

	Title	Authors	Journal	Date
185	Local-scale structures across the morphotropic phase boundary in $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$	N Zhang, H Yokota, A M Glazer, D A Keen, S Gorfman, P A Thomas, W Ren and Z-G Ye	<i>IUCrJ</i> 5 73-81	2017
184	Neutron and X-ray total scattering study of hydrogen disorder in fully hydrated hydrogrossular, $\text{Ca}_3\text{Al}_2(\text{O}_4\text{H}_4)_3$	D A Keen, D S Keeble and T D Bennett	<i>Phys Chem Miner (published online)</i> doi:10.1007/s00269-017-0923-0	2017
183	Liquid metal-organic frameworks	R Gaillac, P Pullumbi, K A Beyer, K W Chapman, D A Keen, T D Bennett and F-X Coudert	<i>Nature Mater</i> 16 1149-1154 doi:10.1038/nmat4998	2017
182	Direct visualization of critical hydrogen atoms in a pyridoxal 5'-phosphate enzyme	S Dajnowicz, R C Johnston, J M Parks, M P Blakeley, D A Keen, K L Weiss, O Gerlits, A Kovalevsky and T C Mueser	<i>Nature Comm</i> 8 955 doi:10.1038/s41467-017-01060-y	2017
181	Magnetic structure and spin wave excitations in the multiferroic magnetic metal organic framework $(\text{CD}_3)\text{ND}_2[\text{Mn}(\text{DCO}_2)_3]$	H C Walker, H D Duncan, M D Le, D A Keen, D J Voneshen and A E Phillips	<i>Phys Rev B</i> 96 094423	2017
180	Focus issue on studies of structural disorder using reverse Monte Carlo methods - Editorial	D A Keen	<i>Physica Scripta</i> 92 070201	2017
179	Local structure study of the orbital order/disorder transition in LaMnO_3	P M M Thygesen, C A Young, E O R Beake, F D Romero, L D Connor, T E Proffen, A E Phillips, M G Tucker, M A Hayward, D A Keen and A L Goodwin	<i>Phys Rev B</i> 95 174107	2017
178	Gel-based morphological design of zirconium metal-organic frameworks	B Bueken, N Van Velthoven, T Willhammar, T Stassin, I Stassen, D A Keen, G V Baron, J F M Denayer, R Ameloot, S Bals, D De Vos and T D Bennett	<i>Chemical Science</i> 8 3939-3948	2017
177	Room temperature neutron crystallography of drug-resistant HIV-1 protease uncovers limitations of X-ray structural analysis at 100K	O Gerlits, D A Keen, M P Blakeley, J M Louis, I T Weber and A Kovalevsky	<i>J Med Chem</i> 60 2018-2025	2017
176	Orbital dimer model for spin-glass state in $\text{Y}_2\text{Mo}_2\text{O}_7$	P M M Thygesen, J A M Paddison, R Zhang, K A Beyer, K W Chapman, H Y Playford, M G Tucker, D A Keen, M A Hayward and A L Goodwin	<i>Phys. Rev. Lett.</i> 118 067201	2017
175	Exploration of antiferromagnetic CoO and NiO using reverse Monte Carlo total neutron scattering refinements	L Timm, M G Tucker, D A Keen, P M M Thygesen, P J Saines and A L Goodwin	<i>Physica Scripta</i> 91 114004	2016

174	In situ studies of materials for high temperature CO ₂ capture and storage	M T Dunstan, S A Maugeri, W Liu, M G Tucker, O O Taiwo, B Gonzalez, P K Allan, M W Gaultois, P R Shearing, D A Keen, A E Phillips, M T Dove, S A Scott, J S Dennis, C P Grey	<i>Faraday Discussions</i> 192 217-240	2016
173	Local structure of crystalline and amorphous materials using reverse Monte Carlo methods	H Playford, D Keen and M Tucker	<i>Neutron News</i> 27 17-21	2016
172	Emergence of long-range order in BaTiO ₃ from local symmetry-breaking distortions	M S Senn, D A Keen, T C A Lucas, J A Hriljac and A L Goodwin	<i>Phys. Rev. Lett.</i> 116 207602	2016
171	Melt-quenched glasses of metal-organic frameworks	T D Bennett, Y Yue, P Li, A Qiao, H Tao, N G Greaves, T Richards, G I Lampronti, S A T Redfern, F Blanc, O K Farha, J T Hupp, A K Cheetham and D A Keen	<i>J. Am. Chem. Soc.</i> 138 3484-3492	2016
170	Long-range electrostatics-induced two-proton transfer captured by neutron crystallography in an enzyme catalytic site	O Gerlits, T Wymore, A Das, C-H Shen, J M Parks, J C Smith, K L Weiss, D A Keen, M P Blakeley, J M Louis, P Langan, I T Weber and A Kovalevsky	<i>Angewandte Chemie</i> 55 4924-4927	2016
169	A comparison of the amorphization of zeolitic imidazolate frameworks (ZIFs) and aluminosilicate zeolites by ball-milling	E F Baxter, T D Bennett, A B Cairns, N J Brownbill, A L Goodwin, D A Keen, P A Chater, F Blanc and A K Cheetham	<i>Dalton Trans.</i> 45 4258-4268	2016
168	Local structure of the metal-organic perovskite dimethylammonium manganese(II) formate	H D Duncan, M T Dove, D A Keen and A E Phillips	<i>Dalton Trans.</i> 45 4380-4391	2016
167	Direct mapping of microscopic polarization in ferroelectric x(BiScO ₃)-(1 - x)(PbTiO ₃) throughout its morphotropic phase boundary	K Datta, A Richter, M Göbbels, D A Keen and R B Neder	<i>Phys Rev B</i> 93 064102	2016
166	Connecting defects and amorphization in UiO-66 and MIL-140 metal-organic frameworks: A combined experimental and computational study	T D Bennett, T K Yordanova, E F Baxter, D G Reid, C Gervais, B Bueken, B Van de Voorde, D De Vos, D A Keen and C Mellot-Draznieks	<i>Phys. Chem. Chem. Phys.</i> 18 2192-2201	2016
165	Perovskites take the lead in local structure analysis (invited open access commentary)	D A Keen	<i>IUCrJ</i> 3 8-9	2016
164	Phase behaviour in the LiBH ₄ -LiBr system and structure of the anion-stabilised fast ionic, high temperature phase	I Cascallana-Matias, D A Keen, E J Cussen and D H Gregory	<i>Chemistry of Materials</i> 27 7780-7787	2015
163	The Crystallography of Correlated Disorder	D A Keen and A L Goodwin	<i>Nature</i> 521 303-309	2015

162	Crystallography and Physics (invited open access comment)	D A Keen	<i>Physica Scripta</i> 89 128003	2014
161	Observation of Interstitial Molecular Hydrogen in Clathrate Hydrates	R G Grim, B C Barnes, P G Lafond, W A Kockelmann, D A Keen, A K Soper, M Hiratsuka, K Yasuoka, C A Koh and A K Sum	<i>Angewandte Chemie.</i> 53 10710-10713	2014
160	L-Arabinose Binding, Isomerization, and Epimerization by D-Xylose Isomerase: X-ray/Neutron Crystallographic and Molecular Simulation Study.	P Langan, A K Sangha, T Wymore, J M Parks, Z K Yang, B L Hanson, Z Fisher, S A Mason, M P Blakeley, V T Forsyth, J P Glusker, H L Carrell, J C Smith, D A Keen, D E Graham, and A Kovalevsky	<i>Structure</i> 22 1287-1300 dx.doi.org/10.1016/j.str.2014.07.002	2014
159	The Missing Boundary in the Phase Diagram of $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$	N Zhang, H Yokota, A M Glazer, Z Ren, D A Keen, D S Keeble, P A Thomas and Z-G Ye	<i>Nature Comm.</i> 5 5231	2014
158	Geometric switching of linear to area negative thermal expansion in uniaxial metal–organic frameworks	I E Collings, M G Tucker, D A Keen and A L Goodwin	<i>Crystal Engineering Comm.</i> 16 3498-3506	2014
157	Systematic and controllable negative, zero and positive thermal expansion in cubic $\text{Zr}_{1-x}\text{Sn}_x\text{Mo}_2\text{O}_8$	S E Tallentire, F Child, I Fall, L Vella-Zarb, I Radosavljevic Evans, M G Tucker, D A Keen, C Wilson and J S O Evans	<i>J. Am. Chem. Soc.</i> 135 12849-12856	2013
156	Preface to “The first 24 years of reverse Monte Carlo modelling, Budapest, Hungary 20-22 September 2012”	D A Keen and L Pusztai	<i>J. Phys. Condensed Matter</i> 25 450301 (issue number 45; 454201-454222)	2013
155	Flexibility of zeolitic imidazolate framework structures studied by neutron total scattering and the Reverse Monte Carlo method	E O R Beake, M T Dove, A E Phillips, D A Keen, M G Tucker, A L Goodwin, T D Bennett and A K Cheetham	<i>J. Phys. Condensed Matter</i> 25 395403	2013
154	Coupling of the local defect and magnetic structure of wüstite, Fe_{1-x}O	P J Saines, M G Tucker, D A Keen, A K Cheetham and A L Goodwin	<i>Phys. Rev. B</i> 88 134418	2013
153	Joint X-ray/neutron crystallographic study of HIV-1 protease with clinical inhibitor amprenavir – insights for drug design	I T Weber, M J Waltman, M Mustyakimov, M P Blakeley, D A Keen, A K Ghosh, P Langan and A Y Kovalevsky	<i>J. Medicinal Chem</i> 56 5631-5635 DOI: 10.1021/jm400684f	2013
152	Ball-Milling-Induced Amorphization of Zeolitic Imidazolate Frameworks (ZIFs) for the Irreversible Trapping of Iodine	T D Bennett, P J Saines, D A Keen, J-C Tan and A K Cheetham	<i>Chem, A Eur.J.</i> 19 7049-55 DOI: 10.1002/chem.201300216	2013
151	Preface ‘Aminoff Prize in crystallography’	D A Keen	<i>Physica Scripta</i> 87 048101	2013
150	Bifurcated polarization rotation in bismuth-based piezoelectrics	D S Keeble, E R Barney, D A Keen, M G Tucker, J Kreisel and P A Thomas	<i>Adv. Funct. Mater.</i> 23 185-190	2013
149	Amorphization of the prototypical zeolitic imidazolate	S Cao, T D Bennett, D A Keen, A L Goodwin	<i>Chem. Comm.</i> 48 7805-7807	2012

- | | | | | |
|-----|---|---|---|------|
| | framework ZIF-8 by ball-milling | and A K Cheetham | | |
| 148 | Inhibition of D-xylose isomerase by polyols: atomic details by joint x-ray/neutron crystallography | A Kovalevsky, B L Hanson, S A Mason, V T Forsyth, Z Fisher, M Mustyakimov, M P Blakeley, D A Keen and P Langan | <i>Acta Cryst D</i> 68 1201-1206 | 2012 |
| 147 | Dynamic disorder and the α - β phase transition in quartz-type FePO ₄ at high temperature investigated by total neutron scattering, Raman spectroscopy, and density functional theory | G M Bhalerao, P Hermet, J Haines, O Cambon, D A Keen, M G Tucker, E Buixaderas, P Simon | <i>Phys. Rev. B</i> 86 134104 | 2012 |
| 146 | From quantum disorder to magnetic order in an s=1/2 Kagome lattice: a structural and magnetic study of Herbertsmithite at high pressure | D P Kozlenko, A F Kusmartseva, E V Lukin, D A Keen, W G Marshall, M de Vries and K V Kamenev | <i>Phys. Rev. Lett.</i> 108 187207 | 2012 |
| 145 | Static disorder and local structure in zinc(II) isonicotinate, a quartzlike metal-organic framework | I E Collings, M G Tucker, D A Keen and A L Goodwin | <i>Z. Krist.</i> 227 313 | 2012 |
| 144 | Reverse Monte Carlo study of apical Cu-O bond distortions in YBa ₂ Cu ₃ O _{6.93} | C A Young, E Dixon, M G Tucker, D A Keen, M A Hayward and A L Goodwin | <i>Z. Krist.</i> 227 280 | 2012 |
| 143 | Facile mechanosynthesis of amorphous zeolitic imidazolate frameworks | T D Bennett, S Cao, J C Tan, D A Keen, E G Bithell, P J Beldon, T Friscic and A K Cheetham | <i>J. Am. Chem. Soc.</i> 133 14546
doi: 10.1021/ja206082s | 2011 |
| 142 | Reversible pressure-induced amorphization of a zeolitic imidazolate framework (ZIF-4) | T D Bennett, P Simoncic, S A Moggach, F Gozzo, P Macchi, D A Keen, J-C Tan and A K Cheetham | <i>Chem. Comm.</i> 47 7983
doi: 10.1039/c1cc11985k | 2011 |
| 141 | Vibrational origin of the thermal stability in the high-performance piezoelectric material GaAsO ₄ | O Cambon, G M Bhalerao, D Bourgogne, J Haines, P Hermet, D A Keen and M G Tucker | <i>J. Am. Chem. Soc.</i> 133 8048
doi: 10.1021/ja202427x | 2011 |
| 140 | The elusive hydronium ion is found in an enzyme exchanging roles with a proton at lower pH | A Y Kovalevsky, B L Hanson, S A Mason, T Yoshida, S Z Fisher, M Mustyakimov, V T Forsyth, M P Blakeley, D A Keen and P Langan | <i>Angew. Chem. Int. Ed.</i> 50 7520
doi: 10.1002/anie.201101753 | 2011 |
| 139 | Thermal amorphization of Zeolitic Imidazolate frameworks | T D Bennett, D A Keen, J-C Tan, E R Barney, A L Goodwin, A K Cheetham | <i>Angew. Chem. Int. Ed.</i> 50 3067
doi: 10.1002/anie.201007303 | 2011 |
| 138 | Diffraction study of pressure-amorphized ZrW ₂ O ₈ using <i>in situ</i> and recovered samples | D A Keen, A L Goodwin, M G Tucker, J A Hriljac, T D Bennett, M T Dove, A K Kleppe, A P Jephcoat and M Brunelli | <i>Phys. Rev. B</i> 83 064109 | 2011 |
| 137 | Structure model of synthetic amorphous calcium carbonate | R J Reeder, A L Goodwin, M Michel, B L Phillips, D A Keen and M T Dove | <i>Geochimica et Cosmochimica Acta</i> 74 A855
(Conf. on Goldschmidt 2010 – Earth Energy and the Environment, Knoxville | 2010 |

- 136 Solving a hydrogen bond puzzle.
Suppressing negative thermal expansion in $\text{H}_3\text{Co}(\text{CN})_6$
through deuteration — a 40-year old structural puzzle
solved using advanced neutron diffraction techniques. D A Keen 13-18/6/10)
J. Phys. Condensed Matter – LabTalk 2010
<http://iopscience.iop.org/0953-8984/labtalk-article/43988>
- 135 Preface to “The first 21 years of reverse Monte Carlo
modelling – a workshop held in Budapest, Hungary (1-3
October 2009)” D A Keen and L Pusztai *J. Phys. Condensed Matter* **22** 400301 2010
(issue number 40; 404201-404216)
- 134 Hydrogen-bonding transition and isotope-dependent
negative thermal expansion in $\text{H}_3\text{Co}(\text{CN})_6$ D A Keen, M T Dove, J S O Evans, A L
Goodwin, L Peters and M G Tucker *J. Phys. Condensed Matter* **22** 404202 2010
- 133 Metal ion roles and the movement of hydrogen during
reaction catalyzed by D-Xylose Isomerase:
A joint X-ray and neutron diffraction study A Y Kovalevsky, L Hanson, S Z Fisher, M
Mustyakimov, S A Mason, V T Forsyth, M P
Blakeley, D A Keen, T Wagner, H L Carrell, A
K Katz, J P Glusker and P Langan *Structure* **18** 688-699 2010
- 132 Reverse Monte Carlo modelling of disordered crystalline
and amorphous materials D A Keen and M G Tucker *‘Diffraction at the Nanoscale:
Nanocrystals, Defects and Amorphous
Materials’* eds A Guagliardi and N
Masciocchi, Insubria University Press
(Como) 2010
- 131 Nanoporous structure and medium-range order in
synthetic amorphous calcium carbonate A L Goodwin, F M Michel, B L Phillips, D A
Keen, M T Dove and R J Reeder *Chemistry of Materials* **22** 3197-3205 2010
- 130 Structure and properties of an amorphous metal-organic
framework T D Bennett, A L Goodwin, M T Dove, D A
Keen, M G Tucker, E R Barney, A K Soper, E G
Bithell, J-C Tan and A K Cheetham *Phys. Rev. Lett.* **104** 115503 2010
- 129 Magnetic order and dynamics of the charge-ordered
antiferromagnet $\text{La}_{1.5}\text{Sr}_{0.5}\text{CoO}_4$ L M Helme, A T Boothroyd, R Coldea, D
Prabhakaran, C D Frost, D A Keen, L P
Regnault, P G Freedman, M Enderle and J Kulda *Phys. Rev. B* **80** 134414 2009
- 128 Topologically ordered amorphous silica obtained from the
collapsed siliceous zeolite, Silicalite-1-F: a step towards
“perfect” glasses J Haines, C Levelut, A Isambert, P Hébert, S
Kohara, D A Keen, T Hammouda and D
Andrault *J. Am. Chem. Soc.* **131** 12333-8 2009
doi: 10.1021/ja904054v
- 127 Effect of Ga-content on the instantaneous structure of
 $\text{Al}_{(1-x)}\text{Ga}_x\text{PO}_4$ solid solutions at high temperature O Cambon, J Haines, M Cambon, D A Keen, M
G Tucker, L C Chapon, N K Hansen, M
Souhassou and F Porcher *Chemistry of Materials* **21** 237-246 2009
doi:10.1021/cm801667p
- 126 Large negative linear compressibility of $\text{Ag}_3[\text{Co}(\text{CN})_6]$ A L Goodwin, D A Keen and M G Tucker *Proc. Natl. Acad. Sci. (USA)* **105** 18708- 2008

			13	
125	Amorphization of faujasite at high pressure: an X-ray diffraction and Raman spectroscopy study	A Isambert, E Angot, P Hébert, J Haines, C Levelut, R Le Parc, Y Ohishi, S Kohara and D A Keen	<i>J. Mater. Chem.</i> 18 5746-5752	2008
124	Argentophilicity-dependent colossal thermal expansion in extended Prussian blue analogues	A L Goodwin, D A Keen, M G Tucker, M T Dove, L Peters and J S O Evans	<i>J. Am. Chem. Soc.</i> 130 9660-9661	2008
123	Local structure in Ag ₃ [Co(CN) ₆]: Colossal thermal expansion, rigid unit modes and argentophilic interactions	M J Conterio, A L Goodwin, M G Tucker, D A Keen, M T Dove, L Peters and J S O Evans	<i>J. Phys.: Condensed Matter</i> 20 255225 http://arxiv.org/abs/0802.4385	2008
122	Colossal positive and negative thermal expansion in the framework material Ag ₃ [Co(CN) ₆]	A L Goodwin, M Calleja, M J Conterio, M T Dove, J S O Evans, D A Keen, L Peters and M G Tucker	<i>Science</i> 319 794-797	2008
121	Development and experimental use of a compact focussing device at ISIS	D A Keen, R M Dalgliesh, M J Gutmann and J R P Webster	<i>Nucl. Inst. and Meth. A</i> 586 64-67	2008
120	Ferroelectric nanoscale domains and the 905K phase transition in SrSnO ₃ : A neutron total scattering study	A L Goodwin, S A T Redfern, M T Dove, D A Keen and M G Tucker	<i>Phys. Rev. B</i> 76 174114	2007
119	Ionic diffusion within the α^* and β phases of Ag ₃ SI	S Hull, D A Keen, P A Madden and M Wilson	<i>J. Phys.: Condensed Matter</i> 19 406214	2007
118	Preface to 'The First Eighteen Years of Reverse Monte Carlo Modelling, a workshop held in Budapest, Hungary (28–30th September 2006)'	D A Keen and L Pusztai	<i>J. Phys.: Condensed Matter</i> 19 330301	2007
117	Neutron total scattering and reverse Monte Carlo study of cation ordering in Ca _x Sr _{1-x} TiO ₃	Q Hui, M T Dove, M G Tucker, S A T Redfern and D A Keen	<i>J. Phys.: Condensed Matter</i> 19 335214	2007
116	Local structure in ZrW ₂ O ₈ from neutron total scattering	M G Tucker, D A Keen, J S O Evans and M T Dove	<i>J. Phys.: Condensed Matter</i> 19 335215	2007
115	RMCPProfile: Reverse Monte Carlo for polycrystalline materials	M G Tucker, D A Keen, M T Dove, A L Goodwin and Q Hui	<i>J. Phys.: Condensed Matter</i> 19 335218	2007
114	A structural description of pressure induced amorphization in ZrW ₂ O ₈	D A Keen, A L Goodwin, M G Tucker, M T Dove, J S O Evans, W A Crichton and M Brunelli	<i>Phys. Rev. Lett.</i> 98 225501	2007
113	MnO spin-wave dispersion curves from neutron powder diffraction data	A L Goodwin, M T Dove, M G Tucker and D A Keen	<i>Phys. Rev. B.</i> 75 075423 <i>arXiv:cond-mat/0601558 and 0601559</i>	2007
112	SXD - The single crystal diffractometer at the ISIS Spallation Neutron Source	D A Keen, M J Gutmann and C C Wilson	<i>J. Appl. Cryst</i> 39 714-722	2006
111	Magnetic structure of MnO at 10K from neutron total scattering	A L Goodwin, M G Tucker, M T Dove and D A Keen	<i>Phys. Rev. Lett.</i> 96 047209	2006

110	Experimental verification of the simulated performance of a compact supermirror focusing device	D A Keen, R M Dalgliesh, M J Gutmann and J R P Webster	<i>Physica B</i> 385-386 1240-1242	2006
109	Dynamics from diffraction	A L Goodwin, M G Tucker, E R Cope, M T Dove and D A Keen	<i>Physica B</i> 385-386 285-287	2006
108	High-temperature structural disorder, phase transitions and piezoelectric properties of GaPO ₄	J Haines, O Cambon, N Prudhomme, G Frayssé, D A Keen, L C Chapon and M G Tucker	<i>Phys. Rev. B</i> 73 014103	2006
107	Model-independent extraction of dynamical information from powder diffraction data	A L Goodwin, M G Tucker, E R Cope, M T Dove and D A Keen	<i>Phys. Rev. B</i> 72 214304	2005
106	Negative thermal expansion in ZrW ₂ O ₈ : mechanisms, rigid unit modes and neutron total scattering	M G Tucker, A L Goodwin, M T Dove, D A Keen, S A Wells and J S O Evans	<i>Phys. Rev. Lett.</i> 95 255501	2005
105	High pressure forms of lithium sulphate: structural determination and computer simulation	D C Parfitt, D A Keen, S Hull, W A Crichton, M Mezouar, M Wilson and P A Madden	<i>Phys. Rev. B</i> 72 054121	2005
104	Piezoelectric properties at high temperature in α -quartz materials	O Cambon, J Haines, G Frayssé, D A Keen and M G Tucker	<i>J. Phys. IV France</i> 126 27-30	2005
103	Total scattering and reverse Monte Carlo study of the 105K displacive phase transition in strontium titanate	Q Hui, M G Tucker, M T Dove, S A Wells and D A Keen	<i>J. Phys.: Condensed Matter</i> 17 S111-S124	2005
102	Refinement of the Si-O-Si bond angle distribution in vitreous silica	M G Tucker, D A Keen, M T Dove and K Trachenko	<i>J. Phys.: Condensed Matter</i> 17 S67-S75	2005
101	Reverse Monte Carlo modelling of crystalline disorder	D A Keen, M G Tucker and M T Dove	<i>J. Phys.: Condensed Matter</i> 17 S15-S22	2005
100	The first fifteen years of reverse Monte Carlo modelling, Budapest, Hungary	D A Keen, L Pusztai and M T Dove	<i>J. Phys.: Condensed Matter</i> 17 U3	2005
99	Neutron powder diffraction and total scattering studies of α -quartz-type piezoelectric materials at high temperature	J Haines, O Cambon and D A Keen	<i>Physica B</i> 350 e979-e981	2004
98	Phonons from powder diffraction: a quantitative model-independent evaluation	A L Goodwin, M G Tucker, M T Dove and D A Keen	<i>Phys. Rev. Lett.</i> 93 075502	2004
97	High pressure dissociation of silver mercury iodide, Ag ₂ HgI ₄	D C Parfitt, S Hull, D A Keen and W A Crichton	<i>J. Sol. State Chem.</i> 177 3715-3720	2004
96	Reply to Comment on 'Quantum correlations between protons in potassium bicarbonate'	D A Keen and S W Lovesey	<i>J. Phys.: Condensed Matter</i> 16 5637-5638	2004
95	The nature of the superionic transition in Ag ⁺ and Cu ⁺ halides	D A Keen, S Hull, A C Barnes, P Berastegui, W A Crichton, P A Madden, M G Tucker and M Wilson	<i>Phys. Rev. B</i> 68 014117	2003
94	Quantum correlations between protons in potassium bicarbonate	D A Keen and S W Lovesey	<i>J. Phys.: Condensed Matter</i> 15 4937-4946	2003

93	New instrumentation for high-pressure single crystal diffraction at ISIS	M J Gutmann, D A Keen and C C Wilson	<i>High Pressure Research</i> 23 313-316	2003
92	Observation of dynamical structure arising from spatially extended quantum entanglement and long-lived quantum coherence in the KHCO ₃ crystal	F Fillaux, A Cousson and D A Keen	<i>Phys. Rev. B</i> 67 054301 & 189901	2003
91	Disordering phenomena in superionic conductors.	D A Keen	<i>J. Phys.: Condensed Matter</i> 14 R819-R857	2002
90	Reverse Monte Carlo methods	M T Dove, M G Tucker, S A Wells and D A Keen	<i>EMU Notes in Mineralogy</i> 4 Ch 4 ed. C M Gramaccioli (Eötvös Univ. Press, Budapest)	2002
89	Structural and superionic properties of Ag ⁺ -rich ternary phases within the AgI-MI ₂ systems	S Hull, D A Keen and P Berastegui	<i>J. Phys.: Condensed Matter</i> 14 13579-13596	2002
88	Structural disorder and loss of piezoelectric properties in alpha-quartz at high temperature	J Haines, O Cambon, D A Keen, M G Tucker and M T Dove	<i>Applied Physics Letters</i> 81 2968-2970	2002
87	Neutron total scattering method: simultaneous determination of long-range and short-range order in disordered materials.	M T Dove, M G Tucker and D A Keen	<i>European. J. Mineralogy.</i> 14 331-348	2002
86	Total scattering and reverse Monte Carlo modelling of disordered crystalline materials.	M G Tucker, M T Dove and D A Keen	in 'From semiconductors to proteins: beyond the average structure' eds S. J. L. Billinge and M. F. Thorpe <i>Fundamental Materials Research Series</i> , Plenum, New York	2002
85	Crystal structures and ionic conductivities of ternary derivatives of the silver and copper monohalides. I. Superionic phases of stoichiometry MA ₄ I ₅ : M=K ⁺ , Rb ⁺ and A=Ag ⁺ , Cu ⁺ .	S. Hull, D. A. Keen and P. Berastegui	<i>J. Solid State Chemistry</i> 165 363-371	2002
84	Structural description of the superionic behaviour in the system (AgI) _x -(PbI ₂) _{1-x} , 2/3<x<4/5.	S. Hull, D. A. Keen and P. Berastegui	<i>Solid State Ionics</i> 147 97-106.	2002
83	The high-temperature superionic behaviour of Ag ₂ S.	S. Hull, D. A. Keen, D. S. Sivia, P. A. Madden and M. Wilson	<i>J. Phys.: Condensed Matter</i> 14 L9-L17.	2002
82	Structural characterisation of further high-temperature superionic phases of Ag ₂ HgI ₄ and Cu ₂ HgI ₄	S. Hull and D. A. Keen	<i>J. Phys.: Condensed Matter</i> 13 5587-5610.	2001
81	A detailed characterisation of quartz on heating through	M. G. Tucker, D. A. Keen and M. T. Dove	<i>Mineralogical Magazine.</i> 65 489-507.	2001

	the α - β phase transition.			
80	Application of the reverse Monte Carlo method to crystalline materials.	M. G. Tucker, M. T. Dove and D. A. Keen	<i>J. Appl. Cryst.</i> 34 630-8.	2001
79	MCGRtof: Monte Carlo G(r) with resolution corrections for time-of-flight neutron diffractometers.	M. G. Tucker, M. T. Dove and D. A. Keen	<i>J. Appl. Cryst.</i> 34 780-2.	2001
78	An x-ray and neutron scattering study of the structure of zinc vanadate glasses.	U. Hoppe, R. Kranold, E. Gattf, J. Neuefeind and D. A. Keen	<i>Z. fur Naturf. A</i> 56 478-488	2001
77	Combined neutron and x-ray scattering study of phosphate glasses.	U. Hoppe, R. Kranold, A. Barz, D. Stachel, J. Neuefeind and D. A. Keen	<i>J. Non-Cryst. Sol.</i> 293-295 158-168.	2001
76	Diffuse neutron scattering from crystalline materials	V. M. Nield & D. A. Keen	Oxford University Press	2001
75	A comparison of various commonly used correlation functions for describing total scattering.	D. A. Keen	<i>J. Appl. Cryst.</i> 34 172-7.	2001
74	Dynamical structural disorder in cristobalite: neutron total scattering measurement and reverse Monte Carlo modelling.	M. G. Tucker, M. P. Squires, M. T. Dove and D. A. Keen	<i>J. Phys.: Condensed Matter</i> 13 403-23.	2001
73	The crystal structures of superionic Ag ₃ SI.	S. Hull, D. A. Keen, N. J. G. Gardner and W. Hayes	<i>J. Phys.: Condensed Matter</i> 13 2295-316.	2001
72	Structural behaviour at the γ - β phase transition of Ag ₃ SI.	D. A. Keen and S. Hull	<i>J. Phys.: Condensed Matter</i> 13 L343-7.	2001
71	Pressure-induced phase transitions in chromium thiospinels.	P. Vaqueiro, A. V. Powell, S. Hull and D. A. Keen	<i>Physical Review B</i> 63 064106.	2001
70	The molecular structure of (PSH ⁺)(nido-7,8-C ₂ B ₉ H ₁₂ ⁻) determined by neutron diffraction (PS=proton sponge, 1,8-bis(dimethylamino)naphthalene)	M. A. Fox, A. E. Goeta, J. A. K. Howard, A. K. Hughes, A. L. Johnson, D. A. Keen, K. Wade and C. C. Wilson	<i>Inorg. Chem.</i> 40 173-5.	2001
69	Structure and dynamics of maleic anhydride.	S. F. Parker, C. C. Wilson, J. Tomkinson, D. A. Keen, A. J. Ramirez-Cuesta, P. C. H. Mitchell, A. J. Florence and N. Shankland	<i>J. Phys. Chem. A</i> 105 3064-70.	2001
68	Simultaneous analysis of changes in long-range and short-range structural order at the displacive phase transition in quartz	M. G. Tucker, M. T. Dove and D. A. Keen	<i>J. Phys.: Condensed Matter</i> 12 L723-30.	2000
67	Aspects of the structure and dynamics of the CMR material Nd _{0.5} Pb _{0.5} MnO ₃	A. Møllergaard, D. A. Keen, M. J. Harris and R. L. McGreevy	<i>Physica B</i> 276-278 , 774-5	2000
66	Direct measurement of the thermal expansion of the Si-O bond by neutron total scattering	M. G. Tucker, M. T. Dove and D. A. Keen	<i>J. Phys.: Condensed Matter</i> 12 , L425-L430.	2000

65	Combined single crystal neutron diffraction and solution NMR relaxation studies of mono- and bis(silyl) substituted niobocene hydrides with nonclassical interligand interactions.	V. I. Bakhmutov, J. A. K. Howard, D. A. Keen, L. G. Kuzmina, M. A. Leech, G. I. Nikonov, E. V. Vorontsov and C. C. Wilson	<i>J. Chem. Soc. Dalton Trans.</i> 10 1631-5.	2000
64	Rigid Unit Modes in framework structures: theory, experiment and applications	M. T. Dove, K. O. Trachenko, M. G. Tucker & D. A. Keen	<i>Reviews in Mineralogy</i> 39 , 1-33	2000
63	Halogen trimer synthons in crystal engineering: low-temperature X-ray and neutron diffraction study of the 1:1 complex of 2,4,6-tris(4-chlorophenoxy)-1,3,5-triazine with tribromobenzene.	C. K. Broder, J. A. K. Howard, D. A. Keen, C. C. Wilson, F. H. Allen, R K R Jetti, A Nangia & G. R. Desiraju	<i>Acta Crystallographica B</i> 56 1080-4.	2000
62	Crystal structure of the high-pressure monoclinic phase-II of cristobalite, SiO ₂	M. T. Dove, D. A. Keen, W. G. Marshall, S. A. T. Redfern, K. Trachenko & M. G. Tucker	<i>Mineralogical Magazine</i> 64 , 569-576	2000
61	Amorphous silica from the Rigid Unit Mode approach	M. T. Dove, K. D. Hammonds, M. J. Harris, V. Heine, D. A. Keen, A. K. A. Pryde, K. Trachenko and M. C. Warren.	<i>Mineralogical Magazine</i> 64 , 377-388	2000
60	Total scattering studies of silica polymorphs: similarities in glass and disordered crystalline local structure	D. A. Keen & M. T. Dove	<i>Mineralogical Magazine</i> 64 , 447-457	2000
59	Structural characterization of the $\beta \rightarrow \alpha$ superionic transition in Ag ₂ HgI ₄ and Cu ₂ HgI ₄	S. Hull & D. A. Keen	<i>J. Phys.: Condensed Matter</i> 12 , 3751-3765	2000
58	Phase transitions in tridymite studied using 'Rigid Unit Mode' theory, reverse Monte carlo methods and molecular dynamics simulation	M. T. Dove, A. K. A. Pryde and D. A. Keen	<i>Mineralogical Magazine</i> 64 , 243-259	2000
57	Modelling the magnetic structure of Dy ₇ Fe ₃ metallic glass	L. Karlsson, A. Wannberg, R. L. McGreevy and D. A. Keen	<i>Physical Review B</i> 61 , 487-491	2000
56	Single crystal diffraction at ISIS. User guide for the SXD instrument	D. A. Keen & C. C. Wilson	<i>SXD instrument manual</i> version 2	1999
55	Atomic structure of disordered materials	M. T. Dove & D. A. Keen	in ' <i>Microscopic Properties and Processes in Minerals</i> ' ed C.R.A.Catlow and K.Wright (Kluwer Academic, The Netherlands) 371-387	1999
54	Local structures of amorphous and crystalline phases of silica, SiO ₂ , by neutron total scattering	D. A. Keen & M. T. Dove	<i>J. Phys.: Condensed Matter</i> 11 , 9263-9273	1999
53	Pressure-induced phase transitions in AgCl, AgBr and AgI	S. Hull and D. A. Keen	<i>Physical Review B</i> 59 , 750-761	1999
52	Effect of hydrostatic pressure on the crystal structure and	S. Hull and D. A. Keen	<i>Physical Review B</i> 58 , 14837-14844	1998

	superionic behaviour of lead(II) fluoride			
51	Superionic behaviour in copper(I) iodide at elevated pressures and temperatures	S. Hull, D. A. Keen, W. Hayes and N. J. G. Gardner	<i>J Phys: Condensed Matter</i> 10 , 10941-10954	1998
50	Determination of structural disorder in superionic Ag ₂ Te by neutron total scattering	D. A. Keen and S. Hull	<i>J Phys: Condensed Matter</i> 10 , 8217-8234	1998
49	User manual for impedance spectroscopy measurements at ISIS	N. J. G. Gardner, S. Hull, D. A. Keen and P. Berastegui	<i>Rutherford Appleton Laboratory Technical Report RAL-TR-1998-032</i>	1998
48	Local structure from diffraction	D. A. Keen	'Local structure from diffraction' Eds S. J. L. Billinge and M. F. Thorpe, Plenum Press New York. 101-119	1998
47	Neutron time-of-flight measurements of diffuse scattering	D. A. Keen, M J Harris and W. I. F. David	<i>Physica B</i> 241-243 , 201-203	1998
46	Direct measurement of the Si-O bond length and orientational disorder in β -cristobalite	M T Dove, D. A. Keen, A. C. Hannon and I. P. Swainson	<i>Physics and Chemistry of Minerals</i> 24 , 311-317	1997
45	Refining disordered structural models using reverse Monte Carlo methods: application to vitreous silica	D. A. Keen	<i>Phase Transitions</i> 61 , 109-124	1997
44	A high temperature, high pressure cell for time-of-flight neutron scattering	S. Hull, D. A. Keen, R. Done, T. Pike and N. J. G. Gardner	<i>Nucl. Inst. Meth. in Phys. Res. A</i> 385 , 354-360	1997
43	Spin configurations in an amorphous random-anisotropy magnet	D. A. Keen, R. I. Bewley, R. Cywinski and R. L. McGreevy	<i>Physical Review B</i> 54 , 1036-1042	1996
42	Structural evidence for a fast-ion transition in the high-pressure rocksalt phase of silver iodide	D. A. Keen, S. Hull, W. Hayes and N. J. G. Gardner	<i>Physical Review Letters</i> 77 , 4914-4917	1996
41	Superionic behaviour in copper(I) chloride at high pressures and high temperatures	S. Hull and D. A. Keen	<i>J Phys: Condensed Matter</i> 8 , 6191-6198	1996
40	Neutron and X-ray diffuse scattering of calcium-stabilized zirconia at temperatures up to 1500K	Th. Proffen, M. Keilholz, R. B. Neder, F. Frey and D. A. Keen	<i>Acta Crystallographica B</i> 52 , 66-71	1996
39	SXD diffuse scattering data analysis manual	D. A. Keen and V. M. Nield	<i>Rutherford Appleton Laboratory Technical Report RAL-TR-96-095</i>	1996
38	Single crystal diffraction at ISIS. User guide for the SXD instrument	D. A. Keen and C. C. Wilson	<i>Rutherford Appleton Laboratory Technical Report RAL-TR-96-083</i>	1996
37	Magnetic structure determination of amorphous materials using RMC modelling of neutron diffraction data	D. A. Keen, R. L. McGreevy, R. I. Bewley and R. Cywinski	<i>Nucl. Inst. Meth. in Phys. Res. A</i> 354 , 48-52	1995
36	The interpretation of single-crystal diffuse scattering using reverse Monte Carlo modelling	V. M. Nield, D. A. Keen and R. L. McGreevy	<i>Acta Crystallographica A</i> 51 , 763-771	1995
35	Anomalies in the normal-state properties of UPd ₂ Al ₃	L. Paolasini, R. Caciuffo, G. H. Lander, J.	<i>J Phys. Chem. Solids</i> 56 , 1323-1329	1995

		Rebizant, D. A. Keen, N. Sato and T. Komatsubara		
34	Meeting report of the U.K. neutron user's meeting	D. A. Keen and D. Kearley	<i>Neutron News</i> 6 , 6-7	1995
33	The high-temperature structural behaviour of copper(I) iodide	D. A. Keen and S. Hull	<i>J Phys: Condensed Matter</i> 7 , 5793-5804	1995
32	High-pressure phase of copper(I) iodide	M. Hofmann, S. Hull and D. A. Keen	<i>Physical Review B</i> 51 , 12022-12025	1995
31	Pressure induced phase transitions in copper and silver halides	S. Hull and D. A. Keen	<i>High Pressure Research</i> 14 , 121-126	1995
30	Pulsed neutron Laue diffraction studies of the magnetic structures of holmium and terbium	C. C. Tang, P. W. Haycock, W. G. Stirling, C. C. Wilson, D. A. Keen and D. Fort	<i>Physica B</i> 205 , 105-114	1995
29	High-pressure polymorphism of the copper(I) halides: A neutron-diffraction study to ~10GPa	S. Hull and D. A. Keen	<i>Physical Review B</i> 50 , 5868-5885	1994
28	Diffuse neutron scattering from an <i>in-situ</i> grown α -AgI single crystal	D. A. Keen, V. M. Nield and R. L. McGreevy	<i>J Appl. Cryst.</i> 27 , 393-398	1994
27	Simultaneous neutron and X-ray refinement of ortho-II superstructure in $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$	R. A. Hadfield, P. Schleger, H. Casalta, N. H. Andersen, H. F. Poulsen, M. v. Zimmerman, J. R. Schneider, M. T. Hutchings, D. A. Keen, Ruixing Liang, P. Dosanjh and W. N. Hardy	<i>Physica C</i> 235-240 , 1267-1268	1994
26	Diffuse neutron-scattering study of deuterated ice Ih	J. C. Li, V. M. Nield, D. K. Ross, R. W. Whitworth, C. C. Wilson and D. A. Keen	<i>Phil. Mag. B</i> 69 , 1173-1181	1994
25	Determination of the structure of β -CuI by high-resolution neutron powder diffraction	D. A. Keen and S. Hull	<i>J Phys: Condensed Matter</i> 6 , 1637-1644	1994
24	Structural disorder in CuBr	V. M. Nield, R. L. McGreevy, D. A. Keen and W. Hayes	<i>Physica B</i> 202 , 159-166	1994
23	Disorder in silver and copper halides	D. A. Keen	<i>InCr - ISIS Crystallography Seminar</i> RAL-94-031, 85-95	1994
22	Structure and fast-ion conduction in α -AgI	V. M. Nield, D. A. Keen, W. Hayes and R. L. McGreevy	<i>Solid State Ionics</i> 66 , 247-258	1993
21	Structural modifications within copper(I) iodide at pressures up to 27kbar	S. Hull and D. A. Keen	<i>Europhys. Lett.</i> 23 , 129-134	1993
20	A powder neutron diffraction study of the pressure-induced phase transitions within silver iodide	D. A. Keen and S. Hull	<i>J Phys: Condensed Matter</i> 5 , 23-32	1993
19	Defect structure and diffuse scattering of zirconia single crystals with 10 and 15mol% CaO at temperatures up to	Th. Proffen, R. B. Neder, F. Frey, D. A. Keen and C. M. E. Zeyen	<i>Acta Crystallographica B</i> 49 , 605-610	1993

	1750K			
18	Diffuse scattering studies using neutron time-of-flight Laue diffraction	D. A. Keen	<i>Transaction Symposia of ACA Annual Meeting, Albuquerque, NM U.S.A.</i> 29 , 43-54	1993
17	Structural changes in silver bromide at the melting point	V. M. Nield, D. A. Keen, R. L. McGreevy and W. Hayes	<i>J Phys: Condensed Matter</i> 4 , 6703-6714	1992
16	Neutron scattering studies of disorder and melting in Ag and Cu halides	D. A. Keen, V. M. Nield, R. L. McGreevy and W. Hayes	<i>Physica B</i> 180-181 , 798-800	1992
15	Determining the structures of disordered materials by diffuse neutron scattering and reverse Monte Carlo modelling	R. L. McGreevy, M. A. Howe, V. M. Nield, J. D. Wicks and D. A. Keen	<i>Physica B</i> 180-181 , 801-804	1992
14	Neutron diffraction study of the low-temperature domain structure in LiKSO ₄	B. N. Savenko, B. Mroz, D. Sangaa, D. A. Keen and C. C. Wilson	<i>Physica B</i> 180-181 , 309-311	1992
13	The observation of phonons in barium fluoride by pulsed neutron diffraction	C. J. Carlile, D A Keen, C. C. Wilson and B. T. M. Willis	<i>Acta Crystallographica A</i> 48 , 826-829	1992
12	On hydrogen atom positions in 3-Deazauracil	C. C. Wilson, D. A. Keen and N. S. Stewart	<i>J Chem. Soc. Chem. Comm.</i> 1992 , 1160-1162	1992
11	Determination of disordered magnetic structures by RMC modelling of neutron diffraction data	D. A. Keen and R. L. McGreevy	<i>J Phys: Condensed Matter</i> 3 , 7383-7394	1991
10	Powder neutron diffraction study of the high pressure phases of silver iodide	S. Hull, D. A. Keen, R. Done and C. N. Uden	<i>Rutherford Appleton Laboratory Report</i> RAL-91-089	1991
9	Single crystal diffraction at ISIS	C. C. Wilson and D. A. Keen	<i>ICANS-XI, Japan ed. N. Watanabe, KEK Report 90-25</i> , 849-860	1991
8	Diffuse scattering studies on SxD	C. C. Wilson, S. Hull and D. A. Keen	<i>ICANS-XI, Japan ed. N. Watanabe, KEK Report 90-25</i> , 1099-1105	1991
7	Structural modelling of glasses using reverse Monte Carlo simulation	D. A. Keen and R. L. McGreevy	<i>Nature</i> 344 , 423-425	1990
6	Structural disorder in AgBr: Reverse Monte Carlo analysis of powder neutron diffraction	D. A. Keen, R. L. McGreevy, W. Hayes and K. N. Clausen	<i>Phil. Mag. Lett.</i> 61 , 349-357	1990
5	Structural disorder in AgBr on the approach to melting	D. A. Keen, W. Hayes and R. L. McGreevy	<i>J Phys: Condensed Matter</i> 2 , 2773-2786	1990
4	Reverse Monte Carlo (RMC) simulation: modelling structural disorder in crystals, glasses and liquids from diffraction data	R. L. McGreevy, M. A. Howe, D. A. Keen and K. N. Clausen	<i>IOP Conference Series</i> 107 , 165-184	1990
3	The neutron diamagnetic form factor of graphite	C. Wilkinson, D. A. Keen, P. J. Brown and J. B.	<i>J Phys: Condensed Matter</i> 1 , 3833-3839	1989

- | | | | |
|---|---|--|---|
| 2 | Neutron scattering and electrical transport in $\text{Nd}_{0.5}\text{Pb}_{0.5}\text{MnO}_3$ | Forsyth
K. N. Clausen, W. Hayes, D. A. Keen, R. M. Kusters, R. L. McGreevy and J. Singleton | <i>J Phys: Condensed Matter</i> 1 , 2721-2726 1989 |
| 1 | Magnetoresistance measurements on the magnetic semiconductor $\text{Nd}_{0.5}\text{Pb}_{0.5}\text{MnO}_3$ | R. M. Kusters, J. Singleton, D. A. Keen, R. L. McGreevy and W. Hayes | <i>Physica B</i> 155 , 362-365 1989 |