Christian Jelsch

List of Publications by Year
in descending order

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156	4,377	134610 34	134545 62
papers	citations	h-index	g-index

159	159	159	3424
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Case of Charge-Assisted Hydrogen Bonding in the Crystal Structure of Sodium Laurate, Lauric Acid. Journal of Chemical Crystallography, 2023, 53, 93-104.	0.5	2
2	Synthesis, crystal structure, Hirshfeld surface analysis and characterization of a new Cd(II) complex with the 4,4â€™-dimethyl-2,2â€™-dipyridine monodentate ligand. Journal of the Iranian Chemical Society, 2022, 19, 319-329.	1.2	1
3	Machine learning-driven identification of drugs inhibiting cytochrome P450 2C9. PLoS Computational Biology, 2022, 18, e1009820.	1.5	11
4	Synthesis, structural characterization, antibacterial activity, DFT computational studies and thermal analysis of two new thiocyanate compounds based on 1-phenylpiperazine. Journal of Molecular Structure, 2022, 1257, 132620.	1.8	8
5	The Coordination Behavior of Two New Complexes, [(C7H10NO2)CdCl3]n(I) and [(C7H9NO2)CuCl2] (II), Based on 2,6-Dimethanolpyridine; Elaboration of the Structure and Hirshfeld Surface, Optical, Spectroscopic and Thermal Analysis. Materials, 2022, 15, 1624.	1.3	11
6	Ï€-Hole bonding in a new co-crystal hydrate of gallic acid and pyrazine: static and dynamic charge density analysis. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 231-246.	0.5	4
7	Probing the Electronic Properties and Interaction Landscapes in a Series of N-(Chlorophenyl)pyridinecarboxamides. Crystal Growth and Design, 2022, 22, 3343-3358.	1.4	2
8	Theoretical search of crystal polymorphs of Temozolomide. Heliyon, 2022, , e09608.	1.4	0
9	Synthesis, structural elucidation, spectroscopic, Hirshfeld surface analysis and theoretical simulation of a new adeninium orthoperiodate (1â˚) bis(hydrate) organicâ€“inorganic hybrid crystals. Journal of Molecular Structure, 2021, 1224, 129034.	1.8	9
10	Structural, NMR, IR, Hirshfeld surface, electrochemical and in vitro biochemical investigations of a new organic cyclohexaphosphate, (C6H6ClFN)4 (Li)2(P6O18)(H2O)4. Journal of the Iranian Chemical Society, 2021, 18, 933-947.	1.2	1
11	Synthesis, crystal structure and antibacterial studies of dihydropyrimidines and their regioselectively oxidized products. RSC Advances, 2021, 11, 6312-6329.	1.7	12
12	Synthesis, Structure and Hirshfeld Surface Analysis of a New Iron Complex [Fe(N4Py)(tcnspr)] (tcnspr). Journal of Inorganic and Organometallic Polymers and Materials, 2021, 31, 3054-3061.	1.9	2
13	Synthesis, crystal structure, computational studies and spectroscopic characterization of a hybrid material self-assembly from tetra(isothiocyanate)cobalt(II) anion and 1-(4-methoxyphenyl)piperazinium. Journal of Molecular Structure, 2021, 1230, 129929.	1.8	7
14	The supramolecular behavior and molecular recognition of adeninium cations on anionic hydrogen selenite/diselenite frameworks: A structural and theoretical analysis. Journal of Molecular Structure, 2021, 1229, 129836.	1.8	6
15	Charge density studies of multicentre two-electron bonding of an anion radical at non-ambient temperature and pressure. IUCrJ, 2021, 8, 644-654.	1.0	8
16	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.	1.9	7
17	A rush to explore proteinâ€“ligand electrostatic interaction energy with Charger. Acta Crystallographica Section D: Structural Biology, 2021, 77, 1292-1304.	1.1	4
18	Synthesis, crystal structure and antibacterial studies of 2,4,6-trimetoxybenzaldehyde based dihydropyrimidine derivatives. Journal of Molecular Structure, 2021, 1241, 130678.	1.8	7

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19	Synthesis, structure and theoretical simulation of a zinc(II) coordination complex with 2,3-pyridinedicarboxylate. Journal of Molecular Structure, 2020, 1199, 127015.	1.8	14
20	Crystal structure, Hirshfeld surface analysis and physicochemical studies of two new Cu(II) complexes with the ligand 2-amino-6-methylpyrimidin-4-(1H)-one. Inorganica Chimica Acta, 2020, 502, 119289.	1.2	3
21	Aceclofenac and interactions analysis in the crystal and COX protein active site. Journal of Molecular Structure, 2020, 1205, 127600.	1.8	12
22	Synthesis, crystal structure determination, DFT calculation, and Hirshfeld surface analysis of a new Zn(II) complex with the guaninium ligand. Journal of Coordination Chemistry, 2020, 73, 3307-3321.	0.8	2
23	Synthesis, structural elucidation, characterization and theoretical DFT study of 1-(o-tolyl)biguanidium chloride. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 572-578.	0.2	2
24	Synthesis, crystal structure and antibacterial properties of 6-methyl-2-oxo-4-(quinolin-2-yl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate. Journal of Molecular Structure, 2020, 1219, 128581.	1.8	9
25	A new 1D Zn(II) coordination polymer containing 2-amino-4,6-dimethoxypyrimidine ligand: crystal structure, Hirshfeld surface analysis, and physicochemical studies. Journal of Molecular Structure, 2020, 1216, 128309.	1.8	2
26	syn and anti polymorphs of 2,6-dimethoxy benzoic acid and its molecular and ionic cocrystals: Structural analysis and energetic perspective. Journal of Molecular Structure, 2020, 1221, 128721.	1.8	7
27	Hirshfeld surface analysis, crystal structure and physicochemical studies of a new Zn(II) complex with the 2,6-dimethylpyrimidin-4-(1H)-one ligand. Solid State Sciences, 2020, 101, 106119.	1.5	3
28	Theoretical crystal structure prediction of aminosalicylic acid: Charge density topological and electrostatic analyses. Journal of Molecular Structure, 2020, 1213, 128139.	1.8	5
29	A new pyrimidinium tetrachloroferrate(III) salt with a low band gap: Hirshfeld surface analysis, crystal structure and physicochemical studies. Journal of the Iranian Chemical Society, 2020, 17, 2317-2326.	1.2	1
30	Morphology of the GdVO₄crystal: first-principles studies. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 749-756.	0.5	4
31	Polarization of Electron Density Databases of Transferable Multipolar Atoms. Journal of Physical Chemistry A, 2019, 123, 7156-7170.	1.1	9
32	At the Interface of Isomorphous Behavior in a 3 Ã— 3 Isomer Grid of Monochlorobenzamides: Analyses of the Interaction Landscapes via Contact Enrichment Studies. Crystal Growth and Design, 2019, 19, 6141-6158.	1.4	7
33	Topological and electrostatic properties of diclofenac molecule as a non-steroidal anti-inflammatory drug: An experimental and theoretical study. Journal of Molecular Structure, 2019, 1196, 42-53.	1.8	17
34	Crystal structure, Hirshfeld surface analysis, and physicochemical studies of a new Cu(II) complex with 2-amino-4-methylpyrimidine. Journal of Molecular Structure, 2019, 1194, 297-304.	1.8	1
35	Malleable Electronic Structure of Chloranilic Acid and Its Species Determined by X-ray Charge Density Studies. Crystal Growth and Design, 2019, 19, 2802-2810.	1.4	18
36	Synthesis, structural elucidation, spectroscopic and Hirshfeld surface analysis of a new organic cyclohexaphosphate, (C12H19N2)4(Li)2(P6O18)(H2O)4. Chemical Data Collections, 2019, 20, 100188.	1.1	1

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37	Partially Covalent Two-Electron/Multicentric Bonding between Semiquinone Radicals. Crystal Growth and Design, 2019, 19, 391-402.	1.4	29
38	Crystal structure and Hirshfeld surface analysis of tris(2,2â€²-bipyridine)nickel(II) bis(1,1,3,3-tetracyano-2-ethoxypropenide) dihydrate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 867-871.	0.2	0
39	Aggregation in isomeric imides: analysis of the weak interactions in six N-(benzoyl)-N-(2-pyridyl)benzamides. Structural Chemistry, 2018, 29, 1153-1164.	1.0	4
40	Synthesis and Reactivity of Copper(I) Complexes Based on C 3 -Symmetric Tripodal HTIM(PR2)3 Ligands. European Journal of Inorganic Chemistry, 2018, 2018, 2612-2620.	1.0	10
41	A method to estimate statistical errors of properties derived from charge-density modelling. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, 170-183.	0.0	19
42	Syn vs Anti Carboxylic Acids in Hybrid Peptides: Experimental and Theoretical Charge Density and Chemical Bonding Analysis. Journal of Physical Chemistry A, 2018, 122, 3665-3679.	1.1	9
43	Hirshfeld Surface Analysis, Crystal Structure and Spectroscopic Studies of a New Cu(II) Halocuprate Salt with Protonated N-Amino-Ethyl-Piperazine. Journal of Structural Chemistry, 2018, 59, 1610-1618.	0.3	5
44	Aggregation in Three Benzamide or Pyridylcarboxamide Hydrates: Formation of 1D Chains Comprising Water Molecules in a Chloro(pyridyl)benzamide Dihydrate. Croatica Chemica Acta, 2018, 91, .	0.1	1
45	Synthesis, structural characterisations, NMR spectroscopy, Hirshfeld surface analysis and electrochemical study of a new organic cyclohexaphosphate, (C 6 H 7 FN) 4 (Li) 2 (P 6 O 18) (H 2 O) 6. Journal of Molecular Structure, 2018, 1170, 30-37.	1.8	3
46	The first Fe(II) complex bearing end-to-end dicyanamide as a double bridging ligand: Crystallography study and Hirshfeld surface analysis; completed with a CSD survey. Journal of Molecular Structure, 2018, 1173, 697-706.	1.8	7
47	Molecular rules for selectivity in lipase-catalysed acylation of lysine. Process Biochemistry, 2018, 74, 50-60.	1.8	17
48	Crystal structure, Hirshfeld surface analysis, thermal behavior and spectroscopic investigations of a new organic cyclohexaphosphate, (C 10 H 15 N 2) 4 (Li) 2 (P 6 O 18)(H 2 O) 6. Journal of Molecular Structure, 2018, 1171, 429-437.	1.8	6
49	Synthesis and Reactivity of Copper(I) Complexes Based on C 3 -Symmetric Tripodal HTIM(PR2)3 Ligands. European Journal of Inorganic Chemistry, 2018, 2018, 2608-2608.	1.0	0
50	A Hirshfeld surface analysis, crystal structure, and physicochemical studies of a new Cu(II) complex with the 1,10-phenanthroline ligand. Journal of Coordination Chemistry, 2018, 71, 2526-2539.	0.8	6
51	Experimental Charge Density Analysis of the Anti-inflammatory Drug Meloxicam [sodium 4-hydroxy-2-methyl-N-(5-methyl-1,3-thiazol-2-yl)-1,1-dioxo-1$l^{6},2-benzothiazine-3-carboxamide Monohydrate]. Croatica Chemica Acta, 2018, 91, .	0.1	1
52	A Hirshfeld surface analysis, crystal structure and infrared characterization of a new organic cyclohexaphosphate, (C8H12N)4(Li)2(P6O18)(H2O)6. Journal of Molecular Structure, 2017, 1134, 828-834.	1.8	4
53	A Hirshfeld surface analysis, crystal structure and spectroscopic properties of new Zn(II) complex with N-aminoethylpiperazine ligand. Journal of Molecular Structure, 2017, 1134, 538-545.	1.8	3
54	Charge density analysis of metformin chloride, a biguanide anti-hyperglycemic agent. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 10-22.	0.5	15

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55	Crystal structure, Hirshfeld surface analysis, quantum mechanical study and spectroscopic characterization of the non-centrosymmetric coordination compound bis(4-fluoroaniline)dichloridozincate. Journal of Molecular Structure, 2017, 1138, 71-80.	1.8	4
56	Bonding in Uranium(V) Hexafluoride Based on the Experimental Electron Density Distribution Measured at 20 K. Inorganic Chemistry, 2017, 56, 1775-1778.	1.9	23
57	Experimental evidence of a 3-centre, 2-electron covalent bond character of the central Oâ€“Hâ€“O fragment on the Zundel cation in crystals of Zundel nitranilate tetrahydrate. CrystEngComm, 2017, 19, 3898-3901.	1.3	11
58	Crystal and geometry-optimized structure, Hirshfeld surface analysis and physicochemical studies of a new Co(II) complex with the ligand 2-amino-6-methoxypyrimidine. Journal of Molecular Structure, 2017, 1146, 347-355.	1.8	2
59	Synthesis, X-ray single crystal structure, likelihood of occurrence of intermolecular contacts, spectroscopic investigation and DFT quantum chemical calculations of zwitterionic complex: 1-Ethylpiperaziniumtrichlorozincate (II). Journal of Molecular Structure, 2017, 1146, 70-79.	1.8	1
60	Directional O...F halogen bonds. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 136-137.	0.5	12
61	Crystal and geometry-optimized structure, Hirshfeld surface analysis and spectroscopic studies of tetrachlorocuprate and nitrate salts of 1-(2-fluorophenyl)piperazine cations, (C10H15FN2)[CuCl4] (I) and (C10H14FN2)[NO3] (II). Inorganic Chemistry Communication, 2017, 86, 118-127.	1.8	2
62	A Hirshfeld surface analysis, synthesis, structure and characterization of a new Ni(II) diamagnetic complex with the bidentate ligand homopiperazine. Journal of Molecular Structure, 2017, 1148, 412-420.	1.8	2
63	A Hirshfeld surface analysis, supramolecular structure and magnetic properties of a new Cu(II) complex with the 4-amino-6-methoxypyrimidine ligand. Journal of Molecular Structure, 2017, 1130, 114-121.	1.8	5
64	A Hirshfeld surface analysis, crystal structure and physicochemical studies of a new Cd(II) complex with the 2-amino-4-methylpyrimidine ligand. Journal of Molecular Structure, 2017, 1128, 378-384.	1.8	11
65	A theoretical-electron-density databank using a model of real and virtual spherical atoms. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 610-625.	0.5	13
66	Atom interaction propensities of oxygenated chemical functions in crystal packings. IUCrJ, 2017, 4, 158-174.	1.0	23
67	Betulin Phosphonates; Synthesis, Structure, and Cytotoxic Activity. Molecules, 2016, 21, 1123.	1.7	27
68	A hirshfeld surface analysis, crystal structure and physicochemical characterization of 1-ethylpiperazinium trichlorocadmate(II). Solid State Sciences, 2016, 57, 49-55.	1.5	10
69	A Hirshfeld surface analysis, crystal structure and physicochemical studies of zwitterionic complex: 1-(2-hydroxyethyl)piperaziniumtrichlorozincate (II). Inorganic Chemistry Communication, 2016, 70, 65-70.	1.8	4
70	Carbohydrate-based peptidomimetics targeting neuropilin-1: Synthesis, molecular docking study and in vitro biological activities. Bioorganic and Medicinal Chemistry, 2016, 24, 5315-5325.	1.4	29
71	Structural, Hirshfeld surface and spectroscopic studies of the noncentrosymmetric 1-ethylpiperazinediium pentachloroantimonate (III) monohydrate. Solid State Sciences, 2016, 58, 94-100.	1.5	7
72	Structural, crystal structure, Hirshfeld surface analysis and physicochemical studies of a new chlorocadmate template by 1-(2-hydroxyethyl)piperazine. Journal of Molecular Structure, 2016, 1123, 66-74.	1.8	10

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73	Experimental and theoretical charge-density analysis of 1,4-bis(5-hexyl-2-thienyl)butane-1,4-dione: applications of a virtual-atom model. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 75-86.	0.5	2
74	Synthesis, structural characterization, Hirshfeld surface analysis and spectroscopic studies of cadmium (II) chloride complex with 4-hydroxy-1-methylpiperidine. Journal of Solid State Chemistry, 2016, 237, 7-13.	1.4	15
75	Libraries of Extremely Localized Molecular Orbitals. 2. Comparison with the Pseudoatoms Transferability. Journal of Chemical Theory and Computation, 2016, 12, 1068-1081.	2.3	48
76	Likelihood of atomâ€“atom contacts in crystal structures of halogenated organic compounds. IUCrJ, 2015, 2, 327-340.	1.0	69
77	Cholesterol oxidase: ultrahigh-resolution crystal structure and multipolar atom model-based analysis. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 954-968.	2.5	17
78	Crystal structure, Hirshfeld surface analysis, quantum mechanical study and spectroscopic studies of noncentrosymmetric (S)nicotiniumtrichloridozincate monohydrate complex. Inorganic Chemistry Communication, 2015, 61, 187-192.	1.8	9
79	A polarÎ€ model of interactions explains face-to-face stacked quinoid rings: a case study of the crystal of potassium hydrogen chloranilate dihydrate. CrystEngComm, 2015, 17, 8645-8656.	1.3	9
80	Synthesis and physico-chemical studies of a novel layered structure with a heptanuclear Cd complex: (C9N4H28)Cd7(H2O)2Cl18Â·nH2O(n=5.89). Journal of Molecular Structure, 2015, 1084, 46-54.	1.8	16
81	The enrichment ratio of atomic contacts in crystals, an indicator derived from the Hirshfeld surface analysis. IUCrJ, 2014, 1, 119-128.	1.0	380
82	Bis(2-amino-4-methyl-6-oxo-3,6-dihydropyrimidin-1-ium) sulfate monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2014, 70, o747-o748.	0.2	0
83	Pseudo-symmetry, rotation- and inversion-twinning of a structure with dinuclear and trinuclear Cd complexes. CP-MAS-NMR and IR spectroscopies characterisation. Journal of Molecular Structure, 2014, 1075, 442-449.	1.8	2
84	Charge-density analysis using multipolar atom and spherical charge models: 2-methyl-1,3-cyclopentanedione, a compound displaying a resonance-assisted hydrogen bond. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2014, 70, 197-211.	0.5	12
85	Poly[diaquatris(Î¼6-4,6-dioxo-1,4,5,6-tetrahydro-1,3,5-triazine-2-carboxylato)tripotassium]. Acta Crystallographica Section E: Structure Reports Online, 2014, 70, m174-m175.	0.2	0
86	Crystal structure of 2-amino-5-methylsulfanyl-1,3,4-thiadiazol-3-ium chloride monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2014, 70, o913-o914.	0.2	0
87	MoProViewer: a tool to study proteins from a charge density science perspective. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C279-C279.	0.0	38
88	Hydrogen atoms in protein structures: high-resolution X-ray diffraction structure of the DFPase. BMC Research Notes, 2013, 6, 308.	0.6	27
89	Experimental and Theoretical Charge Density Analysis of a Bromoethyl Sulfonium Salt. Journal of Physical Chemistry A, 2013, 117, 14267-14275.	1.1	8
90	Relationship between Stereochemistry and Charge Density in Hydrogen Bonds with Oxygen Acceptors. Crystal Growth and Design, 2013, 13, 315-325.	1.4	36

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91	The organicâ€“inorganic hybrid material 1-cyclohexylpiperazine-1,4-diium tetrachloridozincate. Acta Crystallographica Section C: Crystal Structure Communications, 2013, 69, 1304-1306.	0.4	6
92	o-Phenylenediaminium chloride nitrate. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o600-o600.	0.2	2
93	Charge Density Analysis and Topological Properties of Hal₃-Synthons and Their Comparison with Competing Hydrogen Bonds. Crystal Growth and Design, 2012, 12, 5373-5386.	1.4	78
94	A critical analysis of dipole-moment calculations as obtained from experimental and theoretical structure factors. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 715-728.	0.3	18
95	Experimental and database-transferred electron-density analysis and evaluation of electrostatic forces in coumarin-102 dye. Acta Crystallographica Section B: Structural Science, 2012, 68, 646-660.	1.8	10
96	Topological analysis of hydrogen-bonds and weak interactions in protein helices. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, s56-s56.	0.3	0
97	An improved experimental databank of transferable multipolar atom models â€“ ELMAM2. Construction details and applications. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 337-351.	0.3	119
98	Charge-density analysis and electrostatic properties of 2-carboxy-4-methylanilinium chloride monohydrate obtained using a multipolar and a spherical-charges model. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 452-463.	0.3	28
99	Electron and Electrostatic Properties of Three Crystal Forms of Piracetam. Crystal Growth and Design, 2011, 11, 2528-2539.	1.4	11
100	Charge Density Analysis of 2-Methyl-4-nitro-1-phenyl-1H-imidazole-5-carbonitrile: An Experimental and Theoretical Study of Câ‰¡NÂ·Â·Â·Câ‰¡N Interactions. Journal of Physical Chemistry A, 2011, 115, 12941-12952.	1.1	21
101	Experimental and Theoretical Investigation of Topological and Energetic Characteristics of Sb Complexes Reversibly Binding Molecular Oxygen. Journal of Physical Chemistry A, 2011, 115, 8271-8281.	1.1	42
102	Periodic Projector Augmented Wave Density Functional Calculations on the Hexachlorobenzene Crystal and Comparison with the Experimental Multipolar Charge Density Model. Journal of Physical Chemistry A, 2011, 115, 14484-14494.	1.1	43
103	Topological Analysis of Hydrogen Bonds and Weak Interactions in Protein Helices via Transferred Experimental Charge Density Parameters. Journal of Physical Chemistry A, 2011, 115, 12895-12904.	1.1	21
104	Frontier Applications of Experimental Charge Density and Electrostatics to Bio-macromolecules. , 2011, , 527-552.		0
105	2,2â€²-(Ethane-1,2-diyl)bis[2-(5-bromothiophen-2-yl)-1,3-dioxolane] at 100â€…K refined using a multipolar atom model. Acta Crystallographica Section C: Crystal Structure Communications, 2011, 67, o329-o333.	0.4	9
106	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
107	Structural analysis and multipole modelling of quercetin monohydrate â€“ a quantitative and comparative study. Acta Crystallographica Section B: Structural Science, 2011, 67, 63-78.	1.8	70
108	Charge-density analysis of 1-nitroindoline: refinement quality using freeRfactors and restraints. Acta Crystallographica Section B: Structural Science, 2011, 67, 250-262.	1.8	34

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109	R-free factor and experimental charge-density analysis of 1-(2â€²-aminophenyl)-2-methyl-4-nitroimidazole: a crystal structure withZâ€² = 2. Acta Crystallographica Section B: Structural Science, 2011, 67, 365-378.	1.8	41
110	5-(3,4-Dimethoxybenzyl)-7-isopropyl-1,3,5-triazepane-2,6-dione acetonitrile solvate refined using a multipolar atom model. Acta Crystallographica Section C: Crystal Structure Communications, 2010, 66, o292-o294.	0.4	1
111	Experimental and Theoretical Charge Density Analysis of Polymorphic Structures: The Case of Coumarin 314 Dye. Crystal Growth and Design, 2010, 10, 1516-1526.	1.4	35
112	Correction to Experimental and Theoretical Charge Density Analysis of Polymorphic Structures: The Case of Coumarin 314 Dye. Crystal Growth and Design, 2010, 10, 4670-4670.	1.4	1
113	4-Benzoyl-3,4-dihydro-2H-1,4-benzoxazine-2-carbonitrile: refinement using a multipolar atom model. Acta Crystallographica Section C: Crystal Structure Communications, 2009, 65, o342-o344.	0.4	1
114	Charge density and electrostatic potential analyses in paracetamol. Acta Crystallographica Section B: Structural Science, 2009, 65, 363-374.	1.8	43
115	Charge Density and Electrostatic Interactions of Fidarestat, an Inhibitor of Human Aldose Reductase. Journal of the American Chemical Society, 2009, 131, 10929-10941.	6.6	48
116	Elucidation of the Phosphate Binding Mode of DING Proteins Revealed by Subangstrom X-ray Crystallography. Journal of the American Chemical Society, 2009, 131, 7879-7886.	6.6	50
117	(2S,3S)-2-(N,N-Dibenzylamino)butane-1,3-diol refined using a multipolar atom model. Acta Crystallographica Section C: Crystal Structure Communications, 2008, 64, o18-o20.	0.4	0
118	Charge-density analysis of a protein structure at subatomic resolution: the human aldose reductase case. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 567-588.	2.5	51
119	Ultrahigh-resolution crystallography and related electron density and electrostatic properties in proteins. Journal of Synchrotron Radiation, 2008, 15, 202-203.	1.0	15
120	Optimal local axes and symmetry assignment for charge-density refinement. Journal of Applied Crystallography, 2008, 41, 1140-1149.	1.9	50
121	Charge-density analysis of human aldose reductase active site. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, C368-C368.	0.3	3
122	The experimental library multipolar atom model refinement ofL-aspartic acid. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o361-o364.	0.4	29
123	On the application of an experimental multipolar pseudo-atom library for accurate refinement of small-molecule and protein crystal structures. Acta Crystallographica Section A: Foundations and Advances, 2007, 63, 108-125.	0.3	148
124	Advances in protein and small-molecule charge-density refinement methods usingMoPro. Journal of Applied Crystallography, 2005, 38, 38-54.	1.9	285
125	Frontier example in experimental charge density research: Experimental electrostatics of proteins. International Journal of Quantum Chemistry, 2005, 101, 624-634.	1.0	20
126	Charge density research: from inorganic and molecular materials to proteins. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	17

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127	Ultra-high-resolution X-ray structure of proteins. Cellular and Molecular Life Sciences, 2004, 61, 774-782.	2.4	28
128	A comparison between experimental and theoretical aspherical-atom scattering factors for charge-density refinement of large molecules. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 204-208.	0.3	58
129	Experimental and Theoretical Electron Density Studies in Large Molecules:Â NAD+, Î²-Nicotinamide Adenine Dinucleotide. Journal of Physical Chemistry B, 2003, 107, 9109-9121.	1.2	30
130	Electrostatic complementarity in an aldose reductase complex from ultra-high-resolution crystallography and first-principles calculations. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 8742-8747.	3.3	113
131	The Crystal Structure of a Novel, Inactive, Lysine 49 PLA2 from Agkistrodon acutus Venom. Journal of Biological Chemistry, 2003, 278, 41400-41408.	1.6	36
132	Trypsin Revisited. Journal of Biological Chemistry, 2003, 278, 43357-43362.	1.6	57
133	Experimental Electron Density of 1-Phenyl-4-nitroimidazole and Topological Analysis of Câ^'HÂ·Â·Â·O and Câ^'HÂ·Â·Â·N Hydrogen Bonds. Journal of Physical Chemistry B, 2002, 106, 3706-3714.	1.2	46
134	X-ray crystallography at subatomic resolution. Europhysics News, 2002, 33, 113-117.	0.1	11
135	Refinement of proteins at subatomic resolution withMOPRO. Journal of Applied Crystallography, 2001, 34, 214-223.	1.9	149
136	Sparsity of the normal matrix in the refinement of macromolecules at atomic and subatomic resolution. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 558-570.	0.3	6
137	Experimental and theoretical charge density of DL-alanyl-methionine. Acta Crystallographica Section B: Structural Science, 2001, 57, 567-578.	1.8	26
138	High-resolution neutron structure of nicotinamide adenine dinucleotide. Acta Crystallographica Section D: Biological Crystallography, 2001, 57, 981-989.	2.5	13
139	Equilibrium kinetics of lysozyme crystallization under an external electric field. Journal of Crystal Growth, 2001, 232, 250-255.	0.7	66
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