Kenneth Shankland

List of Publications by Year
in descending order

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	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
2	Structure and spectroscopy of methionyl-methionine for aquaculture. Scientific Reports, 2021, 11, 458.	3.3	2
3	GALLOP: accelerated molecular crystal structure determination from powder diffraction data. CrystEngComm, 2021, 23, 6481-6485.	2.6	2
4	Insights into the Mechanochemical Synthesis of MOF-74. Crystal Growth and Design, 2021, 21, 3047-3055.	3.0	51
5	Organocatalytic Access to a cis-Cyclopentyl-Î³-amino Acid: An Intriguing Model of Selectivity and Formation of a Stable 10/12-Helix from the Corresponding Î³/Î±-Peptide. Journal of the American Chemical Society, 2020, 142, 1382-1393.	13.7	11
6	Highly Enantioselective, Organocatalytic, and Scalable Synthesis of a Rare cis,cisâ€Tricyclic Diterpenoid. Chemistry - A European Journal, 2020, 26, 3504-3508.	3.3	6
7	Synthesis of an intriguing steroidal constitutional isomer. Tetrahedron Letters, 2020, 61, 151942.	1.4	2
8	Co-Crystal Structures of Furosemide:Urea and Carbamazepine:Indomethacin Determined from Powder X-Ray Diffraction Data. Crystals, 2020, 10, 42.	2.2	12
9	Experimental Analysis of Powder Diffraction Data. , 2020, , 1-23.		0
10	A new crystalline form of Î±Î²-<scp>D</scp>-lactose prepared by oven drying a concentrated aqueous solution of <scp>D</scp>-lactose. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 904-909.	0.5	4
11	Chasing the â€œKillerâ€•Phonon Mode for the Rational Design of Lowâ€Disorder, Highâ€Mobility Molecular Semiconductors. Advanced Materials, 2019, 31, e1902407.	21.0	126
12	Elucidating an Amorphous Form Stabilization Mechanism for Tenapanor Hydrochloride: Crystal Structure Analysis Using X-ray Diffraction, NMR Crystallography, and Molecular Modeling. Molecular Pharmaceutics, 2018, 15, 1476-1487.	4.6	32
13	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
14	Rietveld-Based Quantitative Phase Analysis of Sugars in Confectionery. Food Analytical Methods, 2018, 11, 2673-2681.	2.6	5
15	Development of a Zeolite Filter for Removing Polycyclic Aromatic Hydrocarbons (PAHs) from Smoke and Smoked Ingredients while Retaining the Smoky Flavor. Journal of Agricultural and Food Chemistry, 2018, 66, 2449-2458.	5.2	18
16	Synthesis and antiviral activity of novel spirocyclic nucleosides. New Journal of Chemistry, 2018, 42, 18363-18380.	2.8	10
17	High potency of lipid conjugated TLR7 agonist requires nanoparticulate or liposomal formulation. European Journal of Pharmaceutical Sciences, 2018, 123, 268-276.	4.0	9
18	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

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19	Improved performance of crystal structure solution from powder diffraction data through parameter tuning of a simulated annealing algorithm. Journal of Applied Crystallography, 2017, 50, 1411-1420.	4.5	20
20	Ruthenium-conjugated chrysin analogues modulate platelet activity, thrombus formation and haemostasis with enhanced efficacy. Scientific Reports, 2017, 7, 5738.	3.3	41
21	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
22	Asymmetric Organocatalytic Synthesis of Cyclopentane Î³-Nitroketones. Synlett, 2015, 27, 17-20.	1.8	3
23	Asymmetric cyclopropanation of conjugated cyanosulfones using a novel cupreine organocatalyst: rapid access to Î´³-amino acids. Chemical Communications, 2015, 51, 13558-13561.	4.1	28
24	Salt and Ionic Cocrystalline Forms of Amides: Protonation of Carbamazepine in Aqueous Media.. Crystal Growth and Design, 2015, 15, 5955-5962.	3.0	7
25	CDASH: a cloud-enabled program for structure solution from powder diffraction data. Journal of Applied Crystallography, 2015, 48, 2033-2039.	4.5	5
26	Detection of nitroaromatic vapours with diketopyrrolopyrrole thin films: exploring the role of structural order and morphology on thin film properties and fluorescence quenching efficiency. Chemical Communications, 2015, 51, 1143-1146.	4.1	22
27	Utilizing organic and organometallic structural data in powder diffraction. Powder Diffraction, 2014, 29, S19-S30.	0.2	7
28	Phosphorescence quantum yield enhanced by intermolecular hydrogen bonds in Cu4I4 clusters in the solid state. Dalton Transactions, 2014, 43, 9448.	3.3	35
29	Synthesis and Antiviral Properties of Spirocyclic [1,2,3]â€Triazolooxazine Nucleosides. Chemistry - A European Journal, 2014, 20, 11685-11689.	3.3	25
30	Structure and stability of two polymorphs of creatine and its monohydrate. CrystEngComm, 2014, 16, 8197.	2.6	17
31	The principles underlying the use of powder diffraction data in solving pharmaceutical crystal structures. Acta Crystallographica Section C: Crystal Structure Communications, 2013, 69, 1251-1259.	0.4	23
32	Zipping and Unzipping of a Paddlewheel Metalâ€“Organic Framework to Enable Twoâ€Step Synthetic and Structural Transformation. Chemistry - A European Journal, 2013, 19, 3552-3557.	3.3	28
33	Organocatalytic Domino Reaction of Cyanosulfones: Access to Complex Cyclohexane Systems with Quaternary Carbon Centers. Organic Letters, 2013, 15, 1386-1389.	4.6	32
34	Application of hydrogen-bond propensity calculations to an indomethacinâ€“nicotinamide (1â€‰:â€‰1) co-crystal. CrystEngComm, 2013, 15, 4041.	2.6	29
35	Salt Forms of Amides: Protonation and Polymorphism of Carbamazepine and Cytenamide. Crystal Growth and Design, 2013, 13, 5121-5127.	3.0	17
36	Structure Solution: Global Optimisation Methods. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 117-124.	0.3	0

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37	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
38	Magnesium, calcium and strontium salts of phenylacetic acid. Acta Crystallographica Section C: Crystal Structure Communications, 2012, 68, m29-m33.	0.4	3
39	Organocatalytic enantioselective construction of nitrocyclohexanes containing multiple chiral centres via a cascade reaction. Chemical Science, 2012, 3, 584-588.	7.4	58
40	Organic Compounds. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 45-52.	0.3	0
41	Conformational polymorphism of the molecular complex of 3-fluorobenzoic acid with 4-acetylpyridine. CrystEngComm, 2011, 13, 3349.	2.6	11
42	A carbamazepine-indomethacin (1â€‰:â€‰1) cocrystal produced by milling. CrystEngComm, 2011, 13, 6327.	2.6	29
43	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
44	A benchmark method for global optimization problems in structure determination from powder diffraction data. Journal of Applied Crystallography, 2010, 43, 401-406.	4.5	9
45	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
46	Asymmetric Phase-Transfer-Catalyzed Synthesis of Five-Membered Cyclic Î³-Amino Acid Precursors. Synlett, 2010, 2010, 3011-3014.	1.8	4
47	High-pressure structural studies of the pharmaceutical, chlorothiazide. CrystEngComm, 2010, 12, 2533.	2.6	23
48	Characterisation of amorphous and nanocrystalline molecular materials by total scattering. CrystEngComm, 2010, 12, 1366-1368.	2.6	78
49	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
50	Vibrational spectroscopy of a compound with a CS₇ ring. Journal of Raman Spectroscopy, 2009, 40, 703-708.	2.5	3
51	GDASH: a grid-enabled program for structure solution from powder diffraction data. Journal of Applied Crystallography, 2009, 42, 356-359.	4.5	9
52	MDASH: a multi-core-enabled program for structure solution from powder diffraction data. Journal of Applied Crystallography, 2009, 42, 360-361.	4.5	12
53	Temperature- and Pressure-Induced Proton Transfer in the 1:1 Adduct Formed between Squaric Acid and 4,4â€²-Bipyridine. Journal of the American Chemical Society, 2009, 131, 3884-3893.	13.7	82
54	Structure determination from powder data: Mogul and CASTEP. Zeitschrift FÃ¼r Kristallographie, Supplement, 2009, 2009, 215-220.	0.5	34

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55	Large-scale distributed computing for accelerated structure solution. Zeitschrift FÃ¼r Kristallographie, Supplement, 2009, 2009, 227-232.	0.5	1
56	Structure determination from powder diffraction data. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, 52-64.	0.3	242
57	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
58	A differential thermal expansion approach to crystal structure determination from powder diffraction data. Journal of Applied Crystallography, 2008, 41, 1089-1094.	4.5	5
59	ExtSym: a program to aid space-group determination from powder diffraction data. Journal of Applied Crystallography, 2008, 41, 1177-1181.	4.5	27
60	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
61	Solid Phases of Cyclopentane:â€‰ Combined Experimental and Simulation Study. Journal of Physical Chemistry B, 2008, 112, 3746-3758.	2.6	39
62	A catemer-to-dimer structural transformation in cyheptamide. CrystEngComm, 2008, 10, 26-28.	2.6	26
63	Two-dimensional similarity between forms I and II of cytenamide, a carbamazepine analogue. CrystEngComm, 2008, 10, 811.	2.6	21
64	The crystal structure of a metastable polymorph of para-azoxyanisole. CrystEngComm, 2008, 10, 279-282.	2.6	14
65	Ureaâ€“N,N-dimethylacetamide (1/1). Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o355-o355.	0.2	2
66	Three-centre hydrogen bonds in triphenylphosphine oxideâ€“hydroquinone (1/1). Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o367-o367.	0.2	0
67	Cytenamide acetic acid solvate. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o1175-o1176.	0.2	0
68	Cytenamide trifluoroacetic acid solvate. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o1215-o1216.	0.2	0
69	Cytenamideâ€“1,4-dioxane (2/1). Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o1345-o1346.	0.2	0
70	Cytenamideâ€“butyric acid (1/1). Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o1295-o1296.	0.2	0
71	Search for a Predicted Hydrogen Bonding Motif â^' A Multidisciplinary Investigation into the Polymorphism of 3-Azabicyclo[3.3.1]nonane-2,4-dione. Journal of the American Chemical Society, 2007, 129, 3649-3657.	13.7	61
72	Crystallization and Crystal Energy Landscape of Hydrochlorothiazide. Crystal Growth and Design, 2007, 7, 705-712.	3.0	41

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73	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
74	Solving Molecular Crystal Structures from X-ray Powder Diffraction Data: The Challenges Posed by Î³-Carbamazepine and Chlorothiazide N,N,-Dimethylformamide (1/2) Solvate. Journal of Pharmaceutical Sciences, 2007, 96, 1192-1202.	3.3	40
75	Hirshfeld surface analysis of two bendroflumethiazide solvates. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o659-o663.	0.4	14
76	A low-temperature redetermination of cyheptamide. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o205-o206.	0.2	3
77	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
78	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
79	10,11-Dihydrocarbamazepine (form III). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o675-o677.	0.2	11
80	6-MethoxyquinolineN-oxideâ€“hydroquinone (2/1). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o2891-o2891.	0.2	1
81	(S)-Trichlormethiazide. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3685-o3685.	0.2	4
82	7-Fluoroisatinâ€“1,4-dioxane (1/1). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3574-o3574.	0.2	9
83	Hydroflumethiazide dimethyl sulfoxide disolvate. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3956-o3956.	0.2	2
84	10,11-Dihydrocarbamazepineâ€“dimethyl sulfoxide (1/1). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3918-o3919.	0.2	3
85	Carbamazepine trifluoroacetic acid solvate. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o4269-o4269.	0.2	6
86	Ureaâ€“N,N-dimethylformamide (3/1). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o4861-o4861.	0.2	5
87	Control and prediction of packing motifs: a rare occurrence of carbamazepine in a catemeric configuration. CrystEngComm, 2006, 8, 746.	2.6	56
88	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
89	Single-crystal X-ray and neutron powder diffraction investigation of the phase transition in tetrachlorobenzene. Acta Crystallographica Section B: Structural Science, 2006, 62, 287-295.	1.8	21
90	Accurate molecular structures and hydrogen bonding in two polymorphs of ortho-acetamidobenzamide by single-crystal neutron diffraction. Acta Crystallographica Section B: Structural Science, 2006, 62, 926-930.	1.8	8

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91	Powder study of chlorothiazideN,N-dimethylformamide solvate. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o2216-o2218.	0.2	8
92	Powder study of 3-azabicyclo[3.3.1]nonane-2,4-dione form 2. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o3046-o3048.	0.2	5
93	Powder study of 3-azabicyclo[3.3.1]nonane-2,4-dione 1-methylnaphthalene hemisolvate. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o3752-o3754.	0.2	1
94	An automated platform for parallel crystallization of small organic molecules. Journal of Applied Crystallography, 2006, 39, 922-924.	4.5	31
95	DASH: a program for crystal structure determination from powder diffraction data. Journal of Applied Crystallography, 2006, 39, 910-915.	4.5	495
96	Polymorphism in Benzamide. Angewandte Chemie - International Edition, 2005, 44, 7032-7035.	13.8	71
97	Powder diffraction study of 1,2:3,4-dibenzanthracene. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o1483-o1485.	0.2	2
98	Powder study of hydrochlorothiazide form II. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2798-o2800.	0.2	14
99	Powder study of hydrochlorothiazideâ€“methyl acetate (1/1). Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2974-o2977.	0.2	3
100	Characterization of a hybrid Monte Carlo search algorithm for structure determination. Journal of Applied Crystallography, 2005, 38, 107-111.	4.5	8
101	Solving molecular crystal structures from laboratory X-ray powder diffraction data withDASH: the state of the art and challenges. Journal of Applied Crystallography, 2005, 38, 249-259.	4.5	82
102	Hydrophobic vs. Hydrophilic:â€‰ Ionic Competition in Remacemide Salt Structures. Crystal Growth and Design, 2005, 5, 427-438.	3.0	9
103	Polymorphism in tetra-aryl biphenyl diamine hole transport materials: resolving the conflicting literature on N, Nâ€²-diphenyl-N, Nâ€²-bis(3,3â€²-methylphenyl)-[(1,1â€²-biphenyl)]-4,4â€²-diamine by high-resolution powder diffraction. Journal of Materials Chemistry, 2005, 15, 4838.	6.7	5
104	Woehler and Liebig Revisited:â€‰ A Small Molecule Reveals Its SecretsThe Crystal Structure of the Unstable Polymorph of Benzamide Solved after 173 Years. Crystal Growth and Design, 2005, 5, 2218-2224.	3.0	40
105	Powder diffraction based structural studies of pharmaceuticals. Zeitschrift Fur Kristallographie - Crystalline Materials, 2004, 219, .	0.8	26
106	Powder study ofN-[2-(4-hydroxy-2-oxo-2,3-dihydro-1,3-benzothiazol-7-yl)ethyl]-3-[2-(2-naphthalen-1-ylethoxy)ethylsulfonyl]propylammonium benzoate. Acta Crystallographica Section E: Structure Reports Online, 2004, 60, o1751-o1753.	0.2	5
107	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
108	Global Rietveld refinement. Journal of Research of the National Institute of Standards and Technology, 2004, 109, 143.	1.2	17

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109	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
110	Indexing Powder Patterns in Physical Form Screening: Instrumentation and Data Quality. Journal of Pharmaceutical Sciences, 2003, 92, 1930-1938.	3.3	66
111	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 precursorsElectronic supplementary information (ESI) available: atomic cooordinates for 6 and 7. See http://www.rsc.org/suppdata/nj/b2/b206946f/. New Journal of Chemistry, 2003, 27, 149-152.	2.8	49
112	Extending the Power of Global Optimisation Methods in Direct Space Structure Determination from Powder Diffraction Data. Crystallography Reviews, 2003, 9, 3-15.	1.5	1
113	Tetraaryl biphenyl diamine hole transport materials: a structural study utilizing both single crystal and high resolution powder diffraction. Journal of Materials Chemistry, 2002, 12, 168-172.	6.7	48
114	Conformational analysis by solid-state NMR and its application to restrained structure determination from powder diffraction data. Chemical Communications, 2002, , 1976-1977.	4.1	42
115	Structure solution and refinement of tetracaine hydrochloride from X-ray powder diffraction data. New Journal of Chemistry, 2002, 26, 469-472.	2.8	47
116	One-Dimensional Spin Chains from CuII Ions and 2,5-Bis(pyrazol-1-yl)-1,4-dihydroxybenzene. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2002, 628, 310-314.	1.2	28
117	Molecular, crystallographic and algorithmic factors in structure determination from powder diffraction data by simulated annealing. Journal of Applied Crystallography, 2002, 35, 443-454.	4.5	45
118	A maximum-likelihood method for global-optimization-based structure determination from powder diffraction data. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, 316-326.	0.3	20
119	A hybrid Monte Carlo method for crystal structure determination from powder diffraction data. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, 441-447.	0.3	32
120	Structure and Dynamics of Maleic Anhydride. Journal of Physical Chemistry A, 2001, 105, 3064-3070.	2.5	15
121	Decafluoroquarterphenyl - crystal and molecular structure solved from X-ray powder data. Zeitschrift Fur Kristallographie - Crystalline Materials, 2001, 216, .	0.8	20
122	A probabilistic approach to space-group determination from powder diffraction data. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 47-54.	0.3	105
123	Chiral Metal-Dithiolene/Viologen Ion Pairs: Synthesis and Electrical Conductivity. Chemistry - A European Journal, 2001, 7, 738-748.	3.3	47
124	Single-crystal neutron diffraction of urea-phosphoric acid: evidence for H-atom migration in a short hydrogen bond between 150 K and 350 K. Zeitschrift Fur Kristallographie - Crystalline Materials, 2001, 216, 303-306.	0.8	39
125	Structural transformations in zopiclone. Chemical Communications, 2001, , 2204-2205.	4.1	26
126	Crystal Structure of the [(C5H4BMe2)2Fe]-4,4â€²-bipyridine Polymer from High Resolution X-Ray Powder Diffraction. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2000, 626, 1400-1405.	1.2	45

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127	Structural Characterization of Three Crystalline Modifications of Telmisartan by Single Crystal and Highâ€Resolution Xâ€ray Powder Diffraction. Journal of Pharmaceutical Sciences, 2000, 89, 1465-1479.	3.3	55
128	The disordered structure of tetraferrocenyl-[3]-cumulene, (Fc)2C=C=C=C(Fc)2, by simulated annealing using synchrotron powder diffraction data. Journal of Applied Crystallography, 2000, 33, 1199-1207.	4.5	9
129	Single-crystal X-ray diffraction analysis of pyrene II at 93K. Journal of Molecular Structure, 2000, 520, 29-32.	3.6	50
130	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
131	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. New Journal of Chemistry, 1999, 23, 565-567.	2.8	24
132	Structure solution of Ibuprofen from powder diffraction data by the application of a genetic algorithm combined with prior conformational analysis. International Journal of Pharmaceutics, 1998, 165, 117-126.	5.2	68
133	Conformational analysis of Ibuprofen by crystallographic database searching and potential energy calculation. International Journal of Pharmaceutics, 1998, 165, 107-116.	5.2	21
134	Routine determination of molecular crystal structures from powder diffraction data. Chemical Communications, 1998, , 931-932.	4.1	187
135	Routineab initiostructure determination of chlorothiazide by X-ray powder diffraction using optimised data collection and analysis strategies. Journal of Materials Chemistry, 1997, 7, 569-572.	6.7	96
136	Crystal structure determination from powder diffraction data by the application of a genetic algorithm. Zeitschrift Fur Kristallographie - Crystalline Materials, 1997, 212, 550-552.	0.8	151
137	The nine modes of complexed water. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 2333-2339.	3.9	10
138	Crystal Structure Solution from Neutron Powder Diffraction Data by a new Monte Carlo Approach Incorporating Restrained Relaxation of the Molecular Geometry. Journal of Applied Crystallography, 1997, 30, 968-974.	4.5	26
139	Constrained Rietveld refinement of [Î²-1H1]decadeuteriodopamine deuteriobromide using powder neutron diffraction data. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 4555-4559.	1.7	5
140	Some observations on the crystal structure of (R,S)-propranolol hydrochloride. International Journal of Pharmaceutics, 1996, 137, 255-259.	5.2	5
141	Unit cell determination of sotalol hydrochloride by powder x-ray diffraction. International Journal of Pharmaceutics, 1996, 139, 9-14.	5.2	1
142	The crystal structure of perdeuterated pyrene II at 4.2 K. Chemical Physics Letters, 1996, 258, 490-494.	2.6	12
143	The use of maximum entropy and likelihood ranking to determine the crystal structure of 4-(4â€²-(N,N-dimethyl)aminobenzylidene)-pyrazolidine-3,5-dione at 1.4 Å... resolution from electron diffraction and high-resolution electron microscopy image data. Ultramicroscopy, 1994, 56, 271-288.	1.9	39
144	Phase extension in electron crystallography using the maximum-entropy method and its application to two-dimensional purple membrane data from Halobacterium halobium. Ultramicroscopy, 1993, 49, 132-146.	1.9	49

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145	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, Mg3BN3. Acta Crystallographica Section A: Foundations and Advances, 1993, 49, 493-501.	0.3	26
146	Applications of the maximum entropy method to powder diffraction and electron crystallography. Proceedings of the Royal Society A, 1993, 442, 97-111.	0.9	44
147	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. Journal of Materials Chemistry, 1992, 2, 1301.	6.7	20
148	Ab initio structure determination of LiCF3SO3 from X-ray powder diffraction data using entropy maximization and likelihood ranking. Journal of Solid State Chemistry, 1992, 100, 191-196.	2.9	66
149	Determination of refractive indices of polyalkylcyanoacrylate particles. Journal of Colloid and Interface Science, 1992, 154, 160-166.	9.4	0
150	Polydispersity evaluation of poly(cyanoacrylate) manoparticles and nanocapsules by photon correlation spectroscopy. Journal of Controlled Release, 1990, 13, 312-313.	9.9	0
151	An efficient treatment of ring conformations during molecular crystal structure determination from powder diffraction data. CrystEngComm, 0, , .	2.6	0