

MercÃ Deumal

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Synthesis, Structure, and Magnetic Properties of an Antiferromagnetic Spin-Ladder Complex: \hat{A} Bis(2,3-dimethylpyridinium) Tetrabromocuprate. <i>Journal of the American Chemical Society</i> , 2007, 129, 952-959.	6.6	121
2	Structure-Magnetism Relationships in $\hat{I}\pm$ -Nitronyl Nitroxide Radicals. <i>Chemistry - A European Journal</i> , 1999, 5, 1631-1642.	1.7	103
3	Magnetic Properties of Organic Molecular Crystals via an Algebraic Heisenberg Hamiltonian. Applications to WLVW, TOLKEK, and KAXHAS Nitronyl Nitroxide Crystals. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1299-1315.	1.1	87
4	Calculation of microscopic exchange interactions and modelling of macroscopic magnetic properties in molecule-based magnets. <i>Chemical Society Reviews</i> , 2011, 40, 3182.	18.7	77
5	On the Validity of the McConnell-I Model of Ferromagnetic Interactions: $\hat{a}\epsilon\%$ The [2.2]Paracyclophane Example. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8404-8412.	1.1	68
6	Origin of the Magnetic Bistability in Molecule-Based Magnets: A First-Principles Bottom-Up Study of the TTTA Crystal. <i>Journal of the American Chemical Society</i> , 2010, 132, 17817-17830.	6.6	61
7	Direct versus Mediated Through-Space Magnetic Interactions: A First Principles, Bottom-Up Reinvestigation of the Magnetism of the Pyridyl-Verdazyl:Hydroquinone Molecular Co-Crystal. <i>Chemistry - A European Journal</i> , 2006, 12, 3995-4005.	1.7	59
8	Synthesis, Structure, and Magnetic Behavior of Bis(2-amino-5-fluoropyridinium) Tetrachlorocuprate(II). <i>Inorganic Chemistry</i> , 2007, 46, 11254-11265.	1.9	57
9	The key role of vibrational entropy in the phase transitions of dithiazolyl-based bistable magnetic materials. <i>Nature Communications</i> , 2014, 5, 4411.	5.8	55
10	Studying the Origin of the Antiferromagnetic to Spin $\hat{a}\epsilon$ Canting Transition in the $\hat{I}^2\hat{a}\epsilon\langle i \rangle p \langle /i \rangle \hat{a}\epsilon\text{NCC} \langle \text{sub} \rangle 6 \langle / \text{sub} \rangle \text{F} \langle \text{sub} \rangle 4 \langle / \text{sub} \rangle \text{CNSSN} \langle \text{sup} \rangle . \langle / \text{sup} \rangle$ Molecular Magnet. <i>Chemistry - A European Journal</i> , 2010, 16, 2741-2750.	1.7	51
11	Structure-Magnetism Relationships in $\hat{I}\pm$ -Nitronyl Nitroxide Radicals: Pitfalls and Lessons to be Learned. <i>Advanced Materials</i> , 1998, 10, 1461-1466.	11.1	48
12	Modeling Photochemical [4 + 4] Cycloadditions: \hat{A} Conical Intersections Located with CASSCF for Butadiene + Butadiene. <i>Journal of the American Chemical Society</i> , 1997, 119, 709-718.	6.6	38
13	The Mechanism of Magnetic Interactions in the Bulk Ferromagnet para-(Methylthio)Phenyl Nitronyl Nitroxide (YUJNEW): A First Principles, Bottom-Up, Theoretical Study. <i>Chemistry - A European Journal</i> , 2004, 10, 6422-6432.	1.7	37
14	The Mechanism of Magnetic Interaction in Spin-Ladder Molecular Magnets: A First-Principles, Bottom-Up, Theoretical Study of the Magnetism in the Two-Legged Spin-Ladder Bis(2-amino-5-nitropyridinium) Tetrabromocuprate Monohydrate. <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 4697-4706.	1.0	35
15	Dynamical effects on the magnetic properties of dithiazolyl bistable materials. <i>Chemical Science</i> , 2015, 6, 2371-2381.	3.7	34
16	First-Principles Bottom-Up Study of 1D to 3D Magnetic Transformation in the Copper Pyrazine Dinitrate $S = 1/2$ Antiferromagnetic Crystal. <i>Inorganic Chemistry</i> , 2010, 49, 1750-1760.	1.9	33
17	A theoretical study of the magnetism of the $\hat{I}\pm$ -p-cyano-tetrafluorophenyl-dithiadiazolyl radical using a first principles bottom-up procedure. <i>Polyhedron</i> , 2007, 26, 1949-1958.	1.0	32
18	The Mechanism of the Through-Space Magnetic Interactions in Purely Organic Molecular Magnets. , 2001, , 33-60.		30

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19	Synthesis, Structure, Magnetic Behavior, and Theoretical Analysis of Diazine-Bridged Magnetic Ladders: Cu(quinoline) ₂ and Cu(2,3-dimethylpyrazine) ₂ (X = Cl, Br). <i>Inorganic Chemistry</i> , 2012, 51, 6315-6325.	1.9	27
20	Insights into the magnetism and phase transitions of organic radical-based materials. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10624-10646.	2.7	27
21	Theoretical analysis of the crystal packing of nitronyl nitroxide radicals: the packing of the $\hat{I}\pm$ -2-hydro nitronyl nitroxide radical. <i>Chemical Physics Letters</i> , 1997, 265, 190-199.	1.2	25
22	The mechanism of the magnetic interaction in the \hat{I}^2 phase of the p-(nitro)phenyl nitronyl nitroxide (KAXHAS). A bottom-up study using only ab initio data. <i>Polyhedron</i> , 2003, 22, 1935-1944.	1.0	23
23	Dividing the Spoils: Role of Pyrazine Ligands and Perchlorate Counterions in the Magnetic Properties of Bis(pyrazine)diperchloratecopper(II), [Cu(pz) ₂](ClO ₄) ₂ . <i>Inorganic Chemistry</i> , 2013, 52, 12923-12932.	1.9	22
24	Bulk ferromagnetism in nitronyl nitroxide crystals: a first principles bottom-up comparative study of four bulk nitronyl nitroxide ferromagnets (KAXHAS, YOMYII, LICMIT and YUJNEW). <i>Molecular Physics</i> , 2006, 104, 857-873.	0.8	20
25	Theoretical Analysis of the Packing and Polimorphism of Molecular Crystals Using Quantum Mechanical Methods: The Packing of the 2-Hydro Nitronyl Nitroxide. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 305, 143-156.	0.3	18
26	Controlling pairing of π -conjugated electrons in 2D covalent organic radical frameworks via in-plane strain. <i>Nature Communications</i> , 2021, 12, 1705.	5.8	18
27	On the existence of temperature induced changes in the magnetic topology of crystals that show no first-order crystallographic phase transitions. <i>Polyhedron</i> , 2009, 28, 1965-1971.	1.0	17
28	Elucidating the 2D Magnetic Topology of the \hat{I}^2 -Metal-Radical TTTA...Cu(hfac) ₂ System. <i>Chemistry - A European Journal</i> , 2014, 20, 7083-7090.	1.7	16
29	The magnetic fingerprint of dithiazolyl-based molecule magnets. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20406-20416.	1.3	16
30	A general study of the spin population of $\hat{I}\pm$ -nitronyl nitroxide radicals: radicals with crystals presenting dominant ferro or antiferromagnetic behavior. <i>Synthetic Metals</i> , 2001, 122, 477-483.	2.1	15
31	Through space magnetic exchange in tetrabromocuprates: theoretical considerations. <i>Polyhedron</i> , 2003, 22, 2235-2239.	1.0	15
32	$\langle S \rangle = 1/2$ One-Dimensional Random-Exchange Ferromagnetic Zigzag Ladder, Which Exhibits Competing Interactions in a Critical Regime. <i>Chemistry - A European Journal</i> , 2014, 20, 8355-8362.	1.7	15
33	Theoretical study of the magnetism in molecular crystals using a first-principles bottom-up methodol. <i>Progress in Theoretical Chemistry and Physics</i> , 2007, , 271-289.	0.2	15
34	Product Distributions from Molecular Mechanics ² Valence Bond Dynamics: Modeling Photochemical [4 + 4] Cycloadditions. <i>Journal of Organic Chemistry</i> , 1998, 63, 4594-4600.	1.7	14
35	2D Hexagonal Covalent Organic Radical Frameworks as Tunable Correlated Electron Systems. <i>Advanced Functional Materials</i> , 2021, 31, 2004584.	7.8	14
36	The Magnetism of (5MAP) ₂ CuBr ₄ [5MAP = 5-Methyl-2-aminopyridinium]: A Quasi-2D or a 3D Magnetic System?. <i>Inorganic Chemistry</i> , 2010, 49, 8017-8024.	1.9	13

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37	A First-Principles Analysis of the Magnetism of Cull Polynuclear Coordination Complexes: the Case of [Cu4(bpy)4(aspartate)2(H2O)3](ClO4)4·2.5H2O. <i>Molecules</i> , 2004, 9, 757-770.	1.7	12
38	Tracing the Sources of the Different Magnetic Behavior in the Two Phases of the Bistable (BDTA) ₂ [Co(mnt) ₂] Compound. <i>Inorganic Chemistry</i> , 2012, 51, 8646-8648.	1.9	12
39	The origin of the bistability in the thiazyl radical 1,3,5-trithia-2,4,6-triazapentalenyl (TTTA): A first principles bottom-up investigation of the magnetic properties of its high temperature polymorph. <i>Polyhedron</i> , 2009, 28, 1614-1619.	1.0	10
40	The quest for rationalizing the magnetism in purely organic semiquinone-bridged bisdithiazolyl molecular magnets. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20738-20749.	1.3	10
41	Does the McConnell-I Model Really Work? An ab Initio Study of the Magnetic Character of Some Intermolecular Contacts. <i>Molecular Crystals and Liquid Crystals</i> , 1999, 335, 603-612.	0.3	8
42	Revising the common understanding of metamagnetism in the molecule-based bisdithiazolyl BDTMe compound. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12184-12191.	1.3	8
43	A Theoretical Analysis of the Packing and Polymorphism of the 2-Hydro Nitronyl Nitroxide Crystal. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 305, 129-141.	0.3	7
44	A first-principles bottom-up study of the magnetic interaction mechanism in the bulk ferromagnet p-O2N-C6F4-CNSSN. <i>Inorganica Chimica Acta</i> , 2008, 361, 3586-3592.	1.2	7
45	Reorganization of Intermolecular Interactions in the Polymorphic Phase Transition of a Prototypical Dithiazolyl-Based Bistable Material. <i>Crystal Growth and Design</i> , 2019, 19, 2329-2339.	1.4	7
46	Two different mechanisms of stabilization of regular Î±-stacks of radicals in switchable dithiazolyl-based materials. <i>Journal of Materials Chemistry C</i> , 2020, 8, 5437-5448.	2.7	7
47	Pitfalls on evaluating pair exchange interactions for modelling molecule-based magnetism. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10647-10660.	2.7	7
48	Architecture of purely organic molecular magnets: Crystal packing rationalization of some Î±-nitronyl nitroxides using the crystal packing functional group analysis. <i>Synthetic Metals</i> , 1999, 103, 2283-2286.	2.1	6
49	The microscopic basis of the intermolecular magnetism. An ab initio study on molecular crystals. <i>Computational and Theoretical Chemistry</i> , 2000, 506, 287-296.	1.5	6
50	Assigning the dimensionality in low-dimensional materials: A rigorous study of the dimensionality of (2,5-dimethylpyrazine)CuCl2. <i>Polyhedron</i> , 2013, 52, 699-705.	1.0	6
51	Quantitative analysis of the magnetism of the meta-(methoxy)phenyl nitronyl nitroxide crystal: A bottom-up analysis of a crystal presenting competing ferro and antiferromagnetic interactions. <i>Polyhedron</i> , 2005, 24, 2368-2376.	1.0	5
52	The origin of the antiferromagnetic behaviour of the charge-transfer compound (HMTTF)[Ni(mnt) ₂]. <i>Dalton Transactions</i> , 2015, 44, 608-614.	1.6	5
53	A Definition of the Magnetic Transition Temperature Using Valence Bond Theory. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2168-2177.	1.1	5
54	Disentangling the magnetic dimensionality of an alleged magnetically isolated cuprate spin-ladder CuHpCl system: a long-lasting issue. <i>Dalton Transactions</i> , 2021, 50, 1754-1765.	1.6	5

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55	A theoretical analysis of the magnetic properties of the low-dimensional copper(II) $X_2(2-X-3\text{-methylpyridine})_2$ ($X = \text{Cl}$ and Br) complexes. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	4
56	Revisiting the Role of Hydrogen Bonding in the Strong Dimer Superexchange of a 2D Copper(II) Halide Honeycomb-Like Lattice: Structural and Magnetic Study. <i>Inorganic Chemistry</i> , 2020, 59, 6319-6331.	1.9	4
57	A theoretical analysis of the magnetic properties of the low dimensional bis(2-chloropyrazine)dichlorocopper(II) molecule-based magnet. <i>Polyhedron</i> , 2013, 64, 163-171.	1.0	2
58	Assessing $\text{Cu}_2\text{L}_2\text{X}_4$ dimeric moieties as ferromagnetic building blocks in double halide-bridged polymers ($X = \text{Cl}^-$, Br^- and $\text{L} = \text{benzamide}$). An experimental and computational study. <i>Polyhedron</i> , 2020, 185, 114603.	1.0	2
59	Approaching the isotropic spin-ladder regime: structure and magnetism of all-pyrazine-bridged copper(scp)-based antiferromagnetic ladders. <i>Dalton Transactions</i> , 2022, 51, 4653-4667.	1.6	2
60	Electronic structure and magnetic coupling in selenium substituted pyridine-bridged bisdithiazolyl multifunctional molecular materials. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12196-12207.	1.3	2
61	Theoretical Study of the Electronic Structure and Magnetic Interactions in Purely Organic Nitronyl Nitroxide Crystals. , 0, , 65-117.		1
62	Structure-Magnetism Relationships in $\hat{1}\pm$ -Nitronyl Nitroxide Radicals. , 1999, 5, 1631.		1
63	Structure-Magnetism Relationships in $\hat{1}\pm$ -Nitronyl Nitroxide Radicals: Pitfalls and Lessons to be Learned. <i>Advanced Materials</i> , 1998, 10, 1461-1466.	11.1	1
64	Theoretical Study of the Electronic Structure and Magnetic Interactions in Purely Organic Nitronyl Nitroxide Crystals. <i>ChemInform</i> , 2003, 34, no.	0.1	0
65	A theoretical analysis of the magnetic properties of the low-dimensional copper(II) $X_2(2-X-3\text{-methylpyridine})_2$ ($X = \text{Cl}$ and Br) complexes. <i>Highlights in Theoretical Chemistry</i> , 2014, , 219-230.	0.0	0
66	Crystal Engineering of Purely Organic Molecular Magnets: What can AB Initio Computations Tell Us?. , 1999, , 105-125.		0