Spinning around in Transition-Metal Chemistry

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Citation Report

#	Article	IF	Citations
2	Catalytic Oxidation of Water with High-Spin Iron(IV)â€“Oxo Species: Role of the Water Solvent. ACS Catalysis, 2017, 7, 4018-4025.	5.5	38
3	Assessment of electronic structure methods for the determination of the ground spin states of Fe(<scp>ii</scp>), Fe(<scp>iii</scp>) and Fe(<scp>iv</scp>) complexes. Physical Chemistry Chemical Physics, 2017, 19, 13049-13069.	1.3	100
4	Structures of dimetallocenes M₂(C₅H₅)₂ (M = Zn, Cu,) Tj ETQq0 0 0 rgBT /Overloch	1.4	1
5	Low-Energy Photoelectron Imaging Spectroscopy of La_n(benzene) (n = 1 and) Tj ETQq1 1 0.784314 rgBT /O	1.1	6
6	NO oxidation catalyzed by Ir4-based nanoclusters: the role of alloying on the catalytic activity. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	1
7	The role of spin states in the catalytic mechanism of the intra- and extradiol cleavage of catechols by O₂. Organic and Biomolecular Chemistry, 2017, 15, 7860-7868.	1.5	9
8	The role of ligand redox non-innocence in ring-opening polymerization reactions catalysed by bis(imino)pyridine iron alkoxide complexes. Dalton Transactions, 2017, 46, 12971-12980.	1.6	43
9	Rational design of Fe catalysts for olefin aziridination through DFT-based mechanistic analysis. Catalysis Science and Technology, 2017, 7, 4388-4400.	2.1	22
10	A Simple Method of Predicting Spin State in Solution. Journal of the American Chemical Society, 2017, 139, 18392-18396.	6.6	68
11	Multireference Electronic Structures of Feâ€“Pyridine(diimine) Complexes over Multiple Oxidation States. Journal of Physical Chemistry A, 2017, 121, 5932-5939.	1.1	18
12	Understanding the Catalase-Like Activity of a Bioinspired Manganese(II) Complex with a Pentadentate NSNSN Ligand Framework. A Computational Insight into the Mechanism. ACS Catalysis, 2018, 8, 2944-2958.	5.5	9
13	Toward Highly Accurate Spin State Energetics in First-Row Transition Metal Complexes: A Combined CASPT2/CC Approach. Journal of Chemical Theory and Computation, 2018, 14, 2446-2455.	2.3	95
14	Experimental and Theoretical Identification of the Origin of Magnetic Anisotropy in Intermediate Spin Iron(III) Complexes. Chemistry - A European Journal, 2018, 24, 5091-5094.	1.7	11
15	Electronic structure and energy decomposition of binuclear transition metal complexes containing Î²-diketiminate and imido ligands: spin state and metalâ€™s nature effects. Structural Chemistry, 2018, 29, 1307-1320.	1.0	11
16	Calculation of Ligand Dissociation Energies in Large Transition-Metal Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2456-2468.	2.3	62
17	Indirect evidence for a Ni^{III}â€“oxyl oxidant in the reaction of a Ni^{II} complex with peracid. Dalton Transactions, 2018, 47, 246-250.	1.6	14
18	Rotating Iron and Titanium Sandwich Complexes. Chemistry - A European Journal, 2018, 24, 5070-5073.	1.7	1
19	Ab initio investigation of magnetic anisotropy in intermediate spin iron(<scp>iii</scp>) complexes. Journal of Chemical Physics, 2018, 149, 234302.	1.2	10

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20	H₂O₂ Oxidation by Fe^{III}â€“OOH Intermediates and Its Effect on Catalytic Efficiency. ACS Catalysis, 2018, 8, 9665-9674.	5.5	53
21	High-Oxidation-State 3d Metal (Tiâ€“Cu) Complexes with N-Heterocyclic Carbene Ligation. Chemical Reviews, 2018, 118, 9930-9987.	23.0	136
22	DFT Study on Fe(IV)-Peroxo Formation and H Atom Transfer Triggered O₂ Activation by NiFe Complex. Organometallics, 2018, 37, 1534-1545.	1.1	11
23	Projected site-occupation embedding theory. Physical Review B, 2019, 100, .	1.1	13
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36	Computational Versus Experimental Spectroscopy for Transition Metals. Challenges and Advances in Computational Chemistry and Physics, 2019, , 161-183.	0.6	1
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39	DFT investigation of homotrinuclear and heterotrinuclear [M3(Phz)2], [MMâ€²2(Phz)2], [M3(CO)2(Phz)2], [MMâ€²2(CO)2(Phz)2] sandwich complexes (Mâ€‰=â€‰Ti, Cr, Fe and Ni; Mâ€²â€‰=â€‰V and Mn, Phzâ€‰=â€‰C12H8N2): p models and electronic structures. Structural Chemistry, 2019, 30, 1859-1871.	1.6	
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50	Density functional approximations for consistent spin and oxidation states of oxoiron complexes. International Journal of Quantum Chemistry, 2020, 120, e26121.	1.0	10
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