

# Mark A Spackman

## List of Publications by Year in descending order

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138  
papers

24,869  
citations

46918

47  
h-index

14156

128  
g-index

139  
all docs

139  
docs citations

139  
times ranked

10813  
citing authors

| #  | ARTICLE  | IF  | CITATIONS |
|----|--|-----|-----------|
| 1  | Hirshfeld surface analysis. <i>CrystEngComm</i> , 2009, 11, 19-32.   | 1.3 | 5,526     |
| 2  | Fingerprinting intermolecular interactions in molecular crystals. <i>CrystEngComm</i> , 2002, 4, 378-392.  | 1.3 | 3,050     |
| 3  | Towards quantitative analysis of intermolecular interactions with Hirshfeld surfaces. <i>Chemical Communications</i> , 2007, , 3814.   | 2.2 | 2,589     |
| 4  | Novel tools for visualizing and exploring intermolecular interactions in molecular crystals. <i>Acta Crystallographica Section B: Structural Science</i> , 2004, 60, 627-668.                      | 1.8 | 2,165     |
| 5  | <i>CrystalExplorer</i> : a program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals. <i>Journal of Applied Crystallography</i> , 2021, 54, 1006-1011. | 1.9 | 1,744     |
| 6  | A novel definition of a molecule in a crystal. <i>Chemical Physics Letters</i> , 1997, 267, 215-220.   | 1.2 | 974       |
| 7  | <i>CrystalExplorer</i> model energies and energy frameworks: extension to metal coordination compounds, organic salts, solvates and open-shell systems. <i>IUCr</i> , 2017, 4, 575-587.            | 1.0 | 848       |
| 8  | Hirshfeld Surfaces: A New Tool for Visualising and Exploring Molecular Crystals. <i>Chemistry - A European Journal</i> , 1998, 4, 2136-2141.   | 1.7 | 710       |
| 9  | Energy frameworks: insights into interaction anisotropy and the mechanical properties of molecular crystals. <i>Chemical Communications</i> , 2015, 51, 3735-3738.                                 | 2.2 | 515       |
| 10 | Comparing entire crystal structures: structural genetic fingerprinting. <i>CrystEngComm</i> , 2007, 9, 648.  | 1.3 | 486       |
| 11 | Visualisation and characterisation of voids in crystalline materials. <i>CrystEngComm</i> , 2011, 13, 1804-1813.   | 1.3 | 397       |
| 12 | Accurate and Efficient Model Energies for Exploring Intermolecular Interactions in Molecular Crystals. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4249-4255.                          | 2.1 | 380       |
| 13 | Three new co-crystals of hydroquinone: crystal structures and Hirshfeld surface analysis of intermolecular interactions. <i>New Journal of Chemistry</i> , 2010, 34, 193-199.                      | 1.4 | 306       |
| 14 | Comparison of Polymorphic Molecular Crystal Structures through Hirshfeld Surface Analysis. <i>Crystal Growth and Design</i> , 2007, 7, 755-769.  | 1.4 | 296       |
| 15 | Accurate prediction of static dipole polarizabilities with moderately sized basis sets. <i>The Journal of Physical Chemistry</i> , 1989, 93, 7594-7603.  | 2.9 | 229       |
| 16 | A simple quantitative model of hydrogen bonding. <i>Journal of Chemical Physics</i> , 1986, 85, 6587-6601.   | 1.2 | 209       |
| 17 | Atom-atom potentials via electron gas theory. <i>Journal of Chemical Physics</i> , 1986, 85, 6579-6586.  | 1.2 | 169       |
| 18 | Accurate Lattice Energies for Molecular Crystals from Experimental Crystal Structures. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1614-1623.                                    | 2.3 | 164       |

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|----|--|-----|-----------|
| 19 | Solvent inclusion in the structural voids of form II carbamazepine: single-crystal X-ray diffraction, NMR spectroscopy and Hirshfeld surface analysis. <i>CrystEngComm</i> , 2007, 9, 728.   | 1.3 | 157       |
| 20 | Electrostatic potentials mapped on Hirshfeld surfaces provide direct insight into intermolecular interactions in crystals. <i>CrystEngComm</i> , 2008, , .   | 1.3 | 133       |
| 21 | Molecules in crystals. <i>Physica Scripta</i> , 2013, 87, 048103.  | 1.2 | 127       |
| 22 | Intermolecular interactions in molecular crystals: whatâ€™s in a name?. <i>Faraday Discussions</i> , 2017, 203, 93-112.  | 1.6 | 121       |
| 23 | Potential derived charges using a geodesic point selection scheme. , 1996, 17, 1-18.   |     | 116       |
| 24 | How Reliable Are Intermolecular Interaction Energies Estimated from Topological Analysis of Experimental Electron Densities?. <i>Crystal Growth and Design</i> , 2015, 15, 5624-5628.  | 1.4 | 105       |
| 25 | The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasiâ€™isotropic Crystal Packing. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 8468-8472.  | 7.2 | 104       |
| 26 | Direct Evidence of Cation Disorder in Thermoelectric Lead Chalcogenides PbTe and PbS. <i>Advanced Functional Materials</i> , 2013, 23, 5477-5483.  | 7.8 | 98        |
| 27 | Hydrogen bond energetics from topological analysis of experimental electron densities: Recognising the importance of the promolecule. <i>Chemical Physics Letters</i> , 1999, 301, 425-429.  | 1.2 | 97        |
| 28 | Introduction and validation of an invariom database for amino-acid, peptide and protein molecules. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2006, 62, 1325-1335.  | 2.5 | 94        |
| 29 | Estimated H-atom anisotropic displacement parameters: a comparison between different methods and with neutron diffraction results. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2008, 64, 465-475.  | 0.3 | 94        |
| 30 | Vibrational averaging of electrical properties. <i>Molecular Physics</i> , 1995, 84, 1239-1255.  | 0.8 | 83        |
| 31 | Influence of intermolecular interactions on multipole-refined electron densities. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1999, 55, 30-47.   | 0.3 | 78        |
| 32 | Anisotropic displacement parameters for H atoms using an ONIOM approach. <i>Acta Crystallographica Section B: Structural Science</i> , 2006, 62, 875-888.  | 1.8 | 69        |
| 33 | Reassessment of Large Dipole Moment Enhancements in Crystals:â€™ A Detailed Experimental and Theoretical Charge Density Analysis of 2-Methyl-4-nitroaniline. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8763-8776.  | 1.1 | 64        |
| 34 | Invarioms for improved absolute structure determination of light-atom crystal structures. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2006, 62, 217-223.   | 0.3 | 64        |
| 35 | Dipole Moment Enhancement in Molecular Crystals from Xâ€™ray Diffraction Data. <i>ChemPhysChem</i> , 2007, 8, 2051-2063.   | 1.0 | 63        |
| 36 | Anisotropic molecular polarizabilities, dipole moments, and quadrupole moments of (CH <sub>2</sub> ) <sub>2</sub> X, (CH <sub>3</sub> ) <sub>2</sub> X, and C <sub>4</sub> H <sub>4</sub> X (X = O, S, Se). Comparison of experimental results and ab initio calculations. <i>The Journal of Physical Chemistry</i> , 1992, 96, 7301-7307. | 2.9 | 60        |

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|----|---|-----|-----------|
| 37 | Basis set choice and basis set superposition error (BSSE) in periodic Hartree-Fock calculations on molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 1518-1523.   | 1.3 | 59        |
| 38 | Electron Distribution and Molecular Motion in Crystalline Benzene: An Accurate Experimental Study Combining CCD X-ray Data on C <sub>6</sub> H <sub>6</sub> with Multitemperature Neutron-Diffraction Results on C <sub>6</sub> D <sub>6</sub> . <i>Chemistry - A European Journal</i> , 2002, 8, 3512. | 1.7 | 59        |
| 39 | Hirshfeld atom refinement for modelling strong hydrogen bonds. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, 483-498.   | 0.0 | 59        |
| 40 | Molecular surfaces from the promolecule: A comparison with Hartree-Fock ab initio electron density surfaces. <i>Journal of Computational Chemistry</i> , 2000, 21, 933-942.   | 1.5 | 58        |
| 41 | Accurate prediction of static dipole polarizabilities with moderately sized basis sets. <i>Molecular Physics</i> , 1994, 82, 193-209.   | 0.8 | 57        |
| 42 | Visualizing Lithium-Ion Migration Pathways in Battery Materials. <i>Chemistry - A European Journal</i> , 2013, 19, 15535-15544.   | 1.7 | 57        |
| 43 | Time-dependent Hartree-Fock second-order molecular properties with a moderately sized basis set. I. The frequency dependence of the dipole polarizability. <i>Journal of Chemical Physics</i> , 1991, 94, 1288-1294.  | 1.2 | 55        |
| 44 | Global Analysis of the Mechanical Properties of Organic Crystals. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .  | 7.2 | 55        |
| 45 | A simple quantitative model of hydrogen bonding: application to more complex systems. <i>The Journal of Physical Chemistry</i> , 1987, 91, 3179-3186.   | 2.9 | 54        |
| 46 | An ab initio study of vibrational corrections to the electrical properties of the second-row hydrides. <i>Molecular Physics</i> , 1997, 90, 251-264.  | 0.8 | 54        |
| 47 | Molecular dynamics simulations of structure and dynamics of organic molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14916.   | 1.3 | 51        |
| 48 | Crystal packing in the 2-R,4-oxo-[1,3-a/b]-naphthodioxanes - Hirshfeld surface analysis and melting point correlation. <i>CrystEngComm</i> , 2012, 14, 1083-1093.   | 1.3 | 49        |
| 49 | Effective molecular polarizabilities and crystal refractive indices estimated from x-ray diffraction data. <i>Journal of Chemical Physics</i> , 2006, 125, 174505.  | 1.2 | 48        |
| 50 | Polymorphism in 3-methyl-4-methoxy-4'-nitrostilbene (MMONS), a highly active NLO material. <i>CrystEngComm</i> , 2008, 10, 197-206.   | 1.3 | 48        |
| 51 | Energy frameworks and a topological analysis of the supramolecular features in in situ cryocrystallized liquids: tuning the weak interaction landscape via fluorination. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31811-31820.  | 1.3 | 48        |
| 52 | The use of the promolecular charge density to approximate the penetration contribution to intermolecular electrostatic energies. <i>Chemical Physics Letters</i> , 2006, 418, 158-162.  | 1.2 | 47        |
| 53 | Synthesis, Crystal Structure, Atomic Hirshfeld Surfaces, and Physical Properties of Hexagonal CeMnNi <sub>4</sub> . <i>Inorganic Chemistry</i> , 2010, 49, 9343-9349.   | 1.9 | 46        |
| 54 | Charge density analysis of two polymorphs of antimony(III) oxide. <i>Dalton Transactions</i> , 2004, , 23.  | 1.6 | 45        |

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|----|--|-----|-----------|
| 55 | Quasi-isostructural polymorphism™ in molecular crystals: inputs from interaction hierarchy and energy frameworks. <i>Chemical Communications</i> , 2016, 52, 2141-2144.  | 2.2 | 44        |
| 56 | Can the interaction density be measured? The example of the non-standard amino acid sarcosine. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2007, 63, 426-436.  | 0.3 | 43        |
| 57 | The use of dipole lattice sums to estimate electric fields and dipole moment enhancement in molecular crystals. <i>Chemical Physics Letters</i> , 2007, 443, 87-91.  | 1.2 | 42        |
| 58 | Refractive indices for molecular crystals from the response of X-ray constrained Hartree-Fock wavefunctions. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 7209.  | 1.3 | 41        |
| 59 | Magnetically recoverable Fe <sub>3</sub> O <sub>4</sub> @Au-coated nanoscale catalysts for the A <sup>3</sup> -coupling reaction. <i>Dalton Transactions</i> , 2017, 46, 5133-5137.  | 1.6 | 40        |
| 60 | Time-dependent Hartree-Fock second-order molecular properties with a moderately sized basis set. II. Dispersion coefficients. <i>Journal of Chemical Physics</i> , 1991, 94, 1295-1305.  | 1.2 | 38        |
| 61 | Accurate <i>ab initio</i> study of acetylene Vibrational and rotational corrections to electrical properties. <i>Molecular Physics</i> , 1996, 88, 1109-1136.  | 0.8 | 36        |
| 62 | Redetermination, invariom-model and multipole refinement of L-ornithine hydrochloride. <i>Acta Crystallographica Section B: Structural Science</i> , 2007, 63, 505-509.  | 1.8 | 36        |
| 63 | Analysis of the compression of molecular crystal structures using Hirshfeld surfaces. <i>CrystEngComm</i> , 2008, , .  | 1.3 | 36        |
| 64 | The Polymorphs of ROY: A Computational Study of Lattice Energies and Conformational Energy Differences. <i>Australian Journal of Chemistry</i> , 2018, 71, 279.  | 0.5 | 36        |
| 65 | Bonded Radii and the Contraction of the Electron Density of the Oxygen Atom by Bonded Interactions. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1632-1640.   | 1.1 | 35        |
| 66 | Measurement of Electric Fields Experienced by Urea Guest Molecules in the 18-Crown-6/Urea (1:5) Host-Guest Complex: An Experimental Reference Point for Electric-Field-Assisted Catalysis. <i>Journal of the American Chemical Society</i> , 2019, 141, 3965-3976. | 6.6 | 35        |
| 67 | Supramolecular Recognition and Energy Frameworks in Host-Guest Complexes of 18-Crown-6 and Sulfonamides. <i>Crystal Growth and Design</i> , 2015, 15, 5892-5900.   | 1.4 | 34        |
| 68 | An Exploration of Theoretical and Experimental Electron Density Distributions and SiO Bonded Interactions for the Silica Polymorph Coesite. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12996-13006.   | 1.2 | 33        |
| 69 | Bond Length and Local Energy Density Property Connections for Non-Transition-Metal Oxide-Bonded Interactions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12259-12266.   | 1.1 | 33        |
| 70 | Chapter 5. Charge densities from X-ray diffraction data. <i>Annual Reports on the Progress of Chemistry Section C</i> , 1998, 94, 177.   | 4.4 | 32        |
| 71 | Electrostatic potential in dehydrated zeolite NaA from low-resolution x-ray diffraction data. <i>The Journal of Physical Chemistry</i> , 1988, 92, 794-796.  | 2.9 | 31        |
| 72 | Supramolecular polymorphism of the 1:1 molecular salt (adamantane-1-carboxylate-3,5,7-tricarboxylic) Tj ETQq0 0 0 rgBT /Ov<br>2012, 48, 1883-1885.   | 2.2 | 31        |

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|----|--|-----|-----------|
| 73 | Effects of Weak Intermolecular Interactions on the Molecular Isomerism of Tricobalt Metal Chains. <i>Journal of the American Chemical Society</i> , 2009, 131, 7580-7591.  | 6.6 | 29        |
| 74 | Multi-temperature Synchrotron Powder X-ray Diffraction Study and Hirshfeld Surface Analysis of Chemical Bonding in the Thermoelectric Zintl Phase $\text{Yb}_{14}\text{MnSb}_{11}$ . <i>Chemistry of Materials</i> , 2011, 23, 3723-3730.                            | 3.2 | 29        |
| 75 | The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasi-Isotropic Crystal Packing. <i>Angewandte Chemie</i> , 2017, 129, 8588-8592.   | 1.6 | 29        |
| 76 | Theoretical Electron Density Distributions for Fe- and Cu-Sulfide Earth Materials: A Connection between Bond Length, Bond Critical Point Properties, Local Energy Densities, and Bonded Interactions. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1923-1931. | 1.2 | 28        |
| 77 | Visualising intermolecular interactions in crystals: naphthalene vs. terephthalic acid. <i>Chemical Communications</i> , 1998, , 2071-2072.  | 2.2 | 26        |
| 78 | Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 16780-16784.   | 7.2 | 26        |
| 79 | Controlling the Confinement and Alignment of Fullerene C <sub>70</sub> in para-Substituted Calix[5]arenes. <i>Chemistry - A European Journal</i> , 2007, 13, 3907-3912.  | 1.7 | 25        |
| 80 | Intermolecular Interactions and Electrostatic Properties of the $\beta$ -Hydroquinone Apohost: Implications for Supramolecular Chemistry. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12962-12972.   | 1.1 | 21        |
| 81 | Intermolecular Interaction Energies in Hydroquinone Clathrates at High Pressure. <i>Crystal Growth and Design</i> , 2017, 17, 3834-3846.   | 1.4 | 21        |
| 82 | Revisiting a Historical Concept by Using Quantum Crystallography: Are Phosphate, Sulfate and Perchlorate Anions Hypervalent?. <i>Chemistry - A European Journal</i> , 2019, 25, 6523-6532.   | 1.7 | 20        |
| 83 | Variable Intercalation of Calcium Ions in Bilayers of Partially Deprotonated p-Phosphonic Acid Calix[4]arene. <i>Crystal Growth and Design</i> , 2009, 9, 3759-3764.   | 1.4 | 19        |
| 84 | Mechanism of Concerted Hydrogen Bond Reorientation in Clathrates of Dianin <sup>TM</sup> s Compound and Hydroquinone. <i>Journal of the American Chemical Society</i> , 2011, 133, 18880-18888.  | 6.6 | 19        |
| 85 | Supramolecular interactions between hexabromoethane and cyclopentadienyl ruthenium bromides: Halogen bonding or electrostatic organisation?. <i>CrystEngComm</i> , 2012, 14, 804-811.  | 1.3 | 19        |
| 86 | Global Analysis of the Mechanical Properties of Organic Crystals. <i>Angewandte Chemie</i> , 2022, 134, .  | 1.6 | 19        |
| 87 | Crystal structure and chemical bonding of the intermetallic Zintl phase $\text{Yb}_{11}\text{AlSb}_9$ . <i>Dalton Transactions</i> , 2012, 41, 10347.  | 1.6 | 18        |
| 88 | Structural Collapse of the Hydroquinone-Formic Acid Clathrate: A Pressure-Dependent Phase Transition. <i>Chemistry - A European Journal</i> , 2016, 22, 4061-4069.   | 1.7 | 18        |
| 89 | Quantifying Mechanical Properties of Molecular Crystals: A Critical Overview of Experimental Elastic Tensors. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .   | 7.2 | 18        |
| 90 | The determination of electric field gradients from X-ray diffraction data. <i>Molecular Physics</i> , 1994, 83, 551-566.   | 0.8 | 17        |

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|-----|--|-----|-----------|
| 91  | An ab initio study of vibrational corrections to the electrical properties of ethylene. <i>Molecular Physics</i> , 2000, 98, 855-865.  | 0.8 | 17        |
| 92  | Electrostatic Potentials in Crystals. , 1981, , 407-425.   |     | 17        |
| 93  | Application of Atomic Hirshfeld Surface Analysis to Intermetallic Systems: Is Mn in Cubic CeMnNi <sub>4</sub> a Thermoelectric Rattler atom?. <i>Inorganic Chemistry</i> , 2012, 51, 1916-1924.  | 1.9 | 16        |
| 94  | Simulations of Guest Transport in Clathrates of Dianin <sup>TM</sup> s Compound and Hydroquinone. <i>Chemistry - A European Journal</i> , 2013, 19, 2676-2684.   | 1.7 | 16        |
| 95  | Molecular Imprisonment: Host Response to Guest Location, Orientation, and Dynamics in Clathrates of Dianin <sup>TM</sup> s Compound. <i>Crystal Growth and Design</i> , 2014, 14, 1296-1306.   | 1.4 | 16        |
| 96  | Ab initio SCF and MP2 calculations of the frequency dependence of the polarizability of cyclohexane. <i>Chemical Physics Letters</i> , 1989, 161, 285-290.   | 1.2 | 15        |
| 97  | Pauling bond strength, bond length and electron density distribution. <i>Physics and Chemistry of Minerals</i> , 2014, 41, 17-25.  | 0.3 | 15        |
| 98  | Si <sup>δ+</sup> O Bonded Interactions in Silicate Crystals and Molecules: A Comparison. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12678-12683.  | 1.1 | 14        |
| 99  | Variable temperature Hirshfeld surface analysis of interdigitated calix[6]arene bearing O-alkyl C18 linear chains. <i>CrystEngComm</i> , 2007, 9, 566.   | 1.3 | 14        |
| 100 | Dipole and quadrupole moments of molecules in crystals: A novel approach based on integration over Hirshfeld surfaces. <i>Journal of Chemical Physics</i> , 2006, 124, 074106.   | 1.2 | 13        |
| 101 | Towards the use of experimental electron densities to estimate reliable lattice energies. <i>CrystEngComm</i> , 2018, 20, 5340-5347.   | 1.3 | 13        |
| 102 | Revised electrostatics from invariom refinement of the 18-residue peptaibol antibiotic trichotoxin A50E. <i>CrystEngComm</i> , 2010, 12, 2419.   | 1.3 | 12        |
| 103 | Properties of atoms under pressure: Bonded interactions of the atoms in three perovskites. <i>Journal of Chemical Physics</i> , 2012, 137, 164313.   | 1.2 | 12        |
| 104 | Quantifying Host-Guest Interaction Energies in Clathrates of Dianin <sup>TM</sup> s Compound. <i>Crystal Growth and Design</i> , 2016, 16, 6858-6866.  | 1.4 | 12        |
| 105 | Comment on On the calculation of the electrostatic potential, electric field and electric field gradient from the aspherical pseudoatom model by Volkov, King, Coppens & Farrugia (2006). <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2007, 63, 198-200. | 0.3 | 11        |
| 106 | An ab initio study of vibrational corrections to the electrical properties of ethane. <i>Molecular Physics</i> , 2000, 98, 867-874.  | 0.8 | 10        |
| 107 | An ab initio study of vibrational corrections to the electrical properties of the fluoromethanes: CH <sub>3</sub> F, CH <sub>2</sub> F <sub>2</sub> , CHF <sub>3</sub> and CF <sub>4</sub> . <i>Molecular Physics</i> , 2000, 98, 633-642.                                       | 0.8 | 10        |
| 108 | Host Perturbation in a Hydroquinone Clathrate Studied by Combined X-ray/Neutron Charge Density Analysis: Implications for Molecular Inclusion in Supramolecular Entities. <i>Chemistry - A European Journal</i> , 2014, 20, 8089-8098.   | 1.7 | 10        |

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|-----|--|-----|-----------|
| 109 | Electrostatic complementarity in pseudoreceptor modeling based on drug molecule crystal structures: the case of loxistatin acid (E64c). <i>New Journal of Chemistry</i> , 2015, 39, 1628-1633.   | 1.4 | 10        |
| 110 | Ab initio cluster calculations of the electron density and electric field gradient in corundum. <i>The Journal of Physical Chemistry</i> , 1992, 96, 9200-9204.  | 2.9 | 9         |
| 111 | Temperature-dependent crystal structure of the isopropanol clathrate of Dianin's compound. <i>Chemical Communications</i> , 2011, 47, 2029.  | 2.2 | 9         |
| 112 | Computational study of methyl group dynamics in the hydroquinoneclathrate of acetonitrile. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1570-1572.   | 1.3 | 9         |
| 113 | Invariom-model refinement of L-valinol. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, o633-o635.   | 0.4 | 8         |
| 114 | Proton switching of polarity in metalloamphiphile crystals. <i>CrystEngComm</i> , 2009, 11, 249-253.   | 1.3 | 8         |
| 115 | Combined structure-factor phase measurement and theoretical calculations for mapping of chemical bonds in GaN. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, 446-450.  | 0.3 | 8         |
| 116 | Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. <i>Angewandte Chemie</i> , 2019, 131, 16936-16940.  | 1.6 | 8         |
| 117 | Investigation of an Unusual Crystal Habit of Hydrochlorothiazide Reveals Large Polar Enantiopure Domains and a Possible Crystal Nucleation Mechanism. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 10255-10259.  | 7.2 | 7         |
| 118 | Quantifying Mechanical Properties of Molecular Crystals: A Critical Overview of Experimental Elastic Tensors. <i>Angewandte Chemie</i> , 2022, 134, .  | 1.6 | 7         |
| 119 | Accurate ab initio study of acetylene Vibrational and rotational corrections to electrical properties. , 0, .  |     | 6         |
| 120 | Phase Measurement for Accurate Mapping of Chemical Bonds in Acentric Space Groups. <i>Physical Review Letters</i> , 2005, 95, 085502.  | 2.9 | 5         |
| 121 | Electric field-derived point charges to mimic the electrostatics in molecular crystals. <i>Journal of Computational Chemistry</i> , 2006, 27, 1063-1070.   | 1.5 | 5         |
| 122 | Tetraiodoallene, I <sub>2</sub> C=C=CI <sub>2</sub> – the missing link between I <sub>2</sub> C=CI <sub>2</sub> and I <sub>2</sub> C=C=C=CI <sub>2</sub> – and the oxidation product, 2,2-diiodoacrylic acid, I <sub>2</sub> C=CH(CO <sub>2</sub> H). <i>Australian Journal of Chemistry</i> , 2018, 71, 70. | 0.5 | 5         |
| 123 | Investigation of an Unusual Crystal Habit of Hydrochlorothiazide Reveals Large Polar Enantiopure Domains and a Possible Crystal Nucleation Mechanism. <i>Angewandte Chemie</i> , 2019, 131, 10361-10365.   | 1.6 | 5         |
| 124 | Single-Crystal High-Pressure X-ray Diffraction Study of Host Structure Compression in Clathrates of Dianin's Compound. <i>Crystal Growth and Design</i> , 2020, 20, 4092-4099.   | 1.4 | 5         |
| 125 | Insights into Host-Guest Binding in Hydroquinone Clathrates: Single-Crystal X-ray and Neutron Diffraction, and Complementary Computational Studies on the Hydroquinone-CO <sub>2</sub> Clathrate. <i>Crystal Growth and Design</i> , 2021, 21, 3477-3486.  | 1.4 | 5         |
| 126 | Physical and crystallographic characterisation of the mGlu5 antagonist MTEP and its monohydrochloride. <i>Journal of Pharmaceutical Sciences</i> , 2010, 99, 234-245.  | 1.6 | 4         |



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|-----|---|-----|-----------|
| 127 | Approaching an experimental electron density model of the biologically active trans $\alpha$ -epoxysuccinyl amide group—Substituent effects vs. crystal packing. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3683.      | 0.9 | 4         |
| 128 | Seemingly simple group 8 cyclopentadienyl dicarbonyl metal halides: From little things, interesting things grow. <i>CrystEngComm</i> , 2012, 14, 812-818.   | 1.3 | 3         |
| 129 | Intermolecular interactions in crystals of small unsubstituted cyclic ethers and substituted epoxides. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2018, 233, 641-648.  | 0.4 | 2         |
| 130 | Facile Synthesis of Pentamethylcyclopentadienyl Ruthenium Half-Sandwich Complexes by Naphthalene Displacement. <i>Australian Journal of Chemistry</i> , 2018, 71, 289.  | 0.5 | 2         |
| 131 | Charge Densities and Crystal Engineering. , 2011, , 553-572.  |     | 1         |
| 132 | Geometries, interaction energies and complexation free energies of 18-crown-6 with neutral molecules. <i>CrystEngComm</i> , 2016, 18, 8653-8663.  | 1.3 | 1         |
| 133 | Contracted basis sets for electrical property calculations derived from Second-order Møller-Plesset theory atomic natural orbitals. <i>Theoretical Chemistry Accounts</i> , 2000, 104, 385-391.                                       | 0.5 | 0         |
| 134 | Robert Farrell Stewart (1936–2015). <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2016, 72, 507-509.  | 0.0 | 0         |
| 135 | Celebrating Professor Graham Chandler’s 80th Birthday. <i>Australian Journal of Chemistry</i> , 2018, 71, 201.  | 0.5 | 0         |
| 136 | Insights from high-pressure crystallography and X-ray charge-density analysis into mechanical flexibility of metal–organic complex crystals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2019, 75, e470-e470. | 0.0 | 0         |
| 137 | Solution-phase decomposition of ferrocene into wüstite-iron oxide core–shell nanoparticles. <i>Dalton Transactions</i> , 2022, , .  | 1.6 | 0         |
| 138 | Structure correlation and dynamics in crystals – a tribute to Hans-Beat Böggi. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2022, 78, 281-282.                                    | 0.5 | 0         |