Graeme Day

List of Publications by Year
in descending order

159	11,871	17405 63	27345 106
papers	citations	h-index	g-index

177	177	177	8719
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Cocrystal Strategy to Tune the Luminescent Properties of Stilbeneâ€Type Organic Solidâ€State Materials. Angewandte Chemie - International Edition, 2011, 50, 12483-12486.	7.2	463
2	Modular and predictable assembly of porous organic molecular crystals. Nature, 2011, 474, 367-371.	13.7	452
3	Improving Mechanical Properties of Crystalline Solids by Cocrystal Formation: New Compressible Forms of Paracetamol. Advanced Materials, 2009, 21, 3905-3909.	11.1	451
4	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
5	A third blind test of crystal structure prediction. Acta Crystallographica Section B: Structural Science, 2005, 61, 511-527.	1.8	373
6	Significant progress in predicting the crystal structures of small organic molecules â€“ a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125.	1.8	371
7	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
8	Functional materials discovery using energyâ€“structureâ€“function maps. Nature, 2017, 543, 657-664.	13.7	348
9	Static and lattice vibrational energy differences between polymorphs. CrystEngComm, 2015, 17, 5154-5165.	1.3	323
10	The Prediction, Morphology, and Mechanical Properties of the Polymorphs of Paracetamol. Journal of the American Chemical Society, 2001, 123, 5086-5094.	6.6	283
11	Modelling organic crystal structures using distributed multipole and polarizability-based model intermolecular potentials. Physical Chemistry Chemical Physics, 2010, 12, 8478.	1.3	268
12	Terahertz time-domain spectroscopy and the quantitative monitoring of mechanochemical cocrystal formation. Nature Materials, 2007, 6, 206-209.	13.3	266
13	Powder Crystallography by Combined Crystal Structure Prediction and High-Resolution ¹H Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2010, 132, 2564-2566.	6.6	201
14	Current approaches to predicting molecular organic crystal structures. Crystallography Reviews, 2011, 17, 3-52.	0.4	196
15	Near-Ideal Xylene Selectivity in Adaptive Molecular Pillar[n]arene Crystals. Journal of the American Chemical Society, 2018, 140, 6921-6930.	6.6	191
16	Onâ€“Off Porosity Switching in a Molecular Organic Solid. Angewandte Chemie - International Edition, 2011, 50, 749-753.	7.2	176
17	De Novo Determination of the Crystal Structure of a Large Drug Molecule by Crystal Structure Prediction-Based Powder NMR Crystallography. Journal of the American Chemical Society, 2013, 135, 17501-17507.	6.6	173
18	Solid-state dynamic combinatorial chemistry: reversibility and thermodynamic product selection in covalent mechanosynthesis. Chemical Science, 2011, 2, 696.	3.7	165

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19	Understanding the Influence of Polymorphism on Phonon Spectra:Â Lattice Dynamics Calculations and Terahertz Spectroscopy of Carbamazepine. Journal of Physical Chemistry B, 2006, 110, 447-456.	1.2	157
20	Powder crystallography of pharmaceutical materials by combined crystal structure prediction and solid-state 1H NMR spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 8069.	1.3	155
21	Machine learning for the structureâ€“energyâ€“property landscapes of molecular crystals. Chemical Science, 2018, 9, 1289-1300.	3.7	153
22	Which conformations make stable crystal structures? Mapping crystalline molecular geometries to the conformational energy landscape. Chemical Science, 2014, 5, 3173-3182.	3.7	148
23	Evaluating the Energetic Driving Force for Cocrystal Formation. Crystal Growth and Design, 2018, 18, 892-904.	1.4	145
24	Interaction of Charge Carriers with Lattice Vibrations in Oligoacene Crystals from Naphthalene to Pentacene. Journal of the American Chemical Society, 2010, 132, 14437-14446.	6.6	128
25	Controlling the Crystallization of Porous Organic Cages: Molecular Analogs of Isoreticular Frameworks Using Shape-Specific Directing Solvents. Journal of the American Chemical Society, 2014, 136, 1438-1448.	6.6	122
26	Reticular synthesis of porous molecular 1D nanotubes and 3D networks. Nature Chemistry, 2017, 9, 17-25.	6.6	122
27	The delicate balance between gelation and crystallisation: structural and computational investigations. Soft Matter, 2010, 6, 4144.	1.2	121
28	Beyond the Isotropic Atom Model in Crystal Structure Prediction of Rigid Molecules:â€‰ Atomic Multipoles versus Point Charges. Crystal Growth and Design, 2005, 5, 1023-1033.	1.4	119
29	The curious case of (caffeine)Â·(benzoic acid): how heteronuclear seeding allowed the formation of an elusive cocrystal. Chemical Science, 2013, 4, 4417.	3.7	115
30	Elastic Constant Calculations for Molecular Organic Crystals. Crystal Growth and Design, 2001, 1, 13-27.	1.4	110
31	Successful prediction of a model pharmaceutical in the fifth blind test of crystal structure prediction. International Journal of Pharmaceutics, 2011, 418, 168-178.	2.6	110
32	Structure Calculation of an Elastic Hydrogel from Sonication of Rigid Small Molecule Components. Angewandte Chemie - International Edition, 2008, 47, 1058-1062.	7.2	107
33	Predicting Intrinsic Aqueous Solubility by a Thermodynamic Cycle. Molecular Pharmaceutics, 2008, 5, 266-279.	2.3	104
34	A strategy for predicting the crystal structures of flexible molecules: the polymorphism of phenobarbital. Physical Chemistry Chemical Physics, 2007, 9, 1693.	1.3	103
35	Interaction of Charge Carriers with Lattice Vibrations in Organic Molecular Semiconductors: Naphthalene as a Case Study. Journal of Physical Chemistry C, 2009, 113, 4679-4686.	1.5	102
36	Testing the Sensitivity of Terahertz Spectroscopy to Changes in Molecular and Supramolecular Structure: A Study of Structurally Similar Cocrystals. Crystal Growth and Design, 2009, 9, 1452-1460.	1.4	99

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37	A Nonempirical Anisotropic Atomâ˜Atom Model Potential for Chlorobenzene Crystals. Journal of the American Chemical Society, 2003, 125, 16434-16443.	6.6	98
38	An Assessment of Lattice Energy Minimization for the Prediction of Molecular Organic Crystal Structures. Crystal Growth and Design, 2004, 4, 1327-1340.	1.4	94
39	Benchmark fragment-based¹H,¹³C,¹⁵N and¹⁷O chemical shift predictions in molecular crystals. Physical Chemistry Chemical Physics, 2016, 18, 21686-21709.	1.3	94
40	Pharmaceutical polymorph control in a drug-mimetic supramolecular gel. Chemical Science, 2017, 8, 78-84.	3.7	94
41	Towards Prediction of Stoichiometry in Crystalline Multicomponent Complexes. Chemistry - A European Journal, 2008, 14, 8830-8836.	1.7	92
42	Prediction and Observation of Isostructurality Induced by Solvent Incorporation in Multicomponent Crystals. Journal of the American Chemical Society, 2006, 128, 14466-14467.	6.6	91
43	Atomistic Calculations of Phonon Frequencies and Thermodynamic Quantities for Crystals of Rigid Organic Molecules. Journal of Physical Chemistry B, 2003, 107, 10919-10933.	1.2	88
44	A study of the known and hypothetical crystal structures of pyridine: why are there four molecules in the asymmetric unit cell?. CrystEngComm, 2002, 4, 348-355.	1.3	86
45	Modeling the interplay of inter- and intramolecular hydrogen bonding in conformational polymorphs. Journal of Chemical Physics, 2008, 128, 244708.	1.2	83
46	Molecular Polarization Effects on the Relative Energies of the Real and Putative Crystal Structures of Valine. Journal of Chemical Theory and Computation, 2008, 4, 1795-1805.	2.3	82
47	Accurate force fields and methods for modelling organic molecular crystals at finite temperatures. Physical Chemistry Chemical Physics, 2016, 18, 15828-15837.	1.3	81
48	Modelling temperature-dependent properties of polymorphic organic molecular crystals. Physical Chemistry Chemical Physics, 2016, 18, 31132-31143.	1.3	81
49	Predicted energyâ€“structureâ€“function maps for the evaluation of small molecule organic semiconductors. Journal of Materials Chemistry C, 2017, 5, 7574-7584.	2.7	81
50	Cocrystallization by Freeze-Drying: Preparation of Novel Multicomponent Crystal Forms. Crystal Growth and Design, 2013, 13, 4599-4606.	1.4	80
51	Large-Scale Computational Screening of Molecular Organic Semiconductors Using Crystal Structure Prediction. Chemistry of Materials, 2018, 30, 4361-4371.	3.2	79
52	Investigating the latent polymorphism of maleic acid. Chemical Communications, 2006, , 54-56.	2.2	78
53	A study into the effect of subtle structural details and disorder on the terahertz spectrum of crystalline benzoic acid. Physical Chemistry Chemical Physics, 2010, 12, 5329.	1.3	78
54	Predicting stoichiometry and structure of solvates. Chemical Communications, 2010, 46, 2224.	2.2	78

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55	Convergence Properties of Crystal Structure Prediction by Quasi-Random Sampling. Journal of Chemical Theory and Computation, 2016, 12, 910-924.	2.3	78
56	In silico Design of Supramolecules from Their Precursors: Oddâ€“Even Effects in Cage-Forming Reactions. Journal of the American Chemical Society, 2013, 135, 9307-9310.	6.6	75
57	Resorcinol Crystallization from the Melt: A New Ambient Phase and New â€œRiddlesâ€• Journal of the American Chemical Society, 2016, 138, 4881-4889.	6.6	74
58	Predicted crystal energy landscapes of porous organic cages. Chemical Science, 2014, 5, 2235-2245.	3.7	73
59	An Expandable Hydrogen-Bonded Organic Framework Characterized by Three-Dimensional Electron Diffraction. Journal of the American Chemical Society, 2020, 142, 12743-12750.	6.6	70
60	Application of computational methods to the design and characterisation of porous molecular materials. Chemical Society Reviews, 2017, 46, 3286-3301.	18.7	68
61	Computationally-Guided Synthetic Control over Pore Size in Isostructural Porous Organic Cages. ACS Central Science, 2017, 3, 734-742.	5.3	68
62	Realizing Predicted Crystal Structures at Extreme Conditions:â€‰ The Low-Temperature and High-Pressure Crystal Structures of 2-Chlorophenol and 4-Fluorophenol. Crystal Growth and Design, 2005, 5, 1055-1071.	1.4	63
63	Solvent inclusion in form II carbamazepine. Chemical Communications, 2007, , 1600.	2.2	62
64	Single-crystal investigation of <scp>L</scp>-tryptophan with Zâ€² = 16. Acta Crystallographica Section B: Structural Science, 2012, 68, 549-557.	1.8	62
65	Predicting Inclusion Behaviour and Framework Structures in Organic Crystals. Chemistry - A European Journal, 2009, 15, 13033-13040.	1.7	61
66	Mining predicted crystal structure landscapes with high throughput crystallisation: old molecules, new insights. Chemical Science, 2019, 10, 9988-9997.	3.7	61
67	Amide Pyramidalization in Carbamazepine:â€‰ A Flexibility Problem in Crystal Structure Prediction?. Crystal Growth and Design, 2006, 6, 1858-1866.	1.4	60
68	Modification of luminescent properties of a coumarin derivative by formation of multi-component crystals. CrystEngComm, 2012, 14, 5121.	1.3	59
69	Importance of Molecular Shape for the Overall Stability of Hydrogen Bond Motifs in the Crystal Structures of Various Carbamazepine-Type Drug Molecules. Crystal Growth and Design, 2007, 7, 100-107.	1.4	52
70	From Concept to Crystals via Prediction: Multiâ€Component Organic Cage Pots by Social Selfâ€Sorting. Angewandte Chemie - International Edition, 2019, 58, 16275-16281.	7.2	52
71	Pseudoracemic amino acid complexes: blind predictions for flexible two-component crystals. Physical Chemistry Chemical Physics, 2010, 12, 8466.	1.3	48
72	Rapid Structure Determination of Molecular Solids Using Chemical Shifts Directed by Unambiguous Prior Constraints. Journal of the American Chemical Society, 2019, 141, 16624-16634.	6.6	47

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73	Determination of the Crystal Structure of a New Polymorph of Theophylline. Chemistry - A European Journal, 2013, 19, 7883-7888.	1.7	46
74	Space group selection for crystal structure prediction of solvates. CrystEngComm, 2007, 9, 556.	1.3	45
75	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€Crystals. Angewandte Chemie - International Edition, 2018, 57, 14906-14910.	7.2	45
76	Photocatalytic proton reduction by a computationally identified, molecular hydrogen-bonded framework. Journal of Materials Chemistry A, 2020, 8, 7158-7170.	5.2	45
77	Energyâ€“Structureâ€“Function Maps: Cartography for Materials Discovery. Advanced Materials, 2018, 30, e1704944.	11.1	44
78	Multifidelity Statistical Machine Learning for Molecular Crystal Structure Prediction. Journal of Physical Chemistry A, 2020, 124, 8065-8078.	1.1	38
79	Structure prediction, disorder and dynamics in a DMSO solvate of carbamazepine. Physical Chemistry Chemical Physics, 2011, 13, 12808.	1.3	36
80	Polymorph Identification and Crystal Structure Determination by a Combined Crystal Structure Prediction and Transmission Electron Microscopy Approach. Chemistry - A European Journal, 2013, 19, 7874-7882.	1.7	34
81	Enhanced NMR Discrimination of Pharmaceutically Relevant Molecular Crystal Forms through Fragment-Based Ab Initio Chemical Shift Predictions. Crystal Growth and Design, 2016, 16, 6479-6493.	1.4	34
82	Minimizing Polymorphic Risk through Cooperative Computational and Experimental Exploration. Journal of the American Chemical Society, 2020, 142, 16668-16680.	6.6	34
83	Computational modelling of solvent effects in a prolific solvatomorphic porous organic cage. Faraday Discussions, 2018, 211, 383-399.	1.6	33
84	Machine-Learned Fragment-Based Energies for Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2019, 15, 2743-2758.	2.3	33
85	Analogy Powered by Prediction and Structural Invariants: Computationally Led Discovery of a Mesoporous Hydrogen-Bonded Organic Cage Crystal. Journal of the American Chemical Society, 2022, 144, 9893-9901.	6.6	33
86	A computational and experimental search for polymorphs of parabanic acid â€“ a salutary tale leading to the crystal structure of oxo-ureido-acetic acid methyl esterElectronic supplementary information (ESI) available: crystal structures of the 16 lattice energy minima in Table 2, in the space group setting used in the minimisation. See http://www.rsc.org/suppdata/ce/b2/b211784c/. CrystEngComm, 2003, 5, 3-9.	1.3	32
87	Dynamics in crystals of rigid organic molecules: contrasting the phonon frequencies calculated by molecular dynamics with harmonic lattice dynamics for imidazole and 5-azauracil. Molecular Physics, 2004, 102, 1067-1083.	0.8	32
88	Crystal packing predictions of the alpha-amino acids: methods assessment and structural observations. CrystEngComm, 2010, 12, 2443.	1.3	32
89	Digital navigation of energyâ€“structureâ€“function maps for hydrogen-bonded porous molecular crystals. Nature Communications, 2021, 12, 817.	5.8	31
90	Database guided conformation selection in crystal structure prediction of alanine. CrystEngComm, 2007, 9, 595.	1.3	30

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91	Substituent interference on supramolecular assembly in urea gelators: synthesis, structure prediction and NMR. Soft Matter, 2016, 12, 4034-4043.	1.2	29
92	Isostructural organic binary-host frameworks with tuneable and diversely decorated inclusion cavities. CrystEngComm, 2012, 14, 7898.	1.3	26
93	Structure prediction of crystals, surfaces and nanoparticles. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190600.	1.6	26
94	Evolutionary chemical space exploration for functional materials: computational organic semiconductor discovery. Chemical Science, 2020, 11, 4922-4933.	3.7	25
95	Structural diversity in imidazolidinone organocatalysts: a synchrotron and computational study. Acta Crystallographica Section C: Crystal Structure Communications, 2008, 64, o10-o14.	0.4	24
96	Rationalization of the Color Properties of Fluorescein in the Solid State: A Combined Computational and Experimental Study. Chemistry - A European Journal, 2016, 22, 10065-10073.	1.7	24
97	An optimized intermolecular force field for hydrogen-bonded organic molecular crystals using atomic multipole electrostatics. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 477-487.	0.5	24
98	Exploring the Multi-minima Behavior of Small Molecule Crystal Polymorphs at Finite Temperature. Crystal Growth and Design, 2019, 19, 5568-5580.	1.4	24
99	Polymorphism of Scyllo-Inositol:â€‰ Joining Crystal Structure Prediction with Experiment to Elucidate the Structures of Two Polymorphs. Crystal Growth and Design, 2006, 6, 2301-2307.	1.4	23
100	From Concept to Crystals via Prediction: Multiâ€Component Organic Cage Pots by Social Selfâ€Sorting. Angewandte Chemie, 2019, 131, 16421-16427.	1.6	23
101	Electronic Excitations in Homopolyatomic Bismuth Cations: Spectroscopic Measurements in Molten Salts and an ab initio CI-Singles Study. Chemistry - A European Journal, 2000, 6, 1078-1086.	1.7	22
102	An Experiment in Crystal Structure Prediction by Popular Vote. Crystal Growth and Design, 2006, 6, 1985-1990.	1.4	22
103	The Plot Thickens: Gelation by Phenylalanine in Water and Dimethyl Sulfoxide. Crystal Growth and Design, 2017, 17, 4100-4109.	1.4	22
104	Solid-State Chemistry and Polymorphism of the Nucleobase Adenine. Crystal Growth and Design, 2016, 16, 3262-3270.	1.4	21
105	Effect of Fluorination on Molecular Conformation in the Solid State: Tuning the Conformation of Cocrystal Formers. Crystal Growth and Design, 2011, 11, 972-981.	1.4	19
106	Is the equilibrium composition of mechanochemical reactions predictable using computational chemistry?. Faraday Discussions, 2014, 170, 41-57.	1.6	19
107	Crystal structure determination of an elusive methanol solvate â€“ hydrate of catechin using crystal structure prediction and NMR crystallography. CrystEngComm, 2020, 22, 4969-4981.	1.3	19
108	Highly Unusual Triangular Crystals of Theophylline: The Influence of Solvent on the Growth Rates of Polar Crystal Faces. Crystal Growth and Design, 2015, 15, 2514-2523.	1.4	18

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109	Clathrate Structure Determination by Combining Crystal Structure Prediction with Computational and Experimental ¹²⁹Xe NMR Spectroscopy. Chemistry - A European Journal, 2017, 23, 5258-5269.	1.7	18
110	Explaining crystallization preferences of two polyphenolic diastereoisomers by crystal structure prediction. CrystEngComm, 2019, 21, 2067-2079.	1.3	18
111	Sensitivity of Morphology Prediction to the Force Field:â€‰ Paracetamol as an Example. Crystal Growth and Design, 2004, 4, 1341-1349.	1.4	17
112	Exploration and Optimization in Crystal Structure Prediction: Combining Basin Hopping with Quasi-Random Sampling. Journal of Chemical Theory and Computation, 2021, 17, 1988-1999.	2.3	17
113	Synthesis, structure, electrostatic properties and spectroscopy of 3-methyl-4,5,6,7-tetrafluoro-1H-indazole. An experimental and ab initio computational studyâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1998, , 2713-2720.	0.9	16
114	Understanding the formation of apremilast cocrystals. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 803-814.	0.5	15
115	The monolayer structure of 1,2-bis(4-pyridyl)ethylene physisorbed on a graphite surface. Molecular Physics, 2013, 111, 73-79.	0.8	14
116	De Novo Crystal Structure Determination from Machine Learned Chemical Shifts. Journal of the American Chemical Society, 2022, 144, 7215-7223.	6.6	14
117	Co-crystallisation of cytosine with 1,10-phenanthroline: computational screening and experimental realisation. CrystEngComm, 2015, 17, 7130-7141.	1.3	13
118	Accelerating computational discovery of porous solids through improved navigation of energy-structure-function maps. Science Advances, 2021, 7, .	4.7	13
119	Introduction to the special issue on crystal structure prediction. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 435-436.	0.5	11
120	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€Crystals. Angewandte Chemie, 2018, 130, 15122-15126.	1.6	10
121	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	1.6	8
122	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	1.6	7
123	Experimental and predicted crystal structures of Pigment Red 168 and other dihalogenated anthanthrones. Acta Crystallographica Section B: Structural Science, 2010, 66, 515-526.	1.8	6
124	Applications of crystal structure prediction â€“ inorganic and network structures: general discussion. Faraday Discussions, 2018, 211, 613-642.	1.6	6
125	Inherent Ethyl Acetate Selectivity in a Trianglimine Molecular Solid. Chemistry - A European Journal, 2021, 27, 10589-10594.	1.7	6
126	Surprising Chemistry of 6-Azidotetrazolo[5,1-a]phthalazine: What a Purported Natural Product Reveals about the Polymorphism of Explosives. Journal of Organic Chemistry, 2022, 87, 6680-6694.	1.7	5

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127	Dynamic behaviour in the solid state. CrystEngComm, 2011, 13, 4303.	1.3	3
128	Computational Methods for the Assignment of Vibrational Modes in Crystalline Materials. Springer Series in Optical Sciences, 2012, , 151-190.	0.5	3
129	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	1.6	3
130	Properties of Crystalline Organic Molecules. , 2001, , 3-50.		3
131	On the effects of basis set truncation and electron correlation in conformers of 2-hydroxy-acetamide. Advances in Quantum Chemistry, 1998, 32, 93-107.	0.4	2
132	Pasteur's tartaramide/malamide quasiracemates: new entries and departures from near inversion symmetry. CrystEngComm, 2018, 20, 4213-4220.	1.3	2
133	Modelling of crystal structure of cis-1,2,3,6 and 3,4,5,6-tetrahydrophthalic anhydrides using lattice energy calculations. Journal of Molecular Modeling, 2015, 21, 211.	0.8	1
134	Correction: Substituent interference on supramolecular assembly in urea gelators: synthesis, structure prediction and NMR. Soft Matter, 2016, 12, 5489-5489.	1.2	1
135	2016 New talent: crystal engineering at its biggest and strongest. CrystEngComm, 2016, 18, 3963-3967.	1.3	1
136	Combining forces: complementary techniques brought together to determine tricky crystal structures. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 294-295.	0.5	1
137	Powder Crystallography by Combining NMR and Crystal Structure Predictions. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C136-C136.	0.0	1
138	Modelling the effect of hydrogen positions on the lattice dynamics calculations of terahertz spectra of benzoic acid. , 2008, , .		0
139	Using terahertz time-domain-spectroscopy to follow the kinetics and mechanism of cocrystal formation. , 2008, , .		0
140	Probing solids through THz spectroscopy: Differentiation of chiral and racemic forms of isostructural and non-isostructural cocrystals. , 2008, , .		0
141	Cover Picture: On-Off Porosity Switching in a Molecular Organic Solid (Angew. Chem. Int. Ed. 3/2011). Angewandte Chemie - International Edition, 2011, 50, 555-555.	7.2	0
142	Towards the computation-led design of porous molecular crystals. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, s108-s108.	0.3	0
143	Finally: the crystal structure ofL-tryptophan. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, s114-s114.	0.3	0
144	Structure prediction of N-heteroacenes as potential organic semiconductors. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1621-C1621.	0.0	0

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145	The exciting life of a small adenine molecule. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s363-s363.	0.0	0
146	Lattice vibrations in molecular crystals: polymorphism and phase transitions. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s127-s127.	0.0	0
147	Computer-guided porous materials design: from rationalization to prediction. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, a289-a289.	0.0	0
148	Crystal energy landscapes of intrinsically porous molecules. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C251-C252.	0.3	0
149	A novel approach to crystal structure determination for organic compounds. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, s109-s109.	0.3	0
150	Mapping crystalline molecular geometries to the conformational energy landscape. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, s154-s154.	0.3	0
151	Towards computer-guided tuning of the crystal packing of porous organic cages. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C667-C667.	0.0	0
152	Insight from energy surfaces: structure prediction by lattice energy exploration. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C28-C28.	0.0	0
153	Predicting Porous Molecular Crystals and Clathrates. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1625-C1625.	0.0	0
154	Ab initio 35Cl solid state NMR-based crystallography of active pharmaceutical ingredients. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s117-s117.	0.0	0
155	Combining experimental and computational techniques for polymorph screening. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a303-a303.	0.0	0
156	Applying fast, accurate lattice energies for molecular crystal structure prediction using CrystalExplorer model energies. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e364-e364.	0.0	0
157	Computation-led discovery of functional molecular materials. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e119-e119.	0.0	0
158	Combining experimental and computational techniques to understand phase transitions of nucleobase adenine. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e158-e158.	0.0	0
159	Determination of elusive crystal structure of solvate-hydrate of catechin by crystal structure prediction and NMR crystallography. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e611-e611.	0.0	0