

Eliseo Ruiz

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.

276 papers	15,532 citations	66 h-index	115 g-index
288 ext. papers	16,410 ext. citations	6.1 avg, IF	6.64 L-index

#	Paper	IF	Citations
276	Room-Temperature Spin-Dependent Transport in Metalloporphyrin-Based Supramolecular Wires. <i>Angewandte Chemie</i> , 2021 , 133, 26162	3.6	3
275	Room-Temperature Spin-Dependent Transport in Metalloporphyrin-Based Supramolecular Wires. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 25958-25965	16.4	5
274	Metal-Organic Nanocapsules with Functionalized s-Heptazine Ligands. <i>Inorganic Chemistry</i> , 2021 , 60, 570-573	5.1	
273	Experimental and Computational Studies on Quadruply Bonded Dimolybdenum Complexes with Terminal and Bridging Hydride Ligands. <i>Chemistry - A European Journal</i> , 2021 , 27, 6569-6578	4.8	3
272	Magnetic anisotropy in Yb complex candidates for molecular qubits: a theoretical analysis. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 1976-1983	3.6	1
271	Slow magnetic relaxation in dinuclear dysprosium and holmium phenoxide bridged complexes: a Dy ₂ single molecule magnet with a high energy barrier. <i>Inorganic Chemistry Frontiers</i> , 2021 , 8, 2532-2541	6.8	5
270	Spin-Phonon Coupling and Slow-Magnetic Relaxation in Pristine Ferrocenium. <i>Chemistry - A European Journal</i> , 2021 , 27, 16440-16447	4.8	1
269	Nickel(II) salicylaldimines: Re-visiting a classic. <i>Polyhedron</i> , 2021 , 205, 115321	2.7	0
268	[Co/Fe(μ-Alkyl-tpdt)]: Alkyl-Substituted Cobalt and Iron Bis-dithiolenethiophenic Complexes. <i>Inorganic Chemistry</i> , 2020 , 59, 9261-9269	5.1	
267	Dysprosium-based complexes with a flat pentadentate donor: a magnetic and ab initio study. <i>Dalton Transactions</i> , 2020 , 49, 8389-8401	4.3	5
266	Spin dynamics in single-molecule magnets and molecular qubits. <i>Dalton Transactions</i> , 2020 , 49, 9916-9928	4.3	37
265	Self-Assembled, Highly Positively Charged, Allyl-Pd Crowns: Cavity-Pocket-Driven Interactions of Fluoroanions. <i>Chemistry - A European Journal</i> , 2020 , 26, 7847-7860	4.8	2
264	Assessment of the SCAN Functional for Spin-State Energies in Spin-Crossover Systems. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 5053-5058	2.8	7
263	Single-Molecule Transport of Fullerene-Based Curcuminoids. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 2698-2704	3.8	5
262	Tuning Single-Molecule Conductance in Metalloporphyrin-Based Wires via Supramolecular Interactions. <i>Angewandte Chemie</i> , 2020 , 132, 19355-19363	3.6	3
261	Tuning Single-Molecule Conductance in Metalloporphyrin-Based Wires via Supramolecular Interactions. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 19193-19201	16.4	11
260	Room temperature conductance switching in a molecular iron(iii) spin crossover junction. <i>Chemical Science</i> , 2020 , 12, 2381-2388	9.4	10

- 259 Dinuclear CoYvs. tetranuclear CoY complexes: the effect of increasing molecular size on magnetic anisotropy and relaxation dynamics. *Dalton Transactions*, **2019**, 48, 14873-14884 4.3 5
- 258 Computational Modeling of Transition Temperatures in Spin-Crossover Systems. *Comments on Inorganic Chemistry*, **2019**, 39, 216-241 3.9 14
- 257 Magnetization Slow Dynamics in Ferrocenium Complexes. *Chemistry - A European Journal*, **2019**, 25, 10625-10632 4.3 10
- 256 Slow-spin relaxation of a low-spin $S = 1/2$ Fe carborane complex. *Chemical Communications*, **2019**, 55, 3825-3828 5.8 10
- 255 [UF] : A Molecular Hexafluorido Actinide(IV) Complex with Compensating Spin and Orbital Magnetic Moments. *Angewandte Chemie - International Edition*, **2019**, 58, 15650-15654 16.4 3
- 254 [UF₆]2A Molecular Hexafluorido Actinide(IV) Complex with Compensating Spin and Orbital Magnetic Moments. *Angewandte Chemie*, **2019**, 131, 15797-15801 3.6
- 253 R  titelbild: [UF₆]2A Molecular Hexafluorido Actinide(IV) Complex with Compensating Spin and Orbital Magnetic Moments (Angew. Chem. 44/2019). *Angewandte Chemie*, **2019**, 131, 16084-16084 3.6
- 252 Control over Near-Ballistic Electron Transport through Formation of Parallel Pathways in a Single-Molecule Wire. *Journal of the American Chemical Society*, **2019**, 141, 240-250 16.4 20
- 251 A Pseudo-Octahedral Cobalt(II) Complex with Bispyrazolylpyridine Ligands Acting as a Zero-Field Single-Molecule Magnet with Easy Axis Anisotropy. *Chemistry - A European Journal*, **2018**, 24, 8857-8868 4.8 40
- 250 Electronic and Steric Control of the Spin-Crossover Behavior in [(Cp)Mn] Manganocenes. *Inorganic Chemistry*, **2018**, 57, 702-709 5.1 13
- 249 Antiferromagnetic Interactions in Copper(II) μ -Oxalato Dinuclear Complexes: The Role of the Counterion. *European Journal of Inorganic Chemistry*, **2018**, 2018, 509-516 2.3 9
- 248 Structure, magnetic properties and DFT calculations of azido-copper(II) complexes with different azido-bonding, nuclearity and dimensionality. *New Journal of Chemistry*, **2018**, 42, 2627-2639 3.6 9
- 247 H-Mediated Magnetic Interactions between Layers in a 2D MnII Dicyanamide Polymer: Neutron Diffraction, DFT, and Quantum Monte Carlo Calculations. *European Journal of Inorganic Chemistry*, **2018**, 2018, 278-288 2.3
- 246 Element-Selective Molecular Charge Transport Characteristics of Binuclear Copper(II)-Lanthanide(III) Complexes. *Inorganic Chemistry*, **2018**, 57, 9274-9285 5.1 5
- 245 Electric-field induced bistability in single-molecule conductance measurements for boron coordinated curcuminoid compounds. *Chemical Science*, **2018**, 9, 6988-6996 9.4 12
- 244 Boosting Self-Assembly Diversity in the Solid-State by Chiral/Non-Chiral Zn -Porphyrin Crystallization. *Chemistry - A European Journal*, **2018**, 24, 12950-12960 4.8 6
- 243 Single-ion magnetic anisotropy in a vacant octahedral Co(ii) complex. *Dalton Transactions*, **2018**, 48, 25-29 4.3 19
- 242 Slow relaxation of magnetization in a bis-mer-tridentate octahedral Co(ii) complex. *Dalton Transactions*, **2018**, 47, 859-867 4.3 29

241	Mononuclear Lanthanide Complexes with 18-Crown-6 Ether: Synthesis, Characterization, Magnetic Properties, and Theoretical Studies. <i>Inorganic Chemistry</i> , 2018 , 57, 13225-13234	5.1	15
240	Benchmarking Density Functional Methods for Calculation of State Energies of First Row Spin-Crossover Molecules. <i>Inorganic Chemistry</i> , 2018 , 57, 14097-14105	5.1	77
239	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> , 2018 , 57, 6362-6375	5.1	40
238	An Unprecedented Stimuli-Controlled Single-Crystal Reversible Phase Transition of a Metal-Organic Framework and Its Application to a Novel Method of Guest Encapsulation. <i>Advanced Materials</i> , 2018 , 30, e1800726	24	25
237	Effect of Heteroatoms on Field-Induced Slow Magnetic Relaxation of Mononuclear Fe (S = 5/2) Ions within Polyoxometalates. <i>Inorganic Chemistry</i> , 2018 , 57, 6957-6964	5.1	13
236	Metal-Controlled Magnetoresistance at Room Temperature in Single-Molecule Devices. <i>Journal of the American Chemical Society</i> , 2017 , 139, 5768-5778	16.4	26
235	Investigation of easy-plane magnetic anisotropy in P-ligand square-pyramidal Co single ion magnets. <i>Chemical Communications</i> , 2017 , 53, 5338-5341	5.8	37
234	Analysis of Magnetic Anisotropy and the Role of Magnetic Dilution in Triggering Single-Molecule Magnet (SMM) Behavior in a Family of Co Y Dinuclear Complexes with Easy-Plane Anisotropy. <i>Chemistry - A European Journal</i> , 2017 , 23, 11649-11661	4.8	39
233	Six States Switching of Redox-Active Molecular Tweezers by Three Orthogonal Stimuli. <i>Journal of the American Chemical Society</i> , 2017 , 139, 9213-9220	16.4	34
232	Quantitative Estimation of Ising-Type Magnetic Anisotropy in a Family of C -Symmetric Co Complexes. <i>Chemistry - A European Journal</i> , 2017 , 23, 12550-12558	4.8	25
231	Models to predict the magnetic properties of single- and multiple-bridged phosphate CuII systems: a theoretical DFT insight. <i>Inorganic Chemistry Frontiers</i> , 2017 , 4, 509-520	6.8	4
230	Single-molecule magnetism arising from cobalt(II) nodes of a crystalline sponge. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 835-841	7.1	51
229	Coming full circle: constructing a [Gd] wheel dimer by dimer and the importance of spin topology. <i>Dalton Transactions</i> , 2017 , 46, 10255-10263	4.3	11
228	Tunable Magnetization Dynamics through Solid-State Ligand Substitution Reaction. <i>Inorganic Chemistry</i> , 2017 , 56, 8829-8836	5.1	10
227	Influence of the Disposition of the Anisotropy Axes into the Magnetic Properties of Mn Dinuclear Compounds with Benzoato Derivative Bridges. <i>Inorganic Chemistry</i> , 2017 , 56, 8135-8146	5.1	2
226	An Unsaturated Four-Coordinate Dimethyl Dimolybdenum Complex with a Molybdenum-Molybdenum Quadruple Bond. <i>Chemistry - A European Journal</i> , 2017 , 23, 194-205	4.8	8
225	Rational Design of Lanthanoid Single-Ion Magnets: Predictive Power of the Theoretical Models. <i>Chemistry - A European Journal</i> , 2016 , 22, 13532-9	4.8	22
224	Exchange Interactions on the Highest-Spin Reported Molecule: the Mixed-Valence Fe42 Complex. <i>Scientific Reports</i> , 2016 , 6, 23847	4.9	12

223	Ferromagnetism in polynuclear systems based on non-linear [MnII2MnIII] building blocks. <i>Inorganic Chemistry Frontiers</i> , 2016 , 3, 1272-1279	6.8	7
222	DFT approaches to transport calculations in magnetic single-molecule devices. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	6
221	Lanthanide Tetrazolate Complexes Combining Single-Molecule Magnet and Luminescence Properties: The Effect of the Replacement of Tetrazolate N3 by β -Diketonate Ligands on the Anisotropy Energy Barrier. <i>Chemistry - A European Journal</i> , 2016 , 22, 14548-59	4.8	37
220	Electronic Structure Modulation in an Exceptionally Stable Non-Heme Nitrosyl Iron(II) Spin-Crossover Complex. <i>Chemistry - A European Journal</i> , 2016 , 22, 12741-51	4.8	13
219	Modeling Magnetic Properties with Density Functional Theory-Based Methods 2016 , 419-446		1
218	Magnetic and transport properties of Fe single-molecule magnets: a theoretical insight. <i>Dalton Transactions</i> , 2016 , 45, 18867-18875	4.3	6
217	Relaxation Dynamics of Identical Trigonal Bipyramidal Cobalt Molecules with Different Local Symmetries and Packing Arrangements: Magnetostructural Correlations and ab initio Calculations. <i>Journal of the American Chemical Society</i> , 2016 , 138, 16407-16416	16.4	68
216	MEPROCS framework for Craniofacial Superimposition: Validation study. <i>Legal Medicine</i> , 2016 , 23, 99-108	9	8
215	Predetermined Ferromagnetic Coupling via Strict Control of M-O-M Angles. <i>Inorganic Chemistry</i> , 2016 , 55, 11707-11715	5.1	9
214	A Low Spin Manganese(IV) Nitride Single Molecule Magnet. <i>Chemical Science</i> , 2016 , 7, 6132-6140	9.4	87
213	Single-Molecule Magnet Properties of Transition-Metal Ions Encapsulated in Lacunary Polyoxometalates: A Theoretical Study. <i>Inorganic Chemistry</i> , 2016 , 55, 6405-13	5.1	17
212	Theoretical Modeling of the Ligand-Tuning Effect over the Transition Temperature in Four-Coordinated Fe(II) Molecules. <i>Inorganic Chemistry</i> , 2016 , 55, 1657-63	5.1	22
211	Pyridinethiolate Titanocene Metalloligands and Their Self-Assembly Reactions To Yield Early-Stage Metallamacrocycles. <i>Organometallics</i> , 2016 , 35, 336-345	3.8	10
210	Sequential Electron Transport and Vibrational Excitations in an Organic Molecule Coupled to Few-Layer Graphene Electrodes. <i>ACS Nano</i> , 2016 , 10, 2521-7	16.7	36
209	Large Conductance Switching in a Single-Molecule Device through Room Temperature Spin-Dependent Transport. <i>Nano Letters</i> , 2016 , 16, 218-26	11.5	118
208	Multiscale study of mononuclear Co SMMs based on curcuminoid ligands. <i>Chemical Science</i> , 2016 , 7, 2793-2803	9.4	43
207	Antiferro- to ferromagnetic crossover in diphenoxido bridged NiII2MnII complexes derived from N2O2 donor Schiff base ligands. <i>Polyhedron</i> , 2016 , 117, 57-63	2.7	11
206	Large magnetic anisotropy in mononuclear metal complexes. <i>Coordination Chemistry Reviews</i> , 2015 , 289-290, 379-392	23.2	280

205	A trinuclear Cu(II) complex with functionalized s-heptazine N-ligands: molecular chemistry from a g-C ₃ N ₄ fragment. <i>Dalton Transactions</i> , 2015 , 44, 15761-3	4.3	8
204	Increasing the effective energy barrier promoted by the change of a counteranion in a Zn-Dy-Zn SMM: slow relaxation via the second excited state. <i>Chemical Communications</i> , 2015 , 51, 12353-6	5.8	53
203	Theoretical modeling of two-step spin-crossover transitions in FeII dinuclear systems. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 7954-7961	7.1	25
202	First evidence of light-induced spin transition in molybdenum(IV). <i>Chemical Communications</i> , 2015 , 51, 8229-32	5.8	49
201	Amending the anisotropy barrier and luminescence behavior of heterometallic trinuclear linear [M(II)-Ln(III)-M(II)] (Ln(III) = Gd, Tb, Dy; M(II) = Mg/Zn) complexes by change from divalent paramagnetic to diamagnetic metal ions. <i>Chemistry - A European Journal</i> , 2015 , 21, 6449-64	4.8	50
200	Neodymium 1D systems: targeting new sources for field-induced slow magnetization relaxation. <i>Dalton Transactions</i> , 2015 , 44, 15774-8	4.3	27
199	Different topologies in three manganese-azido 1D compounds: magnetic behavior and DFT-quantum Monte Carlo calculations. <i>Dalton Transactions</i> , 2015 , 44, 18632-42	4.3	6
198	Modulation of single-molecule magnet behaviour via photochemical [2+2] cycloaddition. <i>Chemical Communications</i> , 2015 , 51, 15358-61	5.8	50
197	Negatively charged metallacarborane redox couples with both members stable to air. <i>Chemistry - A European Journal</i> , 2015 , 21, 6888-97	4.8	16
196	Magnetic Behaviour of Transition Metal Complexes with Functionalized Chiral and C ₆₀ -Filled Nanotubes as Bridging Ligands: A Theoretical Study. <i>Magnetochemistry</i> , 2015 , 1, 62-71	3.1	2
195	All-round robustness of the Mn ₁₉ coordination cluster system: experimental validation of a theoretical prediction. <i>Chemical Communications</i> , 2014 , 50, 5847-50	5.8	15
194	Experimental and theoretical studies on arene-bridged metal-metal-bonded dimolybdenum complexes. <i>Chemistry - A European Journal</i> , 2014 , 20, 6092-102	4.8	29
193	A racemic and enantiopure unsymmetric diiron(III) complex with a chiral o-carborane-based pyridylalcohol ligand: combined chiroptical, magnetic, and nonlinear optical properties. <i>Chemistry - A European Journal</i> , 2014 , 20, 1081-90	4.8	18
192	Huge magnetic anisotropy in a trigonal-pyramidal nickel(II) complex. <i>Inorganic Chemistry</i> , 2014 , 53, 676-8	5.1	38
191	Spin-crossover behavior in two new supramolecular isomers. <i>Inorganic Chemistry</i> , 2014 , 53, 201-8	5.1	22
190	Charge transport properties of spin crossover systems. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 14-22	3.6	92
189	Guest modulation of spin-crossover transition temperature in a porous iron(II) metal-organic framework: experimental and periodic DFT studies. <i>Chemistry - A European Journal</i> , 2014 , 20, 12864-73	4.8	46
188	Ferro- to antiferromagnetic crossover angle in diphenoxido- and carboxylato-bridged trinuclear Ni(II)Mn(II) complexes: experimental observations and theoretical rationalization. <i>Inorganic Chemistry</i> , 2014 , 53, 9296-305	5.1	33

187	Rational electrostatic design of easy-axis magnetic anisotropy in a Zn(II) -Dy(III) -Zn(II) single-molecule magnet with a high energy barrier. <i>Chemistry - A European Journal</i> , 2014 , 20, 14262-9	4.8	84
186	Origin of slow magnetic relaxation in Kramers ions with non-uniaxial anisotropy. <i>Nature Communications</i> , 2014 , 5, 4300	17.4	283
185	Effect of metal complexation on the conductance of single-molecular wires measured at room temperature. <i>Journal of the American Chemical Society</i> , 2014 , 136, 8314-22	16.4	38
184	Two C ₃ -symmetric Dy ³⁺ complexes with triple di- <i>tert</i> -methoxy- <i>tert</i> -phenoxo bridges, magnetic ground state, and single-molecule magnetic behavior. <i>Chemistry - A European Journal</i> , 2014 , 20, 8410-20	4.8	36
183	Slow magnetic relaxation in a Co(II)-Y(III) single-ion magnet with positive axial zero-field splitting. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 9130-4	16.4	242
182	Two 3d-4f nanomagnets formed via a two-step in situ reaction of picolinaldehyde. <i>Chemical Communications</i> , 2013 , 49, 6549-51	5.8	61
181	Spin-polarized transport through single-molecule magnet Mn ₆ complexes. <i>Nanoscale</i> , 2013 , 5, 4751-7	7.7	16
180	A density functional theory approach to the magnetic properties of a coupled single-molecule magnet (Mn ₇) ₂ complex: An entangled qubit pair candidate. <i>Canadian Journal of Chemistry</i> , 2013 , 91, 866-871	0.9	1
179	Exchange Coupling in Di- and Polynuclear Complexes 2013 , 501-549		6
178	A Mn ₁₂ Mn ₁₂ single-strand molecular wheel with a reuleaux triangular topology: synthesis, structure, magnetism, and DFT studies. <i>Inorganic Chemistry</i> , 2013 , 52, 12070-9	5.1	17
177	Shedding light on the single-molecule magnet behavior of mononuclear Dy(III) complexes. <i>Inorganic Chemistry</i> , 2013 , 52, 13770-8	5.1	159
176	Unprecedented ferromagnetic dipolar interaction in a dinuclear holmium(III) complex: a combined experimental and theoretical study. <i>Chemical Communications</i> , 2013 , 49, 9341-3	5.8	30
175	Interconversion of Quadruply and Quintuply Bonded Molybdenum Complexes by Reductive Elimination and Oxidative Addition of Dihydrogen. <i>Angewandte Chemie</i> , 2013 , 125, 3309-3313	3.6	22
174	Interconversion of quadruply and quintuply bonded molybdenum complexes by reductive elimination and oxidative addition of dihydrogen. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 3227-31	16.4	45
173	Mononuclear single-molecule magnets: tailoring the magnetic anisotropy of first-row transition-metal complexes. <i>Journal of the American Chemical Society</i> , 2013 , 135, 7010-8	16.4	335
172	Self-assembly of pentanuclear mesocate versus octanuclear helicate: size effect of the [M(II) ₃ (B-O/X)] _n ⁺ triangle core. <i>Inorganic Chemistry</i> , 2013 , 52, 1099-107	5.1	31
171	Spins on a curved surface: an Fe(III) ₁₄ ferracalixarene. <i>Dalton Transactions</i> , 2013 , 42, 9606-12	4.3	6
170	Magnetic interactions mediated by diamagnetic cations in [Mn ₁₈ M] (M = Sr ²⁺ , Y ³⁺ , Cd ²⁺ , and Lu ³⁺) coordination clusters. <i>Inorganic Chemistry</i> , 2013 , 52, 5764-74	5.1	18

169	Structures, magnetochemistry, spectroscopy, theoretical study, and catechol oxidase activity of dinuclear and dimer-of-dinuclear mixed-valence Mn(III)Mn(II) complexes derived from a macrocyclic ligand. <i>Inorganic Chemistry</i> , 2013 , 52, 7732-46	5.1	56
168	Cu(II)-Gd(III) cryogenic magnetic refrigerants and Cu8Dy9 single-molecule magnet generated by in situ reactions of picolinaldehyde and acetylpyridine: experimental and theoretical study. <i>Chemistry - A European Journal</i> , 2013 , 19, 17567-77	4.8	80
167	Reversible chemisorption of sulfur dioxide in a spin crossover porous coordination polymer. <i>Inorganic Chemistry</i> , 2013 , 52, 12777-83	5.1	61
166	Slow Magnetic Relaxation in a Co(II) Single-Ion Magnet with Positive Axial Zero-Field Splitting. <i>Angewandte Chemie</i> , 2013 , 125, 9300-9304	3.6	44
165	Coherent transport through spin-crossover single molecules. <i>Journal of the American Chemical Society</i> , 2012 , 134, 777-9	16.4	123
164	Self-Assembly of Coordination Compounds: Design Principles 2012 ,		1
163	Enhanced bistability by guest inclusion in Fe(II) spin crossover porous coordination polymers. <i>Chemical Communications</i> , 2012 , 48, 4686-8	5.8	95
162	Field and dilution effects on the slow relaxation of a luminescent DyO9 low-symmetry single-ion magnet. <i>Chemical Communications</i> , 2012 , 48, 7916-8	5.8	189
161	Exchange coupling and magnetic anisotropy of exchanged-biased quantum tunnelling single-molecule magnet Ni3Mn2 complexes using theoretical methods based on Density Functional Theory. <i>Dalton Transactions</i> , 2012 , 41, 2659-66	4.3	6
160	Exchange coupling mediated by N-H...Cl hydrogen bonds: experimental and theoretical study of the frustrated magnetic system in bis(o-phenylenediamine)nickel(II) chloride. <i>Inorganic Chemistry</i> , 2012 , 51, 5487-93	5.1	21
159	Co(II)Ln(III) dinuclear complexes (Ln(III) = Gd, Tb, Dy, Ho and Er) as platforms for 1,5-dicyanamide-bridged tetranuclear Co(II)Ln(III)2 complexes: A magneto-structural and theoretical study. <i>Comptes Rendus Chimie</i> , 2012 , 15, 878-888	2.7	23
158	Charge transfer and tunable ambipolar effect induced by assembly of Cu(II) binuclear complexes on carbon nanotube field effect transistor devices. <i>Journal of the American Chemical Society</i> , 2012 , 134, 7896-901	16.4	24
157	Hexanuclear copper(II) cages built on a central {B-O...H...B-O} moiety, 1,3-bis(dimethylamino)-2-propanolato and capping R-phosphonates: crystal structures, magnetic behavior, and DFT studies. <i>Inorganic Chemistry</i> , 2012 , 51, 6842-50	5.1	18
156	Synthesis, crystal structure and magnetism of new salicylamidoxime-based hexanuclear manganese(III) single-molecule magnets. <i>Dalton Transactions</i> , 2012 , 41, 13668-81	4.3	33
155	Family of carboxylate- and nitrate-diphenoxo triply bridged dinuclear Ni(II)Ln(III) complexes (Ln = Eu, Gd, Tb, Ho, Er, Y): synthesis, experimental and theoretical magneto-structural studies, and single-molecule magnet behavior. <i>Inorganic Chemistry</i> , 2012 , 51, 5857-68	5.1	126
154	Triangular nickel complexes derived from 2-pyridylcyanoxime: an approach to the magnetic properties of the [Ni3(B-OH){pyC(R)NO}3]2+ core. <i>Chemistry - A European Journal</i> , 2012 , 18, 3637-48	4.8	34
153	Theoretical study of exchange coupling in 3d-Gd complexes: large magnetocaloric effect systems. <i>Journal of the American Chemical Society</i> , 2012 , 134, 10532-42	16.4	144
152	Self-Assembly of Heterometallic Metallomacrocycles via Ditopic Fluoroaryl Gold(I) Organometallic Metalloligands. <i>Organometallics</i> , 2012 , 31, 1533-1545	3.8	27

151	S(T) = 22 [Mn10] supertetrahedral building-block to design extended magnetic networks. <i>Inorganic Chemistry</i> , 2011 , 50, 8580-7	5.1	24
150	Mononuclear Fe(II) single-molecule magnets: a theoretical approach. <i>Inorganic Chemistry</i> , 2011 , 50, 4016-20	5.20	35
149	Thermal behavior of Si-doped fullerenes vs their structural stability at T=0K: A density functional study. <i>Chemical Physics Letters</i> , 2011 , 510, 14-17	2.5	16
148	Ni-2,3-thiophenedithiolate Anions in New Architectures: An In-Line Mixed-Valence Ni Dithiolene (Ni4S12) Cluster. <i>European Journal of Inorganic Chemistry</i> , 2011 , 2011, 4807-4815	2.3	9
147	Exchange coupling constants using Density Functional Theory: long-range corrected functionals. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1998-2004	3.5	41
146	The use of a bis(phenylpyrazolyl)pyridyl ligand to prepare [Mn4] and [Mn10] cage complexes. <i>Chemistry - A European Journal</i> , 2011 , 17, 4960-3	4.8	21
145	The dilemma of CrIIINiII exchange interactions: ferromagnetism versus antiferromagnetism. <i>Chemistry - A European Journal</i> , 2011 , 17, 8841-9	4.8	2
144	A molecular pair of [GdNi3] tetrahedra bridged by water molecules. <i>Chemistry - A European Journal</i> , 2011 , 17, 8264-8	4.8	57
143	Design of dinuclear copper species with carboranylcarboxylate ligands: study of their steric and electronic effects. <i>Chemistry - A European Journal</i> , 2011 , 17, 13217-29	4.8	26
142	Synthesis, crystal structure and magnetic properties of two oxalato-bridged dimetallic trinuclear complexes combined with a polar cation. <i>Dalton Transactions</i> , 2010 , 39, 4951-8	4.3	34
141	Electronic structure and localization properties of C60Tan clusters (n=1,3): A first-principles study. <i>Physical Review B</i> , 2010 , 81,	3.3	3
140	Synthesis of a novel heptacoordinated Fe(III) dinuclear complex: experimental and theoretical study of the magnetic properties. <i>Dalton Transactions</i> , 2010 , 39, 4874-81	4.3	32
139	Magneto-structural correlation studies and theoretical calculations of a unique family of single end-to-end azide-bridged Ni(II)4 cyclic clusters. <i>Inorganic Chemistry</i> , 2010 , 49, 9517-26	5.1	51
138	A new family of oxime-based hexanuclear manganese(III) single molecule magnets with high anisotropy energy barriers. <i>Chemical Communications</i> , 2010 , 46, 5106-8	5.8	51
137	Magnetic properties of largest-spin single molecule magnets: Mn17 complexes--a density functional theory approach. <i>Inorganic Chemistry</i> , 2010 , 49, 9641-8	5.1	30
136	Extended FeII butterfly complexes: theoretical analysis of magnetic properties and magnetostructural maps. <i>Dalton Transactions</i> , 2010 , 39, 4832-7	4.3	6
135	Synthesis, crystal structure and magnetic properties of three unprecedented tri-nuclear and one very rare tetra-nuclear copper(II) Schiff-base complexes supported by mixed azido/phenoxo/nitrato or acetato bridges. <i>Dalton Transactions</i> , 2010 , 39, 7474-84	4.3	69
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1	Electronic Structure and Magnetic Behavior in Polynuclear Transition-Metal Compounds 227-279		5