Venkatesha R Hathwar

List of Publications by Year
in descending order

65	1,633	304743 22	289244 40
papers	citations	h-index	g-index

65	65	65	1997
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantitative Investigation of Halogen and Hydrogen Bonding in 2â€Chloro, 4â€Xâ€Benzoic Acids. ChemistrySelect, 2022, 7, .	1.5	2
2	The Relevance of Experimental Charge Density Analysis in Unraveling Noncovalent Interactions in Molecular Crystals. Molecules, 2022, 27, 3690.	3.8	14
3	Structure and ionic conductivity of Na3+Sc2Si P3-O12 (x=0.0, 0.2, 0.4, 0.8) NASICON materials: A combined neutron diffraction, MAS NMR and impedance study. Solid State Sciences, 2021, 111, 106470.	3.2	14
4	A Zinc(II) Coordination Polymer Based on a Chain of {Zn 2 O 7 } Bitetrahedra Bridged by 3â€Methoxybenzoates. ChemistrySelect, 2020, 5, 9820-9824.	1.5	1
5	Investigation of bond topological and electrostatic properties of plumbagin molecule: An experimental and theoretical charge density study. Journal of Molecular Structure, 2020, 1220, 128714.	3.6	2
6	Insights from electron density analysis into the charge transfer mechanism in a photoluminescent cocrystal of phenanthrene and tetrafluoro-1,4-benzoquinone. Journal of Molecular Structure, 2020, 1208, 127864.	3.6	2
7	Low-Temperature Structural Phase Transitions in Thermoelectric Tetrahedrite, Cu₁₂Sb₄S₁₃, and Tennantite, Cu₁₂As₄S₁₃. Crystal Growth and Design, 2019, 19, 3979-3988.	3.0	8
8	Measurement of Electric Fields Experienced by Urea Guest Molecules in the 18-Crown-6/Urea (1:5) Hostâ€“Guest Complex: An Experimental Reference Point for Electric-Field-Assisted Catalysis. Journal of the American Chemical Society, 2019, 141, 3965-3976.	13.7	35
9	Experimental and theoretical charge density, intermolecular interactions and electrostatic properties of metronidazole. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 942-953.	1.1	10
10	X-ray electron density investigation of chemical bonding in van der Waals materials. Nature Materials, 2018, 17, 249-252.	27.5	93
11	Probing the accuracy and precision of Hirshfeld atom refinement with HARt interfaced with Olex2. IUCrJ, 2018, 5, 32-44.	2.2	74
12	Characterization of electronic features of intermolecular interactions involving organic fluorine: Inputs from in situ cryo-crystallization studies on F and CF3 substituted anilines. Journal of Fluorine Chemistry, 2018, 211, 37-51.	1.7	11
13	Charge density and electrostatic potential of hepatitis C anti-viral agent andrographolide: an experimental and theoretical study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2018, 74, 693-704.	1.1	11
14	CHAPTER 5. Experimental Charge Density Analysis in Organic Solids. Monographs in Supramolecular Chemistry, 2018, , 159-188.	0.2	0
15	Neutron and X-ray investigations of the Jahnâ€“Teller switch in partially deuterated ammonium copper Tutton salt, (NH₄)₂[Cu(H₂O)₆](SO₄)₂. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 87-93.	1.1	3
16	Validation of Chemical Bonding by Charge-Density Descriptors: The Current Scenario. Journal of the Indian Institute of Science, 2017, 97, 281-298.	1.9	5
17	Variable-temperature structural studies on valence tautomerism in cobalt bis(dioxolene) molecular complexes. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 304-312.	1.1	4
18	Characterization of fluorine-centred `F...O' Ïƒ-hole interactions in the solid state. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 140-152.	1.1	28

#	ARTICLE	IF	CITATIONS
19	Investigation of Chemical Bonding in In Situ Cryocrystallized Organometallic Liquids. ChemPhysChem, 2017, 18, 2859-2863.	2.1	9
20	â€œConformational lockâ€•via unusual intramolecular Câ€“Fâ‹¯Oî€€ and Câ€“Hâ‹¯Clâ€“C parallel dipoles observed in in situ cryocrystallized liquids. Chemical Communications, 2016, 52, 7225-7228.	4.1	31
21	Electron Density Analysis of the â€œOâ€“Oâ€•Charge-Shift Bonding in Rubrene Endoperoxide. Journal of Physical Chemistry A, 2016, 120, 7510-7518.	2.5	12
22	Quantitative analysis of intermolecular interactions in orthorhombic rubrene. IUCrJ, 2015, 2, 563-574.	2.2	206
23	Accurate atomic displacement parameters from time-of-flight neutron-diffraction data at TOPAZ. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, 679-681.	0.1	12
24	Contemporary X-ray electron-density studies using synchrotron radiation. IUCrJ, 2014, 1, 267-280.	2.2	34
25	Topological analysis of electron density and the electrostatic properties of isoniazid: an experimental and theoretical study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2014, 70, 331-341.	1.1	27
26	Revealing the Polarizability of Organic Fluorine in the Trifluoromethyl Group: Implications in Supramolecular Chemistry. Crystal Growth and Design, 2014, 14, 5366-5369.	3.0	64
27	Relationships between Electron Density and Magnetic Properties in Water-Bridged Dimetal Complexes. Inorganic Chemistry, 2014, 53, 11531-11539.	4.0	8
28	Intermolecular interactions, charge-density distribution and the electrostatic properties of pyrazinamide anti-TB drug molecule: an experimental and theoretical charge-density study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2014, 70, 568-579.	1.1	29
29	Topological Electron Density Analysis and Electrostatic Properties of Aspirin: An Experimental and Theoretical Study. Crystal Growth and Design, 2012, 12, 4357-4366.	3.0	42
30	Superconductivity at Tc = 44 K in LixFe2Se2(NH3)y. European Physical Journal B, 2012, 85, 1.	1.5	89
31	Synthesis, growth, and characterization of a new NLO material 3-(2,3-dimethoxyphenyl)-1-(pyridin-2-yl)prop-2-en-1-one. Journal of Molecular Structure, 2012, 1007, 175-178.	3.6	26
32	Extending the Supramolecular Synthon Based Fragment Approach (SBFA) for Transferability of Multipole Charge Density Parameters to Monofluorobenzoic Acids and their Cocrystals with Isonicotinamide: Importance of Câ€“HÂ·Â·Â·O, Câ€“HÂ·Â·Â·F, and FÂ·Â·Â·F Intermolecular Regions. Journal of Physical Chemistry A, 2011, 115, 12852-12863.	2.5	57
33	Transferability of Multipole Charge Density Parameters for Supramolecular Synthons: A New Tool for Quantitative Crystal Engineering. Crystal Growth and Design, 2011, 11, 616-623.	3.0	65
34	Halogen Bonding in 2,5-Dichloro-1,4-benzoquinone: Insights from Experimental and Theoretical Charge Density Analysis. Crystal Growth and Design, 2011, 11, 1855-1862.	3.0	70
35	Charge Density Analysis of a Pentaborate Ion in an Ammonium Borate: Toward the Understanding of Topological Features in Borate Minerals. Journal of Physical Chemistry A, 2011, 115, 12818-12825.	2.5	19
36	Charge Density Analysis of Heterohalogen (ClÂ·Â·Â·F) and Homohalogen (FÂ·Â·Â·F) Intermolecular Interactions in Molecular Crystals: Importance of the Extent of Polarizability. Crystal Growth and Design, 2011, 11, 1338-1346.	3.0	82

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37	Analysis of Clâ€¦Cl and C-Hâ€¦Cl intermolecular interactions involving chlorine in substituted 2-chloroquinoline derivatives. Journal of Chemical Sciences, 2010, 122, 677-685.	1.5	68
38	2-Chloro-8-methyl-3-[(pyrimidin-4-yloxy)methyl]quinoline. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1010-o1010.	0.2	0
39	5-(4-Chlorophenyl)-3-(2,4-dimethylthiazol-5-yl)-1,2,4-triazolo[3,4-a]isoquinoline. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1056-o1057.	0.2	1
40	5-(4-Chlorophenyl)-3-(2-furyl)-1,2,4-triazolo[3,4-a]isoquinoline. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1061-o1061.	0.2	1
41	3-(4-Chlorophenyl)-5-phenyl-1,2,4-triazolo[3,4-a]isoquinoline. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1094-o1094.	0.2	1
42	(2-Chloro-8-methoxyquinolin-3-yl)methanol monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1542-o1542.	0.2	2
43	3-[(2-Chloro-6-methylquinolin-3-yl)methyl]quinazolin-4(3H)-one. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1545-o1545.	0.2	0
44	4-(5-Phenyl-1,2,4-triazolo[3,4-a]isoquinolin-3-yl)benzonitrile. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1081-o1081.	0.2	1
45	3-tert-Butyl-1H-isochromene-1-thione. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1470-o1470.	0.2	1
46	Charge Density Analysis of Crystals of Nicotinamide with Salicylic Acid and Oxalic Acid: An Insight into the Salt to Cocrystal Continuum. Crystal Growth and Design, 2010, 10, 3306-3310.	3.0	77
47	Experimental and Theoretical Charge Density Analysis of Polymorphic Structures: The Case of Coumarin 314 Dye. Crystal Growth and Design, 2010, 10, 1516-1526.	3.0	35
48	Correction to Experimental and Theoretical Charge Density Analysis of Polymorphic Structures: The Case of Coumarin 314 Dye. Crystal Growth and Design, 2010, 10, 4670-4670.	3.0	1
49	Nature of ClÂ·Â·Â·Cl Intermolecular Interactions via Experimental and Theoretical Charge Density Analysis: Correlation of Polar Flattening Effects with Geometry. Journal of Physical Chemistry A, 2010, 114, 13434-13441.	2.5	122
50	2-Chloro-3-hydroxymethyl-7,8-dimethylquinoline. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o200-o200.	0.2	8
51	2-Chloro-3-hydroxymethyl-6-methoxyquinoline. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o201-o201.	0.2	15
52	1-[3-(4-Chlorophenyl)isoquinolin-1-yl]-3,5-diphenyl-1H-pyrazole. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o369-o369.	0.2	3
53	5-Phenyl-3-(2-thienyl)-1,2,4-triazolo[3,4-a]isoquinoline. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o488-o488.	0.2	11
54	(2-Chlorobenzo[h]quinolin-3-yl)methanol. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o953-o953.	0.2	1

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55	Ethyl 6-chloro-2-[(2-chloro-7,8-dimethylquinolin-3-yl)methoxy]-4-phenylquinoline-3-carboxylate. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o972-o973.	0.2	5
56	1,3,6-Trimethylpyrano[4,3-b]pyrrol-4(1H)-one. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o381-o381.	0.2	0
57	Evaluation of intermolecular interactions in thioisocoumarin derivatives: the role of the sulfur atom in generating packing motifs. CrystEngComm, 2009, 11, 284-291.	2.6	25
58	2-Chloro-6-methylquinoline-3-carbaldehyde. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o2686-o2686.	0.2	6
59	N-Phenylnicotinamide. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o571-o571.	0.2	5
60	3-(4-Methoxyphenyl)-1H-isochromen-1-one. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o128-o128.	0.2	3
61	3-(1,3-Dioxolan-2-yl)-2-hydrazino-7-methylquinoline. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o407-o408.	0.2	1
62	1-(4-Chlorophenyl)-2-phenyl-2-(3-phenyl-1-isoquinolylsulfanyl)ethanone. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o2732-o2732.	0.2	2
63	3-Phenyl-1-[2-(3-phenylisoquinolin-1-yl)diselanyl]isoquinoline. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o2295-o2295.	0.2	9
64	3-Butyl-1H-isochromen-1-one. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3707-o3707.	0.2	16
65	3-Butyl-1H-isochromene-1-thione. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3708-o3708.	0.2	14