SarahÂ L Price

List of Publications by Year
in descending order

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189 papers	13,039 citations	19657 61 h-index	25787 108 g-index
196 all docs	196 docs citations	196 times ranked	7505 citing authors

#	Article	IF	Citations
1	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
2	Predicting crystal structures of organic compounds. Chemical Society Reviews, 2014, 43, 2098-2111.	38.1	421
3	A test of crystal structure prediction of small organic molecules. Acta Crystallographica Section B: Structural Science, 2000, 56, 697-714.	1.8	376
4	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
5	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
6	Crystal structure prediction of small organic molecules: a second blind test. Acta Crystallographica Section B: Structural Science, 2002, 58, 647-661.	1.8	334
7	Computed Crystal Energy Landscapes for Understanding and Predicting Organic Crystal Structures and Polymorphism. Accounts of Chemical Research, 2009, 42, 117-126.	15.6	333
8	Amino/Aromatic Interactions in Proteins: Is the Evidence Stacked Against Hydrogen Bonding?. Journal of Molecular Biology, 1994, 239, 315-331.	4.2	319
9	The Prediction, Morphology, and Mechanical Properties of the Polymorphs of Paracetamol. Journal of the American Chemical Society, 2001, 123, 5086-5094.	13.7	283
10	Role of Electrostatic Interactions in Determining the Crystal Structures of Polar Organic Molecules. A Distributed Multipole Study. The Journal of Physical Chemistry, 1996, 100, 7352-7360.	2.9	280
11	Modelling organic crystal structures using distributed multipole and polarizability-based model intermolecular potentials. Physical Chemistry Chemical Physics, 2010, 12, 8478.	2.8	268
12	Innovation in crystal engineeringÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂ. CrystEngComm, 2002, 4, 500-509.	2.6	235
13	The computational prediction of pharmaceutical crystal structures and polymorphism. Advanced Drug Delivery Reviews, 2004, 56, 301-319.	13.7	215
14	Hydrogen bonding of carbonyl, ether, and ester oxygen atoms with alkanol hydroxyl groups. Journal of Computational Chemistry, 1997, 18, 757-774.	3.3	195
15	Salt or Cocrystal? A New Series of Crystal Structures Formed from Simple Pyridines and Carboxylic Acids. Crystal Growth and Design, 2009, 9, 2881-2889.	3.0	183
16	Role of the crystal-field theory in determining the structures of spinels. Journal of the American Chemical Society, 1982, 104, 92-95.	13.7	181
17	Why don't we find more polymorphs?. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2013, 69, 313-328.	1.1	179
18	A strategy for producing predicted polymorphs: catemeric carbamazepine form V. Chemical Communications, 2011, 47, 7074.	4.1	176

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19	A New Polymorph of 5-Fluorouracil Found Following Computational Crystal Structure Predictions. Journal of the American Chemical Society, 2005, 127, 1116-1117.	13.7	164
20	From crystal structure prediction to polymorph prediction: interpreting the crystal energy landscape. Physical Chemistry Chemical Physics, 2008, 10, 1996.	2.8	159
21	Toward Crystal Structure Prediction for Conformationally Flexible Molecules:â€‰ The Headaches Illustrated by Aspirin. Crystal Growth and Design, 2004, 4, 1119-1127.	3.0	154
22	Can computed crystal energy landscapes help understand pharmaceutical solids?. Chemical Communications, 2016, 52, 7065-7077.	4.1	146
23	Can the Formation of Pharmaceutical Cocrystals Be Computationally Predicted? I. Comparison of Lattice Energies. Crystal Growth and Design, 2009, 9, 442-453.	3.0	141
24	Dimer or Catemer? Low-Energy Crystal Packings for Small Carboxylic Acids. Journal of Physical Chemistry B, 2000, 104, 2647-2655.	2.6	140
25	Grid Service Orchestration Using the Business Process Execution Language (BPEL). Journal of Grid Computing, 2005, 3, 283-304.	3.9	123
26	Exploring the Experimental and Computed Crystal Energy Landscape of Olanzapine. Crystal Growth and Design, 2013, 13, 1602-1617.	3.0	123
27	Ab Initio Calculations on Uracilâ‹¯Water. Journal of Physical Chemistry A, 1999, 103, 1611-1618.	2.5	119
28	Can the Formation of Pharmaceutical Cocrystals Be Computationally Predicted? 2. Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2009, 5, 1432-1448.	5.3	118
29	Molecular Conformations and Relative Stabilities Can Be as Demanding of the Electronic Structure Method as Intermolecular Calculations. Journal of Physical Chemistry A, 2006, 110, 8-12.	2.5	115
30	An Automated Parallel Crystallisation Search for Predicted Crystal Structures and Packing Motifs of Carbamazepine. Journal of Pharmaceutical Sciences, 2006, 95, 1918-1930.	3.3	114
31	Elastic Constant Calculations for Molecular Organic Crystals. Crystal Growth and Design, 2001, 1, 13-27.	3.0	110
32	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
33	A Prolific Solvate Former, Galunisertib, under the Pressure of Crystal Structure Prediction, Produces Ten Diverse Polymorphs. Journal of the American Chemical Society, 2019, 141, 13887-13897.	13.7	109
34	Kinetic Insights into the Role of the Solvent in the Polymorphism of 5-Fluorouracil from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 3323-3329.	2.6	107
35	The nature of the N ? H?O?C hydrogen bond: An intermolecular perturbation theory study of the formamide/formaldehyde complex. Journal of Computational Chemistry, 1990, 11, 1217-1233.	3.3	104
36	An overlap model for estimating the anisotropy of repulsion. Molecular Physics, 1990, 69, 507-533.	1.7	103

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37	Towards an understanding of the arginine-aspartate interaction. Journal of Molecular Biology, 1992, 226, 251-262.	4.2	103
38	Computational prediction of organic crystal structures and polymorphism. International Reviews in Physical Chemistry, 2008, 27, 541-568.	2.3	103
39	A Nonempirical Anisotropic Atomâ˜Atom Model Potential for Chlorobenzene Crystals. Journal of the American Chemical Society, 2003, 125, 16434-16443.	13.7	98
40	Applications of realistic electrostatic modelling to molecules in complexes, solids and proteins. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2997.	1.7	97
41	Complex Polymorphic System of Gallic Acidâ€”Five Monohydrates, Three Anhydrates, and over 20 Solvates. Crystal Growth and Design, 2013, 13, 19-23.	3.0	97
42	The Determination of the Crystal Structure of Anhydrous Theophylline by X-ray Powder Diffraction with a Systematic Search Algorithm, Lattice Energy Calculations, and13C and15N Solid-State NMR:Â A Question of Polymorphism in a Given Unit Cell. Journal of Physical Chemistry B, 2001, 105, 5818-5826.	2.6	92
43	Which, if any, hydrates will crystallise? Predicting hydrate formation of two dihydroxybenzoic acids. Chemical Communications, 2011, 47, 5443-5445.	4.1	92
44	The potential of computed crystal energy landscapes to aid solid-form development. Drug Discovery Today, 2016, 21, 912-923.	6.4	91
45	Ab initio and diffusion Monte Carlo study of uracilâ€“water, thymineâ€“water, cytosineâ€“water, and cytosineâ€“(water)2. Physical Chemistry Chemical Physics, 2000, 2, 1281-1290.	2.8	88
46	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
47	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
48	Crystal structure predictions for acetic acid. Journal of Computational Chemistry, 1998, 19, 459-474.	3.3	85
49	Energy Minimization of Crystal Structures Containing Flexible Molecules. Journal of Chemical Theory and Computation, 2006, 2, 1184-1199.	5.3	83
50	Modeling the interplay of inter- and intramolecular hydrogen bonding in conformational polymorphs. Journal of Chemical Physics, 2008, 128, 244708.	3.0	83
51	A first principles prediction of the crystal structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si4.gif" display="inline" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mspace width="0.35em" height="0.8ex" /><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>6</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mrow	2.6	79
	Chemical Physics Letters, 2008, 456, 105-109.		
52	Is zeroth order crystal structure prediction (CSP_0) coming to maturity? What should we aim for in an ideal crystal structure prediction code?. Faraday Discussions, 2018, 211, 9-30.	3.2	78
53	Accurate Induction Energies for Small Organic Molecules. 2. Development and Testing of Distributed Polarizability Models against SAPT(DFT) Energies. Journal of Chemical Theory and Computation, 2008, 4, 19-32.	5.3	77
54	Toward a Molecular Understanding of Crystal Agglomeration. Crystal Growth and Design, 2005, 5, 3-16.	3.0	75

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55	Carbamazepine Co-crystallization with Pyridine Carboxamides: Rationalization by Complementary Phase Diagrams and Crystal Energy Landscapes. Crystal Growth and Design, 2010, 10, 903-912.	3.0	75
56	The polymorphism of progesterone: Stabilization of a â€˜disappearingâ€™ polymorph by coâ€crystallization. Journal of Pharmaceutical Sciences, 2007, 96, 3419-3431.	3.3	72
57	Contrasting Polymorphism of Related Small Molecule Drugs Correlated and Guided by the Computed Crystal Energy Landscape. Crystal Growth and Design, 2014, 14, 2056-2072.	3.0	72
58	An Experimental and Theoretical Search for Polymorphs of Barbituric Acid:â€‰ The Challenges of Even Limited Conformational Flexibility. Crystal Growth and Design, 2004, 4, 979-987.	3.0	70
59	Factors influencing solid-state structureâ€”an analysis using pseudopotential radii structural maps. Physical Review B, 1981, 24, 2903-2912.	3.2	69
60	On the relative strengths of amideâ€¦amide and amideâ€¦water hydrogen bonds. Chemical Physics Letters, 1991, 180, 517-523.	2.6	64
61	The Thermal Stability of Lattice-Energy Minima of 5-Fluorouracil:Â Metadynamics as an Aid to Polymorph Prediction. Journal of Physical Chemistry B, 2008, 112, 4298-4308.	2.6	64
62	Navigating the Waters of Unconventional Crystalline Hydrates. Molecular Pharmaceutics, 2015, 12, 3069-3088.	4.6	62
63	Electrostatic models for polypeptides: can we assume transferability?. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 1755.	1.7	61
64	Predictions of Crystal Packings for Uracil, 6-Azauracil, and Allopurinol:Â The Interplay between Hydrogen Bonding and Close Packing. Journal of Physical Chemistry A, 1997, 101, 2198-2206.	2.5	61
65	Three Polymorphs of 2-Amino-5-nitropyrimidine:Â Experimental Structures and Theoretical Predictions. Journal of the American Chemical Society, 1998, 120, 8986-8993.	13.7	61
66	Which organic crystal structures are predictable by lattice energy minimisation?. CrystEngComm, 2001, 3, 178-212.	2.6	61
67	Search for a Predicted Hydrogen Bonding Motif â^’ A Multidisciplinary Investigation into the Polymorphism of 3-Azabicyclo[3.3.1]nonane-2,4-dione. Journal of the American Chemical Society, 2007, 129, 3649-3657.	13.7	61
68	Carbonic Acid:â€‰ From Polyamorphism to Polymorphism. Journal of the American Chemical Society, 2007, 129, 13863-13871.	13.7	61
69	Computational prediction of salt and cocrystal structuresâ€”Does a proton position matter?. International Journal of Pharmaceutics, 2011, 418, 187-198.	5.2	60
70	The Complexity of Hydration of Phloroglucinol: A Comprehensive Structural and Thermodynamic Characterization. Journal of Physical Chemistry B, 2012, 116, 3961-3972.	2.6	60
71	Quantifying intermolecular interactions and their use in computational crystal structure prediction. CrystEngComm, 2004, 6, 344.	2.6	59
72	Evaluating a Crystal Energy Landscape in the Context of Industrial Polymorph Screening. Crystal Growth and Design, 2013, 13, 2396-2406.	3.0	58

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73	Are the Crystal Structures of Enantiopure and Racemic Mandelic Acids Determined by Kinetics or Thermodynamics?. Journal of the American Chemical Society, 2015, 137, 11095-11104.	13.7	57
74	Isomorphous template induced crystallisation: a robust method for the targeted crystallisation of computationally predicted metastable polymorphs. Chemical Communications, 2016, 52, 7384-7386.	4.1	57
75	A systematic intermolecular potential method applied to chlorine. Molecular Physics, 1990, 71, 1381-1404.	1.7	56
76	Is the Fenamate Group a Polymorphophore? Contrasting the Crystal Energy Landscapes of Fenamic and Tolfenamic Acids. Crystal Growth and Design, 2012, 12, 4230-4239.	3.0	56
77	Is the Induction Energy Important for Modeling Organic Crystals?. Journal of Chemical Theory and Computation, 2008, 4, 522-532.	5.3	55
78	Solid-State Forms of Î²-Resorcylic Acid: How Exhaustive Should a Polymorph Screen Be?. Crystal Growth and Design, 2011, 11, 210-220.	3.0	55
79	Validation of a search technique for crystal structure prediction of flexible molecules by application to piracetam. Acta Crystallographica Section B: Structural Science, 2005, 61, 558-568.	1.8	54
80	Electrostatic factors in DNA intercalation. Biopolymers, 1999, 52, 84-93.	2.4	53
81	Racemic Naproxen: A Multidisciplinary Structural and Thermodynamic Comparison with the Enantiopure Form. Crystal Growth and Design, 2011, 11, 5659-5669.	3.0	53
82	Characterization of Complicated New Polymorphs of Chlorothalonil by X-ray Diffraction and Computer Crystal Structure Prediction. Journal of the American Chemical Society, 2004, 126, 7071-7081.	13.7	52
83	Calculation of Attachment Energies and Relative Volume Growth Rates As an Aid to Polymorph Prediction. Crystal Growth and Design, 2005, 5, 879-885.	3.0	52
84	Toward the Prediction of Organic Hydrate Crystal Structures. Journal of Chemical Theory and Computation, 2007, 3, 1597-1608.	5.3	52
85	Successful Computationally Directed Templating of Metastable Pharmaceutical Polymorphs. Crystal Growth and Design, 2018, 18, 5322-5331.	3.0	52
86	Amino/aromatic interactions. Nature, 1993, 366, 413-413.	27.8	50
87	Challenges of Crystal Structure Prediction of Diastereomeric Salt Pairs. Journal of Physical Chemistry B, 2005, 109, 17134-17150.	2.6	50
88	Thermal Expansion of Carbamazepine: Systematic Crystallographic Measurements Challenge Quantum Chemical Calculations. Journal of Physical Chemistry Letters, 2017, 8, 4319-4324.	4.6	50
89	Investigating Unused Hydrogen Bond Acceptors Using Known and Hypothetical Crystal Polymorphism. Crystal Growth and Design, 2005, 5, 983-993.	3.0	49
90	Predictable Disorder versus Polymorphism in the Rationalization of Structural Diversity: A Multidisciplinary Study of Eniluracil. Crystal Growth and Design, 2008, 8, 3474-3481.	3.0	49

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91	Substitutional and orientational disorder in organic crystals: a symmetry-adapted ensemble model. Physical Chemistry Chemical Physics, 2011, 13, 9590.	2.8	49
92	The crystal structures of chloro and methyl ortho-benzoic acids and their co-crystal: rationalizing similarities and differences. CrystEngComm, 2008, 10, 1848.	2.6	48
93	Toward the Computational Design of Diastereomeric Resolving Agents:Â An Experimental and Computational Study of 1-Phenylethylammonium-2-phenylacetate Derivatives. Journal of Physical Chemistry B, 2007, 111, 5326-5336.	2.6	47
94	The effect of basis set and electron correlation on the predicted electrostatic interactions of peptides. Journal of the American Chemical Society, 1992, 114, 8268-8276.	13.7	46
95	Morphologies of Organic Crystals:â€‰ Sensitivity of Attachment Energy Predictions to the Model Intermolecular Potential. Crystal Growth and Design, 2001, 1, 447-453.	3.0	46
96	Control and prediction of the organic solid state: a challenge to theory and experiment <sup />. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2018, 474, 20180351.	2.1	46
97	On the lack of hydrogen bonds in the crystal structure of alloxan. Chemical Physics Letters, 1997, 265, 532-537.	2.6	42
98	Crystallization and Crystal Energy Landscape of Hydrochlorothiazide. Crystal Growth and Design, 2007, 7, 705-712.	3.0	41
99	Screening for cocrystals of succinic acid and 4-aminobenzoic acid. CrystEngComm, 2012, 14, 2454.	2.6	41
100	Direct Observation of Templated Two-Step Nucleation Mechanism during Olanzapine Hydrate Formation. Crystal Growth and Design, 2017, 17, 6382-6393.	3.0	41
101	Ab initio calculations on indoleâ€“water, 1-methylindoleâ€“water and indoleâ€“(water)2. Chemical Physics Letters, 2000, 331, 253-261.	2.6	40
102	Groth's Original Concomitant Polymorphs Revisited. Crystal Growth and Design, 2005, 5, 2197-2209.	3.0	40
103	Spontaneous Resolution of Enantiomers by Crystallization: Insights from Computed Crystal Energy Landscapes. Crystal Growth and Design, 2010, 10, 1749-1756.	3.0	40
104	Isomers, Conformers, and Cocrystal Stoichiometry: Insights from the Crystal Energy Landscapes of Caffeine with the Hydroxybenzoic Acids. Crystal Growth and Design, 2010, 10, 3263-3272.	3.0	40
105	Solid Phases of Cyclopentane:â€‰ Combined Experimental and Simulation Study. Journal of Physical Chemistry B, 2008, 112, 3746-3758.	2.6	39
106	The observed and energetically feasible crystal structures of 5-substituted uracils. New Journal of Chemistry, 2008, 32, 1761.	2.8	39
107	Absorbing a Little Water: The Structural, Thermodynamic, and Kinetic Relationship between Pyrogallol and Its Tetarto-Hydrate. Crystal Growth and Design, 2013, 13, 4071-4083.	3.0	39
108	A Non-Empirical Intermolecular Potential for Oxalic Acid Crystal Structures. Journal of Physical Chemistry A, 1999, 103, 6448-6457.	2.5	38

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109	A Systematic Nonempirical Method of Deriving Model Intermolecular Potentials for Organic Molecules:Â Application To Amides. Journal of Physical Chemistry A, 2000, 104, 10958-10971.	2.5	38
110	Colored Polymorphs: Thermochemical and Structural Features of N-Picryl- p-toluidine Polymorphs and Solvates. Crystal Growth and Design, 2008, 8, 1977-1989.	3.0	38
111	The factors influencing cation site-preferences in spinels a new mendelyevian approach. Physics and Chemistry of Minerals, 1982, 8, 69-76.	0.8	37
112	A molecular picture of the problems in ensuring structural purity of tazofelone. Journal of Molecular Structure, 2014, 1078, 26-42.	3.6	37
113	Are Oxygen and Sulfur Atoms Structurally Equivalent in Organic Crystals?. Crystal Growth and Design, 2017, 17, 827-833.	3.0	35
114	Is the Isotropic Atomâ€”Atom Model Potential Adequate?. Molecular Simulation, 1988, 1, 135-156.	2.0	33
115	The matching of electrostatic extrema: A useful method in drug design? A study of phosphodiesterase III inhibitors. Journal of Computer-Aided Molecular Design, 1995, 9, 33-43.	2.9	33
116	Unraveling Complexity in the Solid Form Screening of a Pharmaceutical Salt: Why so Many Forms? Why so Few?. Crystal Growth and Design, 2017, 17, 5349-5365.	3.0	33
117	Thermochemistry of Racemic and Enantiopure Organic Crystals for Predicting Enantiomer Separation. Crystal Growth and Design, 2017, 17, 4676-4686.	3.0	33
118	The errors in lattice energy minimisation studies: sensitivity to experimental variations in the molecular structure of paracetamol. CrystEngComm, 2000, 2, 183.	2.6	30
119	Developments in computational studies of crystallization and morphology applied to urea. Physical Chemistry Chemical Physics, 2000, 2, 3017-3027.	2.8	29
120	Crystal structure prediction of flexible pharmaceutical-like molecules: density functional tight-binding as an intermediate optimisation method and for free energy estimation. Faraday Discussions, 2018, 211, 275-296.	3.2	29
121	Applications Of Dl_poly And Dl_multi To Organic Molecular Crystals. Molecular Simulation, 2006, 32, 985-997.	2.0	27
122	What base pairings can occur in DNA? A distributed multipole study of the electrostatic interactions between normal and alkylated nucleic acid bases. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 3407.	1.7	26
123	A comparison of three theoretical approaches to the study of side-chain interactions in proteins. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 2619.	1.7	25
124	Solvent interactions with n ring systems in proteins. Protein Engineering, Design and Selection, 1995, 8, 109-116.	2.1	24
125	A Systematic Experimental and Theoretical Study of the Crystalline State of Six Chloronitrobenzenes. Crystal Growth and Design, 2008, 8, 24-36.	3.0	24
126	Interference between the Hydrogen Bonds to the Two Rings of Nicotine. Journal of the American Chemical Society, 2003, 125, 5988-5997.	13.7	23

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127	Testing a Variety of Electronic-Structure-Based Methods for the Relative Energies of 5-Formyluracil Crystals. Journal of Chemical Theory and Computation, 2011, 7, 2685-2688.	5.3	23
128	Analysis of the conformational profiles of fenamates shows route towards novel, higher accuracy, force-fields for pharmaceuticals. Physical Chemistry Chemical Physics, 2015, 17, 7936-7948.	2.8	23
129	Anisotropic Repulsion Potentials for Cyanuric Chloride (C3N3Cl3) and Their Application to Modeling the Crystal Structures of Azaaromatic Chlorides. Journal of Physical Chemistry A, 2001, 105, 9961-9971.	2.5	22
130	A predicted dimer-based polymorph of 10,11-dihydrocarbamazepine (Form IV). CrystEngComm, 2010, 12, 64-66.	2.6	21
131	Systematic Finite-Temperature Reduction of Crystal Energy Landscapes. Crystal Growth and Design, 2020, 20, 6847-6862.	3.0	21
132	Diffusion Monte Carlo simulations on uracilâ€“water using an anisotropic atomâ€“atom potential model. Faraday Discussions, 2001, 118, 95-108.	3.2	20
133	Reversible, Two-Step Single-Crystal to Single-Crystal Phase Transitions between Desloratadine Forms I, II, and III. Crystal Growth and Design, 2020, 20, 1800-1810.	3.0	20
134	Relative binding orientations of adenosine A1 receptor ligands â€" A test case for Distributed Multipole Analysis in medicinal chemistry. Journal of Computer-Aided Molecular Design, 1995, 9, 44-54.	2.9	19
135	Use of Crystal Structure Informatics for Defining the Conformational Space Needed for Predicting Crystal Structures of Pharmaceutical Molecules. Journal of Chemical Theory and Computation, 2017, 13, 5163-5171.	5.3	19
136	Serendipitous isolation of a disappearing conformational polymorph of succinic acid challenges computational polymorph prediction. CrystEngComm, 2018, 20, 3971-3977.	2.6	19
137	The orientation of N-H...O=C and N-H...N hydrogen bonds in biological systems: how good is a point charge as a model for a hydrogen bonding atom?. Journal of Computer-Aided Molecular Design, 1997, 11, 479-490.	2.9	18
138	Toward More Accurate Model Intermolecular Potentials for Organic Molecules. Reviews in Computational Chemistry, 2007, , 225-289.	1.5	16
139	From dimers to the solid-state: Distributed intermolecular force-fields for pyridine. Journal of Chemical Physics, 2017, 147, 161722.	3.0	16
140	Molecular Crystal Structure Prediction. , 2017, , 333-363.		16
141	The (Current) Acridine Solid Form Landscape: Eight Polymorphs and a Hydrate. Crystal Growth and Design, 2019, 19, 4884-4893.	3.0	16
142	Application of Woodward-Hoffmann ideas to solid-state polymorphic phase transitions with specific reference to polymerization ofS2N2and the black phosphorus toA7(arsenic) structural transformation. Physical Review B, 1982, 25, 5778-5789.	3.2	15
143	Aza analogues of nucleic acid bases: experimental determination and computational prediction of the crystal structure of anhydrous 5-azauracil. Journal of Molecular Structure, 1999, 485-486, 349-361.	3.6	15
144	Toward Physics-Based Solubility Computation for Pharmaceuticals to Rival Informatics. Journal of Chemical Theory and Computation, 2021, 17, 3700-3709.	5.3	15

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145	Modelling Intermolecular Forces for Organic Crystal Structure Prediction. Structure and Bonding, 2005, , 81-123.	1.0	13
146	The solid state forms of the sex hormone 17-Î²-estradiol. CrystEngComm, 2019, 21, 2154-2163.	2.6	13
147	Charge Distributions of Nitro Groups Within Organic Explosive Crystals: Effects on Sensitivity and Modeling. ACS Omega, 2019, 4, 8614-8625.	3.5	13
148	Anisotropic atom-atom potentials. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1996, 73, 95-106.	0.6	12
149	Computational prediction and X-ray determination of the crystal structures of 3-oxauracil and 5-hydroxyuracilâ€"an informal blind test. CrystEngComm, 2005, 7, 421.	2.6	11
150	Racemic progesterone: predicted in silico and produced in the solid state. Chemical Communications, 2006, , 4921-3.	4.1	10
151	Lattice energy, nailed?. Science, 2014, 345, 619-620.	12.6	10
152	Concomitant conformational dimorphism in 1,2-bis(9-anthryl)acetylene. CrystEngComm, 2015, 17, 4877-4882.	2.6	10
153	Molecular self-assembly and clustering in nucleation processes: general discussion. Faraday Discussions, 2015, 179, 155-197.	3.2	10
154	Blind crystal structure prediction of a novel second polymorph of 1-hydroxy-7-azabenzotriazole. Acta Crystallographica Section B: Structural Science, 2006, 62, 642-650.	1.8	9
155	Experimental and Predicted Crystal Energy Landscapes of Chlorothiazide. Crystal Growth and Design, 2011, 11, 405-413.	3.0	9
156	The unexpected but predictable tetrazole packing in flexible 1-benzyl-1H-tetrazole. CrystEngComm, 2012, 14, 6441.	2.6	9
157	Color Differences Highlight Concomitant Polymorphism of Chalcones. Crystal Growth and Design, 2020, 20, 6346-6355.	3.0	9
158	Surface Structure of a Complex Inorganic Crystal in Aqueous Solution from Classical Molecular Simulation. Journal of Physical Chemistry B, 2004, 108, 12537-12546.	2.6	8
159	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	3.2	8
160	Calculation of Diamagnetic Susceptibility Tensors of Organic Crystals: From Coronene to Pharmaceutical Polymorphs. Journal of Physical Chemistry A, 2020, 124, 1409-1420.	2.5	8
161	On the inversion of thermophysical properties generated from anisotropic potential energy functions. Chemical Physics Letters, 1980, 74, 193-195.	2.6	7
162	An interpretation of structural sorting diagrams for AB type compounds using molecular orbital ideas. Journal of Physics and Chemistry of Solids, 1982, 43, 521-531.	4.0	7

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163	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	3.2	7
164	A non-empirical method of determining atom?atom repulsion parameters: application to the crystal structure prediction of an oxyboryl derivative. CrystEngComm, 1999, 1, 24-32.	2.6	6
165	A computationally inspired investigation of the solid forms of (R)â€1â€phenylethylammoniumâ€(S)â€2â€phenylbutyrate. Chirality, 2010, 22, 447-455.	2.6	6
166	Nucleation in complex multi-component and multi-phase systems: general discussion. Faraday Discussions, 2015, 179, 503-542.	3.2	6
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