

# Peter Comba

## List of Publications by Year in Descending Order

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

186  
papers

6,361  
citations

48  
h-index

66  
g-index

200  
ext. papers

6,844  
ext. citations

5.3  
avg, IF

5.72  
L-index

#	Paper	IF	Citations
186	Exceptional Manganese(II) Stability and Manganese(II) / Zinc(II) Selectivity with Rigid Polydentate Ligands.. <i>Angewandte Chemie - International Edition</i> , <b>2022</b> ,	16.4	3
185	Efficient synthesis for a wide variety of patellamide derivatives and phosphatase activity of copper-patellamide complexes.. <i>Chemistry - A European Journal</i> , <b>2022</b> ,	4.8	1
184	Molecular magnetic properties of a dysprosium(III) complex coordinated to a nonadentate bispidine ligand. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2021</b> , 647, 843-849	1.3	2
183	Validation of Ab-Initio-Predicted Magnetic Anisotropies and Magneto-structural Correlations in Linear Hetero-trinuclear Dy -Ni Compounds. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 9372-9382	4.8	2
182	Excited State Properties of Lanthanide(III) Complexes with a Nonadentate Bispidine Ligand. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 10303-10312	4.8	7
181	Pathways of the Extremely Reactive Iron(IV)-oxido complexes with Tetradentate Bispidine Ligands. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 11377-11390	4.8	3
180	Phosphine-Catalyzed Vinylation at Low Acetylene Pressure. <i>Journal of Organic Chemistry</i> , <b>2021</b> , 86, 13041-13055	4.1	3055
179	Redox Potentials of High-Valent Iron-, Cobalt-, and Nickel-Oxido Complexes: Evidence for Exchange Enhanced Reactivity. <i>Israel Journal of Chemistry</i> , <b>2020</b> , 60, 957-962	3.4	1
178	Mechanistic Investigation of the Nickel-Catalyzed Carbonylation of Alcohols. <i>Organometallics</i> , <b>2020</b> , 39, 870-880	3.8	3
177	Ru or Ru: A Study on Stabilizing the "Activated" Form of Ru-PNP Complexes with Additional Phosphine Ligands in Alcohol Dehydrogenation and Ester Hydrogenation. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 5099-5115	5.1	15
176	First-Generation Bispidine Chelators for Bi Radiopharmaceutical Applications. <i>ChemMedChem</i> , <b>2020</b> , 15, 1591-1600	3.7	14
175	Spin state and reactivity of iron(iv)oxido complexes with tetradentate bispidine ligands. <i>Dalton Transactions</i> , <b>2020</b> , 49, 2888-2894	4.3	14
174	Versatile Bispidine-Based Bifunctional Chelators for Cu -Labelling of Biomolecules. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 1989-2001	4.8	11
173	Characterization and Reactivity of a Tetrahedral Copper(II) Alkylperoxido Complex. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 11157-11165	4.8	6
172	Octadentate Oxine-Armed Bispidine Ligand for Radiopharmaceutical Chemistry. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 8685-8693	5.1	11
171	A Structural and Functional Model for the Tris-Histidine Motif in Cysteine Dioxygenase. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 9540-9547	4.8	6
170	Optimization of Hexadentate Bispidine Ligands as Chelators for Cu PET Imaging. <i>ChemPlusChem</i> , <b>2018</b> , 83, 597-604	2.8	5

169	Correlation of Structural and Magnetic Properties in a Set of Mononuclear Lanthanide Complexes. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 5319-5330	4.8	10
168	Heteroatom-Interchanged Isomers of Lissoclinamide 5: Copper(II) Complexation, Halide Binding, and Biological Activity. <i>European Journal of Organic Chemistry</i> , <b>2018</b> , 2018, 1465-1476	3.2	7
167	Direct Asymmetric Ruthenium-Catalyzed Reductive Amination of Alkyl-Aryl Ketones with Ammonia and Hydrogen. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 355-361	16.4	75
166	Cu selective chelators relieve copper-induced oxidative stress. <i>Chemical Science</i> , <b>2018</b> , 9, 7916-7930	9.4	35
165	Bispidines for radiopharmaceuticals. <i>Dalton Transactions</i> , <b>2018</b> , 47, 9202-9220	4.3	36
164	Iron catalyzed demethylation of acetic acid*. <i>Journal of Coordination Chemistry</i> , <b>2018</b> , 71, 1704-1714	1.6	1
163	Synthesis, structural analysis, solution equilibria and biological activity of rhodium(III) complexes with a quinquedentate polyaminopolycarboxylate. <i>RSC Advances</i> , <b>2017</b> , 7, 5282-5296	3.7	8
162	N-Aryl Groups Are Ubiquitous in Cross-Dehydrogenative Couplings Because They Stabilize Reactive Intermediates. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 9313-9318	4.8	24
161	Nonheme Iron-Oxo-Catalyzed Methane Formation from Methyl Thioethers: Scope, Mechanism, and Relevance for Natural Systems. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 10465-10472	4.8	14
160	Is Cu Coordinated to Patellamides inside Prochloron Cells?. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 12264-12274	4.8	12
159	Octadentate Picolinic Acid-Based Bispidine Ligand for Radiometal Ions. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 15945-15956	4.8	44
158	Dinuclear Copper(II) Complexes with Distant Metal Centers: Weaker Donor Groups Increase Catecholase Activity. <i>European Journal of Inorganic Chemistry</i> , <b>2017</b> , 2017, 56-62	2.3	17
157	Solution and solid state structures and magnetism of a series of linear trinuclear compounds with a hexacoordinate Ln and two terminal Ni centers. <i>Dalton Transactions</i> , <b>2016</b> , 46, 138-149	4.3	15
156	Dinuclear Zn and mixed Cu-Zn complexes of artificial patellamides as phosphatase models. <i>Dalton Transactions</i> , <b>2016</b> , 45, 18931-18945	4.3	11
155	A Bispidine Iron(IV)-Oxo Complex in the Entatic State. <i>Angewandte Chemie</i> , <b>2016</b> , 128, 11295-11299	3.6	7
154	A Bispidine Iron(IV)-Oxo Complex in the Entatic State. <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 11129-33	16.4	32
153	First row transition metal complexes of a hexadentate pyrazole-based bispidine ligand. <i>Polyhedron</i> , <b>2013</b> , 52, 1239-1245	2.7	7
152	Optimization of pentadentate bispidines as bifunctional chelators for <sup>64</sup> Cu positron emission tomography (PET). <i>Inorganic Chemistry</i> , <b>2013</b> , 52, 8131-43	5.1	39

151	An efficient fluctuating charge model for transition metal complexes. <i>Journal of Computational Chemistry</i> , <b>2013</b> , 34, 1598-608	3.5	13
150	Nonheme Oxoiron(IV) Complexes of Pentadentate N5 Ligands: Spectroscopy, Electrochemistry, and Oxidative Reactivity. <i>Chemical Science</i> , <b>2013</b> , 4, 282-291	9.4	123
149	Purple acid phosphatase: A journey into the function and mechanism of a colorful enzyme. <i>Coordination Chemistry Reviews</i> , <b>2013</b> , 257, 473-482	23.2	135
148	Synthesis, magnetic properties, and phosphoesterase activity of dinuclear cobalt(II) complexes. <i>Inorganic Chemistry</i> , <b>2013</b> , 52, 2029-43	5.1	54
147	Ensemble and single-molecule studies on fluorescence quenching in transition metal bipyridine-complexes. <i>PLoS ONE</i> , <b>2013</b> , 8, e58049	3.7	17
146	Tuning of the properties of transition-metal bispidine complexes by variation of the basicity of the aromatic donor groups. <i>Inorganic Chemistry</i> , <b>2013</b> , 52, 6481-501	5.1	47
145	Dinuclear Cobalt(II) Complexes as Metallo- $\beta$ -lactamase Mimics. <i>European Journal of Inorganic Chemistry</i> , <b>2013</b> , 2013, 3082-3089	2.3	9
144	Monoesterase activity of a purple acid phosphatase mimic with a cyclam platform. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 1700-10	4.8	44
143	Cu(II) coordination chemistry of patellamide derivatives: possible biological functions of cyclic pseudopeptides. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 2578-90	4.8	24
142	Spectroscopic characterization of the active Fe(III)Fe(III) and Fe(III)Fe(II) forms of a purple acid phosphatase model system. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 12195-209	5.1	37
141	Structure, bonding, and catecholase mechanism of copper bispidine complexes. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 9214-25	5.1	53
140	Cyanide-bridged Fe(III)-Cu(II) complexes: Jahn-Teller isomerism and its influence on the magnetic properties. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 9357-68	5.1	15
139	Zero-field splitting in a series of structurally related mononuclear Ni(II)-bispidine complexes. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 12324-35	5.1	33
138	Riboflavin carrier protein-targeted fluorescent USPIO for the assessment of vascular metabolism in tumors. <i>Biomaterials</i> , <b>2012</b> , 33, 8822-9	15.6	32
137	Cadmium(II) complexes: mimics of organophosphate pesticide degrading enzymes and metallo- $\beta$ -lactamases. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 7669-81	5.1	19
136	Dioxygen reactivity of new bispidine-copper complexes. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 2841-51	5.1	26
135	Cyano-bridged homodinuclear copper(II) complexes. <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 6890-901	5.1	27
134	Structures, spectroscopy and modeling of a rare set of isomeric copper(II) complexes. <i>Inorganica Chimica Acta</i> , <b>2011</b> , 374, 422-428	2.7	9

133	Synthesis and Cu(II) coordination chemistry of a patellamide derivative: consequences of the change from the natural thiazole/oxazoline to the artificial imidazole heterocycles. <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 5165-74	5.1	23
132	Optimization of the Efficiency of Oxidation Catalysts Based on Iron Bispidine Complexes. <i>European Journal of Inorganic Chemistry</i> , <b>2011</b> , 2011, 2610-2615	2.3	11
131	Oxidation versus Dioxygenation of Catechol: The Iron Bispidine System. <i>European Journal of Inorganic Chemistry</i> , <b>2011</b> , 2011, 5242-5249	2.3	23
130	An oxocobalt(IV) complex stabilized by Lewis acid interactions with scandium(III) ions. <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 1711-5	16.4	119
129	FMN-coated fluorescent iron oxide nanoparticles for RCP-mediated targeting and labeling of metabolically active cancer and endothelial cells. <i>Biomaterials</i> , <b>2011</b> , 32, 5863-71	15.6	53
128	Complex formation and stability of westiellamide derivatives with copper(II). <i>Journal of Biological Inorganic Chemistry</i> , <b>2010</b> , 15, 1129-35	3.7	12
127	Novel Rull Complexes with Bispidine-Based Bridging Ligands: Luminescence Sensing and Photocatalytic Properties. <i>European Journal of Inorganic Chemistry</i> , <b>2010</b> , 2010, 1295-1302	2.3	24
126	Iron-catalyzed halogenation of alkanes: modeling of nonheme halogenases by experiment and DFT calculations. <i>Chemistry - A European Journal</i> , <b>2010</b> , 16, 7293-9	4.8	76
125	Electron-transfer properties of an efficient nonheme iron oxidation catalyst with a tetradentate bispidine ligand. <i>Angewandte Chemie - International Edition</i> , <b>2010</b> , 49, 2622-5	16.4	67
124	Synthesis, structure, and highly efficient copper-catalyzed aziridination with a tetraaza-bispidine ligand. <i>Chemistry - A European Journal</i> , <b>2009</b> , 15, 10880-7	4.8	46
123	Computation of structures and properties of transition metal compounds. <i>Coordination Chemistry Reviews</i> , <b>2009</b> , 253, 564-574	23.2	83
122	Cyanometalate-bridged oligonuclear transition metal complexes Possibilities for a rational design of SMMs. <i>Coordination Chemistry Reviews</i> , <b>2009</b> , 253, 2306-2314	23.2	96
121	Calculation of exchange coupling constants of transition metal complexes with DFT. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 6751-5	2.8	62
120	Oxidation of cyclohexane by high-valent iron bispidine complexes: tetradentate versus pentadentate ligands. <i>Inorganic Chemistry</i> , <b>2009</b> , 48, 10389-96	5.1	74
119	Novel bispidine ligands and their first-row transition metal complexes: trigonal bipyramidal and trigonal prismatic geometries. <i>Inorganic Chemistry</i> , <b>2009</b> , 48, 6604-14	5.1	27
118	Mono- and Dinuclear Copper(II) and Iron(II) Complexes of a Tetradentate Bispidine-diacetate Ligand. <i>Australian Journal of Chemistry</i> , <b>2009</b> , 62, 1238	1.2	10
117	Hexadentate bispidine derivatives as versatile bifunctional chelate agents for copper(II) radioisotopes. <i>Bioconjugate Chemistry</i> , <b>2009</b> , 20, 347-59	6.3	82
116	Modeling of the various minima on the potential energy surface of bispidine copper(II) complexes: a further test for ligand field molecular mechanics. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 9518-27	5.1	41

115	Epoxidation and 1,2-dihydroxylation of alkenes by a nonheme iron model system - DFT supports the mechanism proposed by experiment. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 78-93	5.1	54
114	Combined ligand field and density functional theory analysis of the magnetic anisotropy in oligonuclear complexes based on Fe(III)-CN-M(II) exchange-coupled pairs. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 2449-63	5.1	73
113	Trinuclear {M1}CN{M2}2 complexes (M1 = Cr(III), Fe(III), Co(III); M2 = Cu(II), Ni(II), Mn(II)). Are single molecule magnets predictable?. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 8112-25	5.1	58
112	Hydrophilic oxybathophenanthroline ligands: synthesis and copper(II) complexation. <i>New Journal of Chemistry</i> , <b>2008</b> , 32, 2016	3.6	8
111	Oxidation of cyclohexane by a high-valent iron bispidine complex: a combined experimental and computational mechanistic study. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 13028-36	2.8	52
110	Copper(II)-mediated aromatic ortho-hydroxylation: a hybrid DFT and AB initio exploration. <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 344-57	4.8	44
109	Copper(II) coordination chemistry of westiellamide and its imidazole, oxazole, and thiazole analogues. <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 4393-403	4.8	41
108	The mechanism of the (bispidine)copper(II)-catalyzed aziridination of styrene: a combined experimental and theoretical study. <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 5313-28	4.8	71
107	Stable five- and six-coordinate cobalt(III) complexes with a pentadentate bispidine ligand. <i>Angewandte Chemie - International Edition</i> , <b>2008</b> , 47, 4740-3	16.4	22
106	Electronic structure of bispidine iron(IV) oxo complexes. <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 6420-6	5.1	51
105	A density functional theory study of the reaction of the biomimetic iron(II) complex of a tetradentate bispidine ligand with H <sub>2</sub> O <sub>2</sub> . <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 3826-38	5.1	57
104	Biomimetic high-valent non-heme iron oxidants for the cis-dihydroxylation and epoxidation of olefins. <i>Angewandte Chemie - International Edition</i> , <b>2007</b> , 46, 8067-70	16.4	124
103	Competing Radical and Non-Radical Pathways for the Decomposition of LFe(II)(H <sub>2</sub> O <sub>2</sub> ) Complexes: a Density Functional Study. <i>European Journal of Inorganic Chemistry</i> , <b>2007</b> , 2007, 65-73	2.3	15
102	Synthesis and Oxidation of Vanadyl Complexes Containing Bispidine Ligands. <i>European Journal of Inorganic Chemistry</i> , <b>2007</b> , 2007, 657-664	2.3	19
101	On the ground state Tg <sup>2</sup> g (Tg=2T <sub>2</sub> g, 3T <sub>1</sub> g) Jahn-Teller-coupling in hexacyano complexes of 3d-transition metals. <i>Journal of Molecular Structure</i> , <b>2007</b> , 838, 157-163	3.4	11
100	DFT-based studies on the Jahn-Teller effect in 3d hexacyanometalates with orbitally degenerate ground states. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 9145-63	2.8	41
99	An examination of the binding behavior of histidine-containing peptides with immobilized metal complexes derived from the macrocyclic ligand, 1,4,7-triazacyclononane. <i>Journal of Biological Inorganic Chemistry</i> , <b>2007</b> , 12, 11-21	3.7	13
98	Catecholase activity of dicopper(II)-bispidine complexes: stabilities and structures of intermediates, kinetics and reaction mechanism. <i>Journal of Biological Inorganic Chemistry</i> , <b>2007</b> , 12, 36-48	3.7	41

97	Encapsulation of cyanometalates by a tris-macrocyclic ligand tricopper(II) complex: syntheses, structural variation, and magnetic exchange coupling pathways. <i>Chemistry - A European Journal</i> , <b>2006</b> , 12, 737-48	4.8	28
96	Catalytic epoxidation and 1,2-dihydroxylation of olefins with bispidine-iron(II)/H <sub>2</sub> O <sub>2</sub> systems. <i>Angewandte Chemie - International Edition</i> , <b>2006</b> , 45, 3446-9	16.4	136
95	Formation of an aqueous oxoiron(IV) complex at pH 2-6 from a nonheme iron(II) complex and H <sub>2</sub> O <sub>2</sub> . <i>Angewandte Chemie - International Edition</i> , <b>2006</b> , 45, 5681-4	16.4	101
94	The Reactivity of Hexa(N-methylideneimine)Co(III) Complexes towards Nucleophiles: Structure and Mechanism. <i>European Journal of Inorganic Chemistry</i> , <b>2006</b> , 2006, 2792-2807	2.3	7
93	Synthesis of New Phenanthroline-Based Heteroditopic Ligands [Highly Efficient and Selective Fluorescence Sensors for Copper(II) Ions. <i>European Journal of Inorganic Chemistry</i> , <b>2006</b> , 2006, 4442-4448	2.3	34
92	DFT models for copper(II) bispidine complexes: structures, stabilities, isomerism, spin distribution, and spectroscopy. <i>Journal of Computational Chemistry</i> , <b>2006</b> , 27, 1263-77	3.5	67
91	Determination of the solution structures of melamine-based bis- and tris-macrocyclic ligand copper(II) complexes. <i>Inorganic Chemistry</i> , <b>2006</b> , 45, 3632-8	5.1	27
90	Tuning of inter- versus intrachain magnetic interactions in cyano-bridged Ni(II)/M(III) (M = Cr, Fe, Co) chain complexes. <i>Inorganic Chemistry</i> , <b>2006</b> , 45, 7722-35	5.1	31
89	Spin-crossover in an iron(III)-bispidine-alkylperoxide system. <i>Inorganic Chemistry</i> , <b>2006</b> , 45, 7077-82	5.1	44
88	DFT studies on the magnetic exchange across the cyanide bridge. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 13332-40	2.8	50
87	A new molecular mechanics force field for the design of oxotechnetium(V) and oxorhenium(V) radiopharmaceuticals. <i>Journal of Organometallic Chemistry</i> , <b>2006</b> , 691, 2495-2502	2.3	19
86	Coordination chemistry of a new rigid, hexadentate bispidine-based bis(amine)tetrakis(pyridine) ligand. <i>Inorganic Chemistry</i> , <b>2005</b> , 44, 8145-55	5.1	59
85	Electronic Interactions in Ferrocene- and Ruthenocene-Functionalized Tetraazamacrocyclic Ligand Complexes of Fe(II/III), Co(II), Ni(II), Cu(II) and Zn(II). <i>European Journal of Inorganic Chemistry</i> , <b>2005</b> , 2005, 383-388	2.3	7
84	Synthesis and Binding Properties of Dendritic Oxybathophenanthroline Ligands towards Copper(II). <i>European Journal of Inorganic Chemistry</i> , <b>2005</b> , 2005, 4501-4508	2.3	8
83	Tuning the Properties of Copper(II) Complexes with Tetra- and Pentadentate Bispidine (=3,7-Diazabicyclo[3.3.1]nonane) Ligands. <i>Helvetica Chimica Acta</i> , <b>2005</b> , 88, 647-664	2	46
82	Structural variation in the copper(II) complexes with a tetradentate bis-6-methylpyridine-substituted bispidine ligand. <i>Comptes Rendus Chimie</i> , <b>2005</b> , 8, 1506-1518	2.7	14
81	Interpretation of the temperature-dependent color of blue copper protein mutants. <i>Journal of Inorganic Biochemistry</i> , <b>2004</b> , 98, 896-902	4.2	19
80	Bispidine ligand effects on iron/hydrogen peroxide chemistry. <i>Angewandte Chemie - International Edition</i> , <b>2004</b> , 43, 1283-7	16.4	77

79	Slow Electron Self-Exchange in Spite of a Small Inner-Sphere Reorganisation Energy □ The Electron-Transfer Properties of a Copper Complex with a Tetradentate Bispidine Ligand. <i>European Journal of Inorganic Chemistry</i> , <b>2004</b> , 2004, 4640-4645	2.3	29
78	Density functional investigation of metal-metal interactions in mixed-valence d <sup>2</sup> d <sup>3</sup> (Cr, Mo, W) and d <sup>3</sup> d <sup>4</sup> (Mn, Tc, Re) face-shared [M <sub>2</sub> Cl <sub>9</sub> ] <sup>2-</sup> systems. <i>Inorganic Chemistry</i> , <b>2004</b> , 43, 6734-44	5.1	14
77	Heterotrinnuclear Complexes of the Platinum Group Metals with 2,2'-Biimidazole as a Bridging Ligand. <i>European Journal of Inorganic Chemistry</i> , <b>2003</b> , 2003, 1703-1710	2.3	20
76	Catalytic Aziridination of Styrene with Copper Complexes of Substituted 3,7-Diazabicyclo[3.3.1]nonanones. <i>European Journal of Inorganic Chemistry</i> , <b>2003</b> , 2003, 1711-1718	2.3	59
75	Macrocyclic Melamine-Based Ligand Complexes as Building Blocks for the Metal-Directed Synthesis of Heterometallic Di- and Trinuclear Compounds. <i>European Journal of Inorganic Chemistry</i> , <b>2003</b> , 2003, 34-37	2.3	10
74	Bond-stretch isomerism: trapped isomeric structures of hexacoordinate copper(II) bispidine chromophores along a Jahn-Teller active vibrational coordinate. <i>Angewandte Chemie - International Edition</i> , <b>2003</b> , 42, 4536-40	16.4	48
73	Structure correlation in bispidine coordination compounds □ Isomerism and tuneable reactivity. <i>Crystal Engineering</i> , <b>2003</b> , 6, 197-211		18
72	Structural properties of cyclopentanone-bridged bis-macrocyclic ligand dicopper(II) complexes in the solid and in solution: a successful test of the MM-EPR method. <i>Inorganic Chemistry</i> , <b>2003</b> , 42, 3387-9	5.1	21
71	Synthesis and structural properties of patellamide A derivatives and their copper(II) compounds. <i>Chemistry - A European Journal</i> , <b>2002</b> , 8, 1527-36	4.8	44
70	Structural variation in transition-metal bispidine compounds. <i>Chemistry - A European Journal</i> , <b>2002</b> , 8, 5750-60	4.8	74
69	Cooperative Effects in the Binding of Substrates to Nickel(II) and Nickel(III) Complexes with a Bis(macrocyclic) Ligand. <i>European Journal of Inorganic Chemistry</i> , <b>2002</b> , 2002, 1871-1882	2.3	7
68	A new molecular mechanics force field for the oxidized form of blue copper proteins. <i>Journal of Computational Chemistry</i> , <b>2002</b> , 23, 697-705	3.5	73
67	Structural and mechanistic studies of the copper(II)-assisted ortho-hydroxylation of benzoates by trimethylamine N-oxide. <i>Journal of Organometallic Chemistry</i> , <b>2002</b> , 641, 71-80	2.3	20
66	Iron coordination chemistry with tetra-, penta- and hexadentate bispidine-type ligands. <i>Inorganica Chimica Acta</i> , <b>2002</b> , 337, 407-419	2.7	88
65	Trends in Base Hydrolysis Rates of Chlorocobalt(III) Complexes of a Series of Related Pentaamine Ligands. <i>Inorganic Reaction Mechanisms</i> , <b>2002</b> , 4, 31-47		3
64	Copper-bispidine coordination chemistry: syntheses, structures, solution properties, and oxygenation reactivity. <i>Inorganic Chemistry</i> , <b>2002</b> , 41, 5440-52	5.1	65
63	An amicyanin C-terminal loop mutant where the active-site histidine donor cannot be protonated. <i>Journal of Biological Inorganic Chemistry</i> , <b>2001</b> , 6, 23-6	3.7	25
62	The Role of the Apical Donor in the Decomposition of Copper(II) Benzoate under DOW-Phenol Conditions. <i>European Journal of Inorganic Chemistry</i> , <b>2001</b> , 2001, 3143-3149	2.3	11



61	Catalytic Dehalogenation of Halogenated Pyridine Donors under DOW-Phenol Conditions. <i>European Journal of Inorganic Chemistry</i> , <b>2001</b> , 2001, 3151-3154	2.3	2
60	Hybrid quantum mechanics/molecular mechanics studies of the active site of the blue copper proteins amicyanin and rusticyanin. <i>Inorganica Chimica Acta</i> , <b>2001</b> , 324, 21-26	2.7	27
59	Axial bonds in copper(II) compounds. <i>Inorganica Chimica Acta</i> , <b>2001</b> , 324, 99-107	2.7	25
58	Molecular mechanics: theoretical basis, rules, scope and limits. <i>Coordination Chemistry Reviews</i> , <b>2001</b> , 212, 3-10	23.2	36
57	Template synthesis of a tetraazamacrocyclic ligand with two pendant pyridinyl groups: properties of the isomers of the metal-free ligand and of their first-row transition metal compounds. <i>Inorganic Chemistry</i> , <b>2001</b> , 40, 2335-45	5.1	34
56	Bispidine copper(II) compounds: effects of the rigid ligand backbone. <i>Inorganic Chemistry</i> , <b>2001</b> , 40, 5206-5219	5.1	57
55	A copper(I) oxygenation precursor in the entatic state: two isomers of a copper(I) compound of a rigid tetradentate ligand. <i>Chemistry - A European Journal</i> , <b>2000</b> , 6, 914-9	4.8	56
54	Loop-Directed Mutagenesis of the Blue Copper Protein Amicyanin from <i>Paracoccus versutus</i> and Its Effect on the Structure and the Activity of the Type-1 Copper Site. <i>Journal of the American Chemical Society</i> , <b>2000</b> , 122, 204-211	16.4	69
53	Strains and stresses in coordination compounds. <i>Coordination Chemistry Reviews</i> , <b>1999</b> , 182, 343-371	23.2	87
52	Conformational searching of transition metal compounds. <i>Journal of Computational Chemistry</i> , <b>1999</b> , 20, 1549-1558	3.5	29
51	Isomerism in Copper(I)-Induced Folding of Homoditopic Macrocyclic Ligands with Bis(dithiadiimine) Donor Sets. <i>European Journal of Inorganic Chemistry</i> , <b>1999</b> , 1999, 509-515	2.3	6
50	A Simple New Structural Force Field for the Computation of Linear Metallocenes. <i>European Journal of Inorganic Chemistry</i> , <b>1999</b> , 1999, 1787-1792	2.3	5
49	Structural Variation of Dinuclear Transition Metal Compounds with a Common Type of Ligand: Solid State and Solution Structures and Model Studies. <i>Inorganic Chemistry</i> , <b>1999</b> , 38, 1416-1421	5.1	22
48	Bis-macrocyclic Ligands with Two Ferrocenyl End Groups, and Their Tetranuclear Dicopper(I) Compounds. <i>Inorganic Chemistry</i> , <b>1999</b> , 38, 3316-3320	5.1	11
47	Transition Metal Coordination Compounds of Bisamidobispyridyl Ligands. <i>European Journal of Inorganic Chemistry</i> , <b>1998</b> , 1998, 2041-2049	2.3	21
46	Molecular mechanics modeling of organic backbone of metal-free and coordinated ligands. <i>Journal of Computational Chemistry</i> , <b>1998</b> , 19, 512-523	3.5	65
45	Helical Figure-of-Eight Loop Dicopper(I) Compounds: Syntheses, Structures, and Dynamics. <i>Inorganic Chemistry</i> , <b>1998</b> , 37, 4389-4401	5.1	33
44	The Solution Structure of a Copper(II) Compound of a New Cyclic Octapeptide by EPR Spectroscopy and Force Field Calculations. <i>Inorganic Chemistry</i> , <b>1998</b> , 37, 6721-6727	5.1	40

43	Structural, EPR, and Electrochemical Studies of Binuclear Copper(II) Complexes of Bis(pentadentate) Ligands Derived from Bis(1,4,7-triazacyclonane) Macrocycles. <i>Inorganic Chemistry</i> , <b>1998</b> , 37, 3705-3713	5.1	37
42	Preparation, Structure, and Electronic Properties of a Low-Spin Iron(II) Hexamine Compound. <i>Inorganic Chemistry</i> , <b>1998</b> , 37, 3853-3857	5.1	24
41	Molecular Mechanics Calculations and the Metal Ion Selective Extraction of Lanthanoids. <i>Inorganic Chemistry</i> , <b>1998</b> , 37, 3310-3315	5.1	37
40	Modeling of End-On ( $\eta^2$ -Peroxo)dicopper(II) Complexes. <i>Inorganic Chemistry</i> , <b>1997</b> , 36, 2309-2313	5.1	25
39	Novel Ring Contraction Reaction for the Synthesis of Functionalized Tetrathiamacrocyclic Ligand Molecules. <i>Journal of Organic Chemistry</i> , <b>1997</b> , 62, 8459-8462	4.2	8
38	Modeling of the Redox Properties of (Hexamine)cobalt(III/II) Couples. <i>Inorganic Chemistry</i> , <b>1997</b> , 36, 4500-4507	5.1	53
37	Solution Structures of a Pair of Stable Hexaminecobalt (III/II) Conformers. <i>Angewandte Chemie International Edition in English</i> , <b>1997</b> , 36, 2006-2008		13
36	The Structure of an Isomeric Pair of a (Tetraamine)copper(II) Compound in the solid state and in solution. <i>Helvetica Chimica Acta</i> , <b>1997</b> , 80, 1831-1842	2	16
35	Reduction Potentials of Tetraaminecopper(II/I) Couples. <i>Helvetica Chimica Acta</i> , <b>1997</b> , 80, 1983-1991	2	21
34	Inorganic Molecular Mechanics. <i>Journal of Chemical Education</i> , <b>1996</b> , 73, 108	2.4	15
33	Interpretation of Electronic and EPR Spectra of Copper(II) Amine Complexes: A Test of the MM-AOM Method. <i>Inorganic Chemistry</i> , <b>1995</b> , 34, 3903-3911	5.1	90
32	Double Helical Dinuclear Copper(I) Complexes of Macrocyclic Bis(dithiadiimine) Ligands. <i>Angewandte Chemie International Edition in English</i> , <b>1995</b> , 34, 1883-1885		23
31	The Directionality of d-Orbitals and Molecular-Mechanics Calculations of Octahedral Transition-Metal Compounds. <i>Helvetica Chimica Acta</i> , <b>1995</b> , 78, 2042-2047	2	49
30	Solution Structures of Coordination Compounds. <i>Comments on Inorganic Chemistry</i> , <b>1994</b> , 16, 133-151	3.9	29
29	Prediction and Interpretation of EPR Spectra of Low-Spin Iron(III) Complexes with the MM-AOM Method. <i>Inorganic Chemistry</i> , <b>1994</b> , 33, 4577-4583	5.1	26
28	Solution Structures and Isomer Distributions of Bis( $\beta$ -diketonato) Complexes of Titanium(IV) and Cobalt(III). <i>Inorganic Chemistry</i> , <b>1994</b> , 33, 3396-3400	5.1	40
27	Molecular Mechanics and the Jahn-Teller Effect. <i>Inorganic Chemistry</i> , <b>1994</b> , 33, 5368-5369	5.1	51
26	Metal-Directed Synthesis of Macrocyclic Tetraamines With Pendant Nitro or Amine Groups, Based on trans-Cyclohexane-1,2-diamine. <i>Australian Journal of Chemistry</i> , <b>1994</b> , 47, 1171	1.2	16

25	Prediction and interpretation of electronic spectra of transition metal complexes via the combination of molecular mechanics and angular overlap model calculations. <i>Inorganic Chemistry</i> , <b>1993</b> , 32, 2798-2803	5.1	52
24	Complexation of cis-6,13-dimethyl-1,4,8,11-tetraazacyclotetradecane-6,13-diamine with the first row transition metal ions cobalt(III), chromium(III), and nickel(II). <i>Inorganic Chemistry</i> , <b>1993</b> , 32, 2804-2809	5.1	22
23	The relation between ligand structures, coordination stereochemistry, and electronic and thermodynamic properties. <i>Coordination Chemistry Reviews</i> , <b>1993</b> , 123, 1-48	23.2	141
22	Molecular mechanics calculations of transition metal complexes. <i>Inorganic Chemistry</i> , <b>1992</b> , 31, 2638-2644	5.1	112
21	Determination of solution structures of binuclear copper(II) complexes. <i>Inorganic Chemistry</i> , <b>1992</b> , 31, 2644-2651	5.1	57
20	Transition metal complexes of the novel tridentate di-2-pyridylmethanamine (dipa). <i>Inorganic Chemistry</i> , <b>1992</b> , 31, 4194-4200	5.1	24
19	Predictions and methods of separation of racemic bidentate ligands via stereoselective ligand exchange reactions. <i>Inorganic Chemistry</i> , <b>1992</b> , 31, 1220-1223	5.1	7
18	Chiral Tetraamines Based on (S)-2-(Aminomethyl)pyrrolidine: Template synthesis and properties of copper(II) complexes. <i>Helvetica Chimica Acta</i> , <b>1992</b> , 75, 145-152	2	12
17	Base Hydrolysis of Pentaaminecobalt(III) Complexes: The [CoX(dien) (dapo)] <sup>n+</sup> system. Part 1. Syntheses, structures, configuration, and spectroscopy. <i>Helvetica Chimica Acta</i> , <b>1992</b> , 75, 1130-1146	2	9
16	Base Hydrolysis of Pentaaminecobalt(III) Complexes: The [CoX(dien) (dapo)] <sup>n+</sup> system. Part 2. Structure and reactivity of the pentacoordinate intermediate. <i>Helvetica Chimica Acta</i> , <b>1992</b> , 75, 1147-1171	2	17
15	Base Hydrolysis of Pentaaminecobalt (III) Complexes: The [CoX(dien) (dapo)] <sup>n+</sup> system. Part 3. The internal conjugate base mechanism. <i>Helvetica Chimica Acta</i> , <b>1992</b> , 75, 1172-1184	2	15
14	A Molecular-Mechanics Analysis of Complexes of the Sexidentate Macrocycles cis- and trans-6,13-Dimethyl-1,4,8,11-tetraazacyclotetradecane-6,13-diamine. <i>Helvetica Chimica Acta</i> , <b>1991</b> , 74, 1834-1842	2	17
13	Coordination of the sexidentate macrocycle 6,13-dimethyl-1,4,8,11-tetraazacyclotetradecane-6,13-diamine to iron(III). <i>Inorganic Chemistry</i> , <b>1991</b> , 30, 942-946	5.1	27
12	EPR spectrum and metal-ligand bonding parameters of a low-spin (hexaamine)iron(III) complex. <i>Inorganic Chemistry</i> , <b>1991</b> , 30, 4088-4093	5.1	30
11	Synthesis, Crystal Structure and Magnetism of a Macrocyclic Binuclear Dicopper(II) Amino Alcohol Complex From a Metal Directed Reaction Involving Formaldehyde and Nitroethane. <i>Australian Journal of Chemistry</i> , <b>1990</b> , 43, 69	1.2	18
10	Stereoselective Coordination to Chiral Matrices. Cobalt(III). Chemistry of Simple Facially Coordinating Chiral Triamines. <i>Helvetica Chimica Acta</i> , <b>1990</b> , 73, 874-882	2	6
9	Dicopper(II) Complexes of Spiro Macrobicycles With Aza and Thia Aza Donor Sets. <i>Australian Journal of Chemistry</i> , <b>1990</b> , 43, 2035	1.2	23
8	Coordination of the "pendant-arm" macrocycle 6,13-diamino-6,13-dimethyl-1,4,8,11-tetraazacyclotetradecane to chromium(III). Crystal structure and physical properties of the hexacoordinated complex ion. <i>Inorganic Chemistry</i> , <b>1990</b> , 29, 3208-3213	5.1	17

7	Energy-Minimized Structures and Calculated and Experimental Isomer distributions in the hexaamine-cobalt(III) system $[\text{Co}(\text{L})_2]^{3+}$ with the chiral facially-coordinating triamine (L = butane-1,2,4-triamine). <i>Helvetica Chimica Acta</i> , <b>1989</b> , 72, 1029-1037	2	16
6	Coordination geometries of hexaamine cage complexes. <i>Inorganic Chemistry</i> , <b>1989</b> , 28, 426-431	5.1	45
5	The solution structure and reactivity of decavanadate. <i>Helvetica Chimica Acta</i> , <b>1988</b> , 71, 1406-1420	2	19
4	Energy-Minimized Structures and Calculated and Experimental Isomer Distributions in the Hexaaminocobalt(III) system $[\text{Co}(\text{trap})_2]^{3+}$ (trap = 1,2,3-propanetriamine). <i>Helvetica Chimica Acta</i> , <b>1988</b> , 71, 1875-1880	2	20
3	Synthesis of a Cis-N <sub>2</sub> S <sub>2</sub> Donor Macrocyclic by Metal-Directed Condensation of Formaldehyde, Nitroethane and a Diaminodithiaalkane - Crystal-Structure of the (6-Methyl-6-Nitro-1,11-Dithia-4,8-Diazacyclotetradecane)-Copper(II) Perchlorate Product. <i>Australian Journal of Chemistry</i> , <b>1988</b> , 41, 773	1.2	19
2	The titanyl question revisited. <i>Inorganic Chemistry</i> , <b>1987</b> , 26, 1315-1323	5.1	89
1	Exceptional Manganese(II) Stability and Manganese(II)/Zinc(II) Selectivity with Rigid Polydentate Ligands**. <i>Angewandte Chemie</i> , e202115580	3.6	0