Wiktor Zierkiewicz

List of Publications by Citations

91 papers	1,843 citations	23 h-index	38 g-index
95 ext. papers	2,086 ext. citations	3.5 avg, IF	5.48 L-index

#	Paper	IF	Citations
91	Electronic structures, vibrational spectra, and revised assignment of aniline and its radical cation: Theoretical study. *Journal of Chemical Physics*, **2003**, 118, 10900-10911	3.9	143
90	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, 8499-507	16.4	113
89	Molecular Structures and Infrared Spectra ofp-Chlorophenol andp-Bromophenol. Theoretical and Experimental Studies. *Journal of Physical Chemistry A*, **2000**, 104, 11685-11692	2.8	95
88	On differences between hydrogen bonding and improper blue-shifting hydrogen bonding. *ChemPhysChem*, **2005**, 6, 609-17	3.2	91
87	Study of the nature of improper blue-shifting hydrogen bonding and standard hydrogen bonding in the X3CH...OH2 and XH...OH2 complexes (X = F, Cl, Br, I): A correlated Ab initio study. *ChemPhysChem*, **2002**, 3, 511-8	3.2	83
86	Troublesome Vibrations of Aromatic Molecules in Second-Order Møller Plesset and Density Functional Theory Calculations: Infrared Spectra of Phenol and Phenol-OD Revisited. *Journal of Physical Chemistry A*, **2001**, 105, 8734-8739	2.8	82
85	Molecular Structure and Infrared Spectra of 4-Fluorophenol: A Combined Theoretical and Spectroscopic Study. *Journal of Physical Chemistry A*, **2003**, 107, 4547-4554	2.8	59
84	Implications of monomer deformation for tetrel and pnicogen bonds. *Physical Chemistry Chemical Physics*, **2018**, 20, 8832-8841	3.6	55
83	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	3.8	44
82	Halogen bonded complexes between volatile anaesthetics (chloroform, halothane, enflurane, isoflurane) and formaldehyde: a theoretical study. *Physical Chemistry Chemical Physics*, **2011**, 13, 5105-13	3.6	42
81	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, 16734-40	3.4	42
80	Coordination of anions by noncovalently bonded hole ligands. *Coordination Chemistry Reviews*, **2020**, 405, 213136	23.2	41
79	Doubly chloro bridged dimeric copper(II) complex: magneto-structural correlation and anticancer activity. *Dalton Transactions*, **2015**, 44, 8876-88	4.3	40
78	Comparison between Tetrel Bonded Complexes Stabilized by and Hole Interactions. *Molecules*, **2018**, 23,	4.8	36
77	Regium bonds between M clusters (M = Cu, Ag, Au and n = 2-6) and nucleophiles NH and HCN. *Physical Chemistry Chemical Physics*, **2018**, 20, 22498-22509	3.6	36
76	Theoretical investigation of the conformation, acidity, basicity and hydrogen bonding ability of halogenated ethers. *Physical Chemistry Chemical Physics*, **2010**, 12, 13681-91	3.6	33
75	The dihydrogen bond in X3CH?HM 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	3.6	32

74	Theoretical investigation of the halogen bonded complexes between carbonyl bases and molecular chlorine. *Journal of Computational Chemistry*, **2015**, 36, 821-32	3.5	29
73	Metal□rganic framework in an L-arginine copper(II) ion polymer: structure, properties, theoretical studies and microbiological activity. *RSC Advances*, **2015**, 5, 36295-36306	3.7	26
72	Aerogen bonds formed between AeOF (Ae = Kr, Xe) and diazines: comparisons between □hole and □hole complexes. *Physical Chemistry Chemical Physics*, **2018**, 20, 4676-4687	3.6	24
71	Blue shifts and unusual intensity changes in the infrared spectra of the enflurane□acetone complexes: spectroscopic and theoretical studies. *Journal of Physical Chemistry A*, **2011**, 115, 11362-8	2.8	24
70	On the ability of pnicogen atoms to engage in both □and □hole complexes. Heterodimers of ZFCH (Z = P, As, Sb, Bi) and NH. *Journal of Molecular Modeling*, **2019**, 25, 152	2	23
69	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,	4.8	23
68	The crystal structure, infrared, Raman and density functional studies of bis(2-aminophenyl) diselenide. *Polyhedron*, **2011**, 30, 2466-2472	2.7	23
67	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, 6922-34	2.8	22
66	Anion???Anion Attraction in Complexes of MCl (M=Zn, Cd, Hg) with CN. *ChemPhysChem*, **2020**, 21, 1119-1125	3.2	22
65	Dual Geometry Schemes in Tetrel Bonds: Complexes between TF□(T = Si, Ge, Sn) and Pyridine Derivatives. *Molecules*, **2019**, 24,	4.8	21
64	How Many Pnicogen Bonds can be Formed to a Central Atom Simultaneously?. *Journal of Physical Chemistry A*, **2020**, 124, 2046-2056	2.8	19
63	Hexacoordinated Tetrel-Bonded Complexes between TF (T=Si, Ge, Sn, Pb) and NCH: Competition between □and □Holes. *ChemPhysChem*, **2019**, 20, 959-966	3.2	19
62	On the Stability of Interactions between Pairs of Anions - Complexes of MCl (M=Be, Mg, Ca, Sr, Ba) with Pyridine and CN. *ChemPhysChem*, **2020**, 21, 870-877	3.2	18
61	Triel-Bonded Complexes between TrR (Tr=B, Al, Ga; R=H, F, Cl, Br, CH) and Pyrazine. *ChemPhysChem*, **2018**, 19, 3122-3133	3.2	18
60	Influence of monomer deformation on the competition between two types of □holes in tetrel bonds. *Physical Chemistry Chemical Physics*, **2019**, 21, 10336-10346	3.6	17
59	Pnicogen Bonds Pairing Anionic Lewis Acid with Neutral and Anionic Bases. *Journal of Physical Chemistry A*, **2020**, 124, 4998-5006	2.8	17
58	Atypical calcium coordination number: Physicochemical study, cytotoxicity, DFT calculations and in silico pharmacokinetic characteristics of calcium caffeates. *Journal of Inorganic Biochemistry*, **2009**, 103, 1189-95	4.2	17
57	The barrier to internal rotation and electronic effects in para-halogenophenols: theoretical study. *Chemical Physics Letters*, **2004**, 386, 95-100	2.5	17

56	Pnictogen bonding in pyrazine···PnX (Pn = P, As, Sb and X = F, Cl, Br) complexes. *Journal of Molecular Modeling*, **2017**, 23, 328	2	16
55	Competition between Intra and Intermolecular Triel Bonds. Complexes between Naphthalene Derivatives and Neutral or Anionic Lewis Bases. *Molecules*, **2020**, 25,	4.8	16
54	Chalcogen bonding of two ligands to hypervalent YF (Y = S, Se, Te, Po). *Physical Chemistry Chemical Physics*, **2019**, 21, 20829-20839	3.6	15
53	Noncovalent Bonds between Tetrel Atoms. *ChemPhysChem*, **2020**, 21, 1934-1944	3.2	15
52	Structures and energetics of clusters surrounding diatomic anions stabilized by hydrogen, halogen, and other noncovalent bonds. *Chemical Physics*, **2020**, 530, 110590	2.3	14
51	On the nature of unusual intensity changes in the infrared spectra of the enflurane···acetone complexes. *Physical Chemistry Chemical Physics*, **2013**, 15, 6001-7	3.6	13
50	Reaction of volatile anaesthetic desflurane with chlorine atom. Theoretical investigation. *Chemical Physics Letters*, **2013**, 555, 72-78	2.5	13
49	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	1.9	13
48	Adenine ribbon stabilized by Watson-Crick and Hoogsteen hydrogen bonds: WFT and DFT study. *Physical Chemistry Chemical Physics*, **2010**, 12, 2888-94	3.6	13
47	A computational study of oxidation of ruthenium porphyrins via ORu(IV) and ORu(VI)O species. *Dalton Transactions*, **2006**, 1867-74	4.3	13
46	Structures of clusters surrounding ions stabilized by hydrogen, halogen, chalcogen, and pnicogen bonds. *Chemical Physics*, **2019**, 524, 55-62	2.3	12
45	Ab initio and DFT studies of the interaction between carbonyl and thiocarbonyl groups: the role of S···O chalcogen bonds. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	12
44	S?N chalcogen bonded complexes of carbon disulfide with diazines. Theoretical study. *Chemical Physics*, **2018**, 500, 37-44	2.3	12
43	Anion-anion and anion-neutral triel bonds. *Physical Chemistry Chemical Physics*, **2021**, 23, 4818-4828	3.6	11
42	Nature of the interaction between ammonia derivatives and carbon disulfide. A theoretical investigation. *International Journal of Quantum Chemistry*, **2017**, 117, e25369	2.1	10
41	Spectroscopic and DFT studies of zinc(II) complexes of diamines and thiocyanate; crystal structure of (cis-1,2-diaminocyclohexane)bis(thiocyanato-N)zinc(II). *Journal of Molecular Structure*, **2017**, 1128, 455-461	3.4	10
40	Crystallographic and Theoretical Evidences of Anion???Anion Interaction. *ChemPhysChem*, **2021**, 22, 818-821	3.2	10
39	Modelling of interactions between volatile anaesthetics (halothane, enflurane) and aromatic compounds, ab initio study. *Chemical Physics*, **2010**, 373, 243-250	2.3	9

38	Noncovalent Bonds through Sigma and Pi-Hole Located on the Same Molecule. Guiding Principles and Comparisons. *Molecules*, **2021**, 26,	4.8	9
37	Copper(II) complex with L-arginine □Crystal structure, DFT calculations, spectroscopic, thermal and magnetic properties. *Materials Chemistry and Physics*, **2019**, 228, 272-284	4.4	9
36	Synthesis, characterization, DFT calculations and antibacterial activity of palladium(II) cyanide complexes with thioamides. *Journal of Molecular Structure*, **2017**, 1141, 204-212	3.4	8
35	Synthesis, X-ray structure, DFT calculations and anticancer activity of a selenourea coordinated gold(I)-carbene complex. *Polyhedron*, **2017**, 137, 197-206	2.7	8
34	Theoretical study of the interaction of a proton with the O, F and Cl atoms of enflurane (CHFCl□CF2□O□CHF2). *Computational and Theoretical Chemistry*, **2009**, 911, 58-64		8
33	Structural and spectroscopic properties and density functional theory (DFT) calculations of a linearly bridged zinc(II) l-tyrosinato complex. *Polyhedron*, **2015**, 85, 665-674	2.7	7
32	Synthesis, characterization, DFT optimization and anticancer evaluation of phosphanegold(I) dithiocarbamates. *Journal of Molecular Structure*, **2020**, 1218, 128486	3.4	7
31	Experimental and Theoretical Studies of Dimers Stabilized by Two Chalcogen Bonds in the Presence of a N⋯N Pnicogen Bond. *Journal of Physical Chemistry A*, **2021**, 125, 657-668	2.8	7
30	Magnesium cinnamate complex, [Mg(cinn)2(H2O)2]n; structural, spectroscopic, thermal, biological and pharmacokinetical characteristics. *Journal of Molecular Structure*, **2017**, 1134, 199-207	3.4	6
29	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	3.4	6
28	Structural, spectroscopic, magnetic behavior and DFT investigations of L-tyrosinato nickel(II) coordination polymer. *New Journal of Chemistry*, **2015**, 39, 6813-6822	3.6	6
27	On the nature of halogen bonded complexes between carbonyl bases and chlorotrifluoromethane. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	6
26	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	2.8	6
25	1□ Framework l-arginine zinc(II) units bridged by oxalate: synthesis, structure, properties, and theoretical studies. *Journal of Coordination Chemistry*, **2016**, 69, 886-900	1.6	6
24	The role of hydrogen bonding in □stacking interactions in Ni(II) complex derived from triethanolamine: synthesis, crystal structure, antimicrobial, and DFT studies. *Research on Chemical Intermediates*, **2019**, 45, 5649-5664	2.8	6
23	Anion-Anion Interactions in Aerogen-Bonded Complexes. Influence of Solvent Environment. *Molecules*, **2021**, 26,	4.8	6
22	Anionanion (MX) dimers (M = Zn, Cd, Hg; X = Cl, Br, I) in different environments. *Physical Chemistry Chemical Physics*, **2021**, 23, 13853-13861	3.6	6
21	Theoretical studies of the interaction between enflurane and water. *Journal of Molecular Modeling*, **2013**, 19, 1399-405	2	5

20	Synthesis and molecular structure of polymeric bis(N-methylthiourea-S)bis(thiocyanato-N)nickel(II), [Ni(Metu)2(NCS)2]n; DFT analysis of [Ni(Metu)2(NCS)2]n and [Ni(Thiourea)2(NCS)2]n. *Journal of Molecular Structure*, **2019**, 1189, 66-72	3.4	4
19	Theoretical modeling of argentophilic interactions in [Ag(CN)2]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	2.5	4
18	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	3.4	4
17	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	3.2	3
16	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 S?chalcogen bond. *Journal of Molecular Structure*, **2017**, 1133, 271-277	3.4	3
15	Silver(I) complex with 2-amino-4,4dihydro-4,7-dimethyl-3H-phenoxazin-3-one (Phx-1) ligand: crystal structure, vibrational spectra and biological studies. *Journal of Coordination Chemistry*, **2017**, 70, 3471-3487	1.6	3
14	Deciphering preferred solid-state conformations in nitrogen-containing bisphosphonates and their coordination compounds. A case study of discrete Cu(II) complexes based on C-substituted analogues of zoledronic acid: crystal structures and solid-state characterization. *CrystEngComm*, **2019**, 21, 4340-4353	3.3	3
13	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	1.6	3
12	Crystal structure and theoretical investigation of bis(cis-1,2-diaminocyclohexane)zinc(II) tetrachloridozincate(II). *Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences*, **2017**, 72, 627-630	1	3
11	Ability of Lewis Acids with Shallow -Holes to Engage in Chalcogen Bonds in Different Environments. *Molecules*, **2021**, 26,	4.8	3
10	Picoplatin-based complexes with the bioactive orotate and 5-fluoroorotate ligands: Synthesis, DFT calculations, structure, spectroscopic characterization and in vitro cytotoxicity. *Journal of Molecular Structure*, **2018**, 1171, 155-167	3.4	2
9	Iron (III) complex exhibiting efficient catechol oxidase activity: Experimental, kinetic and theoretical approach. *Journal of Molecular Structure*, **2022**, 1252, 131685	3.4	2
8	Competition between Inter and Intramolecular Tetrel Bonds: Theoretical Studies Complemented by CSD Survey. *ChemPhysChem*, **2021**, 22, 924-934	3.2	2
7	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, [Zn2(Dach)4(CN)][Zn2(CN)7]2CH3OH. *Journal of Molecular Structure*, **2018**, 1169, 110-118	3.4	2
6	Nature of multiple weak interactions between volatile anaesthetic isoflurane and apoferritin: A theoretical study. *Chemical Physics*, **2012**, 400, 137-141	2.3	1
5	Experimental and theoretical evidence of attractive interactions between dianions: [PdCl]?[PdCl]. *Chemical Communications*, **2021**, 57, 13305-13308	5.8	1
4	Triel bonds within anionanion complexes. *Physical Chemistry Chemical Physics*, **2021**, 23, 25097-25106	3.6	1
3	Synthesis, crystal structure and NLO study of two new versatile Ca (II) complexes. *Applied Organometallic Chemistry*, **2018**, 32, e4564	3.1	1

2	Interactions of (MY)6 (M = Zn, Cd; Y = O, S, Se) quantum dots with N-bases. *Structural Chemistry*, **2019**, 30, 1003-1014	1.8	0
1	DFT Calculations and SEM-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	1.2	0