Sarah L Price

List of Publications by Citations

188 papers	11,264 citations	59 h-index	100 g-index
196 ext. papers	12,126 ext. citations	5.4 avg, IF	6.67 L-index

#	Paper	IF	Citations
188	Predicting crystal structures of organic compounds. *Chemical Society Reviews*, **2014**, 43, 2098-111	58.5	345
187	Report on the sixth blind test of organic crystal structure prediction methods. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 439-59	1.8	338
186	A test of crystal structure prediction of small organic molecules. *Acta Crystallographica Section B: Structural Science*, **2000**, 56, 697-714		338
185	Significant progress in predicting the crystal structures of small organic molecules--a report on the fourth blind test. *Acta Crystallographica Section B: Structural Science*, **2009**, 65, 107-25		334
184	Towards crystal structure prediction of complex organic compounds--a report on the fifth blind test. *Acta Crystallographica Section B: Structural Science*, **2011**, 67, 535-51		318
183	Computed crystal energy landscapes for understanding and predicting organic crystal structures and polymorphism. *Accounts of Chemical Research*, **2009**, 42, 117-26	24.3	302
182	Amino/aromatic interactions in proteins: is the evidence stacked against hydrogen bonding?. *Journal of Molecular Biology*, **1994**, 239, 315-31	6.5	297
181	Crystal structure prediction of small organic molecules: a second blind test. *Acta Crystallographica Section B: Structural Science*, **2002**, 58, 647-61		293
180	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		243
179	The prediction, morphology, and mechanical properties of the polymorphs of paracetamol. *Journal of the American Chemical Society*, **2001**, 123, 5086-94	16.4	239
178	Modelling organic crystal structures using distributed multipole and polarizability-based model intermolecular potentials. *Physical Chemistry Chemical Physics*, **2010**, 12, 8478-90	3.6	231
177	Innovation in crystal engineering. *CrystEngComm*, **2002**, 4, 500-509	3.3	210
176	The computational prediction of pharmaceutical crystal structures and polymorphism. *Advanced Drug Delivery Reviews*, **2004**, 56, 301-19	18.5	181
175	Salt or Cocrystal? A New Series of Crystal Structures Formed from Simple Pyridines and Carboxylic Acids. *Crystal Growth and Design*, **2009**, 9, 2881-2889	3.5	169
174	Hydrogen bonding of carbonyl, ether, and ester oxygen atoms with alkanol hydroxyl groups. *Journal of Computational Chemistry*, **1997**, 18, 757-774	3.5	161
173	A strategy for producing predicted polymorphs: catemeric carbamazepine form V. *Chemical Communications*, **2011**, 47, 7074-6	5.8	152
172	Why don't we find more polymorphs?. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2013**, 69, 313-28	1.8	150

171	A new polymorph of 5-fluorouracil found following computational crystal structure predictions. *Journal of the American Chemical Society*, **2005**, 127, 1116-7	16.4	143
170	Toward Crystal Structure Prediction for Conformationally Flexible Molecules: The Headaches Illustrated by Aspirin. *Crystal Growth and Design*, **2004**, 4, 1119-1127	3.5	142
169	Role of the crystal-field theory in determining the structures of spinels. *Journal of the American Chemical Society*, **1982**, 104, 92-95	16.4	138
168	From crystal structure prediction to polymorph prediction: interpreting the crystal energy landscape. *Physical Chemistry Chemical Physics*, **2008**, 10, 1996-2009	3.6	131
167	Dimer or Catemer? Low-Energy Crystal Packings for Small Carboxylic Acids. *Journal of Physical Chemistry B*, **2000**, 104, 2647-2655	3.4	130
166	Can the Formation of Pharmaceutical Cocrystals Be Computationally Predicted? I. Comparison of Lattice Energies. *Crystal Growth and Design*, **2009**, 9, 442-453	3.5	128
165	Can computed crystal energy landscapes help understand pharmaceutical solids?. *Chemical Communications*, **2016**, 52, 7065-77	5.8	116
164	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	2.8	113
163	Ab Initio Calculations on Uracil Water. *Journal of Physical Chemistry A*, **1999**, 103, 1611-1618	2.8	111
162	Exploring the Experimental and Computed Crystal Energy Landscape of Olanzapine. *Crystal Growth and Design*, **2013**, 13, 1602-1617	3.5	106
161	Successful prediction of a model pharmaceutical in the fifth blind test of crystal structure prediction. *International Journal of Pharmaceutics*, **2011**, 418, 168-78	6.5	105
160	Can the Formation of Pharmaceutical Cocrystals Be Computationally Predicted? 2. Crystal Structure Prediction. *Journal of Chemical Theory and Computation*, **2009**, 5, 1432-48	6.4	105
159	Towards an understanding of the arginine-aspartate interaction. *Journal of Molecular Biology*, **1992**, 226, 251-62	6.5	98
158	An overlap model for estimating the anisotropy of repulsion. *Molecular Physics*, **1990**, 69, 507-533	1.7	98
157	An automated parallel crystallisation search for predicted crystal structures and packing motifs of carbamazepine. *Journal of Pharmaceutical Sciences*, **2006**, 95, 1918-30	3.9	97
156	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, 3323-9	3.4	97
155	The nature of the N ? HD?C hydrogen bond: An intermolecular perturbation theory study of the formamide/formaldehyde complex. *Journal of Computational Chemistry*, **1990**, 11, 1217-1233	3.5	96
154	Computational prediction of organic crystal structures and polymorphism. *International Reviews in Physical Chemistry*, **2008**, 27, 541-568	7	95

153	Elastic Constant Calculations for Molecular Organic Crystals. *Crystal Growth and Design*, **2001**, 1, 13-27	3.5	95
152	Grid Service Orchestration Using the Business Process Execution Language (BPEL). *Journal of Grid Computing*, **2005**, 3, 283-304	4.2	91
151	A nonempirical anisotropic atom-atom model potential for chlorobenzene crystals. *Journal of the American Chemical Society*, **2003**, 125, 16434-43	16.4	87
150	Atomistic Calculations of Phonon Frequencies and Thermodynamic Quantities for Crystals of Rigid Organic Molecules. *Journal of Physical Chemistry B*, **2003**, 107, 10919-10933	3.4	82
149	Applications of realistic electrostatic modelling to molecules in complexes, solids and proteins. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 2997		82
148	Ab initio and diffusion Monte Carlo study of uracil·water, thymine·water, cytosine·water, and cytosine·(water)2. *Physical Chemistry Chemical Physics*, **2000**, 2, 1281-1290	3.6	81
147	The Determination of the Crystal Structure of Anhydrous Theophylline by X-ray Powder Diffraction with a Systematic Search Algorithm, Lattice Energy Calculations, and 13C and 15N Solid-State NMR: A Question of Polymorphism in a Given Unit Cell. *Journal of Physical Chemistry B*, **2001**, 105, 5818-5826	3.4	81
146	Which, if any, hydrates will crystallise? Predicting hydrate formation of two dihydroxybenzoic acids. *Chemical Communications*, **2011**, 47, 5443-5	5.8	78
145	Modeling the interplay of inter- and intramolecular hydrogen bonding in conformational polymorphs. *Journal of Chemical Physics*, **2008**, 128, 244708	3.9	78
144	Energy Minimization of Crystal Structures Containing Flexible Molecules. *Journal of Chemical Theory and Computation*, **2006**, 2, 1184-1199	6.4	78
143	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	3.3	78
142	Complex Polymorphic System of Gallic Acid-Five Monohydrates, Three Anhydrates, and over 20 Solvates. *Crystal Growth and Design*, **2013**, 13, 19-23	3.5	77
141	Crystal structure predictions for acetic acid. *Journal of Computational Chemistry*, **1998**, 19, 459-474	3.5	76
140	The potential of computed crystal energy landscapes to aid solid-form development. *Drug Discovery Today*, **2016**, 21, 912-23	8.8	74
139	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	6.4	72
138	A first principles prediction of the crystal structure of . *Chemical Physics Letters*, **2008**, 456, 105-109	2.5	71
137	An Experimental and Theoretical Search for Polymorphs of Barbituric Acid: The Challenges of Even Limited Conformational Flexibility. *Crystal Growth and Design*, **2004**, 4, 979-987	3.5	67
136	Toward a Molecular Understanding of Crystal Agglomeration. *Crystal Growth and Design*, **2005**, 5, 3-16	3.5	65

135	Contrasting Polymorphism of Related Small Molecule Drugs Correlated and Guided by the Computed Crystal Energy Landscape. *Crystal Growth and Design*, **2014**, 14, 2056-2072	3.5	63
134	Carbamazepine Co-crystallization with Pyridine Carboxamides: Rationalization by Complementary Phase Diagrams and Crystal Energy Landscapes. *Crystal Growth and Design*, **2010**, 10, 903-912	3.5	62
133	Factors influencing solid-state structure—an analysis using pseudopotential radii structural maps. *Physical Review B*, **1981**, 24, 2903-2912	3.3	62
132	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	16.4	61
131	The polymorphism of progesterone: stabilization of a "disappearing" polymorph by co-crystallization. *Journal of Pharmaceutical Sciences*, **2007**, 96, 3419-31	3.9	60
130	The thermal stability of lattice-energy minima of 5-fluorouracil: metadynamics as an aid to polymorph prediction. *Journal of Physical Chemistry B*, **2008**, 112, 4298-308	3.4	59
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128	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	3.6	57
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125	Electrostatic models for polypeptides: can we assume transferability?. *Journal of the Chemical Society, Faraday Transactions*, **1992**, 88, 1755		55
124	Three Polymorphs of 2-Amino-5-nitropyrimidine: Experimental Structures and Theoretical Predictions. *Journal of the American Chemical Society*, **1998**, 120, 8986-8993	16.4	54
123	Search for a predicted hydrogen bonding motif--a multidisciplinary investigation into the polymorphism of 3-azabicyclo[3.3.1]nonane-2,4-dione. *Journal of the American Chemical Society*, **2007**, 129, 3649-57	16.4	54
122	Which organic crystal structures are predictable by lattice energy minimisation?. *CrystEngComm*, **2001**, 3, 178-212	3.3	54
121	A systematic intermolecular potential method applied to chlorine. *Molecular Physics*, **1990**, 71, 1381-1404	1.7	54
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118	Navigating the Waters of Unconventional Crystalline Hydrates. *Molecular Pharmaceutics*, **2015**, 12, 3069-88	4.8	52

117	Evaluating a Crystal Energy Landscape in the Context of Industrial Polymorph Screening. *Crystal Growth and Design*, **2013**, 13, 2396-2406	3.5	52
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115	Is the Induction Energy Important for Modeling Organic Crystals?. *Journal of Chemical Theory and Computation*, **2008**, 4, 522-32	6.4	51
114	Predictions of Crystal Packings for Uracil, 6-Azauracil, and Allopurinol:The Interplay between Hydrogen Bonding and Close Packing. *Journal of Physical Chemistry A*, **1997**, 101, 2198-2206	2.8	50
113	Solid-State Forms of Resorcylic Acid: How Exhaustive Should a Polymorph Screen Be?. *Crystal Growth and Design*, **2011**, 11, 210-220	3.5	49
112	Validation of a search technique for crystal structure prediction of flexible molecules by application to piracetam. *Acta Crystallographica Section B: Structural Science*, **2005**, 61, 558-68		49
111	Calculation of Attachment Energies and Relative Volume Growth Rates As an Aid to Polymorph Prediction. *Crystal Growth and Design*, **2005**, 5, 879-885	3.5	48
110	Amino/aromatic interactions. *Nature*, **1993**, 366, 413-413	50.4	48
109	The crystal structures of chloro and methylortho-benzoic acids and their co-crystal: rationalizing similarities and differences. *CrystEngComm*, **2008**, 10, 1848	3.3	47
108	Is the Fenamate Group a Polymorphophore? Contrasting the Crystal Energy Landscapes of Fenamic and Tolfenamic Acids. *Crystal Growth and Design*, **2012**, 12, 4230-4239	3.5	46
107	Toward the Prediction of Organic Hydrate Crystal Structures. *Journal of Chemical Theory and Computation*, **2007**, 3, 1597-608	6.4	46
106	Investigating Unused Hydrogen Bond Acceptors Using Known and Hypothetical Crystal Polymorphism. *Crystal Growth and Design*, **2005**, 5, 983-993	3.5	46
105	Are the Crystal Structures of Enantiopure and Racemic Mandelic Acids Determined by Kinetics or Thermodynamics?. *Journal of the American Chemical Society*, **2015**, 137, 11095-104	16.4	45
104	Thermal Expansion of Carbamazepine: Systematic Crystallographic Measurements Challenge Quantum Chemical Calculations. *Journal of Physical Chemistry Letters*, **2017**, 8, 4319-4324	6.4	44
103	Predictable Disorder versus Polymorphism in the Rationalization of Structural Diversity: A Multidisciplinary Study of Eniluracil. *Crystal Growth and Design*, **2008**, 8, 3474-3481	3.5	44
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99	Characterization of complicated new polymorphs of chlorothalonil by X-ray diffraction and computer crystal structure prediction. *Journal of the American Chemical Society*, **2004**, 126, 7071-81	16.4	43
98	Racemic Naproxen: A Multidisciplinary Structural and Thermodynamic Comparison with the Enantiopure Form. *Crystal Growth and Design*, **2011**, 11, 5659-5669	3.5	42
97	Morphologies of Organic Crystals: Sensitivity of Attachment Energy Predictions to the Model Intermolecular Potential. *Crystal Growth and Design*, **2001**, 1, 447-453	3.5	42
96	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	16.4	41
95	GrothS Original Concomitant Polymorphs Revisited. *Crystal Growth and Design*, **2005**, 5, 2197-2209	3.5	39
94	Spontaneous Resolution of Enantiomers by Crystallization: Insights from Computed Crystal Energy Landscapes. *Crystal Growth and Design*, **2010**, 10, 1749-1756	3.5	38
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90	Isomorphous template induced crystallisation: a robust method for the targeted crystallisation of computationally predicted metastable polymorphs. *Chemical Communications*, **2016**, 52, 7384-6	5.8	37
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88	Crystallization and Crystal Energy Landscape of Hydrochlorothiazide. *Crystal Growth and Design*, **2007**, 7, 705-712	3.5	36
87	Absorbing a Little Water: The Structural, Thermodynamic, and Kinetic Relationship between Pyrogallol and Its Tetarto-Hydrate. *Crystal Growth and Design*, **2013**, 13, 4071-4083	3.5	35
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85	Solid phases of cyclopentane: combined experimental and simulation study. *Journal of Physical Chemistry B*, **2008**, 112, 3746-58	3.4	35
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83	A Non-Empirical Intermolecular Potential for Oxalic Acid Crystal Structures. *Journal of Physical Chemistry A*, **1999**, 103, 6448-6457	2.8	34
82	Direct Observation of Templated Two-Step Nucleation Mechanism during Olanzapine Hydrate Formation. *Crystal Growth and Design*, **2017**, 17, 6382-6393	3.5	33

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80	A molecular picture of the problems in ensuring structural purity of tazofelone. *Journal of Molecular Structure*, **2014**, 1078, 26-42	3.4	32
79	Screening for cocrystals of succinic acid and 4-aminobenzoic acid. *CrystEngComm*, **2012**, 14, 2454	3.3	32
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66	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		21
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61	Diffusion Monte Carlo simulations on uracil□water using an anisotropic atom□atom potential model. *Faraday Discussions*, **2001**, 118, 95-108	3.6	19
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58	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	2.8	18
57	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, 479-90	4.2	17
56	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	3.5	16
55	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	6.4	15
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48	Toward More Accurate Model Intermolecular Potentials for Organic Molecules. *Reviews in Computational Chemistry*, **2007**, 225-289		11
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35	Surface Structure of a Complex Inorganic Crystal in Aqueous Solution from Classical Molecular Simulation. *Journal of Physical Chemistry B*, **2004**, 108, 12537-12546	3.4	7
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27	Applications of crystal structure prediction - organic molecular structures: general discussion. *Faraday Discussions*, **2018**, 211, 493-539	3.6	6
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