HÃ©lÃ¨ne Bolvin

List of Publications by Year
in descending order

58 papers	2,003 citations	257450 24 h-index	243625 44 g-index

60 all docs	60 docs citations	60 times ranked	2087 citing authors

#	Article	IF	Citations
1	Metal-Based Linear Light Upconversion Implemented in Molecular Complexes: Challenges and Perspectives. Accounts of Chemical Research, 2022, 55, 442-456.	15.6	22
2	Molecular light-upconversion: we have had a problem! When excited state absorption (ESA) overcomes energy transfer upconversion (ETU) in Cr(<scp>iii</scp>)/Er(<scp>iii</scp>) complexes. Dalton Transactions, 2021, 50, 7955-7968.	3.3	16
3	Temperature Dependence of 1 H Paramagnetic Chemical Shifts in Actinide Complexes, Beyond Bleaney's Theory: The An VI O 2 2+ â€“Dipicolinic Acid Complexes (An=Np, Pu) as an Example. Chemistry - A European Journal, 2021, 27, 7138-7153.	3.3	9
4	Octahedral Hexachloro Environment of Dy 3+ with Slow Magnetic Relaxation and Luminescent Properties. European Journal of Inorganic Chemistry, 2021, 2021, 2099-2107.	2.0	1
5	Local Structure and Magnetism of La_{1â€“x}M_xPO₄ (M =) Tj ETQq1 1 0.784314 rgB Journal of Physical Chemistry C, 2021, 125, 22163-22174.	3.1	4
6	Crystal Structure and Magnetic Properties of Peacockâ€“Weakley Type Polyoxometalates Na9[Ln(W5O18)2] (Ln = Tm, Yb): Rare Example of Tm(III) SMM. Magnetochemistry, 2020, 6, 53.	2.4	7
7	Crystallographic structure and crystal field parameters in the [AnIV(DPA)3]2â^' series, An = Th, U, Np, Pu. Physical Chemistry Chemical Physics, 2020, 22, 14293-14308.	2.8	10
8	Derivation of Lanthanide Series Crystal Field Parameters From First Principles. Chemistry - A European Journal, 2019, 25, 15112-15122.	3.3	30
9	Insight of the Metalâ€“Ligand Interaction in fâ€Element Complexes by Paramagnetic NMR Spectroscopy. Chemistry - A European Journal, 2019, 25, 4435-4451.	3.3	21
10	Magnetic Coupling in the Ce(III) Dimer Ce₂(COT)₃. Inorganic Chemistry, 2019, 58, 581-593.	4.0	14
11	Crystal Field in Rareâ€Earth Complexes: From Electrostatics to Bonding. Chemistry - A European Journal, 2018, 24, 5538-5550.	3.3	21
12	Complete Active Space Wavefunction-Based Analysis of Magnetization and Electronic Structure. Topics in Organometallic Chemistry, 2018, , 355-390.	0.7	8
13	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
14	Relativistic Methods for Calculating Electron Paramagnetic Resonance (EPR) Parameters. , 2017, , 725-763.		12
15	Hysteresis in a bimetallic holmium complex: A synergy between electronic and nuclear magnetic interactions. Physical Review B, 2017, 96, .	3.2	8
16	Tools for Predicting the Nature and Magnitude of Magnetic Anisotropy in Transition Metal Complexes: Application to Co(II) Complexes. Magnetochemistry, 2016, 2, 31.	2.4	37
17	Unraveling Ïƒ and Ï€ Effects on Magnetic Anisotropy in cisâ€NiA₄B₂ Complexes: Magnetization, HFâ€HFEPR Studies, Firstâ€Principles Calculations, and Orbital Modeling. Chemistry - A European Journal, 2016, 22, 16850-16862.	3.3	15
18	Biâ€Compartmental Schiffâ€Base with Peripheral Ester Functionalization: Synthesis and Magnetic Behavior of Bimetallic Znâ€Ln Complexes (Ln = Dy, Tb, Gd). European Journal of Inorganic Chemistry, 2016, 2016, 4988-4995.	2.0	15

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19	Structure, luminescence and magnetic properties of an erbium(iii) Î²-diketonate homodinuclear complex. New Journal of Chemistry, 2016, 40, 8251-8261.	2.8	17
20	Paramagnetism of Aqueous Actinide Cations. Part II: Theoretical Aspects and New Measurements on An(IV). Inorganic Chemistry, 2016, 55, 12149-12157.	4.0	11
21	Magnetic susceptibility of actinide(<scp>iii</scp>) cations: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2016, 18, 6515-6525.	2.8	19
22	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
23	Relativistic Methods for Calculating Electron Paramagnetic Resonance (EPR) Parameters. , 2015, , 1-39.		2
24	Single-ion 4f element magnetism: an ab-initio look at Ln(COT)₂^{â^'}. Dalton Transactions, 2015, 44, 19886-19900.	3.3	52
25	Magnetic properties of a fourfold degenerate state: Np4+ ion diluted in Cs2ZrCl6 crystal. Journal of Electron Spectroscopy and Related Phenomena, 2014, 194, 74-80.	1.7	25
26	Structural and Electronic Dependence of the Single-Molecule-Magnet Behavior of Dysprosium(III) Complexes. Inorganic Chemistry, 2014, 53, 2598-2605.	4.0	49
27	A Combined Experimental and Theoretical Study of the Ti₂ + N₂O Reaction. Journal of Physical Chemistry A, 2014, 118, 561-572.	2.5	6
28	Magnetic Resonance Properties of Actinyl Carbonate Complexes and Plutonyl(VI)-tris-nitrate. Inorganic Chemistry, 2014, 53, 8577-8592.	4.0	49
29	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
30	Crystal structure diversity in the bis[hydrotris(3,5-dimethylpyrazolyl)borate]iodouranium(iii) complex: from neutral to cationic forms. Dalton Transactions, 2013, 42, 8861.	3.3	26
31	Single-ion magnet behaviour in [U(TpMe2)2I]. Dalton Transactions, 2012, 41, 13568.	3.3	97
32	Ferromagnetic coupling induced by spin-orbit coupling in dipyridylamide linear trinuclear Cu-Pd-Cu and Cu-Pt-Cu complexes. Comptes Rendus Chimie, 2012, 15, 170-175.	0.5	3
33	Case of a Strong Antiferromagnetic Exchange Coupling Induced by Spin Polarization of a Mnâ€“Mn Partial Single Bond. Inorganic Chemistry, 2012, 51, 7112-7118.	4.0	12
34	Zero field splitting of the chalcogen diatomics using relativistic correlated wave-function methods. Journal of Chemical Physics, 2011, 135, 114106.	3.0	32
35	Magnetic Memory Effect in a Transuranic Mononuclear Complex. Angewandte Chemie - International Edition, 2011, 50, 1696-1698.	13.8	153
36	Ab Initio Investigation of Spectroscopic Parameters for CrX63-: The Unexpected Role of Bond Length Variation - Size Really Matters. European Journal of Inorganic Chemistry, 2010, 2010, 2221-2223.	2.0	5

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37	The electronic structure of the triiodide ion from relativistic correlated calculations: A comparison of different methodologies. Journal of Chemical Physics, 2010, 133, 064305.	3.0	29
38	Optical and magnetic properties of the 5f[sup 1]AnX[sub 6][sup qâ^'] series: A theoretical study. Journal of Chemical Physics, 2009, 130, 184310.	3.0	45
39	Unique Definition of the Zeeman-Splitting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>g</mml:mi></mml:math>Tensor of a Kramers Doublet. Physical Review Letters, 2008, 101, 033003.	7.8	58
40	A theoretical study of the excited states of AmO2n+, n=1,2,3. Journal of Chemical Physics, 2008, 128, 164315.	3.0	19
41	Theoretical Determination of the Excited States and ofg-Factors of the Creutzâ^'Taube Ion, [(NH3)5â^'Ruâ^'pyrazineâ^'Ruâ^'(NH3)5]5+. Inorganic Chemistry, 2007, 46, 417-427.	4.0	44
42	An Alternative Approach to the g-Matrix: Theory and Applications. ChemPhysChem, 2006, 7, 1575-1589.	2.1	150
43	Cation templation of Mn2+/[Mo(CN)7]4â^' system: Formation of pseudo-dimorphs (NH4)2Mn3(H2O)4[Mo(CN)7]2Â·nH2O (n=4, 5). Polyhedron, 2005, 24, 1033-1046.	2.2	5
44	Uranyl Complexation in Fluorinated Acids (HF, HBF4, HPF6, HTf2N): A Combined Experimental and Theoretical Study.. ChemInform, 2005, 36, no.	0.0	0
45	Uranyl Complexation in Fluorinated Acids (HF, HBF4, HPF6, HTf2N):Â A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2005, 44, 852-861.	4.0	39
46	Aminomethyl-bipyridine Bearing Two Flexible Nitronyl-nitroxide Arms: A New Podand for Complexation of Transition Metals in a Facial or Meridional Conformation. Inorganic Chemistry, 2003, 42, 2938-2949.	4.0	26
47	From ab Initio Calculations to Model Hamiltonians: The Effective Hamiltonian Technique as an Efficient Tool to Describe Mixed-Valence Molecules. Journal of Physical Chemistry A, 2003, 107, 5071-5078.	2.5	14
48	Ab Initio Study of the Two Iso-electronic Molecules NpO4- and UO42-. Journal of Physical Chemistry A, 2001, 105, 10570-10576.	2.5	28
49	On the Structure of Np(VI) and Np(VII) Species in Alkaline Solution Studied by EXAFS and Quantum Chemical Methods. Journal of Physical Chemistry A, 2001, 105, 11441-11445.	2.5	52
50	AbInitioCalculations of the Magnetic Coupling between a Ni(II) Ion and Two Nitroxide Radicals incisandtransPositions. Inorganic Chemistry, 1999, 38, 6089-6095.	4.0	9
51	d â†' d Spectrum and High-Spin/Low-Spin Competition in d6Octahedral Coordination Compounds:Â ab Initio Study of Potential Energy Curves. Journal of Physical Chemistry A, 1998, 102, 7525-7534.	2.5	48
52	The Neel point for spin-transition systems: toward a two-step transition. Chemical Physics, 1996, 211, 101-114.	1.9	16
53	Ferromagnetism and spin transition: an attempt at a unifying approach. Chemical Physics Letters, 1995, 243, 355-358.	2.6	10
54	Ising model for low-spin high-spin transitions in molecular compounds; within and beyond the mean-field approximation. Chemical Physics, 1995, 192, 295-305.	1.9	46

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55	High-spin-low-spin transitions in Fe(II) complexes by effective Hamiltonian method. Chemical Physics, 1995, 193, 19-26.	1.9	25
56	Cooperativity and Anticooperativity in Spin Transition Compounds; Macroscopic Approach and Orbital Modelization. Molecular Crystals and Liquid Crystals, 1993, 234, 275-282.	0.3	2
57	Two-step spin crossover in the new dinuclear compound [Fe(bt)(NCS)2]2bpym, with bt = 2,2'-bi-2-thiazoline and bpym = 2,2'-bipyrimidine: experimental investigation and theoretical approach. Journal of the American Chemical Society, 1992, 114, 4650-4658.	13.7	281
58	Dipolar and Contact Paramagnetic NMR Chemical Shifts in An^{IV} Complexes with Dipicolinic Acid Derivatives. Inorganic Chemistry, 0, , .	4.0	2