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 analysis of intermolecular interactions in orthorhombic rubrene. IUCrJ, 2015, 2, 563-574.	2.2	206
2	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
3	X-ray electron density investigation of chemical bonding in van der Waals materials. Nature Materials, 2018, 17, 249-252.	27.5	93
4	Superconductivity at Tc = 44 K in LixFe2Se2(NH3)y. European Physical Journal B, 2012, 85, 1.	1.5	89
5	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
6	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
7	Probing the accuracy and precision of Hirshfeld atom refinement with HARt interfaced with Olex2. IUCrJ, 2018, 5, 32-44.	2.2	74
8	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
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	Contemporary X-ray electron-density studies using synchrotron radiation. IUCrJ, 2014, 1, 267-280.	2.2	34
17	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
18	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

#	ARTICLE	IF	CITATIONS
19	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
20	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
21	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
22	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
23	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
24	3-Butyl-1H-isochromen-1-one. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3707-o3707.	0.2	16
25	2-Chloro-3-hydroxymethyl-6-methoxyquinoline. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o201-o201.	0.2	15
26	3-Butyl-1H-isochromene-1-thione. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3708-o3708.	0.2	14
27	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
28	The Relevance of Experimental Charge Density Analysis in Unraveling Noncovalent Interactions in Molecular Crystals. Molecules, 2022, 27, 3690.	3.8	14
29	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
30	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
31	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
32	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
33	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
34	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
35	Investigation of Chemical Bonding in In Situ Cryocrystallized Organometallic Liquids. ChemPhysChem, 2017, 18, 2859-2863.	2.1	9
36	3-Phenyl-1-[2-(3-phenylisoquinolin-1-yl)diselanyl]isoquinoline. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o2295-o2295.	0.2	9

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37	Relationships between Electron Density and Magnetic Properties in Water-Bridged Dimetal Complexes. Inorganic Chemistry, 2014, 53, 11531-11539.	4.0	8
38	Low-Temperature Structural Phase Transitions in Thermoelectric Tetrahedrite, Cu₁₂Sb₄S₁₃, and Tennantite, Cu₁₂As₄S₁₃. Crystal Growth and Design, 2019, 19, 3979-3988.	3.0	8
39	2-Chloro-3-hydroxymethyl-7,8-dimethylquinoline. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o200-o200.	0.2	8
40	2-Chloro-6-methylquinoline-3-carbaldehyde. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o2686-o2686.	0.2	6
41	N-Phenylnicotinamide. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o571-o571.	0.2	5
42	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
43	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
44	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
45	Neutron and X-ray investigations of the Jahna€"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
46	3-(4-Methoxyphenyl)-1H-isochromen-1-one. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o128-o128.	0.2	3
47	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
48	(2-Chloro-8-methoxyquinolin-3-yl)methanol monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1542-o1542.	0.2	2
49	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
50	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
51	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
52	Quantitative Investigation of Halogen and Hydrogen Bonding in 2â€Chloro, 4â€Xâ€Benzoic Acids. ChemistrySelect, 2022, 7, .	1.5	2
53	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
54	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

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55	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
56	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
57	3-tert-Butyl-1H-isochromene-1-thione. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1470-o1470.	0.2	1
58	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
59	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
60	3-(1,3-Dioxolan-2-yl)-2-hydrazino-7-methylquinoline. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o407-o408.	0.2	1
61	(2-Chlorobenzo[h]quinolin-3-yl)methanol. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o953-o953.	0.2	1
62	2-Chloro-8-methyl-3-[(pyrimidin-4-yloxy)methyl]quinoline. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o1010-o1010.	0.2	0
63	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
64	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
65	CHAPTER 5. Experimental Charge Density Analysis in Organic Solids. Monographs in Supramolecular Chemistry, 2018, , 159-188.	0.2	0