Richard I Cooper

List of Publications by Year
in descending order

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53 papers	5,230 citations	430874 18 h-index	302126 39 g-index
56 all docs	56 docs citations	56 times ranked	5428 citing authors

#	Article	IF	Citations
1	CRYSTALSversion 12: software for guided crystal structure analysis. Journal of Applied Crystallography, 2003, 36, 1487-1487.	4.5	2,595
2	Retrieval of Crystallographically-Derived Molecular Geometry Information. Journal of Chemical Information and Computer Sciences, 2004, 44, 2133-2144.	2.8	842
3	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
4	CRYSTALSenhancements: dealing with hydrogen atoms in refinement. Journal of Applied Crystallography, 2010, 43, 1100-1107.	4.5	406
5	The derivation of non-merohedral twin laws during refinement by analysis of poorly fitting intensity data and the refinement of non-merohedrally twinned crystal structures in the programCRYSTALS. Journal of Applied Crystallography, 2002, 35, 168-174.	4.5	168
6	Crystal structures of increasingly large molecules: meeting the challenges with CRYSTALS software. Chemistry Central Journal, 2015, 9, 30.	2.6	93
7	Compositional dependence of anomalous thermal expansion in perovskite-like ABX₃formates. Dalton Transactions, 2016, 45, 4169-4178.	3.3	78
8	ElectroShape: fast molecular similarity calculations incorporating shape, chirality and electrostatics. Journal of Computer-Aided Molecular Design, 2010, 24, 789-801.	2.9	77
9	A hexagonal planar transition-metal complex. Nature, 2019, 574, 390-393.	27.8	72
10	Will it crystallise? Predicting crystallinity of molecular materials. CrystEngComm, 2015, 17, 1927-1934.	2.6	70
11	Will they co-crystallize?. CrystEngComm, 2017, 19, 5336-5340.	2.6	67
12	Beyond Rotatable Bond Counts: Capturing 3D Conformational Flexibility in a Single Descriptor. Journal of Chemical Information and Modeling, 2016, 56, 2347-2352.	5.4	30
13	Charge-ice dynamics in the negative thermal expansion material Cd(CN)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	3.2	29
14	Structure and hydrogen bonding in 2,4-dihydroxybenzoic acid at 90, 100, 110 and 150â€…K; a theoretical and single-crystal X-ray diffraction study. Acta Crystallographica Section B: Structural Science, 2007, 63, 303-308.	1.8	26
15	Structure matching: measures of similarity and pseudosymmetry. Journal of Applied Crystallography, 2006, 39, 842-849.	4.5	24
16	Î±-Azidoesters as divergent intermediates for combinatorial generation of glucofuranose libraries of novel N-linked glycopeptides. Tetrahedron, 1996, 52, 10711-10720.	1.9	21
17	CRYSTALSenhancements: refinement of atoms continuously disordered along a line, on a ring or on the surface of a sphere. Journal of Applied Crystallography, 2004, 37, 545-550.	4.5	21
18	Applications of leverage analysis in structure refinement. Journal of Applied Crystallography, 2012, 45, 417-429.	4.5	20

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19	Controlling Intramolecular Interactions in the Design of Selective, High-Affinity Ligands for the CREBBP Bromodomain. Journal of Medicinal Chemistry, 2021, 64, 10102-10123.	6.4	17
20	Why direct and post-refinement determinations of absolute structure may give different results. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 661-683.	1.1	16
21	A publicly available crystallisation data set and its application in machine learning. CrystEngComm, 2017, 19, 3737-3745.	2.6	15
22	Absolute structure determination usingCRYSTALS. Acta Crystallographica Section C, Structural Chemistry, 2016, 72, 261-267.	0.5	11
23	The partial dehydrogenation of aluminium dihydrides. Chemical Science, 2019, 10, 8083-8093.	7.4	11
24	Howard Flack and the Flack Parameter. Chemistry, 2020, 2, 796-804.	2.2	10
25	Increasing the performance, trustworthiness and practical value of machine learning models: a case study predicting hydrogen bond network dimensionalities from molecular diagrams. CrystEngComm, 2020, 22, 7186-7192.	2.6	9
26	Steviamine, a new class of indolizidine alkaloid [(1R,2S,3R,5R,8aR)-3-hydroxymethyl-5-methyloctahydroindolizine-1,2-diol hydrobromide]. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o2904-o2905.	0.2	9
27	HUG and SQUEEZE: using CRYSTALS to incorporate resonant scattering in the SQUEEZE structure-factor contributions to determine absolute structure. Acta Crystallographica Section C, Structural Chemistry, 2017, 73, 845-853.	0.5	8
28	HAR, TAAM and BODD refinements of model crystal structures using CuÂKÎ± and MoÂKÎ± X-ray diffraction data. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2021, 77, 41-53.	1.1	8
29	The application of inelastic neutron scattering to investigate the interaction of methyl propanoate with silica. Physical Chemistry Chemical Physics, 2016, 18, 17210-17216.	2.8	6
30	CRYSTALSenhancements: asymmetric restraints. Journal of Applied Crystallography, 2012, 45, 1057-1060.	4.5	5
31	Heteroatom substitution effects in spin crossover dinuclear complexes. Dalton Transactions, 2019, 48, 7337-7343.	3.3	5
32	Acetato[1-(oxazolin-2-ylmethyl-ÎºN)-1H-indolyl-ÎºC2](triphenylphosphine)palladium(II) dichloromethane solvate. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, m582-m584.	0.2	3
33	An enhanced set of displacement parameter restraints in CRYSTALS. Journal of Applied Crystallography, 2018, 51, 1059-1068.	4.5	2
34	Recent Developments in the Refinement and Analysis of Crystal Structures. Structure and Bonding, 2020, , 43-67.	1.0	2
35	CIF applications. XVI.CIF2CRY: for CIF input into theCRYSTALSprogram. Journal of Applied Crystallography, 2004, 37, 669-671.	4.5	1
36	Chloro{1-[(dimethylamino)methyl-ÎºN]-1H-indolyl-ÎºC2}(triphenylphosphine-ÎºP)palladium(II) dichloromethane solvate. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, m585-m586.	0.2	1

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37	2-Acetamido-4-nitrotoluene. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2778-o2780.	0.2	1
38	3-Iodo-2,6-dinitrotoluene. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2836-o2838.	0.2	1
39	DetOx: a program for determining anomalous scattering factors of mixed-oxidation-state species. Journal of Synchrotron Radiation, 2013, 20, 200-204.	2.4	1
40	Isopropyl 6-amino-2,5-anhydro-3,6-dideoxy-6-N-(2,5-anhydro-6-azido-3,6-dideoxy-L-arabino-hexonyl)-L-arabino-hexonate. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o1712-o1714.	0.2	0
41	Methyl 3,6-anhydro-4-azido-5,7-O-(S)-benzylidene-2,4-dideoxy-D-talo-heptonate. Acta Crystallographica Section E: Structure Reports Online, 2004, 60, o839-o840.	0.2	0
42	N-(2-Methyl-3,6-dinitrophenyl)acetamide. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o3888-o3890.	0.2	0
43	Software solutions for custom-built X-ray diffractometers and non-standard experimental setups. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s499-s499.	0.1	0
44	Crystal math â€“ when numerical algorithms meet black magic. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s306-s307.	0.1	0
45	CRYSTALS: refinement and validation tools. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, s314-s314.	0.3	0
46	Effective data collection and refinement of pertubated structures. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1750-C1750.	0.1	0
47	Displacement Parameter Restraints for Dealing with Limited Data. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1728-C1728.	0.1	0
48	Fitting ensemble models of disorder usinga priorichemical structure information. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s165-s166.	0.1	0
49	On the application of leverage analysis to parameter precision using area-detector strategies. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s433-s433.	0.1	0
50	Optimizing co-crystal screens using a data-driven machine learning method. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1037-C1037.	0.1	0
51	Co-crystal or salt? A cautionary tale when inferring proton disorder solely from X-ray and computational data. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e220-e220.	0.1	0
52	Crystallographic software for the next generation. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e167-e167.	0.1	0
53	Adventures with CRYSTALS: developing methods and tools with an in-house refinement code. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, a238-a238.	0.1	0