Martin Dove

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6238230/publications.pdf

Version: 2024-02-01

302 papers	13,640 citations	22153 59 h-index	32842 100 g-index
307 all docs	307 docs citations	307 times ranked	10495 citing authors

#	Article	IF	Citations
1	Orientational order and phase transitions in deuterated methane: a neutron total scattering and reverse Monte Carlo study. Journal of Physics Condensed Matter, 2022, 34, 015401.	1.8	4
2	Neutron powder diffraction study of the phase transitions in deuterated methylammonium lead iodide. Journal of Physics Condensed Matter, 2022, 34, 145401.	1.8	2
3	Origin of Ferroelectricity in Two Prototypical Hybrid Organicâ€“Inorganic Perovskites. Journal of the American Chemical Society, 2022, 144, 816-823.	13.7	47
4	Neutron powder-diffraction study of phase transitions in strontium-doped bismuth ferrite: 1. Variation with chemical composition. Journal of Physics Condensed Matter, 2022, 34, 255401.	1.8	1
5	Orientational disorder in sulfur hexafluoride: a neutron total scattering and reverse Monte Carlo study. Journal of Physics Condensed Matter, 2022, 34, 295401.	1.8	2
6	Atomic structure of the continuous random network of amorphous C[(C6H4)2]2 PAF-1. Cell Reports Physical Science, 2022, , 100899.	5.6	0
7	High-pressure neutron diffraction study of magnetite, Fe3O4, nanoparticles. Applied Physics Letters, 2022, 120, .	3.3	1
8	Methane hydrate clathrates: effects in the simulation of melting arising from the assumption of simple combining rules in interatomic potentials. Molecular Simulation, 2021, 47, 161-169.	2.0	0
9	DFT study for the absorption spectra evolution of CdS magic-size clusters. Chemical Physics Letters, 2021, 779, 138870.	2.6	6
10	The ferroelastic phase transition in hydrogen cyanide studied by density functional theory. Journal of Physics Condensed Matter, 2021, , .	1.8	1
11	Phonons and low thermal expansion in sodalite zinc borate <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Zn</mml:mi><mml:mn>4</mml:mn></mml:mr mathvariant="normal">B</mml:mi><mml:mn>6</mml:mn></mml:msub><mml:msub><mml:mi		

#	Article	IF	Citations
19	Colossal Pressure-Induced Softening in Scandium Fluoride. Physical Review Letters, 2020, 124, 255502.	7.8	19
20	Neutron scattering study of the orientational disorder in potassium cyanide. Journal of Physics Communications, 2020, 4, 023001.	1.2	8
21	Negative thermal expansion of cubic silicon dicarbodiimide, Si(NCN)₂, studied by ab initio lattice dynamics. Journal of Physics Condensed Matter, 2020, 32, 465402.	1.8	5
22	Structural phase transitions in malononitrile, CH2(CN)2: crystal structure of the Î´ phase by neutron powder diffraction, and ab initio calculations of the structures and phonons of the Î± and Î´ phases. Journal of Physics Condensed Matter, 2019, 31, 255401.	1.8	0
23	Structural study of bismuth ferrite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub><m neutron total scattering and the reverse Monte Carlo method. Physical Review B, 2019, 100, .	3.2	5
24	The nature of collective excitations and their crossover at extreme supercritical conditions. Scientific Reports, 2019, 9, 755.	3.3	6
25	Hydrogen-bond-mediated structural variation of metal guanidinium formate hybrid perovskites under pressure. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180227.	3.4	15
26	Thermal Disorder and Bond Anharmonicity in Cesium Lead Iodide Studied by Neutron Total Scattering and the Reverse Monte Carlo Method. Journal of Physical Chemistry C, 2019, 123, 14934-14940.	3.1	21
27	Flexibility of network materials and the Rigid Unit Mode model: a personal perspective. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180222.	3.4	25
28	Adsorption and migration of alkali metals (Li, Na, and K) on pristine and defective graphene surfaces. Nanoscale, 2019, 11, 5274-5284.	5.6	149
29	Thermodynamic heterogeneity and crossover in the supercritical state of matter. Journal of Physics Condensed Matter, 2019, 31, 225401.	1.8	3
30	X-ray total scattering study of magic-size clusters and quantum dots of cadmium sulphide. Nanoscale, 2019, 11, 21900-21908.	5.6	17
31	Structures of CdSe and CdS Nanoclusters from Ab Initio Random Structure Searching. Journal of Physical Chemistry C, 2019, 123, 29370-29378.	3.1	22
32	Low-temperature anharmonicity and symmetry breaking in the sodalite |Na8I2|[AlSiO4]6. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 219-228.	0.8	2
33	Magnetic structure of paramagnetic MnO. Physical Review B, 2018, 97, .	3.2	16
34	Emergence of microstructure and oxygen diffusion in yttrium-stabilized cubic zirconia. Physical Review B, 2018, 97, .	3.2	5
35	Yang etÂal. Reply:. Physical Review Letters, 2018, 120, 219602.	7.8	18
36	Thermally-induced reversible structural isomerization in colloidal semiconductor CdS magic-size clusters. Nature Communications, 2018, 9, 2499.	12.8	79

#	Article	IF	Citations
37	Orientational Disorder in Adamantane and Adamantanecarboxylic Acid. ChemPhysChem, 2017, 18, 459-464.	2.1	18
38	Direct links between dynamical, thermodynamic, and structural properties of liquids: Modeling results. Physical Review E, 2017, 95, 032116.	2.1	24
39	A review of drug therapy for sporadic fatal insomnia. Prion, 2017, 11, 293-299.	1.8	8
40	Emergence and Evolution of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>k</mml:mi></mml:math> Gap in Spectra of Liquid and Supercritical States. Physical Review Letters, 2017, 118, 215502.	7.8	85
41	Molecular dynamics study of CO₂ absorption and desorption in zinc imidazolate frameworks. Molecular Systems Design and Engineering, 2017, 2, 457-469.	3.4	8
42	Local structure of a switchable dielectric Prussian blue analogue. CrystEngComm, 2017, 19, 7316-7321.	2.6	17
43	Supercritical GrÃ¼neisen parameter and its universality at the Frenkel line. Physical Review E, 2017, 96, 012107.	2.1	5
44	In situ studies of materials for high temperature CO₂ capture and storage. Faraday Discussions, 2016, 192, 217-240.	3.2	12
45	Negative thermal expansion and associated anomalous physical properties: review of the lattice dynamics theoretical foundation. Reports on Progress in Physics, 2016, 79, 066503.	20.1	211
46	Local structure of the metalâ€“organic perovskite dimethylammonium manganese(<scp>ii</scp>) formate. Dalton Transactions, 2016, 45, 4380-4391.	3.3	44
47	Molecular dynamics simulation study of various zeolitic imidazolate framework structures. Dalton Transactions, 2016, 45, 4289-4302.	3.3	19
48	Electric ordering in metal-organic perovskites from total neutron scattering. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s95-s95.	0.1	0
49	Frenkel line and solubility maximum in supercritical fluids. Physical Review E, 2015, 91, 012112.	2.1	52
50	Simulation study of negative thermal expansion in yttrium tungstate Y₂W₃O₁₂. Journal of Physics Condensed Matter, 2015, 27, 185401.	1.8	14
51	Solid-state diffusion in amorphous zirconolite. Journal of Applied Physics, 2014, 116, 184901.	2.5	3
52	Agâ€“Ag dispersive interaction and physical properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">Ag</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mi>Co</mml:mi><mml:mo>(</mml:mo><mml:mo>/</><mml:mn>6</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	3.2	26
53	High-energy radiation damage in zirconia: Modeling results. Journal of Applied Physics, 2014, 115, .	2.5	27
54	Framework flexibility and the negative thermal expansion mechanism of copper(I) oxide<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:math>. Physical Review B, 2014, 89, .	3.2	34

#	Article	IF	Citations
55	A phenomenological expression to describe the temperature dependence of pressure-induced softening in negative thermal expansion materials. Journal of Physics Condensed Matter, 2014, 26, 115402.	1.8	18
56	Electronic effects in high-energy radiation damage in iron. Journal of Physics Condensed Matter, 2014, 26, 085401.	1.8	44
57	Role of Disorder in the Thermodynamics and Atomic Dynamics of Glasses. Physical Review Letters, 2014, 112, 025502.	7.8	125
58	Computer simulations of cations orderâ€disorder in 2:1 dioctahedral phyllosilicates using cationâ€exchange potentials and monte carlo methods. International Journal of Quantum Chemistry, 2014, 114, 1257-1286.	2.0	10
59	Acoustic phonons and negative thermal expansion in MOF-5. Physical Chemistry Chemical Physics, 2014, 16, 21144-21152.	2.8	61
60	Common origin of negative thermal expansion and other exotic properties in ceramic and hybrid materials. Physical Review B, 2014, 89, .	3.2	42
61	An eâ€Science data infrastructure for simulations within Grid computing environment: methods, approaches and practice. Concurrency Computation Practice and Experience, 2013, 25, 385-409.	2.2	3
62	Structural changes in zirconolite under Î±-decay. Journal of Physics Condensed Matter, 2013, 25, 055401.	1.8	4
63	The heat capacity of matter beyond the Dulongâ€“Petit value. Journal of Physics Condensed Matter, 2013, 25, 235401.	1.8	54
64	Simulation study of pressure and temperature dependence of the negative thermal expansion in Zn(CN)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 88, .	3.2	46
65	Pressure-induced softening as a common feature of framework structures with negative thermal expansion. Physical Review B, 2013, 87, .	3.2	49
66	Local structure correlations in plastic cyclohexaneâ€”a reverse Monte Carlo study. Journal of Physics Condensed Matter, 2013, 25, 454204.	1.8	10
67	The nature of high-energy radiation damage in iron. Journal of Physics Condensed Matter, 2013, 25, 125402.	1.8	74
68	RMCgui: a new interface for the workflow associated with running Reverse Monte Carlo simulations. Journal of Physics Condensed Matter, 2013, 25, 454222.	1.8	5
69	Temperature-dependent pressure-induced softening in Zn(CN)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 88, .	3.2	27
70	Flexibility of zeolitic imidazolate framework structures studied by neutron total scattering and the reverse Monte Carlo method. Journal of Physics Condensed Matter, 2013, 25, 395403.	1.8	28
71	The re-entrant phase transitions in crystalline malononitrile, CH₂(CN)₂: a neutron powder diffraction study. Journal of Physics Condensed Matter, 2011, 23, 225402.	1.8	4
72	ContrastingP- andT-induced amorphization using ZrW2O8and ZIF-4 as case studies. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C54-C55.	0.3	0

#	Article	IF	Citations
73	An examination of the structure of Fe3O4using reverse Monte Carlo refinements. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C401-C402.	0.3	0
74	Geo-visualization Fortran library. Computers and Geosciences, 2011, 37, 65-74.	4.2	8
75	Diffraction study of pressure-amorphized ZrW<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>	3.2	17
76	Implementing a Grid/Cloud eScience Infrastructure for Hydrological Sciences. Computer Communications and Networks, 2011, , 3-28.	0.8	6
77	Developing an End-to-End Scientific Workflow:. Computing in Science and Engineering, 2010, 12, 52-61.	1.2	10
78	Evaluation of domain models for Î²-cristobalite from the pair distribution function. Journal of Physics Condensed Matter, 2010, 22, 125401.	1.8	12
79	Structure Determination of Disordered Materials from Diffraction Data. Physical Review Letters, 2010, 104, 125501.	7.8	97
80	Structure and Properties of an Amorphous Metal-Organic Framework. Physical Review Letters, 2010, 104, 115503.	7.8	246
81	Nanoporous Structure and Medium-Range Order in Synthetic Amorphous Calcium Carbonate. Chemistry of Materials, 2010, 22, 3197-3205.	6.7	160
82	A Service-Oriented Framework for Running Quantum Mechanical Simulations of Material Properties in a Grid Environment. IEEE Transactions on Systems, Man and Cybernetics, Part C: Applications and Reviews, 2010, 40, 485-490.	2.9	4
83	The hydrogen-bonding transition and isotope-dependent negative thermal expansion in H₃Co(CN)₆. Journal of Physics Condensed Matter, 2010, 22, 404202.	1.8	15
84	Aperiodicity, structure, and dynamics inNi(CN)2. Physical Review B, 2009, 80, .	3.2	30
85	Lessons in scientific data interoperability: XML and the e Minerals project. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 1041-1046.	3.4	9
86	Zinc incorporation into hydroxylapatite. Biomaterials, 2009, 30, 2864-2872.	11.4	215
87	Geospatial Visualization Tool Kit for Scientists Using Fortran. Eos, 2009, 90, 249-250.	0.1	3
88	eScience for molecular-scale simulations and the e Minerals project. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 967-985.	3.4	8
89	New tools to support collaboration and virtual organizations. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 1051-1056.	3.4	12
90	Integrating computing, data and collaboration grids: the RMCS tool. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 1047-1050.	3.4	14

#	Article	IF	Citations
91	The compressibility and high pressure structure of diopside from first principles simulation. Physics and Chemistry of Minerals, 2008, 35, 359-366.	0.8	22
92	Job submission to grid computing environments. Concurrency Computation Practice and Experience, 2008, 20, 1329-1340.	2.2	10
93	Colossal Positive and Negative Thermal Expansion in the Framework Material Ag ₃ [Co(CN) ₆]. Science, 2008, 319, 794-797.	12.6	575
94	Argentophilicity-Dependent Colossal Thermal Expansion in Extended Prussian Blue Analogues. Journal of the American Chemical Society, 2008, 130, 9660-9661.	13.7	82
95	Origin of the colossal positive and negative thermal expansion in Ag3[Co(CN)6]: anab initiodensity functional theory study. Journal of Physics Condensed Matter, 2008, 20, 255226.	1.8	23
96	Local structure in Ag₃[Co(CN)₆]: colossal thermal expansion, rigid unit modes and argentophilic interactions. Journal of Physics Condensed Matter, 2008, 20, 255225.	1.8	34
97	Electrostatic versus polarization effects in the adsorption of aromatic molecules of varied polarity on an insulating hydrophobic surface. Journal of Physics Condensed Matter, 2008, 20, 035215.	1.8	16
98	First-principles calculations of structural changes in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>B</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mtext> under pressure. Physical Review B, 2008, 78, .	3.2	22
99	Neutron total scattering and reverse Monte Carlo study of cation ordering in Ca_xSr_{1â^'x}TiO₃. Journal of Physics Condensed Matter, 2007, 19, 335214.	1.8	13
100	Exotic distributions of rigid unit modes in the reciprocal spaces of framework aluminosilicates. Journal of Physics Condensed Matter, 2007, 19, 275209.	1.8	21
101	MnOspin-wave dispersion curves from neutron powder diffraction. Physical Review B, 2007, 75, .	3.2	13
102	Structural Description of Pressure-Induced Amorphization inZrW2O8. Physical Review Letters, 2007, 98, 225501.	7.8	65
103	Ferroelectric nanoscale domains and the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>905</mml:mn><mml:mspace width="0.3em" /><mml:mi mathvariant="normal">K</mml:mi></mml:mrow></mml:math>phase transition in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Sr</mml:mi><mml:mi mathvariant="normal">Sr</mml:mi><mml:msub><mml:mi	3.2	44
104	Local structure in ZrW₂O₈from neutron total scattering. Journal of Physics Condensed Matter, 2007, 19, 335215.	1.8	26
105	Ekhard Salje. Journal of Physics Condensed Matter, 2007, 19, 270301.	1.8	0
106	RMCProfile: reverse Monte Carlo for polycrystalline materials. Journal of Physics Condensed Matter, 2007, 19, 335218.	1.8	351
107	The origin of the compressibility anomaly in amorphous silica: a molecular dynamics study. Journal of Physics Condensed Matter, 2007, 19, 275210.	1.8	22
108	Logarithmic relaxation in radiation-amorphized zircon. Physical Review B, 2007, 76, .	3.2	7

#	Article	IF	Citations
109	Pressure-Induced Structural Transformation in Radiation-Amorphized Zircon. Physical Review Letters, 2007, 98, 135502.	7.8	19
110	Pair distribution functions calculated from interatomic potential models using theGeneral Utility Lattice Program. Journal of Applied Crystallography, 2007, 40, 589-594.	4.5	24
111	Use of massively parallel molecular dynamics simulations for radiation damage in pyrochlores. Journal of Materials Science, 2007, 42, 1920-1930.	3.7	15
112	Molecular dynamics in a grid computing environment: experiences using DL_POLY_3 within theeMinerals escience project. Molecular Simulation, 2006, 32, 945-952.	2.0	9
113	Atomistic simulations of resistance to amorphization by radiation damage. Physical Review B, 2006, 73, .	3.2	68
114	Simulation of radiation damage in gadolinium pyrochlores. Journal of Physics Condensed Matter, 2006, 18, 2217-2234.	1.8	19
115	Synchrotron Radiation, Neutron, and Mass Spectrometry Techniques at User Facilities. Elements, 2006, 2, 15-21.	0.5	11
116	DL_POLY_3: new dimensions in molecular dynamics simulations via massive parallelism. Journal of Materials Chemistry, 2006, 16, 1911.	6.7	1,010
117	Cation substitution and strain screening in framework structures: The role of rigid unit modes. Chemical Geology, 2006, 225, 213-221.	3.3	10
118	Dynamics from diffraction. Physica B: Condensed Matter, 2006, 385-386, 285-287.	2.7	3
119	DFT study of the cation arrangements in the octahedral and tetrahedral sheets of dioctahedral 2:1 phyllosilicates. Physics and Chemistry of Minerals, 2006, 33, 655-666.	0.8	45
120	Magnetic Structure of MnO at 10ÂK from Total Neutron Scattering Data. Physical Review Letters, 2006, 96, 047209.	7.8	74
121	Neutron powder diffraction study of the orientational orderâ€“disorder phase transition in calcite, CaCO3. Physics and Chemistry of Minerals, 2005, 32, 493-503.	0.8	29
122	Computational investigation of Al/Si and Al/Mg ordering in aluminous tremolite amphiboles. Mineralogical Magazine, 2005, 69, 1-20.	1.4	11
123	Total scattering and reverse Monte Carlo study of the 105 K displacive phase transition in strontium titanate. Journal of Physics Condensed Matter, 2005, 17, S111-S124.	1.8	38
124	Model-independent extraction of dynamical information from powder diffraction data. Physical Review B, 2005, 72, .	3.2	32
125	Temperature measurement in a Paris-Edinburgh cell by neutron resonance spectroscopy. Journal of Applied Physics, 2005, 98, 064905.	2.5	27
126	Grid computing and molecular simulations: the vision of theeMinerals project. Molecular Simulation, 2005, 31, 297-301.	2.0	12

#	Article	IF	Citations
127	A computational study of the effect of Liâ€“K solid solutions on the structures and stabilities of layered silicate materialsâ€”an application of the use of Condor pools in molecular simulation. Molecular Simulation, 2005, 31, 339-347.	2.0	6
128	Calculation of the effect of intrinsic point defects and volume swelling in the nuclear magnetic resonance spectra of ZrSiO4. Molecular Simulation, 2005, 31, 349-354.	2.0	10
129	Workflow issues in atomistic simulations. Molecular Simulation, 2005, 31, 323-328.	2.0	1
130	Reverse Monte Carlo modelling of crystalline disorder. Journal of Physics Condensed Matter, 2005, 17, S15-S22.	1.8	52
131	Negative Thermal Expansion inZrW2O8: Mechanisms, Rigid Unit Modes, and Neutron Total Scattering. Physical Review Letters, 2005, 95, 255501.	7.8	164
132	TheeMinerals collaboratory: tools and experience. Molecular Simulation, 2005, 31, 329-337.	2.0	4
133	Collaborative grid infrastructure for molecular simulations: TheeMinerals minigrid as a prototype integrated compute and data grid. Molecular Simulation, 2005, 31, 303-313.	2.0	14
134	Refinement of the Siâ€“Oâ€“Si bond angle distribution in vitreous silica. Journal of Physics Condensed Matter, 2005, 17, S67-S75.	1.8	56
135	How the nature of the chemical bond governs resistance to amorphization by radiation damage. Physical Review B, 2005, 71, .	3.2	104
136	Radiation damage in the bulk and at the surface. Molecular Simulation, 2005, 31, 355-359.	2.0	10
137	Dynamics from diffraction. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c434-c435.	0.3	0
138	Effect of the Tetrahedral Charge on the Order-disorder of the Cation Distribution in the Octahedral Sheet of Smectites and Illites by Computational Methods. Clays and Clay Minerals, 2004, 52, 357-374.	1.3	12
139	Calculating Activation Energies in Diffusion Processes Using a Monte Carlo Approach in a Grid Environment. Lecture Notes in Computer Science, 2004, , 483-490.	1.3	3
140	Phonons from Powder Diffraction: A Quantitative Model-Independent Evaluation. Physical Review Letters, 2004, 93, 075502.	7.8	28
141	Radiation damage effects in the perovskiteCaTiO3and resistance of materials to amorphization. Physical Review B, 2004, 70, .	3.2	35
142	Study of cation order-disorder in MgAl₂O₄spinel by in situ neutron diffraction up to 1600 K and 3.2 GPa. American Mineralogist, 2004, 89, 981-986.	1.9	56
143	Simulations of minerals using density-functional theory based on atomic orbitals for linear scaling. Physics and Chemistry of Minerals, 2004, 31, 12-21.	0.8	15
144	Reverse Monte Carlo with geometric analysis â€“ RMC+GA. Journal of Applied Crystallography, 2004, 37, 536-544.	4.5	40

#	Article	IF	Citations
145	Radiation damage effects and percolation theory. Journal of Physics Condensed Matter, 2004, 16, S2623-S2627.	1.8	39
146	Local events and stretched-exponential relaxation in glasses. Physical Review B, 2004, 70, .	3.2	12
147	Network Rigidity and Properties ofSiO2andGeO2Glasses under Pressure. Physical Review Letters, 2004, 93, 135502.	7.8	82
148	A computational investigation of the Al/Fe/Mg order-disorder behavior in the dioctahedral sheet of phyllosilicates. American Mineralogist, 2004, 89, 164-175.	1.9	30
149	Investigation of Al/Si ordering in tetrahedral phyllosilicate sheets by Monte Carlo simulation. American Mineralogist, 2004, 89, 176-184.	1.9	7
150	Discreteâ€“element modelling: methods and applications in the environmental sciences. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2004, 362, 1797-1816.	3.4	42
151	Advanced analysis of neutron total scattering data: modelling disorder in network structures. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, s104-s104.	0.3	0
152	An interatomic potential model for carbonates allowing for polarization effects. Physics and Chemistry of Minerals, 2003, 30, 416-424.	0.8	58
153	Infrared and Raman spectroscopy studies of the ??? phase transition in cristobalite. Physics and Chemistry of Minerals, 2003, 30, 353-365.	0.8	54
154	Octahedral cation ordering of illite and smectite. Theoretical exchange potential determination and Monte Carlo simulations. Physics and Chemistry of Minerals, 2003, 30, 382-392.	0.8	33
155	Trapping of oxygen vacancies on twin walls of CaTiO3: a computer simulation study. Journal of Physics Condensed Matter, 2003, 15, 2301-2307.	1.8	118
156	Computational study of tetrahedral Alâ€“Si and octahedral Alâ€“Mg ordering in phengite. Physics and Chemistry of Minerals, 2003, 30, 293-304.	0.8	19
157	Rigidity and logarithmic relaxation in network glasses. Journal of Physics Condensed Matter, 2003, 15, L743-L748.	1.8	4
158	RECENT DEVELOPMENTS USING THE PARIS-EDINBURGH CELL FOR NEUTRON DIFFRACTION AT HIGH PRESSURE AND HIGH TEMPERATURE AND SOME APPLICATIONS. High Pressure Research, 2003, 23, 281-287.	1.2	17
159	Impact of self-irradiation damage on the aqueous durability of zircon (ZrSiO4): implications for its suitability as a nuclear waste form. Journal of Physics Condensed Matter, 2003, 15, L597-L605.	1.8	64
160	Compressibility, kinetics, and phase transition in pressurized amorphous silica. Physical Review B, 2003, 67, .	3.2	72
161	Intermediate state in pressurized silica glass: Reversibility window analogue. Physical Review B, 2003, 67, .	3.2	37
162	Monte Carlo simulations of ordering of Al, Fe, and Mg cations in the octahedral sheet of smectites and illites. American Mineralogist, 2003, 88, 1033-1045.	1.9	46

#	Article	IF	Citations
163	Reply to comment on ÂLarge swelling and percolation in irradiated zirconÂ. Journal of Physics Condensed Matter, 2003, 15, 6457-6471.	1.8	10
164	Computer simulation of Al-Mg ordering in glaucophane and a comparison with infrared spectroscopy. European Journal of Mineralogy, 2003, 15, 893-901.	1.3	14
165	Large swelling and percolation in irradiated zircon. Journal of Physics Condensed Matter, 2003, 15, L1-L7.	1.8	45
166	Radiation-induced structural changes, percolation effects and resistance to amorphization by radiation damage. Materials Research Society Symposia Proceedings, 2003, 792, 418.	0.1	0
167	Origin of theT1+Î±dependence of the heat capacity of glasses at low temperature. Physical Review B, 2002, 65, .	3.2	8
168	Structural changes in zircon under Î±-decay irradiation. Physical Review B, 2002, 65, .	3.2	75
169	Publisherâ€™s Note: Structural changes in zircon under Î±-decay irradiation [Phys. Rev. B65, 180102 (2002)]. Physical Review B, 2002, 65, .	3.2	4
170	An introduction to the use of neutron scattering methods in mineral sciences. European Journal of Mineralogy, 2002, 14, 203-224.	1.3	32
171	Computer simulation study of low-energy excitations of silicate glasses. Journal of Physics Condensed Matter, 2002, 14, 4857-4879.	1.8	7
172	Finding best-fit polyhedral rotations with geometric algebra. Journal of Physics Condensed Matter, 2002, 14, 4567-4584.	1.8	45
173	Neutron total scattering method: simultaneous determination of long-range and short-range order in disordered materials. European Journal of Mineralogy, 2002, 14, 331-348.	1.3	109
174	Floppy modes in silica glass under pressure. Journal of Physics Condensed Matter, 2002, 14, 1143-1152.	1.8	28
175	Real-space rigid-unit-mode analysis of dynamic disorder in quartz, cristobalite and amorphous silica. Journal of Physics Condensed Matter, 2002, 14, 4645-4657.	1.8	43
176	Densification of silica glass under pressure. Journal of Physics Condensed Matter, 2002, 14, 7449-7459.	1.8	48
177	Structural disorder and loss of piezoelectric properties in Î±-quartz at high temperature. Applied Physics Letters, 2002, 81, 2968-2970.	3.3	54
178	Short-Range Disorder and Long-Range Order: Implications of the â€œRigid Unit Modeâ€•Picture. , 2002, , 253-271.		0
179	Floppy Modes in Crystalline and Amorphous Silicates. , 2002, , 217-238.		0
180	Total Scattering and Reverse Monte Carlo Modelling of Disordered Crystalline Materials. Fundamental Materials Research, 2002, , 85-103.	0.1	5

#	Article	IF	Citations
181	Recent developments using the Paris-Edinburgh cell for neutron diffraction at high pressure and high temperature. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, c255-c255.	0.3	0
182	Neutron diffraction at simultaneous high temperatures and pressures, with measurement of temperature by neutron radiography. Mineralogical Magazine, 2001, 65, 737-748.	1.4	60
183	Dynamic structural disorder in cristobalite: neutron total scattering measurement and reverse Monte Carlo modelling. Journal of Physics Condensed Matter, 2001, 13, 403-423.	1.8	71
184	A new high P-T cell for neutron diffraction up to 7 GPa and 2000 K with measurement of temperature by neutron radiography. High Pressure Research, 2001, 21, 263-280.	1.2	15
185	Modeling of dioctahedral 2:1 phyllosilicates by means of transferable empirical potentials. Physics and Chemistry of Minerals, 2001, 28, 130-141.	0.8	78
186	Scaling of thermodynamic mixing properties in garnet solid solutions. Physics and Chemistry of Minerals, 2001, 28, 177-187.	0.8	41
187	Theoretical modelling of cis â€Š-vacant and trans â€Š-vacant configurations in the octahedral sheet of illites and smectites. Physics and Chemistry of Minerals, 2001, 28, 322-331.	0.8	39
188	Computational study of tetrahedral Al-Si ordering in muscovite. Physics and Chemistry of Minerals, 2001, 28, 534-544.	0.8	55
189	Application of the reverse Monte Carlo method to crystalline materials. Journal of Applied Crystallography, 2001, 34, 630-638.	4.5	94
190	MCGRtof: Monte CarloG(r) with resolution corrections for time-of-flight neutron diffractometers. Journal of Applied Crystallography, 2001, 34, 780-782.	4.5	19
191	Atomistic modelling of radiation damage in zircon. Journal of Physics Condensed Matter, 2001, 13, 1947-1959.	1.8	54
192	Anisotropic ionic transport in quartz: the effect of twin boundaries. Journal of Physics Condensed Matter, 2001, 13, 9445-9454.	1.8	32
193	Computational methods for the study of energies of cation distributions: applications to cation-ordering phase transitions and solid solutions. Mineralogical Magazine, 2001, 65, 193-219.	1.4	84
194	A detailed structural characterization of quartz on heating through the Î±â€“Î² phase transition. Mineralogical Magazine, 2001, 65, 489-507.	1.4	132
195	Monte Carlo methods for the study of cation ordering in minerals. Mineralogical Magazine, 2001, 65, 221-248.	1.4	67
196	Phase transitions in tridymite studied using â€˜Rigid Unit Modeâ€™ theory, Reverse Monte Carlo methods and molecular dynamics simulations. Mineralogical Magazine, 2000, 64, 267-283.	1.4	34
197	Modelling in relation to cation ordering. Phase Transitions, 2000, 71, 205-226.	1.3	15
198	Simulation studies on the pyrope-grossular garnet solid solution. Physics and Chemistry of Minerals, 2000, 27, 398-418.	0.8	74

#	Article	IF	Citations
199	The inherent displacive flexibility of the hexacelsian tetrahedral framework and its relationship to polymorphism in Ba-hexacelsian. Physics and Chemistry of Minerals, 2000, 27, 747-756.	0.8	9
200	Rigid Unit Modes in disordered nepheline: a study of a displacive incommensurate phase transition. Physics and Chemistry of Minerals, 2000, 27, 285-290.	0.8	24
201	Disordering of MgAl2O4 spinel from first principles. Mineralogical Magazine, 2000, 64, 311-317.	1.4	44
202	Total scattering studies of silica polymorphs: similarities in glass and disordered crystalline local structure. Mineralogical Magazine, 2000, 64, 447-457.	1.4	28
203	1. Rigid Unit Modes in Framework Structures: Theory, Experiment and Applications. , 2000, , 1-34.		0
204	Surface relaxations in hydroxyapatite. Journal of Physics Condensed Matter, 2000, 12, 9829-9841.	1.8	41
205	Structure and dynamics of silicate glasses and melts. Mineralogical Magazine, 2000, 64, 373-376.	1.4	2
206	Floppy modes and the Boson peak in crystalline and amorphous silicates: an inelastic neutron scattering study. Mineralogical Magazine, 2000, 64, 435-440.	1.4	18
207	Crystal structure of the high-pressure monoclinic phase-II of cristobalite, SiO2. Mineralogical Magazine, 2000, 64, 569-576.	1.4	47
208	Amorphous silica from the Rigid Unit Mode approach. Mineralogical Magazine, 2000, 64, 377-388.	1.4	21
209	Simultaneous analysis of changes in long-range and short-range structural order at the displacive phase transition in quartz. Journal of Physics Condensed Matter, 2000, 12, L723-L730.	1.8	51
210	Modelling the percolation-type transition in radiation damage. Journal of Applied Physics, 2000, 87, 7702-7707.	2.5	30
211	Direct measurement of the thermal expansion of the Si-O bond by neutron total scattering. Journal of Physics Condensed Matter, 2000, 12, L425-L430.	1.8	51
212	Ab initiosimulations of cation ordering in oxides: application to spinel. Journal of Physics Condensed Matter, 2000, 12, L43-L48.	1.8	40
213	Rigid Unit Modes in Framework Structures: Theory, Experiment and Applications. Reviews in Mineralogy and Geochemistry, 2000, 39, 1-33.	4.8	38
214	Dynamics of silica glass: two-level tunnelling states and low-energy floppy modes. Journal of Physics Condensed Matter, 2000, 12, 8041-8064.	1.8	51
215	Effect of surface relaxations on the equilibrium growth morphology of crystals: platelet formation. Journal of Physics Condensed Matter, 1999, 11, 7385-7410.	1.8	27
216	Fluctuations and some strain related interaction mechanisms in structural phase transitions. Phase Transitions, 1999, 67, 539-569.	1.3	1

#	Article	IF	Citations
217	Geometrical Origin and Theory of Negative Thermal Expansion in Framework Structures. Journal of the American Ceramic Society, 1999, 82, 1793-1802.	3.8	130
218	Anatomy of a structural phase transition: theoretical analysis of the displacive phase transition in quartz and other silicates. Physics and Chemistry of Minerals, 1999, 26, 344-353.	0.8	38
219	Rigid unit modes and dynamic disorder: SiO 2 cristobalite and quartz. Physics and Chemistry of Minerals, 1999, 26, 484-495.	0.8	32
220	Local structures of amorphous and crystalline phases of silica, SiO2, by neutron total scattering. Journal of Physics Condensed Matter, 1999, 11, 9263-9273.	1.8	78
221	Order/Disorder Phenomena in Minerals: Ordering Phase Transitions and Solid Solutions. , 1999, , 451-475.		9
222	Introduction to the Theory of Displacive Phase Transitions. , 1999, , 427-450.		0
223	Atomic Structure of Disordered Materials. , 1999, , 371-387.		2
224	Introduction to the Theory of Lattice Dynamics. , 1999, , 281-297.		0
225	Thermodynamics of Al/Al avoidance in the ordering of Al/Si tetrahedral framework structures. Physics and Chemistry of Minerals, 1998, 25, 457-464.	0.8	72
226	Negative thermal expansion in beta-quartz. Physics and Chemistry of Minerals, 1998, 26, 63-77.	0.8	107
227	On the Sequence of Phase Transitions in Tridymite. Physics and Chemistry of Minerals, 1998, 26, 171-179.	0.8	52
228	Rigid-Unit Modes and the Quantitative Determination of the Flexibility Possessed by Zeolite Frameworks. Journal of Physical Chemistry B, 1998, 102, 1759-1767.	2.6	117
229	Inelastic neutron scattering, phonon softening, and the phase transition in sodium nitrate,. Journal of Physics Condensed Matter, 1998, 10, 6851-6861.	1.8	8
230	Low Energy Dynamics and Tunneling States in Silica Glass. Physical Review Letters, 1998, 81, 3431-3434.	7.8	54
231	Simulation studies of at high pressure. Journal of Physics Condensed Matter, 1998, 10, 8417-8428.	1.8	25
232	Anomalous dynamical effects in calcite. Journal of Physics Condensed Matter, 1998, 10, L423-L429.	1.8	12
233	Calibration of excess thermodynamic properties and elastic constant variations associated with the alpha <-->beta phase transition in quartz. American Mineralogist, 1998, 83, 2-22.	1.9	197
234	Rigid unit modes in crystal structures with octahedrally coordinated atoms. American Mineralogist, 1998, 83, 476-479.	1.9	67

#	Article	IF	Citations
235	A neutron diffraction study of the order - disorder phase transition in sodium nitrate. Journal of Physics Condensed Matter, 1997, 9, 2423-2432.	1.8	15
236	How Floppy Modes Give Rise to Adsorption Sites in Zeolites. Physical Review Letters, 1997, 78, 3701-3704.	7.8	96
237	Floppy Modes in Crystalline and Amorphous Silicates. Physical Review Letters, 1997, 78, 1070-1073.	7.8	123
238	Structural behavior, crystal chemistry, and phase transitions in substituted leucite; high-resolution neutron powder diffraction studies. American Mineralogist, 1997, 82, 16-29.	1.9	117
239	A one-parameter model of a rigid-unit structure. Phase Transitions, 1997, 61, 125-139.	1.3	7
240	Computational studies of Si/Al ordering in aluminosilicate tetrahedral framework structures. Phase Transitions, 1997, 61, 51-66.	1.3	4
241	Insights into zeolite behaviour from the rigid unit mode model. Phase Transitions, 1997, 61, 155-172.	1.3	21
242	Static lattice simulation of feldspar solid solutions: Ferroelastic instabilities and order/disorder. Phase Transitions, 1997, 61, 173-194.	1.3	4
243	Approaches to modelling the behaviour of ceramics and minerals. Phase Transitions, 1997, 61, 1-17.	1.3	9
244	Rigid unit modes and the negative thermal expansion in ZrW₂O₈. Phase Transitions, 1997, 61, 141-153.	1.3	75
245	Crystal structure and paramagnetic behaviour of. Journal of Physics Condensed Matter, 1997, 9, 6563-6577.	1.8	100
246	The use of 29Si MAS-NMR and Monte Carlo methods in the study of Al/Si ordering in silicates. Geoderma, 1997, 80, 353-368.	5.1	11
247	Theory of displacive phase transitions in minerals. American Mineralogist, 1997, 82, 213-244.	1.9	247
248	Direct measurement of the Si-O bond length and orientational disorder in the high-temperature phase of cristobalite. Physics and Chemistry of Minerals, 1997, 24, 311-317.	0.8	99
249	Silicates and Soft Modes. , 1997, , 349-383.		13
250	Lattice simulation studies of the ferroelastic phase transitions in (Na,K)AlSi₃O₈and (Sr,Ca)Al₂Si₂O₈feldspar solid solutions. American Mineralogist, 1997, 82, 8-15.	1.9	24
251	Distortions of framework structures. Phase Transitions, 1996, 58, 121-143.	1.3	37
252	A computational study of Al/Si ordering in cordierite. Physics and Chemistry of Minerals, 1996, 23, 127.	0.8	35

#	Article	IF	Citations
253	Rigid unit modes in the high-temperature phase of SiO2 tridymite: calculations and electron diffraction. Physics and Chemistry of Minerals, 1996, 23, 56.	0.8	40
254	The use of Monte Carlo methods to determine the distribution of Al and Si cations in framework aluminosilicates from²⁹Si MAS NMR data. American Mineralogist, 1996, 81, 39-44.	1.9	25
255	Rigid-unit phonon modes and structural phase transitions in framework silicates. American Mineralogist, 1996, 81, 1057-1079.	1.9	235
256	The phenomenon of low Al-Si ordering temperatures in aluminosilicate framework structures. American Mineralogist, 1996, 81, 349-362.	1.9	66
257	Origin of the negative thermal expansion in and. Journal of Physics Condensed Matter, 1996, 8, 10973-10982.	1.8	234
258	A single-crystal neutron scattering study of lattice melting in ferroelastic. Journal of Physics Condensed Matter, 1996, 8, 7073-7084.	1.8	9
259	The low-temperature behaviour of analcime. 1: high-resolution neutron powder diffraction. Mineralogical Magazine, 1996, 60, 499-507.	1.4	15
260	Fluctuations in the structure of calcite. Acta Crystallographica Section A: Foundations and Advances, 1996, 52, C439-C439.	0.3	0
261	On the thermal expansion of ?-cristobalite. Physics and Chemistry of Minerals, 1995, 22, 61.	0.8	62
262	Rigid unit modes in framework silicates. Mineralogical Magazine, 1995, 59, 629-639.	1.4	147
263	Observation of lattice melting in a single crystal: The ferroelastic phase transition inNa2CO3. Physical Review B, 1995, 51, 6758-6760.	3.2	6
264	Molecular dynamics simulation of alpha - and beta -cristobalite. Journal of Physics Condensed Matter, 1995, 7, 1771-1788.	1.8	67
265	Neutron powder diffraction study of the ferroelastic phase transition and lattice melting in sodium carbonate, Na2CO3. Journal of Physics Condensed Matter, 1995, 7, 4395-4417.	1.8	44
266	LATTICE MELTING AT STRUCTURAL PHASE TRANSITIONS. Modern Physics Letters B, 1995, 09, 67-85.	1.9	8
267	The Ginzburg interval in soft-mode phase transitions: consequences of the rigid unit mode picture. Journal of Physics Condensed Matter, 1994, 6, 3171-3196.	1.8	26
268	Crystalline potassium perrhenate: a study using molecular dynamics and lattice dynamics. Journal of Physics Condensed Matter, 1994, 6, 9895-9902.	1.8	7
269	A computer simulation study of Al/Si ordering in gehlenite and the paradox of the low transition temperature. Physics and Chemistry of Minerals, 1994, 21, 110.	0.8	34
270	The determination of rigid-unit modes as potential soft modes for displacive phase transitions in framework crystal structures. Acta Crystallographica Section A: Foundations and Advances, 1993, 49, 697-703.	0.3	226

#	Article	IF	Citations
271	Comment on â€˜â€˜First-principles studies on structural properties of Î²-cristobaliteâ€™â€™. Physical Review Letters, 1993, 71, 3610-3610.	7.8	24
272	Observation of lattice melting at the ferroelastic phase transition inNa2CO3. Physical Review Letters, 1993, 71, 2939-2942.	7.8	14
273	Low-frequency floppy modes in Î²-cristobalite. Physical Review Letters, 1993, 71, 193-196.	7.8	122
274	Anomalous inelastic neutron scattering from calcite. Journal of Physics Condensed Matter, 1992, 4, 2761-2774.	1.8	34
275	On the displacive character of the phase transition in quartz: a hard-mode spectroscopy study. Journal of Physics Condensed Matter, 1992, 4, 571-577.	1.8	62
276	Landau free energy and order parameter behaviour of theÎ±/Î²phase transition in cristobalite. Zeitschrift FÃ¼r Kristallographie, 1992, 201, 125-145.	1.1	116
277	Landau theory revisited. Ferroelectrics, 1992, 128, 255-264.	0.6	13
278	On the application of mean-field and landau theory to displacive phase transitions. Ferroelectrics, 1992, 136, 33-49.	0.6	54
279	Thermodynamic properties of MgSiO3 perovskite derived from large scale molecular dynamics simulations. Physics and Chemistry of Minerals, 1992, 18, 407.	0.8	40
280	Neutron powder diffraction study of the ï¿½kermanite-gehlenite solid solution series. Physics and Chemistry of Minerals, 1992, 19, 185.	0.8	99
281	Phonon stabilized polytypism in PbI2: in situ Raman spectroscopy and transferable core-shell model calculations. Journal of Physics Condensed Matter, 1991, 3, 539-550.	1.8	22
282	Bifurcation behaviour in structural phase transitions with multi-well potentials. Journal of Physics Condensed Matter, 1990, 2, 3737-3745.	1.8	13
283	Spontaneous strain energies associated with orientational order-disorder phase transitions. Molecular Physics, 1990, 70, 425-431.	1.7	3
284	The non-analytic nature of landau free energies. Ferroelectrics, 1990, 104, 331-335.	0.6	6
285	Inelastic neutron scattering determination of phonon dispersion curves in the molecular crystal symâ€C6F3Cl3. Journal of Chemical Physics, 1989, 90, 1918-1923.	3.0	11
286	What do Landau free energies really look like for structural phase transitions?. Journal of Physics Condensed Matter, 1989, 1, 8327-8335.	1.8	39
287	The elastic constants of the disordered phase of SF6: A computer simulation calculation. Chemical Physics Letters, 1988, 150, 303-306.	2.6	6
288	Molecular Dynamics Simulations in the Solid State Sciences. , 1988, , 501-590.		6

#	Article	IF	Citations
289	Orientational ordering and the low temperature structure of SF6. Molecular Physics, 1987, 62, 1127-1141.	1.7	41
290	A model of the paraelectric phase of thiourea. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1986, 54, 443-463.	0.6	15
291	Dynamics of orientationally disordered crystals. Journal of Molecular Graphics, 1986, 4, 79-81.	1.1	8
292	A simulation study of the disordered phase of CBr4. II. Collective properties and rotation-translation coupling. Journal of Physics C: Solid State Physics, 1986, 19, 3343-3363.	1.5	16
293	A simulation study of the disordered phase of CBr4. I. Single-particle properties. Journal of Physics C: Solid State Physics, 1986, 19, 3325-3341.	1.5	27
294	SHAMGAR's OXGOAD: A new approach to the problem of resolution corrections for triple-axis neutron inelastic scattering data using parallel processors. Journal of Applied Crystallography, 1985, 18, 493-498.	4.5	6
295	A Raman scattering study of the pressure induced phase transition in sâ€triazine. Journal of Chemical Physics, 1985, 82, 2026-2032.	3.0	11
296	A molecular dynamics simulation study of the orientationally disordered phase of sulphur hexafluoride. Journal of Physics C: Solid State Physics, 1984, 17, 6581-6599.	1.5	47
297	A Neutron Scattering Study of Phonons in Perâ€Deuterated Sâ€Triazine. Physica Status Solidi (B): Basic Research, 1983, 120, 173-181.	1.5	7
298	The re-entrant phase transitions in malononitrile: specific heat capacity measurements. Journal of Physics C: Solid State Physics, 1983, 16, L195-L198.	1.5	12
299	A new theoretical model for the re-entrant phase transitions in malononitrile. Journal of Physics C: Solid State Physics, 1983, 16, 3233-3244.	1.5	16
300	A molecular dynamics simulation study of the plastic crystalline phase of sulphur hexafluoride. Journal of Physics C: Solid State Physics, 1983, 16, 5969-5983.	1.5	60
301	Raman scattering study of the phase transition in s-triazine. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1983, 47, 641-654.	0.6	10
302	Structural phase transitions in malononitrile. Faraday Discussions of the Chemical Society, 1980, 69, 98.	2.2	21