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	Mechanochemistry: opportunities for new and cleaner synthesis. Chemical Society Reviews, 2012, 41, 413-447.	18.7	2,281
2	Contemporary Advances in the Use of Powder X-Ray Diffraction for Structure Determination. Angewandte Chemie - International Edition, 2001, 40, 1626-1651.	7.2	328
3	Crystal Structure Determination from Powder Diffraction Data by Monte Carlo Methods. Journal of the American Chemical Society, 1994, 116, 3543-3547.	6.6	311
4	Triptycene-Based Polymers of Intrinsic Microporosity: Organic Materials That Can Be Tailored for Gas Adsorption. Macromolecules, 2010, 43, 5287-5294.	2.2	275
5	Crystal Structure Determination from Powder Diffraction Data. Chemistry of Materials, 1996, 8, 2554-2570.	3.2	217
6	Structural aspects of urea inclusion compounds and their investigation by X-ray diffraction: a general discussion. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 2985.	1.7	182
7	How to determine structures when single crystals cannot be grown: opportunities for structure determination of molecular materials using powder diffraction data. Chemical Society Reviews, 2004, 33, 526.	18.7	178
8	Meldola Lecture: understanding the properties of urea and thiourea inclusion compounds. Chemical Society Reviews, 1997, 26, 279.	18.7	141
9	Direct Structure Determination of a Multicomponent Molecular Crystal Prepared by a Solid-State Grinding Procedure. Journal of the American Chemical Society, 2003, 125, 14658-14659.	6.6	134
10	Nitrogen and Hydrogen Adsorption by an Organic Microporous Crystal. Angewandte Chemie - International Edition, 2009, 48, 3273-3277.	7.2	132
11	Mechanistic Insights into the Conversion of Cyclohexene to Adipic Acid by H2O2 in the Presence of a TAPO-5 Catalyst. Angewandte Chemie - International Edition, 2003, 42, 1520-1523.	7.2	113
12	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
13	Structure Determination of a Complex Organic Solid from X-Ray Powder Diffraction Data by a Generalized Monte Carlo Method: The Crystal Structure of Red Fluorescein. Angewandte Chemie International Edition in English, 1997, 36, 770-772.	4.4	99
14	Fundamental and Applied Aspects of Urea and Thiourea Inclusion Compounds. Supramolecular Chemistry, 2007, 19, 47-53.	1.5	94
15	Powder Diffraction Crystallography of Molecular Solids. Topics in Current Chemistry, 2011, 315, 133-177.	4.0	86
16	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
17	New families of catalysts for the selective oxidation of methane. Faraday Discussions of the Chemical Society, 1989, 87, 33.	2.2	79
18	A Triphenylphoshine Oxideâ^'Water Aggregate Facilitates an Exceptionally Short Câ^'HÂ·Â·Â·O Hydrogen Bond. Journal of the American Chemical Society, 1997, 119, 12679-12680.	6.6	79

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19	Clustering of Glycine Molecules in Aqueous Solution Studied by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 7280-7288.	1.2	79
20	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
21	Structural properties of Î±,Ï‰-dibromoalkane/urea inclusion compounds: a new type of interchannel guest molecule ordering. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 3423-3429.	1.7	74
22	Weak interactions in crystal engineeringâ€"understanding the recognition properties of the nitro group. New Journal of Chemistry, 2000, 24, 799-806.	1.4	74
23	An Adaptable and Dynamically Porous Organic Salt Traps Unique Tetrahalide Dianions. Angewandte Chemie - International Edition, 2013, 52, 13444-13448.	7.2	73
24	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
25	Direct Structural Understanding of a Topochemical Solid State Photopolymerization Reaction. Journal of Physical Chemistry C, 2008, 112, 19793-19796.	1.5	70
26	The crystal structure of l-arginine. Chemical Communications, 2012, 48, 2761.	2.2	70
27	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
28	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
29	Developments in genetic algorithm techniques for structure solution from powder diffraction data. Zeitschrift Fur Kristallographie - Crystalline Materials, 2004, 219, 838-846.	0.4	68
30	Discovery of a New System Exhibiting Abundant Polymorphism: m-Aminobenzoic Acid. Crystal Growth and Design, 2012, 12, 3104-3113.	1.4	68
31	Crystal Structure Solution from Powder X-ray Diffraction Data:Â The Development of Monte Carlo Methods To Solve the Crystal Structure of the Î³-Phase of 3-Chloro-trans-cinnamic Acidâ€. Chemistry of Materials, 1996, 8, 565-569.	3.2	66
32	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
33	Manometric real-time studies of the mechanochemical synthesis of zeolitic imidazolate frameworks. Chemical Science, 2020, 11, 2141-2147.	3.7	64
34	Evolving Opportunities in Structure Solution from Powder Diffraction Dataâ€"Crystal Structure Determination of a Molecular System with Twelve Variable Torsion Angles. Angewandte Chemie - International Edition, 1999, 38, 831-835.	7.2	62
35	New Opportunities for Structure Determination of Molecular Materials Directly from Powder Diffraction Data. Crystal Growth and Design, 2003, 3, 887-895.	1.4	62
36	Solid-State Supramolecular Organization, Established Directly from Powder Diffraction Data, and Photoluminescence Efficiency of Rigid-Core Oligothiophene-Ś,S-dioxides. Journal of the American Chemical Society, 2003, 125, 12277-12283.	6.6	62

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37	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
38	Structure Determination of an Oligopeptide Directly from Powder Diffraction Data. Angewandte Chemie - International Edition, 2000, 39, 4488-4491.	7.2	61
39	Development of a multipopulation parallel genetic algorithm for structure solution from powder diffraction data. Journal of Computational Chemistry, 2003, 24, 1766-1774.	1.5	60
40	Conformational properties of monosubstituted cyclohexanes in their thiourea inclusion compounds and in solution: variable-temperature one-dimensional and two-dimensional carbon-13 NMR investigations. Journal of the American Chemical Society, 1993, 115, 6369-6377.	6.6	59
41	Structure determination of a steroid directly from powder diffraction dataâ€. Chemical Communications, 1999, , 1677-1678.	2.2	59
42	Intermolecular organisation of triphenyleneÂbased discotic mesogens by interdigitation of alkyl chains. Journal of Materials Chemistry, 2001, 11, 302-311.	6.7	59
43	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
44	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
45	Câ‹¯Hâ‹…â‹…â‹…O Hydrogen Bond Mediated Chain Reversal in a Peptide Containing a Î³-Amino Acid Residue, Determined Directly from Powder X-ray Diffraction Data. Angewandte Chemie - International Edition, 2002, 41, 494-496.	7.2	55
46	<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
47	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
48	Understanding the Structural Properties of a Homologous Series of Bis-diphenylphosphine Oxides. Chemistry - A European Journal, 2000, 6, 2338-2349.	1.7	53
49	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
50	Dynamic Properties of the Tetrahydrofuran Clathrate Hydrate, Investigated by Solid State2H NMR Spectroscopy. Journal of Physical Chemistry B, 2001, 105, 2699-2706.	1.2	51
51	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
52	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
53	Direct observation of a transient polymorph during crystallization. Chemical Communications, 2010, 46, 4982.	2.2	49
54	Structural aspects of the chlorocyclohexane/thiourea inclusion system. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 1095.	1.7	48

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55	Simple technique for temperature calibration of a MAS probe for solid-state NMR spectroscopy. Magnetic Resonance in Chemistry, 1994, 32, 366-369.	1.1	48
56	Observation of the Sliding Mode in Incommensurate Intergrowth Compounds: Brillouin Scattering from the Inclusion Compound of Urea and Heptadecane. Physical Review Letters, 1995, 74, 734-737.	2.9	48
57	Zigzag Channels in the Structure of Sebaconitrile/Urea. Angewandte Chemie International Edition in English, 1994, 33, 649-652.	4.4	46
58	Synthesis of layered nickel phosphonate materials based on a topotactic approach. Journal of Materials Chemistry, 1998, 8, 579-584.	6.7	45
59	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
60	A carbon-13 CP/MAS NMR study of a double tert-butyl group rotation in the solid state using T1.rho. and line shape measurements. Journal of the American Chemical Society, 1993, 115, 1881-1885.	6.6	43
61	Spring-Loading at the Molecular Level:â€‰ Relaxation of Guest-Induced Strain in Channel Inclusion Compounds. Journal of the American Chemical Society, 1999, 121, 9732-9733.	6.6	43
62	Determination of a molecular crystal structure by X-ray powder diffraction on a conventional laboratory instrument. Journal of the Chemical Society Chemical Communications, 1992, , 1012.	2.0	42
63	New Light on an Old Story:Â The Solid-State Transformation of Ammonium Cyanate into Urea. Journal of the American Chemical Society, 1998, 120, 13274-13275.	6.6	42
64	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
65	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
66	How grinding evolves. Nature Chemistry, 2013, 5, 12-14.	6.6	41
67	Conformational and vibrational properties of Î±,Ï‰-dihalogenoalkane/urea inclusion compounds: a Raman scattering investigation. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1313-1322.	1.7	39
68	Topochemical Rationalization of the Solid-State Polymerization Reaction of Sodium Chloroacetate:Â Structure Determination from Powder Diffraction Data by the Monte Carlo Method. Journal of Physical Chemistry B, 1997, 101, 8827-8831.	1.2	39
69	Comparison of the Thermal Stabilities of Diazonium Salts and Their Corresponding Triazenes. Organic Process Research and Development, 2020, 24, 2336-2341.	1.3	39
70	A new approach for indexing powder diffraction data based on whole-profile fitting and global optimization using a genetic algorithm. Journal of Synchrotron Radiation, 1999, 6, 87-92.	1.0	38
71	Vapour Induced Crystalline Transformation Investigated by ab initio Powder X-ray Diffraction Analysis. Crystal Growth and Design, 2009, 9, 1201-1207.	1.4	37
72	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

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73	Contrasting Solid-State Structures of Trithiocyanuric Acid and Cyanuric Acid. Crystal Growth and Design, 2006, 6, 846-848.	1.4	36
74	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
75	Optical phonons in millerite (NiS) from singleâ€crystal polarized Raman spectroscopy. Journal of Raman Spectroscopy, 2008, 39, 1419-1422.	1.2	36
76	Powder X-ray diffraction studies of a low-temperature phase transition in the n-hexadecane/urea inclusion compound. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 3135.	1.7	35
77	A quantitative analysis of guest periodicity in oneâ€dimensional inclusion compounds. Journal of Chemical Physics, 1992, 96, 7117-7124.	1.2	34
78	Theoretical prediction of the guest periodicity of alkane/urea inclusion compounds. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 2023.	1.7	34
79	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
80	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
81	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
82	Dynamic properties of dioctanoyl peroxide guest molecules constrained within the urea tunnel structure: A combined incoherent quasielastic neutron scattering and solid state 2H nuclear magnetic resonance investigation. Journal of Chemical Physics, 1998, 109, 4078-4089.	1.2	33
83	â€œAmorphous Nickel Sulfideâ€•Is Hydrated Nanocrystalline NiS with a Coreâˆ'Shell Structure. Inorganic Chemistry, 2009, 48, 11486-11488.	1.9	32
84	High-Resolution Solid-State²H NMR Spectroscopy of Polymorphs of Glycine. Journal of Physical Chemistry A, 2011, 115, 12201-12211.	1.1	32
85	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
86	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
87	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
88	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
89	Mathematical analysis of intra-stack dimerizations in reactive crystalline solids. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 325.	1.7	30
90	Recognition-Mediated Facilitation of a Disfavored Dielsâˆ'Alder Reaction. Organic Letters, 1999, 1, 1087-1090.	2.4	30

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91	Computational investigation of surface structural relaxation in crystalline urea. Journal of Materials Chemistry, 1995, 5, 133.	6.7	29
92	Structural and dynamic properties of the 1,10-dibromodecane/urea inclusion compound, investigated by variable-temperature powder X-ray diffraction, solid-state2H NMR lineshape analysis and solid-state2H NMR spinâ€“lattice relaxation time measurements. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2179-2185.	1.7	29
93	Design of a Solid Inclusion Compound with Optimal Properties as a Linear Dichroic Filter for X-ray Polarization Analysis. Angewandte Chemie - International Edition, 2003, 42, 2982-2985.	7.2	29
94	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
95	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
96	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
97	Solution of an organic crystal structure from X-ray powder diffraction data by a generalized rigid-body Monte Carlo method: crystal structure determination of 1-methylfluorene. Journal of Materials Chemistry, 1996, 6, 1601.	6.7	26
98	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
99	Crystal engineering of hydrogen-bonded co-crystals between cyanuric acid and â€˜diamideâ€™ molecules. Investigations on the formation and structure of co-crystals containing cyanuric acid and oxalyl dihydrazide. Journal of Materials Chemistry, 1993, 3, 947-952.	6.7	25
100	Dynamics of the Hydrogen-Bonding Arrangement in Solid Triphenylmethanol:â€‰ An Investigation by Solid-State 2H NMR Spectroscopy. Journal of Physical Chemistry B, 1998, 102, 2165-2175.	1.2	25
101	X-ray birefringence imaging. Science, 2014, 344, 1013-1016.	6.0	25
102	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
103	37Cl/35Cl isotope effects in13C NMR spectroscopy of chlorohydrocarbons. Magnetic Resonance in Chemistry, 1993, 31, 54-57.	1.1	24
104	2H NMR lineshape analysis using automated fitting procedures based on local and quasi-global optimization techniques. Magnetic Resonance in Chemistry, 1998, 36, 855-868.	1.1	24
105	Structural understanding of a polymorphic system by structure solution and refinement from powder X-ray diffraction data: the Î± and Î² phases of the latent pigment DPP-Bocâ€Šâ€. Perkin Transactions II RSC, 2000, , 1513-1519.	1.1	24
106	Fine-Tuning the Crystal Morphology of Tunnel Inclusion Compounds:â€‰ A General Strategy. Journal of the American Chemical Society, 2001, 123, 12682-12683.	6.6	24
107	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
108	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

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109	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
110	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
111	Directâ€Space Structure Determination of Covalent Organic Frameworks from 3D Electron Diffraction Data. Angewandte Chemie - International Edition, 2020, 59, 22638-22644.	7.2	23
112	Losing symmetry by design. Nature, 1989, 341, 19-19.	13.7	22
113	High-resolution solid-state 13C and 29Si NMR investigations of the dynamic properties of tetrakis(trimethylsilyl)silane. Journal of the Chemical Society Chemical Communications, 1993, , 251.	2.0	22
114	Ab initio structure determination of a peptide Î²-turn from powder X-ray diffraction data. Chemical Communications, 2001, , 1460-1461.	2.2	22
115	Effects of Polymorphism on Functional Group Dynamics:Â Solid State2H NMR Studies of the Dynamic Properties of the Î± and Î² Phases ofl-Glutamic Acid. Journal of Physical Chemistry A, 2002, 106, 7228-7234.	1.1	22
116	Ammonium Cyanate Shows Nâ^'HÂ·Â·Â·N Hydrogen Bonding, Not Nâ^'HÂ·Â·Â·O. Journal of the American Chemical Society, 2003, 125, 14449-14451.	6.6	22
117	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
118	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
119	The effect of intermolecular hydrogen bonding on the planarity of amides. Physical Chemistry Chemical Physics, 2012, 14, 11944.	1.3	22
120	Structural Properties of the Low-Temperature Phase of the Hexadecane/Urea Inclusion Compound, Investigated by Synchrotron X-ray Powder Diffractionâ€. Journal of Physical Chemistry B, 1997, 101, 9926-9931.	1.2	21
121	Substituent effects on aromatic interactions in the solid state. Chemical Communications, 2001, , 1500-1501.	2.2	21
122	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
123	Probing the Evolution of Adsorption on Nanoporous Solids by In Situ Solid-State NMR Spectroscopy. ChemPhysChem, 2007, 8, 1311-1313.	1.0	21
124	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
125	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
126	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

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127	Polymorphism of l â€Tryptophan. Angewandte Chemie - International Edition, 2019, 58, 18788-18792.	7.2	21
128	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
129	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
130	Materials chemistry communications. Application of the combined maximum entropy and likelihood method to the ab initio determination of an organic crystal structure from X-ray powder diffraction data. Journal of Materials Chemistry, 1992, 2, 1301.	6.7	20
131	Dynamic Properties of Cyclohexane Guest Molecules Constrained within the Zeolite H-ZSM-5 Host Structure:â€‰ A Wide-Line Solid State 2H NMR Investigation. Journal of Physical Chemistry A, 1997, 101, 4541-4547.	1.1	20
132	Unravelling the Disordered Hydrogen Bonding Arrangement in Solid Triphenylmethanol. Journal of Physical Chemistry B, 1999, 103, 6215-6223.	1.2	20
133	A borazaaromatic analogue of isophthalic acid. Perkin Transactions II RSC, 2001, , 2166-2173.	1.1	20
134	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
135	Aluminium-catalysed isocyanate trimerization, enhanced by exploiting a dynamic coordination sphere. Chemical Communications, 2019, 55, 7679-7682.	2.2	20
136	Boronâ€“Nitrogenâ€Doped Nanographenes: A Synthetic Tale from Borazine Precursors. Chemistry - A European Journal, 2020, 26, 6608-6621.	1.7	20
137	Solid-state and solution phase reactivity of 10-hydroxy-10,9-boroxophenanthrene: a model building block for self-assembly processes. New Journal of Chemistry, 2002, 26, 701-710.	1.4	19
138	The Interplay of Aryl-Perfluoroaryl Stacking Interactions and Interstack Hydrogen Bonding in Controlling the Structure of a Molecular Cocrystal. ChemPhysChem, 2003, 4, 766-769.	1.0	19
139	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
140	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
141	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
142	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
143	Significant Conformational Changes Associated with Molecular Transport in a Crystalline Solid. Journal of Physical Chemistry B, 2006, 110, 10708-10713.	1.2	18
144	Structural properties of urea inclusion compounds containing carboxylic acid anhydride guest molecules: anomalous modes of guest-molecule ordering. Journal of Materials Chemistry, 1993, 3, 1085.	6.7	17

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145	Elastic constants of the dioctanoyl peroxide/urea inclusion compound determined by Brillouin scattering. Physical Review B, 1994, 49, 11572-11579.	1.1	17
146	Dynamic properties of the urea molecules in Î±,Ï‰-dibromoalkane/urea inclusion compounds investigated by2H NMR spectroscopy. Journal of Materials Chemistry, 1994, 4, 35-39.	6.7	17
147	Electronic and Local Structural Properties of the Bi2Sr2(Ca1-xYx)Cu2O8+Î´ Family of Materials, Studied by X-ray Absorption Spectroscopy. Chemistry of Materials, 2000, 12, 1115-1121.	3.2	17
148	Polymorphs of a 1:1 Cocrystal with Tunnel and Layer Structures:â€‰ p,pâ€˜-Biphenol/Dimethyl Sulfoxide. Crystal Growth and Design, 2001, 1, 107-111.	1.4	17
149	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
150	Applications of Evolutionary Computation in Structure Determination from Diffraction Data. Structure and Bonding, 0, , 55-94.	1.0	17
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