

Kenneth Shankland

List of Publications by Year in descending order

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151
papers

4,623
citations

94433

37
h-index

114465

63
g-index

155
all docs

155
docs citations

155
times ranked

4240
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|--|------|-----------|
| 1 | DASH: a program for crystal structure determination from powder diffraction data. <i>Journal of Applied Crystallography</i> , 2006, 39, 910-915. | 4.5 | 495 |
| 2 | Structure determination from powder diffraction data. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2008, 64, 52-64. | 0.3 | 242 |
| 3 | Routine determination of molecular crystal structures from powder diffraction data. <i>Chemical Communications</i> , 1998, , 931-932. | 4.1 | 187 |
| 4 | 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 |
| 5 | Crystal structure determination from powder diffraction data by the application of a genetic algorithm. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 1997, 212, 550-552. | 0.8 | 151 |
| 6 | Chasing the "Killer" Phonon Mode for the Rational Design of Low-Disorder, High-Mobility Molecular Semiconductors. <i>Advanced Materials</i> , 2019, 31, e1902407. | 21.0 | 126 |
| 7 | 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 |
| 8 | A probabilistic approach to space-group determination from powder diffraction data. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2001, 57, 47-54. | 0.3 | 105 |
| 9 | Ab initio structure determination of chlorothiazide by X-ray powder diffraction using optimised data collection and analysis strategies. <i>Journal of Materials Chemistry</i> , 1997, 7, 569-572. | 6.7 | 96 |
| 10 | Solving molecular crystal structures from laboratory X-ray powder diffraction data with DASH: the state of the art and challenges. <i>Journal of Applied Crystallography</i> , 2005, 38, 249-259. | 4.5 | 82 |
| 11 | 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 |
| 12 | Temperature- and Pressure-Induced Proton Transfer in the 1:1 Adduct Formed between Squaric Acid and 4,4'-Bipyridine. <i>Journal of the American Chemical Society</i> , 2009, 131, 3884-3893. | 13.7 | 82 |
| 13 | Characterisation of amorphous and nanocrystalline molecular materials by total scattering. <i>CrystEngComm</i> , 2010, 12, 1366-1368. | 2.6 | 78 |
| 14 | Polymorphism in Benzamide. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 7032-7035. | 13.8 | 71 |
| 15 | Structure solution of Ibuprofen from powder diffraction data by the application of a genetic algorithm combined with prior conformational analysis. <i>International Journal of Pharmaceutics</i> , 1998, 165, 117-126. | 5.2 | 68 |
| 16 | Ab initio structure determination of LiCF ₃ SO ₃ from X-ray powder diffraction data using entropy maximization and likelihood ranking. <i>Journal of Solid State Chemistry</i> , 1992, 100, 191-196. | 2.9 | 66 |
| 17 | Indexing Powder Patterns in Physical Form Screening: Instrumentation and Data Quality. <i>Journal of Pharmaceutical Sciences</i> , 2003, 92, 1930-1938. | 3.3 | 66 |
| 18 | Search for a Predicted Hydrogen Bonding Motif "A Multidisciplinary Investigation into the Polymorphism of 3-Azabicyclo[3.3.1]nonane-2,4-dione. <i>Journal of the American Chemical Society</i> , 2007, 129, 3649-3657. | 13.7 | 61 |

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|----|--|------|-----------|
| 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 | Organocatalytic enantioselective construction of nitrocyclohexanes containing multiple chiral centres via a cascade reaction. <i>Chemical Science</i> , 2012, 3, 584-588. | 7.4 | 58 |
| 21 | Control and prediction of packing motifs: a rare occurrence of carbamazepine in a catemeric configuration. <i>CrystEngComm</i> , 2006, 8, 746. | 2.6 | 56 |
| 22 | Structural Characterization of Three Crystalline Modifications of Telmisartan by Single Crystal and High-Resolution X-Ray Powder Diffraction. <i>Journal of Pharmaceutical Sciences</i> , 2000, 89, 1465-1479. | 3.3 | 55 |
| 23 | Insights into the Mechanochemical Synthesis of MOF-74. <i>Crystal Growth and Design</i> , 2021, 21, 3047-3055. | 3.0 | 51 |
| 24 | Single-crystal X-ray diffraction analysis of pyrene II at 93K. <i>Journal of Molecular Structure</i> , 2000, 520, 29-32. | 3.6 | 50 |
| 25 | Phase extension in electron crystallography using the maximum-entropy method and its application to two-dimensional purple membrane data from <i>Halobacterium halobium</i> . <i>Ultramicroscopy</i> , 1993, 49, 132-146. | 1.9 | 49 |
| 26 | Synthesis and optical characterisation of platinum(II) poly-yne polymers incorporating substituted 1,4-diethynylbenzene derivatives and an investigation of the intermolecular interactions in the diethynylbenzene molecular precursors. Electronic supplementary information (ESI) available: atomic coordinates for 6 and 7. See http://www.rsc.org/suppdata/nj/b2/b206946f/ . <i>New Journal of Chemistry</i> , 2003, 27, 140-149. | 2.8 | 49 |
| 27 | Tetraaryl biphenyl diamine hole transport materials: a structural study utilizing both single crystal and high resolution powder diffraction. <i>Journal of Materials Chemistry</i> , 2002, 12, 168-172. | 6.7 | 48 |
| 28 | Chiral Metal-Dithiolene/Viologen Ion Pairs: Synthesis and Electrical Conductivity. <i>Chemistry - A European Journal</i> , 2001, 7, 738-748. | 3.3 | 47 |
| 29 | Structure solution and refinement of tetracaine hydrochloride from X-ray powder diffraction data. <i>New Journal of Chemistry</i> , 2002, 26, 469-472. | 2.8 | 47 |
| 30 | Crystal Structure of the [(C ₅ H ₄ BMe ₂) ₂ Fe]-4,4'-bipyridine Polymer from High Resolution X-Ray Powder Diffraction. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2000, 626, 1400-1405. | 1.2 | 45 |
| 31 | Molecular, crystallographic and algorithmic factors in structure determination from powder diffraction data by simulated annealing. <i>Journal of Applied Crystallography</i> , 2002, 35, 443-454. | 4.5 | 45 |
| 32 | Applications of the maximum entropy method to powder diffraction and electron crystallography. <i>Proceedings of the Royal Society A</i> , 1993, 442, 97-111. | 0.9 | 44 |
| 33 | Conformational analysis by solid-state NMR and its application to restrained structure determination from powder diffraction data. <i>Chemical Communications</i> , 2002, , 1976-1977. | 4.1 | 42 |
| 34 | Crystallization and Crystal Energy Landscape of Hydrochlorothiazide. <i>Crystal Growth and Design</i> , 2007, 7, 705-712. | 3.0 | 41 |
| 35 | Ruthenium-conjugated chrysin analogues modulate platelet activity, thrombus formation and haemostasis with enhanced efficacy. <i>Scientific Reports</i> , 2017, 7, 5738. | 3.3 | 41 |
| 36 | Woehler and Liebig Revisited: A Small Molecule Reveals Its Secrets The Crystal Structure of the Unstable Polymorph of Benzamide Solved after 173 Years. <i>Crystal Growth and Design</i> , 2005, 5, 2218-2224. | 3.0 | 40 |

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| 37 | Solving Molecular Crystal Structures from X-ray Powder Diffraction Data: The Challenges Posed by β -Carbamazepine and Chlorothiazide N,N-Dimethylformamide (1/2) Solvate. <i>Journal of Pharmaceutical Sciences</i> , 2007, 96, 1192-1202. | 3.3 | 40 |
| 38 | The use of maximum entropy and likelihood ranking to determine the crystal structure of 4-(4-(N,N-dimethyl)aminobenzylidene)-pyrazolidine-3,5-dione at 1.4 Å... resolution from electron diffraction and high-resolution electron microscopy image data. <i>Ultramicroscopy</i> , 1994, 56, 271-288. | 1.9 | 39 |
| 39 | Single-crystal neutron diffraction of urea-phosphoric acid: evidence for H-atom migration in a short hydrogen bond between 150 K and 350 K. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2001, 216, 303-306. | 0.8 | 39 |
| 40 | Solid Phases of Cyclopentane: Combined Experimental and Simulation Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 3746-3758. | 2.6 | 39 |
| 41 | Phosphorescence quantum yield enhanced by intermolecular hydrogen bonds in Cu ₄ I ₄ clusters in the solid state. <i>Dalton Transactions</i> , 2014, 43, 9448. | 3.3 | 35 |
| 42 | Structure determination from powder data: Mogul and CASTEP. <i>Zeitschrift Für Kristallographie, Supplement</i> , 2009, 2009, 215-220. | 0.5 | 34 |
| 43 | A hybrid Monte Carlo method for crystal structure determination from powder diffraction data. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2002, 58, 441-447. | 0.3 | 32 |
| 44 | Organocatalytic Domino Reaction of Cyanosulfones: Access to Complex Cyclohexane Systems with Quaternary Carbon Centers. <i>Organic Letters</i> , 2013, 15, 1386-1389. | 4.6 | 32 |
| 45 | Elucidating an Amorphous Form Stabilization Mechanism for Tenapanor Hydrochloride: Crystal Structure Analysis Using X-ray Diffraction, NMR Crystallography, and Molecular Modeling. <i>Molecular Pharmaceutics</i> , 2018, 15, 1476-1487. | 4.6 | 32 |
| 46 | An automated platform for parallel crystallization of small organic molecules. <i>Journal of Applied Crystallography</i> , 2006, 39, 922-924. | 4.5 | 31 |
| 47 | A carbamazepine-indomethacin (1:1) cocrystal produced by milling. <i>CrystEngComm</i> , 2011, 13, 6327. | 2.6 | 29 |
| 48 | Application of hydrogen-bond propensity calculations to an indomethacin-nicotinamide (1:1) co-crystal. <i>CrystEngComm</i> , 2013, 15, 4041. | 2.6 | 29 |
| 49 | One-Dimensional Spin Chains from CuII Ions and 2,5-Bis(pyrazol-1-yl)-1,4-dihydroxybenzene. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2002, 628, 310-314. | 1.2 | 28 |
| 50 | Zippering and Unzippering of a Paddlewheel Metal-Organic Framework to Enable Two-Step Synthetic and Structural Transformation. <i>Chemistry - A European Journal</i> , 2013, 19, 3552-3557. | 3.3 | 28 |
| 51 | Asymmetric cyclopropanation of conjugated cyanosulfones using a novel cupreine organocatalyst: rapid access to β -amino acids. <i>Chemical Communications</i> , 2015, 51, 13558-13561. | 4.1 | 28 |
| 52 | ExtSym: a program to aid space-group determination from powder diffraction data. <i>Journal of Applied Crystallography</i> , 2008, 41, 1177-1181. | 4.5 | 27 |
| 53 | A multisolution method of phase determination by combined maximization of entropy and likelihood. VI. Automatic likelihood analysis via the Student t test, with an application to the powder structure of magnesium boron nitride, Mg ₃ BN ₃ . <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1993, 49, 493-501. | 0.3 | 26 |
| 54 | Crystal Structure Solution from Neutron Powder Diffraction Data by a new Monte Carlo Approach Incorporating Restrained Relaxation of the Molecular Geometry. <i>Journal of Applied Crystallography</i> , 1997, 30, 968-974. | 4.5 | 26 |

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| 55 | Structural transformations in zopiclone. <i>Chemical Communications</i> , 2001, , 2204-2205. | 4.1 | 26 |
| 56 | Powder diffraction based structural studies of pharmaceuticals. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2004, 219, . | 0.8 | 26 |
| 57 | A catemer-to-dimer structural transformation in cyheptamide. <i>CrystEngComm</i> , 2008, 10, 26-28. | 2.6 | 26 |
| 58 | Synthesis and Antiviral Properties of Spirocyclic [1,2,3]- Δ^2 -Triazolooxazine Nucleosides. <i>Chemistry - A European Journal</i> , 2014, 20, 11685-11689. | 3.3 | 25 |
| 59 | A synchrotron X-ray powder diffraction study of 4-(2,3,4-trifluorophenyl)-1,2,3,5-dithiadiazolyl. Crystal structure determination using a global optimisation method. <i>New Journal of Chemistry</i> , 1999, 23, 565-567. | 2.8 | 24 |
| 60 | High-pressure structural studies of the pharmaceutical, chlorothiazide. <i>CrystEngComm</i> , 2010, 12, 2533. | 2.6 | 23 |
| 61 | The principles underlying the use of powder diffraction data in solving pharmaceutical crystal structures. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2013, 69, 1251-1259. | 0.4 | 23 |
| 62 | Detection of nitroaromatic vapours with diketopyrrolopyrrole thin films: exploring the role of structural order and morphology on thin film properties and fluorescence quenching efficiency. <i>Chemical Communications</i> , 2015, 51, 1143-1146. | 4.1 | 22 |
| 63 | Conformational analysis of Ibuprofen by crystallographic database searching and potential energy calculation. <i>International Journal of Pharmaceutics</i> , 1998, 165, 107-116. | 5.2 | 21 |
| 64 | Single-crystal X-ray and neutron powder diffraction investigation of the phase transition in tetrachlorobenzene. <i>Acta Crystallographica Section B: Structural Science</i> , 2006, 62, 287-295. | 1.8 | 21 |
| 65 | Two-dimensional similarity between forms I and II of cytenamide, a carbamazepine analogue. <i>CrystEngComm</i> , 2008, 10, 811. | 2.6 | 21 |
| 66 | Materials chemistry communications. Application of the combined maximum entropy and likelihood method to the ab initio determination of an organic crystal structure from X-ray powder diffraction data. <i>Journal of Materials Chemistry</i> , 1992, 2, 1301. | 6.7 | 20 |
| 67 | Decafluoroquarterphenyl - crystal and molecular structure solved from X-ray powder data. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2001, 216, . | 0.8 | 20 |
| 68 | A maximum-likelihood method for global-optimization-based structure determination from powder diffraction data. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2002, 58, 316-326. | 0.3 | 20 |
| 69 | Improved performance of crystal structure solution from powder diffraction data through parameter tuning of a simulated annealing algorithm. <i>Journal of Applied Crystallography</i> , 2017, 50, 1411-1420. | 4.5 | 20 |
| 70 | Development of a Zeolite Filter for Removing Polycyclic Aromatic Hydrocarbons (PAHs) from Smoke and Smoked Ingredients while Retaining the Smoky Flavor. <i>Journal of Agricultural and Food Chemistry</i> , 2018, 66, 2449-2458. | 5.2 | 18 |
| 71 | Salt Forms of Amides: Protonation and Polymorphism of Carbamazepine and Cytenamide. <i>Crystal Growth and Design</i> , 2013, 13, 5121-5127. | 3.0 | 17 |
| 72 | Structure and stability of two polymorphs of creatine and its monohydrate. <i>CrystEngComm</i> , 2014, 16, 8197. | 2.6 | 17 |

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| 73 | Global Rietveld refinement. Journal of Research of the National Institute of Standards and Technology, 2004, 109, 143. | 1.2 | 17 |
| 74 | The crystal structures of m -xylene and p -xylene, C ₈ D ₁₀ , at 4.5 K. Journal of Molecular Structure, 2000, 524, 121-128. | 3.6 | 15 |
| 75 | Structure and Dynamics of Maleic Anhydride. Journal of Physical Chemistry A, 2001, 105, 3064-3070. | 2.5 | 15 |
| 76 | The crystal structures of three primary products from the selective reduction of 2,4,6-trinitrotoluene. New Journal of Chemistry, 2004, 28, 161. | 2.8 | 15 |
| 77 | Accurate molecular structures of chlorothiazide and hydrochlorothiazide by joint refinement against powder neutron and X-ray diffraction data. Acta Crystallographica Section B: Structural Science, 2008, 64, 101-107. | 1.8 | 15 |
| 78 | Powder study of hydrochlorothiazide form II. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2798-o2800. | 0.2 | 14 |
| 79 | Hirshfeld surface analysis of two bendroflumethiazide solvates. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o659-o663. | 0.4 | 14 |
| 80 | The crystal structure of a metastable polymorph of para-azoxyanisole. CrystEngComm, 2008, 10, 279-282. | 2.6 | 14 |
| 81 | Improved crystal structure solution from powder diffraction data by the use of conformational information. Journal of Applied Crystallography, 2017, 50, 1421-1427. | 4.5 | 14 |
| 82 | The crystal structure of perdeuterated pyrene II at 4.2 K. Chemical Physics Letters, 1996, 258, 490-494. | 2.6 | 12 |
| 83 | <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 |
| 84 | Co-Crystal Structures of Furosemide:Urea and Carbamazepine:Indomethacin Determined from Powder X-Ray Diffraction Data. Crystals, 2020, 10, 42. | 2.2 | 12 |
| 85 | 10,11-Dihydrocarbamazepine (form III). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o675-o677. | 0.2 | 11 |
| 86 | Conformational polymorphism of the molecular complex of 3-fluorobenzoic acid with 4-acetylpyridine. CrystEngComm, 2011, 13, 3349. | 2.6 | 11 |
| 87 | Organocatalytic Access to a <i>cis</i>-Cyclopentyl- ¹³ C-amino Acid: An Intriguing Model of Selectivity and Formation of a Stable 10/12-Helix from the Corresponding ¹³ C- ¹⁵ N-Peptide. Journal of the American Chemical Society, 2020, 142, 1382-1393. | 13.7 | 11 |
| 88 | The nine modes of complexed water. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 2333-2339. | 3.9 | 10 |
| 89 | The Structure of N1-Hydroxylophine N3-Oxide (=1-Hydroxy-2,4,5- triphenyl-1H-imidazole 3-Oxide) in the Solid State. Helvetica Chimica Acta, 2003, 86, 1026-1039. | 1.6 | 10 |
| 90 | Synthesis and antiviral activity of novel spirocyclic nucleosides. New Journal of Chemistry, 2018, 42, 18363-18380. | 2.8 | 10 |

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| 91 | The disordered structure of tetraferrocenyl-[3]-cumulene, (Fc) ₂ C=C=C(Fc) ₂ , by simulated annealing using synchrotron powder diffraction data. <i>Journal of Applied Crystallography</i> , 2000, 33, 1199-1207. | 4.5 | 9 |
| 92 | Hydrophobic vs. Hydrophilic: Ionic Competition in Remacemide Salt Structures. <i>Crystal Growth and Design</i> , 2005, 5, 427-438. | 3.0 | 9 |
| 93 | 7-Fluoroisatin-1,4-dioxane (1/1). <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2007, 63, o3574-o3574. | 0.2 | 9 |
| 94 | 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 |
| 95 | A benchmark method for global optimization problems in structure determination from powder diffraction data. <i>Journal of Applied Crystallography</i> , 2010, 43, 401-406. | 4.5 | 9 |
| 96 | High potency of lipid conjugated TLR7 agonist requires nanoparticulate or liposomal formulation. <i>European Journal of Pharmaceutical Sciences</i> , 2018, 123, 268-276. | 4.0 | 9 |
| 97 | Characterization of a hybrid Monte Carlo search algorithm for structure determination. <i>Journal of Applied Crystallography</i> , 2005, 38, 107-111. | 4.5 | 8 |
| 98 | Accurate molecular structures and hydrogen bonding in two polymorphs of ortho-acetamidobenzamide by single-crystal neutron diffraction. <i>Acta Crystallographica Section B: Structural Science</i> , 2006, 62, 926-930. | 1.8 | 8 |
| 99 | Powder study of chlorothiazide N,N-dimethylformamide solvate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2006, 62, o2216-o2218. | 0.2 | 8 |
| 100 | Utilizing organic and organometallic structural data in powder diffraction. <i>Powder Diffraction</i> , 2014, 29, S19-S30. | 0.2 | 7 |
| 101 | Salt and Ionic Cocrystalline Forms of Amides: Protonation of Carbamazepine in Aqueous Media. <i>Crystal Growth and Design</i> , 2015, 15, 5955-5962. | 3.0 | 7 |
| 102 | Carbamazepine trifluoroacetic acid solvate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2007, 63, o4269-o4269. | 0.2 | 6 |
| 103 | Highly Enantioselective, Organocatalytic, and Scalable Synthesis of a Rare <i>cis,cis</i> -Tricyclic Diterpenoid. <i>Chemistry - A European Journal</i> , 2020, 26, 3504-3508. | 3.3 | 6 |
| 104 | Constrained Rietveld refinement of [² - ¹ H ¹]decadeuteriodopamine deuteriobromide using powder neutron diffraction data. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1996, 92, 4555-4559. | 1.7 | 5 |
| 105 | Some observations on the crystal structure of (R,S)-propranolol hydrochloride. <i>International Journal of Pharmaceutics</i> , 1996, 137, 255-259. | 5.2 | 5 |
| 106 | Powder study of N-[2-(4-hydroxy-2-oxo-2,3-dihydro-1,3-benzothiazol-7-yl)ethyl]-3-[2-(2-naphthalen-1-ylethoxy)ethylsulfonyl]propylammonium benzoate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2004, 60, o1751-o1753. | 0.2 | 5 |
| 107 | Polymorphism in tetra-aryl biphenyl diamine hole transport materials: resolving the conflicting literature on N,N'-diphenyl-N,N'-bis(3,3'-methylphenyl)-[(1,1'-biphenyl)]-4,4'-diamine by high-resolution powder diffraction. <i>Journal of Materials Chemistry</i> , 2005, 15, 4838. | 0.2 | 5 |
| 108 | Powder study of 3-azabicyclo[3.3.1]nonane-2,4-dione form 2. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2006, 62, o3046-o3048. | 0.2 | 5 |

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| 109 | Powder study of (R)-1-phenylethylammonium (R)-2-phenylbutyrate form 2. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o247-o249. | 0.2 | 5 |
| 110 | Urea- <i>N,N</i> -dimethylformamide (3/1). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o4861-o4861. | 0.2 | 5 |
| 111 | A differential thermal expansion approach to crystal structure determination from powder diffraction data. Journal of Applied Crystallography, 2008, 41, 1089-1094. | 4.5 | 5 |
| 112 | CDASH: a cloud-enabled program for structure solution from powder diffraction data. Journal of Applied Crystallography, 2015, 48, 2033-2039. | 4.5 | 5 |
| 113 | Rietveld-Based Quantitative Phase Analysis of Sugars in Confectionery. Food Analytical Methods, 2018, 11, 2673-2681. | 2.6 | 5 |
| 114 | (<i>S</i>)-Trichlormethiazide. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3685-o3685. | 0.2 | 4 |
| 115 | Asymmetric Phase-Transfer-Catalyzed Synthesis of Five-Membered Cyclic β -Amino Acid Precursors. Synlett, 2010, 2010, 3011-3014. | 1.8 | 4 |
| 116 | Pushing the Limits of Molecular Crystal Structure Determination From Powder Diffraction Data in High-Throughput Chemical Environments. Journal of Pharmaceutical Sciences, 2018, 107, 2042-2047. | 3.3 | 4 |
| 117 | A new crystalline form of β -D-lactose prepared by oven drying a concentrated aqueous solution of β -D-lactose. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 904-909. | 0.5 | 4 |
| 118 | Powder study of hydrochlorothiazide-methyl acetate (1/1). Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2974-o2977. | 0.2 | 3 |
| 119 | A low-temperature redetermination of cyheptamide. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o205-o206. | 0.2 | 3 |
| 120 | Powder study of (R)-1-phenylethylammonium (R)-2-phenylbutyrate form 3. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o202-o204. | 0.2 | 3 |
| 121 | 10,11-Dihydrocarbamazepine-dimethyl sulfoxide (1/1). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3918-o3919. | 0.2 | 3 |
| 122 | Discovery of three polymorphs of 7-fluoroisatin reveals challenges in using computational crystal structure prediction as a complement to experimental screening. CrystEngComm, 2008, , . | 2.6 | 3 |
| 123 | Vibrational spectroscopy of a compound with a CS ₇ ring. Journal of Raman Spectroscopy, 2009, 40, 703-708. | 2.5 | 3 |
| 124 | Magnesium, calcium and strontium salts of phenylacetic acid. Acta Crystallographica Section C: Crystal Structure Communications, 2012, 68, m29-m33. | 0.4 | 3 |
| 125 | Asymmetric Organocatalytic Synthesis of Cyclopentane β -Nitroketones. Synlett, 2015, 27, 17-20. | 1.8 | 3 |
| 126 | SDPD-SX: combining a single crystal X-ray diffraction setup with advanced powder data structure determination for use in early stage drug discovery. CrystEngComm, 2022, 24, 4337-4340. | 2.6 | 3 |

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| 127 | Powder diffraction study of 1,2:3,4-dibenzanthracene. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o1483-o1485. | 0.2 | 2 |
| 128 | Hydroflumethiazide dimethyl sulfoxide disolvate. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3956-o3956. | 0.2 | 2 |
| 129 | Ureaâ€“N,N-dimethylacetamide (1/1). Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o355-o355. | 0.2 | 2 |
| 130 | Jpowder: a Java-based program for the display and examination of powder diffraction data. Journal of Applied Crystallography, 2010, 43, 1532-1534. | 4.5 | 2 |
| 131 | A probabilistic approach to space-group determination from powder diffraction data. Corrigendum. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 780-780. | 0.3 | 2 |
| 132 | An Overview of Powder X-ray Diffraction and Its Relevance to Pharmaceutical Crystal Structures. Advances in Delivery Science and Technology, 2016, , 293-314. | 0.4 | 2 |
| 133 | Structure and spectroscopy of methionyl-methionine for aquaculture. Scientific Reports, 2021, 11, 458. | 3.3 | 2 |
| 134 | GALLOP: accelerated molecular crystal structure determination from powder diffraction data. CrystEngComm, 2021, 23, 6481-6485. | 2.6 | 2 |
| 135 | Synthesis of an intriguing steroidal constitutional isomer. Tetrahedron Letters, 2020, 61, 151942. | 1.4 | 2 |
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