Kenneth D M Harris

List of Publications by Year
in descending order

273	10,996	38660 50	42291 92
papers	citations	h-index	g-index

282	282	282	9171
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Solid-State Structural Properties of Alloxazine Determined from Powder XRD Data in Conjunction with DFT-D Calculations and Solid-State NMR Spectroscopy: Unraveling the Tautomeric Identity and Pathways for Tautomeric Interconversion. Crystal Growth and Design, 2022, 22, 524-534.	1.4	8
2	A structure determination protocol based on combined analysis of 3D-ED data, powder XRD data, solid-state NMR data and DFT-D calculations reveals the structure of a new polymorph of<scp>l</scp>-tyrosine. Chemical Science, 2022, 13, 5277-5288.	3.7	15
3	Biogenic Guanine Crystals Are Solid Solutions of Guanine and Other Purine Metabolites. Journal of the American Chemical Society, 2022, 144, 5180-5189.	6.6	26
4	Circumventing a challenging aspect of crystal structure determination from powder diffraction data. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 96-99.	0.5	1
5	Exploiting in situ NMR to monitor the formation of a metalâ€“organic framework. Chemical Science, 2021, 12, 1486-1494.	3.7	17
6	Anderssonâ€MagnÃ©li Phases Ti_nO_{2nâ€1}: Recent Progress Inspired by Swedish Scientists. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2021, 647, 126-133.	0.6	11
7	Structure Determination of Multicomponent Crystalline Phases of (S)-Ibuprofen and l-Proline from Powder X-ray Diffraction Data, Augmented by Complementary Experimental and Computational Techniques. Crystal Growth and Design, 2021, 21, 2498-2507.	1.4	8
8	Monitoring Crystallization Processes in Confined Porous Materials by Dynamic Nuclear Polarization Solid-State Nuclear Magnetic Resonance. Journal of the American Chemical Society, 2021, 143, 6095-6103.	6.6	21
9	Orbital Mapping of Semiconducting Perylenes on Cu(111). Journal of Physical Chemistry C, 2021, 125, 24477-24486.	1.5	2
10	Manometric real-time studies of the mechanochemical synthesis of zeolitic imidazolate frameworks. Chemical Science, 2020, 11, 2141-2147.	3.7	64
11	Polymorphism in a Multicomponent Crystal System of Trimesic Acid and t-Butylamine. Crystal Growth and Design, 2020, 20, 5736-5744.	1.4	9
12	Directâ€Space Structure Determination of Covalent Organic Frameworks from 3D Electron Diffraction Data. Angewandte Chemie - International Edition, 2020, 59, 22638-22644.	7.2	23
13	Directâ€Space Structure Determination of Covalent Organic Frameworks from 3D Electron Diffraction Data. Angewandte Chemie, 2020, 132, 22827-22833.	1.6	2
14	Comparison of the Thermal Stabilities of Diazonium Salts and Their Corresponding Triazenes. Organic Process Research and Development, 2020, 24, 2336-2341.	1.3	39
15	Rationalization of the X-ray photoelectron spectroscopy of aluminium phosphates synthesized from different precursors. RSC Advances, 2020, 10, 8444-8452.	1.7	14
16	Boronâ€“Nitrogenâ€Doped Nanographenes: A Synthetic Tale from Borazine Precursors. Chemistry - A European Journal, 2020, 26, 6608-6621.	1.7	20
17	Polymorphism of l â€Tryptophan. Angewandte Chemie, 2019, 131, 18964-18968.	1.6	5
18	Polymorphism of l â€Tryptophan. Angewandte Chemie - International Edition, 2019, 58, 18788-18792.	7.2	21

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19	Reply to comment on Couzi et al . (2018): a phenomenological model for structural phase transitions in incommensurate alkane/urea inclusion compounds. Royal Society Open Science, 2019, 6, 190518.	1.1	2
20	Spatially resolved mapping of phase transitions in liquid-crystalline materials by X-ray birefringence imaging. Chemical Science, 2019, 10, 3005-3011.	3.7	2
21	Aluminium-catalysed isocyanate trimerization, enhanced by exploiting a dynamic coordination sphere. Chemical Communications, 2019, 55, 7679-7682.	2.2	20
22	Structure and Morphology of Light-Reflecting Synthetic and Biogenic Polymorphs of Isoxanthopterin: A Comparison. Chemistry of Materials, 2019, 31, 4479-4489.	3.2	12
23	Temperature-Dependent Structural Properties, Phase Transition Behavior, and Dynamic Properties of a Benzene Derivative in the Solid State. Crystal Growth and Design, 2019, 19, 2155-2162.	1.4	2
24	A Strategy for Probing the Evolution of Crystallization Processes by Low-Temperature Solid-State NMR and Dynamic Nuclear Polarization. Journal of Physical Chemistry Letters, 2019, 10, 1505-1510.	2.1	21
25	Exploiting in-situ solid-state NMR spectroscopy to probe the early stages of hydration of calcium aluminate cement. Solid State Nuclear Magnetic Resonance, 2019, 99, 1-6.	1.5	25
26	Insights into the Crystallization and Structural Evolution of Glycine Dihydrate by Inâ€…Situ Solidâ€State NMR Spectroscopy. Angewandte Chemie - International Edition, 2018, 57, 6619-6623.	7.2	21
27	Insights into the Crystallization and Structural Evolution of Glycine Dihydrate by Inâ€…Situ Solidâ€State NMR Spectroscopy. Angewandte Chemie, 2018, 130, 6729-6733.	1.6	5
28	Elucidating the Crystal Structure of dl-Arginine by Combined Powder X-ray Diffraction Data Analysis and Periodic DFT-D Calculations. Crystal Growth and Design, 2018, 18, 42-46.	1.4	11
29	A phenomenological model for structural phase transitions in incommensurate alkane/urea inclusion compounds. Royal Society Open Science, 2018, 5, 180058.	1.1	6
30	Establishing the Transitory Existence of Amorphous Phases in Crystallization Pathways by the CLASSIC NMR Technique. ChemPhysChem, 2018, 19, 3341-3345.	1.0	11
31	Polymorphic phase transformations of 3-chloro-trans-cinnamic acid and its solid solution with 3-bromo-trans-cinnamic acid. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 923-928.	0.2	3
32	Structural Diversity of Solid Solutions Formed between 3-Chloro-trans-cinnamic acid and 3-Bromo-trans-cinnamic Acid. Crystal Growth and Design, 2017, 17, 1276-1284.	1.4	16
33	Explorations in the Dynamics of Crystalline Solids and the Evolution of Crystal Formation Processes. Israel Journal of Chemistry, 2017, 57, 154-170.	1.0	2
34	`NMR Crystallization':in-situNMR techniques for time-resolved monitoring of crystallization processes. Acta Crystallographica Section C, Structural Chemistry, 2017, 73, 137-148.	0.2	16
35	Determination of a complex crystal structure in the absence of single crystals: analysis of powder X-ray diffraction data, guided by solid-state NMR and periodic DFT calculations, reveals a new 2â€²-deoxyguanosine structural motif. Chemical Science, 2017, 8, 3971-3979.	3.7	62
36	Complexes of Thiourea with Alkali Metal Bromides and Iodides: Structural Properties, Mixed-Halide and Mixed-Metal Materials, and Halide Exchange Processes. Crystal Growth and Design, 2017, 17, 786-793.	1.4	3

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37	Ab initio random structure searching of organic molecular solids: assessment and validation against experimental data. Physical Chemistry Chemical Physics, 2017, 19, 25949-25960.	1.3	23
38	Assessing the Detection Limit of a Minority Solid-State Form of a Pharmaceutical by 1H Double-Quantum Magic-Angle Spinning Nuclear Magnetic Resonance Spectroscopy. Journal of Pharmaceutical Sciences, 2017, 106, 3372-3377.	1.6	21
39	Novel technique for spatially resolved imaging of molecular bond orientations using x-ray birefringence. AIP Conference Proceedings, 2016, , .	0.3	0
40	New in situ solid-state NMR strategies for exploring materials formation and adsorption processes: prospects in heterogenous catalysis. Applied Petrochemical Research, 2016, 6, 295-306.	1.3	5
41	Determining Molecular Orientations in Disordered Materials from X-ray Linear Dichroism at the Iodine L₁-Edge. Journal of the American Chemical Society, 2016, 138, 16188-16191.	6.6	3
42	The true structural periodicities and superspace group descriptions of the prototypical incommensurate composite materials: Alkane/urea inclusion compounds. Europhysics Letters, 2016, 116, 56001.	0.7	6
43	Calculation of solid-state NMR lineshapes using contour analysis. Solid State Nuclear Magnetic Resonance, 2016, 80, 7-13.	1.5	5
44	Understanding the Solid-State Hydration Behavior of a Common Amino Acid: Identification, Structural Characterization, and Hydration/Dehydration Processes of New Hydrate Phases of <scp>l</scp>-Lysine. Journal of Physical Chemistry C, 2016, 120, 9385-9392.	1.5	19
45	Combining the Advantages of Powder X-ray Diffraction and NMR Crystallography in Structure Determination of the Pharmaceutical Material Cimetidine Hydrochloride. Crystal Growth and Design, 2016, 16, 1798-1804.	1.4	55
46	Some of tomorrow's catalysts for processing renewable and non-renewable feedstocks, diminishing anthropogenic carbon dioxide and increasing the production of energy. Energy and Environmental Science, 2016, 9, 687-708.	15.6	69
47	Discovery of New Metastable Polymorphs in a Family of Urea Co-Crystals by Solid-State Mechanochemistry. Crystal Growth and Design, 2015, 15, 2901-2907.	1.4	34
48	X-ray Birefringence Imaging of Materials with Anisotropic Molecular Dynamics. Journal of Physical Chemistry Letters, 2015, 6, 561-567.	2.1	6
49	<scp>L</scp>â€Lysine: Exploiting Powder Xâ€ray Diffraction to Complete the Set of Crystal Structures of the 20 Directly Encoded Proteinogenic Amino Acids. Angewandte Chemie - International Edition, 2015, 54, 3973-3977.	7.2	55
50	Exploiting Powder X-ray Diffraction to Establish the Solvent-Assisted Solid-State Supramolecular Assembly of Pillar[5]quinone. Crystal Growth and Design, 2015, 15, 1583-1587.	1.4	15
51	Theoretical analysis of the background intensity distribution in X-ray Birefringence Imaging using synchrotron bending-magnet radiation. Journal of Applied Physics, 2015, 117, 164902.	1.1	3
52	New in situ solid-state NMR techniques for probing the evolution of crystallization processes: pre-nucleation, nucleation and growth. Faraday Discussions, 2015, 179, 115-140.	1.6	29
53	Monitoring the evolution of crystallization processes by in-situ solid-state NMR spectroscopy. Solid State Nuclear Magnetic Resonance, 2015, 65, 107-113.	1.5	19
54	X-ray birefringence imaging. Science, 2014, 344, 1013-1016.	6.0	25

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55	Highly Efficient Chiral Resolution of <scp>dl</scp>â€Arginine by Cocrystal Formation Followed by Recrystallization under Preferentialâ€Enrichment Conditions. Chemistry - A European Journal, 2014, 20, 10343-10350.	1.7	31
56	â€œCLASSIC NMRâ€: An Inâ€Situ NMR Strategy for Mapping the Timeâ€Evolution of Crystallization Processes by Combined Liquidâ€State and Solidâ€State Measurements. Angewandte Chemie - International Edition, 2014, 53, 8939-8943.	7.2	57
57	Polymorphism in a trans-Cinnamic Acid Derivative Exhibiting Two Distinct Î²-type Phases: Structural Properties, [2 + 2] Photodimerization Reactions, and Polymorphic Phase Transition Behavior. Crystal Growth and Design, 2013, 13, 4110-4117.	1.4	29
58	An ENDOR and DFT analysis of hindered methyl group rotations in frozen solutions of bis(acetylacetonato)-copper(ii). Physical Chemistry Chemical Physics, 2013, 15, 15214.	1.3	7
59	An NMR crystallography DFT-D approach to analyse the role of intermolecular hydrogen bonding and Ï€â€“Ï€ interactions in driving cocrystallisation of indomethacin and nicotinamide. CrystEngComm, 2013, 15, 8797.	1.3	70
60	How grinding evolves. Nature Chemistry, 2013, 5, 12-14.	6.6	41
61	A Rare Case of Polymorphism in a Three-Component Co-Crystal System, with Each Polymorph Having Ten Independent Molecules in the Asymmetric Unit. Crystal Growth and Design, 2013, 13, 27-30.	1.4	13
62	Exploiting the Synergy of Powder X-ray Diffraction and Solid-State NMR Spectroscopy in Structure Determination of Organic Molecular Solids. Journal of Physical Chemistry C, 2013, 117, 12258-12265.	1.5	81
63	Expanding the Solid-State Landscape of <scp>l</scp>-Phenylalanine: Discovery of Polymorphism and New Hydrate Phases, with Rationalization of Hydration/Dehydration Processes. Journal of Physical Chemistry C, 2013, 117, 12136-12145.	1.5	37
64	Controlling Spatial Distributions of Molecules in Multicomponent Organic Crystals, with Quantitative Mapping by Confocal Raman Microspectrometry. Journal of the American Chemical Society, 2013, 135, 14512-14515.	6.6	12
65	A drifting Markov process on the circle, with physical applications. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2013, 469, 20130092.	1.0	3
66	An Adaptable and Dynamically Porous Organic Salt Traps Unique Tetrahalide Dianions. Angewandte Chemie - International Edition, 2013, 52, 13444-13448.	7.2	73
67	The crystal structure of l-arginine. Chemical Communications, 2012, 48, 2761.	2.2	70
68	Structural Rationalization of the Phase Transition Behavior in a Solid Organic Inclusion Compound: Bromocyclohexane/Thiourea. Crystal Growth and Design, 2012, 12, 577-582.	1.4	16
69	The effect of intermolecular hydrogen bonding on the planarity of amides. Physical Chemistry Chemical Physics, 2012, 14, 11944.	1.3	22
70	Efficient, Scalable, and Solvent-free Mechanochemical Synthesis of the OLED Material Alq₃ (q = 8-Hydroxyquinolinate). Crystal Growth and Design, 2012, 12, 5869-5872.	1.4	51
71	Discovery of a New System Exhibiting Abundant Polymorphism: m-Aminobenzoic Acid. Crystal Growth and Design, 2012, 12, 3104-3113.	1.4	68
72	Exploiting In Situ Solid-State NMR for the Discovery of New Polymorphs during Crystallization Processes. Journal of Physical Chemistry Letters, 2012, 3, 3176-3181.	2.1	28

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73	New Insights into the Preparation of the Low-Melting Polymorph of Racemic Ibuprofen. Crystal Growth and Design, 2012, 12, 5839-5845.	1.4	15
74	X-ray Birefringence: A New Strategy for Determining Molecular Orientation in Materials. Journal of Physical Chemistry Letters, 2012, 3, 3216-3222.	2.1	12
75	Mechanochemistry: opportunities for new and cleaner synthesis. Chemical Society Reviews, 2012, 41, 413-447.	18.7	2,281
76	Structural diversity, but no polymorphism, in a homologous family of co-crystals of urea and Î±,Ï‰-dihydroxyalkanes. New Journal of Chemistry, 2011, 35, 1515.	1.4	24
77	Cooperativity in Solid-State Squaramides. Crystal Growth and Design, 2011, 11, 3725-3730.	1.4	17
78	Natural-Abundance Solid-State2H NMR Spectroscopy at High Magnetic Field. Journal of Physical Chemistry A, 2011, 115, 5568-5578.	1.1	13
79	Structure Determination from Powder X-ray Diffraction Data of a New Polymorph of a High-Density Organic Hydrate Material, with an Assessment of Hydrogen-Bond Disorder by Rietveld Refinement. Crystal Growth and Design, 2011, 11, 5192-5199.	1.4	16
80	X-ray Birefringence from a Model Anisotropic Crystal. Journal of Physical Chemistry Letters, 2011, 2, 2346-2351.	2.1	15
81	High-Resolution Solid-State²H NMR Spectroscopy of Polymorphs of Glycine. Journal of Physical Chemistry A, 2011, 115, 12201-12211.	1.1	32
82	Structural Chemistry of a New Chiral Anhydrous Phase of Ru(bipy)₃(ClO₄)₂Established from Powder X-ray Diffraction Analysis. Crystal Growth and Design, 2011, 11, 3313-3317.	1.4	22
83	Structural Properties of Carboxylic Acid Dimers Confined within the Urea Tunnel Structure: An MD Simulation Study. Journal of Physical Chemistry B, 2011, 115, 2791-2800.	1.2	16
84	Exploiting powder X-ray diffraction for direct structure determination in structural biology: The P2X4 receptor trafficking motif YEQGL. Journal of Structural Biology, 2011, 174, 461-467.	1.3	41
85	Powder Diffraction Crystallography of Molecular Solids. Topics in Current Chemistry, 2011, 315, 133-177.	4.0	86
86	A Strategy for Retrospectively Mapping the Growth History of a Crystal. Angewandte Chemie - International Edition, 2010, 49, 5096-5100.	7.2	10
87	Physicochemical Understanding of Polymorphism and Solid-State Dehydration/Rehydration Processes for the Pharmaceutical Material Acrinol, by Ab Initio Powder X-ray Diffraction Analysis and Other Techniques. Journal of Physical Chemistry C, 2010, 114, 580-586.	1.5	42
88	Triptycene-Based Polymers of Intrinsic Microporosity: Organic Materials That Can Be Tailored for Gas Adsorption. Macromolecules, 2010, 43, 5287-5294.	2.2	275
89	Direct structure elucidation by powder X-ray diffraction of a metalâ€“organic framework material prepared by solvent-free grinding. Chemical Communications, 2010, 46, 7572.	2.2	107
90	A Solid-State Dehydration Process in an Organic Material Associated with Substantial Hydrogen-Bond Reorganization, Investigated by Powder X-ray Diffraction. Crystal Growth and Design, 2010, 10, 3176-3181.	1.4	15

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91	Arrays of Pâ•O Dipoles As a Recurrent Structural Motif in Bis-Diphenylphosphine Oxides, Established from Powder X-ray Diffraction. Crystal Growth and Design, 2010, 10, 3814-3818.	1.4	7
92	Direct observation of a transient polymorph during crystallization. Chemical Communications, 2010, 46, 4982.	2.2	49
93	Nitrogen and Hydrogen Adsorption by an Organic Microporous Crystal. Angewandte Chemie - International Edition, 2009, 48, 3273-3277.	7.2	132
94	In situ solid-state 1H NMR studies of hydration of the solid acid catalyst ZSM-5 in its ammonium form. Solid State Nuclear Magnetic Resonance, 2009, 35, 93-99.	1.5	21
95	Preferential Clustering of Water Molecules During Hydration of the Ammonium Form of the Solid Acid Catalyst ZSM-5. Catalysis Letters, 2009, 131, 16-20.	1.4	5
96	Bidirectional Transport of Guest Molecules through the Nanoporous Tunnel Structure of a Solid Inclusion Compound. Journal of Physical Chemistry C, 2009, 113, 736-743.	1.5	23
97	Structure Solution from Powder X-Ray Diffraction Data by Genetic Algorithm Techniques, Applied to Organic Materials Generated as Polycrystalline Products from Solid State Processes. Materials and Manufacturing Processes, 2009, 24, 293-302.	2.7	24
98	Vapour Induced Crystalline Transformation Investigated by ab initio Powder X-ray Diffraction Analysis. Crystal Growth and Design, 2009, 9, 1201-1207.	1.4	37
99	â€œAmorphous Nickel Sulfideâ€•Is Hydrated Nanocrystalline NiS with a Coreâˆ'Shell Structure. Inorganic Chemistry, 2009, 48, 11486-11488.	1.9	32
100	Lessons on the Discovery and Assignment of Polymorphs, Highlighted by the Case of the Latent Pigment DPP-Boc. Crystal Growth and Design, 2009, 9, 853-857.	1.4	13
101	The effect of deuteration on polymorphic outcome in the crystallization of glycine from aqueous solution. New Journal of Chemistry, 2009, 33, 713.	1.4	34
102	Pathways for hydrogen bond switching in a tetrameric methanol cluster. Physical Chemistry Chemical Physics, 2009, 11, 11340.	1.3	5
103	Optical phonons in millerite (NiS) from singleâ€crystal polarized Raman spectroscopy. Journal of Raman Spectroscopy, 2008, 39, 1419-1422.	1.2	36
104	Clustering of Glycine Molecules in Aqueous Solution Studied by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 7280-7288.	1.2	79
105	Residue-Based Charge Flipping: A New Variant of an Emerging Algorithm for Structure Solution from X-ray Diffraction Data. Journal of Physical Chemistry A, 2008, 112, 4863-4868.	1.1	7
106	Predictable Disorder versus Polymorphism in the Rationalization of Structural Diversity: A Multidisciplinary Study of Eniluracil. Crystal Growth and Design, 2008, 8, 3474-3481.	1.4	49
107	Optimizing the Number of Components in a Molecular Quasicrystal: A Three-Component Material Based on the Penrose Tiling. Journal of Physical Chemistry C, 2008, 112, 16186-16188.	1.5	6
108	Counteracting stagnation in genetic algorithm calculations by implementation of a micro genetic algorithm strategy. Physical Chemistry Chemical Physics, 2008, 10, 7262.	1.3	13

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109	Characterization of a Polymorphic System Exhibiting Substantial Variation of Solubility in a Fluorinated Solvent. Journal of Physical Chemistry C, 2008, 112, 14570-14578.	1.5	5
110	Mapping the Evolution of Adsorption of Water in Nanoporous Silica by in situ Solid-State1H NMR Spectroscopy. Journal of the American Chemical Society, 2008, 130, 5880-5882.	6.6	31
111	Triple-Quantum ²³Na MAS NMR Spectroscopy as a Technique for Probing Polymorphism in Sodium Salts. Crystal Growth and Design, 2008, 8, 6-10.	1.4	20
112	A Technique for In Situ Monitoring of Crystallization from Solution by Solid-State¹³C CPMAS NMR Spectroscopy. Journal of Physical Chemistry A, 2008, 112, 6808-6810.	1.1	52
113	Structural Properties of Low-Temperature Phase Transitions in the Prototypical Thiourea Inclusion Compound:â€‰ Cyclohexane/Thiourea. Journal of Physical Chemistry C, 2008, 112, 839-847.	1.5	12
114	Dynamic Properties of Solid Ammonium Cyanate. Journal of Physical Chemistry C, 2008, 112, 15870-15879.	1.5	7
115	A Solid-State Dehydration Process Associated with a Significant Change in the Topology of Dihydrogen Phosphate Chains, Established from Powder X-ray Diffraction. Crystal Growth and Design, 2008, 8, 3641-3645.	1.4	17
116	Direct Structural Understanding of a Topochemical Solid State Photopolymerization Reaction. Journal of Physical Chemistry C, 2008, 112, 19793-19796.	1.5	70
117	A multi-technique approach for probing the evolution of structural properties during crystallization of organic materials from solution. Faraday Discussions, 2007, 136, 71.	1.6	58
118	Kinetics of Molecular Transport in a Nanoporous Crystal Studied by Confocal Raman Microspectrometry:â€‰ Single-File Diffusion in a Densely Filled Tunnel. Journal of Physical Chemistry B, 2007, 111, 12339-12344.	1.2	21
119	Alteration of Polymorphic Selectivity through Different Crystallization Mechanisms Occurring in the Same Crystallization Solution. Journal of Physical Chemistry B, 2007, 111, 8705-8707.	1.2	36
120	Mechanistic Aspects of the Solid-State Transformation of Ammonium Cyanate to Urea at High Pressure. Journal of Physical Chemistry B, 2007, 111, 3960-3968.	1.2	6
121	Enhanced Efficiency of Direct-Space Structure Solution from Powder X-ray Diffraction Data in the Case of Conformationally Flexible Molecules. Journal of Physical Chemistry B, 2007, 111, 6349-6356.	1.2	8
122	Fundamental and Applied Aspects of Urea and Thiourea Inclusion Compounds. Supramolecular Chemistry, 2007, 19, 47-53.	1.5	94
123	Advantages of a Redefinition of Variable-Space in Direct-Space Structure Solution from Powder X-Ray Diffraction Data. ChemPhysChem, 2007, 8, 650-653.	1.0	14
124	Probing the Evolution of Adsorption on Nanoporous Solids by In Situ Solid-State NMR Spectroscopy. ChemPhysChem, 2007, 8, 1311-1313.	1.0	21
125	Alternative hydrogen bonding modes employed by a helical tubuland diol host molecule. CrystEngComm, 2006, 8, 250.	1.3	9
126	Structureâ^'Reactivity Correlations for Solid-State Enantioselective Photochemical Reactions Established Directly from Powder X-ray Diffraction. Journal of the American Chemical Society, 2006, 128, 15554-15555.	6.6	18

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127	Understanding the Structural Properties of a Dendrimeric Material Directly from Powder X-ray Diffraction Data. Journal of Physical Chemistry B, 2006, 110, 11620-11623.	1.2	31
128	Significant Conformational Changes Associated with Molecular Transport in a Crystalline Solid. Journal of Physical Chemistry B, 2006, 110, 10708-10713.	1.2	18
129	Contrasting Solid-State Structures of Trithiocyanuric Acid and Cyanuric Acid. Crystal Growth and Design, 2006, 6, 846-848.	1.4	36
130	Abundant Polymorphism in a System with Multiple Hydrogen-Bonding Opportunities:Â Oxalyl Dihydrazide. Journal of the American Chemical Society, 2006, 128, 8441-8452.	6.6	76
131	Design of a Molecular Quasicrystal. ChemPhysChem, 2006, 7, 1649-1653.	1.0	17
132	In-situ Monitoring of Alkane-Alkane Guest Exchange in Urea Inclusion Compounds using Confocal Raman Microspectrometry. Molecular Crystals and Liquid Crystals, 2006, 456, 139-147.	0.4	8
133	Structural properties of methoxy derivatives of benzyl bromide, determined from powder X-ray diffraction data. Powder Diffraction, 2005, 20, 345-352.	0.4	3
134	Structural Rationalisation of Co-crystals Formed between Trithiocyanuric Acid and Molecules Containing Hydrogen Bonding Functionality. Chemistry - A European Journal, 2005, 11, 2433-2439.	1.7	34
135	Hydrogen-bonded chains of Î±,Ï‰-diaminoalkane and Î±,Ï‰-dihydroxyalkane guest molecules lead to disrupted tunnel structures in urea inclusion compounds. New Journal of Chemistry, 2005, 29, 1266.	1.4	14
136	Structural and Dynamic Aspects of Hydrogen-Bonded Complexes and Inclusion Compounds Containing Î±,Ï‰-Dicyanoalkanes and Urea, Investigated by Solid-State 13C and 2H NMR Techniques. Journal of Physical Chemistry B, 2005, 109, 23342-23350.	1.2	22
137	Altering the Polymorphic Product Distribution in a Solid-State Dehydration Process by Rapid Sample Rotation in a Solid-State NMR Probe. Journal of the American Chemical Society, 2005, 127, 10832-10833.	6.6	31
138	Prospects for Exploiting 4D Ultrafast Electron Microscopy in Solid-State Organic and Biological Chemistryâ€. Crystal Growth and Design, 2005, 5, 2124-2130.	1.4	12
139	Structural Understanding of a Molecular Material that Is Accessed Only by a Solid-State Desolvation Process:Â The Scope of Modern Powder X-ray Diffraction Techniques. Journal of the American Chemical Society, 2005, 127, 7314-7315.	6.6	66
140	Significantly Contrasting Solid State Dynamics of the Racemic and Enantiomerically Pure Crystalline Forms of an Amino Acid. Journal of Physical Chemistry B, 2005, 109, 22808-22813.	1.2	16
141	A Case Study in Direct-Space Structure Determination from Powder X-ray Diffraction Data:â€‰ Finding the Hydrate Structure of an Organic Molecule with Significant Conformational Flexibilityâ€. Crystal Growth and Design, 2005, 5, 2084-2090.	1.4	19
142	Developments in genetic algorithm techniques for structure solution from powder diffraction data. Zeitschrift Fur Kristallographie - Crystalline Materials, 2004, 219, 838-846.	0.4	68
143	Ammonium cyanate: a DFT study of crystal structure, rotational barriers and vibrational spectrum. Molecular Physics, 2004, 102, 869-876.	0.8	5
144	Challenges in Direct-Space Structure Determination from Powder Diffraction Data: A Molecular Material with Four Independent Molecules in the Asymmetric Unit. ChemPhysChem, 2004, 5, 414-418.	1.0	70

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145	Rationalizing the Structural Properties of Bupivacaine Baseâ€"A Local Anestheticâ€"Directly from Powder X-Ray Diffraction Data. Journal of Pharmaceutical Sciences, 2004, 93, 667-674.	1.6	13
146	Comment on â€œA deuteron NMR study of the tetrahydrofuran clathrate hydrate. Part II: Coupling of rotational and translational dynamics of waterâ€•by T. M. Kirschgen, M. D. Zeidler, B. Geil and F. Fujara, Phys. Chem. Chem. Phys., 2003,5, 5247. Physical Chemistry Chemical Physics, 2004, 6, 871-872.	1.3	6
147	Direct Time-Resolved and Spatially Resolved Monitoring of Molecular Transport in a Crystalline Nanochannel System. Journal of the American Chemical Society, 2004, 126, 11124-11125.	6.6	44
148	Powder Diffraction Indexing as a Pattern Recognition Problem:Â A New Approach for Unit Cell Determination Based on an Artificial Neural Network. Journal of Physical Chemistry A, 2004, 108, 711-716.	1.1	17
149	Structural Aspects of a Dendrimer Precursor Determined Directly from Powder X-ray Diffraction Data. Crystal Growth and Design, 2004, 4, 451-455.	1.4	8
150	Co-crystalline hydrogen bonded solids based on the alcoholâ€“carboxylic acidâ€“alcohol supramolecular motif. CrystEngComm, 2004, 6, 5-10.	1.3	14
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