Christian B HÃ¼bschle

List of Publications by Year
in descending order

47 papers	4,185 citations	361413 20 h-index	265206 42 g-index
49 all docs	49 docs citations	49 times ranked	4054 citing authors

#	Article	IF	Citations
1	ShelXle: a Qt graphical user interface forSHELXL. Journal of Applied Crystallography, 2011, 44, 1281-1284.	4.5	2,798
2	MolIsoâ€“ a program for colour-mapped iso-surfaces. Journal of Applied Crystallography, 2006, 39, 901-904.	4.5	193
3	The invariom model and its application: refinement ofD,L-serine at different temperatures and resolution. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, 314-320.	0.3	136
4	MoleCoolQtâ€“ a molecule viewer for charge-density research. Journal of Applied Crystallography, 2011, 44, 238-240.	4.5	133
5	Automation of invariom and of experimental charge density modelling of organic molecules with the preprocessor programInvariomTool. Journal of Applied Crystallography, 2007, 40, 623-627.	4.5	96
6	Introduction and validation of an invariom database for amino-acid, peptide and protein molecules. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 1325-1335.	2.5	94
7	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
8	Anharmonic Motion in Experimental Charge Density Investigations. Journal of Physical Chemistry A, 2013, 117, 633-641.	2.5	61
9	Towards extracting the charge density from normal-resolution data. Journal of Applied Crystallography, 2009, 42, 1110-1121.	4.5	50
10	Aspherical scattering factors forSHELXLâ€“ model, implementation and application. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 50-62.	0.1	49
11	Reproducibility and transferability of topological data: experimental charge density study of two modifications ofl-alanyl-l-tyrosyl-l-alanine. Organic and Biomolecular Chemistry, 2006, 4, 3242-3251.	2.8	46
12	Electrostatic properties of nine fluoroquinoloneantibiotics derived directly from their crystal structure refinements. CrystEngComm, 2012, 14, 2520-2531.	2.6	39
13	How to easily replace the independent atom model â€“ the example of bergenin, a potential anti-HIV agent of traditional Asian medicine. Acta Crystallographica Section B: Structural Science, 2009, 65, 749-756.	1.8	37
14	Crystal-field effects in<scp>L</scp>-homoserine: multipolesversusquantum chemistry. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 435-442.	0.3	36
15	Experimental charge density of <scp>L</scp>-alanyl-<scp>L</scp>-prolyl-<scp>L</scp>-alanine hydrate: classical multipole and invariom approach, analysis of intra- and intermolecular topological properties. Acta Crystallographica Section B: Structural Science, 2007, 63, 753-767.	1.8	27
16	On QM/MM and MO/MO cluster calculations of all-atom anisotropic displacement parameters for molecules in crystal structures. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 110-116.	0.3	27
17	Mapping the Trajectory of Nucleophilic Substitution at Silicon Using a periâ€Substituted Acenaphthyl Scaffold. Chemistry - A European Journal, 2017, 23, 10568-10579.	3.3	27
18	Bond Orders and Atomic Properties of the Highly Deformed Halogenated Fullerenes C60F18 and C60Cl30 Derived from their Charge Densities. Chemistry - A European Journal, 2007, 13, 1910-1920.	3.3	24

#	Article	IF	Citations
19	Comparative experimental electron density and electron localization function study of thymidine based on 20â€…K X-ray diffraction data. Acta Crystallographica Section B: Structural Science, 2008, 64, 363-374.	1.8	24
20	Cadmium(II) complexes of a hydrazone ligand: Synthesis, characterization, DNA binding, cyto- and genotoxicity studies. Polyhedron, 2019, 171, 237-248.	2.2	23
21	Electron densities of bexarotene and disila-bexarotene from invariom application: a comparative study. Organic and Biomolecular Chemistry, 2013, 11, 2348.	2.8	20
22	Neubestimmung der Ladungsdichte und topologische Analyse vonÎ²-Diboran bei 94 K. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2004, 630, 1313-1316.	1.2	19
23	Experimental Advances for High-Speed Evaluation of Electron Densities. Journal of Physical Chemistry A, 2005, 109, 10177-10179.	2.5	17
24	The electrostatic potential of dynamic charge densities. Journal of Applied Crystallography, 2017, 50, 1627-1636.	4.5	16
25	On the 2-Electron 3-Center Bâ^'Hâ^'B Bond: Charge Density Determination of Tetraborane(10). Inorganic Chemistry, 2008, 47, 1874-1876.	4.0	15
26	Invariom refinement of a new monoclinic solvate of thiostrepton at 0.64â€…Ã… resolution. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 1530-1539.	2.5	14
27	Invariom structure refinement, electrostatic potential and toxicity of 4-O-methylalpinumisoflavone, O,O-dimethylalpinumisoflavone and 5-O-methyl-4-O-(3-methylbut-2-en-1-yl)alpinumisoflavone. Acta Crystallographica Section B: Structural Science, 2006, 62, 843-849.	1.8	12
28	Fundamental Relation between Molecular Geometry and Real-Space Topology. Combined AIM, ELI-D, and ASF Analysis of Hapticities and Intramolecular Hydrogenâ€“Hydrogen Bonds in Zincocene-Related Compounds. Journal of Physical Chemistry A, 2014, 118, 4351-4362.	2.5	12
29	Invariom modeling of disordered structures: case studies on a dipeptide, an amino acid, and cefaclor, a cephalosporin antibiotic. Zeitschrift Fur Kristallographie - Crystalline Materials, 2016, 231, 725-736.	0.8	12
30	Charge density wave and lock-in transitions of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CuV</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2019, 99, .	3.2	11
31	The generalized invariom database (GID). Acta Crystallographica Section B: Structural Science, 2013, 69, 91-104.	1.8	11
32	Examination of intermolecular electronic interactions in the crystal structure of C60(CF3)12 by experimental electron density determination. Chemical Communications, 2007, , 4003.	4.1	8
33	Charge Density of L-Alanyl-glycyl-L-alanine Based on X-Ray Data Collection Periods from 4 to 130 Hours. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2007, 62, 696-704.	0.7	6
34	The Hydroxylated, Tetracyclic Bisquinolizidine Alkaloids Baptifoline and Epibaptifoline: Enantioselective Synthesis and Unambiguous Assignment of their Configuration at Câ€‰13. European Journal of Organic Chemistry, 2019, 2019, 895-899.	2.4	6
35	L-Tryptophan formic acid solvate at 183â€…K. Acta Crystallographica Section C: Crystal Structure Communications, 2002, 58, o540-o542.	0.4	5
36	On avoiding negative electron density in Gram-Charlier refinements of anharmonic motion: the example of glutathione. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 695-706.	0.8	4

#	Article	IF	Citations
37	Local Structure of Ferroic Iron Formates at Low Temperature and High Pressure Studied by MÃ¶ssbauer Spectroscopy. Journal of Physical Chemistry C, 2019, 123, 21676-21684.	3.1	4
38	Charge density of 4-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]thiazole-2(3H)-thione. A comprehensive multipole refinement, maximum entropy method and density functional theory study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 450-468.	1.1	3
39	Boranes: The Boron Subhydride B104.67H3 with a Distorted Î²-Boron Crystal Structure. Inorganic Chemistry, 2020, 59, 13295-13300.	4.0	1
40	IDEAL â€“ invariom-derived electron analysis for APEX3. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a154-a154.	0.1	1
41	ShelXle: a Qt graphical user interface for SHELXL. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, a187-a187.	0.1	1
42	Electrostatic potential of dynamic charge densities. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s86-s86.	0.1	0
43	Electrostatic potential in crystals of Î±-boron, Î³-boron and boron carbide. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 663-673.	0.8	0
44	MoleCoolQt- a molecule viewer for charge-density related science. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, s311-s311.	0.3	0
45	New developments in the BayMEM Suite. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C103-C103.	0.1	0
46	Molecular thermal smeared electrostatic potential. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e307-e307.	0.1	0
47	3D visualization and printing of molecular surfaces. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e365-e365.	0.1	0