Parag Agarwal

List of Publications by Year
in descending order

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12	151	1478505 6	1199594 12
papers	citations	h-index	g-index

12	12	12	178
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	2.2	45
2	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.	3.9	35
3	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.	3.9	19
4	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.	3.6	12
5	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.	2.5	10
6	Characterization and intramolecular bonding patterns of busulfan: Experimental and quantum chemical approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 173, 390-399.	3.9	10
7	Heat capacity and phonon dispersion in polyselenophene in relation to the spectra of oligoselenophenes. Synthetic Metals, 2012, 162, 314-325.	3.9	5
8	Heat capacity and vibrational dynamics of polyvinylidene fluoride (Î²-form). Polymer Science - Series A, 2011, 53, 375-384.	1.0	4
9	Combine experimental and theoretical investigation on an alkaloidâ€“Dimethylisoborreverine. Journal of Molecular Structure, 2016, 1103, 187-201.	3.6	4
10	Structural and spectroscopic analysis of indole alkaloids: Molecular docking and DFT approach. Journal of Molecular Structure, 2018, 1153, 262-274.	3.6	4
11	Vibrational dynamics and heat capacity of polychloroprene. Journal of Applied Polymer Science, 2011, 121, 186-195.	2.6	2
12	Phonon dispersion and specific heat in trans 1,4, poly (2,3-dimethylbutadiene). Journal of Materials Science, 2011, 46, 3452-3463.	3.7	1