Shabbir Ahmad

List of Publications by Year
in descending order

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35	719	471509	580821
papers	citations	17 h-index	25 g-index

35	35	35	704
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Intramolecular charge transfer-based linear and nonlinear optical properties of a Dâ€“Ï€â€“Aâ€“Ï€â€“D type organic chromophore: Experimental and computational approach. Journal of Nonlinear Optical Physics and Materials, 2022, 31, .	1.8	11
2	FTIR and FT-Raman spectra of 6-(dimethylamino)purine and its theoretical studies of anharmonic vibrational analysis using quantum chemical calculations. Vibrational Spectroscopy, 2021, 113, 103224.	2.2	5
3	Experimental and computational investigation of novel dihydrated organic single crystal of 2,4,6-triaminopyrimidine and 3,5-dintrobenzoic acid: Linear and nonlinear optical response with limiting performance. Journal of Solid State Chemistry, 2021, 300, 122255.	2.9	22
4	Experimental thermophysical properties and DFT calculations of imidazolium ionic liquids and 2-butanol mixtures. Fluid Phase Equilibria, 2020, 508, 112447.	2.5	9
5	3Î²-Acetoxy cholest-5-ene crystals: Catalytic synthesis, structural elucidation, contribution of intermolecular interactions and density functional theory calculations. Journal of Molecular Structure, 2020, 1221, 128833.	3.6	0
6	Cocrystallization of 2,3-dimethylquinoxaline with 3,5-dinitrobenzoic acid: Crystal structure, Hirshfeld surface, spectroscopic features and DFT studies. Journal of Molecular Structure, 2019, 1198, 126894.	3.6	16
7	Spectroscopic (FTIR, FT-Raman, 1H NMR and UVâ€“Vis) and DFT/TD-DFT studies on cholesteno [4,6-b,c]-2â€²,5â€²-dihydro-1â€²,5â€²-benzothiazepine. Journal of Molecular Structure, 2019, 1178, 570-582.	3.6	48
8	Structural, vibrational and electronic absorption characteristics of the monohydrate organic salt of 2-amino-5-bromo-6-methyl-4-pyrimidinol and 2,3-pyrazinedicarboxylic acid: A combined experimental and computational study. Journal of Molecular Structure, 2019, 1177, 229-241.	3.6	25
9	DFT/TD-DFT calculations, spectroscopic characterizations (FTIR, NMR, UVâ€“vis), molecular docking and enzyme inhibition study of 7-benzoyloxycoumarin. Computational Biology and Chemistry, 2018, 73, 65-78.	2.3	21
10	Anharmonic vibrational spectra and mode-mode couplings analysis of 2-aminopyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 188, 26-31.	3.9	9
11	Synthesis, spectroscopic, computational (DFT/B3LYP), AChE inhibition and antioxidant studies of imidazole derivative. Journal of Molecular Structure, 2018, 1151, 327-342.	3.6	38
12	Growth, structure, Hirshfeld surface and spectroscopic properties of 2-amino-4-hydroxy-6-methylpyrimidinium-2,3-pyrazinedicorboxylate single crystal. Journal of Molecular Structure, 2018, 1155, 695-710.	3.6	17
13	Experimental vibrational spectroscopy (FTIR and FT-Raman) of D-tryptophan and its anharmonic theoretical studies using density functional theory. Journal of Molecular Structure, 2018, 1171, 315-322.	3.6	14
14	Detailed molecular, structural and spectral studies of bimetallic salt, [Ni(L)][CoCl 4] where LÂ=Â3,7- bis (2-aminoethyl)-1,3,5,7-tetraazabicyclo(3.3.1)nonane. Journal of Molecular Structure, 2017, 1138, 90-101.	3.6	6
15	DFT/B3LYP calculations, in vitro cytotoxicity and antioxidant activities of steroidal pyrimidines and their interaction with HSA using molecular docking and multispectroscopic techniques. Bioorganic Chemistry, 2017, 73, 83-99.	4.1	50
16	Anharmonic vibrational and electronic spectral study of 2-amino-4-hydroxy-6â€“methylpyrimidine: A combined experimental (FTIR, FT-Raman, UVâ€“Vis) and theoretical (DFT, MP2) approach. Journal of Molecular Structure, 2017, 1148, 89-100.	3.6	16
17	Study of molecular structure, anharmonic vibrational dynamic and electronic properties of sulindac using spectroscopic techniques integrated with quantum chemical calculations. Journal of Molecular Structure, 2017, 1147, 603-615.	3.6	11
18	Quantum chemical and spectroscopic investigations of 4-Hydroxy-7-methyl-1,8-naphthyridine-3-carboxylic acid. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650042.	1.8	3

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19	Electron impact ionisation cross section for organoplatinum compounds. Molecular Physics, 2016, 114, 3104-3111.	1.7	6
20	Vibrational and electronic spectral analysis of 2,3-pyrazinedicarboxylic acid: A combined experimental and theoretical study. Spectroscopy Letters, 2016, 49, 449-457.	1.0	9
21	FTIR, FT-Raman and UVâ€“Vis spectral studies of d-tyrosine molecule. Journal of Molecular Structure, 2016, 1105, 169-177.	3.6	15
22	Synthesis, X-ray crystallography, spectroscopic (FT-IR, 1H &13C NMR and UV), computational (DFT/B3LYP) and enzymes inhibitory studies of 7-hydroximinocholest-5-en-3-ol acetate. Journal of Molecular Structure, 2016, 1116, 317-332.	3.6	17
23	Computational and anti-tumor studies of 7a-Aza-B-homostigmast-5-eno [7a, 7-d] tetrazole-3Î²-yl chloride. Journal of Molecular Structure, 2016, 1108, 411-426.	3.6	21
24	Structural elucidation, density functional calculations and contribution of intermolecular interactions in cholest-4-en-3-one crystals: Insights from X-ray and Hirshfeld surface analysis. Journal of Molecular Structure, 2015, 1084, 274-283.	3.6	23
25	Quantum chemical calculations and analysis of FTIR, FTâ€“Raman and UVâ€“Vis spectra of temozolomide molecule. Journal of Molecular Structure, 2015, 1099, 453-462.	3.6	22
26	DFT, Hirshfeld surfaces, spectral and inÂvivo cytotoxic studies of 7a-Aza-B-homostigmast-5-eno [7a,7-d] tetrazole. Journal of Molecular Structure, 2015, 1099, 588-600.	3.6	20
27	FT-IR and FT-Raman spectra, MEP and HOMOâ€“LUMO of 2,5-dichlorobenzonitrile: DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 464-472.	3.9	29
28	FTIR, FT-Raman, UVâ€“Visible spectra and quantum chemical calculations of allantoin molecule and its hydrogen bonded dimers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 961-978.	3.9	49
29	Molecular structure, anharmonic vibrational analysis and electronic spectra of o-, m-, p-iodonitrobenzene using DFT calculations. Journal of Molecular Structure, 2014, 1059, 239-254.	3.6	39
30	Quantum chemical and spectroscopic investigations of 3-methyladenine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 653-664.	3.9	39
31	Anharmonic vibrational studies of l-aspartic acid using HF and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 992-1004.	3.9	54
32	Computational studies of vibrational spectra and molecular properties of 6-methyluracil using HF, DFT and MP2 methods. Indian Journal of Physics, 2011, 85, 239-260.	1.8	24
33	Anharmonic vibrational spectroscopy and investigation of intramolecular mode couplings in adenine. Vibrational Spectroscopy, 2011, 56, 51-59.	2.2	12
34	Approximate solution of the modeâ€“mode coupling integral: Application to cytosine and its deuterated derivative. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 446-456.	3.9	10
35	Anharmonic vibrational analysis of uracil by ab initio Hartreeâ€“Fock and density functional theory calculations. Computational and Theoretical Chemistry, 2009, 895, 18-20.	1.5	9