

# HÃ©lÃ¨ne Bolvin

## List of Publications by Year in descending order

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58  
papers

2,003  
citations

257429

24  
h-index

243610

44  
g-index

60  
all docs

60  
docs citations

60  
times ranked

2087  
citing authors

#	ARTICLE	IF	CITATIONS
1	Two-step spin crossover in the new dinuclear compound [Fe(bt)(NCS) <sub>2</sub> ] <sub>2</sub> bpym, with bt = 2,2'-bi-2-thiazoline and bpym = 2,2'-bipyrimidine: experimental investigation and theoretical approach. <i>Journal of the American Chemical Society</i> , 1992, 114, 4650-4658.	13.7	281
2	Magnetic Memory Effect in a Transuranic Mononuclear Complex. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 1696-1698.	13.8	153
3	An Alternative Approach to the g-Matrix: Theory and Applications. <i>ChemPhysChem</i> , 2006, 7, 1575-1589.	2.1	150
4	Assessing the exchange coupling in binuclear lanthanide( <sup>iii</sup> ) complexes and the slow relaxation of the magnetization in the antiferromagnetically coupled Dy <sub>2</sub> derivative. <i>Chemical Science</i> , 2015, 6, 4148-4159.	7.4	114
5	Single-ion magnet behaviour in [U(TpMe <sub>2</sub> ) <sub>2</sub> ]. <i>Dalton Transactions</i> , 2012, 41, 13568.	3.3	97
6	Magnetic Properties and Electronic Structure of Neptunyl(VI) Complexes: Wavefunctions, Orbitals, and Crystalâ€­Field Models. <i>Chemistry - A European Journal</i> , 2014, 20, 7994-8011.	3.3	85
7	Unique Definition of the Zeeman-Splitting $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \langle \text{mml:mi} \rangle \text{g} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ Tensor of a Kramers Doublet. <i>Physical Review Letters</i> , 2008, 101, 033003.	7.8	58
8	On the Structure of Np(VI) and Np(VII) Species in Alkaline Solution Studied by EXAFS and Quantum Chemical Methods. <i>Journal of Physical Chemistry A</i> , 2001, 105, 11441-11445.	2.5	52
9	Single-ion 4f element magnetism: an ab-initio look at Ln(COT) <sub>2</sub> <sup>âˆ—</sup> . <i>Dalton Transactions</i> , 2015, 44, 19886-19900.	3.3	52
10	Structural and Electronic Dependence of the Single-Molecule-Magnet Behavior of Dysprosium(III) Complexes. <i>Inorganic Chemistry</i> , 2014, 53, 2598-2605.	4.0	49
11	Magnetic Resonance Properties of Actinyl Carbonate Complexes and Plutonyl(VI)-tris-nitrate. <i>Inorganic Chemistry</i> , 2014, 53, 8577-8592.	4.0	49
12	d â† d Spectrum and High-Spin/Low-Spin Competition in d <sub>6</sub> Octahedral Coordination Compounds:â€­ ab Initio Study of Potential Energy Curves. <i>Journal of Physical Chemistry A</i> , 1998, 102, 7525-7534.	2.5	48
13	Ising model for low-spin high-spin transitions in molecular compounds; within and beyond the mean-field approximation. <i>Chemical Physics</i> , 1995, 192, 295-305.	1.9	46
14	Optical and magnetic properties of the 5f <sup>[sup 1]</sup> AnX <sub>[sub 6]</sub> <sup>[sup qâˆ—]</sup> series: A theoretical study. <i>Journal of Chemical Physics</i> , 2009, 130, 184310.	3.0	45
15	Theoretical Determination of the Excited States and of g-Factors of the Creutzâˆ—Taube Ion, [(NH <sub>3</sub> ) <sub>5</sub> âˆ—Ruâˆ—pyrazineâˆ—Ruâˆ—(NH <sub>3</sub> ) <sub>5</sub> ] <sup>5+</sup> . <i>Inorganic Chemistry</i> , 2007, 46, 417-427.	4.0	44
16	Uranyl Complexation in Fluorinated Acids (HF, HBF <sub>4</sub> , HPF <sub>6</sub> , HTf <sub>2</sub> N):â€­ A Combined Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2005, 44, 852-861.	4.0	39
17	Tools for Predicting the Nature and Magnitude of Magnetic Anisotropy in Transition Metal Complexes: Application to Co(II) Complexes. <i>Magnetochemistry</i> , 2016, 2, 31.	2.4	37
18	Zero field splitting of the chalcogen diatomics using relativistic correlated wave-function methods. <i>Journal of Chemical Physics</i> , 2011, 135, 114106.	3.0	32

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19	Derivation of Lanthanide Series Crystal Field Parameters From First Principles. Chemistry - A European Journal, 2019, 25, 15112-15122.	3.3	30
20	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
21	Ab Initio Study of the Two Iso-electronic Molecules NpO <sub>4</sub> <sup>-</sup> and UO <sub>4</sub> <sup>2-</sup> . Journal of Physical Chemistry A, 2001, 105, 10570-10576.	2.5	28
22	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
23	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
24	High-spin-low-spin transitions in Fe(II) complexes by effective Hamiltonian method. Chemical Physics, 1995, 193, 19-26.	1.9	25
25	Magnetic properties of a fourfold degenerate state: Np <sup>4+</sup> ion diluted in Cs <sub>2</sub> ZrCl <sub>6</sub> crystal. Journal of Electron Spectroscopy and Related Phenomena, 2014, 194, 74-80.	1.7	25
26	Metal-Based Linear Light Upconversion Implemented in Molecular Complexes: Challenges and Perspectives. Accounts of Chemical Research, 2022, 55, 442-456.	15.6	22
27	Magnetic circular dichroism of UCl <sub>6</sub> <sup>3-</sup> in the ligand-to-metal charge-transfer spectral region. Physical Chemistry Chemical Physics, 2017, 19, 17300-17313.	2.8	21
28	Crystal Field in Rare-Earth Complexes: From Electrostatics to Bonding. Chemistry - A European Journal, 2018, 24, 5538-5550.	3.3	21
29	Insight of the Metal-Ligand Interaction in f-Element Complexes by Paramagnetic NMR Spectroscopy. Chemistry - A European Journal, 2019, 25, 4435-4451.	3.3	21
30	A theoretical study of the excited states of AmO <sub>2</sub> <sup>n+</sup> , n=1,2,3. Journal of Chemical Physics, 2008, 128, 164315.	3.0	19
31	Magnetic susceptibility of actinide(III) cations: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2016, 18, 6515-6525.	2.8	19
32	Structure, luminescence and magnetic properties of an erbium(III) $\beta^2$ -diketonate homodinuclear complex. New Journal of Chemistry, 2016, 40, 8251-8261.	2.8	17
33	The Neel point for spin-transition systems: toward a two-step transition. Chemical Physics, 1996, 211, 101-114.	1.9	16
34	Molecular light-upconversion: we have had a problem! When excited state absorption (ESA) overcomes energy transfer upconversion (ETU) in Cr(III)/Er(III) complexes. Dalton Transactions, 2021, 50, 7955-7968.	3.3	16
35	Unraveling $\sigma$ and $\pi$ Effects on Magnetic Anisotropy in <i>cis</i> -Ni <sub>4</sub> B <sub>2</sub> Complexes: Magnetization, HF-EPR Studies, First-Principles Calculations, and Orbital Modeling. Chemistry - A European Journal, 2016, 22, 16850-16862.	3.3	15
36	Bimetallic Schiff-Base with Peripheral Ester Functionalization: Synthesis and Magnetic Behavior of Bimetallic Zn-Ln Complexes (Ln = Dy, Tb, Gd). European Journal of Inorganic Chemistry, 2016, 2016, 4988-4995.	2.0	15

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37	From ab Initio Calculations to Model Hamiltonians: The Effective Hamiltonian Technique as an Efficient Tool to Describe Mixed-Valence Molecules. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5071-5078.	2.5	14
38	Magnetic Coupling in the Ce(III) Dimer Ce <sub>2</sub> (COT) <sub>3</sub> . <i>Inorganic Chemistry</i> , 2019, 58, 581-593.	4.0	14
39	Case of a Strong Antiferromagnetic Exchange Coupling Induced by Spin Polarization of a Mn <sup>II</sup> -Mn Partial Single Bond. <i>Inorganic Chemistry</i> , 2012, 51, 7112-7118.	4.0	12
40	Relativistic Methods for Calculating Electron Paramagnetic Resonance (EPR) Parameters. , 2017, , 725-763.		12
41	Paramagnetism of Aqueous Actinide Cations. Part II: Theoretical Aspects and New Measurements on An(IV). <i>Inorganic Chemistry</i> , 2016, 55, 12149-12157.	4.0	11
42	Ferromagnetism and spin transition: an attempt at a unifying approach. <i>Chemical Physics Letters</i> , 1995, 243, 355-358.	2.6	10
43	Crystallographic structure and crystal field parameters in the [AnIV(DPA) <sub>3</sub> ] <sup>2+</sup> series, An = Th, U, Np, Pu. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14293-14308.	2.8	10
44	AbInitioCalculations of the Magnetic Coupling between a Ni(II) Ion and Two Nitroxide Radicals in cis and trans Positions. <i>Inorganic Chemistry</i> , 1999, 38, 6089-6095.	4.0	9
45	Temperature Dependence of <sup>1</sup> H Paramagnetic Chemical Shifts in Actinide Complexes, Beyond Bleaney's Theory: The An VI O <sub>2</sub> <sup>2+</sup> <sup>II</sup> -Dipicolinic Acid Complexes (An=Np, Pu) as an Example. <i>Chemistry - A European Journal</i> , 2021, 27, 7138-7153.	3.3	9
46	Hysteresis in a bimetallic holmium complex: A synergy between electronic and nuclear magnetic interactions. <i>Physical Review B</i> , 2017, 96, .	3.2	8
47	Complete Active Space Wavefunction-Based Analysis of Magnetization and Electronic Structure. <i>Topics in Organometallic Chemistry</i> , 2018, , 355-390.	0.7	8
48	Crystal Structure and Magnetic Properties of Peacock <sup>II</sup> -Weakley Type Polyoxometalates Na <sub>9</sub> [Ln(W <sub>5</sub> O <sub>18</sub> ) <sub>2</sub> ] (Ln = Tm, Yb): Rare Example of Tm(III) SMM. <i>Magnetochemistry</i> , 2020, 6, 53.	2.4	7
49	A Combined Experimental and Theoretical Study of the Ti <sub>2</sub> + N <sub>2</sub> O Reaction. <i>Journal of Physical Chemistry A</i> , 2014, 118, 561-572.	2.5	6
50	Cation templation of Mn <sup>2+</sup> /[Mo(CN) <sub>7</sub> ] <sup>4-</sup> system: Formation of pseudo-dimorphs (NH <sub>4</sub> ) <sub>2</sub> Mn <sub>3</sub> (H <sub>2</sub> O) <sub>4</sub> [Mo(CN) <sub>7</sub> ] <sub>2</sub> ·nH <sub>2</sub> O (n=4, 5). <i>Polyhedron</i> , 2005, 24, 1033-1046.	2.2	5
51	Ab Initio Investigation of Spectroscopic Parameters for CrX <sub>6</sub> <sup>3-</sup> : The Unexpected Role of Bond Length Variation - Size Really Matters. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 2221-2223.	2.0	5
52	Local Structure and Magnetism of La <sub>1-x</sub> M <sub>x</sub> PO <sub>4</sub> (M = Tj ETQq0 0 0 rgBT /Overl <i>Journal of Physical Chemistry C</i> , 2021, 125, 22163-22174.	3.1	4
53	Ferromagnetic coupling induced by spin-orbit coupling in dipyriddyamide linear trinuclear Cu-Pd-Cu and Cu-Pt-Cu complexes. <i>Comptes Rendus Chimie</i> , 2012, 15, 170-175.	0.5	3
54	Cooperativity and Anticooperativity in Spin Transition Compounds; Macroscopic Approach and Orbital Modelization. <i>Molecular Crystals and Liquid Crystals</i> , 1993, 234, 275-282.	0.3	2

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55	Relativistic Methods for Calculating Electron Paramagnetic Resonance (EPR) Parameters. , 2015, , 1-39.		2
56	Dipolar and Contact Paramagnetic NMR Chemical Shifts in An<sup>IV</sup> Complexes with Dipicolinic Acid Derivatives. Inorganic Chemistry, 0, , .	4.0	2
57	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
58	Uranyl Complexation in Fluorinated Acids (HF, HBF <sub>4</sub> , HPF <sub>6</sub> , HTf <sub>2</sub> N): A Combined Experimental and Theoretical Study.. ChemInform, 2005, 36, no.	0.0	0