

Frédéric Gendron

List of Publications by Year in descending order

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51
papers

1,976
citations

304743

22
h-index

254184

43
g-index

60
all docs

60
docs citations

60
times ranked

2292
citing authors

#	ARTICLE	IF	CITATIONS
1	Equatorial Electronic Structure in the Uranyl Ion: Cs ₂ UO ₂ Cl ₄ and Cs ₂ UO ₂ Br ₄ . <i>Inorganic Chemistry</i> , 2022, 61, 3821-3831.	4.0	8
2	Near-infrared circular dichroism of the ytterbium DOTMA complex: an <i>ab initio</i> investigation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 5404-5410.	2.8	3
3	Bis(cyclooctatetraenyl) Thulium(II): Highly Reducing Lanthanide Sandwich Single-Molecule Magnets. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 6042-6046.	13.8	27
4	Solid-state versus solution investigation of a luminescent chiral BINOL-derived bisphosphate single-molecule magnet. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 947-962.	6.0	12
5	Bis(cyclooctatetraenyl) Thulium(II): Highly Reducing Lanthanide Sandwich Single-Molecule Magnets. <i>Angewandte Chemie</i> , 2021, 133, 6107-6111.	2.0	9
6	Luminescence, chiroptical, magnetic and <i>ab initio</i> crystal-field characterizations of an enantiopure helicoidal Yb(III) complex. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 914-926.	6.0	43
7	A new class of Dy ^{III} -SIMs associated with a guanidine-based ligand. <i>Dalton Transactions</i> , 2021, 50, 5146-5153.	3.3	3
8	Solid-State Near-Infrared Circularly Polarized Luminescence from Chiral Yb ^{III} Single-Molecule Magnet. <i>Chemistry - A European Journal</i> , 2021, 27, 7362-7366.	3.3	43
9	Thiophene-Bipyridine Appended Diketopyrrolopyrrole Ligands and Platinum(II) Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 7351-7363.	4.0	4
10	Size-Controlled Hapticity Switching in [Ln(C ₉ H ₉)(C ₈ H ₈)] Sandwiches. <i>Chemistry - A European Journal</i> , 2021, 27, 13558-13567.	3.3	6
11	Single-chain magnet behavior in a finite linear hexanuclear molecule. <i>Chemical Science</i> , 2021, 12, 10613-10621.	7.4	7
12	Combined Experimental/Theoretical Study on the Luminescent Properties of Homoleptic/Heteroleptic Erbium(III) Anilate-Based 2D Coordination Polymers. <i>Inorganic Chemistry</i> , 2021, 60, 17765-17774.	4.0	8
13	Chiral Supramolecular Nanotubes of Single-Chain Magnets. <i>Angewandte Chemie</i> , 2020, 132, 790-794.	2.0	7
14	Chiral Supramolecular Nanotubes of Single-Chain Magnets. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 780-784.	13.8	36
15	Electronic Properties of Polyene Carbon Chains and Derivatives with Transition Metal End Groups. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 667-681.	2.0	20
16	Hysteresis Photomodulation via Single-Crystal-to-Single-Crystal Isomerization of a Photochromic Chain of Dysprosium Single-Molecule Magnets. <i>Journal of the American Chemical Society</i> , 2020, 142, 931-936.	13.7	68
17	Redox-Modulations of Photophysical and Single-molecule Magnet Properties in Ytterbium Complexes Involving Extended-TTF Triads. <i>Molecules</i> , 2020, 25, 492.	3.8	11
18	Luminescence-Driven Electronic Structure Determination in a Textbook Dimeric Dy ^{III} -Based Single-Molecule Magnet. <i>Chemistry - A European Journal</i> , 2020, 26, 4389-4395.	3.3	23

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19	Probing the Local Magnetic Structure of the [Fe III (Tp)(CN) 3] $\hat{\alpha}$ Building Block Via Solid-State NMR Spectroscopy, Polarized Neutron Diffraction, and First-Principle Calculations. Chemistry - A European Journal, 2019, 25, 12120-12136.	3.3	9
20	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
21	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
22	A supramolecular chain of dimeric Dy single molecule magnets decorated with azobenzene ligands. Dalton Transactions, 2019, 48, 16053-16061.	3.3	10
23	Magnetic Coupling in the Ce(III) Dimer Ce ₂ (COT) ₃ . Inorganic Chemistry, 2019, 58, 581-593.	4.0	14
24	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
25	Complete Active Space Wavefunction-Based Analysis of Magnetization and Electronic Structure. Topics in Organometallic Chemistry, 2018, , 355-390.	0.7	8
26	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
27	Similar ligand-metal bonding for transition metals and actinides? 5f ¹ U(C ₇ H ₇) ₂ $\hat{\alpha}$ versus 3d ⁿ metallocenes. Chemical Science, 2018, 9, 6292-6306.	7.4	16
28	Puzzling Lack of Temperature Dependence of the PuO ₂ Magnetic Susceptibility Explained According to Ab Initio Wave Function Calculations. Journal of Physical Chemistry Letters, 2017, 8, 673-678.	4.6	26
29	Structure and Bonding Investigation of Plutonium Peroxocarbonate Complexes Using Cerium Surrogates and Electronic Structure Modeling. Inorganic Chemistry, 2017, 56, 791-801.	4.0	16
30	Electronic Structure and Properties of Berkelium Iodates. Journal of the American Chemical Society, 2017, 139, 13361-13375.	13.7	25
31	Magnetic circular dichroism of UCl ₆ $\hat{\alpha}$ in the ligand-to-metal charge-transfer spectral region. Physical Chemistry Chemical Physics, 2017, 19, 17300-17313.	2.8	21
32	Ligand NMR Chemical Shift Calculations for Paramagnetic Metal Complexes: 5f ¹ vs 5f ² Actinides. Journal of Chemical Theory and Computation, 2016, 12, 5309-5321.	5.3	32
33	Nuclear Magnetic Resonance Measurements and Electronic Structure of Pu(IV) in [(Me) ₄ N] ₂ PuCl ₆ . Inorganic Chemistry, 2016, 55, 8371-8380.	4.0	20
34	Characterization of berkelium(III) dipicolinate and borate compounds in solution and the solid state. Science, 2016, 353, .	12.6	86
35	Assessing the exchange coupling in binuclear lanthanide(ⁱⁱⁱ) complexes and the slow relaxation of the magnetization in the antiferromagnetically coupled Dy ₂ derivative. Chemical Science, 2015, 6, 4148-4159.	7.4	114
36	Calculating NMR Chemical Shifts for Paramagnetic Metal Complexes from First-Principles. Journal of Physical Chemistry Letters, 2015, 6, 2183-2188.	4.6	64

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37	Single-ion 4f element magnetism: an ab-initio look at Ln(COT) ₂ ⁺ . Dalton Transactions, 2015, 44, 19886-19900.	3.3	52
38	Synthesis and Properties of a Mixed-valence Compound with Single-Step Tunneling and Multiple-Step Hopping Behavior. European Journal of Inorganic Chemistry, 2014, 2014, 3899-3911.	2.0	14
39	Magnetic Properties and Electronic Structures of Ar ₃ U ^{IV} L Complexes with Ar = C ₅ (CH ₃) ₄ H ⁺ or C ₅ H ₅ ⁺ and L = CH ₃ , NO, and Cl. Inorganic Chemistry, 2014, 53, 13174-13187.	4.0	29
40	Magnetic Resonance Properties of Actinyl Carbonate Complexes and Plutonyl(VI)-tris-nitrate. Inorganic Chemistry, 2014, 53, 8577-8592.	4.0	49
41	Hexatrienediyl 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
42	Magnetic Properties and Electronic Structure of Neptunyl(VI) Complexes: Wavefunctions, Orbitals, and Crystal Field Models. Chemistry - A European Journal, 2014, 20, 7994-8011.	3.3	85
43	Oxidative Activation of Aryldiynyl Iron Complexes: Regioselective Dimerization. Organometallics, 2013, 32, 1866-1875.	2.3	16
44	Straightforward Access to Tetrametallic Complexes with a Square Array by Oxidative Dimerization of Organometallic Wires. Organometallics, 2013, 32, 5015-5025.	2.3	39
45	Hybrid Molecular Systems Containing Tetrathiafulvalene and Iron Alkynyl Electrophores: Five-Component Functional Molecules Obtained from C≡C-H Bond Activation. Chemistry - A European Journal, 2013, 19, 5742-5757.	3.3	11
46	Oxidative Dimerization of Aryldiynyl Ruthenium Complexes. Organometallics, 2012, 31, 6555-6566.	2.3	15
47	Iron and Ruthenium <i>f</i> -Polyynyls of the General Formula [M(dppe)Cp*] _n (C≡C) _n (M = Fe, Ru): An Experimental and Theoretical Investigation. Organometallics, 2012, 31, 6796-6811.	2.3	37
48	Oxidative Dimerization of Arylalkynyl Ruthenium Complexes. Organometallics, 2011, 30, 2861-2868.	2.3	29
49	New thiocyanato and azido adducts of the redox-active Fe(1-5-C5Me5)(1-2-dppe) center: Synthesis and study of the Fe(II) and Fe(III) complexes. Inorganica Chimica Acta, 2011, 374, 288-301.	2.4	5
50	Coordination-enhanced photochromism in dysprosium dinuclear complexes with photomodulated single-molecule magnet behavior. , 0, 4, 2.		0
51	Cis and trans linkage of spin frustrated copper triangles creating Cu ₆ clusters. , 0, 4, 4.		1