Poonam Tandon

List of Publications by Year in descending order

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		196777	312153
240	3,340	29	41
papers	citations	h-index	g-index

240	240	240	3470
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structural insights, spectral and H-bond analyses, of nitrofurantoin-phenazine cocrystal and comparison of its chemical reactivity with other nitrofurantoin cocrystals. Journal of Molecular Structure, 2022, 1247, 131387.	1.8	1
2	Spectroscopic and quantum chemical study on a non-linear optical material 4-[(1E)-3-(5-chlorothiophen-2-yl)-3-oxoprop-1-en-1-yl] phenyl4-methylbenzene-1-sulfonate. Journal of Molecular Structure, 2022, 1248, 131540.	1.8	4
3	ab-Initio and DFT study of HCN: Role of temperature for the formation of HCN molecule in the interstellar medium. Journal of Molecular Structure, 2022, 1248, 131460.	1.8	1
4	Molecular Structural, Hydrogen Bonding Interactions, and Chemical Reactivity Studies of Ezetimibe-L-Proline Cocrystal Using Spectroscopic and Quantum Chemical Approach. Frontiers in Chemistry, 2022, 10, 848014.	1.8	7
5	Experimental and Quantum Chemical Studies of Nicotinamide-Oxalic Acid Salt: Hydrogen Bonding, AIM and NBO Analysis. Frontiers in Chemistry, 2022, 10, 855132.	1.8	7
6	Molecular structure and quantum descriptors of cefradine by using vibrational spectroscopy (IR and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 and Biomolecular Spectroscopy, 2021, 246, 118976.	2.0	15
7	Quantum chemical study on the formation of isopropyl cyanide and its linear isomer in the interstellar medium. International Journal of Astrobiology, 2021, 20, 62-72.	0.9	5
8	Spectroscopic characterization and structural insights of 4-[(1E)-3-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl] phenyl 4-methylbenzene-1-sulfonate using vibrational, electronic spectra and quantum chemical calculations. Journal of Molecular Structure, 2021, 1225, 129144.	1.8	6
9	Development of polyaniline/ZnO-Ru nanocomposite as a potential LPG sensing material operable at room temperature. Journal of Materials Science: Materials in Electronics, 2021, 32, 6110-6122.	1.1	4
10	Molecular interactions and vibrational properties of ricobendazole: Insights from quantum chemical calculation and spectroscopic methods. Journal of Molecular Structure, 2021, 1230, 129889.	1.8	4
11	Fabrication of nanostructured MgO and Zn-doped MgO as an efficient LPG sensing materials operable at room temperature. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	1.1	5
12	Molecular Structure, Spectral Investigations, Hydrogen Bonding Interactions and Reactivity-Property Relationship of Caffeine-Citric Acid Cocrystal by Experimental and DFT Approach. Frontiers in Chemistry, 2021, 9, 708538.	1.8	13
13	N-Acetylcysteine versus arsenic poisoning: A mechanistic study of complexation by molecular spectroscopy and density functional theory. Journal of Molecular Liquids, 2021, 340, 117168.	2.3	6
14	Structural properties of a novel heterocyclic chalcones derivative, (E)-3-(5-methyl furan-2-yl)-1-phenyl propâ€‘2-en-1-one: A spectroscopic and DFT perception. Journal of Molecular Structure, 2021, 1244, 130973.	1.8	2
15	Vibrational and conformational analysis of structural phase transition in Estradiol 17Î² valerate with temperature. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 263, 120219.	2.0	0
16	Non-covalent interactions and spectroscopic study of chalcone derivative 1-(4-chlorophenyl)-3-(5-methylfuran-2-yl) prop-2-en-1-one. Journal of Molecular Structure, 2020, 1201, 127145.	1.8	12
17	Computational evaluation on molecular stability, reactivity, and drug potential of frovatriptan from DFT and molecular docking approach. Computational and Theoretical Chemistry, 2020, 1191, 113031.	1.1	31
18	Nanostructured cobalt antimonate: a fast responsive and highly stable sensing material for liquefied petroleum gas detection at room temperature. RSC Advances, 2020, 10, 33770-33781.	1.7	10

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19	Attenuating the increased level of creatinine by N â€acetylcysteine: Raman spectroscopy and density functional theoryâ€based monitoring of in vitro complexation in aqueous solution. Journal of Raman Spectroscopy, 2020, 51, 1056-1066.	1.2	3
20	Vibrational spectroscopic, NBO, AIM, and multiwfn study of tectorigenin: A DFT approach. Journal of Molecular Structure, 2020, 1217, 128443.	1.8	43
21	A stable and highly sensitive room-temperature liquefied petroleum gas sensor based on nano-cubes/cuboids of zinc antimonate. RSC Advances, 2020, 10, 20349-20357.	1.7	18
22	Development and characterization of varying percentages of Ru-doped ZnO (xRu:ZnO; 1%â€‰â‰€â€‰xâ€‰â‰€â€‰5%) as a potential material for LPG sensing at room temperature. Applied Physics A: Materials Science and Processing, 2020, 126, 1.	1.1	9
23	Physicochemical and Pharmacokinetic Analysis of Anacardic Acid Derivatives. ACS Omega, 2020, 5, 6021-6030.	1.6	44
24	An efficient room-temperature liquefied petroleum gas sensor based on trirutile copper antimonate nano-polygons. New Journal of Chemistry, 2020, 44, 11949-11958.	1.4	4
25	Molecular Interactions within the Crystal Packing of Busulfan (DNA Cross-Linking Agent) by Hirshfeld Surface Analysis. Current Physical Chemistry, 2020, 10, 199-205.	0.1	0
26	Theoretical approach to study the formation of C₂H₄O₂ isomers in interstellar medium through reaction between interstellar formaldehyde molecules*. Research in Astronomy and Astrophysics, 2020, 20, 014.	0.7	9
27	Structural reactivity analyses of a neoflavonoid 4-methoxydalbergione using vibrational spectroscopy and quantum chemical calculations. Journal of Molecular Structure, 2019, 1175, 28-38.	1.8	7
28	Combined spectroscopic and quantum chemical approach to study the effect of hydrogen bonding interactions in ezetimibe. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 206, 246-253.	2.0	9
29	Structural and Reactivity Analyses of Nitrofurantoinâ€“4-dimethylaminopyridine Salt Using Spectroscopic and Density Functional Theory Calculations. Crystals, 2019, 9, 413.	1.0	7
30	Nitrogen donor ligand for capping ZnS quantum dots: a quantum chemical and toxicological insight. RSC Advances, 2019, 9, 28510-28524.	1.7	13
31	Vibrational spectra, hydrogen bonding interactions and chemical reactivity analysis of nicotinamideâ€“citric acid cocrystals by an experimental and theoretical approach. New Journal of Chemistry, 2019, 43, 15956-15967.	1.4	10
32	A theoretical study on molecular structure, chemical reactivity and molecular docking studies on dalbergin and methyldalbergin. Journal of Molecular Structure, 2019, 1183, 100-106.	1.8	10
33	Fabrication and characterization of polyaniline, polyaniline/MgO(30%) and polyaniline/MgO(40%) nanocomposites for their employment in LPG sensing at room temperature. Journal of Materials Science: Materials in Electronics, 2019, 30, 4487-4498.	1.1	22
34	A novel approach to design febuxostat-salicylic acid eutectic system: evaluation and characterization. CrystEngComm, 2019, 21, 310-320.	1.3	10
35	Theoretical Study of Possible Reaction Mechanisms for the Formation of Carbodiimide in the Interstellar Medium (ISM) and Polarizabilities of Carbodiimide. Origins of Life and Evolution of Biospheres, 2019, 49, 89-103.	0.8	4
36	Nitrofurantoin-melamine monohydrate (cocrystal hydrate): Probing the role of H-bonding on the structure and properties using quantum chemical calculations and vibrational spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 221, 117170.	2.0	11

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37	Study of molecular structure and hydrogen bond interactions in dipfluzine-benzoic acid (DIP-BEN) cocrystal using spectroscopic and quantum chemical method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 216, 7-14.	2.0	11
38	Spectroscopic (FT-IR, FT-Raman, and ¹³C SS-NMR) and quantum chemical investigations to provide structural insights into nitrofurantoinâ€“4-hydroxybenzoic acid cocrystals. New Journal of Chemistry, 2019, 43, 7136-7149.	1.4	6
39	Preparation of Nanostructured Co3O4 and Ru-Doped Co3O4 and Their Applicability in Liquefied Petroleum Gas Sensing. Journal of Materials Engineering and Performance, 2019, 28, 7592-7601.	1.2	4
40	Development of a potential LPG sensor based on a PANIâ€“Co₃O₄ nanocomposite that functions at room temperature. New Journal of Chemistry, 2019, 43, 17340-17350.	1.4	9
41	Formation of Acetaldehyde in the Interstellar Medium from the Reaction of Methanol and Atomic Carbon in Interstellar Water Ice. Springer Proceedings in Physics, 2019, , 415-422.	0.1	2
42	Evaluation of non-covalent interactions of chlorambucil (monomer and dimer) and its interaction with biological targets: Vibrational frequency shift, electron density topological and automated docking analysis. Arabian Journal of Chemistry, 2018, 11, 591-608.	2.3	3
43	Structural and vibrational characteristics of a non-linear optical material 3-(4-nitrophenyl)-1-(pyridine-3-yl) prop-2-en-1-one probed by quantum chemical computation and spectroscopic techniques. Journal of Molecular Structure, 2018, 1164, 180-190.	1.8	12
44	Phase transition analysis of V-shaped liquid crystal: Combined temperature-dependent FTIR and density functional theory approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 188, 561-570.	2.0	8
45	A combined experimental (IR, Raman and UVâ€“Vis) and quantum chemical study of canadine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 191, 249-258.	2.0	4
46	Structural and spectroscopic analysis of indole alkaloids: Molecular docking and DFT approach. Journal of Molecular Structure, 2018, 1153, 262-274.	1.8	4
47	Spectroscopic and theoretical studies of dalbergin and Methyldalbergin. Journal of Molecular Structure, 2018, 1156, 243-254.	1.8	4
48	Molecular structure and hydrogen bond interactions of a paracetamolâ€“4,4â€²-bipyridine cocrystal studied using a vibrational spectroscopic and quantum chemical approach. CrystEngComm, 2018, 20, 213-222.	1.3	18
49	A60 PREDICTIVE FACTORS OF INTENSIVE CARE UNIT ADMISSION AND MORTALITY IN CIRRHOTIC PATIENTS WITH UPPER GASTROINTESTINAL BLEEDS. Journal of the Canadian Association of Gastroenterology, 2018, 1, 95-95.	0.1	0
50	A124 THE DIAGNOSTIC ACCURACY OF BLOOD AND TISSUE-BASED TESTS FOR CYTOMEGALOVIRUS REACTIVATION IN INFLAMMATORY BOWEL DISEASE: A SYSTEMATIC REVIEW AND META-ANALYSIS. Journal of the Canadian Association of Gastroenterology, 2018, 1, 216-216.	0.1	0
51	Monitoring the in Vitro Thiazolidine Ring Formation of Antioxidant Drug N-Acetyl-l-cysteine at Basic pH and Detection of Reaction Intermediates: A Raman Spectroscopic and Ab Initio Study. Journal of Physical Chemistry B, 2018, 122, 10306-10314.	1.2	3
52	Spectroscopic and molecular structure (monomeric and dimeric model) investigation of Febuxostat: A combined experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 1-12.	2.0	11
53	A57 ACUTE VARICEAL GASTROINTESTINAL BLEEDING DOES NOT INFER POOR SURVIVAL COMPARED TO NON-VARICEAL BLEEDING IN PATIENTS WITH CIRRHOSIS: A RETROSPECTIVE, OBSERVATIONAL STUDY. Journal of the Canadian Association of Gastroenterology, 2018, 1, 91-92.	0.1	1
54	Fabrication of copper ferrite porous hierarchical nanostructures for an efficient liquefied petroleum gas sensor. Sensors and Actuators B: Chemical, 2017, 244, 806-814.	4.0	29

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55	Formation of E-cyanomethamine in a nitrile rich environment. Research in Astronomy and Astrophysics, 2017, 17, 1.	0.7	9
56	Study of Cr â†' SmA phase transition and hydrogen bonding in four-ring bent-core liquid crystal. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 178, 142-150.	2.0	6
57	Temperature-dependent infrared study of phase transitions in bent-core liquid crystalline compound 12O(OH)2MeO10. Vibrational Spectroscopy, 2017, 90, 38-45.	1.2	3
58	Experimental and quantum chemical studies on the structure and vibrational spectra of cearoin (a) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.4	1
59	Spectroscopic (far or terahertz, mid-infrared and Raman) investigation, thermal analysis and biological activity of piplartine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 184, 368-381.	2.0	10
60	Structural characterization, spectroscopic signatures, nonlinear optical response, and antioxidant property of 4-benzyloxybenzaldehyde and its binding activity with microtubule-associated tau protein. Journal of Molecular Structure, 2017, 1143, 362-370.	1.8	9
61	Study of molecular interactions and chemical reactivity of the nitrofurantoinâ€"3-aminobenzoic acid cocrystal using quantum chemical and spectroscopic (IR, Raman, ¹³C SS-NMR) approaches. CrystEngComm, 2017, 19, 3921-3930.	1.3	41
62	Structural insights, protein-ligand interactions and spectroscopic characterization of isoformononetin. Journal of Molecular Structure, 2017, 1133, 479-491.	1.8	3
63	Molecular structure, nonlinear optical studies and spectroscopic analysis of chalcone derivative (2E)-3-[4-(methylsulfanyl) phenyl]-1-(3-bromophenyl) prop-2-en-1-one by DFT calculations. Journal of Molecular Structure, 2017, 1150, 166-178.	1.8	33
64	Study of molecular structure, chemical reactivity and H-bonding interactions in the cocrystal of nitrofurantoin with urea. New Journal of Chemistry, 2017, 41, 11069-11078.	1.4	24
65	A theoretical quantum chemical study of alanine formation in interstellar medium. European Physical Journal D, 2017, 71, 1.	0.6	9
66	Study of hydrogen-bonding, vibrational dynamics and structure-activity relationship of genistein using spectroscopic techniques coupled with DFT. Journal of Molecular Structure, 2017, 1130, 929-939.	1.8	6
67	Molecular structure, spectroscopic (FT-IR, FT Raman, UV, NMR and THz) investigation and hyperpolarizability studies of 3-(2-Chloro-6-fluorophenyl)-1-(2-thienyl) prop-2-en-1-one. Journal of Molecular Structure, 2017, 1129, 292-304.	1.8	35
68	Study of vibrational spectra and hydrogen bonding network in dimeric and tetrameric model of ampicillin using DFT and AIM approach. Journal of Molecular Structure, 2017, 1131, 225-235.	1.8	11
69	Characterization and intramolecular bonding patterns of busulfan: Experimental and quantum chemical approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 173, 390-399.	2.0	10
70	Evaluation of Structural Isomers, Molecular Interactions, Reactivity Descriptors, and Vibrational Analysis of Tretinoin. Analytical Sciences, 2017, 33, 83-87.	0.8	2
71	Conformational Study and Vibrational Spectroscopic (FT-IR and FT-Raman) Analysis of an Alkaloid-Borreverine Derivative. Analytical Sciences, 2017, 33, 99-104.	0.8	15
72	An Investigation of nonlinear optical properties, electronic behaviour and structure-NLO relation of 1, 3-Bis(3, 4-dimethoxyphenyl)prop-2-en-1-one: A theoretical and computational study. Asian Journal of Research in Chemistry, 2017, 10, 101.	0.2	4

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73	Combined spectroscopic and quantum chemical studies of ezetimibe. Journal of Molecular Structure, 2016, 1125, 193-203.	1.8	12
74	Computational approaches to find the active binding sites of biological targets against busulfan. Journal of Molecular Modeling, 2016, 22, 142.	0.8	41
75	Preparation and characterization of nanocrystalline nickel ferrite thin films for development of a gas sensor at room temperature. Journal of Materials Science: Materials in Electronics, 2016, 27, 8047-8054.	1.1	18
76	Studies of molecular structure, hydrogen bonding and chemical activity of a nitrofurantoin-<scp>l</scp>-proline cocrystal: a combined spectroscopic and quantum chemical approach. RSC Advances, 2016, 6, 74135-74154.	1.7	37
77	Synthesis, Characterization and Gas Sensing Capability of NixCu1â^'xFe2O4 (0.0Ââ‰ÂxÂâ‰Â0.8) Nanostructures Prepared via Solâ€“Gel Method. Journal of Inorganic and Organometallic Polymers and Materials, 2016, 26, 1392-1403.	1.9	16
78	Spectroscopic, quantum chemical calculation and molecular docking of dipfluzine. Journal of Molecular Structure, 2016, 1125, 751-762.	1.8	11
79	Synthesis and Characterization of Nanostructured Magnesium Oxide: Insight from Solid-State Density Functional Theory Calculations. Journal of Inorganic and Organometallic Polymers and Materials, 2016, 26, 1413-1420.	1.9	21
80	Simplified risk stratification criteria for identification of patients with MRSA bacteremia at low risk of infective endocarditis: implications for avoiding routine transesophageal echocardiography in MRSA bacteremia. European Journal of Clinical Microbiology and Infectious Diseases, 2016, 35, 261-268.	1.3	18
81	Study of phase transitions in a bent-core liquid crystal probed by infrared spectroscopy. Vibrational Spectroscopy, 2016, 86, 24-34.	1.2	9
82	A combined experimental and theoretical approach to study SmC â†' NcybC phase transition in a four-ring bent-core liquid crystal. New Journal of Chemistry, 2016, 40, 6834-6847.	1.4	11
83	Nickel antimony oxide (NiSb2O6): A fascinating nanostructured material for gas sensing application. Chemical Physics Letters, 2016, 646, 41-46.	1.2	28
84	Vibrational analysis and chemical activity of paracetamolâ€“oxalic acid cocrystal based on monomer and dimer calculations: DFT and AIM approach. RSC Advances, 2016, 6, 10024-10037.	1.7	60
85	A computational study on molecular structure, multiple interactions, chemical reactivity and molecular docking studies on 6[D (â^) Î±-amino-phenyl-acetamido] penicillanic acidÂ(ampicillin). Molecular Simulation, 2016, 42, 863-873.	0.9	13
86	Combine experimental and theoretical investigation on an alkaloidâ€“Dimethylisoborreverine. Journal of Molecular Structure, 2016, 1103, 187-201.	1.8	4
87	Fabrication of Cu/Pd bimetallic nanostructures with high gas sorption ability towards development of LPG sensor. Materials Chemistry and Physics, 2015, 154, 16-21.	2.0	26
88	Spectroscopic and quantum chemical analysis of a natural product â€“ Hayatin hydrochloride. Journal of Molecular Structure, 2015, 1093, 101-112.	1.8	3
89	Tip enhanced Raman spectroscopy, DFT and PED calculations of 4â€³-trimethylsilylethylsulfanyl-4,4â€²-di(phenyleneethynylene)benzene thiol adsorbed on silver. Journal of Molecular Structure, 2015, 1099, 534-542.	1.8	3
90	Molecular structure, spectral analysis and hydrogen bonding analysis of ampicillin trihydrate: a combined DFT and AIM approach. New Journal of Chemistry, 2015, 39, 9800-9812.	1.4	53

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91	Molecular structure, spectral investigation (1H NMR, 13C NMR, UVâ€“Visible, FT-IR, FT-Raman), NBO, intramolecular hydrogen bonding, chemical reactivity and first hyperpolarizability analysis of formononetin [7-hydroxy-3(4-methoxyphenyl)chromone]: A quantum chemical study. Journal of Molecular Structure, 2015, 1084, 55-73.	1.8	36
92	Frontal polymerization of acrylamide complex with nanostructured ZnS and PbS: Their characterizations and sensing applications. Sensors and Actuators B: Chemical, 2015, 207, 460-469.	4.0	20
93	Synthesis, characterization and performance of zinc ferrite nanorods for room temperature sensing applications. Journal of Alloys and Compounds, 2015, 618, 475-483.	2.8	90
94	Formation of cyanoallene (buta-2, 3-dienenitrile) in the interstellar medium: a quantum chemical and spectroscopic study. Research in Astronomy and Astrophysics, 2014, 14, 275-284.	0.7	5
95	Molecular structure and vibrational spectra of Nâ€acetylglycine oligomers and polyglycine I using DFT approach. Biopolymers, 2014, 101, 795-813.	1.2	7
96	Reaction Between CH2 and HCCN: A Theoretical Approach to Acrylonitrile Formation in the Interstellar Medium. Origins of Life and Evolution of Biospheres, 2014, 44, 143-157.	0.8	8
97	Quantum chemical and experimental studies on the structure and vibrational spectra of an alkaloidâ€“Corlumine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 470-480.	2.0	9
98	Mechanism for leakage current conduction in manganese doped Bi3.25La0.75Ti3O12 (BLT) ferroelectric thin films. Journal of Alloys and Compounds, 2014, 606, 132-138.	2.8	19
99	Quantum chemical study on influence of intermolecular hydrogen bonding on the geometry, the atomic charges and the vibrational dynamics of 2,6-dichlorobenzonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 121, 464-482.	2.0	35
100	Polymer-matrix nanocomposite gas-sensing materials. Inorganic Materials, 2014, 50, 296-305.	0.2	22
101	Synthesis, characterization, magnetic measurements and liquefied petroleum gas sensing properties of nanostructured cobalt ferrite and ferric oxide. Materials Science in Semiconductor Processing, 2014, 23, 122-135.	1.9	38
102	Synthesis, characterization and liquefied petroleum gas sensing of cobalt acetylenedicarboxylate and its polymer. Sensors and Actuators B: Chemical, 2014, 192, 503-511.	4.0	7
103	Molecular structure (monomeric and dimeric) and hydrogen bonds in 5-benzyl 2-thiohydantoin studied by FT-IR and FT-Raman spectroscopy and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 15-26.	2.0	18
104	Conformational analysis and vibrational study of daidzein by using FT-IR and FT-Raman spectroscopies and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 405-415.	2.0	37
105	Quantum chemical calculations of conformation, vibrational spectroscopic, electronic, NBO and thermodynamic properties of 2,2-dichloro-N-(2,3-dichlorophenyl) acetamide and 2,2-dichloro-N-(2,3-dichlorophenyl) acetamide. Computational and Theoretical Chemistry, 2014, 1032, 27-41.	1.1	10
106	Structural analysis of nanostructured iron antimonate by experimental and quantum chemical simulation and its LPG sensing. Sensors and Actuators B: Chemical, 2014, 195, 373-381.	4.0	19
107	A comparative computational study on molecular structure, NBO analysis, multiple interactions, chemical reactivity and first hyperpolarisability of imatinib mesylate polymorphs using DFT and QTAIM approach. Molecular Simulation, 2014, 40, 1099-1112.	0.9	18
108	Synthesis, characterization, magnetic properties and gas sensing applications of ZnxCu1â^'xFe2O4 (0.0â‰¤xâ‰¤0.8) nanocomposites. Materials Science in Semiconductor Processing, 2014, 27, 934-949.	1.9	47

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109	Fabrication of self-assembled hierarchical flowerlike zinc stannate thin film and its application as liquefied petroleum gas sensor. Sensors and Actuators B: Chemical, 2014, 205, 102-110.	4.0	44
110	Quantum chemical studies of structural, vibrational, NBO and hyperpolarizability of ondansetron hydrochloride. Journal of Molecular Structure, 2014, 1058, 31-40.	1.8	19
111	Experimental and theoretical (FT-IR, FT-Raman, UVâ€“vis, NMR) spectroscopic analysis and first order hyperpolarizability studies of non-linear optical material: (2E)-3-[4-(methylsulfanyl) phenyl]-1-(4-nitrophenyl) prop-2-en-1-one using density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 130, 41-53.	2.0	63
112	Study of conformational stability, structural, electronic and charge transfer properties of cladrin using vibrational spectroscopy and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 615-628.	2.0	5
113	Growth of zinc ferrite aligned nanorods for liquefied petroleum gas sensing. Materials Letters, 2014, 131, 31-34.	1.3	27
114	Quantum-chemical approach to serine formation in the interstellar medium: A possible reaction pathway. Astronomy and Astrophysics, 2014, 563, A55.	2.1	8
115	Comparative vibrational spectroscopic studies, HOMOâ€“LUMO and NBO analysis of N-(phenyl)-2,2-dichloroacetamide, N-(2-chloro phenyl)-2,2-dichloroacetamide and N-(4-chloro) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Chemistry, 2013, 1016, 8-21.	1.1	116
116	Vibrational spectroscopy and density functional theory analysis of 3-O-caffeoylquinic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 104, 358-367.	2.0	12
117	Use of vibrational spectroscopy to study 2-[4-(N-dodecanoylamino)phenyl]-5-(4-nitrophenyl)-1,3,4-oxadiazole: A combined theoretical and experimental approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 114, 236-255.	2.0	19
118	Some new reaction pathways for the formation of cytosine in interstellar space â€“ A quantum chemical study. Advances in Space Research, 2013, 51, 797-811.	1.2	14
119	Density functional theory studies on the structure, spectra (FT-IR, FT-Raman, and UV) and first order molecular hyperpolarizability of 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine: Comparison to experimental data. Vibrational Spectroscopy, 2013, 64, 134-147.	1.2	45
120	Structural, electronic, thermodynamical and charge transfer properties of Chloramphenicol Palmitate using vibrational spectroscopy and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 101, 335-342.	2.0	22
121	Spectroscopic and quantum chemical study of an alkaloid aristolochic acid I. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 258-269.	2.0	9
122	FT-Raman, FT-IR, UV spectroscopic, NBO and DFT quantum chemical study on the molecular structure, vibrational and electronic transitions of clopidogrel hydrogen sulfate form 1: A comparison to form 2. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 104, 409-418.	2.0	11
123	Two-Dimensional Correlation Analysis of Temperature-Dependent FT-IR Spectra of Oleic Acid. Spectroscopy Letters, 2013, 46, 21-27.	0.5	10
124	Study of molecular structure, vibrational, electronic and NMR spectra of oncocalyxone A using DFT and quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 113, 367-377.	2.0	19
125	Study of polymorphism in imatinib mesylate: A quantum chemical approach using electronic and vibrational spectra. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 103, 325-332.	2.0	16
126	Quantum chemical analysis for the formation of glycine in the interstellar medium. Research in Astronomy and Astrophysics, 2013, 13, 912-920.	0.7	21

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127	DFT study of structure and vibrational spectra of ceramide 3: comparison to experimental data. Molecular Simulation, 2012, 38, 872-881.	0.9	6
128	Study of molecular structure and vibrational spectra of poly (Î²,-l-malic acid) [PMLA] using DFT approach. Polymer, 2012, 53, 2681-2690.	1.8	6
129	Heat capacity and phonon dispersion in polyselenophene in relation to the spectra of oligoselenophenes. Synthetic Metals, 2012, 162, 314-325.	2.1	5
130	Formation of 2-imino-malononitrile and diaminomaleonitrile in nitrile rich environments: A quantum chemical study. Computational and Theoretical Chemistry, 2012, 983, 7-15.	1.1	12
131	A computational study on conformational geometries, chemical reactivity and inhibitor property of an alkaloid bicuculline with Î³-aminobutyric acid (GABA) by DFT. Computational and Theoretical Chemistry, 2012, 993, 80-89.	1.1	41
132	Intermolecular charge transfer and vibrational analysis of hydrogen bonding in acetazolamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 99, 150-159.	2.0	9
133	Molecular structure, vibrational spectroscopic, NBO and HOMOâ€“LUMO studies of 2-amino 6-bromo 3-formylchromone. Molecular Simulation, 2012, 38, 567-581.	0.9	9
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