

Azaj Ansari

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Mechanistic Insights on the <i>ortho</i> -Hydroxylation of Aromatic Compounds by Non-heme Iron Complex: A Computational Case Study on the Comparative Oxidative Ability of Ferric-Hydroperoxo and High-Valent Fe ^{IV} =O and Fe ^V =O Intermediates. <i>Journal of the American Chemical Society</i> , 2013, 135, 4235-4249.	13.7	126
2	Oxidation of methane by an N-bridged high-valent diiron=oxo species: electronic structure implications on the reactivity. <i>Dalton Transactions</i> , 2015, 44, 15232-15243.	3.3	43
3	Anticancer properties, apoptosis and catecholase mimic activities of dinuclear cobalt(II) and copper(II) Schiff base complexes. <i>Bioorganic Chemistry</i> , 2020, 95, 103561.	4.1	40
4	<i>ortho</i> -Hydroxylation of aromatic acids by a non-heme Fe ^V =O species: how important is the ligand design?. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14601-14613.	2.8	35
5	Theoretical studies on concerted versus two steps hydrogen atom transfer reaction by non-heme MnIV/III=O complexes: how important is the oxo ligand basicity in the C-H activation step?. <i>Dalton Transactions</i> , 2013, 42, 16518.	3.3	33
6	C-H Bond Activation by Metal=Superoxo Species: What Drives High Reactivity?. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 564-568.	13.8	28
7	Synthesis, characterization, theoretical studies and catecholase like activities of [MO ₆] type complexes. <i>New Journal of Chemistry</i> , 2019, 43, 14074-14083.	2.8	25
8	Exploring solvent dependent catecholase activity in transition metal complexes: an experimental and theoretical approach. <i>New Journal of Chemistry</i> , 2020, 44, 1371-1388.	2.8	25
9	A combined experimental and theoretical approach to investigate the structure, magnetic properties and DNA binding affinity of a homodinuclear Cu(II) complex. <i>New Journal of Chemistry</i> , 2019, 43, 7511-7519.	2.8	23
10	Exploring catecholase activity in dinuclear Mn(II) and Cu(II) complexes: an experimental and theoretical approach. <i>New Journal of Chemistry</i> , 2020, 44, 7998-8009.	2.8	23
11	Interplay of Electronic Cooperativity and Exchange Coupling in Regulating the Reactivity of Diiron(IV)=oxo Complexes towards C-H and O-H Bond Activation. <i>Chemistry - A European Journal</i> , 2017, 23, 10110-10125.	3.3	20
12	Axial vs. Equatorial Ligand Rivalry in Controlling the Reactivity of Iron(IV)=Oxo Species: Single-State vs. Two-State Reactivity. <i>Chemistry - A European Journal</i> , 2018, 24, 6818-6827.	3.3	19
13	Computational Examination on the Active Site Structure of a (Peroxo)diiron(III) Intermediate in the Amine Oxygenase AurF. <i>Inorganic Chemistry</i> , 2015, 54, 11077-11082.	4.0	17
14	Structures, bonding and reactivity of iron and manganese high-valent metal-oxo complexes: A computational investigation. <i>Journal of Chemical Sciences</i> , 2015, 127, 343-352.	1.5	15
15	Unprecedented isolation of a dinuclear tin (II) complex stabilized by pyridine ₂ ,6-dimethanol: structure, DFT and in vitro screening of cytotoxic properties. <i>Applied Organometallic Chemistry</i> , 2019, 33, e5006.	3.5	13
16	How to identify a smoker: a salient crystallographic approach to detect thiocyanate content. <i>RSC Advances</i> , 2021, 11, 16881-16891.	3.6	12
17	Mechanistic insights into the allylic oxidation of aliphatic compounds by tetraamido iron(V) species: A C-H vs. O-H bond activation. <i>New Journal of Chemistry</i> , 2020, 44, 19103-19112.	2.8	11
18	Elucidating the contribution of solvent on the catecholase activity in a mononuclear Cu(II) system: An experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2021, 1244, 130878.	3.6	11

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19	Computational studies on potential new anti-Covid-19 agents with a multi-target mode of action. Journal of King Saud University - Science, 2022, 34, 102086.	3.5	11
20	A side-on Mn(III) η^2 -peroxo supported by a non-heme pentadentate N3Py2 ligand: synthesis, characterization and reactivity studies. Dalton Transactions, 2021, 50, 2824-2831.	3.3	7
21	Electronic structures, bonding, and spin state energetics of biomimetic mononuclear and bridged dinuclear iron complexes: a computational examination. Structural Chemistry, 2021, 32, 1473-1488.	2.0	7
22	Novel {Cu ₄ } and {Cu ₄ Cd ₆ } clusters derived from flexible aminoalcohols: synthesis, characterization, crystal structures, and evaluation of anticancer properties. Dalton Transactions, 2021, 50, 11941-11953.	3.3	5
23	Electronic structures, bonding and energetics of non-heme mono and dinuclear iron-TPA complexes: a computational exploration. Structural Chemistry, 2021, 32, 2007-2018.	2.0	5
24	Effect of the ring size of TMC ligands in controlling C-H bond activation by metal-superoxo species. Dalton Transactions, 2022, 51, 5878-5889.	3.3	5
25	Dataset for Modelling Reaction Mechanisms Using Density Functional Theory: Mechanism of <i>ortho</i> -Hydroxylation by High-Valent Iron-Oxo Species. Dataset Papers in Science, 2014, 2014, 1-7.	1.0	4
26	Electronic structures, bonding aspects and spectroscopic parameters of homo/hetero valent bridged dinuclear transition metal complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 278, 121331.	3.9	3
27	Structure, DFT studies and evaluation of catechol oxidase (CO) mimic activity of mononuclear Co(II) complexes derived from aminoalcohols: an experimental and theoretical approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8740-8751.	3.5	2