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	A Combined Charge and Energy Decomposition Scheme for Bond Analysis. Journal of Chemical Theory and Computation, 2009, 5, 962-975.	5.3	1,350
2	Bond Orbitals from Chemical Valence Theory. Journal of Physical Chemistry A, 2008, 112, 1933-1939.	2.5	508
3	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
4	Donorâ€“Acceptor Properties of Ligands from the Natural Orbitals for Chemical Valence. Organometallics, 2007, 26, 6576-6580.	2.3	367
5	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
6	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
7	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
8	Ï*f*-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
9	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
10	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
11	Extended lead(<scp>ii</scp>) architectures engineered via tetrel bonding interactions. New Journal of Chemistry, 2018, 42, 4959-4971.	2.8	76
12	Multiple Boronâˆ’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
13	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
14	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
15	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
16	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
17	1,3 Geminal Interactions as the Possible Trend Setting Factors for Câˆ’H and Câˆ’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
18	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

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19	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
20	Quasi-aromatic MÃ¶bius Metal Chelates. Inorganic Chemistry, 2018, 57, 4395-4408.	4.0	32
21	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
22	Non-Covalent Interactions in Hydrogen Storage Materials LiN(CH3)2BH3 and KN(CH3)2BH3. Crystals, 2016, 6, 28.	2.2	29
23	Polymorphism driven optical properties of an anil dye. CrystEngComm, 2016, 18, 7249-7259.	2.6	29
24	Origin of Remarkably Different Acidity of Hydroxycoumarinsâ€"Joint Experimental and Theoretical Studies. Journal of Physical Chemistry B, 2017, 121, 4554-4561.	2.6	29
25	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
26	Polar protic solvent-trapping polymorphism of the Hg^{II}-hydrazone coordination polymer: experimental and theoretical findings. CrystEngComm, 2017, 19, 3017-3025.	2.6	27
27	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
28	Chameleon-like Nature of Anagostic Interactions and Its Impact on Metalloaromaticity in Square-Planar Nickel Complexes. Organometallics, 2019, 38, 1973-1981.	2.3	23
29	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
30	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
31	On the asymmetry in molybdenumâ€"oxygen bonding in the MoO3 structure: ETSâ€"NOCV analysis. Structural Chemistry, 2012, 23, 1369-1375.	2.0	19
32	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
33	Modulation of pK_a by cyclodextrins; subtle structural changes induce spectacularly different behaviors. RSC Advances, 2015, 5, 77545-77552.	3.6	19
34	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
35	Aggregationâ€Induced Emissionâ€Based Sensing Platform for Selective Detection of Zn²⁺: Experimental and Theoretical Investigations. ChemPhysChem, 2019, 20, 1630-1639.	2.1	18
36	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

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37	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
38	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
39	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
40	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
41	London Dispersion Forces in Crystal Packing of Thiourea Derivatives. Crystal Growth and Design, 2018, 18, 5385-5397.	3.0	15
42	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
43	Origin of Hydrocarbons Stability from a Computational Perspective: A Case Study of Orthoâ€Xylene Isomers. ChemPhysChem, 2020, 21, 494-502.	2.1	15
44	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
45	Novel sterically demanding Schiff base dyes: An insight from experimental and theoretical calculations. Journal of Luminescence, 2021, 238, 118264.	3.1	12
46	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
47	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
48	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
49	A smart rhodamineâ€“pyridine conjugate for bioimaging of thiocyanate in living cells. RSC Advances, 2015, 5, 103350-103357.	3.6	10
50	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
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	Nature of the water/aromatic parallel alignment interactions. Journal of Computational Chemistry, 2015, 36, 171-180.	3.3	9
53	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
54	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

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55	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
56	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
57	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
58	Formation of active species from ruthenium alkylidene catalystsâ€”an insight from computational perspective. Journal of Molecular Modeling, 2019, 25, 331.	1.8	7
59	Copper(II) acetate structures with benzimidazole derivatives. Inorganica Chimica Acta, 2019, 488, 238-245.	2.4	7
60	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
61	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
62	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
63	Zeolites at the Molecular Level: What Can Be Learned from Molecular Modeling. Molecules, 2021, 26, 1511.	3.8	6
64	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
65	Alternative Route Toward Nitrones: Experimental and Theoretical Findings. Journal of Organic Chemistry, 2017, 82, 1666-1675.	3.2	5
66	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
67	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
68	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
69	Non-covalent Interactions in Selected Transition Metal Complexes. Challenges and Advances in Computational Chemistry and Physics, 2019, , 65-89.	0.6	2
70	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
71	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
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