Azaj Ansari

List of Publications by Year
in descending order

27 papers	587 citations	623734 14 h-index	642732 23 g-index
28 all docs	28 docs citations	28 times ranked	579 citing authors

#	Article	IF	Citations
1	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
2	Effect of the ring size of TMC ligands in controlling Câ€“H bond activation by metal-superoxo species. Dalton Transactions, 2022, 51, 5878-5889.	3.3	5
3	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
4	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
5	A side-on Mn(iii)â€“peroxo supported by a non-heme pentadentate N3Py2 ligand: synthesis, characterization and reactivity studies. Dalton Transactions, 2021, 50, 2824-2831.	3.3	7
6	Novel {Cu4} and {Cu4Cd6} clusters derived from flexible aminoalcohols: synthesis, characterization, crystal structures, and evaluation of anticancer properties. Dalton Transactions, 2021, 50, 11941-11953.	3.3	5
7	How to identify a smoker: a salient crystallographic approach to detect thiocyanate content. RSC Advances, 2021, 11, 16881-16891.	3.6	12
8	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
9	Elucidating the contribution of solvent on the catecholase activity in a mononuclear Cu(II) system: An experimental and theoretical approach. Journal of Molecular Structure, 2021, 1244, 130878.	3.6	11
10	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
11	Exploring solvent dependent catecholase activity in transition metal complexes: an experimental and theoretical approach. New Journal of Chemistry, 2020, 44, 1371-1388.	2.8	25
12	Anticancer properties, apoptosis and catecholase mimic activities of dinuclear cobalt(II) and copper(II) Schiff base complexes. Bioorganic Chemistry, 2020, 95, 103561.	4.1	40
13	Mechanistic insights into the allylic oxidation of aliphatic compounds by tetraamido iron(<scp>v</scp>) species: A Câ€“H <i>vs.</i> Oâ€“H bond activation. New Journal of Chemistry, 2020, 44, 19103-19112.	2.8	11
14	Exploring catecholase activity in dinuclear Mn(<scp>ii</scp>) and Cu(<scp>ii</scp>) complexes: an experimental and theoretical approach. New Journal of Chemistry, 2020, 44, 7998-8009.	2.8	23
15	Synthesis, characterization, theoretical studies and catecholase like activities of [MO₆] type complexes. New Journal of Chemistry, 2019, 43, 14074-14083.	2.8	25
16	Unprecedented isolation of a dinuclear tin (II) complex stabilized by pyridineâ€2,6â€dimethanol: structure, DFT and in vitro screening of cytotoxic properties. Applied Organometallic Chemistry, 2019, 33, e5006.	3.5	13
17	A combined experimental and theoretical approach to investigate the structure, magnetic properties and DNA binding affinity of a homodinuclear Cu(<scp>ii</scp>) complex. New Journal of Chemistry, 2019, 43, 7511-7519.	2.8	23
18	Axial vs. Equatorial Ligand Rivalry in Controlling the Reactivity of Iron(IV)â€Oxo Species: Singleâ€State vs. Twoâ€State Reactivity. Chemistry - A European Journal, 2018, 24, 6818-6827.	3.3	19

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19	Interplay of Electronic Cooperativity and Exchange Coupling in Regulating the Reactivity of Diiron(IV)â€oxo Complexes towards Câˆ'H and Oâˆ'H Bond Activation. Chemistry - A European Journal, 2017, 23, 10110-10125.	3.3	20
20	Cï£¿H Bond Activation by Metalâ€"Superoxo Species: What Drives High Reactivity?. Angewandte Chemie - International Edition, 2015, 54, 564-568.	13.8	28
21	Structures, bonding and reactivity of iron and manganese high-valent metal-oxo complexes: A computational investigation. Journal of Chemical Sciences, 2015, 127, 343-352.	1.5	15
22	Oxidation of methane by an N-bridged high-valent diironâ€"oxo species: electronic structure implications on the reactivity. Dalton Transactions, 2015, 44, 15232-15243.	3.3	43
23	Computational Examination on the Active Site Structure of a (Peroxo)diiron(III) Intermediate in the Amine Oxygenase AurF. Inorganic Chemistry, 2015, 54, 11077-11082.	4.0	17
24	ortho-Hydroxylation of aromatic acids by a non-heme Fe^Vî€O species: how important is the ligand design?. Physical Chemistry Chemical Physics, 2014, 16, 14601-14613.	2.8	35
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	Theoretical studies on concerted versus two steps hydrogen atom transfer reaction by non-heme MnIV/IIIî€O complexes: how important is the oxo ligand basicity in the Câ€"H activation step?. Dalton Transactions, 2013, 42, 16518.	3.3	33
27	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}â•O and Fe^Vâ•O Intermediates. Journal of the American Chemical Society, 2013, 135, 4235-4249.	13.7	126