

# Thomas R Welberry

## List of Publications by Year in descending order

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197  
papers

3,606  
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199  
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199  
docs citations

199  
times ranked

2197  
citing authors

#	ARTICLE	IF	CITATIONS
1	Obtaining diffuse scattering patterns from computer simulations – a retrospective. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 344-355.	1.1	1
2	Simulation of diffuse scattering in $\langle \text{DL} \rangle$ -norleucine. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 393-405.	1.1	0
3	Dynamic Displacement Disorder of Cubic $\text{BaTiO}_3$ . Physical Review Letters, 2018, 120, 167601.	7.8	25
4	Single Crystal Diffuse Neutron Scattering. Quantum Beam Science, 2018, 2, 2.	1.2	4
5	Phase competition and effect of chemical ordering in ferroelectric relaxor $\text{PbSc}_{0.5}\text{Nb}_{0.5}\text{O}_3$ from first principles. Phase Transitions, 2016, 89, 777-784.	1.3	1
6	Total scattering and pair distribution function analysis in modelling disorder in PZN ( $\text{PbZn}_{1/3}\text{Nb}_{2/3}\text{O}_3$ ). IUCrJ, 2016, 3, 20-31.	2.2	13
7	One hundred years of diffuse scattering. Crystallography Reviews, 2016, 22, 2-78.	1.5	87
8	Interpretation of diffuse scattering in the high-Tc superconductor $\text{HgBa}_2\text{CuO}_4 + \delta$ . IUCrJ, 2016, 3, 309-318.	2.2	6
9	Hexagonal paracrystals. Zeitschrift Fur Kristallographie - Crystalline Materials, 2015, 230, 69-74.	0.8	1
10	A neutron diffuse scattering study of $\text{PbZrO}_3$ and Zr-rich $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ . Journal of Applied Crystallography, 2015, 48, 1637-1644.	4.5	32
11	Atomistic modeling of diffuse scattering in cubic $\text{PbZrO}_3$ . Phase Transitions, 2015, 88, 273-282.	1.3	20
12	Nanoscale Order in Molecular Systems from Single Crystal Diffuse Scattering. Australian Journal of Chemistry, 2014, 67, 1807.	0.9	3
13	Approaches to modelling thermal diffuse scattering in triglycine sulfate, $(\text{NH}_2\text{CH}_2\text{COOH})_3 \cdot \text{H}_2\text{SO}_4$ . Journal of Applied Crystallography, 2014, 47, 544-551.	4.5	7
14	Local order in $\sqrt{2}$ stite using a pair distribution function (PDF) approach. Mineralogical Magazine, 2014, 78, 373-385.	1.4	4
15	Diffuse scattering and partial disorder in complex structures. IUCrJ, 2014, 1, 550-562.	2.2	31
16	One Hundred Years of Diffuse X-ray Scattering. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2014, 45, 75-84.	2.2	3
17	Use of bond-valence sums in modelling the diffuse scattering from PZN ( $\text{PbZn}_{1/3}\text{Nb}_{2/3}\text{O}_3$ ). Acta Crystallographica Section A: Foundations and Advances, 2014, 70, 626-635.	0.1	4
18	Diffuse scattering and the mechanism for the phase transition in triglycine sulphate. Journal of Materials Science, 2013, 48, 6605-6612.	3.7	18

#	ARTICLE	IF	CITATIONS
19	Assessing Local Structure in PbZn <sub>1/3</sub> Nb <sub>2/3</sub> O <sub>3</sub> Using Diffuse Scattering and Reverse Monte Carlo Refinement. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2013, 44, 87-93.	2.2	11
20	Reverse Monte Carlo Study of Diffuse Scattering from a Frustrated Protein System. , 2013, , 243-251.		1
21	Polar nanoregions and diffuse scattering in the relaxor ferroelectric PbMg <sub>1-x</sub> Nb <sub>3x</sub> O <sub>7</sub> . Physical Review B, 2012, 85, .	3.2	67
22	Diffuse Scattering as an Aid to the Understanding of Polymorphism in Pharmaceuticals. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2012, 43, 1434-1444.	2.2	4
23	Diffuse scattering and local structure modeling in ferroelectrics. Zeitschrift für Kristallographie, 2011, 226, 113-125.	1.1	21
24	Monte Carlo Modeling of Diffuse Scattering from Single Crystals: The Program ZMC. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2011, 42, 23-31.	2.2	31
25	Monte Carlo and Molecular Dynamics Simulation of Disorder in the Ag <sup>+</sup> Fast Ion Conductors Pearceite and Polybasite. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2011, 42, 6-13.	2.2	9
26	Geometry and Topology of Structure in Amorphous Solids. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2011, 42, 14-22.	2.2	4
27	Diffuse scattering resulting from macromolecular frustration. Acta Crystallographica Section B: Structural Science, 2011, 67, 516-524.	1.8	26
28	Stacking faults and superstructures in a layered brownmillerite. Acta Crystallographica Section B: Structural Science, 2011, 67, 476-485.	1.8	9
29	Monte Carlo Simulation Study of Diffuse Scattering in PZT, Pb(Zr,Ti)O <sub>3</sub> . Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2010, 41, 1110-1118.	2.2	14
30	Approaches to Modeling Diffuse Scattering from Molecular Crystals: Para-Terphenyl (C <sub>18</sub> H <sub>14</sub> ). Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2010, 41, 1119-1129.	2.2	1
31	The geometry, topology and structure of amorphous solids. Acta Materialia, 2010, 58, 615-625.	7.9	32
32	A refinement strategy for Monte Carlo modelling of diffuse scattering from molecular crystal systems. Journal of Applied Crystallography, 2010, 43, 913-915.	4.5	19
33	Precursor effects of the orthorhombic to monoclinic phase transition in benzocaine form (II) revealed by X-ray diffuse scattering. Acta Crystallographica Section B: Structural Science, 2010, 66, 260-270.	1.8	18
34	Diffuse scattering study of aspirin forms (I) and (II). Acta Crystallographica Section B: Structural Science, 2010, 66, 696-707.	1.8	55
35	Advances in Structural Studies of Materials Using Scattering Probes. MRS Bulletin, 2010, 35, 520-530.	3.5	2
36	Use of Monte Carlo simulation for the interpretation and analysis of diffuse scattering. Phase Transitions, 2010, 83, 80-98.	1.3	3

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37	Pb Displacements in $\text{Pb}(\text{ZrTi})\text{O}_{3-x}$ (PZT). Key Engineering Materials, 2009, 421-422, 389-394.	0.4	1
38	Neutron diffuse scattering in deuteratedpara-terphenyl, C18D14. Journal of Physics Condensed Matter, 2009, 21, 124204.	1.8	7
39	Single-crystal diffuse scattering studies on polymorphs of molecular crystals. I. The room-temperature polymorphs of the drug benzocaine. Acta Crystallographica Section B: Structural Science, 2009, 65, 382-392.	1.8	26
40	On the polymorphism of benzocaine; a low-temperature structural phase transition for form (II). Acta Crystallographica Section B: Structural Science, 2009, 65, 509-515.	1.8	27
41	Structured diffuse scattering and the fundamental 1-d dipolar unit in PLZT ( $\text{Pb}_{1-y}\text{La}_y$ ) $\text{Ti}_x(\text{Zr}_{1-x}\text{Ti}_x)$ $\text{O}_3$ (7.5/65/35 and 7.0/60/40) transparent ferroelectric ceramics. Journal of Solid State Chemistry, 2009, 182, 348-355.	2.9	19
42	Structural disorder in BZN-based pyrochlores. Journal of Electroceramics, 2008, 21, 401-404.	2.0	5
43	Diffuse Scattering and Monte Carlo Studies of Relaxor Ferroelectrics. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2008, 39, 3170-3178.	2.2	11
44	The interpretation and analysis of diffuse scattering using Monte Carlo simulation methods. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, 23-32.	0.3	35
45	X-ray diffuse scattering from HMTA: analysis via a Monte Carlo model. Acta Crystallographica Section B: Structural Science, 2008, 64, 456-465.	1.8	2
46	A room-temperature X-ray diffuse scattering study of form (II) of the trimorphic molecular system <i>p</i> -N-methylbenzylidene- <i>p</i> -methylaniline. Acta Crystallographica Section B: Structural Science, 2008, 64, 633-643.	1.8	9
47	Different models for the polar nanodomain structure of PZN and other relaxor ferroelectrics. Journal of Applied Crystallography, 2008, 41, 606-614.	4.5	30
48	An electron diffraction and Monte Carlo simulation study of diffuse scattering in $\text{Pb}(\text{Zr,Ti})\text{O}_3$ . Journal of Applied Crystallography, 2008, 41, 930-938.	4.5	23
49	A composite modulated structure mechanism for $\text{Ag}^+$ fast ion conduction in pearceite and polybasite mineral solid electrolytes. Solid State Ionics, 2008, 179, 2080-2089.	2.7	8
50	Coupled orientational and displacive degrees of freedom in the high-temperature plastic phase of the carbon tetrabromide $\text{CBr}_4$ . $\text{CBr}_4$ . Physical Review B, 2008, 77, .	3.2	22
51	Deformed Penrose tilings. Philosophical Magazine, 2007, 87, 2877-2886.	1.6	5
52	The molecular conformation of Ibuprofen, C <sub>13</sub> H <sub>18</sub> O <sub>2</sub> , through X-ray diffuse scattering. International Journal of Pharmaceutics, 2007, 343, 59-68.	5.2	15
53	Simultaneous fitting of X-ray and neutron diffuse scattering data. Acta Crystallographica Section A: Foundations and Advances, 2007, 63, 30-35.	0.3	6
54	Disorder in pentachloronitrobenzene, C <sub>6</sub> Cl <sub>5</sub> NO <sub>2</sub> : a diffuse scattering study. Acta Crystallographica Section B: Structural Science, 2007, 63, 663-673.	1.8	25

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55	Monte Carlo analysis of neutron diffuse scattering data. <i>Physica B: Condensed Matter</i> , 2006, 385-386, 1352-1354.	2.7	1
56	Crystal chemistry on a lattice: The case of BZN and BZN-related pyrochlores. <i>Journal of Solid State Chemistry</i> , 2006, 179, 2141-2149.	2.9	32
57	Deformed model sets and distorted Penrose tilings. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2006, 221, 621-634.	0.8	21
58	Chemical origin of nanoscale polar domains in $\text{PbZn}_{1-x}\text{Nb}_2\text{O}_3$ . <i>Physical Review B</i> , 2006, 74, .	3.2	61
59	Structural phase transition in deuterated benzil $\text{C}_{14}\text{D}_{10}\text{O}_2$ : Neutron inelastic scattering. <i>Physical Review B</i> , 2006, 73, .	3.2	1
60	“Soft” phonon modes, structured diffuse scattering and the crystal chemistry of Fe-bearing sphalerites. <i>Journal of Solid State Chemistry</i> , 2005, 178, 655-660.	2.9	7
61	Single-crystal neutron diffuse scattering and Monte Carlo study of the relaxor ferroelectric $\text{PbZn}_{1/3}\text{Nb}_{2/3}\text{O}_3$ (PZN). <i>Journal of Applied Crystallography</i> , 2005, 38, 639-647.	4.5	53
62	Problems in measuring diffuse X-ray scattering. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2005, 220, 1052-1058.	0.8	23
63	Diffuse Scattering from Organic Crystals. <i>Molecular Crystals and Liquid Crystals</i> , 2005, 440, 1-21.	0.9	1
64	Disorder and Diffuse Scattering. , 2004, , 457-466.		0
65	The Importance of Multisite Correlations in Disordered Structures. <i>Ferroelectrics</i> , 2004, 305, 117-122.	0.6	6
66	Local crystal chemistry, induced strain and short range order in the cubic pyrochlore $(\text{Bi}_{1.5-x}\text{Zn}_{0.5-x})(\text{Zn}_{0.5-x}\text{Nb}_{1.5-x})\text{O}(7\pm 1.5)$ (BZN). <i>Journal of Solid State Chemistry</i> , 2004, 177, 231-244.	2.9	105
67	Elucidation of zeolite microstructure by synchrotron X-ray diffuse scattering. <i>Journal of Applied Crystallography</i> , 2004, 37, 187-192.	4.5	20
68	Local Strain, Structured Diffuse Scattering and Oxygen/Fluorine Ordering in Transition Metal Oxyfluorides. <i>Ferroelectrics</i> , 2004, 305, 123-126.	0.6	0
69	Effect of High Pressure on the Relaxor Ferroelectrics $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ (NBT) and $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$ (PMN). <i>Ferroelectrics</i> , 2004, 302, 293-298.	0.6	16
70	Oxygen/fluorine ordering, structured diffuse scattering and the local crystal chemistry of $\text{K}_3\text{MoO}_3\text{F}_3$ . <i>Journal of Solid State Chemistry</i> , 2003, 170, 211-220.	2.9	33
71	Diffuse neutron scattering in benzil, $\text{C}_{14}\text{D}_{10}\text{O}_2$ , using the time-of-flight Laue technique. <i>Journal of Applied Crystallography</i> , 2003, 36, 1440-1447.	4.5	22
72	Urotropin azelate: a rather unwilling co-crystal. <i>Acta Crystallographica Section B: Structural Science</i> , 2003, 59, 72-86.	1.8	13

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73	Diffuse X-ray scattering from 4,4-dimethoxybenzil, C <sub>16</sub> H <sub>14</sub> O <sub>4</sub> : analysis via automatic refinement of a Monte Carlo model. Acta Crystallographica Section B: Structural Science, 2003, 59, 760-769.	1.8	5
74	High-energy diffuse scattering on the 1-ID beamline at the Advanced Photon Source. Journal of Synchrotron Radiation, 2003, 10, 284-286.	2.4	16
75	High-pressure x-ray scattering of oxides with a nanoscale local structure: Application to Na <sub>1/2</sub> Bi <sub>1/2</sub> TiO <sub>3</sub> . Physical Review B, 2003, 68, .	3.2	170
76	The Recording and Interpretation of Diffuse X-Ray Scattering. , 2002, , 35-58.		1
77	Personal reflections. Part 91. Zeitschrift Fur Kristallographie - Crystalline Materials, 2002, 217, 379-380.	0.8	0
78	Monte Carlo Study of the quasicrystal-to-crystal transformation using an approach based on the Gummelt covering. Zeitschrift Fur Kristallographie - Crystalline Materials, 2002, 217, 109-118.	0.8	21
79	'Size-effect'-like distortions in quasicrystalline structures. Zeitschrift Fur Kristallographie - Crystalline Materials, 2002, 217, 422-426.	0.8	17
80	Diffuse X-ray scattering from benzil, C <sub>14</sub> H <sub>10</sub> O <sub>2</sub> : analysis via automatic refinement of a Monte Carlo model. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 101-109.	0.3	44
81	Diffuse X-ray scattering and strain effects in disordered crystals. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 244-255.	0.3	24
82	Monte Carlo study of disorder in HMTA. Computer Physics Communications, 2001, 142, 387-390.	7.5	2
83	High-energy X-ray diffuse scattering using Weissenberg flat-cone geometry. Journal of Applied Crystallography, 2000, 33, 1046-1050.	4.5	10
84	Diffuse X-ray scattering and disorder in p-methyl-N-(p-chlorobenzylidene)aniline, C <sub>14</sub> H <sub>12</sub> ClN (ClMe): analysis via automatic refinement of a Monte Carlo model. Acta Crystallographica Section A: Foundations and Advances, 2000, 56, 348-358.	0.3	14
85	Diffuse scattering and Monte Carlo simulations of cyclohexane-perhydrotriphenylene (PHTP) inclusion compounds, C <sub>6</sub> H <sub>12</sub> /C <sub>18</sub> H <sub>30</sub> . Journal of Applied Crystallography, 1999, 32, 464-471.	4.5	12
86	Inter-sublattice ordering correlations and the geometrical locus approach to localized diffuse scattering. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1999, 79, 753-762.	0.6	9
87	Order and Disorder in p-Dialkylbenzene-Urea Inclusion Compounds. Journal of Solid State Chemistry, 1998, 141, 437-451.	2.9	6
88	About short- and long-range orderings in $\sqrt{2}$ stites, Fe 1-x O. Physics and Chemistry of Minerals, 1998, 26, 81-82.	0.8	4
89	Diffuse X-ray Scattering and Short-Range Order in Thallium Antimonyl Germanate, TlSbOGeO <sub>4</sub> . Journal of Applied Crystallography, 1998, 31, 154-162.	4.5	3
90	Analysis of Diffuse Scattering from Single Crystals via the Reverse Monte Carlo Technique. I. Comparison with Direct Monte Carlo. Journal of Applied Crystallography, 1998, 31, 309-317.	4.5	30

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91	Analysis of Diffuse Scattering from Single Crystals via the Reverse Monte Carlo Technique. II. The Defect Structure of Calcium-Stabilized Zirconia. <i>Journal of Applied Crystallography</i> , 1998, 31, 318-326.	4.5	12
92	Analysis of Single-Crystal Diffuse X-ray Scattering via Automatic Refinement of a Monte Carlo Model. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1998, 54, 661-674.	0.3	53
93	Analysis of diffuse scattering of single crystals using monte carlo methods. <i>Phase Transitions</i> , 1998, 67, 373-397.	1.3	33
94	An improved method for analysing single crystal diffuse scattering using the Reverse Monte Carlo technique. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 1997, 212, .	0.8	19
95	Defect distribution and the diffuse X-ray diffraction pattern of $w\text{Al}_{1/4}\text{stite}$ , $\text{Fe}^{1+x}\text{O}$ . <i>Physics and Chemistry of Minerals</i> , 1997, 24, 24-38.	0.8	64
96	Analysis of Diffuse Scattering via the Reverse Monte Carlo Technique: a Systematic Investigation. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1997, 53, 202-216.	0.3	38
97	Diffuse X-ray Scattering and Monte-Carlo Study of Guest-Host Interactions in Urea Inclusion Compounds. <i>Journal of Applied Crystallography</i> , 1996, 29, 353-364.	4.5	50
98	Local structural information of mullite obtained from diffuse X-ray scattering. <i>Journal of the European Ceramic Society</i> , 1996, 16, 187-193.	5.7	9
99	A computer-simulation study of the 'white-line effect' in diffraction patterns of mixed charge-transfer salts. <i>Journal of Applied Crystallography</i> , 1995, 28, 611-614.	4.5	6
100	The fourfold disordered structures of p-chloro-N-(p-methylbenzylidene)aniline and p-methyl-N-(p-chlorobenzylidene)aniline. <i>Acta Crystallographica Section B: Structural Science</i> , 1995, 51, 187-197.	1.8	12
101	A Modulation Wave Approach to Understanding the Disordered Structure of Cubic Stabilized Zirconias (CSZs). <i>Journal of Solid State Chemistry</i> , 1995, 115, 43-54.	2.9	42
102	A TEM and XRD Study of $(\text{BiS})_{1+\delta}(\text{Nb}_{1+\delta}\text{S}_2)_n$ Misfit Layer Structures. <i>Journal of Solid State Chemistry</i> , 1995, 115, 274-282.	2.9	16
103	A Paracrystalline Description of Defect Distributions in $w\text{Al}_{1/4}\text{stite}$ , $\text{Fe}_{1-x}\text{O}$ . <i>Journal of Solid State Chemistry</i> , 1995, 117, 398-406.	2.9	36
104	Microdomains, Solid Solutions and the "Defect Fluorite" to C-Type Sesquioxide Transition in $\text{CeO}_2\text{-RO}_{1.5}$ and $\text{ZrO}_2\text{-RO}_{1.5}$ Systems. <i>Journal of Solid State Chemistry</i> , 1995, 120, 290-298.	2.9	29
105	Diffuse X-ray Scattering from Disordered Crystals. <i>Chemical Reviews</i> , 1995, 95, 2369-2403.	47.7	95
106	The low-temperature phase sequence $\gamma$ - $\delta$ - $\epsilon$ in halide perovskite tetramethylammonium trichlorogermanate(II) studied by X-ray diffraction. <i>Journal of Physics Condensed Matter</i> , 1995, 7, 4983-4998.	1.8	6
107	A TEM and X-Ray Diffraction Study of some Imperfectly Ordered, "Infinitely Adaptive" Crystal Structures and the Principles Underlying their Structural Flexibility. <i>Materials Science Forum</i> , 1994, 150-151, 85-96.	0.3	1
108	Interpretation of diffuse X-ray scattering via models of disorder. <i>Journal of Applied Crystallography</i> , 1994, 27, 205-231.	4.5	101



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109	Analysis of diffuse scattering from the mineral mullite. Journal of Applied Crystallography, 1994, 27, 742-754.	4.5	18
110	Diffuse X-ray scattering in potassium lithium sulfate, KLiSO <sub>4</sub> . Journal of Applied Crystallography, 1994, 27, 733-741.	4.5	10
111	A 3D Model for the Diffuse Scattering in Cubic Stabilized Zirconias. Journal of Solid State Chemistry, 1993, 106, 461-475.	2.9	65
112	Oxygen vacancy ordering and the incommensurate structure of mullite. Physics and Chemistry of Minerals, 1993, 20, 323.	0.8	7
113	Scattering of two-dimensional analogs of disordered lamellae. Colloid and Polymer Science, 1993, 271, 124-132.	2.1	5
114	Response to 'About the diffuse absences and the diffuse planes due to the atomic size effect'. Acta Crystallographica Section A: Foundations and Advances, 1993, 49, 221-221.	0.3	0
115	Interpretation of displacement-caused diffuse scattering using the Taylor expansion. Acta Crystallographica Section A: Foundations and Advances, 1993, 49, 736-743.	0.3	19
116	The effect of second neighbour repulsion on fcc binary alloy phase diagrams: A Monte Carlo study. Pramana - Journal of Physics, 1993, 41, 41-49.	1.8	0
117	Cation ordering and the stability of fluorite-related phases in ZrO <sub>2</sub> -LnO <sub>1.5</sub> systems: a phase diagram simulation study using Monte Carlo methods. Journal of Physics Condensed Matter, 1993, 5, 4251-4262.	1.8	4
118	Molecular dynamics simulation study of solid polyphenyls: Structures determined by the interplay between intra- and intermolecular forces. Molecular Physics, 1992, 75, 867-879.	1.7	11
119	Diffuse Scattering in Disordered Molecular Crystals. Molecular Crystals and Liquid Crystals, 1992, 211, 17-33.	0.3	1
120	Monte Carlo simulation of low temperature phase diagrams of YBa <sub>2</sub> Cu <sub>3</sub> O <sub>6+x</sub> . Physica C: Superconductivity and Its Applications, 1992, 197, 57-63.	1.2	5
121	Diffuse scattering in yttria-stabilized cubic zirconia. Journal of Solid State Chemistry, 1992, 100, 71-89.	2.9	49
122	The effect of low intra-sublattice repulsion on phase diagram of YBa <sub>2</sub> Cu <sub>3</sub> O <sub>6+x</sub> : A Monte Carlo simulation study. Pramana - Journal of Physics, 1992, 39, 329-341.	1.8	1
123	FOURDEM: a program written as an aid to teaching the elements of Fourier synthesis and other crystallographic concepts. Journal of Applied Crystallography, 1992, 25, 443-447.	4.5	2
124	Calculation of diffuse scattering from simulated disordered crystals: a comparison with optical transforms. Journal of Applied Crystallography, 1992, 25, 391-399.	4.5	92
125	QUASI2D: a program written to demonstrate quasiperiodicity and phason fluctuation. Journal of Applied Crystallography, 1992, 25, 648-652.	4.5	0
126	Diffuse absences due to the atomic size effect. Acta Crystallographica Section A: Foundations and Advances, 1992, 48, 737-746.	0.3	28



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127	Molecular dynamics simulation of solid biphenyl. <i>Molecular Physics</i> , 1991, 73, 1317-1334.	1.7	14
128	The rôle of phase in diffuse diffraction patterns and its effect on real-space structure. <i>Journal of Applied Crystallography</i> , 1991, 24, 18-29.	4.5	11
129	Optical transform and Monte-Carlo study of phason fluctuations in quasi-periodic tilings. <i>Journal of Applied Crystallography</i> , 1991, 24, 203-211.	4.5	7
130	Optical transforms of disordered systems containing symmetry-related scattering sites. <i>Journal of Applied Crystallography</i> , 1990, 23, 303-314.	4.5	4
131	A position-sensitive detector system for the measurement of diffuse X-ray scattering. <i>Journal of Applied Crystallography</i> , 1990, 23, 476-484.	4.5	37
132	Computer simulation of size effect from orientationally disordered molecular crystals: monoclinic dibromodiethylmethylbenzene. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1990, 46, 970-975.	0.3	1
133	A computer simulation study of local arrangements in disordered molecular crystals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1990, 46, 975-979.	0.3	3
134	A 'concentration-wave' approach to understanding the disorder diffuse scattering in 1,3-dibromo-2,5-diethyl-4,6-dimethylbenzene, C <sub>12</sub> H <sub>16</sub> Br <sub>2</sub> . <i>Acta Crystallographica Section B: Structural Science</i> , 1990, 46, 267-275.	1.8	10
135	An optical transform and Monte Carlo study of the diffuse X-ray scattering in mullite, Al <sub>2</sub> (Al <sub>2</sub> +2xSi <sub>2</sub> )O <sub>10</sub> x. <i>Physics and Chemistry of Minerals</i> , 1990, 17, 117.	0.8	17
136	The symmetry characterization and structural refinement of displacement modulated NiAs. <i>Phase Transitions</i> , 1989, 16, 47-51.	1.3	2
137	An electron diffraction and lattice dynamical study of thermal diffuse scattering in KCl. <i>Journal of Physics Condensed Matter</i> , 1989, 1, 2305-2311.	1.8	3
138	Lattice dynamics of $\hat{1}\pm$ - and $\hat{1}^2$ -cristobalite, SiO <sub>2</sub> . <i>Journal of Physics and Chemistry of Solids</i> , 1989, 50, 207-213.	4.0	11
139	An optical transform and Monte Carlo study of the disorder in $\hat{1}^2$ -cristobalite SiO <sub>2</sub> . <i>Journal of Applied Crystallography</i> , 1989, 22, 87-95.	4.5	55
140	Diffraction from quasi-crystals and disordered twinned aggregates. <i>Journal of Applied Crystallography</i> , 1989, 22, 308-314.	4.5	6
141	The structure and microstructure of $\hat{1}\pm$ -cristobalite and its relationship to $\hat{1}^2$ -cristobalite. <i>Physics and Chemistry of Minerals</i> , 1989, 16, 517-523.	0.8	63
142	A transmission electron microscopy study of cristobalite. <i>Phase Transitions</i> , 1989, 16, 41-45.	1.3	8
143	An electron diffraction and lattice-dynamical study of the diffuse scattering in $\hat{1}^2$ -cristobalite, SiO <sub>2</sub> . <i>Journal of Applied Crystallography</i> , 1988, 21, 458-465.	4.5	71
144	Scattering of two-dimensional models of microemulsions. <i>Journal of Colloid and Interface Science</i> , 1988, 123, 413-426.	9.4	20

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145	Calculation of elastic constants for crystalline acenaphthylene, C <sub>12</sub> H <sub>8</sub> , using semi-empirical atom-atom potentials. <i>Journal of Physics and Chemistry of Solids</i> , 1988, 49, 421-424.	4.0	11
146	Shear induced anisotropy in two-dimensional liquids. <i>Physica A: Statistical Mechanics and Its Applications</i> , 1988, 149, 406-431.	2.6	28
147	A study of the disordered low-temperature structure of acenaphthylene, C <sub>12</sub> H <sub>8</sub> , using semi-empirical potential-energy calculations. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1988, , 1947.	0.9	2
148	Local order in a dense liquid. <i>Physical Review A</i> , 1988, 38, 1628-1631.	2.5	14
149	Condensed phonon modes and the recently discovered displacive superlattice of nickel arsenide. <i>Journal of Physics C: Solid State Physics</i> , 1988, 21, 309-318.	1.5	13
150	The crystal structure of nickel arsenide. <i>Journal of Physics C: Solid State Physics</i> , 1988, 21, 4007-4015.	1.5	20
151	Diffuse scattering in nickel arsenide, NiAs. <i>Journal of Physics C: Solid State Physics</i> , 1988, 21, 3863-3876.	1.5	12
152	X-ray diffuse scattering study of spatial correlations in para-terphenyl. <i>Journal of Physics C: Solid State Physics</i> , 1987, 20, 4773-4781.	1.5	5
153	Diffuse scattering and long-range order in the octahedral CDW/PLD-bearing transition-metal dichalcogenides. <i>Journal of Physics C: Solid State Physics</i> , 1987, 20, 5975-5982.	1.5	6
154	Optical transforms of disordered systems displaying diffuse intensity loci. <i>Journal of Applied Crystallography</i> , 1987, 20, 280-288.	4.5	11
155	Equations for diffuse scattering from disordered molecular crystals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1987, 43, 718-727.	0.3	2
156	Analysis of the diffuse scattering from disordered molecular crystals: application to 1,3-dibromo-2,5-diethyl-4,6-dimethylbenzene at 295 K. <i>Acta Crystallographica Section B: Structural Science</i> , 1987, 43, 97-106.	1.8	4
157	Multi-site correlations and the atomic size effect. <i>Journal of Applied Crystallography</i> , 1986, 19, 382-389.	4.5	32
158	Analysis of the diffuse scattering from disordered molecular crystals: application to 1,4-dibromo-2,5-diethyl-3,6-dimethylbenzene at 295 K. <i>Acta Crystallographica Section B: Structural Science</i> , 1986, 42, 262-272.	1.8	5
159	Diffuse X-ray scattering and the internal modes of molecular crystals. <i>International Reviews in Physical Chemistry</i> , 1986, 5, 191-196.	2.3	0
160	A lathe-like crystal grinder for grinding pre-aligned crystals into cylindrical cross section. <i>Journal of Applied Crystallography</i> , 1985, 18, 371-372.	4.5	1
161	Moiré patterns in electron diffraction from lanthanum oxide iodide (LaOI). <i>Journal of Applied Crystallography</i> , 1985, 18, 362-364.	4.5	1
162	A comparison of Weissenberg and diffractometer methods for the measurement of diffuse scattering from disordered molecular crystals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1985, 41, 394-399.	0.3	2

#	ARTICLE	IF	CITATIONS
163	Crystal structure of acenaphthylene, C <sub>12</sub> H <sub>8</sub> , at 80 K by neutron diffraction. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1985, , 451.	0.9	22
164	Diffuse x-ray scattering and models of disorder. <i>Reports on Progress in Physics</i> , 1985, 48, 1543-1594.	20.1	156
165	The disordered structures of 1,4-dibromo-2,5-diethyl-3,6-dimethylbenzene (BEMB1) and 1,3-dibromo-2,5-diethyl-4,6-dimethylbenzene (BEMB2), C <sub>12</sub> H <sub>16</sub> Br <sub>2</sub> . <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1984, 40, 1255-1260.	0.4	1
166	Routine recording of diffuse scattering from disordered molecular crystals. <i>Journal of Applied Crystallography</i> , 1983, 16, 192-197.	4.5	6
167	Evidence for the isomorphism of the low-temperature form of hexaamminecobalt(III) iodide with the room-temperature structure of hexaamminecobalt(III) chloride. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1983, 39, 513-514.	0.4	0
168	Disordered structure of 2,3-dichloro-6,7-dimethylantracene, C <sub>16</sub> H <sub>12</sub> Cl <sub>2</sub> , for sublimation-grown (I) and solution-grown (II) crystals. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1983, 39, 1123-1127.	0.4	1
169	Further properties of a Gaussian model of disorder. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1983, 39, 233-245.	0.3	8
170	Least-squares analyses of diffuse scattering from substitutionally disordered molecular crystals: application to 2,3-dichloro-6,7-dimethylantracene. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1983, 39, 882-892.	0.3	7
171	Analysis of the diffuse X-ray scattering from substitutionally disordered molecular crystals: monoclinic 9-bromo-10-methylantracene. <i>The Acta Crystallographica Section A, Crystal Physics, Diffractionoretical and General Crystallography</i> , 1982, 38, 611-618.	0.6	9
172	Gaussian growth-disorder models and optical transform methods. <i>The Acta Crystallographica Section A, Crystal Physics, Diffractionoretical and General Crystallography</i> , 1982, 38, 761-772.	0.6	9
173	Crystals exhibiting disorder " the orthorhombic polymorph of 9-bromo-10-methylantracene. <i>Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry</i> , 1982, 38, 1518-1525.	0.4	8
174	An optical transform study of the disorder in dicalcium barium propionate. <i>Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry</i> , 1982, 38, 1921-1927.	0.4	4
175	Crystals exhibiting disorder " the monoclinic polymorph of 9-chloro-10-methylantracene. <i>Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry</i> , 1981, 37, 1125-1126.	0.4	4
176	Paracrystals and growth-disorder models. <i>The Acta Crystallographica Section A, Crystal Physics, Diffractionoretical and General Crystallography</i> , 1980, 36, 921-929.	0.6	29
177	Crystals exhibiting disorder " the monoclinic polymorph of 9-bromo-10-methylantracene. <i>Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry</i> , 1980, 36, 852-857.	0.4	4
178	Optical transforms of disordered molecular crystals. <i>Journal of Applied Crystallography</i> , 1980, 13, 244-251.	4.5	11
179	Crystal Growth-Disorder Models and Ising Models. <i>Molecular Crystals and Liquid Crystals</i> , 1979, 50, 21-24.	0.8	0
180	A 3-D crystal growth-disorder model with cubic symmetry. <i>Proceedings of the Royal Society of London Series A, Mathematical and Physical Sciences</i> , 1979, 367, 175-192.	1.4	2

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181	A three-dimensional model of crystal-growth disorder. The Acta Crystallographica Section A, Crystal Physics, Diffractionoretical and General Crystallography, 1979, 35, 391-400.	0.6	5
182	A phase transition in a 3D growth-disorder model. The Acta Crystallographica Section A, Crystal Physics, Diffractionoretical and General Crystallography, 1978, 34, 120-123.	0.6	23
183	A phase transition in a 3D growth-disorder model; erratum. The Acta Crystallographica Section A, Crystal Physics, Diffractionoretical and General Crystallography, 1978, 34, 1030-1030.	0.6	0
184	Connections between Ising Models and Various Probability Distributions. Advances in Applied Probability, 1978, 10, 65.	0.7	9
185	An approximation to a two-dimensional binary process. Journal of Applied Probability, 1977, 14, 862-868.	0.7	5
186	Solution of crystal growth disorder models by imposition of symmetry. Proceedings of the Royal Society of London Series A, Mathematical and Physical Sciences, 1977, 353, 363-376.	1.4	19
187	A further solution for a two-dimensional model of crystal-growth disorder. Journal of Applied Crystallography, 1977, 10, 344-348.	4.5	7
188	On Certain Non-circular Zone Plates. Optica Acta, 1976, 23, 237-244.	0.7	17
189	A Fourier-series Approach to Moiré Patterns with Special Reference to Those Produced by Overlapping Zone Plates. Optica Acta, 1975, 22, 409-420.	0.7	5
190	The effect of non-linearity on a two-dimensional model of crystal-growth disorder. Journal of Applied Crystallography, 1975, 8, 636-644.	4.5	22
191	Short-range order in crystals. Nature, 1975, 253, 527-528.	27.8	2
192	Ambiguities in the interpretation of diffuse x-ray scattering. European Polymer Journal, 1974, 10, 19-20.	5.4	2
193	Optical-diffraction screens containing large numbers of apertures. Journal of Applied Crystallography, 1974, 7, 36-38.	4.5	13
194	A two-dimensional model of crystal-growth disorder. Journal of Applied Crystallography, 1973, 6, 87-96.	4.5	49
195	Order and disorder in acenaphthylene. Proceedings of the Royal Society of London Series A, Mathematical and Physical Sciences, 1973, 334, 19-48.	1.4	14
196	A method of producing optical diffraction masks representing static disorder in crystals using computer-generated patterns. Journal of Applied Crystallography, 1972, 5, 133-134.	4.5	0
197	The crystal and molecular structure of the cis-dimer of acenaphthylene. Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry, 1971, 27, 360-365.	0.4	15