

Jacco van de Streek

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3844832/publications.pdf>

Version: 2024-02-01

87
papers

18,044
citations

186265

28
h-index

51608

86
g-index

92
all docs

92
docs citations

92
times ranked

15958
citing authors

#	ARTICLE	IF	CITATIONS
1	Mercury CSD 2.0 – new features for the visualization and investigation of crystal structures. <i>Journal of Applied Crystallography</i> , 2008, 41, 466-470.	4.5	7,887
2	Mercury: visualization and analysis of crystal structures. <i>Journal of Applied Crystallography</i> , 2006, 39, 453-457.	4.5	6,260
3	DASH: a program for crystal structure determination from powder diffraction data. <i>Journal of Applied Crystallography</i> , 2006, 39, 910-915.	4.5	495
4	Significant progress in predicting the crystal structures of small organic molecules – a report on the fourth blind test. <i>Acta Crystallographica Section B: Structural Science</i> , 2009, 65, 107-125.	1.8	371
5	Towards crystal structure prediction of complex organic compounds – a report on the fifth blind test. <i>Acta Crystallographica Section B: Structural Science</i> , 2011, 67, 535-551.	1.8	358
6	Validation of molecular crystal structures from powder diffraction data with dispersion-corrected density functional theory (DFT-D). <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2014, 70, 1020-1032.	1.1	222
7	Combined crystal structure prediction and high-pressure crystallization in rational pharmaceutical polymorph screening. <i>Nature Communications</i> , 2015, 6, 7793.	12.8	193
8	Achieving Polymorphic and Stoichiometric Diversity in Cocrystal Formation: Importance of Solid-State Grinding, Powder X-ray Structure Determination, and Seeding. <i>Crystal Growth and Design</i> , 2005, 5, 2233-2241.	3.0	188
9	Rational Modification of the Hierarchy of Intermolecular Interactions in Molecular Crystal Structures by Using Tunable Halogen Bonds. <i>Chemistry - A European Journal</i> , 2009, 15, 7554-7568.	3.3	164
10	Validation of experimental molecular crystal structures with dispersion-corrected density functional theory calculations. <i>Acta Crystallographica Section B: Structural Science</i> , 2010, 66, 544-558.	1.8	156
11	Reversible Extrusion and Uptake of HCl Molecules by Crystalline Solids Involving Coordination Bond Cleavage and Formation. <i>Journal of the American Chemical Society</i> , 2006, 128, 9584-9585.	13.7	113
12	Searching the Cambridge Structural Database for the 'best' representative of each unique polymorph. <i>Acta Crystallographica Section B: Structural Science</i> , 2006, 62, 567-579.	1.8	92
13	MONTY: Monte Carlo Crystal Growth on Any Crystal Structure in Any Crystallographic Orientation; Application to Fats. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5894-5902.	2.5	82
14	Reversible Gas Uptake by a Nonporous Crystalline Solid Involving Multiple Changes in Covalent Bonding. <i>Journal of the American Chemical Society</i> , 2007, 129, 15606-15614.	13.7	82
15	The Thermodynamically Stable Form of Solid Barbituric Acid: The Enol Tautomer. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 7924-7926.	13.8	81
16	Progress in Crystal Structure Prediction. <i>Chemistry - A European Journal</i> , 2011, 17, 10736-10744.	3.3	79
17	Ligand flexibility and framework rearrangement in a new family of porous metal-organic frameworks. <i>Chemical Communications</i> , 2007, , 1532-1534.	4.1	73
18	New software for searching the Cambridge Structural Database for solvated and unsolvated crystal structures applied to hydrates. <i>CrystEngComm</i> , 2007, 9, 55-64.	2.6	62

#	ARTICLE	IF	CITATIONS
19	Mechanistic Insights into a Gas-Solid Reaction in Molecular Crystals: The Role of Hydrogen Bonding. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 8892-8896.	13.8	59
20	Ab-initio crystal structure analysis and refinement approaches of oligo-p-benzamides based on electron diffraction data. <i>Acta Crystallographica Section B: Structural Science</i> , 2012, 68, 171-181.	1.8	49
21	How many ritonavir cases are there still out there?. <i>Faraday Discussions</i> , 2018, 211, 441-458.	3.2	44
22	Computational polymorph screening reveals late-appearing and poorly-soluble form of rotigotine. <i>Communications Chemistry</i> , 2019, 2, .	4.5	39
23	Searching the Cambridge Structural Database for polymorphs. <i>Acta Crystallographica Section B: Structural Science</i> , 2005, 61, 504-510.	1.8	36
24	Spray drying of fenofibrate loaded nanostructured lipid carriers. <i>Asian Journal of Pharmaceutical Sciences</i> , 2016, 11, 507-515.	9.1	33
25	All series of multiple solvates (including hydrates) from the Cambridge Structural Database. <i>CrystEngComm</i> , 2007, 9, 350-352.	2.6	32
26	Inconvenient Truths about Solid Form Landscapes Revealed in the Polymorphs and Hydrates of Gandotinib. <i>Crystal Growth and Design</i> , 2019, 19, 2947-2962.	3.0	32
27	Complementing High-Throughput X-ray Powder Diffraction Data With Quantum-Chemical Calculations: Application to Piroxicam Form III. <i>Journal of Pharmaceutical Sciences</i> , 2012, 101, 4214-4219.	3.3	30
28	Explanation for the Needle Morphology of Crystals Applied to a Triacylglycerol. <i>Crystal Growth and Design</i> , 2002, 2, 51-54.	3.0	29
29	Crystal-structure prediction of pyridine with four independent molecules. <i>CrystEngComm</i> , 2011, 13, 7135.	2.6	28
30	Structures of six industrial benzimidazolone pigments from laboratory powder diffraction data. <i>Acta Crystallographica Section B: Structural Science</i> , 2009, 65, 200-211.	1.8	25
31	A two-dimensional Hartman-Perdok analysis of polymorphic fat surfaces observed with atomic force microscopy. <i>Surface Science</i> , 2001, 471, 101-113.	1.9	24
32	Structure determination of seven phases and solvates of Pigment Yellow 183 and Pigment Yellow 191 from X-ray powder and single-crystal data. <i>Acta Crystallographica Section B: Structural Science</i> , 2009, 65, 212-222.	1.8	24
33	Dimorphism of the prodrug L-cytosine ethyl ester: Pressure-temperature state diagram and crystal structure of phase II. <i>Journal of Pharmaceutical Sciences</i> , 2011, 100, 4774-4782.	3.3	24
34	Polymorphism of Scyllo-Inositol: Joining Crystal Structure Prediction with Experiment to Elucidate the Structures of Two Polymorphs. <i>Crystal Growth and Design</i> , 2006, 6, 2301-2307.	3.0	23
35	Morphology of and dislocation movement in n-C40H82 paraffin crystals grown from solution. <i>Journal of Crystal Growth</i> , 2003, 249, 600-613.	1.5	22
36	Different structural destinations: comparing reactions of [CuBr2(3-Brpy)2] crystals with HBr and HCl gas. <i>CrystEngComm</i> , 2011, 13, 4400.	2.6	22

#	ARTICLE	IF	CITATIONS
37	Comparing the Morphology of \hat{I}^2 -n.n.nwith \hat{I}^2 -n.n+2.nand \hat{I}^2 -n.n.n-2 Triacylglycerol Crystals. Journal of Physical Chemistry B, 2003, 107, 5680-5689.	2.6	21
38	GRX: a program to search the CSD for functional group exchanges. Journal of Applied Crystallography, 2005, 38, 694-696.	4.5	21
39	On the high-temperature phase of barbituric acid. CrystEngComm, 2012, 14, 3046.	2.6	21
40	The Implication of the Connected Net Topology on the Morphology of \hat{I}^2 -Monoacid Triacylglycerol Crystals. Journal of Physical Chemistry B, 1999, 103, 8301-8309.	2.6	20
41	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
42	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
43	Structural analogy between \hat{I}^2 triacylglycerols and n-alkanes. Toward the crystal structure of \hat{I}^2 -2 p.p+2.p triacylglycerols. JAOCS, Journal of the American Oil Chemists' Society, 1999, 76, 1333-1341.	1.9	18
44	Distinguishing tautomerism in the crystal structure of (<i>Z</i>)-(5-ethyl-2,3-dihydro-1,3,4-thiadiazol-2-ylidene)-4-methylbenzenesulfonamide using DFT-D calculations and ^{13}C solid-state NMR. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 784-789.	0.5	17
45	Ampicillin trihydrate from synchrotron powder diffraction data. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o797-o799.	0.2	16
46	Electron diffraction, X-ray powder diffraction and pair-distribution-function analyses to determine the crystal structures of Pigment Yellow 213, $\text{C}_{23}\text{H}_{21}\text{N}_5\text{O}_9$. Acta Crystallographica Section B: Structural Science, 2009, 65, 189-199.	1.8	16
47	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 für Kristallographie, 2010, 225, 382-387.	1.1	16
48	Amodiaquiniun dichloride dihydrate from laboratory powder diffraction data. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o4196-o4199.	0.2	13
49	The First Crystal Structures of Industrial Laked Yellow Pigments Determined by X-ray Powder Diffraction. Chemistry - A European Journal, 2009, 15, 338-341.	3.3	13
50	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
51	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
52	<i>MDASH</i> : a multi-core-enabled program for structure solution from powder diffraction data. Journal of Applied Crystallography, 2009, 42, 360-361.	4.5	12
53	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
54	Experimental verification of a subtle low-temperature phase transition suggested by DFT-D energy minimisation. CrystEngComm, 2011, 13, 1768.	2.6	12

#	ARTICLE	IF	CITATIONS
55	Crystallographic and Dynamic Aspects of Solid-State NMR Calibration Compounds: Towards ab Initio NMR Crystallography. <i>ChemPhysChem</i> , 2016, 17, 2496-2502.	2.1	12
56	Local structure in the disordered solid solution of <i>cis</i> - and <i>trans</i> -perinones. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 416-433.	1.1	12
57	Revision of the Crystal Structure of the First Molecular Polymorph in History. <i>Crystal Growth and Design</i> , 2016, 16, 1366-1370.	3.0	12
58	Co-Crystal Structures of Furosemide:Urea and Carbamazepine:Indomethacin Determined from Powder X-Ray Diffraction Data. <i>Crystals</i> , 2020, 10, 42.	2.2	12
59	Pamoic acid determined from powder diffraction data. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2006, 62, o1170-o1172.	0.2	11
60	The crystal structure of Pigment Yellow 181 from laboratory powder diffraction data. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2007, 222, 713-717.	0.8	11
61	On the correlation between hydrogen bonding and melting points in the inositols. <i>IUCrJ</i> , 2014, 1, 61-73.	2.2	11
62	Solid-gas reactions between 1,3-dimethylbarbituric acid and amines. A structural and spectroscopic study. <i>New Journal of Chemistry</i> , 2007, 31, 1935.	2.8	10
63	The application of tailor-made force fields and molecular dynamics for NMR crystallography: a case study of free base cocaine. <i>IUCrJ</i> , 2017, 4, 175-184.	2.2	10
64	GDASH: a grid-enabled program for structure solution from powder diffraction data. <i>Journal of Applied Crystallography</i> , 2009, 42, 356-359.	4.5	9
65	The use of dispersion-corrected DFT calculations to prevent an incorrect structure determination from powder data: the case of acetolone, C ₁₁ H ₁₁ N ₃ O ₃ . <i>Zeitschrift für Kristallographie</i> , 2011, 226, 476-482.	1.1	9
66	The crystal structure of an unstable polymorph of ¹² C-d-allose. <i>CrystEngComm</i> , 2004, 6, 535-539.	2.6	8
67	Structures of cefradine dihydrate and cefaclor dihydrate from DFT-D calculations. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2013, 69, 1229-1233.	0.4	8
68	On the influence of thermal motion on the crystal structures and polymorphism of even n-alkanes. <i>Acta Crystallographica Section B: Structural Science</i> , 2002, 58, 677-683.	1.8	7
69	On the irrelevance of electrostatics for the crystal structures and polymorphism of long evenn-alkanes. <i>Journal of Computational Chemistry</i> , 2002, 23, 365-370.	3.3	6
70	Structure of Pigment Yellow 181 dimethylsulfoxide <i>N</i> -methyl-2-pyrrolidone (1:1:1) solvate from XRPD + DFT-D. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2015, 71, 89-94.	1.1	6
71	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. <i>Powder Diffraction</i> , 2021, 36, 2-13.	0.2	5
72	A jumping crystal predicted with molecular dynamics and analysed with TLS refinement against powder diffraction data. <i>IUCrJ</i> , 2019, 6, 136-144.	2.2	5

#	ARTICLE	IF	CITATIONS
73	One hydrogen bond does not a separation make, or does it? Resolution of amines by diacetoneketogluconic acid. <i>Chemical Communications</i> , 2015, 51, 5664-5667.	4.1	4
74	New evidence for $\hat{1}^2\hat{2}$ -p.p+2.p triacylglycerol crystal structure. <i>JAACS, Journal of the American Oil Chemists' Society</i> , 2000, 77, 215-216.	1.9	3
75	Knowledge-based approaches to crystal design. <i>CrystEngComm</i> , 2006, , .	2.6	3
76	Reinterpretation of the monohydrate of clarithromycin from X-ray powder diffraction data as a trihydrate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2012, 68, o369-o372.	0.4	3
77	Structure determinations of three fluorescent organic pigments by powder diffraction and micro-crystal structure analysis. <i>Zeitschrift Für Kristallographie</i> , 2009, 224, 556-562.	1.1	2
78	Validation of missed space-group symmetry in X-ray powder diffraction structures with dispersion-corrected density functional theory. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 756-766.	1.1	2
79	Structure determination of oxamic acid from laboratory powder X-Ray diffraction data and energy minimization by DFT-D. <i>Journal of Molecular Structure</i> , 2019, 1177, 310-316.	3.6	2
80	Crystal structure from X-ray powder diffraction data, DFT-D calculation, Hirshfeld surface analysis, and energy frameworks of (<i>RS</i>)-trichlormethiazide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 140-148.	0.5	2
81	Crystal structure determination of N,N $\hat{2}$ -1,4-phenylene-bis(3-oxobutanamide) from laboratory powder diffraction data. <i>Zeitschrift Für Kristallographie</i> , 2009, 224, 593-597.	1.1	1
82	Crystal structure analysis of a star-shaped triazine compound: a combination of single-crystal three-dimensional electron diffraction and powder X-ray diffraction. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 287-294.	1.1	1
83	Comment on the article <i>Properties and interactions of the melting point of tribromobenzene isomers</i>. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2022, 78, 274-275.	1.1	1
84	Computational pharmaceutical materials science. <i>Journal of Cheminformatics</i> , 2014, 6, O21.	6.1	0
85	Four interpenetrating hydrogen-bonded three-dimensional networks in divanillin. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 1768-1773.	0.5	0
86	Industrial azomethine nickel complex pigments. Four crystal structures from X-ray powder diffraction data. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2021, 236, 105-115.	0.8	0
87	Crystal structure and morphology of the bright orange $\hat{1}^3$ -phase of Pigment Red 53:2 from XRPD, DFT+D and TEM. <i>Dyes and Pigments</i> , 2021, 196, 109456.	3.7	0