Gopalan Rajaraman

List of Publications by Citations

257 papers	7,709 citations	51 h-index	72 g-index
286 ext. papers	8,870 ext. citations	5.6 avg, IF	6.43 L-index

#	Paper	IF	Citations
257	An air-stable Dy(iii) single-ion magnet with high anisotropy barrier and blocking temperature. *Chemical Science*, **2016**, 7, 5181-5191	9.4	404
256	Synthesis and characterization of heterometallic {Cr7M} wheels. *Angewandte Chemie - International Edition*, **2003**, 42, 101-5	16.4	179
255	A family of manganese rods: syntheses, structures, and magnetic properties. *Journal of the American Chemical Society*, **2004**, 126, 15445-57	16.4	159
254	Density functional studies on the exchange interaction of a dinuclear Gd(iii)-Cu(ii) complex: method assessment, magnetic coupling mechanism and magneto-structural correlations. *Dalton Transactions*, **2009**, 3153-61	4.3	129
253	Biomimetic high-valent non-heme iron oxidants for the cis-dihydroxylation and epoxidation of olefins. *Angewandte Chemie - International Edition*, **2007**, 46, 8067-70	16.4	124
252	Density functional studies on dinuclear {Ni(II)Gd(III)} and trinuclear {Ni(II)Gd(III)Ni(II)} complexes: magnetic exchange and magneto-structural maps. *Dalton Transactions*, **2011**, 40, 10897-906	4.3	120
251	Enhancing the effective energy barrier of a Dy(III) SMM using a bridged diamagnetic Zn(II) ion. *Chemical Communications*, **2014**, 50, 8838-41	5.8	110
250	New routes to polymetallic clusters: fluoride-based tri-, deca-, and hexaicosametallic MnIII clusters and their magnetic properties. *Chemistry - A European Journal*, **2004**, 10, 5180-94	4.8	109
249	A classification of spin frustration in molecular magnets from a physical study of large odd-numbered-metal, odd electron rings. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 19113-8	11.5	102
248	Mechanistic insights on the ortho-hydroxylation of aromatic compounds by non-heme iron complex: a computational case study on the comparative oxidative ability of ferric-hydroperoxo and high-valent Fe(IV)?O and Fe(V)?O intermediates. *Journal of the American Chemical Society*, **2013**, 135, 4235-49	16.4	101
247	A synthetic strategy for switching the single ion anisotropy in tetrahedral Co(II) complexes. *Chemical Communications*, **2015**, 51, 3739-42	5.8	95
246	Insight into D Symmetry: Targeting Strong Axiality in Stable Dysprosium(III) Hexagonal Bipyramidal Single-Ion Magnets. *Angewandte Chemie - International Edition*, **2019**, 58, 14146-14151	16.4	88
245	Is a radical bridge a route to strong exchange interactions in lanthanide complexes? A computational examination. *Chemical Communications*, **2012**, 48, 7856-8	5.8	87
244	Studies of an enneanuclear manganese single-molecule magnet. *Journal of the American Chemical Society*, **2005**, 127, 5572-80	16.4	85
243	Low-coordinate mononuclear lanthanide complexes as molecular nanomagnets. *Coordination Chemistry Reviews*, **2018**, 367, 163-216	23.2	84
242	Exploring the Influence of Diamagnetic Ions on the Mechanism of Magnetization Relaxation in {CoLn} (Ln = Dy, Tb, Ho) "Butterfly" Complexes. *Inorganic Chemistry*, **2017**, 56, 2518-2532	5.1	79
241	What Controls the Sign and Magnitude of Magnetic Anisotropy in Tetrahedral Cobalt(II) Single-Ion Magnets?. *Inorganic Chemistry*, **2016**, 55, 9564-9578	5.1	79

240	Fluoride-bridged {Gd(III)3M(III)2} (M = Cr, Fe, Ga) molecular magnetic refrigerants. *Angewandte Chemie - International Edition*, **2014**, 53, 2394-7	16.4	76
239	Resonant Quantum Tunneling in a New Tetranuclear Iron(III)-Based Single-Molecule Magnet. *Advanced Materials*, **2004**, 16, 1101-1105	24	76
238	Magnetic anisotropy and mechanism of magnetic relaxation in Er(III) single-ion magnets. *Inorganic Chemistry*, **2014**, 53, 10835-45	5.1	73
237	What controls the magnetic interaction in bis-□alkoxo Mn(III) dimers? A combined experimental and theoretical exploration. *Chemistry - A European Journal*, **2012**, 18, 5906-18	4.8	72
236	The mechanism of the (bispidine)copper(II)-catalyzed aziridination of styrene: a combined experimental and theoretical study. *Chemistry - A European Journal*, **2008**, 14, 5313-28	4.8	71
235	Effect of Ligand Substitution around the Dy(III) on the SMM Properties of Dual-Luminescent Zn-Dy and Zn-Dy-Zn Complexes with Large Anisotropy Energy Barriers: A Combined Theoretical and Experimental Magnetostructural Study. *Inorganic Chemistry*, **2016**, 55, 4428-40	5.1	71
234	EPR spectroscopy of a family of Cr(III) 7M(II) (M = Cd, Zn, Mn, Ni) "wheels": studies of isostructural compounds with different spin ground states. *Chemistry - A European Journal*, **2009**, 15, 3152-67	4.8	70
233	Theoretical methods enlighten magnetic properties of a family of Mn(6) single-molecule magnets. *Inorganic Chemistry*, **2009**, 48, 8012-9	5.1	67
232	DFT models for copper(II) bispidine complexes: structures, stabilities, isomerism, spin distribution, and spectroscopy. *Journal of Computational Chemistry*, **2006**, 27, 1263-77	3.5	67
231	Single-Molecule Magnetism, Enhanced Magnetocaloric Effect, and Toroidal Magnetic Moments in a Family of Ln4 Squares. *Chemistry - A European Journal*, **2015**, 21, 15639-50	4.8	66
230	Influence of Tuned Linker Functionality on Modulation of Magnetic Properties and Relaxation Dynamics in a Family of Six Isotypic Ln (Ln = Dy and Gd) Complexes. *Inorganic Chemistry*, **2016**, 55, 11283-11298	5.1	66
229	Ferrotoroidic ground state in a heterometallic {CrDy} complex displaying slow magnetic relaxation. *Nature Communications*, **2017**, 8, 1023	17.4	65
228	Magnetic exchange interactions and magneto-structural correlations in heterobridged □phenoxo-□(1,1)-azide dinickel(II) compounds: a combined experimental and theoretical exploration. *Inorganic Chemistry*, **2011**, 50, 7257-67	5.1	65
227	Symmetry and topology determine the MoV-CN-MnII exchange interactions in high-spin molecules. *Angewandte Chemie - International Edition*, **2005**, 44, 2711-2715	16.4	65
226	An unprecedented zero field neodymium(iii) single-ion magnet based on a phosphonic diamide. *Chemical Communications*, **2016**, 52, 7168-71	5.8	65
225	A novel undecametallic iron(III) cluster with an S = (11)/(2) spin ground state. *Inorganic Chemistry*, **2003**, 42, 6601-3	5.1	64
224	An FeIII wheel with a zwitterionic ligand: the structure and magnetic properties of [Fe(OMe)2(proline)]12[ClO4]12. *Chemical Communications*, **2004**, 314-5	5.8	63
223	Analysis of the Role of Peripheral Ligands Coordinated to Zn(II) in Enhancing the Energy Barrier in Luminescent Linear Trinuclear Zn-Dy-Zn Single-Molecule Magnets. *Chemistry - A European Journal*, **2015**, 21, 15785-96	4.8	62

222	Unprecedented magnetic relaxation via the fourth excited state in low-coordinate lanthanide single-ion magnets: a theoretical perspective. *Chemical Communications*, **2014**, 50, 15513-6	5.8	61
221	Magnetic exchange in {Gd(III)-radical} complexes: method assessment, mechanism of coupling and magneto-structural correlations. *Physical Chemistry Chemical Physics*, **2014**, 16, 14568-77	3.6	58
220	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?. *Inorganic Chemistry*, **2008**, 47, 8112-25	5.1	58
219	Large Hexadecametallic {Mn(III) -Ln(III) } Wheels: Synthesis, Structural, Magnetic, and Theoretical Characterization. *Chemistry - A European Journal*, **2015**, 21, 16364-9	4.8	57
218	A density functional theory study of the reaction of the biomimetic iron(II) complex of a tetradentate bispidine ligand with H2O2. *Inorganic Chemistry*, **2007**, 46, 3826-38	5.1	57
217	Studies of an Fe9 tridiminished icosahedron. *Chemistry - A European Journal*, **2006**, 12, 8961-8	4.8	56
216	Structural, magnetic and DFT studies of a hydroxide-bridged [Cr8] wheel. *Dalton Transactions*, **2004**, 1511-3	4.3	56
215	Role of the Diamagnetic Zinc(II) Ion in Determining the Electronic Structure of Lanthanide Single-Ion Magnets. *Chemistry - A European Journal*, **2017**, 23, 4903-4916	4.8	55
214	Chemical and in silico tuning of the magnetisation reversal barrier in pentagonal bipyramidal Dy(iii) single-ion magnets. *Chemical Communications*, **2018**, 54, 8273-8276	5.8	55
213	A family of [Mn6] complexes featuring tripodal ligands. *Inorganic Chemistry*, **2006**, 45, 6782-93	5.1	55
212	Heterometallic 3d-4f single molecule magnets containing diamagnetic metal ions. *Dalton Transactions*, **2018**, 47, 8841-8864	4.3	54
211	Epoxidation and 1,2-dihydroxylation of alkenes by a nonheme iron model system - DFT supports the mechanism proposed by experiment. *Inorganic Chemistry*, **2008**, 47, 78-93	5.1	54
210	Density functional calculations of a tetradecametallic iron(III) cluster with a very large spin ground state. *Chemical Communications*, **2004**, 1476-7	5.8	54
209	Synthesis and studies of a trinuclear Mn(II) carboxylate complex. *Dalton Transactions*, **2004**, 2550-5	4.3	54
208	Record high magnetic exchange and magnetization blockade in Ln2@C79N (Ln = Gd(III) and Dy(III)) molecules: a theoretical perspective. *Chemical Communications*, **2015**, 51, 17732-5	5.8	53
207	Observation of ferromagnetic exchange, spin crossover, reductively induced oxidation, and field-induced slow magnetic relaxation in monomeric cobalt nitroxides. *Inorganic Chemistry*, **2013**, 52, 7557-72	5.1	53
206	Modelling spin Hamiltonian parameters of molecular nanomagnets. *Chemical Communications*, **2016**, 52, 8972-9008	5.8	51
205	Selective C-H halogenation over hydroxylation by non-heme iron(iv)-oxo. *Chemical Science*, **2018**, 9, 7843-7858	9.4	50

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203	Theoretical studies on polynuclear {Cu(II)5Gd(III)n} clusters (n = 4, 2): towards understanding their large magnetocaloric effect. *Inorganic Chemistry*, **2015**, 54, 1661-70	5.1	50
202	A family of ferro- and antiferromagnetically coupled decametallic chromium(III) wheels. *Chemistry - A European Journal*, **2006**, 12, 1385-96	4.8	50
201	Biomimetic High-Valent Non-Heme Iron Oxidants for the cis-Dihydroxylation and Epoxidation of Olefins. *Angewandte Chemie*, **2007**, 119, 8213-8216	3.6	48
200	Magnetic and optical studies on an S = 6 ground-state cluster [Cr12O9(OH)3(O2CCMe3)15]: determination of, and the relationship between, single-ion and cluster spin Hamiltonian parameters. *Inorganic Chemistry*, **2003**, 42, 5293-303	5.1	46
199	Role of Magnetic Exchange Interactions in the Magnetization Relaxation of {3d-4f} Single-Molecule Magnets: A Theoretical Perspective. *Chemistry - A European Journal*, **2016**, 22, 672-80	4.8	46
198	A computational perspective on magnetic coupling, magneto-structural correlations and magneto-caloric effect of a ferromagnetically coupled {GdIIIGdIII} Pair. *Polyhedron*, **2013**, 52, 1299-1305	2.7	44
197	Quenching the Quantum Tunneling of Magnetization in Heterometallic Octanuclear {TM Dy } (TM=Co and Cr) Single-Molecule Magnets by Modification of the Bridging Ligands and Enhancing the Magnetic Exchange Coupling. *Chemistry - A European Journal*, **2017**, 23, 1654-1666	4.8	44
196	CopperII-mediated aromatic ortho-hydroxylation: a hybrid DFT and AB initio exploration. *Chemistry - A European Journal*, **2008**, 14, 344-57	4.8	44
195	Role of Single-Ion Anisotropy and Magnetic Exchange Interactions in Suppressing Zero-Field Tunnelling in {3d-4f} Single Molecule Magnets. *Inorganic Chemistry*, **2016**, 55, 11201-11215	5.1	44
194	Decisive interactions that determine ferro/antiferromagnetic coupling in {3d-4f} pairs: a case study on dinuclear {V(IV)-Gd(III)} complexes. *Dalton Transactions*, **2013**, 42, 3623-30	4.3	43
193	Origin of SMM behaviour in an asymmetric Er(III) Schiff base complex: a combined experimental and theoretical study. *Chemical Communications*, **2015**, 51, 6137-40	5.8	43
192	Discrete {Gd(III)M} (M = Gd(III) or Co(II)) pentanuclear complexes: a new class of metal-organophosphate molecular coolers. *Dalton Transactions*, **2015**, 44, 5961-5	4.3	43
191	Syntheses, structures, magnetic properties, and density functional theory magneto-structural correlations of bis(phenoxo) and bis(phenoxo)-acetate/bis(phenoxo)-bis(acetate) dinuclear Fe(III)Ni(II) compounds. *Inorganic Chemistry*, **2013**, 52, 12881-92	5.1	42
190	Computational insight into a gold(I) N-heterocyclic carbene mediated alkyne hydroamination reaction. *Inorganic Chemistry*, **2012**, 51, 5593-604	5.1	42
189	Synthesis and Characterization of Heterometallic {Cr7M} Wheels. *Angewandte Chemie*, **2003**, 115, 105-109	3.6	42
188	Magnetic anisotropy of mononuclear Ni(II) complexes: on the importance of structural diversity and the structural distortions. *Chemistry - A European Journal*, **2014**, 20, 10305-13	4.8	41
187	Enhancement of Tb(III) -Cu(II) Single-Molecule Magnet Performance through Structural Modification. *Chemistry - A European Journal*, **2016**, 22, 12839-48	4.8	40

186	Designing a Dy Single-Molecule Magnet with Two Well-Differentiated Relaxation Processes by Using a Nonsymmetric Bis-bidentate Bipyrimidine- N-Oxide Ligand: A Comparison with Mononuclear Counterparts. *Inorganic Chemistry*, **2018**, 57, 6362-6375	5.1	40
185	Slow Magnetic Relaxation and Single-Molecule Toroidal Behaviour in a Family of Heptanuclear {Cr Ln } (Ln=Tb, Ho, Er) Complexes. *Angewandte Chemie - International Edition*, **2018**, 57, 779-784	16.4	39
184	Acquiring a record barrier height for magnetization reversal in lanthanide encapsulated fullerene molecules using DFT and ab initio calculations. *Chemical Communications*, **2016**, 52, 14047-14050	5.8	38
183	Halogen Substitution Effects on N O Schiff Base Ligands in Unprecedented Abrupt Fe Spin Crossover Complexes. *Chemistry - A European Journal*, **2017**, 23, 7052-7065	4.8	37
182	Probing the origin of the giant magnetic anisotropy in trigonal bipyramidal Ni(ii) under high pressure. *Chemical Science*, **2018**, 9, 1551-1559	9.4	36
181	Aminotroponiminatogermaacid halides with a Ge(E)X moiety (E = S, Se; X = F, Cl). *Inorganic Chemistry*, **2012**, 51, 9240-8	5.1	34
180	Role of Halide Ions in the Nature of the Magnetic Anisotropy in Tetrahedral Co Complexes. *Chemistry - A European Journal*, **2017**, 23, 9546-9559	4.8	33
179	Boosting axiality in stable high-coordinate Dy(iii) single-molecule magnets. *Chemical Communications*, **2019**, 55, 5950-5953	5.8	33
178	Mechanism of magnetisation relaxation in {MIII2DyIII2} (M = Cr, Mn, Fe, Al) "Butterfly" complexes: how important are the transition metal ions here?. *Chemical Science*, **2019**, 10, 5528-5538	9.4	33
177	Oxidation of methane by an N-bridged high-valent diiron-oxo species: electronic structure implications on the reactivity. *Dalton Transactions*, **2015**, 44, 15232-43	4.3	33
176	Observation of Slow Relaxation and Single-Molecule Toroidal Behavior in a Family of Butterfly-Shaped Ln Complexes. *Chemistry - A European Journal*, **2016**, 22, 18532-18550	4.8	30
175	Probing the origin of magnetic anisotropy in a dinuclear {Mn(III)Cu(II)} single-molecule magnet: the role of exchange anisotropy. *Chemistry - A European Journal*, **2014**, 20, 5214-8	4.8	30
174	Substituted versus Naked Thiourea Ligand Containing Pseudotetrahedral Cobalt(II) Complexes: A Comparative Study on Its Magnetization Relaxation Dynamics Phenomenon. *Inorganic Chemistry*, **2018**, 57, 3371-3386	5.1	29
173	ortho-Hydroxylation of aromatic acids by a non-heme Fe(V)=O species: how important is the ligand design?. *Physical Chemistry Chemical Physics*, **2014**, 16, 14601-13	3.6	29
172	Angular dependence of the exchange interaction in fluoride-bridged Gd(III)-Cr(III) complexes. *Chemical Communications*, **2013**, 49, 5583-5	5.8	29
171	A periodic mixed gaussians-plane waves DFT study on simple thiols on Au(111): adsorbate species, surface reconstruction, and thiols functionalization. *Physical Chemistry Chemical Physics*, **2011**, 13, 3886-95	3.6	29
170	What controls the magnetic exchange interaction in mixed- and homo-valent Mn7 disc-like clusters? A theoretical perspective. *Chemistry - A European Journal*, **2015**, 21, 2881-92	4.8	28
169	From antiferromagnetic to ferromagnetic exchange in a family of oxime-based Mn(III) dimers: a magneto-structural study. *Dalton Transactions*, **2013**, 42, 16510-7	4.3	28

168	How strongly are the magnetic anisotropy and coordination numbers correlated in lanthanide based molecular magnets?. *Journal of Chemical Sciences*, **2014**, 126, 1569-1579	1.8	28
167	Studies of a linear single-molecule magnet. *Dalton Transactions*, **2007**, 5282-9	4.3	28
166	What Controls the Magnetic Exchange and Anisotropy in a Family of Tetranuclear {MnMn} Single-Molecule Magnets?. *Inorganic Chemistry*, **2017**, 56, 1932-1949	5.1	27
165	A cationic aluminium complex: an efficient mononuclear main-group catalyst for the cyanosilylation of carbonyl compounds. *Dalton Transactions*, **2017**, 46, 7672-7676	4.3	27
164	Magneto-Structural Properties and Theoretical Studies of a Family of Simple Heterodinuclear Phenoxide/Alkoxide Bridged MnLn Complexes: On the Nature of the Magnetic Exchange and Magnetic Anisotropy. *Inorganic Chemistry*, **2018**, 57, 3683-3698	5.1	27
163	Deciphering the origin of giant magnetic anisotropy and fast quantum tunnelling in Rhenium(IV) single-molecule magnets. *Nature Communications*, **2016**, 7, 10669	17.4	27
162	Solvate-dependent spin crossover and exchange in cobalt(II) oxazolidine nitroxide chelates. *Inorganic Chemistry*, **2014**, 53, 5055-66	5.1	27
161	A computational examination on the structure, spin-state energetics and spectroscopic parameters of high-valent Fe(IV)=NTs species. *Dalton Transactions*, **2012**, 41, 10430-9	4.3	27
160	Magnetic and theoretical characterization of a ferromagnetic Mn(III) dimer. *Polyhedron*, **2005**, 24, 2450-2454	2.7	26
159	Influence of the Ligand Field on the Slow Relaxation of Magnetization of Unsymmetrical Monomeric Lanthanide Complexes: Synthesis and Theoretical Studies. *Inorganic Chemistry*, **2017**, 56, 14260-14276	5.1	25
158	Crown-linked dipyridylamino-triazine ligands and their spin-crossover iron(II) derivatives: magnetism, photomagnetism and cooperativity. *Dalton Transactions*, **2013**, 42, 16494-509	4.3	25
157	Speciation of uranyl ions in fulvic acid and humic acid: a DFT exploration. *Physical Chemistry Chemical Physics*, **2011**, 13, 18038-46	3.6	25
156	Is a strong axial crystal-field the only essential condition for a large magnetic anisotropy barrier? The case of non-Kramers Ho(iii) versus Tb(iii). *Dalton Transactions*, **2018**, 47, 357-366	4.3	24
155	Self limiting atomic layer deposition of Al2O3 on perovskite surfaces: a reality?. *Nanoscale*, **2016**, 8, 7459-65	7.7	24
154	Theoretical studies on concerted versus two steps hydrogen atom transfer reaction by non-heme Mn(IV/III)=O complexes: how important is the oxo ligand basicity in the C-H activation step?. *Dalton Transactions*, **2013**, 42, 16518-26	4.3	24
153	Role of Coordination Number and Geometry in Controlling the Magnetic Anisotropy in Fe , Co , and Ni Single-Ion Magnets. *Chemistry - A European Journal*, **2020**, 26, 14036-14058	4.8	24
152	Engineering macrocyclic high performance pentagonal bipyramidal Dy(iii) single-ion magnets. *Chemical Communications*, **2020**, 56, 12037-12040	5.8	24
151	Stepwise Reversible Oxidation of N-Peralkyl-Substituted NHC-CAAC Derived Triazaalkenes: Isolation of Radical Cations and Dications. *Organic Letters*, **2017**, 19, 5605-5608	6.2	23

150	Role of (1,3) {Cu-Cu} Interaction on the Magneto-Caloric Effect of Trinuclear {Cu-Gd-Cu} Complexes: Combined DFT and Experimental Studies. *Inorganic Chemistry*, **2018**, 57, 1846-1858	5.1	23
149	Insight into D6h Symmetry: Targeting Strong Axiality in Stable Dysprosium(III) Hexagonal Bipyramidal Single-Ion Magnets. *Angewandte Chemie*, **2019**, 131, 14284-14289	3.6	22
148	Theoretical studies on {3d-Gd} and {3d-Gd-3d} complexes: Effect of metal substitution on the effective exchange interaction. *Polyhedron*, **2013**, 66, 81-86	2.7	22
147	An insight into a base-free Michael addition reaction as catalyzed by a bifunctional nickel N-heterocyclic carbene complex using density functional theory studies. *Journal of Organometallic Chemistry*, **2015**, 775, 109-116	2.3	21
146	Experimental and theoretical exploration of magnetic exchange interactions and single-molecule magnetic behaviour of bis(carboxylate)Gd/Dy systems. *Dalton Transactions*, **2018**, 47, 11455-11469	4.3	21
145	Theoretical studies on di- and tetra-nuclear Ni pivalate complexes. *Chemical Communications*, **2005**, 3053-5	5.8	21
144	Theoretical determination of the exchange coupling constants of a single-molecule magnet Fe10 complex. *Chemical Physics Letters*, **2005**, 415, 6-9	2.5	21
143	The Preparation of Complexes of Germanone from a Germanium Oxo Dimer. *Angewandte Chemie - International Edition*, **2016**, 55, 7742-6	16.4	21
142	Role of Lanthanide-Ligand bonding in the magnetization relaxation of mononuclear single-ion magnets: A case study on Pyrazole and Carbene ligated LnIII(Ln=Tb, Dy, Ho, Er) complexes. *Journal of Chemical Sciences*, **2016**, 128, 1615-1630	1.8	21
141	Digermylene Oxide Stabilized Group 11 Metal Iodide Complexes. *Inorganic Chemistry*, **2015**, 54, 11067-76	5.1	20
140	A DFT exploration of the organization of thiols on Au(111): a route to self-assembled monolayer of magnetic molecules. *Journal of Materials Chemistry*, **2010**, 20, 10747		20
139	High-Pressure Crystallographic and Magnetic Studies of Pseudo- Symmetric Dy(III) and Ho(III) Single-Molecule Magnets. *Inorganic Chemistry*, **2020**, 59, 717-729	5.1	20
138	Pentagonal Bipyramidal Ln(III) Complexes Containing an Axial Phosphine Oxide Ligand: Field-induced Single-ion Magnetism Behavior of the Dy(III) Analogues. *Inorganic Chemistry*, **2020**, 59, 6603-6612	5.1	20
137	Oblate versus Prolate Electron Density of Lanthanide Ions: A Design Criterion for Engineering Toroidal Moments? A Case Study on {Ln } (Ln=Tb, Dy, Ho and Er) Wheels. *Chemistry - A European Journal*, **2019**, 25, 4156-4165	4.8	19
136	Influence of a Counteranion on the Zero-Field Splitting of Tetrahedral Cobalt(II) Thiourea Complexes. *Inorganic Chemistry*, **2019**, 58, 9085-9100	5.1	19
135	Theoretical Studies on Hexanuclear [M(O/OH)] (M = Fe(III), Mn(III), and Ni(II)) Clusters: Magnetic Exchange, Magnetic Anisotropy, and Magneto-Structural Correlations. *Inorganic Chemistry*, **2019**, 58, 3175-3188	5.1	19
134	Magnetic Anisotropy in Co X (X=O, S, Se) Single-Ion Magnets: Role of Structural Distortions versus Heavy Atom Effect. *Chemistry - an Asian Journal*, **2019**, 14, 4696-4704	4.5	19
133	Combining complementary ligands into one framework for the construction of a ferromagnetically coupled [Mn(III)12] wheel. *Chemistry - A European Journal*, **2014**, 20, 3010-3	4.8	19

132	Stability of molecular layer deposited zincone films: experimental and theoretical exploration. *RSC Advances*, **2015**, 5, 29947-29952	3.7	18
131	Can anisotropic exchange be reliably calculated using density functional methods? A case study on trinuclear Mn(III)-M(III)-Mn(III) (M=Fe, Ru, and Os) cyanometalate single-molecule magnets. *Chemistry - A European Journal*, **2014**, 20, 113-23	4.8	18
130	Use of thio and seleno germanones as ligands: silver(I) halide complexes with Ge?E-Ag-I (E = S, Se) moieties and chalcogen-dependent argentophilic interaction. *Inorganic Chemistry*, **2014**, 53, 10054-9	5.1	18
129	Encouraging Chromium(III) Ions to Form Larger Clusters: Syntheses, Structures, Magnetic Properties and Theoretical Studies of Di- and Octametallic Cr Clusters. *European Journal of Inorganic Chemistry*, **2006**, 2006, 3382-3392	2.3	18
128	Design of a Family of Ln Triangles with the HAT Ligand (1,4,5,8,9,12-Hexaazatriphenylene): Single-Molecule Magnetism. *Inorganic Chemistry*, **2017**, 56, 5594-5610	5.1	17
127	Single-step conversion of silathiogermylene to germaacid anhydrides: unusual reactivity. *Chemical Communications*, **2015**, 51, 4310-3	5.8	17
126	Role of oxidation state, ferryl-oxygen, and ligand architecture on the reactivity of popular high-valent FeIV=O species: A theoretical perspective. *Coordination Chemistry Reviews*, **2020**, 419, 213397	23.2	17
125	Solution and Solid-State Study of the Spin-Crossover [FeII(R-bik)3](BF4)2 Complexes (R = Me, Et, Vinyl). *European Journal of Inorganic Chemistry*, **2018**, 2018, 414-428	2.3	17
124	Key role of higher order symmetry and electrostatic ligand field design in the magnetic relaxation of low-coordinate Er(iii) complexes. *Dalton Transactions*, **2017**, 46, 11913-11924	4.3	17
123	Can CH???Interactions be used to design single-chain magnets?. *Chemistry - A European Journal*, **2015**, 21, 980-3	4.8	17
122	Modeling thiols on Au(111): Structural, thermodynamic and magnetic properties of simple thiols and thiol-radicals. *Superlattices and Microstructures*, **2009**, 46, 4-9	2.8	17
121	Thermally-Induced Spin Crossover and LIESST Effect in the Neutral [Fe(bik)(NCX)] Complexes: Variable-Temperature Structural, Magnetic, and Optical Studies (X = S, Se; bik = bis(1-methylimidazol-2-yl)ketone). *Frontiers in Chemistry*, **2018**, 6, 326	5	17
120	Mechanistic insights into intramolecular ortho-amination/hydroxylation by nonheme Fe[double bond, length as m-dash]NTs/Fe[double bond, length as m-dash]O species: the vs. the channels. *Chemical Communications*, **2017**, 53, 3193-3196	5.8	16
119	New examples of triangular terbium(iii) and holmium(iii) and hexagonal dysprosium(iii) single molecule toroics. *Dalton Transactions*, **2019**, 48, 15657-15667	4.3	16
118	Expanding the limits of catalysts with low-valent main-group elements for the hydroboration of aldehydes and ketones using [LSn(ii)][OTf] (L = aminotroponate; OTf = triflate). *Dalton Transactions*, **2019**, 48, 664-672	4.3	16
117	Atomic layer deposition of Zn3N2 thin films: growth mechanism and application in thin film transistor. *RSC Advances*, **2015**, 5, 22712-22717	3.7	16
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