FrÃ©dÃ©ric Gendron

List of Publications by Year
in descending order

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Version: 2024-02-01

51	1,976	304743	254184
papers	citations	22 h-index	43 g-index

60	60	60	2292
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
2	Assessing the exchange coupling in binuclear lanthanide(<scp>iii</scp>) complexes and the slow relaxation of the magnetization in the antiferromagnetically coupled Dy₂ derivative. Chemical Science, 2015, 6, 4148-4159.	7.4	114
3	Characterization of berkelium(III) dipicolinate and borate compounds in solution and the solid state. Science, 2016, 353, .	12.6	86
4	Magnetic Properties and Electronic Structure of Neptunyl(VI) Complexes: Wavefunctions, Orbitals, and Crystalâ€Field Models. Chemistry - A European Journal, 2014, 20, 7994-8011.	3.3	85
5	Hysteresis Photomodulation via Single-Crystal-to-Single-Crystal Isomerization of a Photochromic Chain of Dysprosium Single-Molecule Magnets. Journal of the American Chemical Society, 2020, 142, 931-936.	13.7	68
6	Calculating NMR Chemical Shifts for Paramagnetic Metal Complexes from First-Principles. Journal of Physical Chemistry Letters, 2015, 6, 2183-2188.	4.6	64
7	Single-ion 4f element magnetism: an ab-initio look at Ln(COT)₂^{â^'}. Dalton Transactions, 2015, 44, 19886-19900.	3.3	52
8	Magnetic Resonance Properties of Actinyl Carbonate Complexes and Plutonyl(VI)-tris-nitrate. Inorganic Chemistry, 2014, 53, 8577-8592.	4.0	49
9	Hexatriynediyl Chain Spanning Two Cp*(dppe)M Termini (M = Fe, Ru): Evidence for the Dependence of Electronic and Magnetic Couplings on the Relative Orientation of the Termini. Organometallics, 2014, 33, 2613-2627.	2.3	45
10	Luminescence, chiroptical, magnetic andab initiocrystal-field characterizations of an enantiopure helicoidal Yb(<scp>iii</scp>) complex. Inorganic Chemistry Frontiers, 2021, 8, 914-926.	6.0	43
11	Solidâ€State Nearâ€Infrared Circularly Polarized Luminescence from Chiral Yb^{III}â€Singleâ€Molecule Magnet. Chemistry - A European Journal, 2021, 27, 7362-7366.	3.3	43
12	Straightforward Access to Tetrametallic Complexes with a Square Array by Oxidative Dimerization of Organometallic Wires. Organometallics, 2013, 32, 5015-5025.	2.3	39
13	Iron and Ruthenium Ïƒ-Polyynyls of the General Formula [{M(dppe)Cp*}â€“(Câ‰¡C)_nâ€“R]^{0/+} (M = Fe, Ru): An Experimental and Theoretical Investigation. Organometallics, 2012, 31, 6796-6811.	2.3	37
14	Ab Initio Study of Circular Dichroism and Circularly Polarized Luminescence of Spin-Allowed and Spin-Forbidden Transitions: From Organic Ketones to Lanthanide Complexes. Journal of Chemical Theory and Computation, 2019, 15, 4140-4155.	5.3	37
15	Chiral Supramolecular Nanotubes of Singleâ€Chain Magnets. Angewandte Chemie - International Edition, 2020, 59, 780-784.	13.8	36
16	Low-Spin Fe(III) Macrocyclic Complexes of Imidazole-Appended 1,4,7-Triazacyclononane as Paramagnetic Probes. Inorganic Chemistry, 2018, 57, 8364-8374.	4.0	34
17	Ligand NMR Chemical Shift Calculations for Paramagnetic Metal Complexes: 5f¹ vs 5f² Actinides. Journal of Chemical Theory and Computation, 2016, 12, 5309-5321.	5.3	32
18	Oxidative Dimerization of Arylalkynylâ€“Ruthenium Complexes. Organometallics, 2011, 30, 2861-2868.	2.3	29

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19	Magnetic Properties and Electronic Structures of Ar₃U^{IV}â€“L Complexes with Ar = C₅(CH₃)₄H^{â€“} or C₅H₅^{â€“} and L = CH₃, NO, and Cl. Inorganic Chemistry, 2014, 53, 13174-13187.	4.0	29
20	Bisâ€Cyclooctatetraenyl Thulium(II): Highly Reducing Lanthanide Sandwich Singleâ€Molecule Magnets. Angewandte Chemie - International Edition, 2021, 60, 6042-6046.	13.8	27
21	Puzzling Lack of Temperature Dependence of the PuO₂ Magnetic Susceptibility Explained According to Ab Initio Wave Function Calculations. Journal of Physical Chemistry Letters, 2017, 8, 673-678.	4.6	26
22	Electronic Structure and Properties of Berkelium Iodates. Journal of the American Chemical Society, 2017, 139, 13361-13375.	13.7	25
23	Luminescenceâ€Driven Electronic Structure Determination in a Textbook Dimeric Dy^{III}â€Based Singleâ€Molecule Magnet. Chemistry - A European Journal, 2020, 26, 4389-4395.	3.3	23
24	Magnetic circular dichroism of UCl₆^{â^'}in the ligand-to-metal charge-transfer spectral region. Physical Chemistry Chemical Physics, 2017, 19, 17300-17313.	2.8	21
25	Nuclear Magnetic Resonance Measurements and Electronic Structure of Pu(IV) in [(Me)₄N]₂PuCl₆. Inorganic Chemistry, 2016, 55, 8371-8380.	4.0	20
26	Electronic Properties of Polyâ€Yne Carbon Chains and Derivatives with Transition Metal Endâ€Groups. European Journal of Inorganic Chemistry, 2020, 2020, 667-681.	2.0	20
27	Oxidative Activation of Aryldiynylâ€“Iron Complexes: Regioselective Dimerization. Organometallics, 2013, 32, 1866-1875.	2.3	16
28	Structure and Bonding Investigation of Plutonium Peroxocarbonate Complexes Using Cerium Surrogates and Electronic Structure Modeling. Inorganic Chemistry, 2017, 56, 791-801.	4.0	16
29	Similar ligandâ€“metal bonding for transition metals and actinides? 5f¹ U(C₇H₇)₂^{â^'}versus 3dⁿ metallocenes. Chemical Science, 2018, 9, 6292-6306.	7.4	16
30	Oxidative Dimerization of Aryldiynylâ€“Ruthenium Complexes. Organometallics, 2012, 31, 6555-6566.	2.3	15
31	Synthesis and Properties of a Mixedâ€Valence Compound with Singleâ€Step Tunneling and Multipleâ€Step Hopping Behavior. European Journal of Inorganic Chemistry, 2014, 2014, 3899-3911.	2.0	14
32	Magnetic Coupling in the Ce(III) Dimer Ce₂(COT)₃. Inorganic Chemistry, 2019, 58, 581-593.	4.0	14
33	Solid-stateversussolution investigation of a luminescent chiral BINOL-derived bisphosphate single-molecule magnet. Inorganic Chemistry Frontiers, 2021, 8, 947-962.	6.0	12
34	Hybrid Molecular Systems Containing Tetrathiafulvalene and Ironâ€Alkynyl Electrophores: Fiveâ€Component Functional Molecules Obtained from Cï£¿H Bond Activation. Chemistry - A European Journal, 2013, 19, 5742-5757.	3.3	11
35	Redox-Modulations of Photophysical and Single-molecule Magnet Properties in Ytterbium Complexes Involving Extended-TTF Triads. Molecules, 2020, 25, 492.	3.8	11
36	Calculation of Dipole-Forbidden 5f Absorption Spectra of Uranium(V) Hexa-Halide Complexes. Journal of Physical Chemistry Letters, 2018, 9, 887-894.	4.6	10

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37	A supramolecular chain of dimeric Dy single molecule magnets decorated with azobenzene ligands. Dalton Transactions, 2019, 48, 16053-16061.	3.3	10
38	Probing the Local Magnetic Structure of the [Fe III (Tp)(CN) 3] â^' Building Block Via Solidâ€State NMR Spectroscopy, Polarized Neutron Diffraction, and Firstâ€Principle Calculations. Chemistry - A European Journal, 2019, 25, 12120-12136.	3.3	9
39	Bisâ€Cyclooctatetraenyl Thulium(II): Highly Reducing Lanthanide Sandwich Singleâ€Molecule Magnets. Angewandte Chemie, 2021, 133, 6107-6111.	2.0	9
40	Complete Active Space Wavefunction-Based Analysis of Magnetization and Electronic Structure. Topics in Organometallic Chemistry, 2018, , 355-390.	0.7	8
41	Equatorial Electronic Structure in the Uranyl Ion: Cs₂UO₂Cl₄ and Cs₂UO₂Br₄. Inorganic Chemistry, 2022, 61, 3821-3831.	4.0	8
42	Combined Experimental/Theoretical Study on the Luminescent Properties of Homoleptic/Heteroleptic Erbium(III) Anilate-Based 2D Coordination Polymers. Inorganic Chemistry, 2021, 60, 17765-17774.	4.0	8
43	Chiral Supramolecular Nanotubes of Singleâ€Chain Magnets. Angewandte Chemie, 2020, 132, 790-794.	2.0	7
44	Single-chain magnet behavior in a finite linear hexanuclear molecule. Chemical Science, 2021, 12, 10613-10621.	7.4	7
45	Sizeâ€Controlled Hapticity Switching in [Ln(C₉H₉)(C₈H₈)] Sandwiches. Chemistry - A European Journal, 2021, 27, 13558-13567.	3.3	6
46	New thiocyanato and azido adducts of the redox-active Fe(Î·5-C5Me5)(Î·2-dppe) center: Synthesis and study of the Fe(II) and Fe(III) complexes. Inorganica Chimica Acta, 2011, 374, 288-301.	2.4	5
47	Thiopheneâ€“Bipyridine Appended Diketopyrrolopyrrole Ligands and Platinum(II) Complexes. Inorganic Chemistry, 2021, 60, 7351-7363.	4.0	4
48	A new class of Dy^{III}-SIMs associated with a guanidine-based ligand. Dalton Transactions, 2021, 50, 5146-5153.	3.3	3
49	Near-infrared circular dichroism of the ytterbium DOTMA complex: an ab initio investigation. Physical Chemistry Chemical Physics, 2022, 24, 5404-5410.	2.8	3
50	Cis and trans linkage of spin frustrated copper triangles creating Cu6 clusters. , 0, 4, 4.		1
51	Coordination-enhanced photochromism in dysprosium dinuclear complexes with photomodulated single-molecule magnet behavior. , 0, 4, 2.		0