Jaroslav V Burda

List of Publications by Year
in descending order

100	3,620	126708	143772
papers	citations	33 h-index	57 g-index

106	106	106	3190
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A new grand-canonical potential for the thermodynamic description of the reactions in solutions with constant pH. Journal of Molecular Liquids, 2021, 335, 115979.	2.3	2
2	Estimation of electron absorption spectra and lifetime of the two lowest singlet excited states of pyrimidine nucleobases and their derivatives. Journal of Molecular Structure, 2021, 1250, 131863.	1.8	4
3	QM and QM/MM umbrella sampling MD study of the formation of Hg(II)â€“thymine bond: Model for evaluation of the reaction energy profiles in solutions with constant pH. Journal of Computational Chemistry, 2020, 41, 1509-1520.	1.5	1
4	Zweifel an einem Dogma: Hydrolyse Ãquatorialer Liganden von Pt^{IV}â€Komplexen unter physiologischen Bedingungen. Angewandte Chemie, 2019, 131, 7542-7547.	1.6	5
5	A Dogma in Doubt: Hydrolysis of Equatorial Ligands of Pt^{IV} Complexes under Physiological Conditions. Angewandte Chemie - International Edition, 2019, 58, 7464-7469.	7.2	46
6	Square-Planar Pt(II) and Ir(I) Complexes as the Lewis Bases: Donorâ€“Acceptor Adducts with Group 13 Trihalides and Trihydrides. Inorganic Chemistry, 2019, 58, 3616-3626.	1.9	10
7	Protein environment affects the waterâ€“tryptophan binding mode. MD, QM/MM, and NMR studies of engrailed homeodomain mutants. Physical Chemistry Chemical Physics, 2018, 20, 12664-12677.	1.3	3
8	Formation of chelate structure between His-Met dipeptide and diaqua-cisplatin complex; DFT/PCM computational study. Journal of Biological Inorganic Chemistry, 2018, 23, 363-376.	1.1	3
9	Redox Potentials for Tetraplatin, Satraplatin, Its Derivatives, and Ascorbic Acid: A Computational Study. Inorganic Chemistry, 2018, 57, 951-962.	1.9	15
10	Interactions of Ascorbic Acid with Satraplatin and its trans Analog JM576: DFT Computational Study. European Journal of Inorganic Chemistry, 2018, 2018, 1481-1491.	1.0	6
11	Exploration of selected electronic characteristics of half-sandwich organoruthenium(II) Î²-diketonate complexes. Journal of Molecular Modeling, 2018, 24, 98.	0.8	5
12	Metal Interactions with Nucleobases, Base Pairs, and Oligomer Sequences; Computational Approach. , 2017, , 1827-1874.		1
13	Study on electronic properties, thermodynamic and kinetic parameters of the selected platinum(II) derivatives interacting with guanine. Journal of Inorganic Biochemistry, 2017, 172, 100-109.	1.5	9
14	Side Reactions with an Equilibrium Constraint: Detailed Mechanism of the Substitution Reaction of Tetraplatin with dGMP as a Starting Step of the Platinum(IV) Reduction Process. Journal of Physical Chemistry B, 2017, 121, 4400-4413.	1.2	3
15	The influence of the metal cations and microhydration on the reaction trajectory of the N3 â†" O2 thymine proton transfer: Quantum mechanical study. Journal of Computational Chemistry, 2017, 38, 2680-2692.	1.5	4
16	Interactions of the â€œpianoâ€stoolâ€•[ruthenium(II)(Î·⁶â€arene)(quinolone)Cl]⁺ complexes with water; DFT computational study. Journal of Computational Chemistry, 2016, 37, 1766-1780.	1.5	3
17	International conference on â€œModeling Interaction in Biomolecules VIIâ€• held in Prague, 14â€"18 September 2015. Journal of Molecular Modeling, 2016, 22, 1.	0.8	0
18	Estimation of Transition-Metal Empirical Parameters for Molecular Mechanical Force Fields. Journal of Chemical Theory and Computation, 2016, 12, 3681-3688.	2.3	22

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19	Reduction Process of Tetraplatin in the Presence of Deoxyguanosine Monophosphate (dGMP): A Computational DFT Study. Chemistry - A European Journal, 2016, 22, 1037-1047.	1.7	12
20	Metal Interactions with Nucleobases, Base Pairs, and Oligomer Sequences; Computational Approach. , 2016, , 1-48.		1
21	Reaction mechanism of Ru(II) pianoâ€stool complexes: Umbrella sampling QM/MM MD study. Journal of Computational Chemistry, 2014, 35, 1446-1456.	1.5	20
22	The structure of metallo-DNA with consecutive thymineâ€“HgIIâ€“thymine base pairs explains positive entropy for the metallo base pair formation. Nucleic Acids Research, 2014, 42, 4094-4099.	6.5	106
23	The influence of arene-ring size on stacking interaction with canonical base pairs. Chemical Physics Letters, 2014, 598, 28-34.	1.2	4
24	The IR and Raman spectra of polyaniline adsorbed on the glass surface; comparison of experimental, empirical force field, and quantum chemical results. European Polymer Journal, 2014, 57, 47-57.	2.6	24
25	A double-QM/MM method for investigating donorâ€“acceptor electron-transfer reactions in solution. Physical Chemistry Chemical Physics, 2014, 16, 19530-19539.	1.3	14
26	Energy transfer in aggregates of bacteriochlorophyll c self-assembled with azulene derivatives. Physical Chemistry Chemical Physics, 2014, 16, 16755-16764.	1.3	15
27	Can Satraplatin be hydrated before the reduction process occurs? The DFT computational study. Journal of Molecular Modeling, 2013, 19, 4669-4680.	0.8	12
28	International conference on â€œModeling interaction in biomolecules 2011â€, in KutnÃ¡ Hora, September 4thâ€“9th, 2011. Journal of Molecular Modeling, 2013, 19, 4627-4627.	0.8	0
29	NMR spectroscopic detection of chirality and enantiopurity in referenced systems without formation of diastereomers. Nature Communications, 2013, 4, 2188.	5.8	103
30	Mechanism of the cis-[Pt(1R,2R-DACH)(H₂O)₂]²⁺ Intrastrand Binding to the Double-Stranded (pGpG)Â·(CpC) Dinucleotide in Aqueous Solution: A Computational DFT Study. Inorganic Chemistry, 2013, 52, 5801-5813.	1.9	14
31	Formation of a Thymineâ€Hg^{II}â€Thymine Metalâ€Mediated DNA Base Pair: Proposal and Theoretical Calculation of the Reaction Pathway. Chemistry - A European Journal, 2013, 19, 9884-9894.	1.7	45
32	Exploration of various electronic properties along the reaction coordinate for hydration of Pt(II) and Ru(II) complexes; the CCSD, MPx, and DFT computational study. Journal of Molecular Modeling, 2013, 19, 5245-5255.	0.8	4
33	Exploring the potential energy surface for interaction of a trichloro(diethylenetriamine)gold(III) complex with strong nucleophiles. Chemical Physics Letters, 2012, 548, 64-70.	1.2	14
34	Colorimetric detection of trace water in tetrahydrofuran using N,Nâ€²-substituted oxoporphyrinogens. Chemical Communications, 2012, 48, 3933.	2.2	45
35	Exploring the Potential Energy Surface for the Interaction of Sterically Hindered Trichloro(diethylenetriamine)gold(III) Complexes with Water. Journal of Physical Chemistry A, 2012, 116, 11015-11024.	1.1	14
36	Reactions of cisplatin and glycine in solution with constant pH: a computational study. Physical Chemistry Chemical Physics, 2012, 14, 12571.	1.3	9

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37	Binding of pianoâ€stool Ru(II) complexes to DNA; QM/MM study. Journal of Computational Chemistry, 2012, 33, 2092-2101.	1.5	24
38	Structure and stability of kaolinite/TiO2 nanocomposite: DFT and MM computations. Journal of Molecular Modeling, 2012, 18, 2689-2698.	0.8	22
39	Anthracyclines and ellipticines as DNA-damaging anticancer drugs: Recent advances. , 2012, 133, 26-39.		125
40	Comparison of hydration reactions for â€œpiano-stoolâ€•RAPTA-B and [Ru(Î·6â^' arene)(en)Cl]+ complexes: Density functional theory computational study. Journal of Chemical Physics, 2011, 134, 024520.	1.2	15
41	Exploring a Reaction Mechanism for Acetato Ligand Replacement in Paddlewheel Tetrakisacetatodirhodium (II,II) Complex by Ammonia: Computational Density Functional Theory Study. Journal of Physical Chemistry A, 2011, 115, 784-794.	1.1	6
42	Activation of the cisplatin and transplatin complexes in solution with constant pH and concentration of chloride anions; quantum chemical study. Journal of Molecular Modeling, 2011, 17, 2385-2393.	0.8	31
43	Cisplatin interaction with amino acids cysteine and methionine from gas phase to solutions with constant pH. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 98-114.	2.2	12
44	Reactions of cisplatin with cysteine and methionine at constant pH; a computational study. Dalton Transactions, 2010, 39, 1295-1301.	1.6	28
45	Charge-scaled cavities in polarizable continuum model: Determination of acid dissociation constants for platinum-amino acid complexes. Journal of Chemical Physics, 2009, 131, 135101.	1.2	24
46	Interactions of the â€œpianoâ€stoolâ€•[ruthenium(II) (Î·⁶â€arene)(en)CL]⁺complexes with water and nucleobases; ab initio and DFT study. Journal of Computational Chemistry, 2009, 30, 1758-1770.	1.5	34
47	Reaction Force Analysis of Solvent Effects in the Addition of HCl to Propene. Journal of Physical Chemistry A, 2009, 113, 6500-6503.	1.1	32
48	Cisplatin Interaction with Cysteine and Methionine in Aqueous Solution: Computational DFT/PCM Study. Journal of Physical Chemistry B, 2009, 113, 3139-3150.	1.2	65
49	Comparison of the electronic properties, and thermodynamic and kinetic parameters of the aquation of selected platinum(II) derivatives with their anticancer IC50 indexes. Journal of Molecular Modeling, 2008, 14, 705-716.	0.8	21
50	The trans effect in squareâ€planar platinum(II) complexesâ€”A density functional study. Journal of Computational Chemistry, 2008, 29, 2370-2381.	1.5	69
51	A computational study on DNA bases interactions with dinuclear tetraacetato-diaqua-dirhodium(II,II) complex. Journal of Inorganic Biochemistry, 2008, 102, 53-62.	1.5	15
52	Computational study of redox active centres of blue copper proteins: a computational DFT study. Molecular Physics, 2008, 106, 2733-2748.	0.8	14
53	Theoretical Study of Hydrated Copper(II) Interactions with Guanine:â€‰ A Computational Density Functional Theory Study. Journal of Physical Chemistry A, 2008, 112, 256-267.	1.1	31
54	Computational Study on Spectral Properties of the Selected Pigments from Various Photosystems:Â Structureâ^'Transition Energy Relationship. Journal of Physical Chemistry A, 2007, 111, 5864-5878.	1.1	26

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55	Reaction Force Decomposition of Activation Barriers To Elucidate Solvent Effects. Journal of Physical Chemistry A, 2007, 111, 2455-2457.	1.1	71
56	Pt-bridges in various single-strand and double-helix DNA sequences. DFT and MP2 study of the cisplatin coordination with guanine, adenine, and cytosine. Journal of Molecular Modeling, 2007, 13, 367-379.	0.8	20
57	International conference and workshop: Modeling and Design of Molecular Materials (10â€“15) Tj ETQq1 1 0.784314 rgBT /Overlock 10	0.8	0
58	Can the pH value of water solutions be estimated by quantum chemical calculations of small water clusters?. Journal of Chemical Physics, 2006, 125, 194518.	1.2	19
59	Copper Cation Interactions with Biologically Essential Types of Ligands:Â A Computational DFT Study. Journal of Physical Chemistry A, 2006, 110, 4795-4809.	1.1	40
60	Analysis of the Reaction Force for a Gas Phase SN2 Process:Â CH3Cl + H2O â†' CH3OH + HClâ€. Journal of Physical Chemistry A, 2006, 110, 756-761.	1.1	59
61	Theoretical Study of Interaction of Urate with Li+, Na+, K+, Be2+, Mg2+, and Ca2+Metal Cations. Journal of Physical Chemistry A, 2006, 110, 6139-6144.	1.1	24
62	Towards the Elucidation of the Activation of Cisplatin in Anticancer Treatment. Computational Chemistry - Reviews of Current Trends, 2006, , 265-321.	0.4	2
63	Cisplatin interaction with cysteine and methionine, a theoretical DFT study. Journal of Inorganic Biochemistry, 2005, 99, 2184-2196.	1.5	81
64	Theoretical description of copper Cu(I)/Cu(II) complexes in mixed ammine-aqua environment. DFT and ab initio quantum chemical study. Chemical Physics, 2005, 312, 193-204.	0.9	62
65	Study of electronic spectra of free-base porphin and Mg-porphin: Comprehensive comparison of variety ofab initio, DFT, and semiempirical methods. Journal of Computational Chemistry, 2005, 26, 294-303.	1.5	18
66	Hydration process as an activation of trans- and cisplatin complexes in anticancer treatment. DFT andab initio computational study of thermodynamic and kinetic parameters. Journal of Computational Chemistry, 2005, 26, 907-914.	1.5	88
67	Theoretical model of the aqua-copper [Cu(H2O)5]+cation interactions with guanine. Journal of Molecular Modeling, 2005, 11, 362-369.	0.8	14
68	The international workshop â€œModeling & Design of Molecular Materialsâ€, held 16â€“20 September 2004 in WrocÅ‚aw. Journal of Molecular Modeling, 2005, 11, 257-257.	0.8	2
69	Estimation of Electron Spectra Transitions of Free-Based Porphin and Mg-Porphin Using Various Quantum Chemical Approaches. International Journal of Molecular Sciences, 2004, 5, 196-213.	1.8	10
70	Activation barriers and rate constants for hydration of platinum and palladium square-planar complexes: An ab initio study. Journal of Chemical Physics, 2004, 120, 1253-1262.	1.2	73
71	Theoretical model of copper Cu(I)/Cu(II) hydration. DFT and ab initio quantum chemical study. Computational and Theoretical Chemistry, 2004, 683, 183-193.	1.5	67
72	The influence of a sugar-phosphate backbone on the cisplatin-bridged BpB? models of DNA purine bases. Quantum chemical calculations of Pt(ii) bonding characteristics. Physical Chemistry Chemical Physics, 2004, 6, 3585.	1.3	46

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73	The Influence of N7Guanine Modifications on the Strength of Watsonâ"Crick Base Pairing and Guanine N1Acidity:Â Comparison of Gas-Phase and Condensed-Phase Trends. Journal of Physical Chemistry B, 2003, 107, 5349-5356.	1.2	49
74	How Strong Can the Bend Be on a DNA Helix from Cisplatin? DFT and MP2 Quantum Chemical Calculations of Cisplatin-Bridged DNA Purine Bases. Inorganic Chemistry, 2003, 42, 7162-7172.	1.9	71
75	Density functional study of structural and electronic properties of bimetallic silverâ€"gold clusters: Comparison with pure gold and silver clusters. Journal of Chemical Physics, 2002, 117, 3120-3131.	1.2	305
76	Raman spectroscopy study of acid-base and structural properties of 9-[2-(phosphonomethoxy)ethyl]adenine in aqueous solutions. Biopolymers, 2002, 67, 285-288.	1.2	5
77	The influence of square planar platinum complexes on DNA base pairing. An ab initio DFT study. Physical Chemistry Chemical Physics, 2001, 3, 4404-4411.	1.3	48
78	A Systematic ab Initio Study of the Hydration of Selected Palladium Square-Planar Complexes. A Comparison with Platinum Analogues. Journal of Physical Chemistry A, 2001, 105, 8086-8092.	1.1	53
79	An ab initio quantum chemical study of reactions of hexano-6-lactam peroxy radicals with phenoxy or diphenyl radicals. Polymer Degradation and Stability, 2001, 74, 569-577.	2.7	3
80	The interactions of square platinum(II) complexes with guanine and adenine: a quantum-chemical ab initio study of metalated tautomeric forms. Journal of Biological Inorganic Chemistry, 2000, 5, 178-188.	1.1	64
81	Hydration of cis- and trans-platin: A pseudopotential treatment in the frame of a G3-type theory for platinum complexes. Journal of Chemical Physics, 2000, 113, 2224-2232.	1.2	94
82	Interactions of Hydrated IIa and IIb Group Metal Cations with Thioguanine-Cytosine DNA Base Pair: Ab initio and Density Functional Theory Investigation of Polarization Effects, Differences Among Cations, and Flexibility of the Cation Hydration Shell. Journal of Biomolecular Structure and Dynamics, 1999, 17, 61-77.	2.0	44
83	Metal ions in non-complementary DNA base pairs: an ab initio study of Cu(I), Ag(I), and Au(I) complexes with the cytosine-adenine base pair. Journal of Biological Inorganic Chemistry, 1999, 4, 537-545.	1.1	73
84	Modelling of Aniline-Vermiculite and Tetramethylammonium-Vermiculite; Test of Force Fields. Journal of Molecular Modeling, 1999, 5, 8-16.	0.8	16
85	Interaction of the Adenineâ"Thymine Watsonâ"Crick and Adenineâ"Adenine Reverse-Hoogsteen DNA Base Pairs with Hydrated Group IIa (Mg2+, Ca2+, Sr2+, Ba2+) and IIb (Zn2+, Cd2+, Hg2+) Metal Cations:Â Absence of the Base Pair Stabilization by Metal-Induced Polarization Effects. Journal of Physical Chemistry B, 1999, 103, 2528-2534.	1.2	102
86	(HX)2 species (X=F through At) in the groups of the periodic system:. Chemical Physics Letters, 1998, 288, 20-24.	1.2	12
87	Chemical bonds between noble metals and noble gases.. Chemical Physics Letters, 1998, 288, 635-641.	1.2	36
88	A quantum chemical ab initio study of the interaction between Co+ and Ni+ ions with CO2 and N2O. Chemical Physics, 1998, 230, 13-22.	0.9	6
89	Stabilization of the Purineâ€¢Purineâ€¢Pyrimidine DNA Base Triplets by Divalent Metal Cations. Journal of Biomolecular Structure and Dynamics, 1998, 16, 139-143.	2.0	48
90	Interaction between the Guanineâ"Cytosine Watsonâ"Crick DNA Base Pair and Hydrated Group IIa (Mg2+,) Tj ETQq0 0 0 rgBT /Overlock 102, 5951-5957.	1.1	171

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91	Hydrogen-bonded Trimers of DNA Bases and their Interaction with Metal Cations: Ab initio Quantum-chemical and Empirical Potential Study. Journal of Biomolecular Structure and Dynamics, 1997, 14, 613-628.	2.0	72
92	Interaction of DNA Base Pairs with Various Metal Cations (Mg2+, Ca2+, Sr2+, Ba2+, Cu+, Ag+, Au+, Zn2+,) Tj ETQq0 0 0 rgBT /Overlock Interaction. Journal of Physical Chemistry B, 1997, 101, 9670-9677.	1.2	222
93	Ab Initio Study of the Interaction of Guanine and Adenine with Various Mono- and Bivalent Metal Cations (Li+, Na+, K+, Rb+, Cs+; Cu+, Ag+, Au+; Mg2+, Ca2+, Sr2+, Ba2+; Zn2+, Cd2+, and Hg2+). The Journal of Physical Chemistry, 1996, 100, 7250-7255.	2.9	214
94	Theoretical Study of Thermal Dehydrochlorination of Poly(vinyl chloride) Initiated by Tertiary Chlorine Groupings. Collection of Czechoslovak Chemical Communications, 1995, 60, 1303-1309.	1.0	4
95	Quantum Chemical Study of Thermal Dehydrochlorination of Poly(vinyl chloride) Containing Aldehyde Groups. Collection of Czechoslovak Chemical Communications, 1995, 60, 1310-1315.	1.0	0
96	Dehydrochlorination of Poly(vinyl chloride) in Isotactic Systems. Collection of Czechoslovak Chemical Communications, 1993, 58, 343-353.	1.0	3
97	Oxidizability and Structure of Lactams. Collection of Czechoslovak Chemical Communications, 1993, 58, 354-364.	1.0	1
98	Thermal Dehydrochlorination of Poly(vinyl chloride) in Syndiotactic Systems. Collection of Czechoslovak Chemical Communications, 1992, 57, 93-106.	1.0	2
99	The Effect of Cluster Size on the Characteristics of Chemisorption in the Model Growth of Silicon Crystals. Collection of Czechoslovak Chemical Communications, 1992, 57, 241-247.	1.0	1
100	Interactions of the SiHxCly Silicon Species with the Si4H9 Cluster. Collection of Czechoslovak Chemical Communications, 1992, 57, 248-254.	1.0	0