Jacco van de Streek

List of Publications by Year
in descending order

87	18,044	186265 28	51608 86
papers	citations	h-index	g-index

92	92	92	15958
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Crystal structure from X-ray powder diffraction data, DFT-D calculation, Hirshfeld surface analysis, and energy frameworks of (RS)-trichlormethiazide. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 140-148.	0.5	2
2	Comment on the article Properties and interactions â€“ melting point of tribromobenzene isomers. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 274-275.	1.1	1
3	Industrial azomethine nickel complex pigments. Four crystal structures from X-ray powder diffraction data. Zeitschrift Fur Kristallographie - Crystalline Materials, 2021, 236, 105-115.	0.8	0
4	Crystal structure and morphology of the bright orange Î³-phase of Pigment Red 53:2 from XRPD, DFT+D and TEM. Dyes and Pigments, 2021, 196, 109456.	3.7	0
5	Crystal structure from laboratory X-ray powder diffraction data, DFT-D calculations, Hirshfeld surface analysis, and energy frameworks of a new polymorph of 1-benzothiophene-2-carboxylic acid. Powder Diffraction, 2021, 36, 2-13.	0.2	5
6	Structural analysis of metastable pharmaceutical loratadine form II, by 3D electron diffraction and DFT+D energy minimisation. CrystEngComm, 2020, 22, 7490-7499.	2.6	13
7	Co-Crystal Structures of Furosemide:Urea and Carbamazepine:Indomethacin Determined from Powder X-Ray Diffraction Data. Crystals, 2020, 10, 42.	2.2	12
8	Computational polymorph screening reveals late-appearing and poorly-soluble form of rotigotine. Communications Chemistry, 2019, 2, .	4.5	39
9	Inconvenient Truths about Solid Form Landscapes Revealed in the Polymorphs and Hydrates of Gandotinib. Crystal Growth and Design, 2019, 19, 2947-2962.	3.0	32
10	Structure determination of oxamic acid from laboratory powder X-Ray diffraction data and energy minimization by DFT-D. Journal of Molecular Structure, 2019, 1177, 310-316.	3.6	2
11	A jumping crystal predicted with molecular dynamics and analysed with TLS refinement against powder diffraction data. IUCrJ, 2019, 6, 136-144.	2.2	5
12	Four interpenetrating hydrogen-bonded three-dimensional networks in divanillin. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1768-1773.	0.5	0
13	How many ritonavir cases are there still out there?. Faraday Discussions, 2018, 211, 441-458.	3.2	44
14	Crystal structure analysis of a star-shaped triazine compound: a combination of single-crystal three-dimensional electron diffraction and powder X-ray diffraction. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2018, 74, 287-294.	1.1	1
15	The application of tailor-made force fields and molecular dynamics for NMR crystallography: a case study of free base cocaine. IUCrJ, 2017, 4, 175-184.	2.2	10
16	Validation of missed space-group symmetry in X-ray powder diffraction structures with dispersion-corrected density functional theory. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 756-766.	1.1	2
17	Crystallographic and Dynamic Aspects of Solidâ€State NMR Calibration Compounds: Towards ab Initio NMR Crystallography. ChemPhysChem, 2016, 17, 2496-2502.	2.1	12
18	Local structure in the disordered solid solution ofcis- andtrans-perinones. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 416-433.	1.1	12

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19	Spray drying of fenofibrate loaded nanostructured lipid carriers. Asian Journal of Pharmaceutical Sciences, 2016, 11, 507-515.	9.1	33
20	Crystal structure and tautomerism of Pigment Yellow 138 determined by X-ray powder diffraction and solid-state NMR. Dyes and Pigments, 2016, 131, 364-372.	3.7	20
21	Revision of the Crystal Structure of the First Molecular Polymorph in History. Crystal Growth and Design, 2016, 16, 1366-1370.	3.0	12
22	Structure of Pigment Yellow 181 dimethylsulfoxideN-methyl-2-pyrrolidone (1:1:1) solvate from XRPD + DFT-D. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 89-94.	1.1	6
23	One hydrogen bond does not a separation make, or does it? Resolution of amines by diacetoneketogulonic acid. Chemical Communications, 2015, 51, 5664-5667.	4.1	4
24	Synthesis, characterization, in silico approach and in vitro antiproliferative activity of RPF151, a benzodioxole sulfonamide analogue designed from capsaicin scaffold. Journal of Molecular Structure, 2015, 1088, 138-146.	3.6	13
25	Combined crystal structure prediction and high-pressure crystallization in rational pharmaceutical polymorph screening. Nature Communications, 2015, 6, 7793.	12.8	193
26	Validation of molecular crystal structures from powder diffraction data with dispersion-corrected density functional theory (DFT-D). Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2014, 70, 1020-1032.	1.1	222
27	On the correlation between hydrogen bonding and melting points in the inositols. IUCrJ, 2014, 1, 61-73.	2.2	11
28	Distinguishing tautomerism in the crystal structure of (Z)-N-(5-ethyl-2,3-dihydro-1,3,4-thiadiazol-2-ylidene)-4-methylbenzenesulfonamide using DFT-D calculations and¹³C solid-state NMR. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 784-789.	0.5	17
29	Computational pharmaceutical materials science. Journal of Cheminformatics, 2014, 6, O21.	6.1	0
30	Structures of cefradine dihydrate and cefaclor dihydrate from DFT-D calculations. Acta Crystallographica Section C: Crystal Structure Communications, 2013, 69, 1229-1233.	0.4	8
31	Reinterpretation of the monohydrate of clarithromycin from X-ray powder diffraction data as a trihydrate. Acta Crystallographica Section C: Crystal Structure Communications, 2012, 68, o369-o372.	0.4	3
32	On the high-temperature phase of barbituric acid. CrystEngComm, 2012, 14, 3046.	2.6	21
33	Complementing High-Throughput X-ray Powder Diffraction Data With Quantumâ€“Chemical Calculations: Application to Piroxicam Form III. Journal of Pharmaceutical Sciences, 2012, 101, 4214-4219.	3.3	30
34	Ab-initio crystal structure analysis and refinement approaches of oligo p-benzamides based on electron diffraction data. Acta Crystallographica Section B: Structural Science, 2012, 68, 171-181.	1.8	49
35	Experimental verification of a subtle low-temperature phase transition suggested by DFT-D energy minimisation. CrystEngComm, 2011, 13, 1768.	2.6	12
36	Crystal-structure prediction of pyridine with four independent molecules. CrystEngComm, 2011, 13, 7135.	2.6	28

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37	Different structural destinations: comparing reactions of [CuBr2(3-Brpy)2] crystals with HBr and HCl gas. CrystEngComm, 2011, 13, 4400.	2.6	22
38	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
39	Dimorphism of the prodrug lâ€tyrosine ethyl ester: Pressureâ€“temperature state diagram and crystal structure of phase II. Journal of Pharmaceutical Sciences, 2011, 100, 4774-4782.	3.3	24
40	The Thermodynamically Stable Form of Solid Barbituric Acid: The Enol Tautomer. Angewandte Chemie - International Edition, 2011, 50, 7924-7926.	13.8	81
41	Progress in Crystal Structure Prediction. Chemistry - A European Journal, 2011, 17, 10736-10744.	3.3	79
42	The use of dispersion-corrected DFT calculations to prevent an incorrect structure determination from powder data: the case of acetolone, C₁₁H₁₁N₃O₃. Zeitschrift FÃ¼r Kristallographie, 2011, 226, 476-482.	1.1	9
43	X-ray powder diffraction, solid-state NMR and dispersion-corrected DFT calculations to investigate the solid state structure of 2-ammonio-5-chloro-4-methylbenzenesulfonate. Zeitschrift FÃ¼r Kristallographie, 2010, 225, 382-387.	1.1	16
44	Mechanistic Insights into a Gasâ€“Solid Reaction in Molecular Crystals: The Role of Hydrogen Bonding. Angewandte Chemie - International Edition, 2010, 49, 8892-8896.	13.8	59
45	Validation of experimental molecular crystal structures with dispersion-corrected density functional theory calculations. Acta Crystallographica Section B: Structural Science, 2010, 66, 544-558.	1.8	156
46	H-bonding schemes of di- and tri-p-benzamides assessed by a combination of electron diffraction, X-ray powder diffraction and solid-state NMR. CrystEngComm, 2010, 12, 1824.	2.6	20
47	Validation of dispersion-corrected density functional theory calculations for the crystal structure prediction of molecular salts: a crystal structure prediction study of pyridinium chloride. CrystEngComm, 2010, 12, 3827.	2.6	12
48	Structure determinations of three fluorescent organic pigments by powder diffraction and micro-crystal structure analysis. Zeitschrift FÃ¼r Kristallographie, 2009, 224, 556-562.	1.1	2
49	The First Crystal Structures of Industrial Laked Yellow Pigments Determined by Xâ€ray Powder Diffraction. Chemistry - A European Journal, 2009, 15, 338-341.	3.3	13
50	Rational Modification of the Hierarchy of Intermolecular Interactions in Molecular Crystal Structures by Using Tunable Halogen Bonds. Chemistry - A European Journal, 2009, 15, 7554-7568.	3.3	164
51	Structures of six industrial benzimidazolone pigments from laboratory powder diffraction data. Acta Crystallographica Section B: Structural Science, 2009, 65, 200-211.	1.8	25
52	Structure determination of seven phases and solvates of Pigment Yellow 183 and Pigment Yellow 191 from X-ray powder and single-crystal data. Acta Crystallographica Section B: Structural Science, 2009, 65, 212-222.	1.8	24
53	Electron diffraction, X-ray powder diffraction and pair-distribution-function analyses to determine the crystal structures of Pigment Yellow 213, C₂₃H₂₁N₅O₉. Acta Crystallographica Section B: Structural Science, 2009, 65, 189-199.	1.8	16
54	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

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55	GDASH: a grid-enabled program for structure solution from powder diffraction data. Journal of Applied Crystallography, 2009, 42, 356-359.	4.5	9
56	MDASH: a multi-core-enabled program for structure solution from powder diffraction data. Journal of Applied Crystallography, 2009, 42, 360-361.	4.5	12
57	Crystal structure determination of N,Nâ€²-1,4-phenylene-bis(3-oxobutanamide) from laboratory powder diffraction data. Zeitschrift FÃ¼r Kristallographie, 2009, 224, 593-597.	1.1	1
58	Mercury CSD 2.0â€“ new features for the visualization and investigation of crystal structures. Journal of Applied Crystallography, 2008, 41, 466-470.	4.5	7,887
59	The crystal structure of Pigment Yellow 181 from laboratory powder diffraction data. Zeitschrift Fur Kristallographie - Crystalline Materials, 2007, 222, 713-717.	0.8	11
60	Ligand flexibility and framework rearrangement in a new family of porous metalâ€“organic frameworks. Chemical Communications, 2007, , 1532-1534.	4.1	73
61	New software for searching the Cambridge Structural Database for solvated and unsolvated crystal structures applied to hydrates. CrystEngComm, 2007, 9, 55-64.	2.6	62
62	Reversible Gas Uptake by a Nonporous Crystalline Solid Involving Multiple Changes in Covalent Bonding. Journal of the American Chemical Society, 2007, 129, 15606-15614.	13.7	82
63	All series of multiple solvates (including hydrates) from the Cambridge Structural Database. CrystEngComm, 2007, 9, 350-352.	2.6	32
64	Solidâ€“gas reactions between 1,3-dimethylbarbituric acid and amines. A structural and spectroscopic study. New Journal of Chemistry, 2007, 31, 1935.	2.8	10
65	Knowledge-based approaches to crystal design. CrystEngComm, 2006, , .	2.6	3
66	Polymorphism of Scyllo-Inositol:â€‰ Joining Crystal Structure Prediction with Experiment to Elucidate the Structures of Two Polymorphs. Crystal Growth and Design, 2006, 6, 2301-2307.	3.0	23
67	Reversible Extrusion and Uptake of HCl Molecules by Crystalline Solids Involving Coordination Bond Cleavage and Formation. Journal of the American Chemical Society, 2006, 128, 9584-9585.	13.7	113
68	Searching the Cambridge Structural Database for the `best' representative of each unique polymorph. Acta Crystallographica Section B: Structural Science, 2006, 62, 567-579.	1.8	92
69	Ampicillin trihydrate from synchrotron powder diffraction data. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o797-o799.	0.2	16
70	Pamoic acid determined from powder diffraction data. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o1170-o1172.	0.2	11
71	Amodiaquinium dichloride dihydrate from laboratory powder diffraction data. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o4196-o4199.	0.2	13
72	Mercury: visualization and analysis of crystal structures. Journal of Applied Crystallography, 2006, 39, 453-457.	4.5	6,260

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73	DASH: a program for crystal structure determination from powder diffraction data. Journal of Applied Crystallography, 2006, 39, 910-915.	4.5	495
74	Achieving Polymorphic and Stoichiometric Diversity in Cocrystal Formation:â€‰ Importance of Solid-State Grinding, Powder X-ray Structure Determination, and Seeding. Crystal Growth and Design, 2005, 5, 2233-2241.	3.0	188
75	Searching the Cambridge Structural Database for polymorphs. Acta Crystallographica Section B: Structural Science, 2005, 61, 504-510.	1.8	36
76	GRX: a program to search the CSD for functional group exchanges. Journal of Applied Crystallography, 2005, 38, 694-696.	4.5	21
77	MONTY:Â Monte Carlo Crystal Growth on Any Crystal Structure in Any Crystallographic Orientation; Application to Fats. Journal of Physical Chemistry A, 2004, 108, 5894-5902.	2.5	82
78	The crystal structure of an unstable polymorph of Î²-d-allose. CrystEngComm, 2004, 6, 535-539.	2.6	8
79	Morphology of and dislocation movement in n-C40H82 paraffin crystals grown from solution. Journal of Crystal Growth, 2003, 249, 600-613.	1.5	22
80	Comparing the Morphology of Î²-n.n.nwith Î²â€˜-n.n+2.nand Î²â€˜-n.n.n-2 Triacylglycerol Crystals. Journal of Physical Chemistry B, 2003, 107, 5680-5689.	2.6	21
81	Explanation for the Needle Morphology of Crystals Applied to a Î²â€˜ Triacylglycerol. Crystal Growth and Design, 2002, 2, 51-54.	3.0	29
82	On the irrelevance of electrostatics for the crystal structures and polymorphism of long evenn-alkanes. Journal of Computational Chemistry, 2002, 23, 365-370.	3.3	6
83	On the influence of thermal motion on the crystal structures and polymorphism of even n-alkanes. Acta Crystallographica Section B: Structural Science, 2002, 58, 677-683.	1.8	7
84	A two-dimensional Hartmanâ€“Perdok analysis of polymorphic fat surfaces observed with atomic force microscopy. Surface Science, 2001, 471, 101-113.	1.9	24
85	New evidence for Î²â€²-2 p.p+2.p triacylglycerol crystal structure. JAOCS, Journal of the American Oil Chemists' Society, 2000, 77, 215-216.	1.9	3
86	Structural analogy between Î²â€² triacylglycerols andn-alkanes. Toward the crystal structure of Î²â€²-2 p.p+2.p triacylglycerols. JAOCS, Journal of the American Oil Chemists' Society, 1999, 76, 1333-1341.	1.9	18
87	The Implication of the Connected Net Topology on the Morphology of Î²-Monoacid Triacylglycerol Crystals. Journal of Physical Chemistry B, 1999, 103, 8301-8309.	2.6	20