Poonam Tandon

List of Publications by Year in descending order

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240 papers	3,340 citations	172386 29 h-index	276775 41 g-index
240 all docs	240 docs citations	240 times ranked	3126 citing authors

#	Article	IF	Citations
1	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
2	Phase transitions in oleic acid as studied by X-ray diffraction and FT-Raman spectroscopy. Journal of Molecular Structure, 2000, 524, 201-215.	1.8	99
3	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
4	Structural and spectroscopic studies on 2-pyranones. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 251-260.	2.0	75
5	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
6	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
7	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
8	X-ray diffraction and spectroscopic studies of oleic acidâ€“sodium oleate. Chemistry and Physics of Lipids, 2001, 109, 37-45.	1.5	50
9	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
10	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
11	Phonon dispersion in poly(dimethylsilane). Journal of Organometallic Chemistry, 2006, 691, 2902-2908.	0.8	44
12	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
13	Physicochemical and Pharmacokinetic Analysis of Anacardic Acid Derivatives. ACS Omega, 2020, 5, 6021-6030.	1.6	44
14	Vibrational spectroscopic, NBO, AIM, and multiwfn study of tectorigenin: A DFT approach. Journal of Molecular Structure, 2020, 1217, 128443.	1.8	43
15	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
16	Computational approaches to find the active binding sites of biological targets against busulfan. Journal of Molecular Modeling, 2016, 22, 142.	0.8	41
17	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
18	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

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19	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
20	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
21	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
22	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
23	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
24	An ab initio and DFT study of structure and vibrational spectra of Î³ form of Oleic acid: Comparison to experimental data. Chemistry and Physics of Lipids, 2010, 163, 207-217.	1.5	34
25	A Comparative Ab Initio and DFT Study of Polyaniline Leucoemeraldine Base and Its Oligomers. Journal of Physical Chemistry B, 2009, 113, 14629-14639.	1.2	33
26	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
27	Quantum chemical study of a new reaction pathway for the adenine formation in the interstellar space. Astronomy and Astrophysics, 2011, 528, A129.	2.1	31
28	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
29	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
30	Molecular structure and vibrational spectroscopic investigation of 4-chloro-4â€²dimethylamino-benzylidene aniline using density functional theory. Journal of Molecular Structure, 2010, 981, 1-9.	1.8	28
31	Nickel antimony oxide (NiSb2O6): A fascinating nanostructured material for gas sensing application. Chemical Physics Letters, 2016, 646, 41-46.	1.2	28
32	Vibrational dynamics and heat capacity of Î²-poly(l-serine). Polymer, 1997, 38, 2389-2397.	1.8	27
33	DFT Study and Heat Capacity of Polyaniline Pernigraniline Base. Journal of Physical Chemistry B, 2009, 113, 9702-9707.	1.2	27
34	Growth of zinc ferrite aligned nanorods for liquefied petroleum gas sensing. Materials Letters, 2014, 131, 31-34.	1.3	27
35	Heat capacity and phonon dispersion in poly (L-methionine). Journal of Polymer Science, Part B: Polymer Physics, 1997, 35, 2281-2292.	2.4	26
36	Raman spectroscopic characterization of different regioisomers of monoacyl and diacyl chlorogenic acid. Vibrational Spectroscopy, 2012, 61, 10-16.	1.2	26

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37	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
38	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
39	Molecular Structure and Vibrational Spectroscopic Investigation of Secnidazole Using Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 273-281.	1.1	22
40	Solid state characterization of an antioxidant alkaloid boldine using vibrational spectroscopy and quantum chemical calculations. Vibrational Spectroscopy, 2011, 56, 82-88.	1.2	22
41	Study of vibrational spectra and molecular structure of intermolecular hydrogen bonded 2-thiohydantoin using Density Functional Theory. Journal of Molecular Structure, 2011, 1004, 237-247.	1.8	22
42	Antagonistic properties of a natural product â€“ Bicuculline with the gamma-aminobutyric acid receptor: Studied through electrostatic potential mapping, electronic and vibrational spectra using ab initio and density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 84, 144-155.	2.0	22
43	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
44	Polymer-matrix nanocomposite gas-sensing materials. Inorganic Materials, 2014, 50, 296-305.	0.2	22
45	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
46	Heat capacity and normal modes of poly (L-valine) in relation to spectra of oligovalines. Biopolymers, 1996, 38, 53-67.	1.2	21
47	Quantum chemical analysis for the formation of glycine in the interstellar medium. Research in Astronomy and Astrophysics, 2013, 13, 912-920.	0.7	21
48	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
49	Synthesis of Nanostructured Cobalt Titanate and Its Application as Liquefied Petroleum Gas Sensor at Room Temperature. Sensor Letters, 2011, 9, 533-540.	0.4	21
50	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
51	Phonon dispersion and heat capacity in poly(Îµ-caprolactone). European Polymer Journal, 2004, 40, 1787-1798.	2.6	19
52	Molecular structure and vibrational spectroscopic analysis of an antiplatelet drug; clopidogrel hydrogen sulphate (form 2) â€“ A combined experimental and quantum chemical approach. Journal of Molecular Structure, 2010, 964, 88-96.	1.8	19
53	Molecular structure, vibrational spectra and HOMO, LUMO analysis of yohimbine hydrochloride by density functional theory and ab initio Hartreeâ€“Fock calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 82, 270-278.	2.0	19
54	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

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55	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
56	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
57	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
58	Quantum chemical studies of structural, vibrational, NBO and hyperpolarizability of ondansetron hydrochloride. Journal of Molecular Structure, 2014, 1058, 31-40.	1.8	19
59	Vibrational Dynamics and Heat Capacity of Poly(L-lysine). Polymer Journal, 1997, 29, 914-922.	1.3	18
60	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
61	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
62	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
63	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
64	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
65	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
66	Heat capacity and vibrational dynamics of Îˆ poly(Î²-benzyl-L-aspartate). Journal of Polymer Science, Part B: Polymer Physics, 1996, 34, 1213-1228.	2.4	17
67	Experimental investigations on liquefied petroleum gas sensing of Cd(NO3)2Â·(AAm)4Â·2H2O and CdS/polyacrylamide synthesized via frontal polymerization. Sensors and Actuators B: Chemical, 2011, 160, 826-834.	4.0	17
68	Thermotropic phase behaviour of sodium oleate as studied by FT-Raman spectroscopy and X-ray diffraction. Journal of Molecular Structure, 2000, 526, 49-57.	1.8	16
69	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
70	Synthesis, Characterization and Gas Sensing Capability of NixCu1âˆ’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
71	Normal Modes of Poly(L-valine) in Relation to Spectra of Oligovalines. Polymer Journal, 1995, 27, 481-491.	1.3	15
72	Vibrational dynamics and heat capacity of poly(glycolic acid). Polymer, 2004, 45, 5307-5315.	1.8	15

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73	Quantum chemical and experimental studies on the structure and vibrational spectra of efavirenz. Vibrational Spectroscopy, 2010, 53, 112-116.	1.2	15
74	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
75	Molecular structure and quantum descriptors of cefradine by using vibrational spectroscopy (IR and) Tj ETQq1 1 0.784314 rgBT /Over and Biomolecular Spectroscopy, 2021, 246, 118976.	2.0	15
76	Phonon Dispersion in Ï‰ Helical Poly-L-Phenylalanine. Journal of the Physical Society of Japan, 1995, 64, 308-314.	0.7	14
77	Normal mode analysis of Î³ form of oleic acid. Chemistry and Physics of Lipids, 2006, 142, 70-83.	1.5	14
78	Study on the structure and vibrational spectra of efavirenz conformers using DFT: Comparison to experimental data. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 88, 116-123.	2.0	14
79	Polymer-assisted synthesis of metallopolymer nanocomposites and their applications in liquefied petroleum gas sensing at room temperature. Sensors and Actuators B: Chemical, 2012, 166-167, 281-291.	4.0	14
80	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
81	Phonons and heat capacity of poly(l-leucine). Polymer, 1996, 37, 5401-5410.	1.8	13
82	Vibrational Dynamics of Polyaniline Pernigraniline Base Form: A Conducting Polymer. Macromolecular Symposia, 2008, 265, 111-123.	0.4	13
83	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
84	Nitrogen donor ligand for capping ZnS quantum dots: a quantum chemical and toxicological insight. RSC Advances, 2019, 9, 28510-28524.	1.7	13
85	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
86	Phonons in 72 helical poly(4-methyl-1-pentene). Polymer, 1996, 37, 745-754.	1.8	12
87	Vibrational dynamics and heat capacity of syndiotactic poly(4-methyl-1-pentene). Vibrational Spectroscopy, 2001, 26, 161-178.	1.2	12
88	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
89	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
90	Combined spectroscopic and quantum chemical studies of ezetimibe. Journal of Molecular Structure, 2016, 1125, 193-203.	1.8	12

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91	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
92	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
93	Phonon Dispersion in Ï‰ Helical PolyNÎµ(p-Bromobenzoyl-L-Ornithine). Journal of the Physical Society of Japan, 1995, 64, 315-326.	0.7	11
94	Heat Capacity and Vibrational Dynamics of Poly(L-glutamic acid) (Î± Helix). Polymer Journal, 1997, 29, 33-43.	1.3	11
95	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
96	Spectroscopic, quantum chemical calculation and molecular docking of dipfluzine. Journal of Molecular Structure, 2016, 1125, 751-762.	1.8	11
97	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
98	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
99	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
100	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
101	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
102	Phonon dispersion and heat capacity of poly(l-aspartic acid). European Polymer Journal, 1998, 34, 1781-1791.	2.6	10
103	Vibrational dynamics of syndiotactic poly(1-butene). European Polymer Journal, 2000, 36, 2629-2638.	2.6	10
104	Vibrational dynamics of trans-1,4-polyisoprene (Î²-form). Polymer, 2006, 47, 5154-5160.	1.8	10
105	Vibrational spectroscopic investigation of poly(pâ€phenylene sulfide). Journal of Polymer Science, Part B: Polymer Physics, 2009, 47, 2353-2367.	2.4	10
106	Conformational and vibrational studies of isomeric hydrogen cyanide tetramers by quantum chemical methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 89, 55-66.	2.0	10
107	Two-Dimensional Correlation Analysis of Temperature-Dependent FT-IR Spectra of Oleic Acid. Spectroscopy Letters, 2013, 46, 21-27.	0.5	10
108	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

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109	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
110	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
111	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
112	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
113	A novel approach to design febuxostat-salicylic acid eutectic system: evaluation and characterization. CrystEngComm, 2019, 21, 310-320.	1.3	10
114	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
115	Phonon dispersion in poly(Î±-aminoisobutyric acid). Polymer, 1995, 36, 3739-3743.	1.8	9
116	Conformational Study of Î± Poly(L-valine). A Vibrational Approach. Polymer Journal, 1996, 28, 474-480.	1.3	9
117	Electro-optical Parameters of Bond Polarizability Model for Aluminosilicates. Journal of Physical Chemistry A, 2006, 110, 4516-4523.	1.1	9
118	Vibrational dynamics of poly(Î²â€hydroxybutyrate)â€Î± form. Polymer Engineering and Science, 2009, 49, 850-861.	1.5	9
119	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
120	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
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	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
123	Study of phase transitions in a bent-core liquid crystal probed by infrared spectroscopy. Vibrational Spectroscopy, 2016, 86, 24-34.	1.2	9
124	Formation of E-cyanomethamine in a nitrile rich environment. Research in Astronomy and Astrophysics, 2017, 17, 1.	0.7	9
125	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
126	A theoretical quantum chemical study of alanine formation in interstellar medium. European Physical Journal D, 2017, 71, 1.	0.6	9

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127	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
128	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
129	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
130	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
131	Conformation and phonon dispersion in trans-1,4-polybutadiene. Journal of Macromolecular Science - Physics, 1998, 37, 683-697.	0.4	8
132	Normal Modes and Their Dispersion in Î± Form of Nylon-6 (Î±NY6). Polymer Journal, 2007, 39, 359-368.	1.3	8
133	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
134	Quantum-chemical approach to serine formation in the interstellar medium: A possible reaction pathway. Astronomy and Astrophysics, 2014, 563, A55.	2.1	8
135	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
136	Phase transition and specific heat anomaly in Bâ‡Œ Z and other conformational transitions in poly(dG-dC). Journal of Macromolecular Science - Physics, 1992, 31, 439-454.	0.4	7
137	Drug binding and order-order and order-disorder transitions in DNA triple helices. Journal of Macromolecular Science - Physics, 1999, 38, 349-366.	0.4	7
138	Phonon dispersion and heat capacity in cross-Î² form of poly(O-acetyl, l-serine). Polymer, 2000, 41, 2095-2104.	1.8	7
139	Thermal degradation and theoretical interpretation of vibrational spectra of poly (Î²,l-malic acid). Polymer, 2011, 52, 3118-3126.	1.8	7
140	Molecular structure and vibrational spectra of Nâ€acetylglycine oligomers and polyglycine I using DFT approach. Biopolymers, 2014, 101, 795-813.	1.2	7
141	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
142	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
143	Structural and Reactivity Analyses of Nitrofurantoinâ€“4-dimethylaminopyridine Salt Using Spectroscopic and Density Functional Theory Calculations. Crystals, 2019, 9, 413.	1.0	7
144	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

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