Tejender S Thakur

List of Publications by Year
in descending order

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44 papers	3,048 citations	257101 24 h-index	253896 43 g-index
46 all docs	46 docs citations	46 times ranked	3567 citing authors

#	Article	IF	Citations
1	Polymorphs, Salts, and Cocrystals: Whatâ€™s in a Name?. Crystal Growth and Design, 2012, 12, 2147-2152.	1.4	767
2	Significant progress in predicting the crystal structures of small organic molecules â€“ a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125.	1.8	371
3	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
4	Co-Crystals of the Anti-HIV Drugs Lamivudine and Zidovudine. Crystal Growth and Design, 2009, 9, 951-957.	1.4	148
5	Misassigned Câ€“Hâ‹¯Cu agostic interaction in a copper(ii) ephedrine derivative is actually a weak, multicentred hydrogen bond. Chemical Communications, 2006, , 552-554.	2.2	99
6	Câ€“Hâ‹¯Fâ€“C hydrogen bonding in 1,2,3,5-tetrafluorobenzene and other fluoroaromatic compounds and the crystal structure of alloxan revisited. CrystEngComm, 2010, 12, 2079.	1.3	95
7	Polymorphs, Pseudopolymorphs, and Co-Crystals of Orcinol: Exploring the Structural Landscape with High Throughput Crystallography. Crystal Growth and Design, 2011, 11, 2637-2653.	1.4	92
8	Nature and strength of Câ€“Hâ‹¯O interactions involving formyl hydrogen atoms: computational and experimental studies of small aldehydes. Physical Chemistry Chemical Physics, 2011, 13, 14076.	1.3	83
9	Theoretical investigation of Câ€“Hâ‹¯M interactions in organometallic complexes: A natural bond orbital (NBO) study. Computational and Theoretical Chemistry, 2007, 810, 143-154.	1.5	82
10	Crystal Structure Prediction of a Co-Crystal Using a Supramolecular Synthon Approach: 2-Methylbenzoic Acidâ‹¯2-Amino-4-methylpyrimidine. Crystal Growth and Design, 2008, 8, 4031-4044.	1.4	75
11	Structure-Based Design of DevR Inhibitor Active against Nonreplicating Mycobacterium tuberculosis. Journal of Medicinal Chemistry, 2009, 52, 6324-6334.	2.9	74
12	New Solid State Forms of the Anti-HIV Drug Efavirenz. Conformational Flexibility and High Zâ€² Issues. Crystal Growth and Design, 2010, 10, 3191-3202.	1.4	71
13	Transferability of Multipole Charge Density Parameters for Supramolecular Synthons: A New Tool for Quantitative Crystal Engineering. Crystal Growth and Design, 2011, 11, 616-623.	1.4	65
14	Crystal Structure and Prediction. Annual Review of Physical Chemistry, 2015, 66, 21-42.	4.8	65
15	Intermolecular atomâ€“atom bonds in crystals â€“ a chemical perspective. IUCrJ, 2015, 2, 159-160.	1.0	63
16	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.	1.1	57
17	Crystalline Multicomponent Solids: An Alternative for Addressing the Hygroscopicity Issue in Pharmaceutical Materials. Crystal Growth and Design, 2020, 20, 6245-6265.	1.4	45
18	Third Polymorph of Phenylacetylene. Crystal Growth and Design, 2010, 10, 4246-4249.	1.4	44

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19	Synthesis of Octabromoperylene Dianhydride and Diimides: Evidence of Halogen Bonding and Semiconducting Properties. Organic Letters, 2016, 18, 472-475.	2.4	39
20	New crystalline salt forms of levofloxacin: conformational analysis and attempts towards the crystal structure prediction of the anhydrous form. CrystEngComm, 2014, 16, 4215.	1.3	37
21	Triclabendazole: An Intriguing Case of Coâ€existence of Conformational and Tautomeric Polymorphism. Chemistry - an Asian Journal, 2012, 7, 330-342.	1.7	34
22	Crystalline Supramolecular Nanofibers Based on Dehydrobenzoannulene Derivatives. Chemistry - A European Journal, 2013, 19, 15366-15377.	1.7	28
23	Five varieties of hydrogen bond in 1-formyl-3-thiosemicarbazide: an electron density study. Acta Crystallographica Section B: Structural Science, 2006, 62, 118-127.	1.8	27
24	Preparation of Pyrazinamide Eutectics versus Cocrystals Based on Supramolecular Synthon Variations. Crystal Growth and Design, 2018, 18, 6640-6651.	1.4	24
25	Rational Coformer Selection and the Development of New Crystalline Multicomponent Forms of Resveratrol with Enhanced Water Solubility. Crystal Growth and Design, 2018, 18, 1581-1592.	1.4	22
26	Weak Câ€”H...O hydrogen bonds in anisaldehyde, salicylaldehyde and cinnamaldehyde. Acta Crystallographica Section C: Crystal Structure Communications, 2011, 67, o387-o390.	0.4	20
27	Proton transfer and N(+)â€“Hâ‹¯S(â¯)hydrogen bonds in the crystal structure of 4-aminothiophenol. Chemical Communications, 2004, , 2526-2527.	2.2	19
28	Versatile coordination environment and interplay of metal assisted secondary interactions in the organization of supramolecular motifs in new Hg(II)/PhHg(II) dithiolates. Polyhedron, 2014, 69, 225-233.	1.0	19
29	Correction for Polymorphs, Salts and Cocrystals: Whatâ€™s in a Name?. Crystal Growth and Design, 2012, 12, 4290-4291.	1.4	17
30	Structural Transformation between Supramolecular Nanofibers with Drastic Change of Conductivity by Heat and Ultrasound. Chemistry - an Asian Journal, 2013, 8, 1372-1376.	1.7	13
31	Studying the Role of Câ•OÂ·Â·Â·Câ•O, Câ•OÂ·Â·Â·Nâ€“O, and Nâ€“OÂ·Â·Â·Nâ€“O Dipoleâ€“Dipole Interactions in the Crystal Packing of 4-Nitrobenzoic Acid and 3,3â€²-Dinitrobenzophenone Polymorphs: An Experimental Charge Density Study. Crystal Growth and Design, 2015, 15, 3280-3292.	1.4	13
32	Cationâ‹¯cation hydrogen bonds in synephrine salts: a typical interaction in an unusual environment. Physical Chemistry Chemical Physics, 2019, 21, 20647-20660.	1.3	13
33	Computational Screening of Multicomponent Solid Forms of 2-Aryl-Propionate Class of NSAID, Zaltoprofen, and Their Experimental Validation. Crystal Growth and Design, 2021, 21, 449-461.	1.4	13
34	S-Enantiomer of the Antitubercular Compound S006-830 Complements Activity of Frontline TB Drugs and Targets Biogenesis of Mycobacterium tuberculosis Cell Envelope. ACS Omega, 2017, 2, 8453-8465.	1.6	12
35	Crystal Polymorphism in Pharmaceutical Science. , 2017, , 283-309.		9
36	Photoinstability in Active Pharmaceutical Ingredients: Crystal Engineering as a Mitigating Measure. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2021, 49, 100455.	5.6	7

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37	1,2,3-Trifluorobenzene. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o2670-o2670.	0.2	6
38	1,3-Difluorobenzene. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o2668-o2669.	0.2	5
39	Quinoxaline:Zâ€² = 1 form. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o2789-o2789.	0.2	4
40	Experimental and computational crystal structure landscape study of nigerloxin: a fungal metabolite from Aspergillus niger. CrystEngComm, 2016, 18, 1740-1751.	1.3	4
41	Structural Landscape-Guided Exploration of a New Polymorph of 4-Nitrobenzoic Acid. Crystal Growth and Design, 2019, 19, 952-958.	1.4	3
42	Crystal Engineering in the Desiraju Research Group in Bangalore. Crystal Growth and Design, 2012, 12, 4688-4691.	1.4	2
43	Comment on â€œPolymorphism of levofloxacin: structure, properties and phase transformationâ€•by N. Wei, L. Jia, Z. Shang, J. Gong, S. Wu, J. Wang and W. Tang, CrystEngComm, 2019, 21, 6196â€“6207. CrystEngComm, 2020, 22, 1885-1888.	1.3	2
44	Understanding the guest binding in the cucurbit[7]uril inclusion complexes of CDK4/6 inhibitors, palbociclib, and ribociclib from a combined experimental and computational study. Journal of Molecular Structure, 2021, 1241, 130637.	1.8	2