Wiktor Zierkiewicz

List of Publications by Year in descending order

95 papers	2,284 citations	218592 26 h-index	254106 43 g-index
95 all docs	95 docs citations	95 times ranked	2230 citing authors

#	Article	IF	Citations
1	Electronic structures, vibrational spectra, and revised assignment of aniline and its radical cation: Theoretical study. Journal of Chemical Physics, 2003, 118, 10900-10911.	1.2	163
2	Using Mechanistic and Computational Studies To Explain Ligand Effects in the Palladium-Catalyzed Aerobic Oxidation of Alcohols. Journal of the American Chemical Society, 2005, 127, 8499-8507.	6.6	127
3	Molecular Structures and Infrared Spectra ofp-Chlorophenol andp-Bromophenol. Theoretical and Experimental Studies. Journal of Physical Chemistry A, 2000, 104, 11685-11692.	1.1	99
4	On Differences between Hydrogen Bonding and Improper Blue-Shifting Hydrogen Bonding. ChemPhysChem, 2005, 6, 609-617.	1.0	96
5	Study of the Nature of Improper Blue-Shifting Hydrogen Bonding and Standard Hydrogen Bonding in the X3CHâ‹…â‹…â‹…OH2 and XHâ‹…â‹…â‹…OH2 Complexes (X=F, Cl, Br, I): A Correlated Ab Initio Study. ChemPhysChem, 2002, 3, 511.	1.0	90
6	â€œTroublesomeâ€•Vibrations of Aromatic Molecules in Second-Order MÃ¶llerâ€“Plesset and Density Functional Theory Calculations:â€‰ Infrared Spectra of Phenol and Phenol-OD Revisited. Journal of Physical Chemistry A, 2001, 105, 8734-8739.	1.1	88
7	Implications of monomer deformation for tetrel and pnicogen bonds. Physical Chemistry Chemical Physics, 2018, 20, 8832-8841.	1.3	67
8	Coordination of anions by noncovalently bonded Ïƒ-hole ligands. Coordination Chemistry Reviews, 2020, 405, 213136.	9.5	66
9	Molecular Structure and Infrared Spectra of 4-Fluorophenol:â€‰ A Combined Theoretical and Spectroscopic Study. Journal of Physical Chemistry A, 2003, 107, 4547-4554.	1.1	63
10	A Theoretical Study of the Essential Role of DMSO as a Solvent/Ligand in the Pd(OAc)2/DMSO Catalyst System for Aerobic Oxidation. Organometallics, 2005, 24, 6019-6028.	1.1	52
11	The Amino Group in Adenine: MP2 and CCSD(T) Complete Basis Set Limit Calculations of the Planarization Barrier and DFT/B3LYP Study of the Anharmonic Frequencies of Adenine. Journal of Physical Chemistry B, 2008, 112, 16734-16740.	1.2	46
12	Regium bonds between M_n clusters (M = Cu, Ag, Au and n = 2â€“6) and nucleophiles NH₃ and HCN. Physical Chemistry Chemical Physics, 2018, 20, 22498-22509.	1.3	46
13	Doubly chloro bridged dimeric copper(<scp>ii</scp>) complex: magneto-structural correlation and anticancer activity. Dalton Transactions, 2015, 44, 8876-8888.	1.6	45
14	Comparison between Tetrel Bonded Complexes Stabilized by Ïƒ and Ï€ Hole Interactions. Molecules, 2018, 23, 1416.	1.7	45
15	Halogen bonded complexes between volatile anaesthetics (chloroform, halothane, enflurane,) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.3	44
16	Aerogen bonds formed between AeOF₂ (Ae = Kr, Xe) and diazines: comparisons between Ïƒ-hole and Ï€-hole complexes. Physical Chemistry Chemical Physics, 2018, 20, 4676-4687.	1.3	36
17	The dihydrogen bond in X3Câ€“Hâ¯Hâ€“M complexes (X = F, Cl, Br; M = Li, Na, K). A correlated quantum chemical ab initio and density functional theory study. Physical Chemistry Chemical Physics, 2004, 6, 5288-5296.	1.3	35
18	Theoretical Studies of IR and NMR Spectral Changes Induced by Sigma-Hole Hydrogen, Halogen, Chalcogen, Pnicogen, and Tetrel Bonds in a Model Protein Environment. Molecules, 2019, 24, 3329.	1.7	35

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19	Theoretical investigation of the conformation, acidity, basicity and hydrogen bonding ability of halogenated ethers. Physical Chemistry Chemical Physics, 2010, 12, 13681.	1.3	33
20	Noncovalent Bonds through Sigma and Pi-Hole Located on the Same Molecule. Guiding Principles and Comparisons. Molecules, 2021, 26, 1740.	1.7	32
21	Metalâ€“organic framework in an <scp>l</scp>-arginine copper(<scp>ii</scp>) ion polymer: structure, properties, theoretical studies and microbiological activity. RSC Advances, 2015, 5, 36295-36306.	1.7	31
22	Anionâ‹…â‹…â‹…Anion Attraction in Complexes of MCl₃^{â^'} (M=Zn, Cd, Hg) with CN^{â^'}. ChemPhysChem, 2020, 21, 1119-1125.	1.0	31
23	Theoretical investigation of the halogen bonded complexes between carbonyl bases and molecular chlorine. Journal of Computational Chemistry, 2015, 36, 821-832.	1.5	29
24	On the ability of pnicogen atoms to engage in both Ïƒ and Ï€-hole complexes. Heterodimers of ZF2C6H5 (Zâ€‰=â€‰P, As, Sb, Bi) and NH3. Journal of Molecular Modeling, 2019, 25, 152.	0.8	29
25	How Many Pnicogen Bonds can be Formed to a Central Atom Simultaneously?. Journal of Physical Chemistry A, 2020, 124, 2046-2056.	1.1	29
26	Dual Geometry Schemes in Tetrel Bonds: Complexes between TF4 (T = Si, Ge, Sn) and Pyridine Derivatives. Molecules, 2019, 24, 376.	1.7	28
27	Blue Shifts and Unusual Intensity Changes in the Infrared Spectra of the EnfluraneÂ·Â·Â·Acetone Complexes: Spectroscopic and Theoretical Studies. Journal of Physical Chemistry A, 2011, 115, 11362-11368.	1.1	27
28	Chalcogen bonding of two ligands to hypervalent YF₄ (Y = S, Se, Te, Po). Physical Chemistry Chemical Physics, 2019, 21, 20829-20839.	1.3	27
29	The crystal structure, infrared, Raman and density functional studies of bis(2-aminophenyl) diselenide. Polyhedron, 2011, 30, 2466-2472.	1.0	26
30	Raman and Infrared Spectroscopy, DFT Calculations, and Vibrational Assignment of the Anticancer Agent Picoplatin: Performance of Long-Range Corrected/Hybrid Functionals for a Platinum(II) Complex. Journal of Physical Chemistry A, 2014, 118, 6922-6934.	1.1	25
31	Trielâ€Bonded Complexes between TrR₃ (Tr=B, Al, Ga; R=H, F, Cl, Br, CH₃) and Pyrazine. ChemPhysChem, 2018, 19, 3122-3133.	1.0	25
32	Hexacoordinated Tetrelâ€Bonded Complexes between TF₄ (T=Si, Ge, Sn, Pb) and NCH: Competition between Ïƒâ€•and Ï€â€Holes. ChemPhysChem, 2019, 20, 959-966.	1.0	25
33	On the Stability of Interactions between Pairs of Anions â€“ Complexes of MCl₃^{â^'} (M=Be, Mg, Ca, Sr, Ba) with Pyridine and CN^{â^'}. ChemPhysChem, 2020, 21, 870-877.	1.0	25
34	Crystallographic and Theoretical Evidences of Anionâ‹…â‹…â‹…Anion Interaction. ChemPhysChem, 2021, 22, 818-821.	1.0	25
35	Noncovalent Bonds between Tetrel Atoms. ChemPhysChem, 2020, 21, 1934-1944.	1.0	24
36	Pnicogen Bonds Pairing Anionic Lewis Acid with Neutral and Anionic Bases. Journal of Physical Chemistry A, 2020, 124, 4998-5006.	1.1	24

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37	The barrier to internal rotation and electronic effects in para-halogenophenols: theoretical study. Chemical Physics Letters, 2004, 386, 95-100.	1.2	20
38	Influence of monomer deformation on the competition between two types of Ïƒ-holes in tetrel bonds. Physical Chemistry Chemical Physics, 2019, 21, 10336-10346.	1.3	20
39	Competition between Intra and Intermolecular Triel Bonds. Complexes between Naphthalene Derivatives and Neutral or Anionic Lewis Bases. Molecules, 2020, 25, 635.	1.7	20
40	Atypical calcium coordination number: Physicochemical study, cytotoxicity, DFT calculations and in silico pharmacokinetic characteristics of calcium caffeates. Journal of Inorganic Biochemistry, 2009, 103, 1189-1195.	1.5	19
41	Anionâ€“anion and anionâ€“neutral triel bonds. Physical Chemistry Chemical Physics, 2021, 23, 4818-4828.	1.3	19
42	Pnictogen bonding in pyrazineâ€¢PnX5 (Pn = P, As, Sb and X = F, Cl, Br) complexes. Journal of Molecular Modeling, 2017, 23, 328.	0.8	18
43	Copper(II) complex with L-arginine â€“ Crystal structure, DFT calculations, spectroscopic, thermal and magnetic properties. Materials Chemistry and Physics, 2019, 228, 272-284.	2.0	17
44	Synthesis, X-ray structure, DFT calculations and anticancer activity of a selenourea coordinated gold(I)-carbene complex. Polyhedron, 2017, 137, 197-206.	1.0	16
45	Anionâ¯anion (MX₃^{â”})₂ dimers (M = Zn, Cd, Hg; X = Cl, Br, I) in different environments. Physical Chemistry Chemical Physics, 2021, 23, 13853-13861.	1.3	16
46	Structures and energetics of clusters surrounding diatomic anions stabilized by hydrogen, halogen, and other noncovalent bonds. Chemical Physics, 2020, 530, 110590.	0.9	15
47	Synthesis, crystal structure, DFT calculations, molecular docking study and Hirshfeld surface analysis of alkoxido-bridged dinuclear iron(III) complex. Research on Chemical Intermediates, 2020, 46, 4155-4171.	1.3	15
48	A computational study of oxidation of ruthenium porphyrins via ORuIV and ORuVIO species. Dalton Transactions, 2006, , 1867.	1.6	14
49	On the nature of unusual intensity changes in the infrared spectra of the enfluraneâ¯acetone complexes. Physical Chemistry Chemical Physics, 2013, 15, 6001.	1.3	14
50	On the opposite trends of correlations between interaction energies and electrostatic potentials of chlorinated and methylated amine complexes stabilized by halogen bond. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	14
51	Experimental and Theoretical Studies of Dimers Stabilized by Two Chalcogen Bonds in the Presence of a NÂ·Â·Â·N Pnicogen Bond. Journal of Physical Chemistry A, 2021, 125, 657-668.	1.1	14
52	Adenine ribbon stabilized by Watsonâ€“Crick and Hoogsteen hydrogen Bonds: WFT and DFT study. Physical Chemistry Chemical Physics, 2010, 12, 2888.	1.3	13
53	Reaction of volatile anaesthetic desflurane with chlorine atom. Theoretical investigation. Chemical Physics Letters, 2013, 555, 72-78.	1.2	13
54	Ab initio and DFT studies of the interaction between carbonyl and thiocarbonyl groups: the role of SÂ·Â·Â·O chalcogen bonds. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	13

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55	Structures of clusters surrounding ions stabilized by hydrogen, halogen, chalcogen, and pnicogen bonds. Chemical Physics, 2019, 524, 55-62.	0.9	13
56	Anionâ€“Anion Interactions in Aerogen-Bonded Complexes. Influence of Solvent Environment. Molecules, 2021, 26, 2116.	1.7	13
57	Nature of the interaction between ammonia derivatives and carbon disulfide. A theoretical investigation. International Journal of Quantum Chemistry, 2017, 117, e25369.	1.0	12
58	Sâ‹¯N chalcogen bonded complexes of carbon disulfide with diazines. Theoretical study. Chemical Physics, 2018, 500, 37-44.	0.9	12
59	1â€“D Framework <scp>l</scp>-arginine zinc(II) units bridged by oxalate: synthesis, structure, properties, and theoretical studies. Journal of Coordination Chemistry, 2016, 69, 886-900.	0.8	11
60	Synthesis, characterization, DFT calculations and antibacterial activity of palladium(II) cyanide complexes with thioamides. Journal of Molecular Structure, 2017, 1141, 204-212.	1.8	11
61	Spectroscopic and DFT studies of zinc(II) complexes of diamines and thiocyanate; crystal structure of (cis-1,2-diaminocyclohexane)bis(thiocyanato-ÎºN)zinc(II). Journal of Molecular Structure, 2017, 1128, 455-461.	1.8	11
62	The role of hydrogen bonding in Ï€Â·Â·Â·Ï€ stacking interactions in Ni(II) complex derived from triethanolamine: synthesis, crystal structure, antimicrobial, and DFT studies. Research on Chemical Intermediates, 2019, 45, 5649-5664.	1.3	11
63	Modelling of interactions between volatile anaesthetics (halothane, enflurane) and aromatic compounds, ab initio study. Chemical Physics, 2010, 373, 243-250.	0.9	9
64	Ability of Lewis Acids with Shallow Ïƒ-Holes to Engage in Chalcogen Bonds in Different Environments. Molecules, 2021, 26, 6394.	1.7	9
65	Theoretical study of the interaction of a proton with the O, F and Cl atoms of enflurane (CHFClâ€“CF2â€“Oâ€“CHF2). Computational and Theoretical Chemistry, 2009, 911, 58-64.	1.5	8
66	Structural, spectroscopic, magnetic behavior and DFT investigations of<scp>l</scp>-tyrosinato nickel(<scp>ii</scp>) coordination polymer. New Journal of Chemistry, 2015, 39, 6813-6822.	1.4	8
67	Structural and spectroscopic properties and density functional theory (DFT) calculations of a linearly bridged zinc(II) l-tyrosinato complex. Polyhedron, 2015, 85, 665-674.	1.0	8
68	Synthesis, characterization, DFT optimization and anticancer evaluation of phosphanegold(I) dithiocarbamates. Journal of Molecular Structure, 2020, 1218, 128486.	1.8	8
69	On the nature of halogen bonded complexes between carbonyl bases and chlorotrifluoromethane. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	7
70	IR and Raman spectroscopic analysis, DFT modeling, and magnetic properties of a nickel(II) complex, [Ni(succ)(H2O)4]n. Journal of Coordination Chemistry, 2019, 72, 2215-2232.	0.8	7
71	Competition between Inter and Intramolecular Tetrel Bonds: Theoretical Studies Complemented by CSD Survey. ChemPhysChem, 2021, 22, 924-934.	1.0	7
72	Experimental and theoretical evidence of attractive interactions between dianions: [PdCl₄]^{2â^’}â‹¯[PdCl₄]^{2â^’}. Chemical Communications, 2021, 57, 13305-13308.	2.2	7

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73	Iron (III) complex exhibiting efficient catechol oxidase activity: Experimental, kinetic and theoretical approach. Journal of Molecular Structure, 2022, 1252, 131685.	1.8	7
74	The role of hydrogen bonding in conformational stabilization of 3,5,6- and 3,5-substituted (pyridin-2-yl)aminomethane-1,1-diphosphonic acids and related (pyrimidin-2-yl) derivative. Journal of Molecular Structure, 2010, 980, 182-192.	1.8	6
75	Magnesium cinnamate complex, [Mg(cinn)2(H2O)2]n; structural, spectroscopic, thermal, biological and pharmacokinetical characteristics. Journal of Molecular Structure, 2017, 1134, 199-207.	1.8	6
76	DFT studies of copper(II) complexes of cis -1,2-diaminocyclohexane (Dach) and crystal structure of [Cu(Dach) 2 (H 2 O)]Cl 2. Journal of Molecular Structure, 2017, 1137, 784-791.	1.8	6
77	Triel bonds within anion‹b›Â·Â·Â·‹/b›anion complexes. Physical Chemistry Chemical Physics, 2021, 23, 25097-25106.	1.3	6
78	Theoretical studies of the interaction between enflurane and water. Journal of Molecular Modeling, 2013, 19, 1399-1405.	0.8	5
79	Synthesis and molecular structure of polymeric bis(N-methylthiourea-Î²S)bis(thiocyanato-Î²N)nickel(II), [Ni(Metu)2(NCS)2] ; DFT analysis of [Ni(Metu)2(NCS)2] and [Ni(Thiourea)2(NCS)2]. Journal of Molecular Structure, 2019, 1189, 66-72.	1.8	5
80	Synthesis, Crystal Structure, DFT Modeling and Biological Activity of a Trinuclear Copper(II) Azide Polymer Containing Imidazole and Bridging Imidazolate Ligands, [Cu3(Imz-H)4(Imz)2(N3)4]n. Journal of Inorganic and Organometallic Polymers and Materials, 2017, 27, 510-517.	1.9	4
81	Silver(I) complex with 2-amino-4,4Î±-dihydro-4Î±,7-dimethyl-3H-phenoxazin-3-one (Phx-1) ligand: crystal structure, vibrational spectra andÂbiologicalÂstudies. Journal of Coordination Chemistry, 2017, 70, 3471-3487.	0.8	4
82	Theoretical modeling of argentophilic interactions in [Ag(CN)2â¯]3 trimer found in a copper(II) complex of cis-1,2-diaminocyclohexane (Dach), [Cu(Dach)2-Ag(CN)2-Cu(Dach)2][Ag(CN)2]3. Chemical Physics Letters, 2018, 709, 11-15.	1.2	4
83	Deciphering preferred solid-state conformations in nitrogen-containing bisphosphonates and their coordination compounds. A case study of discrete Cu(ii) complexes based on Cl±-substituted analogues of zoledronic acid: crystal structures and solid-state characterization. CrystEngComm, 2019, 21, 4340-4353.	1.3	4
84	The Role of Hydrogen Bonds in Interactions between [PdCl4]2â¯ Dianions in Crystal. Molecules, 2022, 27, 2144.	1.7	4
85	Competition between Intra and Intermolecular Pnicogen Bonds. Complexes between Naphthalene Derivatives and Neutral or Anionic Bases. ChemPhysChem, 2022, , .	1.0	4
86	Experimental and Theoretical Evidence of a Pbâ‹…â‹…â‹…Pb Ditetrel Bond Without a Ïƒâ€Hole. ChemPhysChem, 2022, 23, .	1.0	4
87	Synthesis, crystal structure and DFT studies of a Zinc(II) complex of 1,3-diaminopropane (Dap), [Zn(Dap)(NCS)2][Zn(Dap)(NCS)2]n. The additional stabilizing role of Sâ‹¯Ï€ chalcogen bond. Journal of Molecular Structure, 2017, 1133, 271-277.	1.8	3
88	Crystal structure and theoretical investigation of bis(‹i›cis‹/i›-1,2-diaminocyclohexane)zinc(II) tetrachloridozincate(II). Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 627-630.	0.3	3
89	Picoplatin-based complexes with the bioactive orotate and 5-fluoroorotate ligands: Synthesis, DFT calculations, structure, spectroscopic characterization and inÂvitro cytotoxicity. Journal of Molecular Structure, 2018, 1171, 155-167.	1.8	3
90	Synthesis, crystal structure and DFT calculations of a cyanido-bridged dinuclear zinc(II) complex of cis -1,2-diaminocyclohexane (Dach) containing a dinuclear cyanidozincate(II) anion, [Zn 2 (Dach) 4 (CN)][Zn 2 (CN) 7]Â·2CH 3 OH. Journal of Molecular Structure, 2018, 1169, 110-118.	1.8	2

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91	Interactions of (MY)6 (M = Zn, Cd; Y = O, S, Se) quantum dots with N-bases. Structural Chemistry, 2019, 30, 1003-1014.	1.0	2
92	Nature of multiple weak interactions between volatile anaesthetic isoflurane and apoferritin: A theoretical study. Chemical Physics, 2012, 400, 137-141.	0.9	1
93	Synthesis, crystal structure and NLO study of two new versatile Ca (II) complexes. Applied Organometallic Chemistry, 2018, 32, e4564.	1.7	1
94	DFT Calculations and SEMâ€“EDX Analysis of Copper(II)-Azide Complexes; [Cu(en)2(N3)2] and [Cu(Tmen)(N3)2]2 (Tmen = N,N,N',N'-Tetramethylethylenediamine). Russian Journal of Physical Chemistry B, 2021, 15, S42-S51.	0.2	1
95	Physicochemical Characterization of the Loganic Acidâ€“IR, Raman, UV-Vis and Luminescence Spectra Analyzed in Terms of Quantum Chemical DFT Approach. Molecules, 2021, 26, 7027.	1.7	0