

Paulina M Dominiak

List of Publications by Year in descending order

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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	Hydrogen atoms can be located accurately and precisely by x-ray crystallography. <i>Science Advances</i> , 2016, 2, e1600192.	10.3	211
2	Corundum, Diamond, and PtS Metal-Organic Frameworks with a Difference: Self-Assembly of a Unique Pair of 3-Connecting D ^{2d} -Symmetric 3,3',5,5'-Tetrakis(4-pyridyl)bimesityl. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2115-2119.	13.8	164
3	Structural Basis for Flip-Flop Action of Thiamin Pyrophosphate-dependent Enzymes Revealed by Human Pyruvate Dehydrogenase. <i>Journal of Biological Chemistry</i> , 2003, 278, 21240-21246.	3.4	144
4	A Theoretical Databank of Transferable Aspherical Atoms and Its Application to Electrostatic Interaction Energy Calculations of Macromolecules. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 232-247.	5.3	134
5	Carbon Monoxide-Promoted Carbene Insertion into the Aryl Substituent of an N-Heterocyclic Carbene Ligand: A Buchner Reaction in a Ruthenium Carbene Complex. <i>Journal of the American Chemical Society</i> , 2005, 127, 15702-15703.	13.7	123
6	Neutral and Ionic Hydrogen Bonding in Schiff Bases. <i>Chemistry - A European Journal</i> , 2003, 9, 963-970.	3.3	109
7	Quantum Crystallography: Current Developments and Future Perspectives. <i>Chemistry - A European Journal</i> , 2018, 24, 10881-10905.	3.3	108
8	New version of the theoretical databank of transferable aspherical pseudoatoms, UBDB2011 "towards nucleic acid modelling. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2012, 68, 139-147.	0.3	94
9	Investigation into Factors Influencing Stereoselectivity in the Reactions of Heterocycles with Donor-Acceptor-Substituted Rhodium Carbenoids. <i>Journal of Organic Chemistry</i> , 2006, 71, 5349-5356.	3.2	91
10	Towards the best model for H atoms in experimental charge-density refinement. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, 300-311.	0.3	83
11	Continua of Interactions between Pairs of Atoms in Molecular Crystals. <i>Chemistry - A European Journal</i> , 2006, 12, 1941-1949.	3.3	73
12	Verification of structural and electrostatic properties obtained by the use of different pseudoatom databases. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2011, 67, 141-153.	0.3	66
13	From a Single Molecule to Molecular Crystal Architectures: Structural and Energetic Studies of Selected Uracil Derivatives. <i>Crystal Growth and Design</i> , 2012, 12, 2508-2524.	3.0	62
14	Hirshfeld atom refinement for modelling strong hydrogen bonds. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, 483-498.	0.1	59
15	Phosphorylation of Serine 264 Impedes Active Site Accessibility in the E1 Component of the Human Pyruvate Dehydrogenase Multienzyme Complex. <i>Biochemistry</i> , 2007, 46, 6277-6287.	2.5	55
16	Validation of X-ray Wavefunction Refinement. <i>ChemPhysChem</i> , 2017, 18, 3334-3351.	2.1	49
17	Combining crystallographic information and an aspherical-atom data bank in the evaluation of the electrostatic interaction energy in an enzyme-substrate complex: influenza neuraminidase inhibition. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 485-499.	2.5	42
18	Structural Variability and the Nature of Intermolecular Interactions in Watson-Crick B-DNA Base Pairs. <i>Journal of Physical Chemistry B</i> , 2010, 114, 9629-9644.	2.6	42

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19	Effect of the Environment on Molecular Properties: Synthesis, Structure, and Photoluminescence of Cu(I) Bis(2,9-dimethyl-1,10-phenanthroline) Nanoclusters in Eight Different Supramolecular Frameworks. <i>Inorganic Chemistry</i> , 2006, 45, 9281-9289.	4.0	39
20	Experimental charge-density study of paracetamol multipole refinement in the presence of a disordered methyl group. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, 490-500.	0.3	35
21	Electrostatic Interactions in Aminoglycoside-RNA Complexes. <i>Biophysical Journal</i> , 2015, 108, 655-665.	0.5	33
22	Finding optimal radial-function parameters for atoms in the Hansen-Coppens multipole model through refinement of theoretical densities. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2006, 62, 224-227.	0.3	32
23	Strong intramolecular hydrogen bonding involving nitro- and acetyl groups. Deuterium isotope effects on chemical shifts. <i>Journal of Molecular Structure</i> , 2006, 789, 81-91.	3.6	32
24	Mechanistic Studies of UV Assisted [4 + 2] Cycloadditions in Synthetic Efforts toward Vibsanin E. <i>Journal of the American Chemical Society</i> , 2007, 129, 10763-10772.	13.7	32
25	Supramolecular solids and time-resolved diffraction. <i>CrystEngComm</i> , 2006, 8, 735.	2.6	31
26	Sunitinib: from charge-density studies to interaction with proteins. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 1257-1270.	2.5	31
27	A Comparative Study of Transferable Aspherical Pseudoatom Databank and Classical Force Fields for Predicting Electrostatic Interactions in Molecular Dimers. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1652-1664.	5.3	25
28	The influence of fluorine position on the properties of fluorobenzoxaboroles. <i>Bioorganic Chemistry</i> , 2015, 60, 130-135.	4.1	25
29	Extension of the transferable aspherical pseudoatom data bank for the comparison of molecular electrostatic potentials in structure-activity studies. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2019, 75, 398-408.	0.1	25
30	H-Bonding Dependent Structures of (NH ₄) ₃ H+(SO ₄) ₂ . <i>Mechanisms of Phase Transitions. Inorganic Chemistry</i> , 2003, 42, 1590-1598.	4.0	24
31	<i>DiSCaMB</i> : a software library for aspherical atom model X-ray scattering factor calculations with CPUs and GPUs. <i>Journal of Applied Crystallography</i> , 2018, 51, 193-199.	4.5	24
32	The PI3K pathway preserves metabolic health through MARCO-dependent lipid uptake by adipose tissue macrophages. <i>Nature Metabolism</i> , 2020, 2, 1427-1442.	11.9	24
33	On the accuracy and precision of X-ray and neutron diffraction results as a function of resolution and the electron density model. <i>IUCr</i> , 2020, 7, 920-933.	2.2	23
34	TAAM: a reliable and user friendly tool for hydrogen-atom location using routine X-ray diffraction data. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 296-306.	1.1	22
35	Interplay between Charge Density Distribution, Crystal Structure Energetic Features, and Crystal Morphology of 6-Methyl-2-thiouracil. <i>Journal of Physical Chemistry C</i> , 2013, 117, 7764-7775.	3.1	21
36	Refinement of organic crystal structures with multipolar electron scattering factors. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2020, 76, 92-109.	0.1	20

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37	Hoogsteenâ€“Watsonâ€“Crick 9-Methyladenine:1-Methylthymine Complex: Charge Density Study in the Context of Crystal Engineering and Nucleic Acid Base Pairing. <i>Crystal Growth and Design</i> , 2013, 13, 239-254.	3.0	19
38	Neutral and ionic multiple hydrogen bonded moieties in crystal structure of a one tripodal Schiff base. <i>Journal of Molecular Structure</i> , 2004, 691, 133-139.	3.6	17
39	Factor Analysis of Deuterium Isotope Effects on ¹³ C NMR Chemical Shifts in Schiff Bases. <i>Chemistry - A European Journal</i> , 2005, 11, 4758-4766.	3.3	17
40	A Universal and Straightforward Approach to Include Penetration Effects in Electrostatic Interaction Energy Estimation. <i>ChemPhysChem</i> , 2016, 17, 2455-2460.	2.1	15
41	Intermolecular Interaction Energies from Experimental Charge Density Studies. , 2011, , 387-433.		13
42	peri-Interactions in Naphthalenes, 6 [1]. On Hypercoordination of Phosphorus in 8-Dialkylamino-naphth-1-yl Phosphonium Salts. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2002, 57, 8-18.	0.7	11
43	Intermolecular Interactions in Ionic Crystals of Nucleobase Chloridesâ€”Combining Topological Analysis of Electron Densities with Energies of Electrostatic Interactions. <i>Crystals</i> , 2019, 9, 668.	2.2	11
44	Universal Method for Electrostatic Interaction Energies Estimation with Charge Penetration and Easily Attainable Point Charges. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6336-6345.	5.3	10
45	Crystal and molecular structure of Î±-hydroxylated analogs of vitamins D. <i>Journal of Molecular Structure</i> , 2005, 734, 149-155.	3.6	9
46	Interplay of point multipole moments and charge penetration for intermolecular electrostatic interaction energies from the University at Buffalo pseudoatom databank model of electron density. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 598-609.	1.1	9
47	Protonated nucleobases are not fully ionized in their chloride salt crystals and form metastable base pairs further stabilized by the surrounding anions. <i>IUCr</i> , 2018, 5, 449-469.	2.2	9
48	Multi-temperature study of potassium uridine-5â€²-monophosphate: electron density distribution and anharmonic motion modelling. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 550-564.	1.1	8
49	peri-Interactions in naphthalenes, 13 8-Dimethylamino-naphth-1-yl carbinols as model systems for potential Nâ€²â€²â€²/Si/P interactions. <i>Journal of Molecular Structure</i> , 2005, 751, 172-183.	3.6	7
50	New lacunar-type and pendant groups containing derivatives of Î²-unsubstituted dibenzotetraaza[14]annulenesâ€”syntheses and crystal structures. <i>Tetrahedron</i> , 2008, 64, 7796-7806.	1.9	7
51	Is it possible to derive quantitative information on polarization of electron density from the multipolar model?. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2012, 68, 705-714.	0.3	7
52	Refinements on electron diffraction data of Î²-glycine in <i>MoPro</i>: a quest for an improved structure model. <i>Journal of Applied Crystallography</i> , 2021, 54, 1234-1243.	4.5	7
53	Transferability of Atomic Multipoles in Amino Acids and Peptides for Various Density Partitions. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1535-1547.	2.5	6
54	Frequency and hydrogen bonding of nucleobase homopairs in small molecule crystals. <i>Nucleic Acids Research</i> , 2020, 48, 8302-8319.	14.5	6

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55	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. <i>Molecules</i> , 2021, 26, 3872.	3.8	6
56	Synthesis, spectral data, and crystal structure of two novel substitution patterns in dithiaporphyrins. <i>Journal of Porphyrins and Phthalocyanines</i> , 2007, 11, 1-8.	0.8	5
57	Di- η^5 -nitrosyl-bis[η^5 -pentamethylcyclopentadienyl]ruthenium(0)](Ru^{Ru}). <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2007, 63, m2596-m2596.	0.2	5
58	Bis- and Tris(tetraazamacrocyclic) Copper Complexes with Disulfide Linkers. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 2295-2301.	2.0	5
59	The influence of refinement strategies on the wavefunctions derived from an experiment. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 715-727.	1.1	5
60	Theoretical 3D electron diffraction electrostatic potential maps of proteins modeled with a multipolar pseudoatom data bank. <i>Acta Crystallographica Section D: Structural Biology</i> , 2022, 78, 1010-1020.	2.3	5
61	Synthesis and structural study on heterocyclic compounds 7-decanoyloxy-3-(4-substitutedphenyl)-4H-1-benzopyran-4-ones: Crystal structure of 7-decanoyloxy-3-(4-methylphenyl)-4H-1-benzopyran-4-one. <i>Journal of Molecular Structure</i> , 2010, 967, 25-33.	3.6	4
62	Refinement of the crystal structure of $[\text{Rb}_x(\text{NH}_4)_{1-x}]_3\text{H}(\text{SO}_4)_2$ ($x = 0.11$) by single-crystal X-ray and neutron diffraction: I. Phase II at 300 K. <i>Crystallography Reports</i> , 2008, 53, 418-427.	0.6	3
63	Differences and similarities among hypoxanthinium nitrate hydrate structures. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 1036-1044.	0.5	3
64	X-ray wavefunction refinement and comprehensive structural studies on bromo-substituted analogues of 2-deoxy-D-glucose in solid state and solution. <i>RSC Advances</i> , 2022, 12, 8345-8360.	3.6	3
65	Tartaric acid and its O-acyl derivatives. 7. Crystal structure of O-p-anisoyl-D-tartaric acid and its dimethylammonium salt trihydrate. <i>Journal of Structural Chemistry</i> , 2013, 54, 155-158.	1.0	2
66	Validation of X-ray Wavefunction Refinement. <i>ChemPhysChem</i> , 2017, 18, 3290-3291.	2.1	2
67	Refinement of hydrogen positions in $(\text{NH}_4)_2\text{SeO}_4$. <i>Journal of Surface Investigation</i> , 2007, 1, 113-119.	0.5	1
68	Molecular tapes in the structure of isoguaninium chloride. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 108-112.	0.5	1
69	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. <i>Chemistry - A European Journal</i> , 2018, 24, .	3.3	1
70	Refinement of the $(\text{NH}_4)_3\text{H}(\text{SO}_4)_2$ crystal structure: II. X-ray and neutron single-crystal diffraction from phase II at room temperature. <i>Journal of Surface Investigation</i> , 2007, 1, 637-644.	0.5	0
71	On quantitative structural and electron-density studies of interactions in molecular crystals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, s84-s84.	0.3	0
72	Di- η^5 -nitrosyl-bis[η^5 -pentamethylcyclopentadienyl]ruthenium(0)](Ru^{Ru}). Corrigendum. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, e25-e25.	0.2	0

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73	Phase Transition of Hypoxanthinium Nitrate Monohydrate. <i>Crystal Growth and Design</i> , 2021, 21, 424-435.	3.0	0
74	Drug-substrate interactions from a theory-based databank of transferable pseudoatoms and potential curves derived from advanced theoretical calculations.. <i>Nihon Kessho Gakkaishi</i> , 2005, 47, 1-2.	0.0	0