Paulina M Dominiak

List of Publications by Year
in descending order

74 papers	2,460 citations	218677 26 h-index	197818 49 g-index
96 all docs	96 docs citations	96 times ranked	2322 citing authors

#	Article	IF	Citations
1	X-ray wavefunction refinement and comprehensive structural studies on bromo-substituted analogues of 2-deoxy-<scp>d</scp>-glucose in solid state and solution. RSC Advances, 2022, 12, 8345-8360.	3.6	3
2	Theoretical 3D electron diffraction electrostatic potential maps of proteins modeled with a multipolar pseudoatom data bank. Acta Crystallographica Section D: Structural Biology, 2022, 78, 1010-1020.	2.3	5
3	Phase Transition of Hypoxanthinium Nitrate Monohydrate. Crystal Growth and Design, 2021, 21, 424-435.	3.0	0
4	Combining Molecular Dynamic Information and an Aspherical-Atom Data Bank in the Evaluation of the Electrostatic Interaction Energy in Multimeric Protein-Ligand Complex: A Case Study for HIV-1 Protease. Molecules, 2021, 26, 3872.	3.8	6
5	Refinements on electron diffraction data of Î²-glycine in MoPro: a quest for an improved structure model. Journal of Applied Crystallography, 2021, 54, 1234-1243.	4.5	7
6	The influence of refinement strategies on the wavefunctions derived from an experiment. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2021, 77, 715-727.	1.1	5
7	Refinement of organic crystal structures with multipolar electron scattering factors. Acta Crystallographica Section A: Foundations and Advances, 2020, 76, 92-109.	0.1	20
8	The PI3K pathway preserves metabolic health through MARCO-dependent lipid uptake by adipose tissue macrophages. Nature Metabolism, 2020, 2, 1427-1442.	11.9	24
9	Frequency and hydrogen bonding of nucleobase homopairs in small molecule crystals. Nucleic Acids Research, 2020, 48, 8302-8319.	14.5	6
10	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.	2.2	23
11	TAAM: a reliable and user friendly tool for hydrogen-atom location using routine X-ray diffraction data. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 296-306.	1.1	22
12	Differences and similarities among hypoxanthinium nitrate hydrate structures. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 1036-1044.	0.5	3
13	Intermolecular Interactions in Ionic Crystals of Nucleobase Chloridesâ€”Combining Topological Analysis of Electron Densities with Energies of Electrostatic Interactions. Crystals, 2019, 9, 668.	2.2	11
14	Extension of the transferable aspherical pseudoatom data bank for the comparison of molecular electrostatic potentials in structureâ€“activity studies. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 398-408.	0.1	25
15	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108
16	DiSCaMB: a software library for aspherical atom model X-ray scattering factor calculations with CPUs and GPUs. Journal of Applied Crystallography, 2018, 51, 193-199.	4.5	24
17	Universal Method for Electrostatic Interaction Energies Estimation with Charge Penetration and Easily Attainable Point Charges. Journal of Chemical Theory and Computation, 2018, 14, 6336-6345.	5.3	10
18	Molecular tapes in the structure of isoguaninium chloride. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 108-112.	0.5	1

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19	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, .	3.3	1
20	Protonated nucleobases are not fully ionized in their chloride salt crystals and form metastable base pairs further stabilized by the surrounding anions. IUCrJ, 2018, 5, 449-469.	2.2	9
21	Multi-temperature study of potassium uridine-5â€²-monophosphate: electron density distribution and anharmonic motion modelling. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 550-564.	1.1	8
22	Validation of Xâ€ray Wavefunction Refinement. ChemPhysChem, 2017, 18, 3290-3291.	2.1	2
23	Validation of Xâ€ray Wavefunction Refinement. ChemPhysChem, 2017, 18, 3334-3351.	2.1	49
24	Interplay of point multipole moments and charge penetration for intermolecular electrostatic interaction energies from the University at Buffalo pseudoatom databank model of electron density. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 598-609.	1.1	9
25	Hydrogen atoms can be located accurately and precisely by x-ray crystallography. Science Advances, 2016, 2, e1600192.	10.3	211
26	A Universal and Straightforward Approach to Include Penetration Effects in Electrostatic Interaction Energy Estimation. ChemPhysChem, 2016, 17, 2455-2460.	2.1	15
27	The influence of fluorine position on the properties of fluorobenzoxaboroles. Bioorganic Chemistry, 2015, 60, 130-135.	4.1	25
28	Electrostatic Interactions in Aminoglycoside-RNA Complexes. Biophysical Journal, 2015, 108, 655-665.	0.5	33
29	Hirshfeld atom refinement for modelling strong hydrogen bonds. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, 483-498.	0.1	59
30	Sunitinib: from charge-density studies to interaction with proteins. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1257-1270.	2.5	31
31	A Comparative Study of Transferable Aspherical Pseudoatom Databank and Classical Force Fields for Predicting Electrostatic Interactions in Molecular Dimers. Journal of Chemical Theory and Computation, 2014, 10, 1652-1664.	5.3	25
32	Tartaric acid and its O-acyl derivatives. 7. Crystal structure of O-p-anisoyl-D-tartaric acid and its dimethylammonium salt trihydrate. Journal of Structural Chemistry, 2013, 54, 155-158.	1.0	2
33	Hoogsteenâ€“Watsonâ€“Crick 9-Methyladenine:1-Methylthymine Complex: Charge Density Study in the Context of Crystal Engineering and Nucleic Acid Base Pairing. Crystal Growth and Design, 2013, 13, 239-254.	3.0	19
34	Interplay between Charge Density Distribution, Crystal Structure Energetic Features, and Crystal Morphology of 6-Methyl-2-thiouracil. Journal of Physical Chemistry C, 2013, 117, 7764-7775.	3.1	21
35	Transferability of Atomic Multipoles in Amino Acids and Peptides for Various Density Partitions. Journal of Physical Chemistry A, 2013, 117, 1535-1547.	2.5	6
36	From a Single Molecule to Molecular Crystal Architectures: Structural and Energetic Studies of Selected Uracil Derivatives. Crystal Growth and Design, 2012, 12, 2508-2524.	3.0	62

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37	Is it possible to derive quantitative information on polarization of electron density from the multipolar model?. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 705-714.	0.3	7
38	New version of the theoretical databank of transferable aspherical pseudoatoms, UBDB2011 â€“ towards nucleic acid modelling. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 139-147.	0.3	94
39	Intermolecular Interaction Energies from Experimental Charge Density Studies. , 2011, , 387-433.		13
40	Verification of structural and electrostatic properties obtained by the use of different pseudoatom databases. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, 141-153.	0.3	66
41	On quantitative structural and electron-density studies of interactions in molecular crystals. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, s84-s84.	0.3	0
42	Synthesis and structural study on heterocyclic compounds 7-decanoyloxy-3-(4â€²-substitutedphenyl)-4H-1-benzopyran-4-ones: Crystal structure of 7-decanoyloxy-3-(4â€²-methylphenyl)-4H-1-benzopyran-4-one. Journal of Molecular Structure, 2010, 967, 25-33.	3.6	4
43	Di-Î¼-nitrosyl-bis[(Î·5-pentamethylcyclopentadienyl)ruthenium(0)](Ruâ€”Ru). Corrigendum. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, e25-e25.	0.2	0
44	Structural Variability and the Nature of Intermolecular Interactions in Watsonâ^'Crick B-DNA Base Pairs. Journal of Physical Chemistry B, 2010, 114, 9629-9644.	2.6	42
45	Towards the best model for H atoms in experimental charge-density refinement. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, 300-311.	0.3	83
46	Experimental charge-density study of paracetamol â€“ multipole refinement in the presence of a disordered methyl group. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, 490-500.	0.3	35
47	Combining crystallographic information and an aspherical-atom data bank in the evaluation of the electrostatic interaction energy in an enzymeâ€“substrate complex: influenza neuraminidase inhibition. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 485-499.	2.5	42
48	Bisâ€•and Tris(tetraazamacrocyclic) Copper Complexes with Disulfide Linkers. European Journal of Inorganic Chemistry, 2008, 2008, 2295-2301.	2.0	5
49	New lacunar-type and pendant groups containing derivatives of Î²-unsubstituted dibenzotetraaza[14]annulenesâ€”syntheses and crystal structures. Tetrahedron, 2008, 64, 7796-7806.	1.9	7
50	Refinement of the crystal structure of [Rb x (NH4)1â^'x]3H(SO4)2(x = 0.11) by single-crystal X-ray and neutron diffraction: I. Phase II at 300 K. Crystallography Reports, 2008, 53, 418-427.	0.6	3
51	Synthesis, spectral data, and crystal structure of two novel substitution patterns in dithiaporphyrins. Journal of Porphyrins and Phthalocyanines, 2007, 11, 1-8.	0.8	5
52	A Theoretical Databank of Transferable Aspherical Atoms and Its Application to Electrostatic Interaction Energy Calculations of Macromolecules. Journal of Chemical Theory and Computation, 2007, 3, 232-247.	5.3	134
53	Phosphorylation of Serine 264 Impedes Active Site Accessibility in the E1 Component of the Human Pyruvate Dehydrogenase Multienzyme Complex. Biochemistry, 2007, 46, 6277-6287.	2.5	55
54	Mechanistic Studies of UV Assisted [4 + 2] Cycloadditions in Synthetic Efforts toward Vibsanin E. Journal of the American Chemical Society, 2007, 129, 10763-10772.	13.7	32

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55	Di-Î¼-nitrosyl-bis[(Î·⁵-pentamethylcyclopentadienyl)ruthenium(0)](Ruâ€”Ru). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, m2596-m2596.	0.2	5
56	Refinement of hydrogen positions in (NH4)2SeO4. Journal of Surface Investigation, 2007, 1, 113-119.	0.5	1
57	Refinement of the (NH4)3H(SO4)2 crystal structure: II. X-ray and neutron single-crystal diffraction from phase II at room temperature. Journal of Surface Investigation, 2007, 1, 637-644.	0.5	0
58	Supramolecular solids and time-resolved diffraction. CrystEngComm, 2006, 8, 735.	2.6	31
59	Effect of the Environment on Molecular Properties:â€‰ Synthesis, Structure, and Photoluminescence of Cu(I) Bis(2,9-dimethyl-1,10-phenanthroline) Nanoclusters in Eight Different Supramolecular Frameworks. Inorganic Chemistry, 2006, 45, 9281-9289.	4.0	39
60	Investigation into Factors Influencing Stereoselectivity in the Reactions of Heterocycles with Donorâ€“Acceptor-Substituted Rhodium Carbenoids. Journal of Organic Chemistry, 2006, 71, 5349-5356.	3.2	91
61	Finding optimal radial-function parameters for SÂatoms in the Hansenâ€“Coppens multipole model through refinement of theoretical densities. Acta Crystallographica Section A: Foundations and Advances, 2006, 62, 224-227.	0.3	32
62	Strong intramolecular hydrogen bonding involving nitro- and acetyl groups. Deuterium isotope effects on chemical shifts. Journal of Molecular Structure, 2006, 789, 81-91.	3.6	32
63	Continua of Interactions between Pairs of Atoms in Molecular Crystals. Chemistry - A European Journal, 2006, 12, 1941-1949.	3.3	73
64	Crystal and molecular structure of 1Î±-hydroxylated analogs of vitamins D. Journal of Molecular Structure, 2005, 734, 149-155.	3.6	9
65	peri-Interactions in naphthalenes, 13 8-Dimethylamino-naphth-1-yl carbinols as model systems for potential Nâ†'Si/P interactions. Journal of Molecular Structure, 2005, 751, 172-183.	3.6	7
66	Corundum, Diamond, and PtS Metal-Organic Frameworks with a Difference: Self-Assembly of a Unique Pair of 3-ConnectingD2d-Symmetric 3,3?,5,5?-Tetrakis(4-pyridyl)bimesityl. Angewandte Chemie - International Edition, 2005, 44, 2115-2119.	13.8	164
67	Factor Analysis of Deuterium Isotope Effects on13C NMR Chemical Shifts in Schiff Bases. Chemistry - A European Journal, 2005, 11, 4758-4766.	3.3	17
68	Carbon Monoxide-Promoted Carbene Insertion into the Aryl Substituent of an N-Heterocyclic Carbene Ligand:Â Buchner Reaction in a Ruthenium Carbene Complex. Journal of the American Chemical Society, 2005, 127, 15702-15703.	13.7	123
69	Drug-substrate interactions from a theory-based databank of transferable pseudoatoms and potential curves derived from advanced theoretical calculations.. Nihon Kessho Gakkaishi, 2005, 47, 1-2.	0.0	0
70	Neutral and ionic multiple hydrogen bonded moieties in crystal structure of a one tripodal Schiff base. Journal of Molecular Structure, 2004, 691, 133-139.	3.6	17
71	Neutral and Ionic Hydrogen Bonding in Schiff Bases. Chemistry - A European Journal, 2003, 9, 963-970.	3.3	109
72	H-Bonding Dependent Structures of (NH4+)3H+(SO42-)2. Mechanisms of Phase Transitions. Inorganic Chemistry, 2003, 42, 1590-1598.	4.0	24

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73	Structural Basis for Flip-Flop Action of Thiamin Pyrophosphate-dependent Enzymes Revealed by Human Pyruvate Dehydrogenase. Journal of Biological Chemistry, 2003, 278, 21240-21246.	3.4	144
74	peri-Interactions in Naphthalenes, 6 [1]. On Hypercoordination of Phosphorus in 8-Dialkylamino-naphth-1-yl Phosphonium Salts. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2002, 57, 8-18.	0.7	11