

Sonja Herres-Pawlis

List of Publications by Year in descending order

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205
papers

4,392
citations

109321

35
h-index

168389

53
g-index

231
all docs

231
docs citations

231
times ranked

2784
citing authors

#	ARTICLE	IF	CITATIONS
1	Geometrical benchmarking and analysis of redox potentials of copper(II) guanidinequinoline complexes: Comparison of semiempirical tight-binding and DFT methods and the challenge of describing the entatic state (part III). <i>Journal of Computational Chemistry</i> , 2023, 44, 319-328.	3.3	1
2	Simple Zn(II) complexes for the production and degradation of polyesters. <i>RSC Advances</i> , 2022, 12, 1416-1424.	3.6	13
3	Master of Chaos and Order: Opposite Microstructures of PCL- <i>g</i> -PGA- <i>g</i> -PLA Accessible by a Single Catalyst**. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	11
4	Kontrolle über Chaos und Ordnung: Gegensätzliche Mikrostrukturen von PCL- <i>g</i> -PGA- <i>g</i> -PLA durch einen einzigen Katalysator zugänglich**. <i>Angewandte Chemie</i> , 2022, 134, e202112853.	2.0	2
5	Innentitelbild: Kontrolle über Chaos und Ordnung: Gegensätzliche Mikrostrukturen von PCL- <i>g</i> -PGA- <i>g</i> -PLA durch einen einzigen Katalysator zugänglich (Angew. Chem. 11/2022). <i>Angewandte Chemie</i> , 2022, 134, .	2.0	0
6	Guanidine Carboxy Zinc Complexes for the Chemical Recycling of Renewable Polyesters. <i>ChemPlusChem</i> , 2022, 87, e202200029.	2.8	11
7	Sharing is Caring: Guidelines for Sharing in the Electronic Laboratory Notebook (ELN) Chemotion as applied by a Synthesis-oriented Working Group**. <i>Chemistry Methods</i> , 2022, 2, .	3.8	5
8	Manipulating electron transfer – the influence of substituents on novel copper guanidine quinolinyl complexes. <i>Chemical Science</i> , 2022, 13, 8274-8288.	7.4	6
9	Determination of Kinetics for Reactive Bubbly Flows Using SuperFocus Mixers. <i>Fluid Mechanics and Its Applications</i> , 2021, , 479-506.	0.2	0
10	Visualization and Quantitative Analysis of Consecutive Reactions in Taylor Bubble Flows. <i>Fluid Mechanics and Its Applications</i> , 2021, , 507-543.	0.2	2
11	Control of the Formation and Reaction of Copper-Oxygen Adduct Complexes in Multiphase Streams. <i>Fluid Mechanics and Its Applications</i> , 2021, , 7-38.	0.2	1
12	Chemical Reactions at Freely Ascending Single Bubbles. <i>Fluid Mechanics and Its Applications</i> , 2021, , 545-581.	0.2	0
13	Shot noise limited soft x-ray absorption spectroscopy in solution at a SASE-FEL using a transmission grating beam splitter. <i>Structural Dynamics</i> , 2021, 8, 014303.	2.3	7
14	Room temperature stable multivalent: highly reactive and versatile copper guanidine complexes in oxygenation reactions. <i>Journal of Biological Inorganic Chemistry</i> , 2021, 26, 249-263.	2.6	9
15	Increasing the Activity of Copper Guanidine Quinoline Catalysts: Substitution at the Quinoline Backbone Leads to Highly Active Complexes for ATRP. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2021, 647, 832-842.	1.2	6
16	Chemogenetic Evolution of a Peroxidase-like Artificial Metalloenzyme. <i>ACS Catalysis</i> , 2021, 11, 5079-5087.	11.2	21
17	In celebration of the 70 th birthday of Peter Kläfers. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2021, 647, 801-802.	1.2	1
18	Small-Scale Phenomena in Reactive Bubbly Flows: Experiments, Numerical Modeling, and Applications. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2021, 12, 625-643.	6.8	9

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19	Nachtaktiv: Eisen-Guanidin-Komplex katalysiert ROP auf der schlafenden Seite der ATRP. Angewandte Chemie, 2021, 133, 21965-21971.	2.0	6
20	The Green toxicology approach: Insight towards the eco-toxicologically safe development of benign catalysts. Journal of Hazardous Materials, 2021, 416, 125889.	12.4	16
21	Active in Sleep: Iron Guanidine Catalyst Performs ROP on Dormant Side of ATRP. Angewandte Chemie - International Edition, 2021, 60, 21795-21800.	13.8	18
22	Influence of the amine donor on hybrid guanidine-stabilized Bis(1/4-oxido) dicopper(III) complexes and their tyrosinase-like oxygenation activity towards polycyclic aromatic alcohols. Journal of Inorganic Biochemistry, 2021, 224, 111541.	3.5	7
23	A new generation of terminal copper nitrenes and their application in aromatic C-H amination reactions. Dalton Transactions, 2021, 50, 6444-6462.	3.3	10
24	Chiral bis(pyrazolyl)methane copper(I) complexes and their application in nitrene transfer reactions. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2021, .	0.7	2
25	Undiscovered Potential: Ge Catalysts for Lactide Polymerization. Chemistry - A European Journal, 2020, 26, 212-221.	3.3	34
26	Mononuclear zinc(II) Schiff base complexes as catalysts for the ring-opening polymerization of lactide. European Polymer Journal, 2020, 122, 109302.	5.4	33
27	Interplay of Spin Crossover and Coordination-Induced Spin State Switch for Iron Bis(pyrazolyl)methanes in Solution. Inorganic Chemistry, 2020, 59, 15343-15354.	4.0	9
28	Kinetic Investigation of the Reaction of Dioxygen with the Copper(I) Complex [Cu(Pim i Pr2)(CH 3) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Chemistry, 2020, 2020, 3143-3150.	2.0	9
29	Innen-1/4-cktitelbild: Mit der n-Ächsten Generation von Zink-ÄBisguanidin-ÄPolymerisationskatalysatoren zu hochkristallinen, biologisch abbaubaren Polyestern (Angew. Chem. 48/2020). Angewandte Chemie, 2020, 132, 21971-21971.	2.0	0
30	Mit der n-Ächsten Generation von Zink-ÄBisguanidin-ÄPolymerisationskatalysatoren zu hochkristallinen, biologisch abbaubaren Polyestern. Angewandte Chemie, 2020, 132, 21962-21968.	2.0	17
31	Next Generation of Zinc Bisguanidine Polymerization Catalysts towards Highly Crystalline, Biodegradable Polyesters. Angewandte Chemie - International Edition, 2020, 59, 21778-21784.	13.8	63
32	Frontispiece: Exceptional Substrate Diversity in Oxygenation Reactions Catalyzed by a Bis(1/4-Äoxo) Copper Complex. Chemistry - A European Journal, 2020, 26, .	3.3	0
33	Forschungsdatenmanagement -Zeit f-Ä1/4r den Abschied vom analogen Laborbuch. Nachrichten Aus Der Chemie, 2020, 68, 20-23.	0.0	2
34	Research Data in Chemistry -Ä- Results of the first NFDI4Chem Community Survey. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 1748-1757.	1.2	11
35	Robust Guanidine Metal Catalysts for the Ring-ÄOpening Polymerization of Lactide under Industrially Relevant Conditions. ChemPlusChem, 2020, 85, 1044-1052.	2.8	38
36	Exceptional Substrate Diversity in Oxygenation Reactions Catalyzed by a Bis(1/4-Äoxo) Copper Complex. Chemistry - A European Journal, 2020, 26, 7556-7562.	3.3	20

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37	New stereocontrol on the block. <i>Nature Chemistry</i> , 2020, 12, 107-109.	13.6	3
38	Enhanced catalytic activity of copper complexes in microgels for aerobic oxidation of benzyl alcohols. <i>Chemical Communications</i> , 2020, 56, 5601-5604.	4.1	10
39	Catalytically Active Iron(IV)oxo Species Based on a Bis(pyridinyl)phenanthrolinylmethane. <i>Israel Journal of Chemistry</i> , 2020, 60, 987-998.	2.3	4
40	Tyrosinase Models: Synthesis, Spectroscopy, Theory and Catalysis. , 2019, , .		6
41	Towards New Robust Zn(II) Complexes for the Ring-Opening Polymerization of Lactide Under Industrially Relevant Conditions. <i>ChemistryOpen</i> , 2019, 8, 1020-1026.	1.9	17
42	NFDI4Chem: Shaping a Digital and Cultural Change in Chemistry. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 10766-10768.	13.8	19
43	How coherent structures dominate the residence time in a bubble wake: An experimental example. <i>Chemical Engineering Science</i> , 2019, 207, 317-326.	3.8	16
44	Using a bio-inspired copper complex to investigate reactive mass transfer around an oxygen bubble rising freely in a thin-gap cell. <i>Chemical Engineering Science</i> , 2019, 207, 1256-1269.	3.8	13
45	One-Pot Two-Step Chemoenzymatic Cascade for the Synthesis of a Bis-benzofuran Derivative. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 6341-6346.	2.4	17
46	Heterolepic λ^2 -Ketoiminate Zinc Phenoxide Complexes as Efficient Catalysts for the Ring Opening Polymerization of Lactide. <i>ChemistryOpen</i> , 2019, 8, 951-960.	1.9	20
47	Tuning a robust system: N,O zinc guanidine catalysts for the ROP of lactide. <i>Dalton Transactions</i> , 2019, 48, 6071-6082.	3.3	31
48	Dual oxidase/oxygenase reactivity and resonance Raman spectra of {Cu3O2} moiety with perfluoro-t-butoxide ligands. <i>Dalton Transactions</i> , 2019, 48, 6899-6909.	3.3	8
49	New Kids in Lactide Polymerization: Highly Active and Robust Iron Guanidine Complexes as Superior Catalysts. <i>ChemSusChem</i> , 2019, 12, 2161-2165.	6.8	53
50	Stepwise Growth of Ruthenium Terpyridine Complexes on Au Surfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6537-6548.	3.1	8
51	NFDI4Chem: Digitalen und kulturellen Wandel in der Chemie gestalten. <i>Angewandte Chemie</i> , 2019, 131, 10880-10882.	2.0	7
52	The MASi repository service – Comprehensive, metadata-driven and multi-community research data management. <i>Future Generation Computer Systems</i> , 2019, 94, 879-894.	7.5	12
53	Renaissance of the entatic state principle. <i>Coordination Chemistry Reviews</i> , 2018, 365, 103-121.	18.8	45
54	Reaction Systems for Bubbly Flows. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 2101-2124.	2.0	17

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55	Reactivity of a Nâ†Sn Coordinated Distannyne: Reduction and Hydrogen Abstraction. European Journal of Inorganic Chemistry, 2018, 2018, 2038-2044. Rational Syntheses and Serendipity: Complexes	2.0	12
56	[LSnPtCl₂(SMe₂)]₂, [LSnPtCl(SMe₂)]₂SnCl₂, [(LSn₃(PtCl₂)(PtClSnCl){LSn(Cl)OH}], and [O(SnCl)₂(SnL)₂] with L=MeN(CH₂CMe₂O)₂. Chemistry - A European Journal, 2018, 24, 5551	3.3	5
57	Transferring the entatic-state principle to copper photochemistry. Nature Chemistry, 2018, 10, 355-362.	13.6	59
58	Next Generation of Guanidine Quinoline Copper Complexes for Highly Controlled ATRP: Influence of Backbone Substitution on Redox Chemistry and Solubility. European Journal of Inorganic Chemistry, 2018, 2018, 3164-3175.	2.0	14
59	Gathering requirements for advancing simulations in HPC infrastructures via science gateways. Future Generation Computer Systems, 2018, 82, 544-554.	7.5	7
60	A cryostat for low temperature resonance Raman measurements on operando oxygenated bioinorganic model complexes. Inorganica Chimica Acta, 2018, 481, 176-180.	2.4	6
61	The Curious Case of a Phenylated Guanidinoquinoline Ligand: Synthesis, Complexes and ATRP Properties of DMEG6phqu. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2018, 644, 1317-1328.	1.2	4
62	Fluorescent Bis(guanidine) Copper Complexes as Precursors for Hydroxylation Catalysis. Inorganics, 2018, 6, 114.	2.7	8
63	Influence of Functionalized Substituents on the Electronâ€transfer Abilities of Copper Guanidinoquinoline Complexes. European Journal of Inorganic Chemistry, 2018, 2018, 4997-5006.	2.0	10
64	MaÃgeschneiderte terminale Kupfernitrene fÃ¼r katalytische Câ€Aminierungen. Angewandte Chemie, 2018, 130, 9294-9299.	2.0	7
65	Imaging of copper oxygenation reactions in a bubble flow. Magnetic Resonance in Chemistry, 2018, 56, 826-830.	1.9	7
66	Synthesis, Structures, and Catalytic Activity of Homoâ€and Heteroleptic Ketoiminate Zinc Complexes in Lactide Polymerization. European Journal of Inorganic Chemistry, 2018, 2018, 4014-4021.	2.0	17
67	Designed To React: Terminal Copper Nitrenes and Their Application in Catalytic Câ”H Aminations. Angewandte Chemie - International Edition, 2018, 57, 9154-9159.	13.8	35
68	A Study on Fe^{II}, Zn^{II} and Cu^{II} Complexes with Novel Tridentate Bis(pyrazolyl)methane Ligands. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2018, 644, 1576-1592.	1.2	4
69	Metadata Management in the MoSGrid Science Gateway - Evaluation and the Expansion of Quantum Chemistry Support. Journal of Grid Computing, 2017, 15, 41-53.	3.9	4
70	On the Way to a Trisanionic {Cu 3 O 2 } Core for Oxidase Catalysis: Evidence of an Asymmetric Trinuclear Precursor Stabilized by Perfluoropinacolate Ligands. Chemistry - A European Journal, 2017, 23, 8212-8224.	3.3	12
71	Atmospheric pressure photo-ionization mass spectrometry for the detection of labile end groups in poly(styrene). European Polymer Journal, 2017, 90, 209-219.	5.4	1
72	Copper(I) Complexes with Thiourea Derivatives as Ligands: Revealing Secrets of Their Bonding Scheme. European Journal of Inorganic Chemistry, 2017, 2017, 1266-1279.	2.0	18

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73	[Cu ₆ (NGuaS) ₆] ²⁺ and its oxidized and reduced derivatives: Confining electrons on a torus. <i>Journal of Computational Chemistry</i> , 2017, 38, 1752-1761.	3.3	1
74	Record Broken: A Copper Peroxide Complex with Enhanced Stability and Faster Hydroxylation Catalysis. <i>Chemistry - A European Journal</i> , 2017, 23, 12171-12183.	3.3	32
75	Oxygen Activation by Copper Complexes with an Aromatic Bis(guanidine) Ligand. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 3350-3359.	2.0	19
76	Iron(II) and Zinc(II) Complexes with Tetradentate Bis(pyrazolyl)methane Ligands as Catalysts for the Ring-Opening Polymerisation of <i>rac</i> -Lactide. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 1341-1354.	2.0	34
77	Direct Electrochemical Synthesis of an Unusual Complex Salt: Almost Structural Identity - Different Charge. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2017, 643, 266-275.	1.2	3
78	Reactive Bubbly Flows. <i>Chemical Engineering and Technology</i> , 2017, 40, 1384-1384.	1.5	0
79	Copper Guanidinoquinoline Complexes as Entatic State Models of Electron-Transfer Proteins. <i>Chemistry - A European Journal</i> , 2017, 23, 15738-15745.	3.3	21
80	Frontispiece: Record Broken: A Copper Peroxide Complex with Enhanced Stability and Faster Hydroxylation Catalysis. <i>Chemistry - A European Journal</i> , 2017, 23, .	3.3	0
81	Relativistic effects at the Cu ₂ O ₂ core – a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26880-26889.	2.8	8
82	Test System for the Investigation of Reactive Taylor Bubbles. <i>Chemical Engineering and Technology</i> , 2017, 40, 1494-1501.	1.5	20
83	Detection of Copper Bisguanidine NO Adducts by UV-Vis Spectroscopy and a SuperFocus Mixer. <i>Chemical Engineering and Technology</i> , 2017, 40, 1475-1483.	1.5	2
84	Highly Active N,O Zinc Guanidine Catalysts for the Ring-Opening Polymerization of Lactide. <i>ChemSusChem</i> , 2017, 10, 3547-3556.	6.8	60
85	ZnII Chlorido Complexes with Aliphatic, Chiral Bisguanidine Ligands as Catalysts in the Ring-Opening Polymerisation of <i>rac</i> -Lactide Using FT-IR Spectroscopy in Bulk. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 5557-5570.	2.0	22
86	Reactivity of Zinc Halide Complexes Containing Camphor-Derived Guanidine Ligands with Technical <i>rac</i> -Lactide. <i>Inorganics</i> , 2017, 5, 85.	2.7	12
87	Addressing Hydrogen Bonding Motifs by Suited Substitution of Thioureas. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2016, 642, 660-669.	1.2	5
88	Multi-level meta-workflows: new concept for regularly occurring tasks in quantum chemistry. <i>Journal of Cheminformatics</i> , 2016, 8, 58.	6.1	3
89	Homolytic, Heterolytic, Mesolytic – As You Like It: Steering the Cleavage of a HC(sp ³)–C(sp ³)H Bond in Bis(1 <i>H</i> -1-benzazaborole) Derivatives. <i>Chemistry - A European Journal</i> , 2016, 22, 15340-15349.	3.3	7
90	Decay kinetics of sensitive bioinorganic species in a SuperFocus mixer at ambient conditions. <i>Reaction Chemistry and Engineering</i> , 2016, 1, 485-493.	3.7	23

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91	Optical response of the Cu ₂ S ₂ diamond core in (NGuaS) ₂ Cl ₂ . Journal of Computational Chemistry, 2016, 37, 2181-2192.	3.3	10
92	A Comprehensive Study of Copper Guanidine Quinoline Complexes: Predicting the Activity of Catalysts in ATRP with DFT. Chemistry - A European Journal, 2016, 22, 13550-13562.	3.3	28
93	Implications of Guanidine Substitution on Copper Complexes as Entatic-State Models. European Journal of Inorganic Chemistry, 2016, 2016, 4731-4743.	2.0	36
94	Hand in Hand: Experimental and Theoretical Investigations into the Reactions of Copper(I) Mono- and Bis(guanidine) Complexes with Dioxygen. European Journal of Inorganic Chemistry, 2016, 2016, 4744-4751.	2.0	27
95	Implications of Guanidine Substitution on Copper Complexes as Entatic-State Models. European Journal of Inorganic Chemistry, 2016, 2016, 4722-4722.	2.0	1
96	Using Science Gateways for Bridging the Differences between Research Infrastructures. Journal of Grid Computing, 2016, 14, 545-557.	3.9	12
97	Zinc Chloride Complexes with Aliphatic and Aromatic Guanidine Hybrid Ligands and Their Activity in the Ring-Opening Polymerisation of ϵ -lactide. European Journal of Inorganic Chemistry, 2016, 2016, 4974-4987.	2.0	29
98	Copper(I) Thiolate Heteroadamantane Cage Structures with Relevance to Metalloproteins. European Journal of Inorganic Chemistry, 2016, 2016, 3744-3755.	2.0	5
99	Experimental and Theoretical High-Energy-Resolution X-ray Absorption Spectroscopy: Implications for the Investigation of the Entatic State. Inorganic Chemistry, 2016, 55, 11694-11706.	4.0	25
100	Insights into Copper-Poly(pyrazolyl)methane-Catalyzed Reactions for Organic Transformations. Synthesis, 2016, 49, 225-236.	2.3	1
101	Jet delivery system for Raman scattering on bio-inorganic compounds. Applied Physics Letters, 2016, 109, 213502.	3.3	2
102	Donor-driven conformational flexibility in a real-life catalytic dicopper(II) peroxo complex. Physical Chemistry Chemical Physics, 2016, 18, 6430-6440.	2.8	21
103	Efficient Biomimetic Hydroxylation Catalysis with a Bis(pyrazolyl)imidazolylmethane Copper Peroxide Complex. Chemistry - A European Journal, 2015, 21, 17639-17649.	3.3	41
104	Quantum chemical meta-workflows in MoSGrid. Concurrency Computation Practice and Experience, 2015, 27, 344-357.	2.2	19
105	Less Is More: Three-Coordinate C,N-Chelated Distannynes and Digermynes. Chemistry - A European Journal, 2015, 21, 7820-7829.	3.3	36
106	Bis(pyrazolyl)methane Copper Complexes as Robust and Efficient Catalysts for Sonogashira Couplings. European Journal of Organic Chemistry, 2015, 2015, 7475-7483.	2.4	16
107	Formation of Hybrid Guanidine-Stabilized Bis(μ -oxo)dicopper Cores in Solution: Electronic and Steric Perturbations. European Journal of Inorganic Chemistry, 2015, 2015, 5426-5436.	2.0	30
108	The Cu ₂ O ₂ torture track for a real-life system: [Cu ₂ (btmgp) ₂ O ₂] ₂ +oxo and peroxo species in density functional calculations. Journal of Computational Chemistry, 2015, 36, 1672-1685.	3.3	33

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109	Zinc Complexes with Guanidine-Pyridine Hybrid Ligands: Anion Effect and Catalytic Activity. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2015, 641, 2147-2156.	1.2	9
110	Transition Metal Complexes Containing C_2 -Symmetric Bis(imidazolin-2-ylidene) Ligands Derived from a 1-Alkyl-3-arylimidazolin-2-ylidene. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2015, 641, 2204-2214.	1.2	10
111	Managing Complexity in Distributed Data Life Cycles Enhancing Scientific Discovery. , 2015, , .		10
112	Multi-layer Meta-metaworkflows for the Evaluation of Solvent and Dispersion Effects in Transition Metal Systems Using the MoSGrid Science Gateways. , 2015, , .		0
113	Challenges and Modifications for Creating a MoSGrid Science Gateway for US and European Infrastructures. , 2015, , .		3
114	Science gateways - leveraging modeling and simulations in HPC infrastructures via increased usability. , 2015, , .		0
115	Low Temperature Syntheses and Reactivity of Cu_2O_2 Active-Site Models. Accounts of Chemical Research, 2015, 48, 2424-2433.	15.6	105
116	Guanidine Metal Complexes for Bioinorganic Chemistry and Polymerisation Catalysis. Topics in Heterocyclic Chemistry, 2015, , 95-164.	0.2	13
117	Biomimetic Hydroxylation Catalysis Through Self-Assembly of a Bis(pyrazolyl)methane Copper-Peroxo Complex. European Journal of Inorganic Chemistry, 2015, 2015, 494-502.	2.0	27
118	Antimony(III) and bismuth(III) amides containing pendant N-donor groups - a combined experimental and theoretical study. Dalton Transactions, 2015, 44, 395-400.	3.3	10
119	Catching an Entatic State - A Pair of Copper Complexes. Angewandte Chemie - International Edition, 2014, 53, 299-304.	13.8	65
120	Molecular Simulation Grid (MosGrid): A Science Gateway Tailored to the Molecular Simulation Community. , 2014, , 151-165.		4
121	New Guanidine-Pyridine Copper Complexes and Their Application in ATRP. Polymers, 2014, 6, 995-1007.	4.5	32
122	Performance Studies on Distributed Virtual Screening. BioMed Research International, 2014, 2014, 1-7.	1.9	8
123	Standards-based metadata management for molecular simulations. Concurrency Computation Practice and Experience, 2014, 26, 1744-1759.	2.2	26
124	Meta-Metaworkflows for Combining Quantum Chemistry and Molecular Dynamics in the MoSGrid Science Gateway. , 2014, , .		6
125	Geometrical and optical benchmarking of copper(II) guanidine-quinoline complexes: Insights from TD-DFT and many-body perturbation theory (part II). Journal of Computational Chemistry, 2014, 35, 2146-2161.	3.3	31
126	Neue aromatische Bisguanidin-Kupfer-Komplexe und ihre Anwendung in der ATRP / New Aromatic Bisguanidine Copper Complexes and Their Application in ATRP. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2014, 69, 589-595.	0.7	15

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127	N-Donor Competition in Iron Bis(chelate) Bis(pyrazolyl)pyridinylmethane Complexes. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2014, 69, 1206-1214.	0.7	7
128	Geometrical and optical benchmarking of copper guanidine-quinoline complexes: Insights from TD-DFT and many-body perturbation theory. Journal of Computational Chemistry, 2014, 35, 1-17.	3.3	62
129	Insights into Different Donor Abilities in Bis(pyrazolyl)pyridinylmethane Transition Metal Complexes. European Journal of Inorganic Chemistry, 2014, 2014, 2296-2306.	2.0	15
130	Insights into the influence of dispersion correction in the theoretical treatment of guanidine-quinoline copper(I) complexes. Journal of Computational Chemistry, 2014, 35, 1943-1950.	3.3	55
131	Expansion of Quantum Chemical Metadata for Workflows in the MoSGrid Science Gateway. , 2014, , . Syntheses and Molecular Structures of		1
132	[RSn{W(CO) ₃ Cp} ₂][W(CO) ₃ Cp], [RSn{W(CO) ₃ Cp}Cl ₂], and [RSn{W(CO) ₃ Cp}Cr(CO) ₅] (R = [4- <i>t</i> -Bu-2,6-{P(O)(OR) ₂ } ₂ C ₆ H ₂], R ² = Et,) Tj	2.3	11
133	4433-4441. Hiking on the potential energy surface of a functional tyrosinase model - implications of singlet, broken-symmetry and triplet description. Chemical Communications, 2014, 50, 403-405.	4.1	27
134	The MoSGrid Science Gateway - A Complete Solution for Molecular Simulations. Journal of Chemical Theory and Computation, 2014, 10, 2232-2245.	5.3	58
135	A Conformationally Flexible Dinuclear Pt ^{II} Complex with Differential Behavior of its Two States toward Quadruplex DNA. Chemistry - A European Journal, 2013, 19, 11429-11438.	3.3	13
136	Simple is best: Diamine zinc complexes as unexpected catalysts in lactide polymerisation. Polyhedron, 2013, 49, 151-157.	2.2	19
137	Oxalic Amidines - Protonation Studies and Activity in Lactide Polymerisation. European Journal of Inorganic Chemistry, 2013, 2013, 99-108.	2.0	2
138	Insights into the Intramolecular Donor Stabilisation of Organostannylene Palladium and Platinum Complexes: Syntheses, Structures and DFT Calculations. Chemistry - A European Journal, 2013, 19, 6695-6708.	3.3	22
139	Catalytic Phenol Hydroxylation with Dioxygen: Extension of the Tyrosinase Mechanism beyond the Protein Matrix. Angewandte Chemie - International Edition, 2013, 52, 5398-5401.	13.8	122
140	Synergistic Empirical and Theoretical Study on the Stereoselective Mechanism for the Aluminum Salalen Complex Mediated Polymerization of Lactide. Chemistry - A European Journal, 2013, 19, 4712-4716.	3.3	44
141	Bis(μ ₂ -oxo and μ ₂ -peroxy dicopper complexes studied within (time-dependent) density-functional and many-body perturbation theory. Journal of Computational Chemistry, 2013, 34, 1035-1045.	3.3	29
142	User-friendly metaworkflows in quantum chemistry. , 2013, , .		4
143	Extending the Family of N-Heterocyclic Heavy Carbene Analogues: Synthesis and Crystal and Molecular Structures of MeN[CH ₂ C(O)N(R)] ₂ Sn (R = Me ₂ NCH ₂ CH ₂ , PhCH ₂ , Me ₃ CCH ₂). European Journal of Inorganic Chemistry, 2013, 2013, 5808-5808.	2.0	0
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