Jacqueline M Cole

List of Publications by Year
in descending order

149 papers	5,779 citations	108046 37 h-index	100535 70 g-index
151 all docs	151 docs citations	151 times ranked	7185 citing authors

#	Article	IF	Citations
1	Characterizing Interfacial Structures of Dye-Sensitized Solar Cell Working Electrodes. Langmuir, 2022, 38, 871-890.	1.6	3
2	Single Model for Organic and Inorganic Chemical Named Entity Recognition in ChemDataExtractor. Journal of Chemical Information and Modeling, 2022, 62, 1207-1213.	2.5	15
3	PDFDataExtractor: A Tool for Reading Scientific Text and Interpreting Metadata from the Typeset Literature in the Portable Document Format. Journal of Chemical Information and Modeling, 2022, 62, 1633-1643.	2.5	11
4	Clustering a database of optically absorbing organic molecules via a hierarchical fingerprint scheme that categorizes similar functional molecular fragments. Journal of Chemical Physics, 2022, 156, 154110.	1.2	3
5	Structural Capture of Î·¹-OSO to Î·²-(OS)O Coordination Isomerism in a New Ruthenium-Based SO₂-Linkage Photoisomer That Exhibits Single-Crystal Optical Actuation. Journal of Physical Chemistry C, 2022, 126, 6047-6059.	1.5	0
6	A database of refractive indices and dielectric constants auto-generated using ChemDataExtractor. Scientific Data, 2022, 9, 192.	2.4	15
7	Auto-generated database of semiconductor band gaps using ChemDataExtractor. Scientific Data, 2022, 9, 193.	2.4	21
8	BatteryBERT: A Pretrained Language Model for Battery Database Enhancement. Journal of Chemical Information and Modeling, 2022, 62, 6365-6377.	2.5	24
9	Reconstructing Chromatic-Dispersion Relations and Predicting Refractive Indices Using Text Mining and Machine Learning. Journal of Chemical Information and Modeling, 2022, 62, 2670-2684.	2.5	7
10	Calculating small-angle scattering intensity functions from electron-microscopy images. RSC Advances, 2022, 12, 16656-16662.	1.7	0
11	Perovskite- and Dye-Sensitized Solar-Cell Device Databases Auto-generated Using ChemDataExtractor. Scientific Data, 2022, 9, .	2.4	24
12	Auto-generating databases of Yield Strength and Grain Size using ChemDataExtractor. Scientific Data, 2022, 9, .	2.4	13
13	Electrolyte/Dye/TiO₂ Interfacial Structures of Dye-Sensitized Solar Cells Revealed by <i>In Situ</i> Neutron Reflectometry with Contrast Matching. Langmuir, 2021, 37, 1970-1982.	1.6	6
14	Data-driven materials discovery for solar photovoltaics. , 2021, , 129-164.		0
15	Low-energy optical switching of SO₂ linkage isomerisation in single crystals of a ruthenium-based coordination complex. RSC Advances, 2021, 11, 13183-13192.	1.7	6
16	How the Shape of Chemical Data Can Enable Data-Driven Materials Discovery. Trends in Chemistry, 2021, 3, 111-119.	4.4	9
17	Bayesian Particle Instance Segmentation for Electron Microscopy Image Quantification. Journal of Chemical Information and Modeling, 2021, 61, 1136-1149.	2.5	16
18	Nanooptomechanical Transduction in a Single Crystal with 100% Photoconversion. Journal of Physical Chemistry C, 2021, 125, 8907-8915.	1.5	9

#	ARTICLE	IF	CITATIONS
19	Assigning Optical Absorption Transitions with Light-Induced Crystal Structures: Case Study of a Single-Crystal Nanooptomechanical Transducer. Journal of Physical Chemistry C, 2021, 125, 15711-15723.	1.5	4
20	Inverse Design of Materials That Exhibit the Magnetocaloric Effect by Text-Mining of the Scientific Literature and Generative Deep Learning. Chemistry of Materials, 2021, 33, 7217-7231.	3.2	21
21	ChemDataExtractor 2.0: Autopopulated Ontologies for Materials Science. Journal of Chemical Information and Modeling, 2021, 61, 4280-4289.	2.5	43
22	Single-Crystal Optical Actuation Generated by 100% SO2 Linkage Photoisomerization in a Ruthenium-Based Coordination Complex. Journal of Physical Chemistry C, 2021, 125, 20059-20066.	1.5	2
23	ReactionDataExtractor: A Tool for Automated Extraction of Information from Chemical Reaction Schemes. Journal of Chemical Information and Modeling, 2021, 61, 4962-4974.	2.5	9
24	Rapid build up of nanooptomechanical transduction in single crystals of a ruthenium-based SO₂ linkage photoisomer. Chemical Communications, 2021, 57, 1320-1323.	2.2	8
25	Modeling dark- and light-induced crystal structures and single-crystal optical absorption spectra of ruthenium-based complexes that undergo SO2-linkage photoisomerization. Journal of Chemical Physics, 2021, 155, 234111.	1.2	0
26	ImageDataExtractor: A Tool To Extract and Quantify Data from Microscopy Images. Journal of Chemical Information and Modeling, 2020, 60, 2492-2509.	2.5	29
27	Dye Nanoaggregate Structures in MK-2, N3, and N749 DyeÂ·Â·Â·TiO₂Interfaces That Represent Dye-Sensitized Solar Cell Working Electrodes. ACS Applied Energy Materials, 2020, 3, 900-914.	2.5	13
28	Dye Aggregation, Photostructural Reorganization and Multiple Concurrent DyeÂ·Â·Â·TiO₂ Binding Modes in Dye-Sensitized Solar Cell Working Electrodes Containing Benzothiadiazole-Based Dye RK-1. ACS Applied Energy Materials, 2020, 3, 423-430.	2.5	17
29	Enumerating Intramolecular Charge Transfer in Conjugated Organic Compounds. Journal of Chemical Information and Modeling, 2020, 60, 6095-6108.	2.5	5
30	A database of battery materials auto-generated using ChemDataExtractor. Scientific Data, 2020, 7, 260.	2.4	76
31	3-D Inorganic Crystal Structure Generation and Property Prediction via Representation Learning. Journal of Chemical Information and Modeling, 2020, 60, 4518-4535.	2.5	50
32	Data-driven materials research enabled by natural language processing and information extraction. Applied Physics Reviews, 2020, 7, .	5.5	117
33	Systems Approach of Photoisomerization Metrology for Single-Crystal Optical Actuators: A Case Study of [Ru(SO₂)(NH₃)₄Cl]Cl. Journal of Physical Chemistry C, 2020, 124, 28230-28243.	1.5	7
34	Local Atomic Structure in Photoisomerized Ruthenium Sulfur Dioxide Complexes Revealed by Pair Distribution Function Analysis. Journal of Physical Chemistry C, 2020, 124, 10094-10104.	1.5	10
35	Dye-Anchoring Modes at the DyeÂ·Â·Â·TiO₂ Interface of N3- and N749-Sensitized Solar Cells Revealed by Glancing-Angle Pair Distribution Function Analysis. Journal of Physical Chemistry C, 2020, 124, 11935-11945.	1.5	20
36	Magnetic and superconducting phase diagrams and transition temperatures predicted using text mining and machine learning. Npj Computational Materials, 2020, 6, .	3.5	58

#	ARTICLE	IF	CITATIONS
37	ChemSchematicResolver: A Toolkit to Decode 2D Chemical Diagrams with Labels and R-Groups into Annotated Chemical Named Entities. Journal of Chemical Information and Modeling, 2020, 60, 2059-2072.	2.5	25
38	A Design-to-Device Pipeline for Data-Driven Materials Discovery. Accounts of Chemical Research, 2020, 53, 599-610.	7.6	59
39	Imaging Dye Aggregation in MK-2, N3, N749, and SQ-2 dyeÂ·Â·Â·TiO₂ Interfaces That Represent Dye-Sensitized Solar Cell Working Electrodes. ACS Applied Energy Materials, 2020, 3, 3230-3241.	2.5	16
40	Predicting Device Parameters for Dye-Sensitized Solar Cells from Electronic Structure Calculations to Reproduce Experiment. ACS Applied Energy Materials, 2020, 3, 4367-4376.	2.5	6
41	Multiphase structural models and hyperpolarizability calculations explain second-order nonlinear optical properties of stilbazolium ions. Physical Review Materials, 2020, 4, .	0.9	4
42	Molecular engineering of organic and organometallic second-order nonlinear optical materials. , 2019, , 139-176.		6
43	Light-Induced Macroscopic Peeling of Single Crystal Driven by Photoisomeric Nano-Optical Switching. Chemistry of Materials, 2019, 31, 4927-4935.	3.2	27
44	Cosensitization in Dye-Sensitized Solar Cells. Chemical Reviews, 2019, 119, 7279-7327.	23.0	190
45	Comparative dataset of experimental and computational attributes of UV/vis absorption spectra. Scientific Data, 2019, 6, 307.	2.4	63
46	Generic Classification Scheme for Second-Order Dipolar Nonlinear Optical Organometallic Complexes That Exhibit Second Harmonic Generation. Journal of Physical Chemistry A, 2019, 123, 702-714.	1.1	2
47	Molecular Origins of the Nonlinear Optical Responses of a Series of Î±-(X-2-Pyridylamino)-<i>o</i>-cresol Chromophores from Concerted X-ray Diffraction, Hyper-Rayleigh Scattering, and <i>Ab Initio</i> Calculations. Journal of Physical Chemistry C, 2019, 123, 665-676.	1.5	7
48	Designâ€toâ€Device Approach Affords Panchromatic Coâ€Sensitized Solar Cells. Advanced Energy Materials, 2019, 9, 1802820.	10.2	40
49	Î·²-SO₂ Linkage Photoisomer of an Osmium Coordination Complex. Inorganic Chemistry, 2018, 57, 2673-2677.	1.9	21
50	Photoexcited Phenyl Ring Twisting in Quinodimethane Dyes Enhances Photovoltaic Performance in Dye-Sensitized Solar Cells. ACS Applied Energy Materials, 2018, 1, 1127-1139.	2.5	7
51	Data-Driven Molecular Engineering of Solar-Powered Windows. Computing in Science and Engineering, 2018, 20, 84-87.	1.2	0
52	Rational Design of Dithienopicenocarbazole-Based Dyes and a Prediction of Their Energy-Conversion Efficiency Characteristics for Dye-Sensitized Solar Cells. ACS Applied Energy Materials, 2018, 1, 1435-1444.	2.5	36
53	Modulation of N3 and N719 dyeÂ·Â·Â·TiO₂ Interfacial Structures in Dye-Sensitized Solar Cells As Influenced by Dye Counter Ions, Dye Deprotonation Levels, and Sensitizing Solvent. ACS Applied Energy Materials, 2018, 1, 2821-2831.	2.5	31
54	Auto-generated materials database of Curie and NÃ©el temperatures via semi-supervised relationship extraction. Scientific Data, 2018, 5, 180111.	2.4	84

#	Article	IF	Citations
55	Host-guest prospects of neodymium and gadolinium ultraphosphate frameworks for nuclear waste storage: Multi-temperature topological analysis of nanoporous cages in RP5O14. Journal of Solid State Chemistry, 2018, 266, 250-257.	1.4	1
56	Multiple rare-earth ion environments in amorphous(Gd2O3)0.230(P2O5)0.770revealed by gadoliniumK-edge anomalous x-ray scattering. Physical Review Materials, 2018, 2, .	0.9	1
57	Removal or storage of environmental pollutants and alternative fuel sources with inorganic adsorbents via hostâ€“guest encapsulation. Journal of Materials Chemistry A, 2017, 5, 10746-10771.	5.2	35
58	Substantial Intramolecular Charge Transfer Induces Long Emission Wavelengths and Mega Stokes Shifts in 6-Aminocoumarins. Journal of Physical Chemistry C, 2017, 121, 13274-13279.	1.5	55
59	Dye aggregation in dye-sensitized solar cells. Journal of Materials Chemistry A, 2017, 5, 19541-19559.	5.2	240
60	Dyeâ‹¯TiO₂ interfacial structure of dye-sensitised solar cell working electrodes buried under a solution of I^{âˆ’}/I₃^{âˆ’} redox electrolyte. Nanoscale, 2017, 9, 11793-11805.	2.8	15
61	Discovery of SÂ·Â·Â·Câ‰¡N Intramolecular Bonding in a Thiophenylcyanoacrylate-Based Dye: Realizing Charge Transfer Pathways and DyeÂ·Â·Â·TiO₂ Anchoring Characteristics for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2017, 9, 25952-25961.	4.0	20
62	Relating the Structure of Geminal Amido Esters to their Molecular Hyperpolarizability. Journal of Physical Chemistry C, 2016, 120, 29439-29448.	1.5	6
63	Molecular engineering of cyanine dyes to design a panchromatic response in co-sensitized dye-sensitized solar cells. Molecular Systems Design and Engineering, 2016, 1, 86-98.	1.7	24
64	ChemDataExtractor: A Toolkit for Automated Extraction of Chemical Information from the Scientific Literature. Journal of Chemical Information and Modeling, 2016, 56, 1894-1904.	2.5	297
65	Molecular engineering of fluorescein dyes as complementary absorbers in dye co-sensitized solar cells. Molecular Systems Design and Engineering, 2016, 1, 402-415.	1.7	17
66	Solid-state photochemistry. CrystEngComm, 2016, 18, 7175-7179.	1.3	17
67	Rationalizing the suitability of rhodamines as chromophores in dye-sensitized solar cells: a systematic molecular design study. Molecular Systems Design and Engineering, 2016, 1, 416-435.	1.7	15
68	Topological Analysis of Void Space in Phosphate Frameworks: Assessing Storage Properties for the Environmentally Important Guest Molecules and Ions: CO2, H2O, UO2, PuO2, U, Pu, Sr2+, Cs+, CH4, and H2. ACS Sustainable Chemistry and Engineering, 2016, 4, 4094-4112.	3.2	6
69	Can nitro groups really anchor onto TiO₂? Case study of dye-to-TiO₂adsorption using azo dyes with NO₂substituents. Physical Chemistry Chemical Physics, 2016, 18, 19062-19069.	1.3	28
70	Discovery of Black Dye Crystal Structure Polymorphs: Implications for Dye Conformational Variation in Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 27646-27653.	4.0	15
71	On the accuracy of density functional theory and wave function methods for calculating vertical ionization energies. Journal of Chemical Physics, 2015, 142, 194114.	1.2	44
72	Concerted Mitigation of OÂ·Â·Â·H and C(Ï€)Â·Â·Â·H Interactions Prospects Sixfold Gain in Optical Nonlinearity of Ionic Stilbazolium Derivatives. ACS Applied Materials & Interfaces, 2015, 7, 4693-4698.	4.0	21

#	Article	IF	Citations
73	Transforming Benzophenoxazine Laser Dyes into Chromophores for Dyeâ€Sensitized Solar Cells: A Molecular Engineering Approach. Advanced Energy Materials, 2015, 5, 1401728.	10.2	11
74	Coumarin 545: an emission reference dye with a record-low temperature coefficient for ratiometric fluorescence based temperature measurements. Analyst, The, 2015, 140, 1008-1013.	1.7	14
75	Anchoring Groups for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 3427-3455.	4.0	654
76	Preferred Molecular Orientation of Coumarin 343 on TiO₂ Surfaces: Application to Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 16404-16409.	4.0	27
77	Data mining with molecular design rules identifies new class of dyes for dye-sensitised solar cells. Physical Chemistry Chemical Physics, 2014, 16, 26684-26690.	1.3	55
78	Temperature insensitive fluorescence intensity in a coumarin monomerâ€"aggregate coupled system. Chemical Communications, 2014, 50, 9329-9332.	2.2	11
79	Black silicon: fabrication methods, properties and solar energy applications. Energy and Environmental Science, 2014, 7, 3223-3263.	15.6	396
80	SO₂ Phototriggered Crystalline Nanomechanical Transduction of Aromatic Rotors in Tosylates: Rationalization via Photocrystallography of [Ru(NH₃)₄SO₂X]tosylate₂ (X = pyridine, 3-Cl-pyridine,) Tj ETQq0 0 0 rgBT /Overlock	1.5	22
81	TiO₂-Assisted Photoisomerization of Azo Dyes Using Self-Assembled Monolayers: Case Study on <i>para</i>-Methyl Red Towards Solar-Cell Applications. ACS Applied Materials & Interfaces, 2014, 6, 3742-3749.	4.0	43
82	Adsorption Properties of <i>p</i>-Methyl Red Monomeric-to-Pentameric Dye Aggregates on Anatase (101) Titania Surfaces: First-Principles Calculations of Dye/TiO₂ Photoanode Interfaces for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2014, 6, 15760-15766.	4.0	42
83	Predicting Solar-Cell Dyes for Cosensitization. Journal of Physical Chemistry C, 2014, 118, 14082-14090.	1.5	15
84	Variation in Optoelectronic Properties of Azo Dye-Sensitized TiO₂ Semiconductor Interfaces with Different Adsorption Anchors: Carboxylate, Sulfonate, Hydroxyl and Pyridyl Groups. ACS Applied Materials & Interfaces, 2014, 6, 7535-7546.	4.0	95
85	Dye Aggregation and Complex Formation Effects in 7-(Diethylamino)-coumarin-3-carboxylic Acid. Journal of Physical Chemistry C, 2014, 118, 13042-13051.	1.5	29
86	Solvent Effects on the UVâ€"vis Absorption and Emission of Optoelectronic Coumarins: a Comparison of Three Empirical Solvatochromic Models. Journal of Physical Chemistry C, 2013, 117, 14731-14741.	1.5	98
87	Molecular Design of UVâ€"vis Absorption and Emission Properties in Organic Fluorophores: Toward Larger Bathochromic Shifts, Enhanced Molar Extinction Coefficients, and Greater Stokes Shifts. Journal of Physical Chemistry C, 2013, 117, 16584-16595.	1.5	209
88	Material Profiling for Photocrystallography: Relating Single-Crystal Photophysical and Structural Properties of Luminescent Bis-Cyclometalated Iridium-Based Complexes. Crystal Growth and Design, 2013, 13, 1826-1837.	1.4	13
89	Relating Electron Donor and Carboxylic Acid Anchoring Substitution Effects in Azo Dyes to Dye-Sensitized Solar Cell Performance. ACS Sustainable Chemistry and Engineering, 2013, 1, 1440-1452.	3.2	83
90	Modeling electron density distributions from X-ray diffraction to derive optical properties: Constrained wavefunction versus multipole refinement. Journal of Chemical Physics, 2013, 139, 064108.	1.2	30

#	Article	IF	Citations
91	Molecular Origins of Dye Aggregation and Complex Formation Effects in Coumarin 343. Journal of Physical Chemistry C, 2013, 117, 14723-14730.	1.5	43
92	Molecular Origins of Optoelectronic Properties in Coumarins 343, 314T, 445, and 522B. Journal of Physical Chemistry C, 2013, 117, 14130-14141.	1.5	36
93	Tuning Solvatochromism of Azo Dyes with Intramolecular Hydrogen Bonding in Solution and on Titanium Dioxide Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 26316-26323.	1.5	35
94	Effects of rare-earth co-doping on the local structure of rare-earth phosphate glasses using high and low energy X-ray diffraction. Physical Chemistry Chemical Physics, 2013, 15, 8529.	1.3	9
95	Molecular Origins of the High-Performance Nonlinear Optical Susceptibility in a Phenolic Polyene Chromophore: Electron Density Distributions, Hydrogen Bonding, and ab Initio Calculations. Journal of Physical Chemistry C, 2013, 117, 9416-9430.	1.5	34
96	Molecular and Supramolecular Origins of Optical Nonlinearity in <i>N</i>-Methylurea. Journal of Physical Chemistry C, 2013, 117, 25669-25676.	1.5	3
97	Quantifying Crystallographically Independent Optical Switching Dynamics in Ru SO₂ Photoisomers via Lock-and-Key Crystalline Environment. Journal of Physical Chemistry Letters, 2013, 4, 3221-3226.	2.1	24
98	Photochemistry: Solarâ€Powered Nanomechanical Transduction from Crystalline Molecular Rotors (Adv. Mater. 24/2013). Advanced Materials, 2013, 25, 3388-3388.	11.1	3
99	L_{2,3}-edge x-ray absorption near-edge spectroscopy analysis of photoisomerism in solid rutheniumâ€“sulfur dioxide complexes. Journal of Physics Condensed Matter, 2013, 25, 085505.	0.7	5
100	Molecular origins of nonlinear optical activity in zinc tris(thiourea)sulfate revealed by high-resolution x-ray diffraction data and<i>ab initio</i>calculations. Physical Review B, 2013, 88, .	1.1	18
101	Solarâ€Powered Nanomechanical Transduction from Crystalline Molecular Rotors. Advanced Materials, 2013, 25, 3324-3328.	11.1	23
102	Solid-State Dilution of Dihydroxybenzophenones with 4,13-Diaza-18-crown-6 for Photocrystallographic Studies. Crystal Growth and Design, 2012, 12, 2277-2287.	1.4	10
103	Solid-state effects of monofluorophenyl substitution in dithiadiazolyl radicals: Impact on SÂ·Â·Â·S and SÂ·Â·Â·N interactions and their classification via Hirshfeld surfaces and fingerprint plots. Polyhedron, 2012, 45, 61-70.	1.0	6
104	Molecular Origins of Optoelectronic Properties in Coumarin Dyes: Toward Designer Solar Cell and Laser Applications. Journal of Physical Chemistry A, 2012, 116, 727-737.	1.1	244
105	Ruâ€“OSO Coordination Photogenerated at 100 K in Tetraammineaqua(sulfur dioxide)ruthenium(II) (Â±)-Camphorsulfonate. Inorganic Chemistry, 2012, 51, 1204-1206.	1.9	44
106	Photoconversion Bonding Mechanism in Ruthenium Sulfur Dioxide Linkage Photoisomers Revealed by in Situ Diffraction. Journal of the American Chemical Society, 2012, 134, 11860-11863.	6.6	56
107	Bayesian analysis of the evidence for minor components in crystallographic models: an alternative to the Hamilton {cal R} test. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 324-330.	0.3	3
108	Rationalizing the molecular origins of Ru- and Fe-based dyes for dye-sensitized solar cells. Acta Crystallographica Section B: Structural Science, 2012, 68, 137-149.	1.8	26

#	ARTICLE	IF	CITATIONS
109	A new form of analytical chemistry: distinguishing the molecular structure of photo-induced states from ground-states. Analyst, The, 2011, 136, 448-455.	1.7	30
110	Effects of the [OC₆F₅] moiety upon structural geometry: crystal structures of half-sandwich tantalum(V) aryloxide complexes from reaction of Cp*Ta(N<sup> <i>t</i>) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 702 Tc Section B: Structural Science, 2011, 67, 416-424.	1.8	4
111	Distinction of disorder, classical and quantum vibrational contributions to atomic mean-square amplitudes in dielectric pentachloronitrobenzene. Physical Review B, 2011, 83, .	1.1	5
112	The 4-(3-chloro-4-methylphenyl)-1,2,3,5-dithiadiazol-3-yl radical. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2514-o2514.	0.2	2
113	Discovery of High-Performance Organic Non-Linear Optical Molecules by Systematic â€˜Smart Materialâ€™ Design Strategies. Advanced Materials Research, 2010, 123-125, 959-962.	0.3	8
114	Effects of the reaction cavity on metastable optical excitation in ruthenium-sulfur dioxide complexes. Physical Review B, 2010, 82, .	1.1	41
115	Photocrystallography. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, 259-271.	0.3	63
116	Conformational variability of molecules in different crystal environments: a database study. Acta Crystallographica Section B: Structural Science, 2008, 64, 348-362.	1.8	36
117	<i>Tormat</i>: a program for the automated structural alignment of molecular conformations. Journal of Applied Crystallography, 2008, 41, 955-957.	1.9	17
118	Applications of photocrystallography: a future perspective. Zeitschrift Fur Kristallographie - Crystalline Materials, 2008, 223, 363-369.	0.4	22
119	X-Ray Diffraction of Photolytically Induced Molecular Species in Single Crystals. , 2008, , 29-61.		3
120	The structure of the rare-earth phosphate glass (Sm2O3)0.205(P2O5)0.795studied by anomalous dispersion neutron diffraction. Journal of Physics Condensed Matter, 2007, 19, 056002.	0.7	18
121	The neutron diffraction anomalous dispersion technique and its application to vitreous Sm2O3Â·4P2O5. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2007, 571, 622-635.	0.7	14
122	Disorder in pentachloronitrobenzene, C6Cl5NO2: a diffuse scattering study. Acta Crystallographica Section B: Structural Science, 2007, 63, 663-673.	1.8	25
123	C-type CeP3O9. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, i138-i139.	0.2	4
124	Direct observation ofRâ€¦Rdistances in rare-earth(R)phosphate glasses by magnetic difference neutron diffraction. Physical Review B, 2006, 73, .	1.1	22
125	Photocrystallographic structure determination of a new geometric isomer of [Ru(NH3)4(H2O)(Î·1-OSO)][MeC6H4SO3]2. Chemical Communications, 2006, , 2448-2450.	2.2	78
126	Matrix dependence of blue light emission from a novel NH2-functionalized dicyanoquinodimethane derivative. Journal of Physical Organic Chemistry, 2006, 19, 206-213.	0.9	7

#	ARTICLE	IF	CITATIONS
127	Neutron and X-ray Diffraction and Spectroscopic Investigations of Intramolecular [Cï£¿Hâ‹…â‹…â‹…Fï£¿C] Contacts in Post-Metallocene Polyolefin Catalysts: Modeling Weak Attractive Polymerâ€“Ligand Interactions. Chemistry - A European Journal, 2006, 12, 2607-2619.	1.7	82
128	Single-Crystal X-Ray Diffraction Studies of Photo-Induced Molecular Species. ChemInform, 2005, 36, no.	0.1	0
129	Molecular rearrangements of diynes coordinated to triosmium carbonyl clusters: reactions of [Os3(Î¼-H)2(CO)10] and [Os3(CO)10(MeCN)2] with 1,4-dipyridylbuta-1,3-diyne. New Journal of Chemistry, 2005, 29, 145-153.	1.4	11
130	A new polymorph of terpyridine: variable temperature X-ray diffraction studies and solid state photophysical properties. CrystEngComm, 2005, 7, 269.	1.3	42
131	\`In-situ' charge-density studies of photoinduced phenomena: possibilities for the future?. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 472-479.	0.3	4
132	Hydride Encapsulation by a Molecular Main-Group-Metal Cluster:Â Single-Crystal Neutron Diffraction Structure of [{Ph(2-C5H4N)N}6HLi8]+. Organometallics, 2004, 23, 4527-4530.	1.1	23
133	Single-crystal X-ray diffraction studies of photo-induced molecular species. Chemical Society Reviews, 2004, 33, 501.	18.7	81
134	Light-Induced Metastable Linkage Isomers of Ruthenium Sulfur Dioxide Complexes. Inorganic Chemistry, 2003, 42, 140-147.	1.9	105
135	Organic materials for second-harmonic generation: advances in relating structure to function. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 2751-2770.	1.6	69
136	Reaction of metallophosphanide anions with MLnX (X = halide) species as a simple route to heterometallic transition metal complexes. Dalton Transactions, 2003, , 1389-1395.	1.6	11
137	Nanosecond time-resolved crystallography of photo-induced species: case study and instrument development for high-resolution excited-state single-crystal structure determination. Faraday Discussions, 2003, 122, 119-129.	1.6	17
138	STRUCTURE AND DEVITRIFICATION CHEMISTRY OF RE(PO₃)₃ (RE=La, Pr, Nd, Gd, Dy, Y) METAPHOSPHATE GLASSES. Phosphorus Research Bulletin, 2002, 13, 137-146.	0.1	6
139	Charge-density study of the nonlinear optical precursor DED-TCNQ at 20 K. Physical Review B, 2002, 65, .	1.1	41
140	Exploiting structure/property relationships in organic non-linear optical materials: developing strategies to realize the potential of TCNQ derivatives. CrystEngComm, 2002, 4, 232-238.	1.3	12
141	X-ray and neutron diffraction studies of the non-linear optical compounds MBANP and MBADNP at 20â€…K: charge-density and hydrogen-bonding analyses. Acta Crystallographica Section B: Structural Science, 2002, 58, 690-700.	1.8	33
142	Rapid neutron-diffraction data collection for hydrogen-bonding studies: application of the Laue diffractometer (LADI) to the case study zinc (tris)thiourea sulfate. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 429-434.	0.3	21
143	Influence of hydrogen bonding on the second harmonic generation effect: neutron diffraction study of 4-nitro-4â€²-methylbenzylidene aniline. Acta Crystallographica Section B: Structural Science, 2001, 57, 410-414.	1.8	42
144	An x-ray diffraction and31P MAS NMR study of rare-earth phosphate glasses, (R2O3)x(P2O5)1-x,x= 0.175-0.263, R = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er. Journal of Physics Condensed Matter, 2001, 13, 4105-4122.	0.7	58

#	Article	IF	Citations
145	A rare-earth K-edge EXAFS study of rare-earth phosphate glasses, (R2O3)x(P2O5)1-x,x= 0.187-0.239, R = La, Nd, Sm, Eu, Gd, Dy, Er. Journal of Physics Condensed Matter, 2001, 13, 6659-6674.	0.7	29
146	Quantitative analysis of hydrogen bonding and atomic thermal motion in the organic non-linear optical material DCNP using X-ray and neutron diffraction. Acta Crystallographica Section B: Structural Science, 2000, 56, 1085-1093.	1.8	25
147	A neutron diffraction and27Al MQMAS NMR study of rare-earth phosphate glasses, (R2O3)x(P2O5)1-x,x= 0.187-0.263, R = Ce, Nd, Tb containing Al impurities. Journal of Physics Condensed Matter, 1999, 11, 9165-9178.	0.7	27
148	Multiple Î±-agostic interactions in a metalâ€“methyl complex: the neutron structure of [Mo(NC6H3Pri2-2,6)2Me2]. Chemical Communications, 1998, , 1829-1830.	2.2	11
149	Using Neutrons to See Whatâ€™s Happening Inside a Transparent Solar Cell. Neutron News, 0, , 1-2.	0.1	0