

Sonja Herres-Pawlis

List of Publications by Citations

Source: <https://exaly.com/author-pdf/4480647/sonja-herres-pawlis-publications-by-citations.pdf>

Version: 2024-04-10

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

198
papers

3,870
citations

33
h-index

51
g-index

231
ext. papers

4,406
ext. citations

4.2
avg, IF

5.55
L-index

#	Paper	IF	Citations
198	Phenolate hydroxylation in a bis(mu-oxo)dicopper(III) complex: lessons from the guanidine/amine series. <i>Journal of the American Chemical Society</i> , 2009 , 131, 1154-69	16.4	146
197	Lactide polymerisation with air-stable and highly active zinc complexes with guanidine-pyridine hybrid ligands. <i>Chemistry - A European Journal</i> , 2009 , 15, 2362-76	4.8	139
196	Catalytic phenol hydroxylation with dioxygen: extension of the tyrosinase mechanism beyond the protein matrix. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 5398-401	16.4	108
195	Lactide Polymerisation with Complexes of Neutral N-Donors I New Strategies for Robust Catalysts. <i>European Journal of Inorganic Chemistry</i> , 2012 , 2012, 765-774	2.3	98
194	Low temperature syntheses and reactivity of Cu ₂ O ₂ active-site models. <i>Accounts of Chemical Research</i> , 2015 , 48, 2424-33	24.3	94
193	Tuning of Copper(I) Dioxygen Reactivity by Bis(guanidine) Ligands. <i>European Journal of Inorganic Chemistry</i> , 2005 , 2005, 3815-3824	2.3	86
192	A Library of Peralkylated Bis-guanidine Ligands for Use in Biomimetic Coordination Chemistry. <i>European Journal of Organic Chemistry</i> , 2005 , 2005, 4879-4890	3.2	83
191	Molecular simulation grid. <i>Journal of Cheminformatics</i> , 2011 , 3,	8.6	78
190	Studies on the mechanism of the lactide polymerization with highly active zinc guanidine catalysts. <i>Journal of Cheminformatics</i> , 2011 , 3,	8.6	78
189	Dissecting the role of guanidine copper complexes in atom transfer radical polymerization by density functional theory. <i>Journal of Cheminformatics</i> , 2011 , 3,	8.6	78
188	Mechanistic studies on the ring-opening polymerisation of D,L-lactide with zinc guanidine complexes. <i>Journal of Cheminformatics</i> , 2010 , 2,	8.6	78
187	Mechanism of the living lactide polymerization mediated by robust zinc guanidine complexes. <i>Chemistry - A European Journal</i> , 2011 , 17, 4507-12	4.8	77
186	Hydroxylation of a methyl group: synthesis of [Cu ₂ (btmmO)2I] ⁺ and of [Cu ₂ (btmmO)2]^{2+} containing the novel ligand {bis(trimethylmethoxy)guanidino}propane (btmmO) by copper-assisted oxygen activation. <i>Inorganica Chimica Acta</i> , 2005 , 358, 1089-1095	2.7	68
185	[Bis(guanidine)]zinc Complexes and Their Application in Lactide Polymerisation. <i>European Journal of Inorganic Chemistry</i> , 2007 , 2007, 5645-5651	2.3	67
184	(Guanidine)copper complexes: structural variety and application in bioinorganic chemistry and catalysis. <i>Reviews in Inorganic Chemistry</i> , 2011 , 31, 83-108	2.4	57
183	New insights into the lactide polymerisation with neutral N-donor stabilised zinc complexes: Comparison of imidazolin-2-imine vs. guanidine complexes. <i>Journal of Molecular Catalysis A</i> , 2010 , 316, 139-145	54	
182	Catching an entatic state--a pair of copper complexes. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 299-304	16.4	53

181	Geometrical and optical benchmarking of copper guanidine-quinoline complexes: insights from TD-DFT and many-body perturbation theory. <i>Journal of Computational Chemistry</i> , 2014 , 35, 1-17	3.5	52
180	Synthesis and properties of guanidine-pyridine hybridligands and structural characterisation of their mono- and bis(chelated) cobalt complexes. <i>Inorganica Chimica Acta</i> , 2009 , 362, 1185-1193	2.7	47
179	The MoSGrid Science Gateway - A Complete Solution for Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2232-45	6.4	46
178	Highly Active N,O Zinc Guanidine Catalysts for the Ring-Opening Polymerization of Lactide. <i>ChemSusChem</i> , 2017 , 10, 3547-3556	8.3	46
177	Stabilisation of a highly reactive bis(mu-oxo)dicopper(III) species at room temperature by electronic and steric constraint of an unconventional nitrogen donor ligand. <i>Chemistry - A European Journal</i> , 2009 , 15, 8678-82	4.8	45
176	Transferring the entatic-state principle to copper photochemistry. <i>Nature Chemistry</i> , 2018 , 10, 355-362	17.6	43
175	Insights into the influence of dispersion correction in the theoretical treatment of guanidine-quinoline copper(I) complexes. <i>Journal of Computational Chemistry</i> , 2014 , 35, 1943-50	3.5	43
174	Außergewöhnliche Donoren und synthetische Vielfalt: Guanidine. <i>Nachrichten Aus Der Chemie</i> , 2009 , 57, 20-23	0.1	40
173	Synergistic empirical and theoretical study on the stereoselective mechanism for the aluminum salalen complex mediated polymerization of rac-lactide. <i>Chemistry - A European Journal</i> , 2013 , 19, 4712-6	4.8	39
172	Katalytische Phenolhydroxylierung mit Sauerstoff: Substratvielfalt jenseits der Proteinmatrix von Tyrosinase. <i>Angewandte Chemie</i> , 2013 , 125, 5508-5512	3.6	38
171	Den entatischen Zustand im Griff Ein Duo von Kupfer-Komplexen. <i>Angewandte Chemie</i> , 2014 , 126, 305-310	37	
170	Zinc Complexes with GuanidinePyridine Hybrid Ligands Guanidine Effect and Catalytic Activity. <i>European Journal of Inorganic Chemistry</i> , 2011 , 2011, 4441-4456	2.3	37
169	Intramolecularly coordinated organotin tellurides: stable or unstable?. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 3478-82	16.4	36
168	Efficient Biomimetic Hydroxylation Catalysis with a Bis(pyrazolyl)imidazolylmethane Copper Peroxide Complex. <i>Chemistry - A European Journal</i> , 2015 , 21, 17639-49	4.8	35
167	Bidentate guanidine ligands with ethylene spacer in copper-dioxygen chemistry: Structural characterization of bis[hydroxo] dicopper complexes. <i>Inorganica Chimica Acta</i> , 2011 , 374, 546-557	2.7	35
166	New Kids in Lactide Polymerization: Highly Active and Robust Iron Guanidine Complexes as Superior Catalysts. <i>ChemSusChem</i> , 2019 , 12, 2161-2165	8.3	33
165	Implications of Guanidine Substitution on Copper Complexes as Entatic-State Models. <i>European Journal of Inorganic Chemistry</i> , 2016 , 2016, 4731-4743	2.3	33
164	A Single Sign-On Infrastructure for Science Gateways on a Use Case for Structural Bioinformatics. <i>Journal of Grid Computing</i> , 2012 , 10, 769-790	4.2	32

163	Systematische Studie zu den Koordinationseigenschaften des Guanidin-Liganden N1,N2-Bis(1,3-dimethylimidazolidin-2-yliden)-ethan-1,2-diamin mit den Metallen Mn, Co, Ni, Ag und Cu. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2008 , 634, 2511-2517	1.3	32
162	Synthesis and Application of New Guanidine Copper Complexes in Atom Transfer Radical Polymerisation. <i>European Journal of Inorganic Chemistry</i> , 2011 , 2011, 2367-2379	2.3	31
161	Intramolecularly coordinated [{2,6-(Me ₂ NCH ₂) ₂ C ₆ H ₃ }Sn(II)] ⁺ : a strong π-honor for Pt(II). <i>Chemistry - A European Journal</i> , 2011 , 17, 7423-7	4.8	31
160	Formation of hybrid guanidine-stabilized bis(EBXO)dicopper cores in solution: Electronic and steric perturbations. <i>European Journal of Inorganic Chemistry</i> , 2015 , 2015, 5426-5436	2.3	29
159	New Guanidine-Pyridine Copper Complexes and Their Application in ATRP. <i>Polymers</i> , 2014 , 6, 995-1007	4.5	29
158	Next Generation of Zinc Bisguanidine Polymerization Catalysts towards Highly Crystalline, Biodegradable Polyesters. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 21778-21784	16.4	28
157	Iron(II) and Zinc(II) Complexes with Tetradentate Bis(pyrazolyl)methane Ligands as Catalysts for the Ring-Opening Polymerisation of rac-Lactide. <i>European Journal of Inorganic Chemistry</i> , 2017 , 2017, 1341-1354	2.3	27
156	Less is more: three-coordinate c,n-chelated distannynes and digermynes. <i>Chemistry - A European Journal</i> , 2015 , 21, 7820-9	4.8	27
155	The Cu ₂ O ₂ torture track for a real-life system: [Cu ₂ (btmgp) ₂ O ₂] ⁽²⁺⁾ oxo and peroxy species in density functional calculations. <i>Journal of Computational Chemistry</i> , 2015 , 36, 1672-85	3.5	27
154	Zinc Chloride Complexes with Aliphatic and Aromatic Guanidine Hybrid Ligands and Their Activity in the Ring-Opening Polymerisation of d,l-Lactide. <i>European Journal of Inorganic Chemistry</i> , 2016 , 2016, 4974-4987	2.3	26
153	Geometrical and optical benchmarking of copper(II) guanidine-quinoline complexes: insights from TD-DFT and many-body perturbation theory (part II). <i>Journal of Computational Chemistry</i> , 2014 , 35, 2146-2151	3.5	26
152	Tin(II) and Tin(IV) Compounds with Scorpion-Shaped Ligands – Intramolecular N-Sn vs. Intermolecular O-Sn Coordination. <i>European Journal of Inorganic Chemistry</i> , 2012 , 2012, 3191-3199	2.3	26
151	Bis-EBXO and 1:1-peroxy dicopper complexes studied within (time-dependent) density-functional and many-body perturbation theory. <i>Journal of Computational Chemistry</i> , 2013 , 34, 1035-45	3.5	26
150	Biomimetic Hydroxylation Catalysis Through Self-Assembly of a Bis(pyrazolyl)methane CopperPeroxo Complex. <i>European Journal of Inorganic Chemistry</i> , 2015 , 2015, 494-502	2.3	25
149	Renaissance of the entatic state principle. <i>Coordination Chemistry Reviews</i> , 2018 , 365, 103-121	23.2	25
148	Hand in Hand: Experimental and Theoretical Investigations into the Reactions of Copper(I) Mono- and Bis(guanidine) Complexes with Dioxygen. <i>European Journal of Inorganic Chemistry</i> , 2016 , 2016, 4744-4751	2.3	24
147	Hiking on the potential energy surface of a functional tyrosinase model–implications of singlet, broken-symmetry and triplet description. <i>Chemical Communications</i> , 2014 , 50, 403-5	5.8	24
146	Systematische Studie zu den Koordinationseigenschaften des Guanidin-Liganden Bis(tetramethylguanidino)propan mit den Metallen Mangan, Cobalt, Nickel, Zink, Cadmium, Quecksilber und Silber. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2010 , 636, 2641-2649	1.3	24

145	Syntheses and X-ray Structure Analyses of the First Bis(chelated) Copper and Iron Bisguanidine Complexes. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2008 , 634, 295-298	1.3	24
144	A Comprehensive Study of Copper Guanidine Quinoline Complexes: Predicting the Activity of Catalysts in ATRP with DFT. <i>Chemistry - A European Journal</i> , 2016 , 22, 13550-62	4.8	24
143	Experimental and Theoretical High-Energy-Resolution X-ray Absorption Spectroscopy: Implications for the Investigation of the Entatic State. <i>Inorganic Chemistry</i> , 2016 , 55, 11694-11706	5.1	22
142	Synthesis and Characterisation of Novel (Guanidine)manganese Complexes and Their Application in the Epoxidation of 1-Octene. <i>European Journal of Inorganic Chemistry</i> , 2011 , 2011, 121-130	2.3	22
141	Neue Bisguanidin-Kupfer-Komplexe und ihre Anwendung in der ATRP/ New Bisguanidine-Copper Complexes and their Application in ATRP. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2010 , 65, 798-806	1	22
140	Undiscovered Potential: Ge Catalysts for Lactide Polymerization. <i>Chemistry - A European Journal</i> , 2020 , 26, 212-221	4.8	22
139	Record Broken: A Copper Peroxide Complex with Enhanced Stability and Faster Hydroxylation Catalysis. <i>Chemistry - A European Journal</i> , 2017 , 23, 12171-12183	4.8	21
138	Designed To React: Terminal Copper Nitrenes and Their Application in Catalytic C-H Aminations. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 9154-9159	16.4	21
137	Structural Aspects of Copper-Mediated Atom Transfer Radical Polymerization with a Novel Tetradentate Bisguanidine Ligand. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2012 , 638, 1683-1690	13	21
136	Intramolekular koordinierte Organozinntelluride: stabil oder labil?. <i>Angewandte Chemie</i> , 2012 , 124, 3535-3540	20	20
135	Unexpected activity of novel 9-oxabispidine zinc complexes in lactide polymerization. <i>Inorganic Chemistry Communication</i> , 2010 , 13, 369-371	3.1	20
134	Decay kinetics of sensitive bioinorganic species in a SuperFocus mixer at ambient conditions. <i>Reaction Chemistry and Engineering</i> , 2016 , 1, 485-493	4.9	20
133	Tuning a robust system: N,O zinc guanidine catalysts for the ROP of lactide. <i>Dalton Transactions</i> , 2019 , 48, 6071-6082	4.3	19
132	Test System for the Investigation of Reactive Taylor Bubbles. <i>Chemical Engineering and Technology</i> , 2017 , 40, 1494-1501	2	19
131	Insights into the intramolecular donor stabilisation of organostannylene palladium and platinum complexes: syntheses, structures and DFT calculations. <i>Chemistry - A European Journal</i> , 2013 , 19, 6695-708	4.8	19
130	Novel Synthetic Strategy towards the Efficient Synthesis of Substituted Bis(pyrazolyl)(2-pyridyl)methane Ligands. <i>European Journal of Organic Chemistry</i> , 2010 , 2010, 4136-4144	3.2	19
129	Oxygen sensing by fluorescence quenching of [Cu(btmgp)]. <i>Journal of Luminescence</i> , 2010 , 130, 1958-1968	19	19
128	Synthese und Strukturen der ersten mehrkernigen Mangan-Guanidin-Komplexe und der ersten Mangan-Komplexe mit mono-protonierten Bis-Guanidinliganden. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2008 , 634, 771-777	1.3	19

127	Donor-driven conformational flexibility in a real-life catalytic dicopper(II) peroxy complex. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 6430-40	3.6	18
126	Simple is best: Diamine zinc complexes as unexpected catalysts in lactide polymerisation. <i>Polyhedron</i> , 2013 , 49, 151-157	2.7	18
125	[{2,6-(Me ₂ NCH ₂) ₂ C ₆ H ₃ }Sn(OH)W(CO) ₅] ₂ : A Transition-Metal-Coordinated Organotin(II) Hydroxide. <i>European Journal of Inorganic Chemistry</i> , 2011 , 2011, 344-348	2.3	18
124	New Challenge for Classics: Neutral Zinc Complexes Stabilised by 2,2'-Bipyridine and 1,10-Phenanthroline and Their Application in the Ring-Opening Polymerisation of Lactide. <i>Sustainability</i> , 2009 , 1, 1226-1239	3.6	18
123	Robust Guanidine Metal Catalysts for the Ring-Opening Polymerization of Lactide under Industrially Relevant Conditions. <i>ChemPlusChem</i> , 2020 , 85, 1044-1052	2.8	17
122	Zn ^{II} Chlorido Complexes with Aliphatic, Chiral Bisguanidine Ligands as Catalysts in the Ring-Opening Polymerisation of rac-Lactide Using FT-IR Spectroscopy in Bulk. <i>European Journal of Inorganic Chemistry</i> , 2017 , 2017, 5557-5570	2.3	17
121	Mononuclear zinc(II) Schiff base complexes as catalysts for the ring-opening polymerization of lactide. <i>European Polymer Journal</i> , 2020 , 122, 109302	5.2	17
120	Oxygen Activation by Copper Complexes with an Aromatic Bis(guanidine) Ligand. <i>European Journal of Inorganic Chemistry</i> , 2017 , 2017, 3350-3359	2.3	16
119	Reaction Systems for Bubbly Flows. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 2101-2124	2.3	16
118	Copper Guanidinoquinoline Complexes as Entatic State Models of Electron-Transfer Proteins. <i>Chemistry - A European Journal</i> , 2017 , 23, 15738-15745	4.8	16
117	Quantum chemical meta-workflows in MoSGrid. <i>Concurrency Computation Practice and Experience</i> , 2015 , 27, 344-357	1.4	16
116	From Pseudo-octahedral to Pseudo-trigonal Bipyramidal Configuration: Syntheses and Molecular Structures of 4-t-Bu-2,6-[(EtO) ₂ P(O)] ₂ C ₆ H ₂ BiCl ₂ and [1(Bi),3(P)-Bi(Cl)OP(O)(OEt)-5-t-Bu-7-P(O)(OEt) ₂]C ₆ H ₂ . <i>Organometallics</i> , 2011 , 30, 5181-5187	3.8	16
115	Heteroleptic Organostannylene and an Organoplumbylene Bearing Phosphorus-Containing Pincer-Type Ligands Structural Variations and Insights into the Configurational Stability. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2011 , 637, n/a-n/a	1.3	16
114	Standards-based metadata management for molecular simulations. <i>Concurrency Computation Practice and Experience</i> , 2014 , 26, 1744-1759	1.4	15
113	Neue aromatische Bisguanidin-Kupfer-Komplexe und ihre Anwendung in der ATRP / New Aromatic Bisguanidine Copper Complexes and Their Application in ATRP. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2014 , 69, 589-595	1	15
112	Stabilization of an Intramolecularly Coordinated Stannylidenium Cation. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2012 , 638, 1672-1675	1.3	15
111	Copper(I) Complexes with Thiourea Derivatives as Ligands: Revealing Secrets of Their Bonding Scheme. <i>European Journal of Inorganic Chemistry</i> , 2017 , 2017, 1266-1279	2.3	14
110	Insights into Different Donor Abilities in Bis(pyrazolyl)pyridinylmethane Transition Metal Complexes. <i>European Journal of Inorganic Chemistry</i> , 2014 , 2014, 2296-2306	2.3	14

109	Bis(pyrazolyl)methane Copper Complexes as Robust and Efficient Catalysts for Sonogashira Couplings. <i>European Journal of Organic Chemistry</i> , 2015 , 2015, 7475-7483	3.2	14
108	A conformationally flexible dinuclear Pt(II) complex with differential behavior of its two states toward quadruplex DNA. <i>Chemistry - A European Journal</i> , 2013 , 19, 11429-38	4.8	13
107	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). <i>European Journal of Inorganic Chemistry</i> , 2013 , 2013, 5836-5842	2.3	13
106	Synthese und Charakterisierung von Cobalt(II)- und Kupfer(I)-Komplexen mit Guanidin-Pyridin-Hybridliganden. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2009 , 635, 64-69	1.3	13
105	Synthesis, Structures, and Catalytic Activity of Homo- and Heteroleptic Ketoiminate Zinc Complexes in Lactide Polymerization. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 4014-4021	2.3	12
104	How coherent structures dominate the residence time in a bubble wake: An experimental example. <i>Chemical Engineering Science</i> , 2019 , 207, 317-326	4.4	12
103	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	3.2	12
102	Tracking the Structure-Reactivity Relationship of Zinc Guanidine-Pyridine Hybrid Complexes Initiating Lactide Polymerisation. <i>Macromolecular Symposia</i> , 2010 , 296, 354-365	0.8	12
101	Novel Guanidine-Quinoline Hybrid Ligands and the Application of their Zinc Complexes in Lactide Polymerisation. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2012 , 67, 0320	1	12
100	On the Way to a Trisanionic {Cu O } Core for Oxidase Catalysis: Evidence of an Asymmetric Trinuclear Precursor Stabilized by Perfluoropinacolate Ligands. <i>Chemistry - A European Journal</i> , 2017 , 23, 8212-8224	4.8	11
99	Heterolepic -Ketoiminate Zinc Phenoxide Complexes as Efficient Catalysts for the Ring Opening Polymerization of Lactide. <i>ChemistryOpen</i> , 2019 , 8, 951-960	2.3	11
98	Syntheses and Molecular Structures of [RSn{W(CO)3Cp}2][W(CO)3Cp], [RSn{W(CO)3Cp}Cl ₂], and [RSn{W(CO)3Cp}Cr(CO) ₅] (R = [4-t-Bu-2,6-{P(O)(OR?) ₂ } ₂ C ₆ H ₂], R? = Et, i-Pr). Autoionization Induced by Intramolecular P?O-?n Coordination. <i>Organometallics</i> , 2014 , 33, 4433-4441	3.8	11
97	Reactivity of 2,2?-Bis(2N-(1,1?,3,3?-tetramethyl-guanidino))diphenylene-amine with Cul and [Cu(MeCN) ₄][PF ₆]: Benzimidazole Formation vs. Cu Oxidation. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2009 , 635, 1209-1214	1.3	11
96	Antimony(III) and bismuth(III) amides containing pendant N-donor groups--a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2015 , 44, 395-400	4.3	10
95	Next Generation of Guanidine Quinoline Copper Complexes for Highly Controlled ATRP: Influence of Backbone Substitution on Redox Chemistry and Solubility. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 3164-3175	2.3	10
94	Using Science Gateways for Bridging the Differences between Research Infrastructures. <i>Journal of Grid Computing</i> , 2016 , 14, 545-557	4.2	10
93	Towards New Robust Zn(II) Complexes for the Ring-Opening Polymerization of Lactide Under Industrially Relevant Conditions. <i>ChemistryOpen</i> , 2019 , 8, 1020-1026	2.3	10
92	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	4.4	10

91	Reactivity of Zinc Halide Complexes Containing Camphor-Derived Guanidine Ligands with Technical rac-Lactide. <i>Inorganics</i> , 2017 , 5, 85	2.9	10
90	Optical response of the Cu ₂ S ₂ diamond core in Cu ₂ II(NGuaS) ₂ Cl ₂ . <i>Journal of Computational Chemistry</i> , 2016 , 37, 2181-92	3.5	10
89	Exceptional Substrate Diversity in Oxygenation Reactions Catalyzed by a Bis(E^{box}) Copper Complex. <i>Chemistry - A European Journal</i> , 2020 , 26, 7556-7562	4.8	9
88	Zinc Complexes with Guanidine-Pyridine Hybrid Ligands: Anion Effect and Catalytic Activity. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2015 , 641, 2147-2156	1.3	9
87	Synthesis and Characterization of Iron(II) Thiocyanate Complexes with Derivatives of the Tris(pyridine-2-ylmethyl)amine (tmpa) Ligand. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2012 , 638, 2069-2077	1.3	9
86	Dissection of Different Donor Abilities Within Bis(pyrazolyl)pyridinylmethane Transition Metal Complexes. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2013 , 639, 1426-1432	1.3	9
85	NFDI4Chem - Towards a National Research Data Infrastructure for Chemistry in Germany. <i>Research Ideas and Outcomes</i> , 6 ,	2.5	9
84	Stepwise Growth of Ruthenium Terpyridine Complexes on Au Surfaces. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 6537-6548	3.8	8
83	Transition Metal Complexes Containing C ₂ -Symmetric Bis(imidazolin-2-imine) Ligands Derived from a 1-Alkyl-3-arylimidazolin-2-ylidene. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2015 , 641, 2204-2214	1.3	8
82	Managing Complexity in Distributed Data Life Cycles Enhancing Scientific Discovery 2015 ,		8
81	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	8
80	Dual oxidase/oxygenase reactivity and resonance Raman spectra of {CuO} moiety with perfluoro-t-butoxide ligands. <i>Dalton Transactions</i> , 2019 , 48, 6899-6909	4.3	7
79	Reactivity of a N- $\ddot{\sigma}$ n Coordinated Distannyne: Reduction and Hydrogen Abstraction. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 2038-2044	2.3	7
78	N-Donor Competition in Iron Bis(chelate) Bis(pyrazolyl)pyridinylmethane Complexes. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2014 , 69, 1206-1214	1	7
77	Palladium(II)-catalyzed cycloisomerization of substituted 1,5-hexadienes: a combined experimental and computational study on an open and an interrupted hydropalladation/carbopalladation/ $\text{E}^{\text{hydride}}$ elimination (HCH _e) catalytic cycle. <i>Journal of Organic Chemistry</i> , 2012 , 77, 4980-95	4.2	7
76	Mit der n $\ddot{\sigma}$ hsten Generation von Zink-Bisguanidin-Polymerisationskatalysatoren zu hochkristallinen, biologisch abbaubaren Polyestern. <i>Angewandte Chemie</i> , 2020 , 132, 21962-21968	3.6	7
75	Chemogenetic Evolution of a Peroxidase-like Artificial Metalloenzyme. <i>ACS Catalysis</i> , 2021 , 11, 5079-5087	1.1	7
74	Fluorescent Bis(guanidine) Copper Complexes as Precursors for Hydroxylation Catalysis. <i>Inorganics</i> , 2018 , 6, 114	2.9	7

73	Influence of Functionalized Substituents on the Electron-Transfer Abilities of Copper Guanidinoquinoline Complexes. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 4997-5006	2.3	7
72	Guanidine Metal Complexes for Bioinorganic Chemistry and Polymerisation Catalysis. <i>Topics in Heterocyclic Chemistry</i> , 2015 , 95-164	0.2	6
71	Tyrosinase Models: Synthesis, Spectroscopy, Theory and Catalysis 2019 ,		6
70	Performance studies on distributed virtual screening. <i>BioMed Research International</i> , 2014 , 2014, 624024	3	6
69	Interplay of Spin Crossover and Coordination-Induced Spin State Switch for Iron Bis(pyrazolyl)methanes in Solution. <i>Inorganic Chemistry</i> , 2020 , 59, 15343-15354	5.1	6
68	Homolytic, Heterolytic, Mesolytic - As You Like It: Steering the Cleavage of a HC(sp ²)-C(sp ²)H Bond in Bis(1H-2,1-benzaborole) Derivatives. <i>Chemistry - A European Journal</i> , 2016 , 22, 15340-15349	4.8	6
67	Maßeschneiderte terminale Kupfernitrile für katalytische C-H-Aminierungen. <i>Angewandte Chemie</i> , 2018 , 130, 9294-9299	3.6	6
66	Imaging of copper oxygenation reactions in a bubble flow. <i>Magnetic Resonance in Chemistry</i> , 2018 , 56, 826-830	2.1	6
65	The Green toxicology approach: Insight towards the eco-toxicologically safe development of benign catalysts. <i>Journal of Hazardous Materials</i> , 2021 , 416, 125889	12.8	6
64	A cryostat for low temperature resonance Raman measurements on operando oxygenated bioinorganic model complexes. <i>Inorganica Chimica Acta</i> , 2018 , 481, 176-180	2.7	5
63	Copper(I) Thiolate Heteroadamantane Cage Structures with Relevance to Metalloproteins. <i>European Journal of Inorganic Chemistry</i> , 2016 , 2016, 3744-3755	2.3	5
62	Relativistic effects at the CuO core - a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 26880-26889	3.6	5
61	Metadata Management in the MoSGrid Science Gateway - Evaluation and the Expansion of Quantum Chemistry Support. <i>Journal of Grid Computing</i> , 2017 , 15, 41-53	4.2	4
60	Rational Syntheses and Serendipity: Complexes [LSnPtCl (SMe) ₃] _n , [{LSnPtCl(SMe) ₃ } SnCl], [(LSn)(PtCl)(PtClSnCl){LSn(Cl)OH}], and [O(SnCl) ₃ (SnL)] with L=MeN(CH ₂ CH ₂ O). <i>Chemistry - A European Journal</i> , 2018 , 24, 5551-5561	4.8	4
59	Gathering requirements for advancing simulations in HPC infrastructures via science gateways. <i>Future Generation Computer Systems</i> , 2018 , 82, 544-554	7.5	4
58	N,N,N?,N?-Tetraethylchloroformamidinium chloride, the first acyclic diaminocarbene?I2 adduct. <i>Inorganic Chemistry Communication</i> , 2006 , 9, 996-998	3.1	4
57	catena-Poly[[Ecyano-[1,3-bis(tetramethylguanidino)propane]dicopper(I)]-Ecyano]. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2005 , 61, m79-m81		4
56	Kinetic Investigation of the Reaction of Dioxygen with the Copper(I) Complex [Cu(PimiPr ₂)(CH ₃ CN)]CF ₃ SO ₃ {PimiPr ₂ = Tris[2-(1,4-diisopropylimidazolyl)]phosphine}. <i>European Journal of Inorganic Chemistry</i> , 2020 , 2020, 3143-3150	2.3	4

55	Addressing Hydrogen Bonding Motifs by Suited Substitution of Thioureas. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2016 , 642, 660-669	1.3	4
54	Katalysatoren f \ddot{u} die Produktion von Biokunststoffen. <i>Chemie in Unserer Zeit</i> , 2016 , 50, 316-325	0.2	4
53	Catalytically Active Iron(IV)oxo Species Based on a Bis(pyridinyl)phenanthrolinylmethane. <i>Israel Journal of Chemistry</i> , 2020 , 60, 987-998	3.4	4
52	Room temperature stable multitalent: highly reactive and versatile copper guanidine complexes in oxygenation reactions. <i>Journal of Biological Inorganic Chemistry</i> , 2021 , 26, 249-263	3.7	4
51	Direct Electrochemical Synthesis of an Unusual Complex Salt: Almost Structural Identity \pm Different Charge. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2017 , 643, 266-275	1.3	3
50	Molecular Simulation Grid (MoSGrid): A Science Gateway Tailored to the Molecular Simulation Community 2014 , 151-165		3
49	Meta-Metaworkflows for Combining Quantum Chemistry and Molecular Dynamics in the MoSGrid Science Gateway 2014 ,		3
48	Tris-phenyl substituted tris(pyrazolyl)methane: Victim of a novel rearrangement in a cobalt(II) complex. <i>Inorganic Chemistry Communication</i> , 2012 , 22, 154-157	3.1	3
47	User-friendly metaworkflows in quantum chemistry 2013 ,		3
46	Zinc Complexes with Mono- and Polydentate Behaving Guanidine Ligands and Their Application in Lactide Polymerization. <i>ACS Symposium Series</i> , 2011 , 169-200	0.4	3
45	Novel Guanidine-Quinoline Hybrid Ligands and the Application of their Zinc Complexes in Lactide Polymerisation. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2012 , 67, 320-330 ¹		3
44	Rare examples of base pairing via a protonated pyridine N atom in two salts of N ₂ ,N ₆ -bis(1,3-dimethylimidazolin-2-ylidene)pyridine-2,6-diamine. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2008 , 64, m194-7		3
43	Di- F luoro-bis[(acetonitrile){N,N'-bis[(dimethylamino)(morpholino)methylene]propane-1,3-diamine}copper(II)] bis(hexafluorophosphate): the first di- F luoro-bridged dicopper bisguanidine compound. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2006 , 62, m2138-m2140		3
42	Simple Zn(II) complexes for the production and degradation of polyesters.. <i>RSC Advances</i> , 2022 , 12, 14165-14243		3
41	A Science Gateway Getting Ready for Serving the International Molecular Simulation Community 2012 ,		3
40	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	1.3	3
39	Multi-level meta-workflows: new concept for regularly occurring tasks in quantum chemistry. <i>Journal of Cheminformatics</i> , 2016 , 8, 58	8.6	3
38	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	3.2	3

37	The Curious Case of a Phenylated Guanidinoquinoline Ligand: Synthesis, Complexes and ATRP Properties of DMEG6phqu. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2018 , 644, 1317-1328	1.3	3
36	Active in Sleep: Iron Guanidine Catalyst Performs ROP on Dormant Side of ATRP. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 21795-21800	16.4	3
35	Research Data in Chemistry Results of the first NFDI4Chem Community Survey. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020 , 646, 1748-1757	1.3	2
34	Jet delivery system for Raman scattering on bio-inorganic compounds. <i>Applied Physics Letters</i> , 2016 , 109, 213502	3.4	2
33	A Study on Fell, ZnII and Cull Complexes with Novel Tridentate Bis(pyrazolyl)methane Ligands. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2018 , 644, 1576-1592	1.3	2
32	Oxalic Amidines Protonation Studies and Activity in Lactide Polymerisation. <i>European Journal of Inorganic Chemistry</i> , 2013 , 2013, 99-108	2.3	2
31	Detection of Copper Bisguanidine NO Adducts by UV-vis Spectroscopy and a SuperFocus Mixer. <i>Chemical Engineering and Technology</i> , 2017 , 40, 1475-1483	2	2
30	[Me ₂ (i-PrO)SiCH ₂] ₂ SnBr ₂ : Evidence for Intramolecular Si D Bond Activation. <i>Organometallics</i> , 2012 , 31, 4716-4721	3.8	2
29	Novel Tin(IV) Complexes with the Hybrid Guanidine Ligand DMEGqu. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2013 , 68, 653-665	1	2
28	Syntheses and characterisation of tris(3-(pyridin-2-yl)-1H-pyrazol-1-yl)methane and its bis(D-hydroxo) dicobalt(II) complex. <i>Arkivoc</i> , 2012 , 2012, 343-355	0.9	2
27	Towards a metadata-driven multi-community research data management service		2
26	A new generation of terminal copper nitrenes and their application in aromatic C-H amination reactions. <i>Dalton Transactions</i> , 2021 , 50, 6444-6462	4.3	2
25	Workflow-enhanced conformational analysis of guanidine zinc complexes via a science gateway. <i>Studies in Health Technology and Informatics</i> , 2012 , 175, 142-51	0.5	2
24	Atmospheric pressure photo-ionization mass spectrometry for the detection of labile end groups in poly(styrene). <i>European Polymer Journal</i> , 2017 , 90, 209-219	5.2	1
23	[Cu (NGuaS)] and its oxidized and reduced derivatives: Confining electrons on a torus. <i>Journal of Computational Chemistry</i> , 2017 , 38, 1752-1761	3.5	1
22	New stereocontrol on the block. <i>Nature Chemistry</i> , 2020 , 12, 107-109	17.6	1
21	Enhanced catalytic activity of copper complexes in microgels for aerobic oxidation of benzyl alcohols. <i>Chemical Communications</i> , 2020 , 56, 5601-5604	5.8	1
20	Implications of Guanidine Substitution on Copper Complexes as Entatic-State Models. <i>European Journal of Inorganic Chemistry</i> , 2016 , 2016, 4722-4722	2.3	1

19	Expansion of Quantum Chemical Metadata for Workflows in the MoSGrid Science Gateway 2014 ,	1
18	Theoretical Studies on Tyrosinase Models 2017 , 1-15	1
17	Rücktitelbild: Katalytische Phenolhydroxylierung mit Sauerstoff: Substratvielfalt jenseits der Proteinmatrix von Tyrosinase (Angew. Chem. 20/2013). <i>Angewandte Chemie</i> , 2013 , 125, 5518-5518	3.6 1
16	MoSGrid - molecular simulation grid as a new tool in computational chemistry, biology and material science. <i>Journal of Cheminformatics</i> , 2011 , 3,	8.6 1
15	The diprotonated 2,2-(propane-1,3-diy)bis(1,1,3,3-tetramethylguanidinium) cation: packing and conformational changes. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006 , 62, m234-7	1
14	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	8.9 1
13	Visualization and Quantitative Analysis of Consecutive Reactions in Taylor Bubble Flows. <i>Fluid Mechanics and Its Applications</i> , 2021 , 507-543	0.2 1
12	Nachtaktiv: Eisen-Guanidin-Komplex katalysiert ROP auf der schlafenden Seite der ATRP. <i>Angewandte Chemie</i> , 2021 , 133, 21965-21971	3.6 1
11	Influence of the amine donor on hybrid guanidine-stabilized Bis(E xido) dicopper(III) complexes and their tyrosinase-like oxygenation activity towards polycyclic aromatic alcohols. <i>Journal of Inorganic Biochemistry</i> , 2021 , 224, 111541	4.2 1
10	Forschungsdatenmanagement - Zeit f $\ddot{\text{u}}$ r den Abschied vom analogen Laborbuch. <i>Nachrichten Aus Der Chemie</i> , 2020 , 68, 20-23	0.1 0
9	Characterization of the optically excited state of a bis (E xo)-dicopper(III) species mimicking the hemocyanin and tyrosinase active sites. <i>Journal of Physics: Conference Series</i> , 2009 , 190, 012201	0.3 0
8	Guanidine Carboxy Zinc Complexes for the Chemical Recycling of Renewable Polyesters.. <i>ChemPlusChem</i> , 2022 , e202200029	2.8 0
7	Chemiker im Grid. <i>Nachrichten Aus Der Chemie</i> , 2013 , 61, 136-138	0.1
6	Kontrolle $\ddot{\text{u}}$ ber Chaos und Ordnung: Gegensätzliche Mikrostrukturen von PCL-co-PGA-co-PLA durch einen einzigen Katalysator zugänglich**. <i>Angewandte Chemie</i> , e202112853	3.6
5	Innenrücktitelbild: Mit der nächsten Generation von Zink-Bisguanidin-Polymerisationskatalysatoren zu hochkristallinen, biologisch abbaubaren Polyestern (Angew. Chem. 48/2020). <i>Angewandte Chemie</i> , 2020 , 132, 21971-21971	3.6
4	In celebration of the 70th birthday of Peter Klüfers. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2021 , 647, 801-802	1.3
3	Determination of Kinetics for Reactive Bubbly Flows Using SuperFocus Mixers. <i>Fluid Mechanics and Its Applications</i> , 2021 , 479-506	0.2
2	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 Chemical Reactions at Freely Ascending Single Bubbles. *Fluid Mechanics and Its Applications*, **2021**, 545-5812