

C Arunagiri

List of Publications by Year in descending order

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papers

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#	ARTICLE	IF	CITATIONS
1	Synthesis, X-ray crystal structure, vibrational spectroscopy, DFT calculations, electronic properties and Hirshfeld analysis of (E)-4-Bromo-N'-(2,4-dihydroxy-benzylidene) benzohydrazide. Journal of Molecular Structure, 2018, 1163, 368-378.	3.6	38
2	A new chalcone structure of (E)-1-(4-Bromophenyl)-3-(naphthalen-2-yl)prop-2-en-1-one: Synthesis, structural characterizations, quantum chemical investigations and biological evaluations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 149, 90-102.	3.9	37
3	Vibrational spectra (experimental and theoretical), molecular structure, natural bond orbital, HOMO-LUMO energy, Mulliken charge and thermodynamic analysis of N ² -hydroxy-pyrimidine-2-carboximidamide by DFT approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 144, 215-225.	3.9	28
4	Vibrational spectroscopic (FT-IR and FT-Raman), first-order hyperpolarizability, HOMO, LUMO, NBO, Mulliken charges and structure determination of 2-bromo-4-chlorotoluene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1747-1756.	3.9	22
5	Synthesis, crystal structure and theoretical studies of a Schiff base 2-[4-hydroxy benzylidene]-amino naphthalene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 307-316.	3.9	22
6	Synthesis, X-ray structure analysis, thermodynamic and electronic properties of 4-acetamido benzaldehyde using vibrational spectroscopy and DFT calculations. Journal of Molecular Structure, 2017, 1130, 244-250.	3.6	12
7	Crystal structure, hydrogen bonding, Hirshfeld surface analysis and inhibition efficiency of a Schiff base 2-methoxy-6-(naphthalene-2-yliminomethyl)-phenol. Chemical Data Collections, 2020, 25, 100337.	2.3	12
8	Synthesis, single crystal, structure and Hirshfeld surface analysis of (E)-4-toluic-N ² -(2,4-dihydroxy-benzylidene) benzohydrazide. Chemical Data Collections, 2018, 17-18, 169-177.	2.3	7
9	Theoretical and experimental calculations, Mulliken charges and thermodynamic properties of 4-chloro-2-nitroanisole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 131, 647-656.	3.9	6
10	Crystal structure, Hirshfeld surface analysis, PIXEL energy and molecular electronic properties on [2-(2-nitrobenzylidene)-amino naphthalene]. Chemical Data Collections, 2020, 30, 100549.	2.3	6
11	X-ray crystal structure, Hirshfeld surface analysis, DFT and electronic properties of (E)-4-chloro-N ² -(2,4-dihydroxy-benzylidene) benzohydrazide. Chemical Data Collections, 2019, 19, 100174.		4
12	Crystal structure, hydrogen bonding interactions, Hirshfeld surface analysis and DFT Studies of 4,4'-dicarboxy-2,2'-bipyridinium chloride. Chemical Data Collections, 2020, 29, 100502.	2.3	2
13	Crystal structure, spectroscopic, quantum chemical and Hirshfeld surface analysis of [2-(3, Tj ETQq 1 0.784314 rgBT /Overlock 1 study. Chemical Data Collections, 2021, 33, 100679.	2.3	0
14	Structural, Optical, Spectral, Thermal and Third-order NLO Behaviour of 4-Chlorobenzhydrazide Trichloro Acetate Single Crystal. Brazilian Journal of Physics, 2022, 52, 1.	1.4	0