

# Garry J McIntyre

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8962985/publications.pdf>

Version: 2024-02-01

213  
papers

6,561  
citations

70961

41  
h-index

91712

69  
g-index

220  
all docs

220  
docs citations

220  
times ranked

7178  
citing authors

#	ARTICLE	IF	CITATIONS
1	Stabilized Magnesium(I) Dimers and Magnesium(II) Hydride Complexes: Synthesis, Characterization, Adduct Formation, and Reactivity Studies. <i>Chemistry - A European Journal</i> , 2010, 16, 938-955.	1.7	387
2	Integration of single-crystal reflections using area multidetectors. <i>Journal of Applied Crystallography</i> , 1988, 21, 471-478.	1.9	219
3	Polarized-Neutron Scattering Study of the Cooper-Pair Moment in Sr <sub>2</sub> RuO <sub>4</sub> . <i>Physical Review Letters</i> , 2000, 85, 5412-5415.	2.9	213
4	Ferroelectric Order of Parallel Bistable Hydrogen Bonds. <i>Physical Review Letters</i> , 2002, 89, 215507.	2.9	213
5	Magnetic structure of the quasi-two-dimensional antiferromagnet NiPS <sub>3</sub> . <i>Physical Review B</i> , 2015, 92, .	4.6	166
6	Crystal Engineering and Correspondence between Molecular and Crystal Structures. Are 2- and 3-Aminophenols Anomalous?. <i>Journal of the American Chemical Society</i> , 1997, 119, 3477-3480.	6.6	146
7	Determination of the hydrogen absorption sites in Zn <sub>4</sub> O(1,4-benzenedicarboxylate) by single crystal neutron diffraction. <i>Chemical Communications</i> , 2006, , 278-280.	2.2	132
8	Incommensurate antiferromagnetic order in the quantum chain compound LiCuVO <sub>4</sub> . <i>Physica B: Condensed Matter</i> , 2004, 350, E253-E256.	1.3	127
9	Magnetic structure and magnon dynamics of the quasi-two-dimensional antiferromagnet FePS <sub>3</sub> . <i>Physical Review B</i> , 2016, 94, .	1.1	102
10	Accurate Molecular Structures of 16-Electron Rhodium Hydrido Boryl Complexes: A Low-Temperature Single-Crystal X-ray and Neutron Diffraction and Computational Studies of [(PR <sub>3</sub> ) <sub>2</sub> RhHCl(Boryl)] (Boryl = Bpin, Bcat). <i>Organometallics</i> , 2003, 22, 4557-4568.	1.1	102
11	Magnetic structure and magnetocalorics of GdPO <sub>4</sub> . <i>Physical Review B</i> , 2014, 90, .	1.0	100
12	The antiferromagnetic structures of IrMn <sub>3</sub> and their influence on exchange-bias. <i>Scientific Reports</i> , 2013, 3, 2412.	1.6	98
13	Hydrogen-Bonded Polyrotaxane-like Structure Containing Cyclic (H <sub>2</sub> O) <sub>4</sub> in [Zn(OAc) <sub>2</sub> (?bpe)] <sub>2</sub> ·2 H <sub>2</sub> O: X-ray and Neutron Diffraction Studies. <i>Chemistry - A European Journal</i> , 2004, 10, 5853-5859.	1.7	96
14	Variable-temperature neutron diffraction studies of the short, strong N...O hydrogen bonds in the 1:2 co-crystal of benzene-1,2,4,5-tetracarboxylic acid and 4,4'-bipyridyl. <i>Acta Crystallographica Section B: Structural Science</i> , 2003, 59, 794-801.	1.8	82
15	Neutron and X-ray Diffraction and Spectroscopic Investigations of Intramolecular [C <sub>12</sub> H <sub>8</sub> ...F <sub>12</sub> C] Contacts in Post-Metallocene Polyolefin Catalysts: Modeling Weak Attractive Polymer-Ligand Interactions. <i>Chemistry - A European Journal</i> , 2006, 12, 2607-2619.	1.7	82
16	The magnetic properties and structure of the quasi-two-dimensional antiferromagnet CoPS <sub>3</sub> . <i>Journal of Physics Condensed Matter</i> , 2017, 29, 455801.	0.7	81
17	The crystal structure of tetragonal KH <sub>2</sub> PO <sub>4</sub> and KD <sub>2</sub> PO <sub>4</sub> as a function of temperature and pressure. <i>Journal of Physics C: Solid State Physics</i> , 1982, 15, 37-58.	1.5	78
18	Magnetic ordering of the antiferromagnet Cu <sub>2</sub> MnSnS <sub>4</sub> from magnetization and neutron-scattering measurements. <i>Physical Review B</i> , 1997, 56, 5424-5431.	1.1	76

#	ARTICLE	IF	CITATIONS
19	Paraelectric and ferroelectric phases of betaine phosphite: Structural, thermodynamic, and dielectric properties. <i>Ferroelectrics</i> , 1993, 138, 1-10.	0.3	73
20	Single-crystal and powder neutron diffraction experiments on $\text{FeP}_3\text{S}$ . Search for the magnetic structure. <i>Physical Review B</i> , 2007, 76, .	1.1	73
21	VIVALDI "A thermal-neutron laue diffractometer for physics, chemistry and materials science. <i>Neutron News</i> , 2002, 13, 37-41.	0.1	72
22	Molecular heterometallic hydride clusters composed of rare-earth and d-transition metals. <i>Nature Chemistry</i> , 2011, 3, 814-820.	6.6	66
23	Cooperative Hydrogen-Bonding Effects in a Water Square: A Single-Crystal Neutron and Partial Atomic Charges and Hardness Analysis Study. <i>Journal of the American Chemical Society</i> , 2005, 127, 11063-11074.	6.6	64
24	Hidden Degrees of Freedom in Aperiodic Materials. <i>Science</i> , 2008, 319, 69-71.	6.0	63
25	High-speed neutron Laue diffraction comes of age. <i>Physica B: Condensed Matter</i> , 2006, 385-386, 1055-1058.	1.3	62
26	Scrutinizing negative thermal expansion in MOF-5 by scattering techniques and ab initio calculations. <i>Dalton Transactions</i> , 2013, 42, 1996-2007.	1.6	59
27	Experimental and Theoretical Charge Density Study of Polymorphic Isonicotinamide Oxalic Acid Molecular Complexes with Strong O-H...N Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13985-13997.	1.1	54
28	Variable-temperature neutron diffraction studies of the short, strong hydrogen bonds in the crystal structure of pyridine-3,5-dicarboxylic acid. <i>Acta Crystallographica Section B: Structural Science</i> , 2005, 61, 724-730.	1.8	53
29	Study of ethanol-lysozyme interactions using neutron diffraction. <i>Biochemistry</i> , 1985, 24, 5862-5869.	1.2	52
30	New Insights into an Old Molecule: Interaction Energies of Theophylline Crystal Forms. <i>Crystal Growth and Design</i> , 2012, 12, 1395-1401.	1.4	51
31	Reentrant behavior of the charge and orbital ordering and antiferromagnetism in $\text{LaSr}_2\text{Mn}_2\text{O}_7$ . <i>Physical Review B</i> , 2000, 61, 570-574.	1.1	48
32	The magnetic structure of holmium. II. <i>Journal of Physics C: Solid State Physics</i> , 1988, 21, 4125-4141.	1.5	47
33	Neutron Diffraction Studies on a 4-Coordinate Hydrogen Atom in an Yttrium Cluster. <i>Journal of the American Chemical Society</i> , 2008, 130, 3888-3891.	6.6	47
34	On the use of a small two-dimensional position-sensitive detector in neutron diffraction. <i>Journal of Applied Crystallography</i> , 1989, 22, 562-568.	1.9	46
35	Experimental and theoretical characterization of the Zn-Zn bond in $[\text{Zn}_2(\text{I}^5\text{C}_5\text{Me}_5)_2]_2$ . <i>Acta Crystallographica Section B: Structural Science</i> , 2007, 63, 862-868.	1.8	46
36	The magnetic structures and transitions of a potential multiferroic orthoferrite $\text{ErFeO}_3$ . <i>Journal of Applied Physics</i> , 2015, 117, 164105.	1.1	45

#	ARTICLE	IF	CITATIONS
37	H $\alpha$ -X Bond Activation via Hydrogen Transfer to Hydride in Ruthenium N-Heterocyclic Carbene Complexes: A Density Functional and Synthetic Studies. <i>Organometallics</i> , 2006, 25, 99-110.	1.1	44
38	The Structure of Nitromalonamide: A Combined Neutron-Diffraction and Computational Study of a Very Short Hydrogen Bond. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8684-8690.	1.1	43
39	The Formation of Defect Pairs for Highly Efficient Visible-Light Catalysts. <i>Advanced Materials</i> , 2017, 29, 1605123.	11.1	43
40	Influence of hydrogen bonding on the second harmonic generation effect: neutron diffraction study of 4-nitro-4-methylbenzylidene aniline. <i>Acta Crystallographica Section B: Structural Science</i> , 2001, 57, 410-414.	1.8	42
41	Neutron Diffraction Investigations of Magnetism in BiFeO <sub>3</sub> Epitaxial Films. <i>Advanced Functional Materials</i> , 2011, 21, 1567-1574.	7.8	42
42	Emergent Frustration in Co-doped $\text{Mn}^{2+}$ -Mn. <i>Physical Review Letters</i> , 2013, 110, 267207.	2.9	42
43	Glass and phase transitions in (KBr) $_{1-x}$ (KCN) $_x$ . <i>Physical Review B</i> , 1988, 37, 389-398.	1.1	41
44	Magnetic Excitations of CsMn(SO <sub>4</sub> ) $_2$ ·12D <sub>2</sub> O, Measured by Inelastic Neutron Scattering. <i>Journal of the American Chemical Society</i> , 2001, 123, 3377-3378.	6.6	41
45	Charge-density study of the nonlinear optical precursor DED-TCNQ at 20 K. <i>Physical Review B</i> , 2002, 65,	1.1	41
46	Spin dynamics and magnetoelectric coupling mechanism of $\text{Ca}_4\text{Mn}_2\text{N}_2\text{O}_{10}$ .	1.1	41
47	Evidence for a devil's staircase in holmium produced by an applied magnetic field. <i>Physical Review Letters</i> , 1991, 66, 1521-1524.	2.9	40
48	Magnetic structure of Gd-Y single-crystal alloys from neutron diffraction and magnetization measurements. <i>Physical Review Letters</i> , 1985, 55, 2968-2971.	2.9	39
49	Neutron scattering investigation of the static critical properties of Rb <sub>2</sub> CrCl <sub>4</sub> . <i>Journal of Physics Condensed Matter</i> , 1993, 5, 7871-7892.	0.7	39
50	Structure and Bonding of the Vanadium(III) Hexa-Aqua Cation. 1. Experimental Characterization and Ligand-Field Analysis. <i>Inorganic Chemistry</i> , 2004, 43, 8049-8060.	1.9	38
51	Antiferromagnetic phase transition and spin correlations in NiO. <i>Physical Review B</i> , 2009, 79, .	1.1	38
52	Minerals in cement chemistry: A single-crystal neutron diffraction and Raman spectroscopic study of thaumasite, Ca <sub>3</sub> Si(OH) <sub>6</sub> (CO <sub>3</sub> )(SO <sub>4</sub> )·12H <sub>2</sub> O. <i>American Mineralogist</i> , 2012, 97, 1060-1069.	0.9	37
53	New Apatite-Type Oxide Ion Conductor, Bi <sub>2</sub> La <sub>8</sub> [(GeO <sub>4</sub> ) <sub>6</sub> ]O <sub>3</sub> : Structure, Properties, and Direct Imaging of Low-Level Interstitial Oxygen Atoms Using Aberration-Corrected Scanning Transmission Electron Microscopy. <i>Advanced Functional Materials</i> , 2017, 27, 1605625.	7.8	37
54	Long-Range Ferromagnetism of Mn <sub>12</sub> Acetate Single-Molecule Magnets under a Transverse Magnetic Field. <i>Physical Review Letters</i> , 2005, 95, 227202.	2.9	36

#	ARTICLE	IF	CITATIONS
55	Proton Disorder in NH <sub>4</sub> <sup>+</sup> -N Bonded [dabcoH] <sup>+</sup> Relaxor: New Insights into H-Disordering in a One-Dimensional H <sub>2</sub> O Ice Analogue. <i>Crystal Growth and Design</i> , 2010, 10, 4334-4338.	1.4	36
56	Simultaneous variation of multipole parameters and Gram-Charlier coefficients in a charge-density study of tetrafluoroterephthalonitrile based on X-ray and neutron data. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2003, 59, 540-550.	0.3	35
57	Electronic and Molecular Structure of High-Spin d <sup>4</sup> Complexes: Experimental and Theoretical Study of the [Cr(D <sub>2</sub> O) <sub>6</sub> ] <sup>2+</sup> Cation in Tutton's Salts. <i>Journal of the American Chemical Society</i> , 2004, 126, 16639-16652.	6.6	35
58	Domain and crystal structure of superconducting Ba <sub>2</sub> YCu <sub>3</sub> O <sub>8</sub> at 40 and 100 K by single-crystal neutron diffraction. <i>Physical Review B</i> , 1988, 37, 5148-5157.	1.1	34
59	Neutron Laue diffraction on the spin crossover crystal [Fe(1-propyltetrazole) <sub>6</sub> ](BF <sub>4</sub> ) <sub>2</sub> showing continuous photoinduced transformation. <i>Physical Review B</i> , 2006, 73, .	1.1	34
60	On the crystal structure and crystal chemistry of pollucite, (Cs,Na) <sub>16</sub> Al <sub>16</sub> Si <sub>32</sub> O <sub>96</sub> ·nH <sub>2</sub> O: A natural microporous material of interest in nuclear technology. <i>American Mineralogist</i> , 2009, 94, 1560-1568.	0.9	34
61	CYCLOPS – a reciprocal-space explorer based on CCD neutron detectors. <i>Journal of Applied Crystallography</i> , 2011, 44, 392-397.	1.9	34
62	X-ray and neutron diffraction studies of the non-linear optical compounds MBANP and MBADNP at 20 K: charge-density and hydrogen-bonding analyses. <i>Acta Crystallographica Section B: Structural Science</i> , 2002, 58, 690-700.	1.8	33
63	YCa <sub>3</sub> (VO) <sub>3</sub> (BO) <sub>3</sub> : A Kagomé Compound Based on Vanadium(III) with a Highly Frustrated Ground State. <i>Chemistry of Materials</i> , 2011, 23, 1315-1322.	3.2	33
64	Aqua Ions. 2. Structural Manifestations of the Jahn-Teller Effect in the $\hat{I}^2$ -Alums. <i>Inorganic Chemistry</i> , 2003, 42, 1350-1365.	1.9	32
65	First accurate location of two proton sites in tourmaline: A single-crystal neutron diffraction study of oxy-dravite. <i>Mineralogical Magazine</i> , 2014, 78, 681-692.	0.6	32
66	Neutron scattering from mixtures of isotopically labelled molecules. A new method for determining the orientational distribution function in liquid crystals. <i>Liquid Crystals</i> , 1990, 7, 701-719.	0.9	31
67	Temperature-induced phase transitions in the giant-piezoelectric-effect material PZN-4.5%PT. <i>Journal of Physics Condensed Matter</i> , 2001, 13, L825-L833.	0.7	31
68	Uranium and Thorium Hydride Complexes as Multielectron Reductants: A Combined Neutron Diffraction and Quantum Chemical Study. <i>Inorganic Chemistry</i> , 2012, 51, 3613-3624.	1.9	31
69	Single-crystal neutron-diffraction study of a structural phase transition induced by a magnetic field in La <sub>1-x</sub> Sr <sub>x</sub> MnO <sub>3</sub> . <i>Physical Review B</i> , 1997, 55, R8622-R8625.	1.1	30
70	Octahedral cation ordering in olivine at high temperature. I: in situ neutron single-crystal diffraction studies on natural mantle olivines (Fa <sub>12</sub> and Fa <sub>10</sub> ). <i>Physics and Chemistry of Minerals</i> , 2000, 27, 623-629.	0.3	30
71	Tuning Proton Disorder in 3,5-Dinitrobenzoic Acid Dimers: the Effect of Local Environment. <i>Crystal Growth and Design</i> , 2013, 13, 497-509.	1.4	30
72	K-edge resonant x-ray magnetic scattering from RbMnF <sub>3</sub> . <i>Physical Review B</i> , 1999, 60, 10170-10179.	1.1	29

#	ARTICLE	IF	CITATIONS
73	On the Nature of the Spin Frustration in the $\text{CuO}_{2/3}$ Ribbon Chains of $\text{LiCuVO}_4$ : Crystal Structure Determination at 1.6 K, Magnetic Susceptibility Analysis, and Density Functional Evaluation of the Spin Exchange Constants. <i>Inorganic Chemistry</i> , 2011, 50, 3582-3588.	1.9	29
74	“Glass-like” thermal conductivity gradually induced in thermoelectric $\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$ clathrate by off-centered guest atoms. <i>Journal of Applied Physics</i> , 2016, 119, 185102.	1.1	29
75	Direct Location of the Hydrido Ligands in the Dianion $[\text{H}_4\text{Os}_{10}(\text{CO})_{24}]^{2-}$ by a Neutron Diffraction Study of Its $[(\text{Ph}_3\text{P})_2\text{N}]^+$ Salt at 20 K. <i>Angewandte Chemie International Edition in English</i> , 1991, 30, 1164-1167.	4.4	28
76	A (3 + 3)-Dimensional “Hypercubic” Oxide-Ionic Conductor: Type II $\text{Bi}_2\text{O}_3$ “ $\text{Nb}_2\text{O}_5$ ”. <i>Journal of the American Chemical Society</i> , 2013, 135, 6477-6484.	6.6	28
77	Neutron-diffraction study of the metamagnetic phases in $\text{HoNi}_2\text{B}_2\text{C}$ . <i>Physical Review B</i> , 2000, 61, 5872-5875.	1.1	27
78	Field-driven magnetisation steps in $\text{Ca}_3\text{Co}_2\text{O}_6$ : A single-crystal neutron-diffraction study. <i>Europhysics Letters</i> , 2010, 90, 67006.	0.7	27
79	Temperature-pressure phase diagram of an aperiodic host guest compound. <i>Europhysics Letters</i> , 2011, 93, 16003.	0.7	27
80	Engineering short, strong hydrogen bonds in urea di-carboxylic acid complexes. <i>CrystEngComm</i> , 2014, 16, 8177-8184.	1.3	27
81	The Low-Barrier Hydrogen Bond of Deuterated Benzoylacetone Probed by Very Low Temperature Neutron and X-ray Diffraction Studies and Theoretical Calculations. <i>Chemistry - A European Journal</i> , 2007, 13, 5539-5547.	1.7	26
82	Magnetic properties of tapiolite ( $\text{FeTa}_2\text{O}_6$ ); a quasi two-dimensional (2D) antiferromagnet. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 7837-7852.	0.7	25
83	A Neutron Diffraction Study of $[\text{OsClH}_3(\text{PPh}_3)_3]$ : A Complex Containing a Highly “Stretched” Dihydrogen Ligand. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 7227-7230.	7.2	25
84	Spin gaps and magnetic structure of $\text{Na}_x\text{CoO}_2$ . <i>Physical Review B</i> , 2006, 73, .	1.1	25
85	Use of a miniature diamond-anvil cell in high-pressure single-crystal neutron Laue diffraction. <i>IUCr</i> , 2016, 3, 168-179.	1.0	25
86	Cooperative Jahn-Teller distortion in $\text{PrO}_2$ . <i>Physical Review B</i> , 2004, 70, .	1.1	24
87	Understanding magnetic interactions in the series $\text{A}_2\text{FeX}_5 \cdot n\text{H}_2\text{O}$ (A=K, Rb; X=Cl, Br). II. Inelastic neutron scattering and DFT studies. <i>Physical Review B</i> , 2008, 78, .	1.1	24
88	The Magnetic Structure of Holmium in an Easy-Axis Magnetic Field. <i>Europhysics Letters</i> , 1992, 17, 553-558.	0.7	23
89	Low-energy magnetic excitations in double-layered manganite $\text{La}_{1.2}\text{Sr}_{1.8}\text{Mn}_2\text{O}_7$ . <i>Europhysics Letters</i> , 1999, 46, 801-807.	0.7	23
90	Hydride Encapsulation by a Molecular Main-Group-Metal Cluster: A Single-Crystal Neutron Diffraction Structure of $[\{\text{Ph}(\text{C}_5\text{H}_4\text{N})\}_6\text{HLi}_8]^+$ . <i>Organometallics</i> , 2004, 23, 4527-4530.	1.1	23

#	ARTICLE	IF	CITATIONS
91	Neutron Diffraction Study of $[H_4Co_4(C_5Me_4Et)_4]$ , a Tetrahedral Metal Cluster Complex with Four Face-Bridging Hydride Ligands. <i>Inorganic Chemistry</i> , 2004, 43, 555-558.	1.9	22
92	Synthesis and X-ray and Neutron Structures of $Zr\{\frac{1}{4}H\}_2BC_8H_{14}\}_4$ . <i>Inorganic Chemistry</i> , 2005, 44, 2459-2464.	1.9	22
93	Hydrogen-bond and cation partitioning in muscovite: A single-crystal neutron-diffraction study at 295 and 20 K. <i>American Mineralogist</i> , 2011, 96, 34-41.	0.9	22
94	A general Lorentz correction for single-crystal diffractometers. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1988, 44, 257-262.	0.3	21
95	A single-crystal neutron diffraction study of the magnetization density in $Fe_2Zr$ . <i>Journal of Physics Condensed Matter</i> , 1992, 4, 5795-5800.	0.7	21
96	Comparison of the $\int I(\theta)/\sin^2\theta$ and Least-Squares Methods for Integration of Bragg Reflections. <i>Journal of Applied Crystallography</i> , 1997, 30, 133-137.	1.9	21
97	Rapid neutron-diffraction data collection for hydrogen-bonding studies: application of the Laue diffractometer (LADI) to the case study zinc (tris)thiourea sulfate. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2001, 57, 429-434.	0.3	21
98	One picture says it all—high-pressure cells for neutron Laue diffraction on VIVALDI. <i>Journal of Physics Condensed Matter</i> , 2005, 17, S3017-S3024.	0.7	21
99	Spectroscopic, Magnetochemical, and Crystallographic Study of Cesium Iron Phosphate Hexahydrate: Characterization of the Electronic Structure of the Iron(II) Hexa-aqua Cation in a Quasicubic Environment. <i>Inorganic Chemistry</i> , 2006, 45, 4695-4705.	1.9	21
100	A non-topological mechanism for negative linear compressibility. <i>Chemical Communications</i> , 2016, 52, 7486-7489.	2.2	21
101	$U(As_{1-x}S_x)$ solid solutions. Resonant x-ray and neutron scattering study of the magnetic phase diagram. <i>Physical Review B</i> , 2001, 63, .	1.1	20
102	Understanding magnetic interactions in the series $U(As_{1-x}S_x)$ solid solutions. <a href="http://www.w3.org/1998/Math/MathML">http://www.w3.org/1998/Math/MathML</a>		

#	ARTICLE	IF	CITATIONS
109	A neutron diffraction study of the superionic transition in $\text{Li}_x\text{S}$ with $x = 0.06$ . <i>Journal of Physics Condensed Matter</i> , 1997, 9, 845-857.	0.7	18
110	Spin-density distribution in the new molecular magnet $\text{p-O}_2\text{N-C}_6\text{F}_4\text{-CNSSN}$ . <i>Physica B: Condensed Matter</i> , 2003, 335, 1-5.	1.3	18
111	Field induced magnetic order in the frustrated magnet gadolinium gallium garnet. <i>Journal of Physics: Conference Series</i> , 2009, 145, 012026.	0.3	18
112	Giant Deuteron Migration During the Isosymmetric Phase Transition in Deuterated 3,5-Pyridinedicarboxylic Acid. <i>Chemistry - A European Journal</i> , 2011, 17, 14942-14951.	1.7	18
113	Long-Range-Ordered Coexistence of 4-, 5-, and 6-Coordinate Niobium in the Mixed Ionic-Electronic Conductor $\text{Ba}_{1-x}\text{Nb}_x\text{O}_{9-x}$ . <i>Chemistry of Materials</i> , 2013, 25, 3154-3161.	3.2	18
114	Insights into the Crystallisation Process from Anhydrous, Hydrated and Solvated Crystal Forms of Diatrizoic Acid. <i>Chemistry - A European Journal</i> , 2015, 21, 1036-1047.	1.7	18
115	On the magnetic phase diagram of erbium in a c axis magnetic field. <i>Journal of Physics Condensed Matter</i> , 1992, 4, 8599-8608.	0.7	17
116	Neutron Laue diffraction study of the complex low-temperature magnetic behaviour of brownmillerite-type $\text{Ca}_2\text{Fe}_2\text{O}_5$ . <i>Journal of Applied Crystallography</i> , 2015, 48, 273-279.	1.9	17
117	Susceptible Ferroelectric/Antiferroelectric Phase Transition near the Surface of Nb-Doped Lead Zirconate Titanate from Surface Processing. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 14313-14317.	4.0	17
118	Elastic and quasielastic neutron scattering studies in $\text{KBr:KCN}$ mixed crystals. <i>European Physical Journal B</i> , 1989, 75, 81-99.	0.6	16
119	Neutron diffraction studies of nuclear and magnetic structures in the $S=1$ Heisenberg antiferromagnets $(\text{d}_6\text{CAP})_2\text{Cu}_4\text{X}$ ( $\text{X}=\text{Br, Cl}$ ). <i>Physical Review B</i> , 2007, 75, .	1.1	16
120	Spin density studies on $\text{p-O}_2\text{N-C}_6\text{F}_4\text{-CNSSN}$ . <i>Physical Review B</i> , 2010, 81, .	1.1	16
121	Dominance of Charge-Assisted Hydrogen Bonding on Short Contacts and Structures that Crystallize with $Z^2 > 1$ . <i>Crystal Growth and Design</i> , 2011, 11, 4904-4919.	1.4	16
122	Proton Cascade in a Molecular Solid: H/D Exchange on Mobile and Immobile Water. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 13463-13467.	7.2	16
123	Engineering Short, Strong, Charge-Assisted Hydrogen Bonds in Benzoic Acid Dimers through Cocrystallization with Proton Sponge. <i>Crystal Growth and Design</i> , 2016, 16, 2112-2122.	1.4	16
124	Manipulation of planar oxygen defect arrangements in multifunctional magn <sup>li</sup> titanium oxide hybrid systems: from energy conversion to water treatment. <i>Energy and Environmental Science</i> , 2020, 13, 5080-5096.	15.6	15
125	Effect of High Pressure on the Crystal Structures of Polymorphs of $\text{L-Histidine}$ . <i>Crystal Growth and Design</i> , 2020, 20, 7788-7804.	1.4	15
126	Bonding-deformation and superposition effects in the electron density of tetragonal nickel sulfate hexadeuterate $\text{NiSO}_4 \cdot 6\text{D}_2\text{O}$ . <i>Acta Crystallographica Section B: Structural Science</i> , 1990, 46, 27-39.	1.8	14



#	ARTICLE	IF	CITATIONS
127	Low-Temperature Single-Crystal Raman and Neutron-Diffraction Study of the Hydrogenous Ammonium Copper(II) Tutton Salt and the Deuterated Analogue in the Metastable State. <i>Inorganic Chemistry</i> , 2003, 42, 8524-8533.	1.9	14
128	Perpendicular Antiferromagnetic Ordering of Mn and Exchange Anisotropy in $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline">\langle \text{mml:mi} \rangle \text{Fe} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle \langle \text{mml:mi} \rangle \text{Mn} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle \text{Multilayers.}$ Physical Review Letters, 2007, 99, 037204.	2.9	14
129	Ab initio study of the magnetic behavior of four dithiadiazolyl radical compounds. <i>Polyhedron</i> , 2005, 24, 2579-2583.	1.0	13
130	Propagation of magnetic and superconducting order in Gd/La superlattices. <i>Journal of Physics Condensed Matter</i> , 2005, 17, 3305-3315.	0.7	13
131	Light-induced phase separation (LIPS) into like-spin phases observed by Laue neutron diffraction on a single crystal of $[\text{Fe}(\text{ptz})_6](\text{BF}_4)_2$ . <i>Zeitschrift für Kristallographie</i> , 2008, 223, .	1.1	13
132	The space between: Neutron diffraction studies reveal multiple hydrogen atom coordination numbers in an anionic dysprosium hydride cluster. <i>Inorganica Chimica Acta</i> , 2010, 363, 562-566.	1.2	13
133	On the crystal chemistry of londonite $[(\text{Cs},\text{K},\text{Rb})\text{Al}_4\text{Be}_5\text{B}_{11}\text{O}_{28}]$ : A single-crystal neutron diffraction study at 300 and 20 K. <i>American Mineralogist</i> , 2010, 95, 1467-1472.	0.9	13
134	A single-crystal neutron diffraction study of hambergite, $\text{Be}_2\text{BO}_3(\text{OH},\text{F})$ . <i>American Mineralogist</i> , 2012, 97, 1891-1897.	0.9	13
135	Polarized neutron Laue diffraction on a crystal containing dynamically polarized proton spins. <i>Journal of Applied Crystallography</i> , 2013, 46, 30-34.	1.9	13
136	A neutron diffraction study of the initial ordering regime in Gd-Y alloys. <i>Journal of Physics F: Metal Physics</i> , 1987, 17, 1973-1982.	1.6	12
137	Bonding deformation and superposition in the electron density of tetragonal $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$ at 25 K. <i>Acta Crystallographica Section B: Structural Science</i> , 1993, 49, 192-201.	1.8	12
138	Fine-tuning of the spin-density-wave state in Cr/V heterostructures via hydrogen uptake. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 336004.	0.7	12
139	Neutron Diffraction Characterization of $\text{H}^{\cdot\cdot}\text{Li}$ Interactions in a Lithium Aluminate Polymer. <i>Organometallics</i> , 2014, 33, 3919-3923.	1.1	12
140	Accurate hydrogen parameters for the amino acid $\text{L}$ -leucine. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 885-892.	0.5	12
141	The Magnetic Structure of Gd-Sc Alloys. <i>Europhysics Letters</i> , 1988, 6, 725-730.	0.7	11
142	Single-crystal neutron-diffraction study of the orientational glass state of $(\text{NaCN})_{1-x}(\text{KCN})_x$ . <i>Physical Review B</i> , 1990, 42, 3711-3718.	1.1	11
143	Multiple $\hat{\text{L}}\text{-agostic}$ interactions in a metal- $\hat{\text{L}}$ -methyl complex: the neutron structure of $[\text{Mo}(\text{NC}_6\text{H}_3\text{Pri}_2\text{-}2,6)_2\text{Me}_2]$ . <i>Chemical Communications</i> , 1998, , 1829-1830.	2.2	11
144	Onset of spin-density-wave antiferromagnetism in $\text{Cr}^{\cdot\cdot}\text{V}$ multilayers. <i>Physical Review B</i> , 2007, 76, .	1.1	11

#	ARTICLE	IF	CITATIONS
145	4-Phenoxyphenol: A Porous Molecular Material. <i>Crystal Growth and Design</i> , 2012, 12, 1746-1751.	1.4	11
146	Structure and dynamics studies of the short strong hydrogen bond in the 3,5-dinitrobenzoic acid–nicotinic acid molecular complex. <i>CrystEngComm</i> , 2013, 15, 7576.	1.3	11
147	Intermolecular Interactions in Solid-State Metalloporphyrins and Their Impacts on Crystal and Molecular Structures. <i>Inorganic Chemistry</i> , 2014, 53, 11552-11562.	1.9	11
148	Synthesis and characterisation of new Bi(iii)-containing apatite-type oxide ion conductors: the influence of lone pairs. <i>Dalton Transactions</i> , 2017, 46, 12494-12499.	1.6	11
149	Symmetry-mode analysis for intuitive observation of structure–property relationships in the lead-free antiferroelectric (1-x)AgNbO <sub>3</sub> (x)LiTaO <sub>3</sub> . <i>IUCr</i> , 2019, 6, 740-750.	1.0	11
150	Neutron Laue and X-ray diffraction study of a new crystallographic superspace phase inn-nonadecane–urea. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2015, 71, 293-299.	0.5	10
151	Bi <sup>2+</sup> NbO <sub>1.5+</sub> (x=0.0625, 0.12) fast ion conductors: Structures, stability and oxide ion migration pathways. <i>Journal of Solid State Chemistry</i> , 2015, 225, 383-390.	1.4	10
152	Extensive Sequential Polymorphic Interconversion in the Solid State: Two Hydrates and Ten Anhydrous Phases of Hexamidine Diisethionate. <i>Crystal Growth and Design</i> , 2019, 19, 7280-7289.	1.4	10
153	Field-induced magnetic and structural domain alignment in PrO <sub>2</sub> . <i>Physical Review B</i> , 2004, 70, .	1.1	9
154	Neutron diffraction studies of the 1:1 and 2:1 cocrystals of benzene-1,2,4,5-tetracarboxylic acid and 4,4'-bipyridine. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, o157-o161.	0.4	9
155	Re-investigation of the structure and crystal chemistry of the Bi <sub>2</sub> W <sub>2</sub> O <sub>6</sub> 'type (Ib)' solid solution using single-crystal neutron and synchrotron X-ray diffraction. <i>Acta Crystallographica Section B: Structural Science</i> . 2010, 66, 165-172.	1.8	9
156	Kagome staircase compound $\text{Co}_3\text{Mn}_9$ an applied magnetic field: Single-crystal neutron diffraction study. <i>Physical Review B</i> , 2010, 82, .	1.1	9
157	NdRhSn: A ferromagnet with an antiferromagnetic precursor. <i>Physical Review B</i> , 2011, 83, .	1.1	9
158	A multi-domain gem-grade Brazilian apatite. <i>American Mineralogist</i> , 2012, 97, 1574-1581.	0.9	9
159	Single-crystal neutron diffraction and Raman spectroscopic study of hydroxylherderite, CaBePO <sub>4</sub> (OH,F). <i>Mineralogical Magazine</i> , 2014, 78, 723-737.	0.6	9
160	Temperature- and pressure-dependent structural study of {Fe(pmd) <sub>2</sub> [Ag(CN) <sub>2</sub> ] <sub>2</sub> } spin-crossover compound by neutron Laue diffraction. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2014, 70, 436-443.	0.5	9
161	Tuning the magnetic anisotropy via Mn substitution in single crystal Co <sub>4</sub> Nb <sub>2</sub> O <sub>9</sub> . <i>Ceramics International</i> , 2019, 45, 1093-1097.	2.3	9
162	Element-specific magnetic order and competing interactions in Gd <sub>0.8</sub> Eu <sub>0.2</sub> S. <i>Europhysics Letters</i> , 2000, 49, 92-98.	0.7	8

#	ARTICLE	IF	CITATIONS
163	Metal distribution and disorder in the crystal structure of $[\text{NH}_2\text{Et}_2][\text{Cr}_7\text{M}_8\text{F}_8](\text{BuCO}_2)_{16}$ wheel molecules for $\text{M} = \text{Mn, Fe, Co, Ni, Cu, Zn}$ and $\text{Cd}$ . <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2014, 70, 932-941.	0.5	8
164	Phase transition sequences in tetramethylammonium tetrachlorometallates by X-ray diffraction and spectroscopic measurements. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 844-855.	0.5	8
165	Large easy-plane anisotropy induced spin reorientation in magnetoelectric materials $(\text{Co}_4\text{Mn}_2\text{Nb}_2\text{O}_9)$ . <i>Journal of Physics Condensed Matter</i> , 2019, 31, 235801.	0.7	8
166	Neutron diffraction studies on a system with a 4-coordinate hydrogen atom in an yttrium cluster. <i>Physica B: Condensed Matter</i> , 2006, 385-386, 231-233.	1.3	7
167	On the use of crystal vibrational modes in the estimation of the anisotropic displacement parameters of hydrogen atoms in molecular crystals: para-Nitroaniline as a test case. <i>Chemical Physics</i> , 2013, 423, 85-91.	0.9	7
168	The Effect of Local Crystalline Environment on Hydrogen Atom Behavior in Molecular Complexes of a Proton Sponge. <i>Crystal Growth and Design</i> , 2016, 16, 2123-2129.	1.4	7
169	Magnetic phases of $\text{GdSc}$ alloys in the multicritical regime. <i>Journal of Applied Physics</i> , 1988, 64, 5889-5891.	1.1	6
170	The Neutron Structure of the Formyl Peptide Receptor Antagonist Cyclosporin H ( $\text{CsH}$ ) Unambiguously Determines the Solvent and Hydrogen-Bonding Structure for Crystal Form II. <i>Journal of Chemical Crystallography</i> , 2011, 41, 470-480.	0.5	6
171	Single-crystal neutron diffraction and Mössbauer spectroscopic study of hureaulite, $(\text{Mn,Fe})_5(\text{PO}_4)_2(\text{HPO}_4)_2(\text{H}_2\text{O})_4$ . <i>European Journal of Mineralogy</i> , 2016, 28, 93-103.	0.4	6
172	Order of $[\text{6Ti}^{4+}]$ in a Ti-rich calcium amphibole from Kaersut, Greenland: a combined X-ray and neutron diffraction study. <i>Physics and Chemistry of Minerals</i> , 2017, 44, 83-94.	0.3	6
173	Inner-sphere water and hydrogen bonds in lanthanide DOTAM complexes. A neutron diffraction study. <i>Inorganica Chimica Acta</i> , 2018, 470, 433-438.	1.2	6
174	Magnetic ordering in the stacked triangular antiferromagnet $\text{CsMnBr}_3$ in the presence of an electric field. <i>Ferroelectrics</i> , 1994, 162, 147-152.	0.3	5
175	Spin-density distribution of the high $T_c$ $\text{p-O}_2\text{N}_2\text{C}_6\text{F}_4\text{-CNSSN}$ free radical studied by polarised neutron diffraction. <i>Polyhedron</i> , 2003, 22, 2301-2305.	1.0	5
176	A neutron diffraction study of ytterbium(II) cyclic organohydroborates. <i>Journal of Molecular Structure</i> , 2008, 890, 277-280.	1.8	5
177	Distinction of disorder, classical and quantum vibrational contributions to atomic mean-square amplitudes in dielectric pentachloronitrobenzene. <i>Physical Review B</i> , 2011, 83, .	1.1	5
178	Area detectors in single-crystal neutron diffraction. <i>Journal Physics D: Applied Physics</i> , 2015, 48, 504002.	1.3	5
179	Chemical pressure effects on crystal and magnetic structures of bilayer manganites $\text{Pr}_{1-x}\text{A}_x\text{Mn}_2\text{O}_7$ ( $\text{A} = \text{Sr, Tl}$ )	1.1	5
180	Neutron and high-pressure X-ray diffraction study of hydrogen-bonded ferroelectric rubidium hydrogen sulfate. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 855-863.	0.5	5

#	ARTICLE	IF	CITATIONS
181	Driving forces for the phase transition of CuQ <sub>2</sub> -TCNQ molecular crystals. CrystEngComm, 2016, 18, 5070-5073.	1.3	5
182	Subpicometer-scale atomic displacements and magnetic properties in the oxygen-isotope substituted multiferroic $\text{DyMnO}_3$ . Physical Review B, 2017, 95, .		5
183	Spin dynamics of edge-sharing spin chains in SrCa <sub>13</sub> Cu <sub>24</sub> O <sub>41</sub> . Physical Review B, 2018, 98, .	1.1	5
184	INTEGRATION OF OVERLAPPING PEAKS IN POSITION-SENSITIVE-DETECTOR (PSD) DATA BY LEAST-SQUARES FITTING. Journal De Physique Colloque, 1986, 47, C5-75-C5-85.	0.2	5
185	The helical-ferromagnetic phase transition in Gd-Y alloys. Journal of Physics Condensed Matter, 1992, 4, 10045-10052.	0.7	4
186	Position-sensitive detectors in single-crystal diffractometry. Neutron News, 1992, 3, 15-19.	0.1	4
187	Effect of spin delocalisation in K <sub>2</sub> FeCl <sub>5</sub> ·H <sub>2</sub> O on its superexchange pathways. Physica B: Condensed Matter, 2003, 335, 15-18.	1.3	4
188	Reorientation of spin-density waves in Cr films induced by proximity effect of vanadium. Journal of Physics Condensed Matter, 2005, 17, 3143-3152.	0.7	4
189	Direct observation of phase coherence in 3-kmagnetic configurations. Philosophical Magazine, 2006, 86, 2553-2565.	0.7	4
190	The crystal structure of tetragonal KH <sub>2</sub> PO <sub>4</sub> and KD <sub>2</sub> PO <sub>4</sub> as a function of temperature and pressure. Journal of Physics C: Solid State Physics, 1982, 15, 3040-3040.	1.5	3
191	Accurate H-atom parameters for the two polymorphs of <i>L</i> -histidine at 5, 105 and 295 K. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2021, 77, 785-800.	0.5	3
192	Quenched chirality in RbNiCl <sub>3</sub> : Linear birefringence and neutron diffraction. Physical Review B, 2004, 70, .	1.1	2
193	Neutron scattering's influence on crystallography. Neutron News, 2014, 25, 19-22.	0.1	2
194	Evolution of the neutron-scattering capability on the OPAL reactor at ANSTO. Neutron News, 2016, 27, 5-8.	0.1	2
195	Understanding the Unusual Response to High Pressure in KBe <sub>2</sub> BO <sub>3</sub> F <sub>2</sub> . Scientific Reports, 2017, 7, 4027.	1.6	2
196	Phonons observed by Laue diffraction on a continuous neutron source. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C129-C130.	0.3	2
197	Use of a miniature diamond-anvil cell in a joint X-ray and neutron high-pressure study on copper sulfate pentahydrate. IUCr, 2022, 9, 73-85.	1.0	2
198	Laue diffraction: The key to neutron crystallography from submillimetric-volume single crystals. European Physical Journal Special Topics, 2005, 131, 335-338.	0.2	1

#	ARTICLE	IF	CITATIONS
199	A neutron/X-Ray diffraction, IR, and $^1\text{H}/^{29}\text{Si}$ NMR Spectroscopic investigation of armenite: behavior of extra framework Ca cations and $\text{H}_2\text{O}$ molecules in microporous silicates. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2012, 227, 411-426.	0.4	1
200	Modulated crystal structures of phases VII and V in $(\text{NH}_4)_3\text{H}(\text{SO}_4)_2$ . <i>Neutron Laue diffraction. Crystallography Reports</i> , 2013, 58, 78-80.	0.1	1
201	Neutron scattering at the OPAL research reactor. <i>Journal of Physics: Conference Series</i> , 2016, 746, 012001.	0.3	1
202	The Martensitic Transformation in Indium-Thallium Alloys. <i>Minerals, Metals and Materials Series</i> , 2018, , 291-297.	0.3	1
203	Simulation and implementation of multiplexing modes on cold-neutron triple-axis spectrometer SIKA. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2020, 959, 163509.	0.7	1
204	Empirical and calculated thermal diffuse-scattering corrections for single-crystal diffraction data collected with a two-dimensional position-sensitive detector. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1993, 49, c46-c46.	0.3	1
205	Defect structure and property consequence when small $\text{Li}^+$ ions meet $\text{BaTiO}_3$ . <i>Physical Review Materials</i> , 2020, 4, .	0.9	1
206	On the pressure dependence of the crystal structure of $\text{PbHPO}_4$ . <i>Journal of Physics C: Solid State Physics</i> , 1987, 20, L881-L881.	1.5	0
207	Magnetic ordering in triangular antiferromagnets: A neutron scattering study (abstract). <i>Journal of Applied Physics</i> , 1991, 69, 5968-5968.	1.1	0
208	The phase diagram of $(\text{NH}_4)_x(\text{Kl})_{1-x}$ . <i>Zeitschrift Für Physik B-Condensed Matter</i> , 1995, 99, 333-338.	1.1	0
209	The multicritical region of the Gd - Lu alloy system. <i>Journal of Physics Condensed Matter</i> , 1996, 8, 3661-3670.	0.7	0
210	Structure of $\text{BiRe}_2\text{O}_6$ re-investigated using single-crystal neutron Laue diffraction. <i>Journal of Physics: Conference Series</i> , 2010, 251, 012028.	0.3	0
211	Journal of Applied Crystallography: the first 50 years and beyond. <i>Journal of Applied Crystallography</i> , 2018, 51, 233-234.	1.9	0
212	Ubiquity of amplitude-modulated magnetic ordering in the $\text{H}-T$ phase diagram of the frustrated non-Fermi-liquid $\text{YbAgGe}$ . <i>Physical Review B</i> , 2021, 104, .	1.1	0
213	Teaching and Education highlighted. <i>Journal of Applied Crystallography</i> , 2022, 55, 215-217.	1.9	0