Dylan Jayatilaka

List of Publications by Year
in descending order

145	18,326	46984 47	12933 131
papers	citations	h-index	g-index

155	155	155	10495
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hirshfeld surface analysis. CrystEngComm, 2009, 11, 19-32.	1.3	5,526
2	Towards quantitative analysis of intermolecular interactions with Hirshfeld surfaces. Chemical Communications, 2007, , 3814.	2.2	2,589
3	CrystalExplorer: a program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals. Journal of Applied Crystallography, 2021, 54, 1006-1011.	1.9	1,744
4	CrystalExplorermodel energies and energy frameworks: extension to metal coordination compounds, organic salts, solvates and open-shell systems. IUCrJ, 2017, 4, 575-587.	1.0	848
5	Energy frameworks: insights into interaction anisotropy and the mechanical properties of molecular crystals. Chemical Communications, 2015, 51, 3735-3738.	2.2	515
6	Comparing entire crystal structures: structural genetic fingerprinting. CrystEngComm, 2007, 9, 648.	1.3	486
7	Visualisation and characterisation of voids in crystalline materials. CrystEngComm, 2011, 13, 1804-1813.	1.3	397
8	Accurate and Efficient Model Energies for Exploring Intermolecular Interactions in Molecular Crystals. Journal of Physical Chemistry Letters, 2014, 5, 4249-4255.	2.1	380
9	Ab initio calculation of anharmonic constants for a transition state, with application to semiclassical transition state tunneling probabilities. Chemical Physics Letters, 1990, 172, 62-68.	1.2	221
10	Hydrogen atoms can be located accurately and precisely by x-ray crystallography. Science Advances, 2016, 2, e1600192.	4.7	211
11	Hirshfeld atom refinement. IUCrJ, 2014, 1, 361-379.	1.0	200
12	Openâ€shell coupledâ€cluster theory. Journal of Chemical Physics, 1993, 98, 9734-9747.	1.2	182
13	Wavefunctions derived from experiment. I. Motivation and theory. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 76-86.	0.3	178
14	X-ray structure refinement using aspherical atomic density functions obtained from quantum-mechanical calculations. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, 383-393.	0.3	172
15	Accurate Lattice Energies for Molecular Crystals from Experimental Crystal Structures. Journal of Chemical Theory and Computation, 2018, 14, 1614-1623.	2.3	164
16	Higher analytic derivatives. IV. Anharmonic effects in the benzene spectrum. Journal of Chemical Physics, 1992, 97, 4233-4254.	1.2	150
17	An open-shell restricted Hartreeâ€”Fock perturbation theory based on symmetric spin orbitals. Chemical Physics Letters, 1993, 201, 1-10.	1.2	150
18	Accurate crystal structures and chemical properties from NoSpherA2. Chemical Science, 2021, 12, 1675-1692.	3.7	147

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19	Electrostatic potentials mapped on Hirshfeld surfaces provide direct insight into intermolecular interactions in crystals. CrystEngComm, 2008, , .	1.3	133
20	Anharmonic corrections to vibrational transition intensities. The Journal of Physical Chemistry, 1990, 94, 5608-5616.	2.9	132
21	Wave Function for Beryllium from X-Ray Diffraction Data. Physical Review Letters, 1998, 80, 798-801.	2.9	131
22	Intermolecular interactions in molecular crystals: whatâ€™s in a name?. Faraday Discussions, 2017, 203, 93-112.	1.6	121
23	Tonto: A Fortran Based Object-Oriented System for Quantum Chemistry and Crystallography. Lecture Notes in Computer Science, 2003, , 142-151.	1.0	119
24	Anharmonic vibrational properties of CH2F2: A comparison of theory and experiment. Journal of Chemical Physics, 1991, 95, 8323-8336.	1.2	115
25	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	1.7	108
26	The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasiâ€isotropic Crystal Packing. Angewandte Chemie - International Edition, 2017, 56, 8468-8472.	7.2	104
27	The prediction of spectroscopic properties from quartic correlated force fields: HCCF, HFCO, SiH+3. Journal of Chemical Physics, 1990, 93, 4965-4981.	1.2	101
28	The Predominant Role of Coordination Number in Potassium Channel Selectivity. Biophysical Journal, 2007, 93, 2635-2643.	0.2	101
29	The Significance of Ionic Bonding in Sulfur Dioxide: Bond Orders from Xâ€ray Diffraction Data. Angewandte Chemie - International Edition, 2012, 51, 6776-6779.	7.2	99
30	Openâ€shell restricted Hartreeâ€“Fock perturbation theory: Some considerations and comparisons. Journal of Chemical Physics, 1994, 100, 7400-7409.	1.2	92
31	Spin contamination in single-determinant wavefunctions. Chemical Physics Letters, 1991, 183, 423-431.	1.2	91
32	Wavefunctions derived from experiment. II. A wavefunction for oxalic acid dihydrate. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 87-100.	0.3	89
33	A Flexible Approach to the Calculation of Resonance Energy Transfer Efficiency between Multiple Donors and Acceptors in Complex Geometries. Biophysical Journal, 2005, 89, 3822-3836.	0.2	83
34	Electron spin resonance g tensors from general Hartreeâ€“Fock calculations. Journal of Chemical Physics, 1998, 108, 7587-7594.	1.2	77
35	Sâ‹¯O chalcogen bonding in sulfa drugs: insights from multipole charge density and X-ray wavefunction of acetazolamide. Physical Chemistry Chemical Physics, 2015, 17, 25411-25420.	1.3	74
36	Probing the accuracy and precision of Hirshfeld atom refinement with HARt interfaced with Olex2. IUCrJ, 2018, 5, 32-44.	1.0	74

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37	Tuning the hydrogen storage properties of defect-engineered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="bold">C</mml:mi></mml:mrow><mml:mrow><mml:mn mathvariant="bold">4</mml:mn></mml:mrow></mml:msub><mml:mi mathvariant="bold">N</mml:mi></mml:mrow></mml:math> nanosheets under ambient conditions.	5.4	69
38	Wave functions derived from experiment. V. Investigation of electron densities, electrostatic potentials, and electron localization functions for noncentrosymmetric crystals. Journal of Computational Chemistry, 2003, 24, 470-483.	1.5	59
39	Hirshfeld atom refinement for modelling strong hydrogen bonds. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, 483-498.	0.0	59
40	Importance of Relativistic Effects and Electron Correlation in Structure Factors and Electron Density of Diphenyl Mercury and Triphenyl Bismuth. Journal of Physical Chemistry A, 2016, 120, 6650-6669.	1.1	57
41	Higher analytic derivatives. II. The fourth derivative of selfâ€consistentâ€field energy. Journal of Chemical Physics, 1991, 95, 7409-7417.	1.2	55
42	Wavefunctions derived from experiment. IV. Investigation of the crystal environment of ammonia. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, 244-251.	0.3	55
43	Wavefunctions derived from experiment. III. Topological analysis of crystal fragments. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, 232-243.	0.3	51
44	Determination of the Orientational Distribution and Orientation Factor for Transfer between Membrane-Bound Fluorophores using a Confocal Microscope. Biophysical Journal, 2006, 91, 1032-1045.	0.2	50
45	Structural Investigation of MscL Gating Using Experimental Data and Coarse Grained MD Simulations. PLoS Computational Biology, 2012, 8, e1002683.	1.5	50
46	Basis set convergence of CCSD(T) equilibrium geometries using a large and diverse set of molecular structures. Journal of Chemical Physics, 2016, 145, 104101.	1.2	50
47	Ab initio prediction of fundamental, overtone and combination band infrared intensities. Chemical Physics Letters, 1990, 169, 127-137.	1.2	49
48	Validation of Xâ€ray Wavefunction Refinement. ChemPhysChem, 2017, 18, 3334-3351.	1.0	49
49	Effective molecular polarizabilities and crystal refractive indices estimated from x-ray diffraction data. Journal of Chemical Physics, 2006, 125, 174505.	1.2	48
50	Some fundamental problems with zero flux partitioning of electron densities. Theoretical Chemistry Accounts, 2001, 105, 213-218.	0.5	46
51	Electron localization functions obtained from X-ray constrained Hartreeâ€“Fock wavefunctions for molecular crystals of ammonia, urea and alloxanWork presented at the Microsymposium on Quantum Crystallography, XIX IUCr Congress, Geneva, Switzerland, August 2002.. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 111-119.	0.3	46
52	The form of spin orbitals for open-shell restricted Hartreeâ€”Fock reference functions. Chemical Physics Letters, 1992, 199, 211-219.	1.2	44
53	X-ray constrained unrestricted Hartreeâ€“Fock and Douglasâ€“Krollâ€“Hess wavefunctions. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, 78-92.	0.3	44
54	Higher analytic derivatives. I. A new implementation for the third derivative of theSCF energy. International Journal of Quantum Chemistry, 1991, 40, 179-199.	1.0	43

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55	The use of dipole lattice sums to estimate electric fields and dipole moment enhancement in molecular crystals. Chemical Physics Letters, 2007, 443, 87-91.	1.2	42
56	Refractive indices for molecular crystals from the response of X-ray constrained Hartreeâ€“Fock wavefunctions. Physical Chemistry Chemical Physics, 2009, 11, 7209.	1.3	41
57	Covalency and Ionicity Do Not Oppose Each Otherâ€”Relationship Between Siâ‹¯O Bond Character and Basicity of Siloxanes. Chemistry - A European Journal, 2018, 24, 15275-15286.	1.7	40
58	Simulation of Structure, Orientation, and Energy Transfer between AlexaFluor Molecules Attached to MscL. Biophysical Journal, 2008, 95, 2711-2721.	0.2	39
59	Metal functionalized inorganic nano-sheets as promising materials for clean energy storage. Applied Surface Science, 2019, 471, 887-892.	3.1	39
60	Crystal-field effects in<scp>L</scp>-homoserine: multipolesversusquantum chemistry. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 435-442.	0.3	36
61	Measurement of Electric Fields Experienced by Urea Guest Molecules in the 18-Crown-6/Urea (1:5) Hostâ€“Guest Complex: An Experimental Reference Point for Electric-Field-Assisted Catalysis. Journal of the American Chemical Society, 2019, 141, 3965-3976.	6.6	35
62	Bond Length and Local Energy Density Property Connections for Non-Transition-Metal Oxide-Bonded Interactions. Journal of Physical Chemistry A, 2006, 110, 12259-12266.	1.1	33
63	A Variety of Bond Analysis Methods, One Answer? An Investigation of the Elementâ‹¯Oxygen Bond of Hydroxides H_nXOH. Chemistry - A European Journal, 2018, 24, 6248-6261.	1.7	33
64	Higher analytic derivatives. Molecular Physics, 1992, 75, 271-291.	0.8	31
65	The Electron Localizability Indicator from Xâ€Ray Diffraction Dataâ€”A First Application to a Series of Epoxide Derivatives. Chemistry - A European Journal, 2010, 16, 12818-12821.	1.7	31
66	A definition for the covalent and ionic bond index in a molecule. Theoretical Chemistry Accounts, 2008, 119, 275-290.	0.5	30
67	Modeling electron density distributions from X-ray diffraction to derive optical properties: Constrained wavefunction versus multipole refinement. Journal of Chemical Physics, 2013, 139, 064108.	1.2	30
68	The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasiâ€isotropic Crystal Packing. Angewandte Chemie, 2017, 129, 8588-8592.	1.6	29
69	A comparison of electron density from Hirshfeld-atom refinement, X-ray wavefunction refinement and multipole refinement on three urea derivatives. CrystEngComm, 2013, 15, 2084.	1.3	28
70	High Throughput Profiling of Molecular Shapes in Crystals. Scientific Reports, 2016, 6, 22204.	1.6	26
71	Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. Angewandte Chemie - International Edition, 2019, 58, 16780-16784.	7.2	26
72	Reactivity Differences between Î±,Î²-Unsaturated Carbonyls and Hydrazones Investigated by Experimental and Theoretical Electron Density and Electron Localizability Analyses. Journal of Physical Chemistry A, 2011, 115, 12715-12732.	1.1	25

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73	Bond orders for intermolecular interactions in crystals: charge transfer, ionicity and the effect on intramolecular bonds. IUCrJ, 2018, 5, 635-646.	1.0	25
74	Hydrogen atoms in bridging positions from quantum crystallographic refinements: influence of hydrogen atom displacement parameters on geometry and electron density. CrystEngComm, 2020, 22, 4778-4789.	1.3	25
75	A challenge for density functional theory: the XONO and XNO 2 (X=F, Cl, and Br) molecules. Theoretical Chemistry Accounts, 1997, 97, 185-194.	0.5	24
76	Fourier transforms of property densities with Gaussian functions. Chemical Physics Letters, 1994, 230, 228-230.	1.2	23
77	Relativistic quantum crystallography of diphenyl- and dicyanomercury. Theoretical structure factors and Hirshfeld atom refinement. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 705-717.	0.0	23
78	On the accuracy and precision of X-ray and neutron diffraction results as a function of resolution and the electron density model. IUCrJ, 2020, 7, 920-933.	1.0	23
79	Post-Hartree-Fock methods for Hirshfeld atom refinement: are they necessary? Investigation of a strongly hydrogen-bonded molecular crystal. Journal of Molecular Structure, 2020, 1209, 127934.	1.8	22
80	Intermolecular Interactions and Electrostatic Properties of the Î²-Hydroquinone Apohost: Implications for Supramolecular Chemistry. Journal of Physical Chemistry A, 2011, 115, 12962-12972.	1.1	21
81	Testing the use of molecular dynamics to simulate fluorophore motions and FRET. Physical Chemistry Chemical Physics, 2011, 13, 11045.	1.3	20
82	Mapping the Importance of Four Factors in Creating Monovalent Ion Selectivity in Biological Molecules. Biophysical Journal, 2011, 100, 60-69.	0.2	19
83	Reliable Measurements of Dipole Moments from Single-Crystal Diffraction Data and Assessment of an In-Crystal Enhancement. Structure and Bonding, 2012, , 27-45.	1.0	18
84	Predicting the Position of the Hydrogen Atom in the Short Intramolecular Hydrogen Bond of the Hydrogen Maleate Anion from Geometric Correlations. Crystal Growth and Design, 2017, 17, 3812-3825.	1.4	18
85	Comparison of semiempirical and ab initio QM decomposition analyses for the interaction energy between molecules. Chemical Physics Letters, 2002, 352, 245-251.	1.2	17
86	ExiFRET: flexible tool for understanding FRET in complex geometries. Journal of Biomedical Optics, 2012, 17, 011005.	1.4	17
87	Linear MgCp*₂ vs Bent CaCp*₂: London Dispersion, Ligand-Induced Charge Localizations, and Pseudo-Pregostic Câ€“HÂ·Â·Â·Ca Interactions. Inorganic Chemistry, 2018, 57, 4906-4920.	1.9	17
88	The Advent of Quantum Crystallography: Form and Structure Factors from Quantum Mechanics for Advanced Structure Refinement and Wavefunction Fitting. Structure and Bonding, 2020, , 65-144.	1.0	17
89	A problematic issue for atoms in molecules: Impact of (quasi-)degenerate states on Quantum Theory Atoms in Molecules and Hirshfeld-I properties. Computational and Theoretical Chemistry, 2015, 1053, 106-111.	1.1	15
90	Siâ€'O Bonded Interactions in Silicate Crystals and Molecules:Â A Comparison. Journal of Physical Chemistry A, 2006, 110, 12678-12683.	1.1	14

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91	Picture change error correction of radon atom electron density. Journal of Chemical Physics, 2010, 133, 174125.	1.2	14
92	Study of the picture change error at the 2nd order Douglas Kroll Hess level of theory. Electron and spin density and structure factors of the Bis[bis(methoxycarbimido) aminato] copper (II) complex. Chemical Physics, 2012, 395, 44-53.	0.9	14
93	Picture change error in quasirelativistic electron/spin density, Laplacian and bond critical points. Chemical Physics, 2014, 438, 37-47.	0.9	14
94	An ab initio calculation of magnetic structure factors for Cs3CoCl5 including spinâ€“orbit and finite magnetic field effects. Journal of Chemical Physics, 1995, 103, 4562-4571.	1.2	13
95	Are intramolecular dynamic electron correlation effects detectable in X-ray diffraction experiments on molecular crystals?. Acta Crystallographica Section A: Foundations and Advances, 2007, 63, 135-145.	0.3	13
96	Revised electrostatics from invariom refinement of the 18-residue peptaibol antibiotic trichotoxin A50E. CrystEngComm, 2010, 12, 2419.	1.3	12
97	An Entropic Mechanism of Generating Selective Ion Binding in Macromolecules. PLoS Computational Biology, 2013, 9, e1002914.	1.5	12
98	Predicting the primary fragments in mass spectrometry using ab initio Robyâ€“Gould bond indices. International Journal of Quantum Chemistry, 2018, 118, e25603.	1.0	12
99	Cyclopropa-Fused Quinones. The Generation and Trapping of Bicyclo[4.1.0]hepta-1(6),3-diene-2,5-dione and 1H-Cyclopropa[b]naphthalene-2,7-dione. Australian Journal of Chemistry, 1997, 50, 505.	0.5	12
100	Analytic second derivatives with model potentials at SCF and MP2 levels. Chemical Physics Letters, 1989, 163, 151-156.	1.2	11
101	A complement to "Some fundamental problems with zero flux partitioning of electron densities". Theoretical Chemistry Accounts, 2002, 107, 383-384.	0.5	11
102	Picture change error correction in the radial distributions of canonical orbital densities and total electron density of radon atom: the effect of the size of nucleus and the basis set limit. Theoretical Chemistry Accounts, 2011, 129, 181-197.	0.5	11
103	Can Experimental Electronâ€Density Studies be Used as a Tool to Predict Biologically Relevant Properties of Lowâ€Molecular Weight Enzyme Ligands?. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 1905-1921.	0.6	11
104	Quantum chemical electron impact mass spectrum prediction for de novo structure elucidation: Assessment against experimental reference data and comparison to competitive fragmentation modeling. International Journal of Quantum Chemistry, 2018, 118, e25460.	1.0	11
105	The advanced treatment of hydrogen bonding in quantum crystallography. Journal of Applied Crystallography, 2021, 54, 718-729.	1.9	11
106	Solid-State Dilution of Dihydroxybenzophenones with 4,13-Diaza-18-crown-6 for Photocrystallographic Studies. Crystal Growth and Design, 2012, 12, 2277-2287.	1.4	10
107	Spin contamination analogy, Kramers pairs symmetry and spin density representations at the 2-component unrestricted Hartreeâ€“Fock level of theory. Computational and Theoretical Chemistry, 2015, 1065, 27-41.	1.1	10
108	Electrostatic complementarity in pseudoreceptor modeling based on drug molecule crystal structures: the case of loxistatin acid (E64c). New Journal of Chemistry, 2015, 39, 1628-1633.	1.4	10

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109	Similarities and Differences between Crystal and Enzyme Environmental Effects on the Electron Density of Drug Molecules. Chemistry - A European Journal, 2021, 27, 3407-3419.	1.7	10
110	fragHAR: towardsab initioquantum-crystallographic X-ray structure refinement for polypeptides and proteins. IUCrJ, 2020, 7, 158-165.	1.0	10
111	X-ray constrained wavefunctions based on Hirshfeld atoms. I. Method and review. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 312-332.	0.5	10
112	X-ray constrained wavefunctions based on Hirshfeld atoms. II. Reproducibility of electron densities in crystals of Î±-oxalic acid dihydrate. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 397-415.	0.5	9
113	Investigating the Resonance in Nitric Acid and the Nitrate Anion Based on a Modern Bonding Analysis. Australian Journal of Chemistry, 2018, 71, 227.	0.5	8
114	Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. Angewandte Chemie, 2019, 131, 16936-16940.	1.6	8
115	Implications of unitary invariance for gradient theory. International Journal of Quantum Chemistry, 1992, 42, 445-458.	1.0	6
116	A theoretical study of the polarized neutron scattering from Cs3CoCl5. Journal of Chemical Physics, 2001, 114, 2687-2697.	1.2	6
117	How does overcoordination create ion selectivity?. Biophysical Chemistry, 2013, 172, 37-42.	1.5	6
118	Spatial symmetry and equivalence with unrestricted Hartree-Fock wavefunctions: application to the prediction of spin densities. Molecular Physics, 1997, 92, 471-476.	0.8	6
119	Ab initio study of the cyclic isomers of N2S4. Chemical Physics, 1995, 198, 169-181.	0.9	4
120	The quasirelativistic contact interaction and effective electron and spin densities at the nucleus: A model based on weighting the electron density with the finite Gaussian nucleus model. Chemical Physics Letters, 2013, 580, 152-159.	1.2	4
121	Is it Reasonable to Obtain Information on the Polarizability and Hyperpolarizability Only from the Electron Density?. Australian Journal of Chemistry, 2018, 71, 295.	0.5	4
122	HgH₂meets relativistic quantum crystallography. How to teach relativity to a non-relativistic wavefunction. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, 54-66.	0.0	4
123	Contributions of the electronic spin and orbital current to the ${m CoCl}_4^{2-}$ CoCl 42â˚' magnetic field probed in polarised neutron diffraction experiments. Journal of Chemical Physics, 2012, 137, 064107.	1.2	3
124	Glycyl-<scp>L</scp>-alanine: a multi-temperature neutron study. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 949-952.	0.2	3
125	Analytic SCF third and fourth derivatives with model potentials. Chemical Physics Letters, 1993, 212, 18-26.	1.2	2
126	Comment on â€œInter/Intramolecular Bonds in TH₅⁺ (T = C/Si/Ge): H₂ as Tetrel Bond Acceptor and the Uniqueness of Carbon Bondsâ€• Journal of Physical Chemistry A, 2019, 123, 9242-9243.	1.1	2

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127	Roby-Gould bond indices as a tool for understanding chemical bonding from a mathematical and quantum mechanical perspective. Results in Chemistry, 2020, 2, 100053.	0.9	2
128	Quantitative approaches to crystal engineering: applications to mechanical properties. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C849-C849.	0.0	2
129	Using Wavefunctions to Get More Information Out of Diffraction Experiments. , 2011, , 213-257.		1
130	A Model of the Open Pore MscL Based on Experimental Data and Restrained Coarse Grained Simulations. Biophysical Journal, 2012, 102, 121a-122a.	0.2	1
131	Structure Factors and Charge Density Description of Aluminum: A Quantum Crystallographic Study. Journal of Physical Chemistry A, 2022, 126, 2042-2049.	1.1	1
132	Mapping the Common Origins of Ion Selectivity in Biological Molecules. Biophysical Journal, 2009, 96, 660a-661a.	0.2	0
133	Determination of Fluorophore Orientation and Energy Transfer from MD Simulations. Biophysical Journal, 2010, 98, 582a.	0.2	0
134	Interpreting FRET in Complex Geometries. Biophysical Journal, 2010, 98, 584a.	0.2	0
135	Mapping the Importance of 4 factors in Creating Monovalent Ion Selectivity in Biological Molecules. Biophysical Journal, 2011, 100, 578a.	0.2	0
136	X-ray wavefunction refinement â€“ introduction, examples, validation. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, s589-s589.	0.3	0
137	Hirshfeld atom refinement for determining hydrogen positions in routine X-ray experiments. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s107-s107.	0.0	0
138	A technique for the comparison and analysis of decorated molecular surfaces. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s474-s475.	0.0	0
139	Quantum mechanical synthon interaction energies. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C682-C682.	0.0	0
140	Applications of X-ray Wavefunction Refinement. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1343-C1343.	0.0	0
141	Hydrogen maleate salts: precise and accurate determination of the hydrogen atom position in short hydrogen bonds using X-ray diffraction at extremely low temperatures. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s89-s89.	0.0	0
142	Precision and accuracy of single-crystal X-ray results. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1388-C1388.	0.0	0
143	Waverfunction refinement-derived spin density of two cAAC-SiCl₃ polymorphs. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C571-C571.	0.0	0
144	Introducing iterative X-ray wavefunction refinement. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C702-C702.	0.0	0

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145	Quantum crystallography towards 'quantitative crystal engineering'. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e78-e78.	0.0	0