

Jacob Overgaard

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/714174/publications.pdf>

Version: 2024-02-01

169
papers

5,714
citations

70961

41
h-index

95083

68
g-index

205
all docs

205
docs citations

205
times ranked

5847
citing authors

#	ARTICLE	IF	CITATIONS
1	Pronounced Magnetic Bistability in Highly Cooperative Mononuclear [Fe(L ⁿ pdztz) ₂ (NCX) ₂] Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 3141-3151.	1.9	9
2	An experimental and theoretical charge density study of theophylline and malonic acid cocrystallization. <i>RSC Advances</i> , 2022, 12, 15670-15684.	1.7	5
3	Catalytic Enantioselective Entry to Triflones Featuring a Quaternary Stereocenter. <i>Organic Letters</i> , 2022, 24, 4371-4376.	2.4	6
4	Exploring the Solubility of the Carbamazepine-Saccharin Cocrystal: A Charge Density Study. <i>Crystal Growth and Design</i> , 2021, 21, 4259-4275.	1.4	8
5	Magnetic anisotropies of Ho(III) and Dy(III) single-molecule magnets experimentally determined via polarized neutron diffraction. <i>Dalton Transactions</i> , 2021, 50, 14207-14215.	1.6	2
6	Diastereoselective Synthesis of Functionalized 5-Amino-4-Dihydro-1H-Pyrrole-2-Carboxylic Acid Esters: One-Pot Approach Using Commercially Available Compounds and Benign Solvents. <i>Chemistry - A European Journal</i> , 2021, 27, 4573-4577.	1.7	3
7	Structure-property correlation in stabilizing axial magnetic anisotropy in octahedral Co(II) complexes. <i>Cell Reports Physical Science</i> , 2021, 2, 100404.	2.8	23
8	The Quest for Optimal 3d Orbital Splitting in Tetrahedral Cobalt Single-Molecule Magnets Featuring Colossal Anisotropy and Hysteresis. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3108-3114.	1.0	13
9	Quantifying magnetic anisotropy using X-ray and neutron diffraction. <i>IUCr</i> , 2021, 8, 833-841.	1.0	2
10	Observation of the asphericity of 4f-electron density and its relation to the magnetic anisotropy axis in single-molecule magnets. <i>Nature Chemistry</i> , 2020, 12, 213-219.	6.6	50
11	High-Pressure Crystallographic and Magnetic Studies of Pseudo-D _{5h} Symmetric Dy(III) and Ho(III) Single-Molecule Magnets. <i>Inorganic Chemistry</i> , 2020, 59, 717-729.	1.9	38
12	Influence of anion induced geometry change in Zn(II) on the magnetization relaxation dynamics of Dy(III) in Zn-Dy-Zn complexes. <i>Dalton Transactions</i> , 2020, 49, 10580-10593.	1.6	5
13	Experimental Charge Densities from Multipole Modeling: Moving into the Twenty-First Century. <i>Structure and Bonding</i> , 2020, , 145-182.	1.0	3
14	Quantification of the Magnetic Anisotropy of a Single-Molecule Magnet from the Experimental Electron Density. <i>Angewandte Chemie</i> , 2020, 132, 21389-21395.	1.6	2
15	Quantification of the Magnetic Anisotropy of a Single-Molecule Magnet from the Experimental Electron Density. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 21203-21209.	7.2	11
16	Investigating Complex Magnetic Anisotropy in a Co(II) Molecular Compound: A Charge Density and Correlated Ab Initio Electronic Structure Study. <i>Inorganic Chemistry</i> , 2020, 59, 13190-13200.	1.9	12
17	Accurate high-resolution single-crystal diffraction data from a Pilatus 3000 X CdTe detector. <i>Journal of Applied Crystallography</i> , 2020, 53, 635-649.	1.9	28
18	High-Pressure Crystallography as a Guide in the Design of Single-Molecule Magnets. <i>Inorganic Chemistry</i> , 2020, 59, 1682-1691.	1.9	14

#	ARTICLE	IF	CITATIONS
19	Single-Crystal High-Pressure X-ray Diffraction Study of Host Structure Compression in Clathrates of Dianinâ€™s Compound. <i>Crystal Growth and Design</i> , 2020, 20, 4092-4099.	1.4	5
20	Chemical Bonding in Colossal Thermopower FeSb ₂ . <i>Chemistry - A European Journal</i> , 2020, 26, 8651-8662.	1.7	6
21	Direct Î±-Imination of <i>N</i> -Acyl Pyrazoles with Nitrosoarenes. <i>Organic Letters</i> , 2019, 21, 5305-5309.	2.4	7
22	Low-Barrier Hydrogen Bonds in Negative Thermal Expansion Material H ₃ [Co(CN) ₆]. <i>Chemistry - A European Journal</i> , 2019, 25, 6814-6822.	1.7	14
23	Molten metal <i>clo</i> -borate solvates. <i>Chemical Communications</i> , 2019, 55, 3410-3413.	2.2	12
24	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
25	Insights into Single-Molecule-Magnet Behavior from the Experimental Electron Density of Linear Two-Coordinate Iron Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 3211-3218.	1.9	28
26	Accessing the rich carbon nitride materials chemistry by heat treatments of ammonium thiocyanate, NH ₄ SCN. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 621-633.	0.5	2
27	Experimental X-ray Electron Density Study of Atomic Charges, Oxidation States, and Inverted Ligand Field in Cu(CF ₃) ₄ ⁺ . <i>Inorganic Chemistry</i> , 2019, 58, 2133-2139.	1.9	28
28	Exploring the Binding of Barbitol to a Synthetic Macrocyclic Receptor. A Charge Density Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3031-3044.	1.1	3
29	X-ray electron density investigation of chemical bonding in van der Waals materials. <i>Nature Materials</i> , 2018, 17, 249-252.	13.3	93
30	Probing Cyclic Î€-Electron Delocalization in an Imidazolâ€¦ylidene and a Corresponding Imidazolium Salt. <i>Chemistry - A European Journal</i> , 2018, 24, 4973-4981.	1.7	8
31	Using Electron Density to Predict Synthon Formation in a 4-Hydroxybenzoic Acid: 4,4-â€²-Bipyridine Cocrystal. <i>Crystal Growth and Design</i> , 2018, 18, 1786-1798.	1.4	20
32	Probing the accuracy and precision of Hirshfeld atom refinement with <i>HART</i> interfaced with <i>Olex2</i> . <i>IUCr</i> , 2018, 5, 32-44.	1.0	74
33	Organocatalyzed Decarboxylative Trichloromethylation of Morita-Baylis-Hillman Adducts in Batch and Continuous Flow. <i>Chemistry - A European Journal</i> , 2018, 24, 1204-1208.	1.7	6
34	Mapping the Magnetic Anisotropy at the Atomic Scale in Dysprosium Single-Molecule Magnets. <i>Chemistry - A European Journal</i> , 2018, 24, 16456-16456.	1.7	1
35	A linear cobalt(II) complex with maximal orbital angular momentum from a non-Aufbau ground state. <i>Science</i> , 2018, 362, .	6.0	254
36	Monoclinic Paracetamol vs. Paracetamol-4,4-â€²-Bipyridine Co-Crystal; What Is the Difference? A Charge Density Study. <i>Crystals</i> , 2018, 8, 46.	1.0	6

#	ARTICLE	IF	CITATIONS
37	Mapping the Magnetic Anisotropy at the Atomic Scale in Dysprosium Single-Molecule Magnets. <i>Chemistry - A European Journal</i> , 2018, 24, 16576-16581.	1.7	18
38	Determination of d-Orbital Populations in a Cobalt(II) Single-Molecule Magnet Using Single-Crystal X-ray Diffraction. <i>Inorganic Chemistry</i> , 2018, 57, 6913-6920.	1.9	22
39	Evidence for Single-Electron Pathways in the Reaction between Palladium(II) Dialkyl Complexes and Alkyl Bromides under Thermal and Photoinduced Conditions. <i>Organometallics</i> , 2017, 36, 2058-2066.	1.1	17
40	Amine Thiourea Catalysed Double Michael Reaction: An Approach for the Asymmetric Synthesis of Spiro[pyrazolone-4,3-tetrahydrothiophenes]. <i>Synthesis</i> , 2017, 49, 1509-1518.	1.2	15
41	Tunable <i>Cinchona</i> -Based Thioureas-Catalysed Asymmetric Epoxidation to Synthetically Important Glycidic Ester Derivatives. <i>Advanced Synthesis and Catalysis</i> , 2017, 359, 913-918.	2.1	20
42	Intermolecular Interaction Energies in Hydroquinone Clathrates at High Pressure. <i>Crystal Growth and Design</i> , 2017, 17, 3834-3846.	1.4	21
43	Crystal structure across the \hat{I}^2 to $\hat{I}\pm$ phase transition in thermoelectric Cu_{2-x}Se . <i>IUCr</i> , 2017, 4, 476-485.	1.0	65
44	Variable-temperature structural studies on valence tautomerism in cobalt bis(dioxolene) molecular complexes. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 304-312.	0.5	4
45	Efficient Water Reduction with $\text{sp}^3\text{-sp}^3$ Diboron(4) Compounds: Application to Hydrogenations, H/D Exchange Reactions, and Carbonyl Reductions. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 15910-15915.	7.2	54
46	Diastereodivergent and Enantioselective Access to Spiroepoxides via Organocatalytic Epoxidation of Unsaturated Pyrazolones. <i>Organic Letters</i> , 2017, 19, 5030-5033.	2.4	42
47	Efficient Water Reduction with $\text{sp}^3\text{-sp}^3$ Diboron(4) Compounds: Application to Hydrogenations, H/D Exchange Reactions, and Carbonyl Reductions. <i>Angewandte Chemie</i> , 2017, 129, 16126-16131.	1.6	15
48	Charge-density study of van der Waals layered MoS_2 and TiS_2 . <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C1390-C1390.	0.0	0
49	Charge density and magnetic anisotropy of Dy-based single-molecule magnet. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C1365-C1365.	0.0	0
50	Anisotropic compressibility of the coordination polymer $\text{emim}[\text{Mn}(\text{btc})]$. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 389-394.	0.5	8
51	A Concise Route to the Strongylophorines. <i>Angewandte Chemie</i> , 2016, 128, 8434-8438.	1.6	4
52	X-ray Diffraction and Mössbauer Spectroscopy Studies of Pressure-Induced Phase Transitions in a Mixed-Valence Trinuclear Iron Complex. <i>Chemistry - A European Journal</i> , 2016, 22, 9616-9623.	1.7	4
53	A Concise Route to the Strongylophorines. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8294-8298.	7.2	20
54	Structural Collapse of the Hydroquinone-Formic Acid Clathrate: A Pressure-Medium-Dependent Phase Transition. <i>Chemistry - A European Journal</i> , 2016, 22, 4061-4069.	1.7	18

#	ARTICLE	IF	CITATIONS
55	Electron Density Analysis of the σ -O π -Charge-Shift Bonding in Rubrene Endoperoxide. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7510-7518.	1.1	12
56	A comparison of the experimental and theoretical charge density distributions in two polymorphic modifications of piroxicam. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28802-28818.	1.3	15
57	An analysis of the experimental and theoretical charge density distributions of the piroxicam-saccharin co-crystal and its constituents. <i>RSC Advances</i> , 2016, 6, 81578-81590.	1.7	18
58	Magnetism and variable temperature and pressure crystal structures of a linear oligonuclear cobalt bis-semiquinonate. <i>Dalton Transactions</i> , 2016, 45, 12924-12932.	1.6	5
59	Expanding the usage of the Source Function to experimental electron densities. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 169-170.	0.5	2
60	Elucidating the magnetic behaviour of a unique linear Fe(II)-complex using the electron density. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2016, 72, s90-s91.	0.0	0
61	Quantifying intermolecular interaction energies in organic clathrates at high pressure. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2016, 72, s347-s347.	0.0	0
62	Electron density of a layered transition metal dichalcogenide. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2016, 72, s85-s85.	0.0	0
63	Pressure-induced structural collapse of the hydroquinone-formic acid clathrate; a pressure-medium dependent non-linear optical phase transition. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2015, 71, s361-s361.	0.0	0
64	Chemical Bonding and Electronic Localization in a Ga ^I Amide. <i>Chemistry - A European Journal</i> , 2015, 21, 14460-14470.	1.7	5
65	Does the thermal evolution of molecular structures critically affect the magnetic anisotropy?. <i>Chemical Science</i> , 2015, 6, 4587-4593.	3.7	61
66	High pressure induced charge transfer in 3d ⁴ bimetallic photomagnetic materials. <i>Chemical Communications</i> , 2015, 51, 8868-8871.	2.2	13
67	Expanding the structural versatility of thioannate(^{iv}) complexes. <i>CrystEngComm</i> , 2015, 17, 2413-2420.	1.3	15
68	Quantitative analysis of intermolecular interactions in orthorhombic rubrene. <i>IUCr</i> , 2015, 2, 563-574.	1.0	206
69	Accurate atomic displacement parameters from time-of-flight neutron-diffraction data at TOPAZ. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, 679-681.	0.0	12
70	Contemporary X-ray electron-density studies using synchrotron radiation. <i>IUCr</i> , 2014, 1, 267-280.	1.0	34
71	Metal distribution and disorder in the crystal structure of [NH ₂ Et ₂][Cr ₇ M ₈](t)BuCO ₂ ₁₆ wheel molecules for M = Mn, Fe, Co, Ni, Cu, Zn and Cd. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2014, 70, 932-941.	0.5	8
72	Chemical Bonding in a Linear Chromium Metal String Complex. <i>Inorganic Chemistry</i> , 2014, 53, 12489-12498.	1.9	21

#	ARTICLE	IF	CITATIONS
73	A structural study of a three-membered linear metal chain compound at elevated pressure. Dalton Transactions, 2014, 43, 1313-1320.	1.6	10
74	Relationships between Electron Density and Magnetic Properties in Water-Bridged Dimetal Complexes. Inorganic Chemistry, 2014, 53, 11531-11539.	1.9	8
75	Atomic properties and chemical bonding in the pyrite and marcasite polymorphs of FeS ₂ : a combined experimental and theoretical electron density study. Chemical Science, 2014, 5, 1408-1421.	3.7	65
76	Alkali Metal Ion Templated Transition Metal Formate Framework Materials: Synthesis, Crystal Structures, Ion Migration, and Magnetism. Inorganic Chemistry, 2014, 53, 10178-10188.	1.9	30
77	(NH ₄) ₄ Sn ₂ S ₆ ·3H ₂ O: Crystal Structure, Thermal Decomposition, and Precursor for Textured Thin Film. Chemistry of Materials, 2014, 26, 4494-4504.	3.2	19
78	Host Perturbation in a γ -Hydroquinone Clathrate Studied by Combined X-ray/Neutron Charge Density Analysis: Implications for Molecular Inclusion in Supramolecular Entities. Chemistry - A European Journal, 2014, 20, 8089-8098.	1.7	10
79	Anisotropic thermal expansion in a metal-organic framework. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2014, 70, 595-601.	0.5	6
80	Access to 1,2-dihydroisoquinolines through Gold-Catalyzed Formal [4+2] Cycloaddition. Chemistry - A European Journal, 2014, 20, 7926-7930.	1.7	42
81	Non-Nuclear Attractor in a Molecular Compound under External Pressure. European Journal of Inorganic Chemistry, 2014, 2014, 5536-5540.	1.0	20
82	Material Design Inputs from Charge Density Analysis in Organic Semiconductors. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1552-C1552.	0.0	0
83	High-pressure Single-crystal X-ray Diffraction Study of the Photomagnetic Switching Complex $[Y(DMF)_4(H_2O)_3(1/4CN)Fe(CN)_5] \cdot H_2O$. Journal of the Chinese Chemical Society, 2013, 60, 929-934.	0.8	6
84	Experimental and Theoretical Charge Densities of a Zinc-Containing Coordination Polymer, Zn(HCOO) ₂ (H ₂ O) ₂ . Inorganic Chemistry, 2013, 52, 297-305.	1.9	24
85	Pushing X-ray Electron Densities to the Limit: Thermoelectric CoSb ₃ . Angewandte Chemie - International Edition, 2013, 52, 1503-1506.	7.2	30
86	Pressure versus Temperature Effects on Intramolecular Electron Transfer in Mixed-Valence Complexes. Chemistry - A European Journal, 2013, 19, 195-205.	1.7	13
87	Comparative study of X-ray charge-density data on CoSb ₃ . Acta Crystallographica Section A: Foundations and Advances, 2013, 69, 570-582.	0.3	36
88	Experimental Electron Density Studies of Inorganic Materials. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 1922-1932.	0.6	24
89	Electron Localisation in Ga-Heterocyclic Compounds. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 1979-1984.	0.6	4
90	Synthesis and Structural Investigation of Zr(BH ₄) ₄ . Journal of Physical Chemistry C, 2012, 116, 20239-20245.	1.5	43

#	ARTICLE	IF	CITATIONS
91	On the significance of Bragg reflections. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 301-303.	0.3	16
92	Testing the Concept of Hypervalency: Charge Density Analysis of K_2SO_4 . Inorganic Chemistry, 2012, 51, 8607-8616.	1.9	93
93	Glucose-assisted continuous flow synthesis of Bi_2Te_3 nanoparticles in supercritical/near-critical water. Journal of Supercritical Fluids, 2012, 67, 84-88.	1.6	15
94	Temperature-dependent crystal structure of the isopropanol clathrate of Dianin's compound. Chemical Communications, 2011, 47, 2029.	2.2	9
95	Experimental Charge Density Analysis of a Gallium(I) N-Heterocyclic Carbene Analogue. Inorganic Chemistry, 2011, 50, 8418-8426.	1.9	33
96	First Experimental Characterization of a Non-nuclear Attractor in a Dimeric Magnesium(I) Compound. Journal of Physical Chemistry A, 2011, 115, 194-200.	1.1	106
97	A photo-induced excited state structure of a hetero-bimetallic ionic pair complex, $Nd(DMA)_4(H_2O)_4Fe(CN)_6 \cdot 3H_2O$, analyzed by single crystal X-ray diffraction. Chemical Communications, 2011, 47, 9486.	2.2	9
98	Charge Density in Materials and Energy Science. , 2011, , 469-504.		0
99	Intermolecular Interactions and Electrostatic Properties of the \hat{I}^2 -Hydroquinone Apohost: Implications for Supramolecular Chemistry. Journal of Physical Chemistry A, 2011, 115, 12962-12972.	1.1	21
100	Analysis of the Photomagnetic Properties of Cyano-Bridged Heterobimetallic Complexes by X-Ray Diffraction. Inorganic Chemistry, 2011, 50, 10974-10984.	1.9	19
101	Enamine-Mediated Addition of Aldehydes to Cyclic Enones. Advanced Synthesis and Catalysis, 2011, 353, 2648-2652.	2.1	13
102	Crystal Structures and Physical Properties of Three New Manganese-Based Coordination Polymers with <i>p</i> -Biphenyldicarboxylic Acid Linkers. European Journal of Inorganic Chemistry, 2011, 2011, 549-555.	1.0	6
103	Practical Synthesis of \hat{I}^2 -Carbonyl Phenyltetrazolesulfones and Investigations of Their Reactivities in Organocatalysis. European Journal of Organic Chemistry, 2011, 2011, 47-52.	1.2	31
104	Taking Advantage of the Ambivalent Reactivity of Ynamides in Gold Catalysis: A Rare Case of Alkyne Dimerization. Angewandte Chemie - International Edition, 2011, 50, 5090-5094.	7.2	105
105	<i>trans</i> -Dibromidobis(1-ethyl-3-methylimidazol-2-ylidene)palladium(II). Acta Crystallographica Section E: Structure Reports Online, 2011, 67, m1205-m1205.	0.2	1
106	In Situ Generated Bulky Palladium Hydride Complexes as Catalysts for the Efficient Isomerization of Olefins. Selective Transformation of Terminal Alkenes to 2-Alkenes. Journal of the American Chemical Society, 2010, 132, 7998-8009.	6.6	196
107	Photomagnetic Switching of Heterometallic Complexes $[M(dmf)_4(H_2O)_3(\hat{I}^2CN)Fe(CN)_5] \cdot H_2O$ ($M=Nd, Tj$) $ETQq1$ 1 0 72 Journal, 2010, 16, 7215-7223.	1.7	24
108	Multicomponent asymmetric reactions mediated by proline lithium salt. Organic and Biomolecular Chemistry, 2010, 8, 980.	1.5	26

#	ARTICLE	IF	CITATIONS
109	Synthesis, Crystal Structure, Atomic Hirshfeld Surfaces, and Physical Properties of Hexagonal CeMnNi ₄ . <i>Inorganic Chemistry</i> , 2010, 49, 9343-9349.	1.9	46
110	Charge Density Methods in Hydrogen Bond Studies. <i>Structure and Bonding</i> , 2010, , 53-74.	1.0	10
111	Characterization of a non-nuclear attractor in a dimeric magnesium(I) compound. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, s93-s93.	0.3	0
112	Photomagnetic Switching of the Complex [Nd(dmf) ₄ (H ₂ O) ₃ (½CN)Fe(CN) ₅]·2H ₂ O Analyzed by Single-Crystal X-Ray Diffraction. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 2780-2783.	7.2	32
113	Experimental and theoretical charge-density study of a tetranuclear cobalt carbonyl complex. <i>Acta Crystallographica Section B: Structural Science</i> , 2009, 65, 715-723.	1.8	20
114	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
115	Fast Preparation and Characterization of Quarternary Thermoelectric Clathrates. <i>Chemistry of Materials</i> , 2009, 21, 122-127.	3.2	27
116	Experimental Electron Density Study of the Mg ⁺ Mg Bonding Character in a Magnesium(I) Dimer. <i>Journal of the American Chemical Society</i> , 2009, 131, 4208-4209.	6.6	63
117	Experimental charge density in an oxidized trinuclear iron complex using 15 K synchrotron and 100 K conventional single-crystal X-ray diffraction. <i>Dalton Transactions</i> , 2009, , 664-671.	1.6	10
118	Helium cryostat synchrotron charge densities determined using a large CCD detector – the upgraded beamline D3 at DESY. <i>Journal of Applied Crystallography</i> , 2008, 41, 846-853.	1.9	21
119	Organocatalytic Asymmetric Synthesis of Versatile β -Lactams. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 4687-4690.	7.2	41
120	Organocatalytic Asymmetric Conjugate Addition to Allenic Esters and Ketones. <i>Journal of the American Chemical Society</i> , 2008, 130, 4897-4905.	6.6	101
121	Organocatalytic asymmetric vinylogous addition to quinones – formation of optically active \pm -aryl ketones. <i>Chemical Communications</i> , 2008, , 632-634.	2.2	74
122	Synchrotron X-ray Charge Density Study of Coordination Polymer Co ₃ (C ₈ H ₄ O ₄) ₄ (C ₄ H ₁₂ N ₂) ₄ (C ₂ H ₄) ₂ at 16 K. <i>Journal of the American Chemical Society</i> , 2008, 130, 7988-7996.	6.6	24
123	Experimental and Theoretical Charge Density Study of Chemical Bonding in a Co Dimer Complex. <i>Journal of the American Chemical Society</i> , 2008, 130, 3834-3843.	6.6	78
124	Tetrakis(½-pivalato-½O ²⁻)bis[(2-methylpyridine-½N)iron(II)](Fe ⁺ Fe). <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2008, 64, m497-m497.	0.2	5
125	Experimental electron density study of a complex between copper(ii) and the antibacterial quinolone family member ciprofloxacin. <i>Dalton Transactions</i> , 2007, , 2171.	1.6	27
126	Electronic Structure of the Alkyne-Bridged Dicobalt Hexacarbonyl Complex Co ₂ (½-C ₂ H ₂ (CO) ₆ :½ Evidence for Singlet Diradical Character and Implications for Metal ⁺ Metal Bonding. <i>Inorganic Chemistry</i> , 2007, 46, 6291-6298.	1.9	29

#	ARTICLE	IF	CITATIONS
127	Short Strong Hydrogen Bonds in 2-Acetyl-1,8-dihydroxy-3,6-dimethylnaphthalene: An Outlier to Current Hydrogen Bonding Theory?. <i>Journal of Physical Chemistry A</i> , 2007, 111, 345-351.	1.1	34
128	Organocatalytic Asymmetric Direct $\hat{\text{I}}^2$ -Alkynylation of Cyclic $\hat{\text{I}}^2$ -Ketoesters. <i>Journal of the American Chemical Society</i> , 2007, 129, 441-449.	6.6	153
129	Experimental and Theoretical Charge Density Distribution in Two Ternary Cobalt(III) Complexes of Aromatic Amino Acids. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10123-10133.	1.1	19
130	Sml2-Promoted Radical Addition Reactions with N-(2-Indolylacetyl)oxazolidinones: Synthesis of Bisindole Compounds. <i>Journal of Organic Chemistry</i> , 2007, 72, 4181-4188.	1.7	19
131	Organocatalytic asymmetric $\hat{\text{I}}^2$ -Michael reaction of $\hat{\text{I}}^2$ -ketoesters. <i>Chemical Communications</i> , 2007, , 3921.	2.2	41
132	Synchrotron X-ray Charge Density Study of Coordination Polymer [Mn(HCOO) ₂ (H ₂ O) ₂]. <i>Chemistry - A European Journal</i> , 2007, 13, 9775-9790.	1.7	38
133	Asymmetric Organocatalytic $\hat{\text{I}}^2$ -Arylation of Aldehydes. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 5520-5523.	7.2	174
134	Cover Picture: Organocatalytic Highly Enantioselective $\hat{\text{I}}^2$ -Arylation of $\hat{\text{I}}^2$ -Ketoesters / Asymmetric Organocatalytic $\hat{\text{I}}^2$ -Arylation of Aldehydes (Angew. Chem. Int. Ed. 29/2007). <i>Angewandte Chemie - International Edition</i> , 2007, 46, 5449-5449.	7.2	2
135	Crystal Structures of Thermoelectric n-and p-type Ba ₈ Ca ₁₆ Ge ₃₀ Studied by Single Crystal, Multitemperature, Neutron Diffraction, Conventional X-ray Diffraction and Resonant Synchrotron X-ray Diffraction. <i>Journal of the American Chemical Society</i> , 2006, 128, 15657-15665.	6.6	167
136	Hexaaqua-1 $\hat{\text{I}}^3$ O ₃ $\hat{\text{I}}^3$ O-tri- $\hat{\text{I}}^4$ -cyano-1:2 $\hat{\text{I}}^2$ N:C;2:3 $\hat{\text{I}}^2$ C:N;3:4 $\hat{\text{I}}^2$ N:C-nonacyano-2 $\hat{\text{I}}^4$ C,4 $\hat{\text{I}}^5$ C-pentakis(N,N-dimethylacetamide)-1 $\hat{\text{I}}^3$ O ₃ $\hat{\text{I}}^2$ O-diiron(III)diytterbium(III) dihydrate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2006, 62, m793-m795.	0.2	0
137	Triaquatetrakis(dimethylacetamide- $\hat{\text{I}}^2$ O)gadolinium(III) hexacyanoferrate(III) dihydrate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2006, 62, m989-m991.	0.2	3
138	An Eu-based metal-organic framework: poly[[tris($\hat{\text{I}}^4$ -benzene-1,4-dicarboxylato)bis($\hat{\text{I}}^4$ -N,N-diethylformamide)dieuropium(III)] 0.7-hydrate]. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2006, 62, m3333-m3335.	0.2	3
139	Non-Biaryl Atropisomers in Organocatalysis. <i>Chemistry - A European Journal</i> , 2006, 12, 6039-6052.	1.7	206
140	Studies of a Molecular Hourglass: Synthesis and Magnetic Characterisation of a Cyclic Dodecanuclear {Cr ₁₀ Cu ₂ } Complex. <i>Chemistry - A European Journal</i> , 2006, 12, 8267-8275.	1.7	20
141	A family of heterometallic wheels containing potentially fourteen hundred siblings. <i>Chemical Communications</i> , 2005, , 1125-1127.	2.2	59
142	Tetraquatetrakis(dimethylacetamide- $\hat{\text{I}}^2$ O)neodymium(III) hexacyanoferrate(III) trihydrate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2005, 61, m268-m270.	0.2	5
143	Bis($\hat{\text{I}}^4$ -diacetylacetonato)bis[pyridinecopper(II)]. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2005, 61, m922-m924.	0.2	3
144	A gadolinium-based metal-organic framework, poly[[tris($\hat{\text{I}}^4$ -benzene-1,4-dicarboxylato)bis($\hat{\text{I}}^4$ -N,N-diethylformamide)digadolinium(III)] monohydrate]. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2005, 61, m1337-m1339.	0.2	4

#	ARTICLE	IF	CITATIONS
145	Diethanolaminiumcyclo-octa-1/42-fluoro-hexadeca-1/42-trimethylacetato-32O:O ²⁻ -heptachromium(III)nickel(II) ethyl acetate 0.5-solvate. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, m1525-m1527.	0.2	2
146	Poly[sesqui(1/44-biphenyl-4,4 ²⁻ -dicarboxylato-4O:O ²⁻ :O ²⁻ :O ²⁻ :O ²⁻ :O ²⁻)(diethylformamide-1O)gadolinium], Acta Crystallographica Section E: Structure Reports Online, 2005, 61, m2308-m2310.	0.2	4
147	Experimental charge density of a potential DHO synthetase inhibitor: dimethyl-trans-2-oxohexahydro-pyrimidine-4,6-dicarboxylate. Organic and Biomolecular Chemistry, 2005, 3, 441.	1.5	14
148	Influencing the nuclearity and constitution of heterometallic rings via templates. Chemical Communications, 2005, , 3649.	2.2	63
149	Testing theory beyond molecular structure: Electron density distributions of complex molecules. International Journal of Quantum Chemistry, 2004, 96, 23-31.	1.0	9
150	The experimental electron density in polymorphs A and B of the anti-ulcer drug famotidine. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 480-487.	0.3	52
151	The Magnetic Möbius Strip: Synthesis, Structure, and Magnetic Studies of Odd-Numbered Antiferromagnetically Coupled Wheels. Angewandte Chemie - International Edition, 2004, 43, 5196-5200.	7.2	120
152	Structural and Magnetic Investigations of the Mixed-Valence Fe ^{I,III} Two-Dimensional Layer Complex, [Fe ^{II} Fe ^{III} (HCOO) ₁₀ (C ₆ H ₇ N) ₆] _n . ChemPhysChem, 2004, 5, 1755-1761.	1.0	6
153	Experimental and Theoretical Charge Density Studies of Tetrafluorophthalonitrile and Tetrafluoroisophthalonitrile. Journal of Physical Chemistry B, 2004, 108, 3663-3672.	1.2	48
154	Synthesis and Characterization of Heterometallic {Cr ₇ M} Wheels. Angewandte Chemie, 2003, 115, 105-109.	1.6	54
155	Experimental and Theoretical Charge Density Study of the Neurotransmitter Taurine. Chemistry - A European Journal, 2003, 9, 1075-1084.	1.7	48
156	Horseshoes, Rings, and Distorted Rings: Studies of Cyclic Chromium-Fluoride Cages. Angewandte Chemie - International Edition, 2003, 42, 5978-5981.	7.2	72
157	Synthesis and Characterization of Heterometallic{Cr ₇ M} Wheels. Angewandte Chemie - International Edition, 2003, 42, 101-105.	7.2	205
158	Flavone. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o767-o768.	0.2	13
159	Influence of Crystal Effects on Molecular Charge Densities in a Study of 9-Ethynyl-9-fluorenol. Journal of Physical Chemistry A, 2003, 107, 11201-11208.	1.1	12
160	Experimental and Theoretical Electron Density Distribution and Magnetic Properties of the Butterfly-like Complex [Fe ₄ O ₂ (O ₂ CCMe ₃) ₈ (NC ₅ H ₄ Me) ₂]-2CH ₃ CN. Inorganic Chemistry, 2003, 42, 7593-7601.	1.9	37
161	Electron Density Distributions of Redox Active Mixed Valence Carboxylate Bridged Trinuclear Iron Complexes. Journal of the American Chemical Society, 2003, 125, 11088-11099.	6.6	66
162	The electron density in flavones I. Baicalein. New Journal of Chemistry, 2003, 27, 1392-1398.	1.4	20

#	ARTICLE	IF	CITATIONS
163	Experimental and theoretical charge distribution in (Z)-N-methyl-C-phenylnitrone. <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 1034-1040.	1.5	20
164	X-ray Charge density analysis of the hydrogen bonding motif in 1-(2-hydroxy-5-nitrophenyl)ethanone. Electronic supplementary information (ESI) available: multipole population coefficients and pseudoatom parameterization. See http://www.rsc.org/suppdata/ob/b2/b211683a/ . <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 1191-1198.	1.5	36
165	Multi-temperature X-ray diffraction, Mössbauer spectroscopy and magnetic susceptibility studies of a solvated mixed-valence trinuclear iron formate, $[\text{Fe}_3\text{O}(\text{HCO}_2)_6(\text{NC}_5\text{H}_4\text{CH}_3)_3] \cdot 1.3(\text{NC}_5\text{H}_4\text{CH}_3)$. <i>Dalton Transactions RSC</i> , 2002, , 2981.	2.3	19
166	Host-Guest Chemistry of the Chromium-Wheel Complex $[\text{Cr}_8\text{F}_8(\text{tBuCO}_2)_{16}]$: Prediction of Inclusion Capabilities by Using an Electrostatic Potential Distribution Determined by Modeling Synchrotron X-ray Structure Factors at 16 K. <i>Chemistry - A European Journal</i> , 2002, 8, 2775.	1.7	63
167	The Charge Density Distribution in a Model Compound of the Catalytic Triad in Serine Proteases. <i>Chemistry - A European Journal</i> , 2001, 7, 3756-3767.	1.7	71
168	Multi-Temperature Crystallographic Studies of Mixed-Valence Polynuclear Complexes; Valence Trapping Process in the Trinuclear Oxo-Bridged Iron Compound, $[\text{Fe}_3\text{O}(\text{O}_2\text{CC}(\text{CH}_3)_3)_6(\text{C}_5\text{H}_5\text{N})_3]$. <i>Journal of the American Chemical Society</i> , 2000, 122, 11370-11379.	6.6	73
169	Strong N-H...O Hydrogen Bonding in a Model Compound of the Catalytic Triad in Serine Proteases. <i>Angewandte Chemie - International Edition</i> , 1999, 38, 1239-1242.	7.2	62