

Rakesh Kumar

List of Publications by Year in descending order

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27
papers

477
citations

687363

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h-index

713466

21
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27
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27
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27
times ranked

404
citing authors

#	ARTICLE	IF	CITATIONS
1	Interaction Between New Anti-cancer Drug Syndros and CNT(6,6-6) Nanotube for Medical Applications: Geometry Optimization, Molecular Structure, Spectroscopic (NMR, UV/Vis, Excited state), FMO, MEP and HOMO-LUMO Investigation. Applied Surface Science, 2018, 434, 504-513.	6.1	57
2	Polarization, excited states, trans - cis properties and anisotropy of thermal and electrical conductivity of the 4-(phenyldiazenyl)aniline in PVA matrix. Journal of Molecular Structure, 2017, 1141, 703-709.	3.6	47
3	Molecular structure and UV-Vis spectral analysis of new synthesized azo dyes for application in polarizing films. Dyes and Pigments, 2016, 129, 9-17.	3.7	39
4	Synthesis, crystal structure investigation, DFT analyses and antimicrobial studies of silver(I) complexes with N,N,N',N'-tetrakis(2-hydroxyethyl)propyl ethylenediamine and tris(2-hydroxyethyl)amine. New Journal of Chemistry, 2014, 38, 1186.	2.8	31
5	Molecular structure and spectroscopic investigation of sodium(E)-2-hydroxy-5-((4-sulfonatophenyl)diazenyl)benzoate: A DFT study. Journal of Molecular Structure, 2015, 1083, 198-203.	3.6	30
6	Synthesis, geometry optimization, spectroscopic investigations (UV/Vis, excited states, FT-IR) and application of new azomethine dyes. Journal of Molecular Structure, 2017, 1148, 134-149.	3.6	26
7	A study of molecular structure, UV, IR, and ¹ H NMR spectra of a new dichroic dye on the basis of quinoline derivative. Journal of Molecular Structure, 2015, 1088, 105-110.	3.6	25
8	Photochromic properties of the molecule Azure A chloride in polyvinyl alcohol matrix. Journal of Molecular Structure, 2015, 1101, 109-115.	3.6	22
9	DFT analysis and DNA binding, cleavage of copper(II) complexes. Journal of Molecular Liquids, 2016, 221, 1045-1053.	4.9	22
10	DFT studies of structural and some spectral parameters of copper(II) complexes with N,N,N',N'-tetrakis(2-hydroxyethyl)propyl ethylenediamine and tris(2-hydroxyethyl)amine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 244-249.	3.9	21
11	Geometry optimization and excited state properties of the new symmetric (E)-Stilbene derivative for application in thermostable polarizing PVA-films: A combined experimental and DFT approach. Journal of Molecular Structure, 2016, 1119, 423-430.	3.6	18
12	Design of geometry, synthesis, spectroscopic (FT-IR, UV/Vis, excited state, polarization) and anisotropy (thermal conductivity and electrical) properties of new synthesized derivatives of (E,E)-azomethines in colored stretched poly (vinyl alcohol) matrix. Journal of Molecular Structure, 2018, 1157, 536-550.	3.6	18
13	Anisotropy (optical, electrical and thermal conductivity) in thin polarizing films for UV/Vis regions of spectrum: Experimental and theoretical investigations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 192, 343-360.	3.9	17
14	Synthesis of biphenyl derivative and its application as dichroic materials in poly (vinyl alcohol) polarizing films. Journal of Molecular Structure, 2016, 1107, 19-24.	3.6	14
15	Synthesis, crystal structure, DNA interaction, DFT analysis and molecular docking studies of copper(II) complexes with 1-methyl-L-tryptophan and phenanthroline units. Journal of Molecular Structure, 2021, 1224, 129236.	3.6	14
16	Investigation of the Adsorption Rubraca Anticancer Drug on the CNT(4,4-8) Nanotube as a Factor of Drug Delivery: A Theoretical Study Based on DFT Method. Current Molecular Medicine, 2019, 19, 473-486.	1.3	12
17	Broad band thermostable polarizing film based on poly (vinyl alcohol), a quinoline derivative and ZnO nanoparticles. RSC Advances, 2016, 6, 42062-42068.	3.6	9
18	DFT study of physisorption effect of CO and CO ₂ on furanocoumarins for air purification. Journal of Environmental Chemical Engineering, 2018, 6, 4784-4796.	6.7	9

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19	Molecular Investigations of the Newly Synthesized Azomethines as Antioxidants: Theoretical and Experimental Studies. <i>Current Molecular Medicine</i> , 2019, 19, 419-433.	1.3	8
20	Supramolecular architectures of N,N,N',N'-tetrakis-(2-hydroxyethyl)ethylenediamine and tris(2-hydroxyethyl)amine with La(III) picrate. <i>RSC Advances</i> , 2014, 4, 59248-59264.	3.6	7
21	Solvothermal synthesis, structural characterization, DFT and magnetic studies of a dinuclear paddlewheel Cu(II)-metallamacrocycle. <i>Journal of Molecular Structure</i> , 2020, 1201, 127193.	3.6	7
22	Synthesis, structural characterization and DFT analysis of an unusual tryptophan copper(II) complex bound via carboxylate monodentate coordination: Tetraaquabis(l-tryptophan) copper(II) picrate. <i>Inorganica Chimica Acta</i> , 2018, 482, 324-332.	2.4	6
23	DFT studies of calcium(II), strontium(II) and barium(II) benzoates with N,N,N',N'-Tetrakis(2-hydroxyethyl/propyl)ethylenediamine. <i>Journal of Molecular Structure</i> , 2016, 1113, 18-23.	3.6	5
24	Triethylammonium salt of dimethyl diphenyldithiophosphates: Single crystal X-ray and DFT analysis. <i>Journal of Chemical Sciences</i> , 2016, 128, 921-928.	1.5	4
25	Photochromic properties of the N-Salicylideneaniline in Polyvinyl Butyral matrix: Experimental and theoretical investigations. <i>Journal of Molecular Structure</i> , 2017, 1134, 530-537.	3.6	4
26	IR-polarizing film containing a new quinoline dye and Fe ₃ O ₄ nanoparticles: optical and thermophysical investigations. <i>RSC Advances</i> , 2016, 6, 114613-114622.	3.6	3
27	Charge Transfer Interaction Between the Antibiotic Drug Ciprofloxacin with Picric Acid: Experimental and Theoretical Investigations. <i>Science of Advanced Materials</i> , 2018, 10, 879-888.	0.7	2