i>Journal of Molecular Structure</i> , 2014 , 1076, 358-372	3.4	15
90	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. <i>Journal of Molecular Structure</i> , 2014 , 1076, 639-650	3.4	7
89	Identification of structural and spectral features of synthesized cyano-stilbene dye derivatives: a comparative experimental and DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 120, 144-50	4.4	15
88	FT-IR, FT-Raman, NMR, UV and quantum chemical studies on monomeric and dimeric conformations of 3,5-dimethyl-4-methoxybenzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 123, 352-62	4.4	22

87	FT-IR, FT-Raman and UV spectroscopic investigation, electronic properties, electric moments, and NBO analysis of anethole using quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 133, 165-77	4.4	16
86	The spectroscopic (FT-IR, FT-Raman, UV and NMR) first order hyperpolarizability and HOMO-LUMO analysis of dansyl chloride. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 117, 234-44	4.4	11
85	Experimental and theoretical FTIR and FT-Raman spectroscopic analysis of 1-pyrenecarboxylic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 114, 509-19	4.4	25
84	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 115, 753-66	4.4	23
83	Molecular structure, spectroscopic characterization (FT-IR, FT-Raman, UV and NMR), HOMO and LUMO analysis of 3-ethynylthiophene with DFT quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 115, 709-18	4.4	13
82	Multi-photon absorption effect and intra-molecular charge transfer of donor-acceptor chromophore ethyl p-amino benzoate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 108, 197-210	4.4	12
81	FT-IR and FT-Raman, NMR and UV spectroscopic investigation and hybrid computational (HF and DFT) analysis on the molecular structure of mesitylene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 116, 622-34	4.4	15
80	Determination of conformational and spectroscopic features of ethyl trans-alfa-cyano-3-indole-acrylate compound: an experimental and quantum chemical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 104, 428-36	4.4	12
79	Synthesis, conformational and spectroscopic characterization of monomeric styrene derivatives having pendant p-substituted benzylic ether groups. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 111, 97-103	4.4	1
78	The infrared, Raman, NMR and UV spectra, ab initio calculations and spectral assignments of 2-amino-4-chloro-6-methoxypyrimidine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 116, 451-9	4.4	8
77	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 114, 38-45	4.4	6
76	Molecular structure, electronic properties, NLO, NBO analysis and spectroscopic characterization of Gabapentin with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 109, 298-307	4.4	30
75	Determination of structural, spectrometric and nonlinear optical features of 2-(4-hydroxyphenylazo)benzoic acid by experimental techniques and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 105, 80-7	4.4	11
74	FT-IR, FT-Raman and UV spectral investigation; computed frequency estimation analysis and electronic structure calculations on 4-hydroxypteridine. <i>Journal of Molecular Structure</i> , 2013 , 1038, 114-125	4.4	7
73	Ultrafast optical nonlinearity, electronic absorption, vibrational spectra and solvent effect studies of ninhydrin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 109, 331-43	4.4	14
72	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 103, 101-11	4.4	37
71	FT-IR, FT-Raman and UV spectral investigation: computed frequency estimation analysis and electronic structure calculations on 1-bromo-2-methylnaphthalene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 101, 314-24	4.4	10
70	Spectroscopic (FT-IR/FT-Raman) and computational (HF/DFT) investigation and HOMO/LUMO/MEP analysis on 2-amino-4-chlorophenol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 104, 337-51	4.4	20

69	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 85, 43-52	4.4	36
68	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 85, 145-54	4.4	44
67	FT-IR, FT-Raman, NMR and UV-vis spectra, vibrational assignments and DFT calculations of 4-butyl benzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 85, 179-89	4.4	85
66	A structural and spectroscopic study on para-aminohippuric acid with experimental and theoretical approaches. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 85, 241-50	4.4	11
65	FT-IR, FT-Raman and UV spectral investigation; computed frequency estimation analysis and electronic structure calculations on 1-nitronaphthalene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 85, 251-60	4.4	28
64	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 87, 261-70	4.4	19
63	Spectroscopic (FT-IR, FT-Raman and UV-vis) investigation and frontier molecular orbitals analysis on 3-methyl-2-nitrophenol using hybrid computational calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 86, 139-51	4.4	23
62	FT-IR, FT-Raman, UV spectra and DFT calculations on monomeric and dimeric structure of 2-amino-5-bromobenzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 86, 590-9	4.4	78
61	Molecular structure, spectroscopic (FT-IR, FT-Raman, ¹³ C and ¹ H NMR, UV), polarizability and first-order hyperpolarizability, HOMO and LUMO analysis of 4-methylbiphenyl-2-carbonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 87, 273-85	4.4	26
60	FT-IR, FT-Raman and UV spectral investigation: computed frequency estimation analysis and electronic structure calculations on chlorobenzene using HF and DFT. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 88, 37-48	4.4	36
59	FT-IR, FT-Raman, ab initio, HF and DFT studies, NBO, HOMO-LUMO and electronic structure calculations on 4-chloro-3-nitrotoluene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 89, 137-48	4.4	58
58	Neural network consistent empirical physical formula construction for density functional theory based nonlinear vibrational absorbance and intensity of 6-chloronicotinic acid molecule. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 90, 55-62	4.4	0
57	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 91, 83-96	4.4	37
56	The spectroscopic (FTIR, FT-Raman, NMR and UV), first-order hyperpolarizability and HOMO-LUMO analysis of methylboronic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 92, 67-77	4.4	30
55	The spectroscopic (FT-IR, FT-Raman, UV) and first order hyperpolarizability, HOMO and LUMO analysis of 3-aminobenzophenone by density functional method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 92, 365-76	4.4	25
54	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 93, 22-31	4.4	83
53	Spectroscopic analysis (FT-IR/FT-Raman) and molecular structure investigation on m-fluoronitrobenzene using hybrid computational calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 94, 318-30	4.4	3
52	Analysis of vibrational spectra (FT-IR and FT-Raman) and nonlinear optical properties of organic 2-chloro-p-xylene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 94, 36-47	4.4	13

51	Synthesis, FT-IR, FT-Raman, dispersive Raman and NMR spectroscopic study of a host molecule which potential applications in sensor devices. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 94, 126-33	4.4	6
50	Vibrational spectroscopic studies, NLO, HOMO-LUMO and electronic structure calculations of trichlorotoluene using HF and DFT. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 94, 53-64	4.4	20
49	Spectroscopic (infrared, Raman, UV and NMR) analysis, Gaussian hybrid computational investigation (MEP maps/HOMO and LUMO) on cyclohexanone oxime. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 96, 207-20	4.4	58
48	Spectroscopic properties, NLO, HOMO-LUMO and NBO analysis of 2,5-Lutidine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 96, 421-35	4.4	66
47	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. <i>Journal of Molecular Structure</i> , 2012 , 1017, 1-13	3.4	28
46	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 97, 556-67	4.4	49
45	Spectroscopic (FT-IR, FT-Raman, UV and NMR) investigation and NLO, HOMO-LUMO, NBO analysis of organic 2,4,5-trichloroaniline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 97, 231-45	4.4	56
44	Synthesis, spectroscopic characterization and quantum chemical computational studies of (S)-N-benzyl-1-phenyl-5-(pyridin-2-yl)-pent-4-yn-2-amine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 97, 435-48	4.4	25
43	A comparative experimental and quantum chemical study on monomeric and dimeric structures of 3,5-dibromoanthranilic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 96, 644-56	4.4	2
42	Vibrational spectra, UV and NMR, first order hyperpolarizability and HOMO-LUMO analysis of 2-amino-4-chloro-6-methylpyrimidine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 97, 811-24	4.4	9
41	Molecular structure investigation and spectroscopic studies on 2,3-difluorophenylboronic acid: a combined experimental and theoretical analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 97, 892-908	4.4	41
40	The spectroscopic (FTIR, FT-Raman, UV and NMR), first-order hyperpolarizability and HOMO-LUMO analysis of 4-amino-5-chloro-2-methoxybenzoic acid. <i>Journal of Molecular Structure</i> , 2012 , 1024, 1-12	3.4	32
39	FT-Raman, FT-IR, UV spectra and DFT and ab initio calculations on monomeric and dimeric structures of 3,5-pyridinedicarboxylic acid. <i>Journal of Molecular Structure</i> , 2012 , 1027, 1-14	3.4	50
38	Neural network consistent empirical physical formula construction for DFT based nonlinear vibrational spectra intensities of N-(2-methylphenyl) and N-(3-methylphenyl) methanesulfonamides. <i>Journal of Molecular Structure</i> , 2011 , 1006, 642-649	3.4	2
37	Natural bond orbital analysis, electronic structure, non-linear properties and vibrational spectral analysis of L-histidinium bromide monohydrate: a density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 81, 85-98	4.4	98
36	FT-IR and FT-Raman vibrational analysis, ab initio HF and DFT simulations of isocyanic acid 1-naphthyl ester. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 81, 504-18	4.4	16
35	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 82, 79-90	4.4	6
34	FT-IR, FT-Raman, ab initio and DFT structural, vibrational frequency and HOMO-LUMO analysis of 1-naphthaleneacetic acid methyl ester. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 82, 169-80	4.4	30

33	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 82, 444-55	4.4	89
32	FT-IR and FT-Raman, UV spectroscopic investigation of 1-bromo-3-fluorobenzene using DFT (B3LYP, B3PW91 and MPW91PW91) calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 82, 481-92	4.4	16
31	Spectroscopic (NMR, UV, FT-IR and FT-Raman) analysis and theoretical investigation of nicotinamide N-oxide with density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 83, 250-8	4.4	26
30	Vibrational spectroscopy (FT-IR and FT-Raman) investigation, and hybrid computational (HF and DFT) analysis on the structure of 2,3-naphthalenediol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 83, 540-52	4.4	37
29	FT-IR, UV-vis, ¹ H and ¹³ C NMR spectra and the equilibrium structure of organic dye molecule disperse red 1 acrylate: a combined experimental and theoretical analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 83, 561-9	4.4	53
28	Experimental (FT-IR, FT-Raman) and theoretical (HF and DFT) investigation and HOMO and LUMO analysis on the structure of p-fluoronitrobenzene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 83, 575-86	4.4	17
27	Molecular structure, vibrational spectroscopic, first-order hyperpolarizability and HOMO, LUMO studies of 2-aminobenzimidazole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 84, 184-95	4.4	60
26	Synthesis, molecular conformation, vibrational, electronic transition, and chemical shift assignments of 4-(thiophene-3-ylmethoxy)phthalonitrile: a combined experimental and theoretical analysis. <i>Structural Chemistry</i> , 2011 , 22, 45-56	1.8	41
25	Molecular structure, vibrational, UV and NBO analysis of 4-chloro-7-nitrobenzofurazan by DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 79, 1162-70	4.4	86
24	FT-IR and FT-Raman spectra, vibrational assignments, NBO analysis and DFT calculations of 2-amino-4-chlorobenzonitrile. <i>Journal of Molecular Structure</i> , 2011 , 985, 148-156	3.4	56
23	Experimental (FT-IR and FT-Raman), electronic structure and DFT studies on 1-methoxynaphthalene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 79, 646-53	4.4	46
22	Structural and spectroscopic characterization of 2,3-difluorobenzoic acid and 2,4-difluorobenzoic acid with experimental techniques and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 79, 1511-9	4.4	30
21	Vibrational spectroscopic analysis of 2-chlorotoluene and 2-bromotoluene: a combined experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010 , 77, 1005-13	4.4	40
20	Experimental vibrational spectra (Raman, infrared) and DFT calculations on monomeric and dimeric structures of 2- and 6-bromonicotinic acid. <i>Journal of Raman Spectroscopy</i> , 2010 , 41, 98-105	2.3	49
19	FT-Raman, FT-IR spectra and DFT calculations on monomeric and dimeric structures of 5-fluoro- and 5-chloro-salicylic acid. <i>Journal of Raman Spectroscopy</i> , 2010 , 41, 1085-1097	2.3	71
18	FT-IR, FT-Raman, NMR spectra and DFT calculations on 4-chloro-N-methylaniline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010 , 75, 1523-9	4.4	67
17	DFT based computational study on the molecular conformation, NMR chemical shifts and vibrational transitions for N-(2-methylphenyl) methanesulfonamide and N-(3-methylphenyl) methanesulfonamide. <i>Journal of Molecular Structure</i> , 2010 , 968, 108-114	3.4	52
16	FT-IR, UV spectroscopic and DFT quantum chemical study on the molecular conformation, vibrational and electronic transitions of 2-aminoterephthalic acid. <i>Journal of Molecular Structure</i> , 2010 , 982, 22-27	3.4	91

15	Experimental (UV, NMR, IR and Raman) and theoretical spectroscopic properties of 2-chloro-6-methylaniline. <i>Molecular Physics</i> , 2009 , 107, 253-264	1.7	67
14	Theoretical investigation on the molecular structure, Infrared, Raman and NMR spectra of para-halogen benzenesulfonamides, 4-X-C ₆ H ₄ SO ₂ NH ₂ (X = Cl, Br or F). <i>Journal of Molecular Structure</i> , 2009 , 919, 26-33	3.4	44
13	The spectroscopic (FT-IR and FT-Raman) and theoretical studies of 5-bromo-salicylic acid. <i>Journal of Molecular Structure</i> , 2009 , 919, 215-222	3.4	70
12	Experimental and theoretical FT-IR and FT-Raman spectroscopic analysis of N1-methyl-2-chloroaniline. <i>Journal of Physical Organic Chemistry</i> , 2009 , 22, 321-330	2.1	56
11	Infrared and Raman spectrum, molecular structure and theoretical calculation of 3,4-dichlorophenylboronic acid. <i>Journal of Molecular Structure</i> , 2009 , 921, 178-187	3.4	39
10	FT-IR, FT-Raman vibrational spectra and molecular structure investigation of 2-chloro-4-methylaniline: a combined experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 72, 1076-83	4.4	37
9	Molecular structure and vibrational assignments of hippuric acid: a detailed density functional theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009 , 74, 1197-203	4.4	46
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7	X-ray, FT-Raman, FT-IR spectra and ab initio HF, DFT calculations of 2-[(5-methylisoxazol-3-yl)amino]-2-oxo-ethyl methacrylate. <i>Journal of Molecular Structure</i> , 2008 , 886, 148-157	3.4	63
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