Byru Venkatram Reddy

List of Publications by Year
in descending order

39 papers	505 citations	758635 12 h-index	752256 20 g-index
39 all docs	39 docs citations	39 times ranked	415 citing authors

#	Article	IF	Citations
1	Transferable valence force fields for substituted benzenes. Vibrational Spectroscopy, 1994, 6, 231-250.	1.2	74
2	Synthesis, Structural, Biological Evaluation, Molecular Docking and DFT Studies of Co(II), Ni(II), Cu(II), Zn(II), Cd(II) and Hg(II) Complexes bearing Heterocyclic Thiosemicarbazone ligand. Applied Organometallic Chemistry, 2018, 32, e4415.	1.7	45
3	Molecular geometry, NBO analysis, Hyperpolarizability and HOMO-LUMO energies of 2-azido-1-phenylethanone using Quantum chemical calculations. Materials Today: Proceedings, 2016, 3, 3761-3769.	0.9	33
4	Vibrational analysis of mononitro substituted benzamides, benzaldehydes and toluenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 279-290.	2.0	28
5	Molecular Structure, Vibrational Analysis and First Order Hyperpolarizability of 4-Methyl-3-Nitrobenzoic Acid Using Density Functional Theory. Optics and Photonics Journal, 2015, 05, 91-107.	0.3	27
6	Spectroscopic investigation on structure (monomer and dimer), molecular characteristics and comparative study on vibrational analysis of picolinic and isonicotinic acids using experimental and theoretical (DFT & IVP) methods. Journal of Molecular Structure, 2018, 1160, 271-292.	1.8	25
7	Synthesis, crystal and molecular structure, and characterization of 2-((2-aminopyridin-3-yl)methylene)-N-ethylhydrazinecarbothioamide using spectroscopic (1H and 13C) Tj ETQq1 1 0.784314 rgBT /Ov Molecular Structure, 2019, 1184, 405-417.	1.8	25
8	Synthesis, structural, spectroscopic, anti-cancer and molecular docking studies on novel 2-[(Anthracene-9-ylmethylene)amino]-2-methylpropane-1,3-diol using XRD, FTIR, NMR, UVâ€“Vis spectra and DFT. Journal of Molecular Structure, 2017, 1147, 406-426.	1.8	23
9	Vibrational analysis and valence force field for nitrotoluenes, dimethylanilines and some substituted methylbenzenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 632-643.	2.0	22
10	Experimental (FTIR and FT-Raman) and theoretical investigation of some pyridine-dicarboxylic acids. Journal of Molecular Structure, 2015, 1100, 43-58.	1.8	16
11	Study on structure, vibrational analysis and molecular characteristics of some halogen substituted azido-phenylethanones using FTIR spectra and DFT. Journal of Molecular Structure, 2018, 1155, 582-597.	1.8	15
12	Investigation of torsional potentials, hindered rotation, molecular structure and vibrational properties of some biphenyl carboxaldehydes using spectroscopic techniques and density functional formalism. Journal of Molecular Structure, 2019, 1196, 139-161.	1.8	14
13	Investigation of torsional potentials, molecular structure, vibrational properties, molecular characteristics and NBO analysis of some bipyridines using experimental and theoretical tools. Journal of Molecular Structure, 2016, 1117, 79-104.	1.8	13
14	Vibrational spectroscopic (FT-IR, FT-Raman), anti-inflammatory, docking and molecular characteristic studies of Ni(II) complex of 2-aminonicotinaldehyde using theoretical and experimental methods. Journal of Molecular Structure, 2019, 1175, 769-781.	1.8	13
15	Molecular structure, vibrational spectra, natural bond orbital and thermodynamic analysis of 3,6-dichloro-4-methylpyridazine and 3,6-dichloropyridazine-4-carboxylic acid by dft approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1134-1148.	2.0	11
16	Synthesis and evaluation of molecular structure from torsional scans, study of molecular characteristics using spectroscopic and DFT methods of some thiosemicarbazones, and investigation of their anticancer activity. Chemical Papers, 2021, 75, 3635-3647.	1.0	11
17	Barrier potentials, molecular structure, force filed calculations and quantum chemical studies of some bipyridine di-carboxylic acids using the experimental and theoretical using (DFT, IVP) approach. Molecular Simulation, 2019, 45, 1353-1383.	0.9	10
18	Structural and vibrational properties of pentabromophenol and pentafluorophenol: A spectroscopic investigation using density functional theory. Journal of Molecular Structure, 2019, 1180, 665-675.	1.8	10

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19	Theoretical and experimental study of torsional potentials, molecular structure (monomer and) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Molecular Structure, 2020, 1200, 127089.	1.8	10
20	Molecular Structure, Vibrational Analysis, Hyperpolarizability and NBO Analysis of 3-Methyl-Picolinic Acid Using SQM Calculations. Journal of Structural Chemistry, 2018, 59, 1022-1031.	0.3	9
21	Barrier Potential, Structure (Monomer and Dimer), Inter- and Intra-Molecular Interactions, Vibrational Analysis, Fukui Functions, MESP, NBO, UV and NMR Analysis of Pyridine-3-Carboxylic Acid Using Spectroscopic and DFT Approach. Polycyclic Aromatic Compounds, 2023, 43, 2488-2505.	1.4	8
22	Synthesis, spectroscopic, and DFT quantum chemical studies of 3- and 4-pyridylacetonitriles. Journal of Molecular Structure, 2019, 1176, 447-460.	1.8	7
23	Synthesis of Sr1-xBaxBi2B2O7 glass ceramics: A study for structure and characterization using experimental techniques and DFT method. Journal of Molecular Structure, 2020, 1220, 128660.	1.8	7
24	Investigation of Barrier Potential, Structure (Monomer & Dimer), Chemical Reactivity, NLO, MEP, and NPA Analysis of Pyrrole-2- Carboxaldehyde Using Quantum Chemical Calculations. Polycyclic Aromatic Compounds, 2023, 43, 4216-4230.	1.4	7
25	Vibrational analysis of substituted anilines, anisoles and anisidines. Vibrational Spectroscopy, 1992, 4, 67-75.	1.2	6
26	Transferable valence force fields for substituted benzenes. Vibrational Spectroscopy, 1994, 6, 251-257.	1.2	6
27	Experimental and theoretical determination of structural and vibrational properties of pentachlorophenol and pentachlorothiophenol. Journal of Molecular Structure, 2019, 1178, 142-154.	1.8	6
28	Synthesis, DFT computations, molecular docking studies and anticancer activity of 2-(4-fluorophenyl)-3-(5-methylisoxazol-3-yl)thiazolidin-4-one. Chemical Data Collections, 2022, 39, 100859.	1.1	5
29	Transferable valence force fields for substituted benzenes Part III. Trisubstituted benzenes. Vibrational Spectroscopy, 1994, 6, 259-265.	1.2	4
30	Theoretical (DFT) and experimental (FT-IR & FT Raman) approach to investigate the molecular geometry and vibrational properties of 2,5- and 2,6-dihydroxytoluenes. Journal of Molecular Structure, 2021, 1240, 130617.	1.8	4
31	DFT simulation of barrier heights, infrared and Raman spectra, and investigation of vibrational characteristics of 2-((2-aminopyridin-3-yl) methylene) hydrazinecarbothioamide and its N-methyl variant. Molecular Simulation, 2022, 48, 1315-1329.	0.9	4
32	Experimental and theoretical study of 3-methyl-4- nitrobenzoic acid using DFT and IVP methods. Journal of Physics: Conference Series, 2016, 759, 012057.	0.3	3
33	Synthesis, single-crystal X-ray diffraction, NLO and DFT studies of centrosymmetric 4-amino-3,5-dimethyl-1H-pyrazolium citrate monohydrate salt. Molecular Physics, 2022, 120, .	0.8	2
34	Vibrational analysis of mononitro substituted benzamides, benzaldehydes and toluenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 291-295.	2.0	1
35	Vibrational Analysis of Some Substituted Methylbenzenes Part II. Transferability of Force Constantsâ€"The Case of Tetra-, Tri-methylbenzenes and Nitro-para-toluidine. , 2011, , .		1
36	Molecular structure and vibrational analysis of 2,5-pyridine-dicarboxylic acid using experimental and theoretical methods. IOP Conference Series: Materials Science and Engineering, 2018, 360, 012028.	0.3	0

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37	NMR & Electronic Spectra, NLO, FMO, NBO and Thermodynamic Properties of Pentachlorophenol: An Experimental and Theoretical Investigation. Asian Journal of Chemistry, 2020, 32, 3057-3062.	0.1	0
38	Synthesis, antimicrobial activity and DFT studies of 4,5-dihydro-9-methoxy-4-(5-methylisoxazol-3-yl)benzo[f][1,4]oxazepin-3(2H)-one. Materials Today: Proceedings, 2021, , .	0.9	0
39	Experimental and density functional theory study on structure, vibrational and molecular characteristics of 2-chloro-5-methylpyrimidine and 2,4-dichloro-5-methylpyrimidine. Molecular Simulation, 0, , 1-14.	0.9	0