Mariusz P Mitoraj

List of Publications by Year
in descending order

73 papers	4,630 citations	218677 26 h-index	98798 67 g-index
75 all docs	75 docs citations	75 times ranked	3050 citing authors

#	Article	IF	Citations
1	Zeolites at the Molecular Level: What Can Be Learned from Molecular Modeling. Molecules, 2021, 26, 1511.	3.8	6
2	Exploring â€œTriazole-Thioureaâ€•Based Ligands for the Self-Assembly of Photoluminescent Hg(II) Coordination Compounds. Crystal Growth and Design, 2021, 21, 3562-3581.	3.0	5
3	Solvent-Induced Formation of Novel Ni(II) Complexes Derived from Bis-Thiosemicarbazone Ligand: An Insight from Experimental and Theoretical Investigations. International Journal of Molecular Sciences, 2021, 22, 5337.	4.1	6
4	Supramolecular structures of Ni^{II} and Cu^{II} with the sterically demanding Schiff base dyes driven by cooperative action of preagostic and other non-covalent interactions. IUCrJ, 2021, 8, 351-361.	2.2	0
5	Differentiation of isomeric metabolites of carbamazepine based on acid-base properties; Experimental vs theoretical approach. Journal of Chromatography A, 2021, 1651, 462275.	3.7	1
6	Novel sterically demanding Schiff base dyes: An insight from experimental and theoretical calculations. Journal of Luminescence, 2021, 238, 118264.	3.1	12
7	Substituent Effect on Conformational Preferences in Ground and Excited States of Selected Schiff Bases: An Insight from Theoretical Calculations. Journal of Physical Chemistry A, 2020, 124, 63-73.	2.5	6
8	Lead(<scp>ii</scp>) coordination polymers driven by pyridine-hydrazine donors: from anion-guided self-assembly to structural features. Dalton Transactions, 2020, 49, 11238-11248.	3.3	16
9	Resonance Assisted Hydrogen Bonding Phenomenon Unveiled through Both Experiments and Theory: A New Family of Ethyl Nâ€Salicylideneglycinate Dyes. Chemistry - A European Journal, 2020, 26, 12987-12995.	3.3	18
10	Origin of Hydrocarbons Stability from a Computational Perspective: A Case Study of Orthoâ€Xylene Isomers. ChemPhysChem, 2020, 21, 494-502.	2.1	15
11	Structural versatility of the quasi-aromatic MÃ¶bius type zinc(ii)-pseudohalide complexes â€“ experimental and theoretical investigations. RSC Advances, 2019, 9, 23764-23773.	3.6	10
12	Formation of active species from ruthenium alkylidene catalystsâ€”an insight from computational perspective. Journal of Molecular Modeling, 2019, 25, 331.	1.8	7
13	Effect of Solvent on the Structural Diversity of Quasi-Aromatic MÃ¶bius Cadmium(II) Complexes Fabricated from the Bulky N6 Tetradentate Helical Ligand. Crystal Growth and Design, 2019, 19, 1649-1659.	3.0	11
14	Chameleon-like Nature of Anagostic Interactions and Its Impact on Metalloaromaticity in Square-Planar Nickel Complexes. Organometallics, 2019, 38, 1973-1981.	2.3	23
15	Kinetic and Potential Energy Contributions to a Chemical Bond from the Charge and Energy Decomposition Scheme of Extended Transition State Natural Orbitals for Chemical Valence. Journal of Physical Chemistry A, 2019, 123, 4616-4622.	2.5	9
16	Non-covalent Interactions in Selected Transition Metal Complexes. Challenges and Advances in Computational Chemistry and Physics, 2019, , 65-89.	0.6	2
17	Aggregationâ€Induced Emissionâ€Based Sensing Platform for Selective Detection of Zn²⁺: Experimental and Theoretical Investigations. ChemPhysChem, 2019, 20, 1630-1639.	2.1	18
18	Metal chelates constructed from CdHal2 (HalÂ= Cl, Br, I) and 1,2-diphenyl-1,2-bis((phenyl(pyridin-2-yl)methylene)hydrazono)ethane. Journal of Molecular Structure, 2019, 1176, 743-750.	3.6	9

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19	Copper(II) acetate structures with benzimidazole derivatives. Inorganica Chimica Acta, 2019, 488, 238-245.	2.4	7
20	Photobleaching of pheomelanin increases its phototoxic potential: Physicochemical studies of synthetic pheomelanin subjected to aerobic photolysis. Pigment Cell and Melanoma Research, 2019, 32, 359-372.	3.3	16
21	Nâ€Thiophosphorylthioureas RNHC(S)NHP(S)(OiPr)₂ as an Excellent Platform for Studying the Synergy between Hydrogenâ€Hydrogen Bonding and Other Families of Nonâ€Covalent Interactions. European Journal of Organic Chemistry, 2019, 2019, 493-503.	2.4	15
22	MÃ¶bius-like metal chelates constructed from CdHal2 (Halâ€¯=â€¯Cl, Br, I) and benzilbis(pyridin-2-yl)methylidenehydrazone. Inorganica Chimica Acta, 2019, 484, 481-490.	2.4	9
23	Extended lead(<scp>ii</scp>) architectures engineered via tetrel bonding interactions. New Journal of Chemistry, 2018, 42, 4959-4971.	2.8	76
24	Thermodynamics of acid-base dissociation of several cathinones and 1â€phenylethylamine, studied by an accurate capillary electrophoresis method free from the Joule heating impact. Journal of Chromatography A, 2018, 1539, 78-86.	3.7	18
25	Quasi-aromatic MÃ¶bius Metal Chelates. Inorganic Chemistry, 2018, 57, 4395-4408.	4.0	32
26	Cyclodextrin-induced acidity modification of substituted cathinones studied by capillary electrophoresis supported by density functional theory calculations. Journal of Chromatography A, 2018, 1580, 142-151.	3.7	9
27	London Dispersion Forces in Crystal Packing of Thiourea Derivatives. Crystal Growth and Design, 2018, 18, 5385-5397.	3.0	15
28	Azide-rich complexes of cobalt(III) with the rare 5-phenyl-2,2â€²-bipyridine ligand. Inorganica Chimica Acta, 2017, 459, 63-72.	2.4	2
29	Alternative Route Toward Nitrones: Experimental and Theoretical Findings. Journal of Organic Chemistry, 2017, 82, 1666-1675.	3.2	5
30	Origin of Remarkably Different Acidity of Hydroxycoumarinsâ€"Joint Experimental and Theoretical Studies. Journal of Physical Chemistry B, 2017, 121, 4554-4561.	2.6	29
31	Polar protic solvent-trapping polymorphism of the Hg^{II}-hydrazone coordination polymer: experimental and theoretical findings. CrystEngComm, 2017, 19, 3017-3025.	2.6	27
32	Anion-driven tetrel bond-induced engineering of lead(<scp>ii</scp>) architectures with Nâ€²-(1-(2-pyridyl)ethylidene)nicotinohydrazide: experimental and theoretical findings. Inorganic Chemistry Frontiers, 2017, 4, 171-182.	6.0	44
33	Complexes and salts of the nitrogen-rich triazoleâ€"tetrazole hybrid ligand with alkali and alkaline earth metal cations: experimental and theoretical findings. New Journal of Chemistry, 2017, 41, 6210-6218.	2.8	6
34	Ligand-Driven Coordination Sphere-Induced Engineering of Hybride Materials Constructed from PbCl₂ and Bis-Pyridyl Organic Linkers for Single-Component Light-Emitting Phosphors. Inorganic Chemistry, 2017, 56, 9698-9709.	4.0	56
35	Non-Covalent Interactions in Hydrogen Storage Materials LiN(CH3)2BH3 and KN(CH3)2BH3. Crystals, 2016, 6, 28.	2.2	29
36	CdS Nanoparticles Fabricated from the Single-Source Precursor [Cd{Et₂NC(S)NP(S)(OiPr)₂}₂]: In Depth Experimental and Theoretical Studies. Crystal Growth and Design, 2016, 16, 3287-3296.	3.0	8

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37	An intermolecular pyrene excimer in the pyrene-labeled N-thiophosphorylated thiourea and its nickel(<scp>ii</scp>) complex. Inorganic Chemistry Frontiers, 2016, 3, 1419-1431.	6.0	14
38	Polymorphism driven optical properties of an anil dye. CrystEngComm, 2016, 18, 7249-7259.	2.6	29
39	Influence of the Homopolar Dihydrogen Bonding Cï£¿Hâ‹…â‹…â‹…Hï£¿C on Coordination Geometry: Experimental and Theoretical Studies. Chemistry - A European Journal, 2015, 21, 16679-16687.	3.3	35
40	Metal ion influences distortion of the ligand in the structure of [M{2-MeO(O)CC₆H₄NHC(S)NP(S)(OiPr)₂}₂] (M =) Tj ETQq0 0 0 rgBT /Overlock 10 Transactions, 2015, 44, 14101-14109.	3.3	6
41	Determination of acid dissociation constants of warfarin and hydroxywarfarins by capillary electrophoresis. Journal of Pharmaceutical and Biomedical Analysis, 2015, 112, 89-97.	2.8	28
42	Modulation of pK_a by cyclodextrins; subtle structural changes induce spectacularly different behaviors. RSC Advances, 2015, 5, 77545-77552.	3.6	19
43	Luminescent mononuclear mixed ligand complexes of copper(<scp>i</scp>) with 5-phenyl-2,2â€²-bipyridine and triphenylphosphine. Dalton Transactions, 2015, 44, 16824-16832.	3.3	43
44	A smart rhodamineâ€“pyridine conjugate for bioimaging of thiocyanate in living cells. RSC Advances, 2015, 5, 103350-103357.	3.6	10
45	Nature of the water/aromatic parallel alignment interactions. Journal of Computational Chemistry, 2015, 36, 171-180.	3.3	9
46	Nucleic Acid Quadruplexes Based on 8-Halo-9-deazaxanthines: Energetics and Noncovalent Interactions in Quadruplex Stems. Journal of Chemical Theory and Computation, 2014, 10, 5353-5365.	5.3	19
47	Physical Nature of Interactions in Zn^{II} Complexes with 2,2â€²-Bipyridyl: Quantum Theory of Atoms in Molecules (QTAIM), Interacting Quantum Atoms (IQA), Noncovalent Interactions (NCI), and Extended Transition State Coupled with Natural Orbitals for Chemical Valence (ETS-NOCV) Comparative Studies. Journal of Physical Chemistry A, 2014, 118, 623-637.	2.5	81
48	Supramolecular Coordination Complexes of the Nâ€Thiophosphorylated 2,5â€Dithiobiurea [NHC(S)NHP(S)(OiPr)₂]₂ with Zn^{II} and Cd^{II} Ions â€“ Cationâ€Induced Dinuclear Mesocate Structure versus Tetranuclear Nanoscaled Aggregate. European Journal of Inorganic Chemistry, 2014, 2014, 5522-5529.	2.0	11
49	Experimental and theoretical investigations of the NiII complex with N-phosphorylated thiourea iPrNHC(S)NHP(O)(OPh)2. CrystEngComm, 2013, 15, 7845.	2.6	16
50	Crucial Influence of the Intramolecular Hydrogen Bond on the Coordination Mode of RC(S)NHP(S)(OiPr)2in Homoleptic Complexes with NiII. European Journal of Inorganic Chemistry, 2013, 2013, 545-555.	2.0	17
51	Complexation properties of N-thiophosphorylated thiourea 2-PyNHC(S)NHP(S)(OiPr)2 towards NiII. Dalton Transactions, 2013, 42, 5252.	3.3	9
52	Theoretical description of halogen bonding â€“ an insight based on the natural orbitals for chemical valence combined with the extended-transition-state method (ETS-NOCV). Journal of Molecular Modeling, 2013, 19, 4681-4688.	1.8	37
53	Influence of CH₂Cl₂for the structure stabilization of the Ni^{II}complex [Ni{6-MeO(O)CC₆H₄NHC(S)NP(S)(OiPr)₂-1,5-S,Sâ€²}₂]Â·CH₂Cl<sub /><sub />. CrystEngComm, 2012, 14, 370-373.	2.6	10
54	On the asymmetry in molybdenumâ€“oxygen bonding in the MoO3 structure: ETSâ€“NOCV analysis. Structural Chemistry, 2012, 23, 1369-1375.	2.0	19

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55	Solvent-induced 1,3-N,S- vs. 1,5-S,Sâ€²-coordination in the NiII complex [Ni{p-Me2NC6H4NHC(S)NP(S)(OiPr)2}2]. CrystEngComm, 2011, 13, 5321.	2.6	22
56	Intramolecular hydrogen bonding controls 1,3-N,S- vs. 1,5-S,Sâ€²-coordination in NiII complexes of N-thiophosphorylated thioureas RNHC(S)NHP(S)(OiPr)2. Dalton Transactions, 2011, 40, 3142.	3.3	30
57	Multiple Boronâ^'Boron Bonds in Neutral Molecules: An Insight from the Extended Transition State Method and the Natural Orbitals for Chemical Valence Scheme. Inorganic Chemistry, 2011, 50, 2168-2174.	4.0	73
58	QTAIM and ETS-NOCV Analyses of Intramolecular CHÂ·Â·Â·HC Interactions in Metal Complexes. Journal of Physical Chemistry A, 2011, 115, 12746-12757.	2.5	45
59	Theoretical description of bonding in cis-W(CO)4(piperidine)2 and its dimer. Journal of Molecular Modeling, 2010, 16, 337-342.	1.8	4
60	Theoretical description of hydrogen bonding in oxalic acid dimer and trimer based on the combined extended-transition-state energy decomposition analysis and natural orbitals for chemical valence (ETS-NOCV). Journal of Molecular Modeling, 2010, 16, 1789-1795.	1.8	24
61	Theoretical Analysis of the Resonance Assisted Hydrogen Bond Based on the Combined Extended Transition State Method and Natural Orbitals for Chemical Valence Scheme^{â€}. Journal of Physical Chemistry A, 2010, 114, 8581-8590.	2.5	94
62	Ïƒ-Donor and Ï€-Acceptor Properties of Phosphorus Ligands: An Insight from the Natural Orbitals for Chemical Valence. Inorganic Chemistry, 2010, 49, 578-582.	4.0	88
63	On the origin of the transâ€influence in square planar d⁸â€complexes: A theoretical study. International Journal of Quantum Chemistry, 2009, 109, 3379-3386.	2.0	77
64	A Combined Charge and Energy Decomposition Scheme for Bond Analysis. Journal of Chemical Theory and Computation, 2009, 5, 962-975.	5.3	1,350
65	On the Nature of the Agostic Bond between Metal Centers and Î²-Hydrogen Atoms in Alkyl Complexes. An Analysis Based on the Extended Transition State Method and the Natural Orbitals for Chemical Valence Scheme (ETS-NOCV). Organometallics, 2009, 28, 3727-3733.	2.3	150
66	Applications of natural orbitals for chemical valence in a description of bonding in conjugated molecules. Journal of Molecular Modeling, 2008, 14, 681-687.	1.8	253
67	Bond Orbitals from Chemical Valence Theory. Journal of Physical Chemistry A, 2008, 112, 1933-1939.	2.5	508
68	Donorâ€“Acceptor Properties of Ligands from the Natural Orbitals for Chemical Valence. Organometallics, 2007, 26, 6576-6580.	2.3	367
69	Natural orbitals for chemical valence as descriptors of chemical bonding in transition metal complexes. Journal of Molecular Modeling, 2007, 13, 347-355.	1.8	493
70	1,3 Geminal Interactions as the Possible Trend Setting Factors for Câ^'H and Câ^'C Bond Energies in Alkanes. Support from a Density Functional Theory Based Bond Energy Decomposition Study. Journal of Organic Chemistry, 2006, 71, 9208-9211.	3.2	42
71	DFT studies on isomerization reactions in the copolymerization of ethylene and methyl acrylate catalyzed by Ni-diimine and Pd-diimine complexes. Journal of Molecular Modeling, 2005, 11, 341-350.	1.8	21
72	Quasi-aromatic MÃ¶bius chelates of Cadmium(II) nitrite and/or nitrate.. CrystEngComm, 0, , .	2.6	0

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73	Coordination polymers fabricated from Cd(NO3)2 and N,N',O-pincer type isonicotinoylhydrazone based polytopyc ligands â€“ an insight from experimental and theoretical investigations. CrystEngComm, 0, , .	2.6	0