

R Meenakshi

List of Publications by Year in descending order

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1163117

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#	ARTICLE	IF	CITATIONS
1	Vibrational spectroscopic (FTIR and FT-Raman), first-order hyperpolarizability, HOMO, LUMO, NBO, Mulliken charge analyses of 2-ethylimidazole based on Hartree-Fock and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 134, 493-501.	3.9	44
2	Spectral investigations, DFT based global reactivity descriptors, Inhibition efficiency and analysis of 5-chloro-2-nitroanisole as a spacer with donor-acceptor variations effect for DSSCs performance. <i>Journal of Molecular Structure</i> , 2017, 1127, 694-707.	3.6	41
3	Quantum chemical studies on structure of 1,3-dibromo-5-chlorobenzene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 316-326.	3.9	26
4	Vibrational spectroscopic studies and DFT calculations of 4-bromo-o-xylene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 419-430.	3.9	25
5	PCM/TD-DFT analysis of 1-bromo-2,3-dichlorobenzene – A combined study of experimental (FT-IR and Tj ETQq1) and theoretical calculations (dimerization, UV-vis, multinuclear NMR and pes). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 105, 497-508.	3.9	25
6	Synthesis, growth, structure and spectroscopic characterization of a new organic nonlinear optical hydrogen bonding complex crystal: 3-Carboxyl anilinium p-toluene sulfonate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 125, 114-119.	3.9	22
7	Vibrational spectra and theoretical calculations (dimerization, UV-vis, multinuclear NMR and pes) Tj ETQq1	1.0	784314 rgBT /Overl...
	Molecular and Biomolecular Spectroscopy, 2014, 117, 739-753.	3.9	19
8	Vibrational spectroscopic investigations, first hyperpolarizability, HOMO-LUMO and NMR analyzes of p-fluorobenzonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 102, 59-65.	3.9	13
9	Growth and combined experimental and quantum chemical study of glycyl-L-Valine crystal. <i>Heliyon</i> , 2019, 5, e01574.	3.2	10
10	Experimental (FT-IR and FT-Raman) and spectroscopic investigations, electronic properties and conformational analysis by PES scan on 2-methoxy-5-nitrophenol and 2-methoxy-4-methylphenol. <i>RSC Advances</i> , 2016, 6, 21822-21831.	3.6	7
11	Synthesis, Crystal Structure and Vibrational Spectral Analysis of Guanidinium Hydrogen L-aspartate Single Crystal. <i>Journal of Physical Science</i> , 2017, 28, 27-47.	0.9	7
12	Spectral investigations, inhibition efficiency analysis and a TD-DFT study on tuning the light harvesting efficiency (LHE) of heterocyclic 5-nitro-1,3-benzodioxole as a photosensitizer for dye sensitized solar cells (DSSCs). <i>RSC Advances</i> , 2016, 6, 63690-63703.	3.6	6
13	Vibrational, electronic absorption, thermal and mechanical analyses of organic nonlinear optical material guanidinium phthalate. <i>Journal of Molecular Structure</i> , 2017, 1130, 472-479.	3.6	6
14	FT-IR and FT-RAMAN analysis and light-harvesting efficiency (LHE) enhancement for DSSC applications of hydrazide derivatives. <i>Journal of the Iranian Chemical Society</i> , 2021, 18, 1179-1198.	2.2	3
15	Synthesis, Crystal Growth, Vibrational Spectral Analysis, Optical Thermal and Antimicrobial Properties of Guanidinium Oxalate Monohydrate Single Crystal. <i>Journal of Physical Science</i> , 2017, 28, 31-56.	0.9	3
16	Growth, spectral, density functional theory (DFT) and Hirshfeld surface analysis on 4-aminopyridinium adipate monohydrate nonlinear optical single crystal. <i>Materials Science-Poland</i> , 2018, 36, 177-184.	1.0	2
17	Growth, density functional theory (DFT) and spectral studies on L-2-aminobutyric acid –biologically active material. <i>Journal of Molecular Structure</i> , 2017, 1149, 655-661.	3.6	0