

Khurram Shahzad Munawar

List of Publications by Year in descending order

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69
papers

2,110
citations

201385

27
h-index

276539

41
g-index

69
all docs

69
docs citations

69
times ranked

880
citing authors

#	ARTICLE	IF	CITATIONS
1	Synthesis of carbon nanotubes anchored with mesoporous Co ₃ O ₄ nanoparticles as anode material for lithium-ion batteries. <i>Electrochimica Acta</i> , 2013, 105, 481-488.	2.6	89
2	Synthesis, crystal structure, theoretical calculation, spectroscopic and antibacterial activity studies of copper(II) complexes bearing bidentate schiff base ligands derived from 4-aminoantipyrine: Influence of substitutions on antibacterial activity. <i>Journal of Molecular Structure</i> , 2021, 1230, 129908.	1.8	87
3	Synthesis, spectral characterization, crystal structure determination and antimicrobial activity of Ni(II), Cu(II) and Zn(II) complexes with the Schiff base ligand derived from 3,5-dibromosalicylaldehyde. <i>Journal of Molecular Structure</i> , 2021, 1229, 129842.	1.8	82
4	Synthesis, characterization, crystal structures, DFT, TD-DFT, molecular docking and DNA binding studies of novel copper(II) and zinc(II) complexes bearing halogenated bidentate N,O-donor Schiff base ligands. <i>Polyhedron</i> , 2021, 195, 114988.	1.0	76
5	Synthesis, spectral characterization, crystal structure and antibacterial activity of nickel(II), copper(II) and zinc(II) complexes containing ONNO donor Schiff base ligands. <i>Journal of Molecular Structure</i> , 2021, 1233, 130112.	1.8	75
6	Synthesis, Crystal Structure, Hirshfeld Surface Analysis, and Computational Study of a Novel Organic Salt Obtained from Benzylamine and an Acidic Component. <i>ACS Omega</i> , 2021, 6, 22357-22366.	1.6	66
7	Synthesis, characterization, crystal structures, Hirshfeld surface analysis, DFT computational studies and catalytic activity of novel oxovanadium and dioxomolybdenum complexes with ONO tridentate Schiff base ligand. <i>Polyhedron</i> , 2021, 202, 115194.	1.0	62
8	Synthesis, crystal structures, antimicrobial properties and enzyme inhibition studies of zinc(II) complexes of thiones. <i>Inorganica Chimica Acta</i> , 2011, 376, 207-211.	1.2	56
9	Novel oxovanadium and dioxomolybdenum complexes of tridentate ONO-donor Schiff base ligand: Synthesis, characterization, crystal structures, Hirshfeld surface analysis, DFT computational studies and catalytic activity for the selective oxidation of benzylic alcohols. <i>Inorganica Chimica Acta</i> , 2021, 523, 120414.	1.2	56
10	Synthesis, spectroscopic characterization, DFT optimization and biological activities of Schiff bases and their metal (II) complexes. <i>Journal of Molecular Structure</i> , 2017, 1145, 132-140.	1.8	51
11	Ultrasound-based synthesis, SC-XRD, NMR, DFT, HSA of new Schiff bases derived from 2-aminopyridine: Experimental and theoretical studies. <i>Journal of Molecular Structure</i> , 2021, 1233, 130105.	1.8	50
12	Some new Cu(II) complexes containing O,N-donor Schiff base ligands derived from 4-aminoantipyrine: synthesis, characterization, crystal structure and substitution effect on antimicrobial activity. <i>Journal of Coordination Chemistry</i> , 2021, 74, 1534-1549.	0.8	49
13	Nickel(II), copper(II) and zinc(II) complexes containing symmetrical Tetradentate Schiff base ligand derived from 3,5-diiodosalicylaldehyde: Synthesis, characterization, crystal structure and antimicrobial activity. <i>Journal of the Iranian Chemical Society</i> , 2021, 18, 2493-2503.	1.2	48
14	Titanium(IV) complex containing ONO-tridentate Schiff base ligand: Synthesis, crystal structure determination, Hirshfeld surface analysis, spectral characterization, theoretical and computational studies. <i>Journal of Molecular Structure</i> , 2021, 1241, 130653.	1.8	47
15	Schiff base triphenylphosphine palladium (II) complexes: Synthesis, structural elucidation, electrochemical and biological evaluation. <i>Journal of Molecular Structure</i> , 2016, 1118, 250-258.	1.8	46
16	Synthesis, spectroscopic characterization, X-ray crystal structure, antimicrobial, DNA-binding, alkaline phosphatase and insulin-mimetic studies of oxidovanadium(IV) complexes of azomethine precursors. <i>Journal of Coordination Chemistry</i> , 2020, 73, 2275-2300.	0.8	46
17	Synthesis, spectral characterization, SC-XRD, HSA, DFT and catalytic activity of novel dioxovanadium(V) complex with aminobenzohydrazone Schiff base ligand: An experimental and theoretical approach. <i>Inorganica Chimica Acta</i> , 2021, 526, 120535.	1.2	46
18	Binuclear Zn(II) Schiff base complexes: Synthesis, spectral characterization, theoretical studies and antimicrobial investigations. <i>Inorganica Chimica Acta</i> , 2022, 530, 120677.	1.2	46

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19	Single-Crystal Investigation, Hirshfeld Surface Analysis, and DFT Study of Third-Order NLO Properties of Unsymmetrical Acyl Thiourea Derivatives. <i>ACS Omega</i> , 2021, 6, 31211-31225.	1.6	46
20	Synthesis, physicochemical elucidation, biological screening and molecular docking studies of a Schiff base and its metal(II) complexes. <i>Arabian Journal of Chemistry</i> , 2020, 13, 1130-1141.	2.3	44
21	Diverse coordination of isoniazid hydrazone Schiff base ligand towards iron(III): Synthesis, characterization, SC-XRD, HSA, QTAIM, MEP, NCI, NBO and DFT study. <i>Journal of Molecular Structure</i> , 2022, 1250, 131691.	1.8	44
22	Schiff Bases: Multipurpose Pharmacophores with Extensive Biological Applications. <i>Journal of Basic & Applied Sciences</i> , 0, 14, 217-229.	0.8	41
23	Synthesis and spectroscopic and thermogravimetric characterization of heterobimetallic complexes with Sn(IV) and Pd(II); DNA binding, alkaline phosphatase inhibition and biological activity studies. <i>Journal of Coordination Chemistry</i> , 2015, 68, 662-677.	0.8	35
24	Synthesis, spectra (FT-IR, NMR) investigations, DFT, FMO, MEP, NBO analysis and catalytic activity of MoO ₂ (VI) complex with ONO tridentate hydrazone Schiff base ligand. <i>Journal of Molecular Structure</i> , 2021, 1245, 131259.	1.8	34
25	Unsymmetrical Ni(II) Schiff base complex: Synthesis, spectral characterization, crystal structure analysis, Hirshfeld surface investigation, theoretical studies, and antibacterial activity. <i>Journal of Molecular Structure</i> , 2022, 1265, 133381.	1.8	34
26	Selective oxidation of benzyl alcohols to benzaldehydes catalyzed by dioxomolybdenum Schiff base complex: synthesis, spectral characterization, crystal structure, theoretical and computational studies. <i>Transition Metal Chemistry</i> , 2021, 46, 437.	0.7	33
27	Sonication-assisted synthesis of new Schiff bases derived from 3-ethoxysalicylaldehyde: Crystal structure determination, Hirshfeld surface analysis, theoretical calculations and spectroscopic studies. <i>Journal of Molecular Structure</i> , 2021, 1243, 130782.	1.8	32
28	Synthesis, spectral characterization, crystal structures, biological activities, theoretical calculations and substitution effect of salicylidene ligand on the nature of mono and dinuclear Zn(II) Schiff base complexes. <i>Polyhedron</i> , 2022, 213, 115636.	1.0	30
29	Synthesis, spectral characterization, SC-XRD, HSA, DFT and catalytic activity of a dioxidomolybdenum complex with aminosalicyl-hydrazone Schiff base ligand: An experimental and theoretical approach. <i>Polyhedron</i> , 2021, 208, 115428.	1.0	29
30	Experimental and theoretical studies of new dioxomolybdenum complex: Synthesis, characterization and application as an efficient homogeneous catalyst for the selective sulfoxidation. <i>Inorganica Chimica Acta</i> , 2021, 527, 120568.	1.2	28
31	Synthesis, crystal structure, spectral characterization, theoretical and computational studies of Ni(II), Cu(II) and Zn(II) complexes incorporating Schiff base ligand derived from 4-(diethylamino)salicylaldehyde. <i>Inorganica Chimica Acta</i> , 2022, 536, 120878.	1.2	28
32	Facile synthesis of carbon nanotubes supported NiO nanocomposite and its high performance as lithium-ion battery anode. <i>Materials Letters</i> , 2013, 107, 158-161.	1.3	27
33	Oxovanadium and dioxomolybdenum complexes: synthesis, crystal structure, spectroscopic characterization and applications as homogeneous catalysts in sulfoxidation. <i>Journal of Coordination Chemistry</i> , 2021, 74, 1563-1583.	0.8	27
34	Zn(II) complexes containing O,N,N,O-donor Schiff base ligands: synthesis, crystal structures, spectral investigations, biological activities, theoretical calculations and substitution effect on structures. <i>Journal of Coordination Chemistry</i> , 2021, 74, 2720-2740.	0.8	27
35	Synthesis, spectral characterization, crystal structure and catalytic activity of a novel dioxomolybdenum Schiff base complex containing 4-aminobenzhydrazone ligand: A combined experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2022, 1249, 131645.	1.8	27
36	Synthesis, spectroscopy, single crystal XRD and biological studies of multinuclear organotin dicarboxylates. <i>Polyhedron</i> , 2016, 117, 64-72.	1.0	26

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37	Symmetrical Pd(II) and Ni(II) Schiff base complexes: Synthesis, crystal structure determination, spectral characterization, and theoretical studies. <i>Journal of Molecular Structure</i> , 2022, 1251, 132037.	1.8	26
38	Synthesis of new cadmium(II) complexes of Schiff bases as alkaline phosphatase inhibitors and their antimicrobial activity. <i>Arabian Journal of Chemistry</i> , 2021, 14, 103308.	2.3	25
39	Synthesis, characterization and pharmacological evaluation of mixed ligand-metal complexes containing omeprazole and 8-hydroxyquinoline. <i>Tropical Journal of Pharmaceutical Research</i> , 2017, 16, 1137.	0.2	23
40	Spectroscopic investigation, molecular structure, catalytic activity with computational studies of a novel Pd(II) complex incorporating unsymmetrical tetradentate Schiff base ligand. <i>Inorganic Chemistry Communication</i> , 2022, 142, 109697.	1.8	23
41	New oxovanadium and dioxomolybdenum complexes as catalysts for sulfoxidation: experimental and theoretical investigations of E and Z isomers of ONO tridentate Schiff base ligand. <i>Journal of Sulfur Chemistry</i> , 2022, 43, 22-36.	1.0	22
42	Single crystal inspection, Hirshfeld surface investigation and DFT study of a novel derivative of 4-fluoroaniline: 4-((4-fluorophenyl)amino)-4-oxobutanoic acid (BFAOB). <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 1953-1961.	1.2	21
43	Pd(II) and Ni(II) complexes containing ONNO tetradentate Schiff base ligand: Synthesis, crystal structure, spectral characterization, theoretical studies, and use of PdL as an efficient homogeneous catalyst for Suzuki-Miyaura cross-coupling reaction. <i>Polyhedron</i> , 2022, 213, 115622.	1.0	21
44	Synthesis, characterization, SC-XRD, HSA and DFT study of a novel copper(I) iodide complex with 2-(thiophen-2-yl)-4,5-dihydro-1H-imidazole ligand: An experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2022, 1253, 132264.	1.8	20
45	Synthesis, crystal structure determination, Hirshfeld surface analysis, spectral characterization, theoretical and computational studies of titanium(IV) Schiff base complex. <i>Journal of Coordination Chemistry</i> , 2021, 74, 2682-2700.	0.8	19
46	Shedding Light on the Synthesis, Crystal Structure, Characterization, and Computational Study of Optoelectronic Properties and Bioactivity of Imine derivatives. <i>ACS Omega</i> , 2022, 7, 5217-5230.	1.6	18
47	Synthesis, crystal structure, spectral characterization, catalytic studies and computational studies of Ni(II) and Pd(II) complexes of symmetrical tetradentate Schiff base ligand. <i>Journal of Coordination Chemistry</i> , 2022, 75, 972-993.	0.8	18
48	One-pot synthesis, structural elucidation, DNA binding and alkaline phosphatase inhibition studies of zinc(II) complexes with 4-nitrocinnamic acid and ethylenediamine. <i>Journal of Coordination Chemistry</i> , 2014, 67, 2479-2495.	0.8	17
49	Syntheses, characterization, and catalytic potential of novel vanadium and molybdenum Schiff base complexes for the preparation of benzimidazoles, benzoxazoles, and benzothiazoles under thermal and ultrasonic conditions. <i>Monatshefte für Chemie</i> , 2021, 152, 593-605.	0.9	17
50	Synthesis, characterization, semi-empirical study, and biological activities of organotin(IV) and transition metal complexes with <i>o</i> -methyl carbonodithioate. <i>Journal of Coordination Chemistry</i> , 2014, 67, 2795-2808.	0.8	16
51	Synthesis, crystal structure, Hirshfeld surface analysis and theoretical investigation of polynuclear coordination polymers of cobalt and manganese complexes with nitrobenzene and pyrazine. <i>Journal of Molecular Structure</i> , 2022, 1250, 131851.	1.8	16
52	Synthesis, characterization, crystal structures, enzyme inhibition, DNA binding, and electrochemical studies of zinc(II) complexes. <i>Journal of Coordination Chemistry</i> , 2014, 67, 1290-1308.	0.8	14
53	Synthesis, single-crystal exploration, hirshfeld surface analysis, and DFT investigation of the thiosemicarbazones. <i>Journal of Molecular Structure</i> , 2022, 1262, 133088.	1.8	14
54	DFT study of structural, electronic, thermo-elastic properties and plausible origin of superconductivity due to quantum degenerate states in LaTiO ₃ . <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650044.	1.8	13

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55	Single crystal exploration, supramolecular behaviour, Hirshfeld surface analysis, linear and non-linear theoretical optical properties of Schiff bases derived from Benzene sulfonamides. <i>Journal of Molecular Structure</i> , 2022, 1261, 132952.	1.8	13
56	One-pot synthesis, characterization, DNA binding and enzymatic studies of 4-methyl trans-cinnamate zinc(II)-mixed ligand complexes. <i>Journal of Coordination Chemistry</i> , 2015, 68, 3636-3650.	0.8	11
57	Theoretical studies, Hirshfeld surface analysis, and crystal structure determination of a newly synthesized benzothiazole copper(II) complex. <i>Journal of Molecular Structure</i> , 2022, 1261, 132905.	1.8	10
58	Structural and computational analysis, spectroscopic and electrochemical elucidation of a Schiff base. <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 3845-3860.	1.2	10
59	Synthesis, crystal structure, Hirshfeld surface and void analysis of bis(1/4-4-aminobenzoato- λ^2 -O,O') Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 582 Td (O_2 : O_2) \cdot 2H ₂ O. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 282-286.		
60	Synthesis, crystal structure, spectral characterization, theoretical studies, and investigation of catalytic activity in selective oxidation of sulfides by oxo-peroxo tungsten(VI) Schiff base complex. <i>Journal of Molecular Structure</i> , 2022, 1257, 132608.	1.8	9
61	Synthesis, spectral characterization, and theoretical investigation of Ni(II) and Pd(II) complexes incorporating symmetrical tetradentate Schiff base ligand: Suzuki-Miyaura cross-coupling reaction using PdLSym. <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 3981-3992.	1.2	9
62	Integration of an aminopyridine derived cobalt based homogenous cocatalyst with a composite photocatalyst to promote H ₂ evolution from water. <i>New Journal of Chemistry</i> , 2021, 45, 5561-5567.	1.4	7
63	Dioxovanadium(V) Complex Incorporating Tridentate ONO Donor Aminobenzohydrazone Ligand: Synthesis, Spectral Characterization and Application as a Homogeneous Lewis Acid Catalyst in the Friedländer Synthesis of Substituted Quinolines. <i>Polycyclic Aromatic Compounds</i> , 2022, 42, 6485-6500.	1.4	4
64	4-Phenylbutyric acid based homo-heteroleptic Zn(II) carboxylates: Synthesis, structural elucidation, DNA interaction through spectroscopic and computational methods as well as ALP inhibition study. <i>Journal of Molecular Liquids</i> , 2022, 356, 119031.	2.3	4
65	Synthesis, characterization, geometric optimization and multi-target therapeutic evaluation of new homoleptic and heteroleptic Cd(II) carboxylates. <i>Journal of Molecular Structure</i> , 2020, 1212, 128088.	1.8	3
66	Aminosalicylic Acid Hydrazone Dioxomolybdenum(VI) Complex: Synthesis, Spectral Characterization and Application as a Green Homogeneous Lewis Acid Catalyst for the One-Pot Three-Component Synthesis of 2-Amino-3-Cyano-4-H-Pyrans. <i>Polycyclic Aromatic Compounds</i> , 2022, 42, 6780-6793.	1.4	3
67	Oxovanadium complexes with multidentate ligands. <i>Review Journal of Chemistry</i> , 2013, 3, 304-322.	1.0	2
68	Synthesis, Spectroscopic Characterization and Biological Applications of Novel Zinc Complexes with Schiff Bases. <i>Key Engineering Materials</i> , 0, 778, 293-300.	0.4	2
69	2-(2-Methoxyphenyl)-1H-isoindole-1,3(2H)-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012, 68, o2589-o2589.	0.2	1