Ignacy Cukrowski

List of Publications by Year
in descending order

101	1,549	304743	377865
papers	citations	22 h-index	34 g-index

102	102	102	1376
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A unified molecularâ€wide and electron density based concept of chemical bonding. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	6
2	A Molecular-Wide and Electron Density-Based Approach in Exploring Chemical Reactivity and Explicit Dimethyl Sulfoxide (DMSO) Solvent Molecule Effects in the Proline Catalyzed Aldol Reaction. Molecules, 2022, 27, 962.	3.8	2
3	The CHÂ·Â·Â·HC interaction in biphenyl is a delocalized, molecularâ€wide and entirely nonâ€classical interaction: Results from FALDI analysis. Journal of Computational Chemistry, 2021, 42, 706-718.	3.3	7
4	A REP-FAMSEC Method as a Tool in Explaining Reaction Mechanisms: A Nucleophilic Substitution of 2-Phenylquinoxaline as a DFT Case Study. Molecules, 2021, 26, 1570.	3.8	2
5	Characterization of bonding modes in metal complexes through electron density crossâ€sections. Journal of Computational Chemistry, 2020, 41, 2695-2706.	3.3	1
6	Molecular Orbitals Support Energy-Stabilizing â€œBondingâ€•Nature of Baderâ€™s Bond Paths. Journal of Physical Chemistry A, 2020, 124, 5523-5533.	2.5	2
7	Origin of Hydrocarbons Stability from a Computational Perspective: A Case Study of Orthoâ€Xylene Isomers. ChemPhysChem, 2020, 21, 494-502.	2.1	15
8	A reaction energy profile and fragment attributed molecular system energy change (FAMSEC)-based protocol designed to uncover reaction mechanisms: a case study of the proline-catalysed aldol reaction. Physical Chemistry Chemical Physics, 2019, 21, 16694-16705.	2.8	7
9	Quantifying individual (anti)bonding molecular orbitalsâ€™ contributions to chemical bonding. Physical Chemistry Chemical Physics, 2019, 21, 20988-20998.	2.8	10
10	Reliability of HF/IQA, B3LYP/IQA, and MP2/IQA data in interpreting the nature and strength of interactions. Physical Chemistry Chemical Physics, 2019, 21, 10244-10260.	2.8	7
11	Exact and exclusive electron localization indices within QTAIM atomic basins. Journal of Computational Chemistry, 2018, 39, 1517-1530.	3.3	7
12	FALDIâ€based decomposition of an atomic interaction line leads to 3D representation of the multicenter nature of interactions. Journal of Computational Chemistry, 2018, 39, 973-985.	3.3	10
13	FALDIâ€based criterion for and the origin of an electron density bridge with an associated (3,â€“1) critical point on Bader's molecular graph. Journal of Computational Chemistry, 2018, 39, 2283-2299.	3.3	8
14	Toward deformation densities for intramolecular interactions without radical reference states using the fragment, atom, localized, delocalized, and interatomic (FALDI) charge density decomposition scheme. Journal of Computational Chemistry, 2017, 38, 981-997.	3.3	12
15	Synthesis, structure and DFT study of asymmetrical NHC complexes of cymantrene derivatives and their application in the dehydrogenative dimerization reaction of thiols. Journal of Organometallic Chemistry, 2017, 840, 11-22.	1.8	16
16	Solventâ€directed Regioselective Benzylation of Adenine: Characterization of N9â€benzyladenine and N3â€benzyladenine. Journal of Heterocyclic Chemistry, 2017, 54, 2946-2950.	2.6	3
17	Gold(I) Hydrides as Proton Acceptors in Dihydrogen Bond Formation. ChemPhysChem, 2017, 18, 2288-2294.	2.1	3
18	Reliability of interacting quantum atoms (IQA) data computed from post-HF densities: impact of the approximation used. Physical Chemistry Chemical Physics, 2017, 19, 16375-16386.	2.8	11

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19	Exploring fundamental differences between red- and blue-shifted intramolecular hydrogen bonds using FAMSEC, FALDI, IQA and QTAIM. Structural Chemistry, 2017, 28, 1429-1444.	2.0	13
20	CpNiBr(NHC) complexes as pre-catalysts in the chemoselective anaerobic oxidation of secondary aryl alcohols: Experimental and DFT studies. Molecular Catalysis, 2017, 432, 47-56.	2.0	9
21	On the origin of the relative stability of Zn^{II}NTA and Zn^{II}NTPA metal complexes. An insight from the IQA, IQF, and I€â€FARMS methods. International Journal of Quantum Chemistry, 2017, 117, e25321.	2.0	5
22	Application of Protocols Devised to Study Bi(III) Complex Formation by Voltammetry: The Bi(III)â€“Picolinic Acid System. Journal of Physical Chemistry B, 2016, 120, 12972-12980.	2.6	0
23	Measurements and Modeling To Determine the Reduction Potential of Uncomplexed Bi(III) in Nitrate Solutions for Application in Bi(III)-Ligand Equilibria Studies by Voltammetry. Journal of Physical Chemistry B, 2016, 120, 4268-4278.	2.6	5
24	On the Stability of Cisâ€ and Transâ€2â€Butene Isomers. An Insight Based on the FAMSEC, IQA, and ETSâ€NOCV Schemes. Journal of Computational Chemistry, 2016, 37, 2783-2798.	3.3	33
25	Competition reaction-based prediction of polyaminesâ€™ stepwise protonation constants: a case study involving 1,4,7,10-tetraazadecane (2,2,2-tet). Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	0
26	Interacting quantum fragmentsâ€rooted preorganizedâ€interacting fragments attributed relative molecular stability of the Be^{II} complexes of nitrilotriacetic acid and nitrilotriâ€3â€propionic acid. Journal of Computational Chemistry, 2016, 37, 1373-1387.	3.3	11
27	A Novel Approach to Monitoring of the Diffusion Junction Potential in Speciation Studies by Polarography under very Acidic Conditions. Part II: The Quasiâ€Reversible Cu(II)â€Picolinic Acid System. Electroanalysis, 2015, 27, 494-502.	2.9	3
28	IQA-embedded fragment attributed molecular system energy change in exploring intramolecular interactions. Computational and Theoretical Chemistry, 2015, 1066, 62-75.	2.5	26
29	Structural-topological preferences and protonation sequence of aliphatic polyamines: a theoretical case study of tetramine trien. Journal of Molecular Modeling, 2015, 21, 162.	1.8	5
30	Evaluating common QTAIM and NCI interpretations of the electron density concentration through IQA interaction energies and 1D cross-sections of the electron and deformation density distributions. Computational and Theoretical Chemistry, 2015, 1053, 60-76.	2.5	50
31	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
32	Physicoâ€“chemical Modelling of Adlayer Phase Formation via Surfaceâ€“limited Reactions of Copper in Relation to Sequential Electrodeposition of Multilayered Platinum on Crystalline Gold. Electrochimica Acta, 2014, 147, 432-441.	5.2	11
33	Solubility, Activity Coefficients, and Protonation Sequence of Risedronic Acid. Journal of Chemical & Engineering Data, 2014, 59, 3728-3740.	1.9	14
34	Multilayered Nanoclusters of Platinum and Gold: Insights on Electrodeposition Pathways, Electrocatalysis, Surface and Bulk Compositional Properties. Journal of the Electrochemical Society, 2013, 160, H529-H546.	2.9	9
35	A Novel Approach to Monitoring of the Diffusion Junction Potential in Speciation Studies by Polarography Under very Acidic Conditions. Partâ€…I: The Reversible Cd(II)â€Picolinic Acid System. Electroanalysis, 2013, 25, 2221-2230.	2.9	4
36	3,6-Diazaoctane-1,8-diaminium diiodide. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o2387-o2387.	0.2	2

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37	2,2â€²-(Piperazine-1,4-diyl)diethanaminium bis(2-hydroxybenzoate). Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o2388-o2388.	0.2	1
38	2,2â€²-(Piperazine-1,4-diyl)diethanaminium dibenzoate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o2389-o2389.	0.2	0
39	A Density Functional Theory and Quantum Theory of Atoms-in-Molecules Analysis of the Stability of Ni(II) Complexes of Some Amino Alcohol Ligands. Journal of Physical Chemistry A, 2011, 115, 6629-6640.	2.5	8
40	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
41	Protonation sequence of linear aliphatic polyamines from intramolecular atomic energies and charges. Computational and Theoretical Chemistry, 2011, 966, 213-219.	2.5	5
42	N,N-Dimethylethane-1,2-diaminium bis(3-hydroxybenzoate). Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2901-o2901.	0.2	0
43	Tris(dicyclohexylammonium) hydrogen [1-hydroxy-2-(1H-imidazol-1-yl)-1-phosphonatoethane]phosphonate ethanol monosolvate monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2980-o2980.	0.2	5
44	99mTc-labelled biguanide derivatives: chemical speciation modelling thereof and evaluation in vervets. Journal of Radioanalytical and Nuclear Chemistry, 2010, 283, 123-131.	1.5	2
45	Hydrogenâ€“hydrogen bonding: A stabilizing interaction in strained chelating rings of metal complexes in aqueous phase. Chemical Physics Letters, 2010, 499, 66-69.	2.6	54
46	Synthesis of Platinum and Ruthenium Nanostructures on Au Films and Au Nanoparticles: Use of Mixed Sacrificial Metals in Surface-Limited Redox-Replacement Reactions in Electrochemical Atomic Layer Deposition. ECS Meeting Abstracts, 2010, , .	0.0	0
47	A Density Functional Theory- and Atoms in Molecules-based Study of NiNTA and NiNTPA Complexes toward Physical Properties Controlling their Stability. A New Method of Computing a Formation Constant. Inorganic Chemistry, 2010, 49, 6931-6941.	4.0	20
48	Density Functional Theory and Isodesmic Reaction Based Prediction of Four Stepwise Protonation Constants, as log K_H⁽ⁿ⁾, for Nitrilotriacetic Acid. The Importance of a Kind and Protonated Form of a Reference Molecule Used. Journal of Physical Chemistry A, 2010, 114, 1868-1878.	2.5	19
49	Electrodeposition of Multilayered Bimetallic Nanoclusters of Ruthenium and Platinum via Surface-Limited Redoxâ^'Replacement Reactions for Electrocatalytic Applications. Langmuir, 2010, 26, 570-580.	3.5	37
50	Automated Electrodeposition of Bimetallic Noble-Metal Nanoclusters via Redox-Replacement Reactions for Electrocatalysis. ECS Transactions, 2009, 19, 97-113.	0.5	2
51	The analysis of pH-dependent protonated conformers of 1-hydroxyethylidene-1,1-diphosphonic acid by means of FT-Raman spectroscopy, multivariate curve resolution and DFT modelling. Journal of Raman Spectroscopy, 2009, 40, 1935-1941.	2.5	7
52	Low-spin complexes of Ni2+ with six NH3 and H2O ligands: A DFTâ€“RX3LYP study. Computational and Theoretical Chemistry, 2009, 902, 21-32.	1.5	9
53	DFT RX3LYP and RPBEPBE studies on the structural, electronic, and vibrational properties of some amino-alcohol ligands. Computational and Theoretical Chemistry, 2009, 915, 20-32.	1.5	12
54	Density Functional Theory in Prediction of Four Stepwise Protonation Constants for Nitrilotripropanoic Acid (NTPA). Journal of Physical Chemistry A, 2009, 113, 3639-3647.	2.5	23

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55	Sc(III) porphyrins. The molecular structure of two Sc(III) porphyrins and a re-evaluation of the parameters for the molecular mechanics modelling of Sc(III) porphyrins. Journal of Molecular Structure, 2008, 872, 47-55.	3.6	7
56	DFT-UX3LYP Studies on the Coordination Chemistry of Ni²⁺. Part 1: Six Coordinate [Ni(NH₃)_n(H₂O)_{6â^'n}]²⁺Complexes. Journal of Physical Chemistry A, 2008, 112, 10657-10666.	2.5	61
57	Electrochemical Performance of Coated Titanium Anodes in Concentrated Chromium VI Solutions. ECS Transactions, 2007, 6, 1-13.	0.5	2
58	Modeling and spectroscopic studies of bisphosphonateâ€“bone interactions. The Raman, NMR and crystallographic investigations of Caâ€“HEDP complexes. Bone, 2007, 41, 668-678.	2.9	51
59	Influence of electronic and steric effects on stability constants and electrochemical reversibility of divalent ion complexes with glycine and sarcosine. Analytica Chimica Acta, 2007, 590, 203-216.	5.4	5
60	Interpretation of nonâ€“Nernstian slopes in graphic analysis of data collected in pH range close to deprotonation of a ligandPart I. A glass electrode potentiometric and polarographic study of Cdâ€“(TAPSO)xâ€“(OH)y and Znâ€“(TAPSO)xâ€“(OH)y systems. Talanta, 2006, 68, 819-830.	5.5	4
61	Modelling the interaction of several bisphosphonates with hydroxyapatite using the generalised AMBER force field. Journal of Molecular Structure, 2006, 825, 134-142.	3.6	29
62	Using artificial neural networks to develop molecular mechanics parameters for the modelling of metalloporphyrins: Part IV. Five-, six-coordinate metalloporphyrins of Mn, Co, Ni and Cu. Journal of Molecular Structure, 2006, 783, 21-33.	3.6	9
63	Voltammetry as Virtual Potentiometric Sensor in Modelling of a Metal/Ligand System and Refinement of Stability Constants. Part 5. Helvetica Chimica Acta, 2006, 89, 2934-2952.	1.6	8
64	Complex Formation in the Region of Metal Hydrolysis and M(OH)2 Precipitation. A Glass Electrode Potentiometric and Polarographic Study of Cdâ€“(AMPSO)xâ€“(OH)y and Znâ€“(AMPSO)xâ€“(OH)y Systems. Electroanalysis, 2006, 18, 719-729.	2.9	8
65	Voltammetry as a virtual potentiometric sensor in modelling of a metalâ€“ligand system and refinement of stability constants. Part 4. An electrochemical study of NiII complexes with methylene diphosphonic acid. Journal of Inorganic Biochemistry, 2005, 99, 2308-2321.	3.5	4
66	Using artificial neural networks to develop molecular mechanics parameters for the modelling of metalloporphyrins. III. Five coordinate Zn(II) porphyrins and the metalloprophyrins of the early 3d metals. Journal of Molecular Structure, 2005, 738, 67-78.	3.6	16
67	Graphic Data Analysis and Complex Formation Curves as Modelling and Optimization Tools in Potentiometric and Voltammetric Speciation Studies of a Pbï£¿(TAPSO)xï£¿(OH)y System. Electroanalysis, 2005, 17, 1291-1301.	2.9	3
68	Voltammetry as a Virtual Potentiometric Sensor in Modeling of a Metal-Ligand System and Refinement of Stability Constants. Part 1. Polarographic and Glass Electrode Potentiometric Study of a Dynamic Cd-Glycine System. Electroanalysis, 2004, 16, 612-626.	2.9	7
69	Voltammetry as a Virtual Potentiometric Sensor in Modelling of a Metal/Ligand System and Refinement of Stability Constants. Part 2. Helvetica Chimica Acta, 2004, 87, 2135-2158.	1.6	7
70	Challenges in modelling and optimisation of stability constants in the study of metal complexes with monoprotonated ligands. Analytica Chimica Acta, 2004, 518, 117-126.	5.4	8
71	Challenges in Modelling and Optimization of Stability Constants in the Study of Metal Complexes with Monoprotonated Ligands. Part II. Helvetica Chimica Acta, 2003, 86, 3288-3304.	1.6	10
72	Solution Equilibria. A Unified Mathematical Treatment of Experimental Polarographic and Potentiometric Data from Acidï£¿Base and Ligand Titrations. A Polarographic and Ion Selective Electrode Study of CdIIï£¿(N-(2-hydroxyethyl)iminodiacetic acid)ï£¿OH System. Electroanalysis, 2003, 15, 1377-1388.	2.9	4

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73	Molecular mechanics parameters for the modelling of four-coordinate Zn(ii) porphyrins. Physical Chemistry Chemical Physics, 2003, 5, 5499-5506.	2.8	17
74	Molecular mechanics modelling of porphyrins. Using artificial neural networks to develop metal parameters for four-coordinate metalloporphyrinsElectronic supplementary information (ESI) available: Molecular mechanics parameters, comparisons between crystallographic and molecular mechanics geometries, error response surfaces, and crystal structures. See http://www.rsc.org/suppdata/cp/b2/b203360g/. Physical Chemistry Chemical Physics, 2002, 4, 5878-5887.	2.8	19
75	Evaluation of Equilibria with Use of Artificial Neural Networks (ANN). II. ANN and Experimental Design as a Tool in Electrochemical Data Evaluation for Fully Dynamic (Labile) Metal Complexes. Electroanalysis, 2001, 13, 295-308.	2.9	12
76	Solution Equilibria. A Unified Mathematical Treatment of Potentiometric and Polarographic Data in a Metal-Ligand Equilibrium Study at a Fixed Ligand to Metal Ratio and Various pH Values. Electroanalysis, 2001, 13, 1242-1252.	2.9	7
77	Evaluation of Equilibria with a Use of Artificial Neural Networks (ANN): I. Artificial Neural Networks and Experimental Design as a Tool in Electrochemical Data Evaluation for Fully Inert Metal Complexes. Electroanalysis, 2000, 12, 1481-1492.	2.9	12
78	Co-ordination of weak field ligands by N-acetylmicroperoxidase-8 (NAcMP8), a ferric haempeptide from cytochrome c, and the influence of the axial ligand on the reduction potential of complexes of NAcMP8â€Šâ€. Dalton Transactions RSC, 2000, , 1335-1342.	2.3	20
79	Experimental and calculated complex formation curves for mixed, dynamic and semi-dynamic, metalâ€“ligand systems.. Journal of Electroanalytical Chemistry, 1999, 460, 197-206.	3.8	15
80	Metal-ion speciation in blood plasma incorporating the bisphosphonate, 1-hydroxy-4-aminopropilydenediphosphonate (APD), in therapeutic radiopharmaceuticals. Journal of Inorganic Biochemistry, 1999, 73, 265-272.	3.5	27
81	A potentiometric and differential pulse polarographic study of CdII with 1-hydroxyethylenediphosphonic acid. Analytica Chimica Acta, 1999, 379, 217-226.	5.4	17
82	Polarographic Complex Formation Curves for Fully Inert Metal-Ligand System. Electroanalysis, 1999, 11, 606-613.	2.9	10
83	A differential pulse polarographic study of bismuthIII complexes with macrocyclic ligands 1,4,7,10-tetraazacyclododecane and 1,4,7,10-tetrakis (2-hydroxypropyl)-1,4,7,10-tetraazacyclododecane. An out-of-cell determination of stability constants of polarographically active and inactive bismuth complexes at fixed ligand to metal ratio and various pH values. Analytica Chimica Acta, 1998, 372, [illegible]	5.4	6
84	Evaluation of a Peak Potential of an Uncomplexed Metal Ion in Speciation Study of Labile Metal-Ligand Systems by Polarography. Stability Constant Determination of CdII and PbII with Picolinic Acid at a Fixed LT:MT Ratio and Varied pH. Electroanalysis, 1998, 10, 877-885.	2.9	18
85	Protonation constant of monoaza-12-crown-4 ether and stability constants with selected metal ions in aqueous solution in the presence of an excess of sodium ion: a potentiometric and differential pulse polarographic study at fixed ligand to metal ratio and varied pH. Talanta, 1998, 47, 1175-1189.	5.5	9
86	Synthesis, stability and structure of the complex of bismuth(III) with the nitrogen-donor macrocycle 1,4,7,10-tetraazacyclododecane. The role of the lone pair on bismuth(III) and lead(II) in determining co-ordination geometry. Journal of the Chemical Society Dalton Transactions, 1997, , 901-908.	1.1	60
87	Modelling of Cadmium(II) Species Formed With N,Nâ€²-Bis(2-pyridylmethyl)-1,2-diaminoethane and Optimisation of Stability Constants by the Use of Polarographic Complex Formation Curves for Labile Metalâ€“Ligand Systems. Analyst, The, 1997, 122, 827-833.	3.5	14
88	Experimental and calculated complex formation curves for a labile metal-ligand system a differential		

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91	The unusual protonation constants of cyclam. A potentiometric, crystallographic and molecular mechanics study. Journal of the Chemical Society Perkin Transactions II, 1996, , 1925.	0.9	54
92	Formation constant calculation for non-labile complexes based on a labile part of the metal-ligand system. A differential pulse polarographic study at fixed ligand to metal ratio and varied pH: application to polarographically inactive complexes. Analytica Chimica Acta, 1996, 319, 39-48.	5.4	31
93	Study of protonation of 1,4,7-tris(2-hydroxyethyl)-1,4,7-triazacyclononane, and its complexes with metal ions, by crystallography, polarography, potentiometry, molecular mechanics and NMR. Inorganica Chimica Acta, 1996, 246, 159-169.	2.4	26
94	A polarographic method of speciation for labile metal-ligand systems based on mass-balance equations. A differential pulse polarographic study at fixed ligand to metal ratio and varied pH. Analytica Chimica Acta, 1996, 336, 23-36.	5.4	48
95	The effect of chelate ring size on metal ion size-based selectivity in polyamine ligands containing pyridyl and saturated nitrogen donor groups. Analytica Chimica Acta, 1995, 312, 307-321.	5.4	49
96	Pulse polarography study of the complexes of lead with azacrown [2,2,2]cryptand in the presence of an excess of competing sodium ion. Electroanalysis, 1995, 7, 763-769.	2.9	8
97	The neutral oxygen donor in complexes of lead and cadmium: A differential pulse polarographic, potentiometric and calorimetric study. Polyhedron, 1995, 14, 1661-1674.	2.2	24
98	Complexation of BiIII by nitrogen donor ligands. A polarographic study. Polyhedron, 1995, 14, 1699-1707.	2.2	24
99	Design of ligands containing the o-hydroxybenzyl group. Metal-complexing properties of N,Nâ€³-bis(2-hydroxybenzyl)diethylenetriamine-N,Nâ€²,Nâ€³-triacetic acid. Journal of the Chemical Society Dalton Transactions, 1994, , 2679-2685.	1.1	6
100	The affinity of bismuth(III) for nitrogen-donor ligands. Journal of the Chemical Society Dalton Transactions, 1993, , 2895.	1.1	51
101	Studies of the process of catalytic hydrogen evolution on the epoxy-resin-impregnated graphite-based mercury film electrode. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1986, 213, 127-134.	0.1	3