ZdenÄ›k Chval

List of Publications by Year in descending order

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21	523	687220 13	752573 20
papers	citations	h-index	g-index

22	22	22	794
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computer Simulations of Quartz (101)â€“Water Interface over a Range of pH Values. Journal of Physical Chemistry C, 2015, 119, 9274-9286.	1.5	99
2	The trans effect in squareâ€planar platinum(II) complexesâ€”A density functional study. Journal of Computational Chemistry, 2008, 29, 2370-2381.	1.5	69
3	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
4	Pentacoordinated transition states of cisplatin hydrolysisâ€”ab initio study. Computational and Theoretical Chemistry, 2000, 532, 59-68.	1.5	63
5	Transition States of Cisplatin Binding to Guanine and Adenine: ab initio Reactivity Study. Collection of Czechoslovak Chemical Communications, 2003, 68, 1105-1118.	1.0	34
6	The C4H6â€¢+Potential Energy Surface. 2. The Reaction of Ethylene Radical Cation with Acetylene. Journal of Physical Chemistry A, 1998, 102, 9297-9307.	1.1	25
7	Cy3 and Cy5 Dyes Terminally Attached to 5â€²C End of DNA: Structure, Dynamics, and Energetics. Journal of Physical Chemistry B, 2014, 118, 13564-13572.	1.2	19
8	A comparative study of the binding of QSY 21 and Rhodamine 6G fluorescence probes to DNA: structure and dynamics. Physical Chemistry Chemical Physics, 2010, 12, 9677.	1.3	18
9	Force Field for Platinum Binding to Adenine and Guanine Taking into Account Flexibility of Nucleic Acids Bases. Journal of Physical Chemistry B, 1998, 102, 1659-1661.	1.2	16
10	Towards molecular dynamics simulations of chiral room-temperature ionic liquids. Journal of Molecular Liquids, 2014, 189, 85-94.	2.3	16
11	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
12	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
13	Surface segregation in a binary mixture of ionic liquids: Comparison between high-resolution RBS measurements and moleculardynamics simulations. Journal of Chemical Physics, 2016, 145, 184704.	1.2	14
14	Modeling the RNA 2â€²OH Activation: Possible Roles of Metal Ion and Nucleobase as Catalysts in Self-Cleaving Ribozymes. Journal of Physical Chemistry B, 2011, 115, 10943-10956.	1.2	13
15	PtÂ·Â·Â·H Nonclassical Interaction in Water-Dissolved Pt(II) Complexes: Coaction of Electronic Effects with Solvent-Assisted Stabilization. Inorganic Chemistry, 2016, 55, 3252-3264.	1.9	13
16	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
17	Tuning the Reactivity and Bonding Properties of Metal Square-Planar Complexes by the Substitution(s) on the Trans-Coordinated Pyridine Ring. ACS Omega, 2020, 5, 11768-11783.	1.6	9
18	Influence of the Environment on the Specificity of the Mg(II) Binding to Uracil. Journal of Physical Chemistry A, 2012, 116, 1786-1793.	1.1	4

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19	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
20	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
21	Tuning the Reactivity and Bonding Properties of the Pt(II) Complexes by the Substitution(s) on the Transâ€Coordinated Nonâ€Aromatic Amine Ligand. ChemistrySelect, 2021, 6, 3162-3168.	0.7	0