Graeme Day

List of Publications by Year
in descending order

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159 papers	11,871 citations	17440 63 h-index	27406 106 g-index
177 all docs	177 docs citations	177 times ranked	8719 citing authors

#	Article	IF	Citations
1	De Novo Crystal Structure Determination from Machine Learned Chemical Shifts. Journal of the American Chemical Society, 2022, 144, 7215-7223.	13.7	14
2	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.	3.2	5
3	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.	13.7	33
4	Digital navigation of energyâ€“structureâ€“function maps for hydrogen-bonded porous molecular crystals. Nature Communications, 2021, 12, 817.	12.8	31
5	Exploration and Optimization in Crystal Structure Prediction: Combining Basin Hopping with Quasi-Random Sampling. Journal of Chemical Theory and Computation, 2021, 17, 1988-1999.	5.3	17
6	Inherent Ethyl Acetate Selectivity in a Trianglimine Molecular Solid. Chemistry - A European Journal, 2021, 27, 10589-10594.	3.3	6
7	Accelerating computational discovery of porous solids through improved navigation of energy-structure-function maps. Science Advances, 2021, 7, .	10.3	13
8	Structure prediction of crystals, surfaces and nanoparticles. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190600.	3.4	26
9	Multifidelity Statistical Machine Learning for Molecular Crystal Structure Prediction. Journal of Physical Chemistry A, 2020, 124, 8065-8078.	2.5	38
10	Minimizing Polymorphic Risk through Cooperative Computational and Experimental Exploration. Journal of the American Chemical Society, 2020, 142, 16668-16680.	13.7	34
11	Photocatalytic proton reduction by a computationally identified, molecular hydrogen-bonded framework. Journal of Materials Chemistry A, 2020, 8, 7158-7170.	10.3	45
12	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.	1.1	1
13	Crystal structure determination of an elusive methanol solvate â€“ hydrate of catechin using crystal structure prediction and NMR crystallography. CrystEngComm, 2020, 22, 4969-4981.	2.6	19
14	An Expandable Hydrogen-Bonded Organic Framework Characterized by Three-Dimensional Electron Diffraction. Journal of the American Chemical Society, 2020, 142, 12743-12750.	13.7	70
15	Evolutionary chemical space exploration for functional materials: computational organic semiconductor discovery. Chemical Science, 2020, 11, 4922-4933.	7.4	25
16	Exploring the Multi-minima Behavior of Small Molecule Crystal Polymorphs at Finite Temperature. Crystal Growth and Design, 2019, 19, 5568-5580.	3.0	24
17	From Concept to Crystals via Prediction: Multiâ€Component Organic Cage Pots by Social Selfâ€Sorting. Angewandte Chemie, 2019, 131, 16421-16427.	2.0	23
18	From Concept to Crystals via Prediction: Multiâ€Component Organic Cage Pots by Social Selfâ€Sorting. Angewandte Chemie - International Edition, 2019, 58, 16275-16281.	13.8	52

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19	Mining predicted crystal structure landscapes with high throughput crystallisation: old molecules, new insights. Chemical Science, 2019, 10, 9988-9997.	7.4	61
20	Explaining crystallization preferences of two polyphenolic diastereoisomers by crystal structure prediction. CrystEngComm, 2019, 21, 2067-2079.	2.6	18
21	Rapid Structure Determination of Molecular Solids Using Chemical Shifts Directed by Unambiguous Prior Constraints. Journal of the American Chemical Society, 2019, 141, 16624-16634.	13.7	47
22	Machine-Learned Fragment-Based Energies for Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2019, 15, 2743-2758.	5.3	33
23	Understanding the formation of apremilast cocrystals. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 803-814.	1.1	15
24	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.	0.1	0
25	Energyâ€“Structureâ€“Function Maps: Cartography for Materials Discovery. Advanced Materials, 2018, 30, e1704944.	21.0	44
26	Machine learning for the structureâ€“energyâ€“property landscapes of molecular crystals. Chemical Science, 2018, 9, 1289-1300.	7.4	153
27	Evaluating the Energetic Driving Force for Cocrystal Formation. Crystal Growth and Design, 2018, 18, 892-904.	3.0	145
28	Applications of crystal structure prediction â€“ inorganic and network structures: general discussion. Faraday Discussions, 2018, 211, 613-642.	3.2	6
29	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€Crystals. Angewandte Chemie, 2018, 130, 15122-15126.	2.0	10
30	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€Crystals. Angewandte Chemie - International Edition, 2018, 57, 14906-14910.	13.8	45
31	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	3.2	3
32	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	3.2	7
33	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	3.2	8
34	Computational modelling of solvent effects in a prolific solvatomorphic porous organic cage. Faraday Discussions, 2018, 211, 383-399.	3.2	33
35	Pasteur's tartaramide/malamide quasiracemates: new entries and departures from near inversion symmetry. CrystEngComm, 2018, 20, 4213-4220.	2.6	2
36	Near-Ideal Xylene Selectivity in Adaptive Molecular Pillar[n]arene Crystals. Journal of the American Chemical Society, 2018, 140, 6921-6930.	13.7	191

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37	Large-Scale Computational Screening of Molecular Organic Semiconductors Using Crystal Structure Prediction. Chemistry of Materials, 2018, 30, 4361-4371.	6.7	79
38	Combining experimental and computational techniques for polymorph screening. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a303-a303.	0.1	0
39	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.	0.1	0
40	Computation-led discovery of functional molecular materials. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e119-e119.	0.1	0
41	Combining experimental and computational techniques to understand phase transitions of nucleobase adenine. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e158-e158.	0.1	0
42	Clathrate Structure Determination by Combining Crystal Structure Prediction with Computational and Experimental ¹²⁹Xe NMR Spectroscopy. Chemistry - A European Journal, 2017, 23, 5258-5269.	3.3	18
43	Application of computational methods to the design and characterisation of porous molecular materials. Chemical Society Reviews, 2017, 46, 3286-3301.	38.1	68
44	Computationally-Guided Synthetic Control over Pore Size in Isostructural Porous Organic Cages. ACS Central Science, 2017, 3, 734-742.	11.3	68
45	Functional materials discovery using energyâ€“structureâ€“function maps. Nature, 2017, 543, 657-664.	27.8	348
46	Predicted energyâ€“structureâ€“function maps for the evaluation of small molecule organic semiconductors. Journal of Materials Chemistry C, 2017, 5, 7574-7584.	5.5	81
47	The Plot Thickens: Gelation by Phenylalanine in Water and Dimethyl Sulfoxide. Crystal Growth and Design, 2017, 17, 4100-4109.	3.0	22
48	Pharmaceutical polymorph control in a drug-mimetic supramolecular gel. Chemical Science, 2017, 8, 78-84.	7.4	94
49	Reticular synthesis of porous molecular 1D nanotubes and 3D networks. Nature Chemistry, 2017, 9, 17-25.	13.6	122
50	Computer-guided porous materials design: from rationalization to prediction. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, a289-a289.	0.1	0
51	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.	3.3	24
52	Correction: Substituent interference on supramolecular assembly in urea gelators: synthesis, structure prediction and NMR. Soft Matter, 2016, 12, 5489-5489.	2.7	1
53	The exciting life of a small adenine molecule. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s363-s363.	0.1	0
54	Substituent interference on supramolecular assembly in urea gelators: synthesis, structure prediction and NMR. Soft Matter, 2016, 12, 4034-4043.	2.7	29

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55	Accurate force fields and methods for modelling organic molecular crystals at finite temperatures. Physical Chemistry Chemical Physics, 2016, 18, 15828-15837.	2.8	81
56	2016 New talent: crystal engineering at its biggest and strongest. CrystEngComm, 2016, 18, 3963-3967.	2.6	1
57	Solid-State Chemistry and Polymorphism of the Nucleobase Adenine. Crystal Growth and Design, 2016, 16, 3262-3270.	3.0	21
58	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.	3.0	34
59	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.	1.1	445
60	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.	1.1	24
61	Introduction to the special issue on crystal structure prediction. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 435-436.	1.1	11
62	Benchmark fragment-based¹H,¹³C,¹⁵N and¹⁷O chemical shift predictions in molecular crystals. Physical Chemistry Chemical Physics, 2016, 18, 21686-21709.	2.8	94
63	Modelling temperature-dependent properties of polymorphic organic molecular crystals. Physical Chemistry Chemical Physics, 2016, 18, 31132-31143.	2.8	81
64	Lattice vibrations in molecular crystals: polymorphism and phase transitions. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s127-s127.	0.1	0
65	Convergence Properties of Crystal Structure Prediction by Quasi-Random Sampling. Journal of Chemical Theory and Computation, 2016, 12, 910-924.	5.3	78
66	Resorcinol Crystallization from the Melt: A New Ambient Phase and New â€œRiddlesâ€• Journal of the American Chemical Society, 2016, 138, 4881-4889.	13.7	74
67	Ab initio 35Cl solid state NMR-based crystallography of active pharmaceutical ingredients. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s117-s117.	0.1	0
68	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.	1.8	1
69	Static and lattice vibrational energy differences between polymorphs. CrystEngComm, 2015, 17, 5154-5165.	2.6	323
70	Co-crystallisation of cytosine with 1,10-phenanthroline: computational screening and experimental realisation. CrystEngComm, 2015, 17, 7130-7141.	2.6	13
71	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.	3.0	18
72	Is the equilibrium composition of mechanochemical reactions predictable using computational chemistry?. Faraday Discussions, 2014, 170, 41-57.	3.2	19

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73	Predicted crystal energy landscapes of porous organic cages. Chemical Science, 2014, 5, 2235-2245.	7.4	73
74	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.	13.7	122
75	Which conformations make stable crystal structures? Mapping crystalline molecular geometries to the conformational energy landscape. Chemical Science, 2014, 5, 3173-3182.	7.4	148
76	Structure prediction of N-heteroacenes as potential organic semiconductors. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1621-C1621.	0.1	0
77	Powder Crystallography by Combining NMR and Crystal Structure Predictions. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C136-C136.	0.1	1
78	Towards computer-guided tuning of the crystal packing of porous organic cages. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C667-C667.	0.1	0
79	Insight from energy surfaces: structure prediction by lattice energy exploration. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C28-C28.	0.1	0
80	Predicting Porous Molecular Crystals and Clathrates. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1625-C1625.	0.1	0
81	Cocrystallization by Freeze-Drying: Preparation of Novel Multicomponent Crystal Forms. Crystal Growth and Design, 2013, 13, 4599-4606.	3.0	80
82	The curious case of (caffeine)Â·(benzoic acid): how heteronuclear seeding allowed the formation of an elusive cocrystal. Chemical Science, 2013, 4, 4417.	7.4	115
83	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.	13.7	173
84	The monolayer structure of 1,2-bis(4-pyridyl)ethylene physisorbed on a graphite surface. Molecular Physics, 2013, 111, 73-79.	1.7	14
85	Powder crystallography of pharmaceutical materials by combined crystal structure prediction and solid-state 1H NMR spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 8069.	2.8	155
86	Determination of the Crystal Structure of a New Polymorph of Theophylline. Chemistry - A European Journal, 2013, 19, 7883-7888.	3.3	46
87	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.	13.7	75
88	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.	3.3	34
89	Mapping crystalline molecular geometries to the conformational energy landscape. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, s154-s154.	0.3	0
90	Towards the computation-led design of porous molecular crystals. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, s108-s108.	0.3	0

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91	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
92	Isostructural organic binary-host frameworks with tuneable and diversely decorated inclusion cavities. CrystEngComm, 2012, 14, 7898.	2.6	26
93	Computational Methods for the Assignment of Vibrational Modes in Crystalline Materials. Springer Series in Optical Sciences, 2012, , 151-190.	0.7	3
94	Finally: the crystal structure ofL-tryptophan. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, s114-s114.	0.3	0
95	Modification of luminescent properties of a coumarin derivative by formation of multi-component crystals. CrystEngComm, 2012, 14, 5121.	2.6	59
96	A novel approach to crystal structure determination for organic compounds. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, s109-s109.	0.3	0
97	Structure prediction, disorder and dynamics in a DMSO solvate of carbamazepine. Physical Chemistry Chemical Physics, 2011, 13, 12808.	2.8	36
98	Dynamic behaviour in the solid state. CrystEngComm, 2011, 13, 4303.	2.6	3
99	Current approaches to predicting molecular organic crystal structures. Crystallography Reviews, 2011, 17, 3-52.	1.5	196
100	Effect of Fluorination on Molecular Conformation in the Solid State: Tuning the Conformation of Cocrystal Formers. Crystal Growth and Design, 2011, 11, 972-981.	3.0	19
101	Solid-state dynamic combinatorial chemistry: reversibility and thermodynamic product selection in covalent mechanosynthesis. Chemical Science, 2011, 2, 696.	7.4	165
102	Successful prediction of a model pharmaceutical in the fifth blind test of crystal structure prediction. International Journal of Pharmaceutics, 2011, 418, 168-178.	5.2	110
103	Modular and predictable assembly of porous organic molecular crystals. Nature, 2011, 474, 367-371.	27.8	452
104	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
105	Onâ€“Off Porosity Switching in a Molecular Organic Solid. Angewandte Chemie - International Edition, 2011, 50, 749-753.	13.8	176
106	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.	13.8	0
107	A Cocrystal Strategy to Tune the Luminescent Properties of Stilbeneâ€Type Organic Solidâ€State Materials. Angewandte Chemie - International Edition, 2011, 50, 12483-12486.	13.8	463
108	Crystal energy landscapes of intrinsically porous molecules. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C251-C252.	0.3	0

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109	Modelling organic crystal structures using distributed multipole and polarizability-based model intermolecular potentials. Physical Chemistry Chemical Physics, 2010, 12, 8478.	2.8	268
110	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.	13.7	201
111	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
112	Pseudoracemic amino acid complexes: blind predictions for flexible two-component crystals. Physical Chemistry Chemical Physics, 2010, 12, 8466.	2.8	48
113	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.	2.8	78
114	Crystal packing predictions of the alpha-amino acids: methods assessment and structural observations. CrystEngComm, 2010, 12, 2443.	2.6	32
115	Predicting stoichiometry and structure of solvates. Chemical Communications, 2010, 46, 2224.	4.1	78
116	The delicate balance between gelation and crystallisation: structural and computational investigations. Soft Matter, 2010, 6, 4144.	2.7	121
117	Interaction of Charge Carriers with Lattice Vibrations in Oligoacene Crystals from Naphthalene to Pentacene. Journal of the American Chemical Society, 2010, 132, 14437-14446.	13.7	128
118	Improving Mechanical Properties of Crystalline Solids by Cocrystal Formation: New Compressible Forms of Paracetamol. Advanced Materials, 2009, 21, 3905-3909.	21.0	451
119	Predicting Inclusion Behaviour and Framework Structures in Organic Crystals. Chemistry - A European Journal, 2009, 15, 13033-13040.	3.3	61
120	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
121	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.	3.0	99
122	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.	3.1	102
123	Structural diversity in imidazolidinone organocatalysts: a synchrotron and computational study. Acta Crystallographica Section C: Crystal Structure Communications, 2008, 64, o10-o14.	0.4	24
124	Towards Prediction of Stoichiometry in Crystalline Multicomponent Complexes. Chemistry - A European Journal, 2008, 14, 8830-8836.	3.3	92
125	Structure Calculation of an Elastic Hydrogel from Sonication of Rigid Small Molecule Components. Angewandte Chemie - International Edition, 2008, 47, 1058-1062.	13.8	107
126	Modeling the interplay of inter- and intramolecular hydrogen bonding in conformational polymorphs. Journal of Chemical Physics, 2008, 128, 244708.	3.0	83

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127	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.	5.3	82
128	Predicting Intrinsic Aqueous Solubility by a Thermodynamic Cycle. Molecular Pharmaceutics, 2008, 5, 266-279.	4.6	104
129	Modelling the effect of hydrogen positions on the lattice dynamics calculations of terahertz spectra of benzoic acid. , 2008, , .		0
130	Using terahertz time-domain-spectroscopy to follow the kinetics and mechanism of cocrystal formation. , 2008, , .		0
131	Probing solids through THz spectroscopy: Differentiation of chiral and racemic forms of isostructural and non-isostructural cocrystals. , 2008, , .		0
132	Solvent inclusion in form II carbamazepine. Chemical Communications, 2007, , 1600.	4.1	62
133	Database guided conformation selection in crystal structure prediction of alanine. CrystEngComm, 2007, 9, 595.	2.6	30
134	Space group selection for crystal structure prediction of solvates. CrystEngComm, 2007, 9, 556.	2.6	45
135	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.	3.0	52
136	A strategy for predicting the crystal structures of flexible molecules: the polymorphism of phenobarbital. Physical Chemistry Chemical Physics, 2007, 9, 1693.	2.8	103
137	Terahertz time-domain spectroscopy and the quantitative monitoring of mechanochemical cocrystal formation. Nature Materials, 2007, 6, 206-209.	27.5	266
138	Prediction and Observation of Isostructurality Induced by Solvent Incorporation in Multicomponent Crystals. Journal of the American Chemical Society, 2006, 128, 14466-14467.	13.7	91
139	Investigating the latent polymorphism of maleic acid. Chemical Communications, 2006, , 54-56.	4.1	78
140	An Experiment in Crystal Structure Prediction by Popular Vote. Crystal Growth and Design, 2006, 6, 1985-1990.	3.0	22
141	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.	3.0	23
142	Amide Pyramidalization in Carbamazepine:â€‰ A Flexibility Problem in Crystal Structure Prediction?. Crystal Growth and Design, 2006, 6, 1858-1866.	3.0	60
143	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.	2.6	157
144	A third blind test of crystal structure prediction. Acta Crystallographica Section B: Structural Science, 2005, 61, 511-527.	1.8	373

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145	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.	3.0	63
146	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.	3.0	119
147	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.	1.7	32
148	Sensitivity of Morphology Prediction to the Force Field:â€‰ Paracetamol as an Example. Crystal Growth and Design, 2004, 4, 1341-1349.	3.0	17
149	An Assessment of Lattice Energy Minimization for the Prediction of Molecular Organic Crystal Structures. Crystal Growth and Design, 2004, 4, 1327-1340.	3.0	94
150	A Nonempirical Anisotropic Atomâ^'Atom Model Potential for Chlorobenzene Crystals. Journal of the American Chemical Society, 2003, 125, 16434-16443.	13.7	98
151	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.	2.6	32
152	Atomistic Calculations of Phonon Frequencies and Thermodynamic Quantities for Crystals of Rigid Organic Molecules. Journal of Physical Chemistry B, 2003, 107, 10919-10933.	2.6	88
153	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.	2.6	86
154	The Prediction, Morphology, and Mechanical Properties of the Polymorphs of Paracetamol. Journal of the American Chemical Society, 2001, 123, 5086-5094.	13.7	283
155	Elastic Constant Calculations for Molecular Organic Crystals. Crystal Growth and Design, 2001, 1, 13-27.	3.0	110
156	Properties of Crystalline Organic Molecules. , 2001, , 3-50.		3
157	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.	3.3	22
158	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
159	On the effects of basis set truncation and electron correlation in conformers of 2-hydroxy-acetamide. Advances in Quantum Chemistry, 1998, 32, 93-107.	0.8	2