Sarah L Price

List of Publications by Year in Descending Order

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	Packing Preferences of Chalcones: A Model Conjugated Pharmaceutical Scaffold.. *Crystal Growth and Design*, **2022**, 22, 1801-1816	3.5	1
187	A non-empirical intermolecular force-field for trinitrobenzene and its application in crystal structure prediction. *Journal of Chemical Physics*, **2021**, 154, 094123	3.9	3
186	Toward Physics-Based Solubility Computation for Pharmaceuticals to Rival Informatics. *Journal of Chemical Theory and Computation*, **2021**, 17, 3700-3709	6.4	4
185	The Crystal Structure of 5-Aminouracil and the Ambiguity of Alternative Polymorphs. *Israel Journal of Chemistry*, **2021**, 61, 590	3.4	0
184	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
183	Calculation of Diamagnetic Susceptibility Tensors of Organic Crystals: From Coronene to Pharmaceutical Polymorphs. *Journal of Physical Chemistry A*, **2020**, 124, 1409-1420	2.8	4
182	Diabat method for polymorph free energies: Extension to molecular crystals. *Journal of Chemical Physics*, **2020**, 153, 244105	3.9	1
181	Color Differences Highlight Concomitant Polymorphism of Chalcones. *Crystal Growth and Design*, **2020**, 20, 6346-6355	3.5	5
180	Systematic Finite-Temperature Reduction of Crystal Energy Landscapes. *Crystal Growth and Design*, **2020**, 20, 6847-6862	3.5	7
179	The solid state forms of the sex hormone 17-β-estradiol. *CrystEngComm*, **2019**, 21, 2154-2163	3.3	7
178	Charge Distributions of Nitro Groups Within Organic Explosive Crystals: Effects on Sensitivity and Modeling. *ACS Omega*, **2019**, 4, 8614-8625	3.9	5
177	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
176	The (Current) Acridine Solid Form Landscape: Eight Polymorphs and a Hydrate. *Crystal Growth and Design*, **2019**, 19, 4884-4893	3.5	9
175	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	3.6	14
174	Successful Computationally Directed Templating of Metastable Pharmaceutical Polymorphs. *Crystal Growth and Design*, **2018**, 18, 5322-5331	3.5	29
173	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
172	Applications of crystal structure prediction - inorganic and network structures: general discussion. *Faraday Discussions*, **2018**, 211, 613-642	3.6	4

171	Toward Computational Polymorph Prediction **2018**, 133-157		3
170	Control and prediction of the organic solid state: a challenge to theory and experiment. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2018**, 474, 20180351	2.4	28
169	Structure searching methods: general discussion. *Faraday Discussions*, **2018**, 211, 133-180	3.6	3
168	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. *Faraday Discussions*, **2018**, 211, 325-381	3.6	6
167	Applications of crystal structure prediction - organic molecular structures: general discussion. *Faraday Discussions*, **2018**, 211, 493-539	3.6	6
166	Serendipitous isolation of a disappearing conformational polymorph of succinic acid challenges computational polymorph prediction. *CrystEngComm*, **2018**, 20, 3971-3977	3.3	12
165	Are Oxygen and Sulfur Atoms Structurally Equivalent in Organic Crystals?. *Crystal Growth and Design*, **2017**, 17, 827-833	3.5	25
164	Direct Observation of Templated Two-Step Nucleation Mechanism during Olanzapine Hydrate Formation. *Crystal Growth and Design*, **2017**, 17, 6382-6393	3.5	33
163	Thermal Expansion of Carbamazepine: Systematic Crystallographic Measurements Challenge Quantum Chemical Calculations. *Journal of Physical Chemistry Letters*, **2017**, 8, 4319-4324	6.4	44
162	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	3.5	23
161	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
160	Thermochemistry of Racemic and Enantiopure Organic Crystals for Predicting Enantiomer Separation. *Crystal Growth and Design*, **2017**, 17, 4676-4686	3.5	33
159	From dimers to the solid-state: Distributed intermolecular force-fields for pyridine. *Journal of Chemical Physics*, **2017**, 147, 161722	3.9	15
158	Molecular Crystal Structure Prediction **2017**, 333-363		9
157	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
156	The potential of computed crystal energy landscapes to aid solid-form development. *Drug Discovery Today*, **2016**, 21, 912-23	8.8	74
155	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
154	Can computed crystal energy landscapes help understand pharmaceutical solids?. *Chemical Communications*, **2016**, 52, 7065-77	5.8	116

153	Concomitant conformational dimorphism in 1,2-bis(9-anthryl)acetylene. *CrystEngComm*, **2015**, 17, 4877-4882	3.8	9
152	Molecular self-assembly and clustering in nucleation processes: general discussion. *Faraday Discussions*, **2015**, 179, 155-97	3.6	8
151	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
150	Navigating the Waters of Unconventional Crystalline Hydrates. *Molecular Pharmaceutics*, **2015**, 12, 3069-88	4.8	52
149	Nucleation in complex multi-component and multi-phase systems: general discussion. *Faraday Discussions*, **2015**, 179, 503-42	3.6	1
148	Analysis of the conformational profiles of fenamates shows route towards novel, higher accuracy, force-fields for pharmaceuticals. *Physical Chemistry Chemical Physics*, **2015**, 17, 7936-48	3.6	19
147	Crystal Energy Landscapes for Aiding Crystal Form Selection **2015**, 7-29		2
146	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
145	Chemistry. Lattice energy, nailed?. *Science*, **2014**, 345, 619-20	33.3	8
144	Predicting crystal structures of organic compounds. *Chemical Society Reviews*, **2014**, 43, 2098-111	58.5	345
143	A molecular picture of the problems in ensuring structural purity of tazofelone. *Journal of Molecular Structure*, **2014**, 1078, 26-42	3.4	32
142	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
141	Exploring the Experimental and Computed Crystal Energy Landscape of Olanzapine. *Crystal Growth and Design*, **2013**, 13, 1602-1617	3.5	106
140	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
139	Evaluating a Crystal Energy Landscape in the Context of Industrial Polymorph Screening. *Crystal Growth and Design*, **2013**, 13, 2396-2406	3.5	52
138	Why don't we find more polymorphs?. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2013**, 69, 313-28	1.8	150
137	Screening for cocrystals of succinic acid and 4-aminobenzoic acid. *CrystEngComm*, **2012**, 14, 2454	3.3	32
136	The unexpected but predictable tetrazole packing in flexible 1-benzyl-1H-tetrazole. *CrystEngComm*, **2012**, 14, 6441	3.3	9

135	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
134	The complexity of hydration of phloroglucinol: a comprehensive structural and thermodynamic characterization. *Journal of Physical Chemistry B*, **2012**, 116, 3961-72	3.4	56
133	A strategy for producing predicted polymorphs: catemeric carbamazepine form V. *Chemical Communications*, **2011**, 47, 7074-6	5.8	152
132	Computational Polymorph Prediction **2011**, 427-450		7
131	Substitutional and orientational disorder in organic crystals: a symmetry-adapted ensemble model. *Physical Chemistry Chemical Physics*, **2011**, 13, 9590-600	3.6	43
130	Experimental and Predicted Crystal Energy Landscapes of Chlorothiazide. *Crystal Growth and Design*, **2011**, 11, 405-413	3.5	8
129	Testing a Variety of Electronic-Structure-Based Methods for the Relative Energies of 5-Formyluracil Crystals. *Journal of Chemical Theory and Computation*, **2011**, 7, 2685-8	6.4	20
128	Racemic Naproxen: A Multidisciplinary Structural and Thermodynamic Comparison with the Enantiopure Form. *Crystal Growth and Design*, **2011**, 11, 5659-5669	3.5	42
127	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
126	Computational prediction of salt and cocrystal structures--does a proton position matter?. *International Journal of Pharmaceutics*, **2011**, 418, 187-98	6.5	52
125	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
124	Which, if any, hydrates will crystallise? Predicting hydrate formation of two dihydroxybenzoic acids. *Chemical Communications*, **2011**, 47, 5443-5	5.8	78
123	Solid-State Forms of Resorcylic Acid: How Exhaustive Should a Polymorph Screen Be?. *Crystal Growth and Design*, **2011**, 11, 210-220	3.5	49
122	Spontaneous Resolution of Enantiomers by Crystallization: Insights from Computed Crystal Energy Landscapes. *Crystal Growth and Design*, **2010**, 10, 1749-1756	3.5	38
121	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	3.5	35
120	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
119	A predicted dimer-based polymorph of 10,11-dihydrocarbamazepine (Form IV). *CrystEngComm*, **2010**, 12, 64-66	3.3	20
118	A computationally inspired investigation of the solid forms of (R)-1-phenylethylammonium-(S)-2-phenylbutyrate. *Chirality*, **2010**, 22, 447-55	2.1	6

117	Modelling organic crystal structures using distributed multipole and polarizability-based model intermolecular potentials. *Physical Chemistry Chemical Physics*, **2010**, 12, 8478-90	3.6	231
116	The representation of molecular electrostatics using interactive graphics. *International Journal of Quantum Chemistry*, **2009**, 36, 73-85	2.1	1
115	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
114	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
113	Computed crystal energy landscapes for understanding and predicting organic crystal structures and polymorphism. *Accounts of Chemical Research*, **2009**, 42, 117-26	24.3	302
112	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
111	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
110	From crystal structure prediction to polymorph prediction: interpreting the crystal energy landscape. *Physical Chemistry Chemical Physics*, **2008**, 10, 1996-2009	3.6	131
109	Is the Induction Energy Important for Modeling Organic Crystals?. *Journal of Chemical Theory and Computation*, **2008**, 4, 522-32	6.4	51
108	A Systematic Experimental and Theoretical Study of the Crystalline State of Six Chloronitrobenzenes. *Crystal Growth and Design*, **2008**, 8, 24-36	3.5	23
107	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
106	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
105	Discovery of three polymorphs of 7-fluoroisatin reveals challenges in using computational crystal structure prediction as a complement to experimental screening. *CrystEngComm*, **2008**,	3.3	2
104	The crystal structures of chloro and methylortho-benzoic acids and their co-crystal: rationalizing similarities and differences. *CrystEngComm*, **2008**, 10, 1848	3.3	47
103	Solid phases of cyclopentane: combined experimental and simulation study. *Journal of Physical Chemistry B*, **2008**, 112, 3746-58	3.4	35
102	Colored Polymorphs: Thermochemical and Structural Features of N-Picryl- p-toluidine Polymorphs and Solvates. *Crystal Growth and Design*, **2008**, 8, 1977-1989	3.5	36
101	The observed and energetically feasible crystal structures of 5-substituted uracils. *New Journal of Chemistry*, **2008**, 32, 1761	3.6	37
100	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

99	A first principles prediction of the crystal structure of . *Chemical Physics Letters*, **2008**, 456, 105-109	2.5	71
98	Modeling the interplay of inter- and intramolecular hydrogen bonding in conformational polymorphs. *Journal of Chemical Physics*, **2008**, 128, 244708	3.9	78
97	Computational prediction of organic crystal structures and polymorphism. *International Reviews in Physical Chemistry*, **2008**, 27, 541-568	7	95
96	Toward More Accurate Model Intermolecular Potentials for Organic Molecules. *Reviews in Computational Chemistry*, **2007**, 225-289		11
95	Toward the computational design of diastereomeric resolving agents: an experimental and computational study of 1-phenylethylammonium-2-phenylacetate derivatives. *Journal of Physical Chemistry B*, **2007**, 111, 5326-36	3.4	44
94	Carbonic acid: from polyamorphism to polymorphism. *Journal of the American Chemical Society*, **2007**, 129, 13863-71	16.4	58
93	The polymorphism of progesterone: stabilization of a disappearing polymorph by co-crystallization. *Journal of Pharmaceutical Sciences*, **2007**, 96, 3419-31	3.9	60
92	Toward the Prediction of Organic Hydrate Crystal Structures. *Journal of Chemical Theory and Computation*, **2007**, 3, 1597-608	6.4	46
91	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
90	Crystallization and Crystal Energy Landscape of Hydrochlorothiazide. *Crystal Growth and Design*, **2007**, 7, 705-712	3.5	36
89	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
88	Racemic progesterone: predicted in silico and produced in the solid state. *Chemical Communications* , **2006**, 4921-3	5.8	6
87	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
86	Applications Of Dl_poly And Dl_multi To Organic Molecular Crystals. *Molecular Simulation*, **2006**, 32, 985-997		25
85	Energy Minimization of Crystal Structures Containing Flexible Molecules. *Journal of Chemical Theory and Computation*, **2006**, 2, 1184-1199	6.4	78
84	Blind crystal structure prediction of a novel second polymorph of 1-hydroxy-7-azabenzotriazole. *Acta Crystallographica Section B: Structural Science*, **2006**, 62, 642-50		9
83	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
82	Computational prediction and X-ray determination of the crystal structures of 3-oxauracil and 5-hydroxyuracil: an informal blind test. *CrystEngComm*, **2005**, 7, 421	3.3	10

81	Challenges of crystal structure prediction of diastereomeric salt pairs. *Journal of Physical Chemistry B*, **2005**, 109, 17134-50	3.4	44
80	Investigating Unused Hydrogen Bond Acceptors Using Known and Hypothetical Crystal Polymorphism. *Crystal Growth and Design*, **2005**, 5, 983-993	3.5	46
79	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
78	Groth's Original Concomitant Polymorphs Revisited. *Crystal Growth and Design*, **2005**, 5, 2197-2209	3.5	39
77	Toward a Molecular Understanding of Crystal Agglomeration. *Crystal Growth and Design*, **2005**, 5, 3-16	3.5	65
76	Modelling Intermolecular Forces for Organic Crystal Structure Prediction. *Structure and Bonding*, **2005**, 81-123	0.9	11
75	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
74	Grid Service Orchestration Using the Business Process Execution Language (BPEL). *Journal of Grid Computing*, **2005**, 3, 283-304	4.2	91
73	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
72	Crystal Structure Prediction **2004**, 371-379		4
71	The computational prediction of pharmaceutical crystal structures and polymorphism. *Advanced Drug Delivery Reviews*, **2004**, 56, 301-19	18.5	181
70	Towards a Fundamental Understanding of the Mechanics of Crystal Agglomeration: A Microscopic and Molecular Approach. *Particle and Particle Systems Characterization*, **2004**, 21, 276-283	3.1	5
69	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
68	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
67	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
66	Toward Crystal Structure Prediction for Conformationally Flexible Molecules: The Headaches Illustrated by Aspirin. *Crystal Growth and Design*, **2004**, 4, 1119-1127	3.5	142
65	Quantifying intermolecular interactions and their use in computational crystal structure prediction. *CrystEngComm*, **2004**, 6, 344	3.3	53
64	Interference between the hydrogen bonds to the two rings of nicotine. *Journal of the American Chemical Society*, **2003**, 125, 5988-97	16.4	20

63	A nonempirical anisotropic atom-atom model potential for chlorobenzene crystals. *Journal of the American Chemical Society*, **2003**, 125, 16434-43	16.4	87
62	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
61	Crystal structure prediction of small organic molecules: a second blind test. *Acta Crystallographica Section B: Structural Science*, **2002**, 58, 647-61		293
60	Innovation in crystal engineering. *CrystEngComm*, **2002**, 4, 500-509	3.3	210
59	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
58	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
57	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
56	Which organic crystal structures are predictable by lattice energy minimisation?. *CrystEngComm*, **2001**, 3, 178-212	3.3	54
55	The prediction, morphology, and mechanical properties of the polymorphs of paracetamol. *Journal of the American Chemical Society*, **2001**, 123, 5086-94	16.4	239
54	Diffusion Monte Carlo simulations on uracil□water using an anisotropic atom□atom potential model. *Faraday Discussions*, **2001**, 118, 95-108	3.6	19
53	Elastic Constant Calculations for Molecular Organic Crystals. *Crystal Growth and Design*, **2001**, 1, 13-27	3.5	95
52	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
51	Ab initio calculations on indole□water, 1-methylindole□water and indole□(water)2. *Chemical Physics Letters*, **2000**, 331, 253-261	2.5	37
50	A test of crystal structure prediction of small organic molecules. *Acta Crystallographica Section B: Structural Science*, **2000**, 56, 697-714		338
49	Dimer or Catemer? Low-Energy Crystal Packings for Small Carboxylic Acids. *Journal of Physical Chemistry B*, **2000**, 104, 2647-2655	3.4	130
48	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
47	Developments in computational studies of crystallization and morphology applied to urea. *Physical Chemistry Chemical Physics*, **2000**, 2, 3017-3027	3.6	27
46	A Systematic Nonempirical Method of Deriving Model Intermolecular Potentials for Organic Molecules: Application To Amides. *Journal of Physical Chemistry A*, **2000**, 104, 10958-10971	2.8	35

45	The errors in lattice energy minimisation studies: sensitivity to experimental variations in the molecular structure of paracetamol. *CrystEngComm*, **2000**, 2, 183	3.3	28
44	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	3.4	14
43	Electrostatic factors in DNA intercalation. *Biopolymers*, **1999**, 52, 84-93	2.2	53
42	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	3.3	6
41	Ab Initio Calculations on Uracil Water. *Journal of Physical Chemistry A*, **1999**, 103, 1611-1618	2.8	111
40	A Non-Empirical Intermolecular Potential for Oxalic Acid Crystal Structures. *Journal of Physical Chemistry A*, **1999**, 103, 6448-6457	2.8	34
39	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
38	Crystal structure predictions for acetic acid. *Journal of Computational Chemistry*, **1998**, 19, 459-474	3.5	76
37	Crystal structure predictions for acetic acid **1998**, 19, 459		1
36	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
35	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
34	Hydrogen bonding of carbonyl, ether, and ester oxygen atoms with alkanol hydroxyl groups. *Journal of Computational Chemistry*, **1997**, 18, 757-774	3.5	161
33	On the lack of hydrogen bonds in the crystal structure of alloxan. *Chemical Physics Letters*, **1997**, 265, 532-537	2.5	37
32	Anisotropic atom-atom potentials. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1996**, 73, 95-106		12
31	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
30	Applications of realistic electrostatic modelling to molecules in complexes, solids and proteins. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 2997		82
29	A Computational Investigation of the Dynamics of Urea Molecules in Solids. *Molecular Simulation*, **1996**, 18, 303-323	2	1
28	Modelling the interactions of protein side-chains. *Molecular Engineering*, **1995**, 5, 89-105		1

27	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	4.2	31
26	Relative binding orientations of adenosine A1 receptor ligands--a test case for Distributed Multipole Analysis in medicinal chemistry. *Journal of Computer-Aided Molecular Design*, **1995**, 9, 44-54	4.2	19
25	Solvent interactions with pi ring systems in proteins. *Protein Engineering, Design and Selection*, **1995**, 8, 109-16	1.9	24
24	Modelling the Interactions of Protein Side-Chains. *Jerusalem Symposia on Quantum Chemistry and Biochemistry*, **1995**, 119-135		1
23	Structural and dynamic properties of hydrogen bonding in a tetrahedral arrangement of methanol molecules. A theoretical investigation. *Chemical Physics Letters*, **1994**, 225, 273-279	2.5	5
22	Amino/aromatic interactions in proteins: is the evidence stacked against hydrogen bonding?. *Journal of Molecular Biology*, **1994**, 239, 315-31	6.5	297
21	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		19
20	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
19	Amino/aromatic interactions. *Nature*, **1993**, 366, 413-413	50.4	48
18	Electrostatic models for polypeptides: can we assume transferability?. *Journal of the Chemical Society, Faraday Transactions*, **1992**, 88, 1755		55
17	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
16	Towards an understanding of the arginine-aspartate interaction. *Journal of Molecular Biology*, **1992**, 226, 251-62	6.5	98
15	On the relative strengths of amide–amide and amide–water hydrogen bonds. *Chemical Physics Letters*, **1991**, 180, 517-523	2.5	57
14	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	3.5	96
13	A systematic intermolecular potential method applied to chlorine. *Molecular Physics*, **1990**, 71, 1381-1404	1.7	54
12	An overlap model for estimating the anisotropy of repulsion. *Molecular Physics*, **1990**, 69, 507-533	1.7	98
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