

# Gopalan Rajaraman

## 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.

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	Synergistic Experimental and Theoretical Studies of Luminescent-Magnetic LnZn Clusters.. <i>Inorganic Chemistry</i> , <b>2022</b> ,	5.1	2
256	Deciphering the Role of Symmetry and Ligand Field in Designing Three-Coordinate Uranium and Plutonium Single-Molecule Magnets.. <i>Inorganic Chemistry</i> , <b>2022</b> ,	5.1	2
255	A theoretical perspective on the reactivity of high-valent Mn-Oxo/nitrene species towards oxidative transformations. <i>Inorganica Chimica Acta</i> , <b>2022</b> , 529, 120654	2.7	
254	Electric-Field-Induced Solid-Gas Interfacial Chemical Reaction in Carbon Nanotube Ensembles: Route toward Ultra-sensitive Gas Detectors.. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2022</b> ,	9.5	1
253	The Decisive Role of Spin States and Spin Coupling in Dictating Selective O Adsorption in Chromium(II) Metal-Organic Frameworks.. <i>Chemistry - A European Journal</i> , <b>2022</b> , e202200661	4.8	
252	Oxidation state variation in bis-calix[4]arene supported decametallc Mn clusters. <i>Dalton Transactions</i> , <b>2021</b> , 50, 17566-17572	4.3	
251	Strategies to Design Single-Molecule Toroids Using Triangular {Ln} Motifs.. <i>ACS Omega</i> , <b>2021</b> , 6, 32349-32364	3.64	1
250	Deciphering the Role of Anions and Secondary Coordination Sphere in Tuning Anisotropy in Dy(III) Air-Stable D SIMs*. <i>Chemistry - A European Journal</i> , <b>2021</b> , 28, e202103585	4.8	3
249	A six-coordinate high-spin Fe <sup>2+</sup> O species of cucurbit[5]uril: a highly potent catalyst for C-H hydroxylation of methane, if synthesised. <i>Chemical Communications</i> , <b>2021</b> ,	5.8	1
248	Attaining record-high magnetic exchange, magnetic anisotropy and blocking barriers in dilanthanofullerenes. <i>Chemical Science</i> , <b>2021</b> , 12, 14207-14216	9.4	3
247	Tuning the Ferrotoroidic Coupling and Magnetic Hysteresis in Double-Triangle Complexes {Dy <sub>3</sub> MIIIIDy <sub>3</sub> } via the MIII-linker. <i>European Journal of Inorganic Chemistry</i> , <b>2021</b> , 2021, 435-444	2.3	7
246	Structure-property correlation in stabilizing axial magnetic anisotropy in octahedral Co(II) complexes. <i>Cell Reports Physical Science</i> , <b>2021</b> , 2, 100404	6.1	6
245	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
244	Effect of the Ligand Backbone on the Reactivity and Mechanistic Paradigm of Non-Heme Iron(IV)-Oxo during Olefin Epoxidation. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 14149-14158	3.6	2
243	Ligand-Constraint-Induced Peroxide Activation for Electrophilic Reactivity. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 15081-15086	3.6	
242	Effect of the Ligand Backbone on the Reactivity and Mechanistic Paradigm of Non-Heme Iron(IV)-Oxo during Olefin Epoxidation. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 14030-14039	16.4	5
241	Ligand-Constraint-Induced Peroxide Activation for Electrophilic Reactivity. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 14954-14959	16.4	4

240	Azide-Coordination in Homometallic Dinuclear Lanthanide(III) Complexes Containing Nonequivalent Lanthanide Metal Ions: Zero-Field SMM Behavior in the Dysprosium Analogue. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 8530-8545	5.1	4
239	Enantiopure Polyradical Tetrahedral Pd L Cages. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 10012-10015	4.8	1
238	Record High Magnetic Anisotropy in Three-Coordinate Mn and Cr Complexes: A Theoretical Perspective. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 9680-9687	5.1	0
237	Insights into the Dual Shuttle Catalytic Mechanism of Guanine Deaminase. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 8814-8826	3.4	1
236	Mechanistic Insights into the Oxygen Atom Transfer Reactions by Nonheme Manganese Complex: A Computational Case Study on the Comparative Oxidative Ability of Manganese-Hydroperoxo vs High-Valent Mn <sup>2+</sup> O and Mn-OH Intermediates. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 12085-12099	5.1	2
235	Modulation of Magnetic Anisotropy and Exchange Interaction in Phenoxide-Bridged Dinuclear Co(II) Complexes. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 11948-11956	5.1	4
234	[(VO)MII5] (M = Ni, Co) Anderson wheels. <i>Dalton Transactions</i> , <b>2021</b> , 50, 12495-12501	4.3	0
233	Are lanthanide-transition metal direct bonds a route to achieving new generation {3d-4f} SMMs?. <i>Dalton Transactions</i> , <b>2021</b> , 50, 16099-16109	4.3	3
232	Exploiting host-guest chemistry to manipulate magnetic interactions in metallocupramolecular ML tetrahedral cages. <i>Chemical Science</i> , <b>2021</b> , 12, 5134-5142	9.4	5
231	design to enhance the barrier height for magnetization reversal in Dy(III) sandwich complexes by stitching them under the umbrella of corannulene. <i>Chemical Science</i> , <b>2021</b> , 12, 11506-11514	9.4	1
230	Magnetic coupling in oximate bridged {MnIII6} clusters bridged by diamagnetic dicyano-metallato linkers: A theoretical perspective. <i>Polyhedron</i> , <b>2021</b> , 206, 115346	2.7	
229	Arjunetin as a promising drug candidate against SARS-CoV-2: molecular dynamics simulation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 1-22	3.6	1
228	A high-frequency EPR study of magnetic anisotropy and intermolecular interactions of Co(II) ions. <i>Polyhedron</i> , <b>2021</b> , 208, 115389	2.7	1
227	strategy to boost stability, axiality, and barrier heights in dysprosium SIMs SWCNT encapsulation. <i>Chemical Communications</i> , <b>2021</b> , 57, 11350-11353	5.8	1
226	Enhancing the barrier height for magnetization reversal in 4d/4f RulII2LnIII2 "butterfly" single molecule magnets (Ln = Gd, Dy) targeted structural alterations. <i>Dalton Transactions</i> , <b>2021</b> , 50, 12265-12274	4.3	1
225	A large axial magnetic anisotropy in trigonal bipyramidal Fe(II). <i>Chemical Communications</i> , <b>2020</b> , 56, 6826-6829	5.8	2
224	Role of oxidation state, ferryl-oxygen, and ligand architecture on the reactivity of popular high-valent FeIV=O species: A theoretical perspective. <i>Coordination Chemistry Reviews</i> , <b>2020</b> , 419, 213397	3.2	17
223	Deciphering the origin of million-fold reactivity observed for the open core diiron [HO-Fe-O-Fe[double bond, length as m-dash]O] species towards C-H bond activation: role of spin-states, spin-coupling, and spin-cooperation. <i>Chemical Science</i> , <b>2020</b> , 11, 10669-10687	9.4	7

222	Deciphering the mechanism of oxygen atom transfer by non-heme Mn-oxo species: an ab initio and DFT exploration. <i>Dalton Transactions</i> , <b>2020</b> , 49, 10380-10393	4-3	4
221	Mechanistic Insights on the Formation of High-Valent Mn(III/IV)=O Species Using Oxygen as Oxidant: A Theoretical Perspective. <i>Israel Journal of Chemistry</i> , <b>2020</b> , 60, 973-986	3-4	3
220	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
219	Influence of ligand field on magnetic anisotropy in a family of pentacoordinate Co complexes. <i>Dalton Transactions</i> , <b>2020</b> , 49, 4785-4796	4-3	6
218	A Design Criteria to Achieve Giant Ising-Type Anisotropy in Co -Encapsulated Metallofullerenes. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 464-477	4-8	10
217	There is nothing wrong with being soft: using sulfur ligands to increase axiality in a Dy(III) single-ion magnet. <i>Chemical Communications</i> , <b>2020</b> , 56, 1533-1536	5-8	12
216	The effect of the electronic structure and flexibility of the counteranions on magnetization relaxation in [Dy(L) <sub>2</sub> (H <sub>2</sub> O) <sub>5</sub> ] <sup>3+</sup> (L = phosphine oxide derivative) pentagonal bipyramidal SIMs. <i>Inorganic Chemistry Frontiers</i> , <b>2020</b> , 7, 689-699	6-8	15
215	High-Pressure Crystallographic and Magnetic Studies of Pseudo- Symmetric Dy(III) and Ho(III) Single-Molecule Magnets. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 717-729	5-1	20
214	Lanthanoid pyridyl-diketonate 'triangles'. New examples of single molecule toroics. <i>Dalton Transactions</i> , <b>2020</b> , 49, 17421-17432	4-3	1
213	An approach to estimate the barrier height for magnetisation reversal in {Dy} SMMs using calculations. <i>Dalton Transactions</i> , <b>2020</b> , 49, 14781-14785	4-3	10
212	Role of Coordination Number and Geometry in Controlling the Magnetic Anisotropy in Fe , Co , and Ni Single-Ion Magnets. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 14036-14058	4-8	24
211	Engineering macrocyclic high performance pentagonal bipyramidal Dy(III) single-ion magnets. <i>Chemical Communications</i> , <b>2020</b> , 56, 12037-12040	5-8	24
210	Enhancing the barrier height for Yb(III) single-ion magnets by modulating axial ligand fields. <i>Chemical Communications</i> , <b>2020</b> , 56, 11879-11882	5-8	4
209	Modulating magnetic anisotropy in Ln(III) single-ion magnets using an external electric field. <i>Chemical Science</i> , <b>2020</b> , 11, 10324-10330	9-4	4
208	Pentagonal Bipyramidal Ln(III) Complexes Containing an Axial Phosphine Oxide Ligand: Field-induced Single-ion Magnetism Behavior of the Dy(III) Analogues. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 6603-6612	5-1	20
207	New examples of triangular terbium(III) and holmium(III) and hexagonal dysprosium(III) single molecule toroics. <i>Dalton Transactions</i> , <b>2019</b> , 48, 15657-15667	4-3	16
206	Magnetic Properties of a Family of [MnLn] Wheel Complexes: An Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 13815-13825	5-1	9
205	Lanthanide complexes as molecular dopants for realizing air-stable n-type graphene logic inverters with symmetric transconductance. <i>Materials Horizons</i> , <b>2019</b> , 6, 743-750	14-4	6

204	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). <i>Dalton Transactions</i> , <b>2019</b> , 48, 664-672	4.3	16
203	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. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 4156-4165	4.8	19
202	{MnIII2LnIII2} (Ln = Gd, La or Y) butterfly complexes: Ferromagnetic exchange observed between bis-alkoxo bridged manganese(III) ions. <i>Polyhedron</i> , <b>2019</b> , 170, 508-514	2.7	3
201	Deciphering the origin of variation in the spin ground state and oxidation state of a {Mn} cluster on a Au(111) surface: is the Au(111) surface innocent?. <i>Chemical Communications</i> , <b>2019</b> , 55, 8238-8241	5.8	3
200	Influence of a Counteranion on the Zero-Field Splitting of Tetrahedral Cobalt(II) Thiourea Complexes. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 9085-9100	5.1	19
199	Influence of -Substitution on the Formation and Oxidation of NHC-CAAC-Derived Triazaalkenes. <i>Journal of Organic Chemistry</i> , <b>2019</b> , 84, 8899-8909	4.2	10
198	In-depth investigation of large axial magnetic anisotropy in monometallic 3d complexes using frequency domain magnetic resonance and methods: a study of trigonal bipyramidal Co(ii). <i>Chemical Science</i> , <b>2019</b> , 10, 6354-6361	9.4	12
197	How important is the coordinating atom in controlling magnetic anisotropy in uranium(iii) single-ion magnets? A theoretical perspective. <i>Dalton Transactions</i> , <b>2019</b> , 48, 8976-8988	4.3	13
196	Boosting axiality in stable high-coordinate Dy(iii) single-molecule magnets. <i>Chemical Communications</i> , <b>2019</b> , 55, 5950-5953	5.8	33
195	Mechanism of magnetisation relaxation in {MIII2DyIII2} (M = Cr, Mn, Fe, Al) "Butterfly" complexes: how important are the transition metal ions here?. <i>Chemical Science</i> , <b>2019</b> , 10, 5528-5538	9.4	33
194	Phosphonate-assisted tetranuclear lanthanide assemblies: observation of the toroidic ground state in the Tb analogue. <i>Dalton Transactions</i> , <b>2019</b> , 48, 6421-6434	4.3	8
193	Theoretical Studies on Hexanuclear [M(EO/OH)] (M = Fe(III), Mn(III), and Ni(II)) Clusters: Magnetic Exchange, Magnetic Anisotropy, and Magneto-Structural Correlations. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 3175-3188	5.1	19
192	Theoretical Studies on Trinuclear {MnGd} and Tetranuclear {MnGd} Clusters: Magnetic Exchange, Mechanism of Magnetic Coupling, Magnetocaloric Effect, and Magneto-Structural Correlations. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 11927-11940	5.1	12
191	Slow Magnetic Relaxation in Dinuclear CoY Complexes. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 10725-10735	5.1	9
190	A single-ion single-electron cerrous magnet. <i>Dalton Transactions</i> , <b>2019</b> , 48, 15928-15935	4.3	7
189	Microwave assisted synthesis of heterometallic 3d-4f MLn complexes. <i>Dalton Transactions</i> , <b>2019</b> , 48, 12440-12450	4.3	14
188	Insight into D6h Symmetry: Targeting Strong Axiality in Stable Dysprosium(III) Hexagonal Bipyramidal Single-Ion Magnets. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 14284-14289	3.6	22
187	Insight into D Symmetry: Targeting Strong Axiality in Stable Dysprosium(III) Hexagonal Bipyramidal Single-Ion Magnets. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 14146-14151	16.4	88

186	Investigation of the magnetic anisotropy in a series of trigonal bipyramidal Mn(ii) complexes. <i>Dalton Transactions</i> , <b>2019</b> , 48, 15480-15486	4.3	6
185	Unprecedented Copper(II) Complex with a Topoquinone-like Moiety as a Structural and Functional Mimic for Copper Amine Oxidase: Role of Copper(II) in the Genesis and Amine Oxidase Activity. <i>ACS Catalysis</i> , <b>2019</b> , 9, 10940-10950	13.1	6
184	Role of Ab Initio Calculations in the Design and Development of Organometallic Lanthanide-Based Single-Molecule Magnets. <i>Chemistry - an Asian Journal</i> , <b>2019</b> , 14, 4056-4073	4.5	8
183	Magnetic Anisotropy in Co X (X=O, S, Se) Single-Ion Magnets: Role of Structural Distortions versus Heavy Atom Effect. <i>Chemistry - an Asian Journal</i> , <b>2019</b> , 14, 4696-4704	4.5	19
182	An [FeIII34] Molecular Metal Oxide. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 17059-17062	3.6	2
181	An [Fe ] Molecular Metal Oxide. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 16903-16906	16.4	12
180	Donor-acceptor-stabilised germanium analogues of acid chloride, ester, and acyl pyrrole compounds: synthesis and reactivity. <i>Chemical Science</i> , <b>2019</b> , 10, 4402-4411	9.4	8
179	In silico design of pseudo D5h actinide based molecular magnets: role of covalency in magnetic anisotropy. <i>Journal of Chemical Sciences</i> , <b>2019</b> , 131, 1	1.8	8
178	Pseudohalogenogermynes versus Halogenogermynes: Difference in their Complexation Behavior towards Group 6 Metal Carbonyls. <i>Chemistry - an Asian Journal</i> , <b>2018</b> , 13, 1357-1365	4.5	7
177	Substituted versus Naked Thiourea Ligand Containing Pseudotetrahedral Cobalt(II) Complexes: A Comparative Study on Its Magnetization Relaxation Dynamics Phenomenon. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 3371-3386	5.1	29
176	Axial vs. Equatorial Ligand Rivalry in Controlling the Reactivity of Iron(IV)-Oxo Species: Single-State vs. Two-State Reactivity. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 6818-6827	4.8	9
175	Role of (1,3) {Cu-Cu} Interaction on the Magneto-Caloric Effect of Trinuclear {Cu-Gd-Cu} Complexes: Combined DFT and Experimental Studies. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 1846-1858	5.1	23
174	Probing the origin of the giant magnetic anisotropy in trigonal bipyramidal Ni(ii) under high pressure. <i>Chemical Science</i> , <b>2018</b> , 9, 1551-1559	9.4	36
173	Understanding the Mechanism of Magnetic Relaxation in Pentanuclear {MnMnLn} Single-Molecule Magnets. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 1158-1170	5.1	15
172	Low-coordinate mononuclear lanthanide complexes as molecular nanomagnets. <i>Coordination Chemistry Reviews</i> , <b>2018</b> , 367, 163-216	23.2	84
171	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. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 3683-3698	5.1	27
170	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). <i>Dalton Transactions</i> , <b>2018</b> , 47, 357-366	4.3	24
169	Solution and Solid-State Study of the Spin-Crossover [FeII(R-bik)3](BF4)2 Complexes (R = Me, Et, Vinyl). <i>European Journal of Inorganic Chemistry</i> , <b>2018</b> , 2018, 414-428	2.3	17



168	Structure, Bonding, Reactivity and Spectral Features of Putative NiIII=O Species: A Theoretical Perspective. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2018</b> , 644, 790-800	1.3	2
167	Experimental and theoretical exploration of magnetic exchange interactions and single-molecule magnetic behaviour of bis(μ <sub>3</sub> -carboxylate)Gd/Dy systems. <i>Dalton Transactions</i> , <b>2018</b> , 47, 11455-11469	4.3	21
166	Chemical and in silico tuning of the magnetisation reversal barrier in pentagonal bipyramidal Dy(iii) single-ion magnets. <i>Chemical Communications</i> , <b>2018</b> , 54, 8273-8276	5.8	55
165	Selective C-H halogenation over hydroxylation by non-heme iron(iv)-oxo. <i>Chemical Science</i> , <b>2018</b> , 9, 7843-7858	5.0	50
164	Heterometallic 3d-4f single molecule magnets containing diamagnetic metal ions. <i>Dalton Transactions</i> , <b>2018</b> , 47, 8841-8864	4.3	54
163	Deciphering the origin of invariance in magnetic anisotropy in {FeS} complexes: a theoretical perspective. <i>Dalton Transactions</i> , <b>2018</b> , 47, 9980-9984	4.3	9
162	Rationalizing the sign and magnitude of the magnetic coupling and anisotropy in dinuclear manganese(iii) complexes. <i>Dalton Transactions</i> , <b>2018</b> , 47, 11820-11833	4.3	13
161	Slow Magnetic Relaxation and Single-Molecule Toroidal Behaviour in a Family of Heptanuclear {Cr Ln } (Ln=Tb, Ho, Er) Complexes. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 779-784	16.4	39
160	Comparison on atomic/molecular layer deposition grown aluminum alkoxide polymer films using alkane and alkyne organic precursors. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , <b>2018</b> , 36, 01A108	2.9	6
159	A Chiral Bipyrimidine-Bridged Dy SMM: A Comparative Experimental and Theoretical Study of the Correlation Between the Distortion of the DyO <sub>6</sub> N <sub>2</sub> Coordination Sphere and the Anisotropy Barrier. <i>Frontiers in Chemistry</i> , <b>2018</b> , 6, 537	5	12
158	Trapping of a Pseudotetrahedral CoO Core in Mixed-Valence Mixed-Geometry [Co] Coordination Aggregates: Synthetic Marvel, Structures, and Magnetism. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 13176-13187	5.1	12
157	Nucleophilic versus Electrophilic Reactivity of Bioinspired Superoxido Nickel(II) Complexes. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 15099-15103	3.6	2
156	Nucleophilic versus Electrophilic Reactivity of Bioinspired Superoxido Nickel(II) Complexes. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 14883-14887	16.4	16
155	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). <i>Frontiers in Chemistry</i> , <b>2018</b> , 6, 326	5	17
154	Mononuclear Dysprosium(III) Complexes with Triphenylphosphine Oxide Ligands: Controlling the Coordination Environment and Magnetic Anisotropy. <i>Inorganics</i> , <b>2018</b> , 6, 61	2.9	14
153	Role of Ab Initio Calculations in the Design and Development of Lanthanide Based Single Molecule Magnets. <i>Topics in Organometallic Chemistry</i> , <b>2018</b> , 281-354	0.6	2
152	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. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 6362-6375	5.1	40
151	"Abnormal" Addition of NHC to a Conjugate Acid of CAAC: Formation of N-Alkyl-Substituted CAAC. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 12722-12727	4.8	6

150	A simple methodology for constructing ferromagnetically coupled Cr(iii) compounds. <i>Dalton Transactions</i> , <b>2018</b> , 47, 8100-8109	4.3	7
149	Magnetic Anisotropy, MagnetoStructural Correlations and Mechanism of Magnetic Relaxation in {DyIIIIN8} Complexes: A Theoretical Perspective. <i>European Journal of Inorganic Chemistry</i> , <b>2018</b> , 2018, 3402-3412	2.3	7
148	Slow Magnetic Relaxation and Single-Molecule Toroidal Behaviour in a Family of Heptanuclear {CrIII LnIII6} (Ln=Tb, Ho, Er) Complexes. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 787-792	3.6	11
147	What Controls the Magnetic Exchange and Anisotropy in a Family of Tetranuclear {MnMn} Single-Molecule Magnets?. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 1932-1949	5.1	27
146	Exploring the Influence of Diamagnetic Ions on the Mechanism of Magnetization Relaxation in {CoLn} (Ln = Dy, Tb, Ho) "Butterfly" Complexes. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 2518-2532	5.1	79
145	Role of the Diamagnetic Zinc(II) Ion in Determining the Electronic Structure of Lanthanide Single-Ion Magnets. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 4903-4916	4.8	55
144	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 $\sigma$ vs. the $\pi$ channels. <i>Chemical Communications</i> , <b>2017</b> , 53, 3193-3196	5.8	16
143	Interplay of Electronic Cooperativity and Exchange Coupling in Regulating the Reactivity of Diiron(IV)-oxo Complexes towards C-H and O-H Bond Activation. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 10110-10125	4.8	14
142	Design of a Family of Ln Triangles with the HAT Ligand (1,4,5,8,9,12-Hexaazatriphenylene): Single-Molecule Magnetism. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 5594-5610	5.1	17
141	Halogen Substitution Effects on N O Schiff Base Ligands in Unprecedented Abrupt Fe Spin Crossover Complexes. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 7052-7065	4.8	37
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23	Studies of an Fe <sub>9</sub> tridiminished icosahedron. <i>Chemistry - A European Journal</i> , <b>2006</b> , 12, 8961-8	4.8	56
22	Encouraging Chromium(III) Ions to Form Larger Clusters: Syntheses, Structures, Magnetic Properties and Theoretical Studies of Di- and Octametallc Cr Clusters. <i>European Journal of Inorganic Chemistry</i> , <b>2006</b> , 2006, 3382-3392	2.3	18
21	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
20	A family of [Mn <sub>6</sub> ] complexes featuring tripodal ligands. <i>Inorganic Chemistry</i> , <b>2006</b> , 45, 6782-93	5.1	55
19	Theoretical studies on di- and tetra-nuclear Ni pivalate complexes. <i>Chemical Communications</i> , <b>2005</b> , 3053-5	3.5	21
18	Studies of an enneanuclear manganese single-molecule magnet. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 5572-80	16.4	85
17	Magnetic and theoretical characterization of a ferromagnetic Mn(III) dimer. <i>Polyhedron</i> , <b>2005</b> , 24, 2450-2454	4.5	26
16	Theoretical determination of the exchange coupling constants of a single-molecule magnet Fe <sub>10</sub> complex. <i>Chemical Physics Letters</i> , <b>2005</b> , 415, 6-9	2.5	21
15	Symmetry and topology determine the MoV-CN-MnII exchange interactions in high-spin molecules. <i>Angewandte Chemie - International Edition</i> , <b>2005</b> , 44, 2711-2715	16.4	65
14	Symmetry and Topology Determine the MoV-CN-MnII Exchange Interactions in High-Spin Molecules. <i>Angewandte Chemie</i> , <b>2005</b> , 117, 2771-2775	3.6	15
13	Single-crystal parallel-mode EPR spectroscopy of an S=6 ground-state transition-metal cluster. <i>Physical Review B</i> , <b>2004</b> , 69,	3.3	11
12	A family of manganese rods: syntheses, structures, and magnetic properties. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 15445-57	16.4	159
11	Resonant Quantum Tunneling in a New Tetranuclear Iron(III)-Based Single-Molecule Magnet. <i>Advanced Materials</i> , <b>2004</b> , 16, 1101-1105	24	76
10	New routes to polymetallic clusters: fluoride-based tri-, deca-, and hexaicosametallc MnIII clusters and their magnetic properties. <i>Chemistry - A European Journal</i> , <b>2004</b> , 10, 5180-94	4.8	109
9	Density functional calculations of a tetradecametallic iron(III) cluster with a very large spin ground state. <i>Chemical Communications</i> , <b>2004</b> , 1476-7	5.8	54
8	Structural, magnetic and DFT studies of a hydroxide-bridged [Cr <sub>8</sub> ] wheel. <i>Dalton Transactions</i> , <b>2004</b> , 1511-3	4.3	56
7	Synthesis and studies of a trinuclear Mn(II) carboxylate complex. <i>Dalton Transactions</i> , <b>2004</b> , 2550-5	4.3	54

6	An FeIII wheel with a zwitterionic ligand: the structure and magnetic properties of [Fe(OMe) <sub>2</sub> (proline)] <sub>12</sub> [ClO <sub>4</sub> ] <sub>12</sub> . <i>Chemical Communications</i> , <b>2004</b> , 314-5	5.8	63
5	Magnetic and optical studies on an S = 6 ground-state cluster [Cr <sub>12</sub> O <sub>9</sub> (OH) <sub>3</sub> (O <sub>2</sub> CCMe <sub>3</sub> ) <sub>15</sub> ]: determination of, and the relationship between, single-ion and cluster spin Hamiltonian parameters. <i>Inorganic Chemistry</i> , <b>2003</b> , 42, 5293-303	5.1	46
4	Synthesis and Characterization of Heterometallic {Cr <sub>7</sub> M} Wheels. <i>Angewandte Chemie</i> , <b>2003</b> , 115, 105-109	9.6	42
3	Synthesis and characterization of heterometallic {Cr <sub>7</sub> M} wheels. <i>Angewandte Chemie - International Edition</i> , <b>2003</b> , 42, 101-5	16.4	179
2	A novel undecametallic iron(III) cluster with an S = (11)/(2) spin ground state. <i>Inorganic Chemistry</i> , <b>2003</b> , 42, 6601-3	5.1	64
1	In Silico Design Criteria for High Blocking Barrier Uranium(III) SIMs. <i>Chemical Communications</i> ,	5.8	1