

Graeme Day

List of Publications by Citations

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140
papers

9,716
citations

58
h-index

96
g-index

177
ext. papers

10,905
ext. citations

7.2
avg, IF

6.35
L-index

#	Paper	IF	Citations
140	Improving Mechanical Properties of Crystalline Solids by Cocrystal Formation: New Compressible Forms of Paracetamol. <i>Advanced Materials</i> , 2009 , 21, 3905-3909	24	404
139	Modular and predictable assembly of porous organic molecular crystals. <i>Nature</i> , 2011 , 474, 367-71	50.4	396
138	A cocrystal strategy to tune the luminescent properties of stilbene-type organic solid-state materials. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 12483-6	16.4	396
137	Report on the sixth blind test of organic crystal structure prediction methods. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016 , 72, 439-59	1.8	338
136	Significant progress in predicting the crystal structures of small organic molecules--a report on the fourth blind test. <i>Acta Crystallographica Section B: Structural Science</i> , 2009 , 65, 107-25		334
135	A third blind test of crystal structure prediction. <i>Acta Crystallographica Section B: Structural Science</i> , 2005 , 61, 511-27		326
134	Towards crystal structure prediction of complex organic compounds--a report on the fifth blind test. <i>Acta Crystallographica Section B: Structural Science</i> , 2011 , 67, 535-51		318
133	Static and lattice vibrational energy differences between polymorphs. <i>CrystEngComm</i> , 2015 , 17, 5154-5155	16.5	249
132	The prediction, morphology, and mechanical properties of the polymorphs of paracetamol. <i>Journal of the American Chemical Society</i> , 2001 , 123, 5086-94	16.4	239
131	Functional materials discovery using energy-structure-function maps. <i>Nature</i> , 2017 , 543, 657-664	50.4	238
130	Modelling organic crystal structures using distributed multipole and polarizability-based model intermolecular potentials. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 8478-90	3.6	231
129	Terahertz time-domain spectroscopy and the quantitative monitoring of mechanochemical cocrystal formation. <i>Nature Materials</i> , 2007 , 6, 206-9	27	225
128	Powder crystallography by combined crystal structure prediction and high-resolution ¹ H solid-state NMR spectroscopy. <i>Journal of the American Chemical Society</i> , 2010 , 132, 2564-6	16.4	175
127	Current approaches to predicting molecular organic crystal structures. <i>Crystallography Reviews</i> , 2011 , 17, 3-52	1.3	169
126	On-off porosity switching in a molecular organic solid. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 749-53	16.4	153
125	Understanding the influence of polymorphism on phonon spectra: lattice dynamics calculations and terahertz spectroscopy of carbamazepine. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 447-56	3.4	145
124	De novo determination of the crystal structure of a large drug molecule by crystal structure prediction-based powder NMR crystallography. <i>Journal of the American Chemical Society</i> , 2013 , 135, 17501-7	16.4	142

123	Powder crystallography of pharmaceutical materials by combined crystal structure prediction and solid-state ¹ H NMR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 8069-80	3.6	134
122	Near-Ideal Xylene Selectivity in Adaptive Molecular Pillar[n]arene Crystals. <i>Journal of the American Chemical Society</i> , 2018 , 140, 6921-6930	16.4	130
121	Solid-state dynamic combinatorial chemistry: reversibility and thermodynamic product selection in covalent mechanosynthesis. <i>Chemical Science</i> , 2011 , 2, 696	9.4	129
120	Which conformations make stable crystal structures? Mapping crystalline molecular geometries to the conformational energy landscape. <i>Chemical Science</i> , 2014 , 5, 3173-3182	9.4	125
119	Interaction of charge carriers with lattice vibrations in oligoacene crystals from naphthalene to pentacene. <i>Journal of the American Chemical Society</i> , 2010 , 132, 14437-46	16.4	113
118	The delicate balance between gelation and crystallisation: structural and computational investigations. <i>Soft Matter</i> , 2010 , 6, 4144	3.6	108
117	Beyond the Isotropic Atom Model in Crystal Structure Prediction of Rigid Molecules: Atomic Multipoles versus Point Charges. <i>Crystal Growth and Design</i> , 2005 , 5, 1023-1033	3.5	106
116	Successful prediction of a model pharmaceutical in the fifth blind test of crystal structure prediction. <i>International Journal of Pharmaceutics</i> , 2011 , 418, 168-78	6.5	105
115	Evaluating the Energetic Driving Force for Cocrystal Formation. <i>Crystal Growth and Design</i> , 2018 , 18, 892-904	3.5	102
114	Structure calculation of an elastic hydrogel from sonication of rigid small molecule components. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 1058-62	16.4	100
113	A strategy for predicting the crystal structures of flexible molecules: the polymorphism of phenobarbital. <i>Physical Chemistry Chemical Physics</i> , 2007 , 9, 1693-704	3.6	98
112	Machine learning for the structure-energy-property landscapes of molecular crystals. <i>Chemical Science</i> , 2018 , 9, 1289-1300	9.4	98
111	The curious case of (caffeine)(benzoic acid): how heteronuclear seeding allowed the formation of an elusive cocrystal. <i>Chemical Science</i> , 2013 , 4, 4417	9.4	97
110	Interaction of Charge Carriers with Lattice Vibrations in Organic Molecular Semiconductors: Naphthalene as a Case Study. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 4679-4686	3.8	97
109	Elastic Constant Calculations for Molecular Organic Crystals. <i>Crystal Growth and Design</i> , 2001 , 1, 13-27	3.5	95
108	Controlling the crystallization of porous organic cages: molecular analogs of isorecticular frameworks using shape-specific directing solvents. <i>Journal of the American Chemical Society</i> , 2014 , 136, 1438-48	16.4	94
107	Predicting intrinsic aqueous solubility by a thermodynamic cycle. <i>Molecular Pharmaceutics</i> , 2008 , 5, 266-296	3.6	91
106	Reticular synthesis of porous molecular 1D nanotubes and 3D networks. <i>Nature Chemistry</i> , 2017 , 9, 17-25	7.6	90

105	A nonempirical anisotropic atom-atom model potential for chlorobenzene crystals. <i>Journal of the American Chemical Society</i> , 2003 , 125, 16434-43	16.4	87
104	An Assessment of Lattice Energy Minimization for the Prediction of Molecular Organic Crystal Structures. <i>Crystal Growth and Design</i> , 2004 , 4, 1327-1340	3.5	84
103	Testing the Sensitivity of Terahertz Spectroscopy to Changes in Molecular and Supramolecular Structure: A Study of Structurally Similar Cocrystals. <i>Crystal Growth and Design</i> , 2009 , 9, 1452-1460	3.5	83
102	Atomistic Calculations of Phonon Frequencies and Thermodynamic Quantities for Crystals of Rigid Organic Molecules. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 10919-10933	3.4	82
101	A Cocrystal Strategy to Tune the Luminescent Properties of Stilbene-Type Organic Solid-State Materials. <i>Angewandte Chemie</i> , 2011 , 123, 12691-12694	3.6	81
100	Prediction and observation of isostructurality induced by solvent incorporation in multicomponent crystals. <i>Journal of the American Chemical Society</i> , 2006 , 128, 14466-7	16.4	80
99	Towards prediction of stoichiometry in crystalline multicomponent complexes. <i>Chemistry - A European Journal</i> , 2008 , 14, 8830-6	4.8	79
98	Modeling the interplay of inter- and intramolecular hydrogen bonding in conformational polymorphs. <i>Journal of Chemical Physics</i> , 2008 , 128, 244708	3.9	78
97	A study of the known and hypothetical crystal structures of pyridine: why are there four molecules in the asymmetric unit cell?. <i>CrystEngComm</i> , 2002 , 4, 348-355	3.3	78
96	Molecular Polarization Effects on the Relative Energies of the Real and Putative Crystal Structures of Valine. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 1795-805	6.4	74
95	Pharmaceutical polymorph control in a drug-mimetic supramolecular gel. <i>Chemical Science</i> , 2017 , 8, 78-84	8.4	72
94	Predicting stoichiometry and structure of solvates. <i>Chemical Communications</i> , 2010 , 46, 2224-6	5.8	72
93	Investigating the latent polymorphism of maleic acid. <i>Chemical Communications</i> , 2006 , 54-6	5.8	72
92	Benchmark fragment-based (1)H, (13)C, (15)N and (17)O chemical shift predictions in molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 21686-709	3.6	70
91	Accurate force fields and methods for modelling organic molecular crystals at finite temperatures. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 15828-37	3.6	67
90	Cocrystallization by Freeze-Drying: Preparation of Novel Multicomponent Crystal Forms. <i>Crystal Growth and Design</i> , 2013 , 13, 4599-4606	3.5	65
89	In silico design of supramolecules from their precursors: odd-even effects in cage-forming reactions. <i>Journal of the American Chemical Society</i> , 2013 , 135, 9307-10	16.4	65
88	A study into the effect of subtle structural details and disorder on the terahertz spectrum of crystalline benzoic acid. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 5329-40	3.6	63

87	Predicted crystal energy landscapes of porous organic cages. <i>Chemical Science</i> , 2014 , 5, 2235-2245	9.4	62
86	On/Off Porosity Switching in a Molecular Organic Solid. <i>Angewandte Chemie</i> , 2011 , 123, 775-779	3.6	61
85	Predicting inclusion behaviour and framework structures in organic crystals. <i>Chemistry - A European Journal</i> , 2009 , 15, 13033-40	4.8	60
84	Modelling temperature-dependent properties of polymorphic organic molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 31132-31143	3.6	59
83	Realizing Predicted Crystal Structures at Extreme Conditions: The Low-Temperature and High-Pressure Crystal Structures of 2-Chlorophenol and 4-Fluorophenol. <i>Crystal Growth and Design</i> , 2005 , 5, 1055-1071	3.5	59
82	Solvent inclusion in form II carbamazepine. <i>Chemical Communications</i> , 2007 , 1600-2	5.8	56
81	Amide Pyramidalization in Carbamazepine: A Flexibility Problem in Crystal Structure Prediction?. <i>Crystal Growth and Design</i> , 2006 , 6, 1858-1866	3.5	56
80	Resorcinol Crystallization from the Melt: A New Ambient Phase and New "Riddles". <i>Journal of the American Chemical Society</i> , 2016 , 138, 4881-9	16.4	55
79	Predicted energy structure function maps for the evaluation of small molecule organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 7574-7584	7.1	55
78	Modification of luminescent properties of a coumarin derivative by formation of multi-component crystals. <i>CrystEngComm</i> , 2012 , 14, 5121	3.3	55
77	Large-Scale Computational Screening of Molecular Organic Semiconductors Using Crystal Structure Prediction. <i>Chemistry of Materials</i> , 2018 , 30, 4361-4371	9.6	53
76	Computationally-Guided Synthetic Control over Pore Size in Isostructural Porous Organic Cages. <i>ACS Central Science</i> , 2017 , 3, 734-742	16.8	51
75	Convergence Properties of Crystal Structure Prediction by Quasi-Random Sampling. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 910-24	6.4	51
74	Application of computational methods to the design and characterisation of porous molecular materials. <i>Chemical Society Reviews</i> , 2017 , 46, 3286-3301	58.5	50
73	Importance of Molecular Shape for the Overall Stability of Hydrogen Bond Motifs in the Crystal Structures of Various Carbamazepine-Type Drug Molecules. <i>Crystal Growth and Design</i> , 2007 , 7, 100-107	3.5	48
72	Single-crystal investigation of L-tryptophan with ZR= 16. <i>Acta Crystallographica Section B: Structural Science</i> , 2012 , 68, 549-57		46
71	Pseudoracemic amino acid complexes: blind predictions for flexible two-component crystals. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 8466-77	3.6	45
70	Determination of the crystal structure of a new polymorph of theophylline. <i>Chemistry - A European Journal</i> , 2013 , 19, 7883-8	4.8	40

69	Mining predicted crystal structure landscapes with high throughput crystallisation: old molecules, new insights. <i>Chemical Science</i> , 2019 , 10, 9988-9997	9.4	36
68	From Concept to Crystals via Prediction: Multi-Component Organic Cage Pots by Social Self-Sorting. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 16275-16281	16.4	35
67	Polymorph identification and crystal structure determination by a combined crystal structure prediction and transmission electron microscopy approach. <i>Chemistry - A European Journal</i> , 2013 , 19, 7874-82	4.8	31
66	Crystal packing predictions of the alpha-amino acids: methods assessment and structural observations. <i>CrystEngComm</i> , 2010 , 12, 2443	3.3	31
65	Dynamics in crystals of rigid organic molecules: contrasting the phonon frequencies calculated by molecular dynamics with harmonic lattice dynamics for imidazole and 5-azauracil. <i>Molecular Physics</i> , 2004 , 102, 1067-1083	1.7	31
64	Structure prediction, disorder and dynamics in a DMSO solvate of carbamazepine. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 12808-16	3.6	30
63	Space group selection for crystal structure prediction of solvates. <i>CrystEngComm</i> , 2007 , 9, 556	3.3	30
62	An Expandable Hydrogen-Bonded Organic Framework Characterized by Three-Dimensional Electron Diffraction. <i>Journal of the American Chemical Society</i> , 2020 , 142, 12743-12750	16.4	28
61	Database guided conformation selection in crystal structure prediction of alanine. <i>CrystEngComm</i> , 2007 , 9, 595	3.3	28
60	A computational and experimental search for polymorphs of parabanic acid 1 a salutary tale leading to the crystal structure of oxo-ureido-acetic acid methyl ester. <i>CrystEngComm</i> , 2003 , 5, 3-9	3.3	28
59	Enhanced NMR Discrimination of Pharmaceutically Relevant Molecular Crystal Forms through Fragment-Based Ab Initio Chemical Shift Predictions. <i>Crystal Growth and Design</i> , 2016 , 16, 6479-6493	3.5	27
58	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acid-Base Co-Crystals. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 14906-14910	16.4	27
57	Rapid Structure Determination of Molecular Solids Using Chemical Shifts Directed by Unambiguous Prior Constraints. <i>Journal of the American Chemical Society</i> , 2019 , 141, 16624-16634	16.4	26
56	Photocatalytic proton reduction by a computationally identified, molecular hydrogen-bonded framework. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 7158-7170	13	26
55	Computational modelling of solvent effects in a prolific solvatomorphic porous organic cage. <i>Faraday Discussions</i> , 2018 , 211, 383-399	3.6	26
54	Energy-Structure-Function Maps: Cartography for Materials Discovery. <i>Advanced Materials</i> , 2018 , 30, e1704944	24	24
53	Structural diversity in imidazolidinone organocatalysts: a synchrotron and computational study. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2008 , 64, o10-4		23
52	Isostructural organic binary-host frameworks with tuneable and diversely decorated inclusion cavities. <i>CrystEngComm</i> , 2012 , 14, 7898	3.3	22

51	Multifidelity Statistical Machine Learning for Molecular Crystal Structure Prediction. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 8065-8078	2.8	22
50	Electronic excitations in homopolyatomic bismuth cations: spectroscopic measurements in molten salts and an ab initio CI-singles study. <i>Chemistry - A European Journal</i> , 2000 , 6, 1078-86	4.8	21
49	Rationalization of the Color Properties of Fluorescein in the Solid State: A Combined Computational and Experimental Study. <i>Chemistry - A European Journal</i> , 2016 , 22, 10065-73	4.8	21
48	An Experiment in Crystal Structure Prediction by Popular Vote. <i>Crystal Growth and Design</i> , 2006 , 6, 1985-1990	3.9	20
47	Machine-Learned Fragment-Based Energies for Crystal Structure Prediction. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 2743-2758	6.4	19
46	An optimized intermolecular force field for hydrogen-bonded organic molecular crystals using atomic multipole electrostatics. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016 , 72, 477-87	1.8	19
45	Effect of Fluorination on Molecular Conformation in the Solid State: Tuning the Conformation of Cocrystal Formers. <i>Crystal Growth and Design</i> , 2011 , 11, 972-981	3.5	19
44	Substituent interference on supramolecular assembly in urea gelators: synthesis, structure prediction and NMR. <i>Soft Matter</i> , 2016 , 12, 4034-43	3.6	19
43	Polymorphism of Scyllo-Inositol: Joining Crystal Structure Prediction with Experiment to Elucidate the Structures of Two Polymorphs. <i>Crystal Growth and Design</i> , 2006 , 6, 2301-2307	3.5	18
42	From Concept to Crystals via Prediction: Multi-Component Organic Cage Pots by Social Self-Sorting. <i>Angewandte Chemie</i> , 2019 , 131, 16421-16427	3.6	17
41	Is the equilibrium composition of mechanochemical reactions predictable using computational chemistry?. <i>Faraday Discussions</i> , 2014 , 170, 41-57	3.6	17
40	Solid-State Chemistry and Polymorphism of the Nucleobase Adenine. <i>Crystal Growth and Design</i> , 2016 , 16, 3262-3270	3.5	17
39	Exploring the Multi-minima Behavior of Small Molecule Crystal Polymorphs at Finite Temperature. <i>Crystal Growth and Design</i> , 2019 , 19, 5568-5580	3.5	16
38	The Plot Thickens: Gelation by Phenylalanine in Water and Dimethyl Sulfoxide. <i>Crystal Growth and Design</i> , 2017 , 17, 4100-4109	3.5	16
37	Synthesis, structure, electrostatic properties and spectroscopy of 3-methyl-4,5,6,7-tetrafluoro-1H-indazole. An experimental and ab initio computational study. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1998 , 2713-2720		16
36	Clathrate Structure Determination by Combining Crystal Structure Prediction with Computational and Experimental Xe NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2017 , 23, 5258-5269	4.8	14
35	Highly Unusual Triangular Crystals of Theophylline: The Influence of Solvent on the Growth Rates of Polar Crystal Faces. <i>Crystal Growth and Design</i> , 2015 , 15, 2514-2523	3.5	14
34	Sensitivity of Morphology Prediction to the Force Field: Paracetamol as an Example. <i>Crystal Growth and Design</i> , 2004 , 4, 1341-1349	3.5	14

33	Explaining crystallization preferences of two polyphenolic diastereoisomers by crystal structure prediction. <i>CrystEngComm</i> , 2019 , 21, 2067-2079	3.3	13
32	Minimizing Polymorphic Risk through Cooperative Computational and Experimental Exploration. <i>Journal of the American Chemical Society</i> , 2020 , 142, 16668-16680	16.4	13
31	Evolutionary chemical space exploration for functional materials: computational organic semiconductor discovery. <i>Chemical Science</i> , 2020 , 11, 4922-4933	9.4	12
30	The monolayer structure of 1,2-bis(4-pyridyl)ethylene physisorbed on a graphite surface. <i>Molecular Physics</i> , 2013 , 111, 73-79	1.7	12
29	Structure prediction of crystals, surfaces and nanoparticles. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2020 , 378, 20190600	3	12
28	Co-crystallisation of cytosine with 1,10-phenanthroline: computational screening and experimental realisation. <i>CrystEngComm</i> , 2015 , 17, 7130-7141	3.3	11
27	Digital navigation of energy-structure-function maps for hydrogen-bonded porous molecular crystals. <i>Nature Communications</i> , 2021 , 12, 817	17.4	11
26	Understanding the formation of apremilast cocrystals. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019 , 75, 803-814	1.8	10
25	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acid-Base Co-Crystals. <i>Angewandte Chemie</i> , 2018 , 130, 15122-15126	3.6	8
24	Crystal structure determination of an elusive methanol solvate hydrate of catechin using crystal structure prediction and NMR crystallography. <i>CrystEngComm</i> , 2020 , 22, 4969-4981	3.3	7
23	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. <i>Faraday Discussions</i> , 2018 , 211, 325-381	3.6	6
22	Applications of crystal structure prediction - organic molecular structures: general discussion. <i>Faraday Discussions</i> , 2018 , 211, 493-539	3.6	6
21	Experimental and predicted crystal structures of Pigment Red 168 and other dihalogenated anthanthrones. <i>Acta Crystallographica Section B: Structural Science</i> , 2010 , 66, 515-26		5
20	Exploration and Optimization in Crystal Structure Prediction: Combining Basin Hopping with Quasi-Random Sampling. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1988-1999	6.4	5
19	Computational Crystal Structure Prediction: Towards In Silico Solid Form Screening		43-66
18	Applications of crystal structure prediction - inorganic and network structures: general discussion. <i>Faraday Discussions</i> , 2018 , 211, 613-642	3.6	4
17	Computational Methods for the Assignment of Vibrational Modes in Crystalline Materials. <i>Springer Series in Optical Sciences</i> , 2012 , 151-190	0.5	3
16	Inherent Ethyl Acetate Selectivity in a Trianglimine Molecular Solid. <i>Chemistry - A European Journal</i> , 2021 , 27, 10589-10594	4.8	3

15	Structure searching methods: general discussion. <i>Faraday Discussions</i> , 2018 , 211, 133-180	3.6	3
14	Advances in Crystal Structure Prediction and Applications to Pharmaceutical Materials 2016 , 87-115		2
13	Pasteur's tartaramide/malamide quasiracemates: new entries and departures from near inversion symmetry. <i>CrystEngComm</i> , 2018 , 20, 4213-4220	3.3	2
12	Properties of Crystalline Organic Molecules 2001 , 3-50		2
11	Accelerating computational discovery of porous solids through improved navigation of energy-structure-function maps. <i>Science Advances</i> , 2021 , 7,	14.3	2
10	Surprising Chemistry of 6-Azidotetrazolo[5,1-]phthalazine: What a Purported Natural Product Reveals about the Polymorphism of Explosives.. <i>Journal of Organic Chemistry</i> , 2022 , 87, 6680-6694	4.2	2
9	Modelling of crystal structure of cis-1,2,3,6 and 3,4,5,6-tetrahydrophthalic anhydrides using lattice energy calculations. <i>Journal of Molecular Modeling</i> , 2015 , 21, 211	2	1
8	Crystal Structure Prediction 2012 ,		1
7	On the effects of basis set truncation and electron correlation in conformers of 2-hydroxy-acetamide. <i>Advances in Quantum Chemistry</i> , 1998 , 32, 93-107	1.4	1
6	Correction: Substituent interference on supramolecular assembly in urea gelators: synthesis, structure prediction and NMR. <i>Soft Matter</i> , 2016 , 12, 5489	3.6	1
5	Combining forces: complementary techniques brought together to determine tricky crystal structures. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020 , 76, 294-295	1.8	0
4	Finally: the crystal structure of L-tryptophan. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2012 , 68, s114-s114		
3	Titelbild: On-Off Porosity Switching in a Molecular Organic Solid (Angew. Chem. 3/2011). <i>Angewandte Chemie</i> , 2011 , 123, 579-579	3.6	
2	Cover Picture: On-Off Porosity Switching in a Molecular Organic Solid (Angew. Chem. Int. Ed. 3/2011). <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 555-555	16.4	
1	Towards the computation-led design of porous molecular crystals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2012 , 68, s108-s108		