Willian R Rocha

List of Publications by Year
in descending order

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107	2,140	172457	289244
papers	citations	29 h-index	40 g-index

108	108	108	2506
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis, Magnetostructural Correlation, and Catalytic Promiscuity of Unsymmetric Dinuclear Copper(II) Complexes: Models for Catechol Oxidases and Hydrolases. Inorganic Chemistry, 2012, 51, 1569-1589.	4.0	103
2	Pyridine-derived thiosemicarbazones and their tin(IV) complexes with antifungal activity against Candida spp.. European Journal of Medicinal Chemistry, 2011, 46, 1473-1482.	5.5	69
3	The hydrolysis process of the cis-dichloro(ethylenediamine)platinum(II): A theoretical study. Journal of Chemical Physics, 2003, 118, 10584-10592.	3.0	67
4	N4-Phenyl-substituted 2-acetylpyridine thiosemicarbazones: Cytotoxicity against human tumor cells, structureâ€“activity relationship studies and investigation on the mechanism of action. Bioorganic and Medicinal Chemistry, 2012, 20, 3396-3409.	3.0	66
5	Improved quantum mechanical study of the potential energy surface for the bithiophene molecule. Journal of Chemical Physics, 2000, 113, 4206-4215.	3.0	61
6	2-Acetylpyridine- and 2-benzoylpyridine-derived hydrazones and their gallium(III) complexes are highly cytotoxic to glioma cells. European Journal of Medicinal Chemistry, 2012, 50, 163-172.	5.5	58
7	Hydroxylamine as an Oxygen Nucleophile. Structure and Reactivity of Ammonia Oxide. Journal of the American Chemical Society, 2006, 128, 12374-12375.	13.7	57
8	Monte Carlo Simulation of Cisplatin Molecule in Aqueous Solution. Journal of Physical Chemistry B, 2006, 110, 12047-12054.	2.6	55
9	The solvent effect on the aquation processes of the cis-dichloro(ethylenediammine)platinum(II) using continuum solvation models. Chemical Physics Letters, 2004, 387, 182-187.	2.6	43
10	Theoretical Study of the Olefin Insertion Reaction in the Heterobimetallic Pt(H)(PH3)2(SnCl3)(C2H4) Compound. Organometallics, 1998, 17, 1961-1967.	2.3	42
11	A Monte Carloâ€“quantum mechanical study of the solvatochromism of pyrimidine in water and in carbon tetrachloride. Physical Chemistry Chemical Physics, 2001, 3, 1583-1587.	2.8	42
12	An efficient quantum mechanical/molecular mechanics Monte Carlo simulation of liquid water. Chemical Physics Letters, 2001, 335, 127-133.	2.6	42
13	Reaction Mechanism and Tautomeric Equilibrium of 2-Mercaptopyrimidine in the Gas Phase and in Aqueous Solution:Â A Combined Monte Carlo and Quantum Mechanics Study. Journal of Physical Chemistry A, 2006, 110, 7253-7261.	2.5	42
14	Design, structural and spectroscopic elucidation, and the inÂvitro biological activities of new diorganotin dithiocarbamates. European Journal of Medicinal Chemistry, 2012, 58, 493-503.	5.5	42
15	HNO Is Produced by the Reaction of NO with Thiols. Journal of the American Chemical Society, 2017, 139, 14483-14487.	13.7	41
16	Rhodium catalyzed hydroformylation of Î²-pinene and camphene: effect of phosphorous ligands and reaction conditions on diastereoselectivity. Journal of Organometallic Chemistry, 2003, 671, 150-157.	1.8	40
17	A radical rebound mechanism for the methane oxidation reaction promoted by the dicopper center of a pMMO enzyme: a computational perspective. Dalton Transactions, 2016, 45, 2492-2504.	3.3	40
18	Solvent effects on the electronic absorption spectrum of formamide studied by a sequential Monte Carlo/quantum mechanical approach. Theoretical Chemistry Accounts, 2002, 108, 31-37.	1.4	39

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19	Bismuth(III) complexes with 2-acetylpyridine- and 2-benzoylpyridine-derived hydrazones: Antimicrobial and cytotoxic activities and effects on the clonogenic survival of human solid tumor cells. Bioorganic and Medicinal Chemistry, 2016, 24, 2988-2998.	3.0	39
20	Cytotoxic and antimicrobial effects of indium(<scp>iii</scp>) complexes with 2-acetylpyridine-derived thiosemicarbazones. Dalton Transactions, 2017, 46, 918-932.	3.3	37
21	NO/H₂S â€œCrosstalkâ€•Reactions. The Role of Thionitrites (SNO^{â€“}) and Perthionitrites (SSNO^{â€“}). Inorganic Chemistry, 2019, 58, 14981-14997.	4.0	37
22	2-Acetylpyridine- and 2-benzoylpyridine-derived thiosemicarbazones and their antimony(III) complexes exhibit high anti-trypanosomal activity. Polyhedron, 2012, 31, 614-621.	2.2	36
23	The electronic spectrum of N-methylacetamide in aqueous solution: a sequential Monte Carlo/quantum mechanical study. Chemical Physics Letters, 2001, 345, 171-178.	2.6	35
24	On the evaluation of thermal corrections to gas phase ab initio relative energies: implications to the conformational analysis study of cyclooctane. Chemical Physics, 2002, 280, 31-42.	1.9	35
25	Kinetics and structural aspects of the cisplatin interactions with guanine: A quantum mechanical description. International Journal of Quantum Chemistry, 2006, 106, 2129-2144.	2.0	35
26	Ab initio conformational analysis of cyclooctane molecule. Journal of Computational Chemistry, 1998, 19, 524-534.	3.3	33
27	Insertion reaction of propene into Rh?H bond in HRh(CO)(PH3)2(C3H6) compound: A density functional study. International Journal of Quantum Chemistry, 2000, 78, 42-51.	2.0	32
28	Theoretical investigation of the reaction mechanism for the phosphate diester hydrolysis using an asymmetric dinuclear metal complex as a biomimetic model of the purple acid phosphatase enzyme. Physical Chemistry Chemical Physics, 2008, 10, 7039.	2.8	30
29	Theoretical study of the potential energy surface for the interaction of cisplatin and their aquated species with water. Journal of Chemical Physics, 2008, 128, 165103.	3.0	30
30	DNA photonuclease activity of four new copper(ii) complexes under UV and red light: theoretical/experimental correlations with active species generation. Dalton Transactions, 2010, 39, 2027-2035.	3.3	28
31	Water Solvent Effect on Theoretical Evaluation of ¹H NMR Chemical Shifts: o-Methyl-Inositol Isomer. Journal of Physical Chemistry A, 2017, 121, 2839-2846.	2.5	27
32	Theoretical analysis of the oxocarbons: structure and spectroscopic properties of croconate ion and its coordination compound with lithium. Physical Chemistry Chemical Physics, 2001, 3, 3499-3505.	2.8	26
33	Theoretical analysis of the oxocarbons: The solvent and counter-ion effects on the structure and spectroscopic properties of the squarate ion. Physical Chemistry Chemical Physics, 2003, 5, 437-445.	2.8	26
34	Reaction path for the insertion reaction of SnCl2 into the Pt(SINGLE BOND)Cl bond: An ab initio study. International Journal of Quantum Chemistry, 1997, 65, 643-650.	2.0	25
35	Linear free energy relationship for 4-substituted (o-phenylenediamine)platinum(II) dichloride derivatives using quantum mechanical descriptors. Journal of Inorganic Biochemistry, 2005, 99, 575-583.	3.5	25
36	[Ag(L)NO₃] Complexes with 2-Benzoylpyridine-Derived Hydrazones: Cytotoxic Activity and Interaction with Biomolecules. ACS Omega, 2018, 3, 7027-7035.	3.5	24

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37	The electronic spectrum of Fe2+ ion in aqueous solution: A sequential Monte Carlo/quantum mechanical study. Chemical Physics Letters, 2007, 449, 144-148.	2.6	22
38	Hydrogen activation and aldehyde elimination promoted by homogeneous Ptâ€“Sn catalyst: a theoretical study. Computational and Theoretical Chemistry, 2004, 677, 133-143.	1.5	21
39	DFT Study of the Homogeneous Hydroformylation of Propene Promoted by a Heterobimetallic Ptâ€“Sn Catalyst. Organometallics, 2011, 30, 4257-4268.	2.3	21
40	Structure and Nature of the Metalâ^'Ligand Interactions in Mixed Iron(II) Phosphametallocenes. Organometallics, 2004, 23, 5308-5313.	2.3	20
41	Quantum-mechanical and molecular mechanics conformational analysis of 1,5-cyclooctadiene. Journal of Computational Chemistry, 1997, 18, 254-259.	3.3	18
42	Design, structural and spectroscopic elucidation, and the in vitro biological activities of new triorganotin dithiocarbamates â€“ Part II. Polyhedron, 2014, 79, 161-169.	2.2	18
43	Carbonyl insertion reaction into the Pt?C bond in heterobimetallic Pt(SnCl3)(PH3)2(CO)(CH3) compound: Theoretical study. Journal of Computational Chemistry, 2000, 21, 668-674.	3.3	17
44	Theoretical analysis of the oxocarbons: The role played by the solvent and counter-ions in the electronic spectrum of the deltate ion. Physical Chemistry Chemical Physics, 2002, 4, 2517-2523.	2.8	17
45	On the isomerization of Î²-pinene: a theoretical study. Computational and Theoretical Chemistry, 2001, 544, 213-220.	1.5	16
46	Phosphorane lifetime and stereo-electronic effects along the alkaline hydrolysis of phosphate esters. Physical Chemistry Chemical Physics, 2016, 18, 18255-18267.	2.8	16
47	On the origin of diastereofacial selectivity in the interaction of Î²-pinene with rhodium carbonyl: A density functional study. Computational and Theoretical Chemistry, 2007, 816, 109-117.	1.5	15
48	Quantum Mechanical/Effective Fragment Potential (QM/EFP) Study of Phosphate Monoester Aminolysis in Aqueous Solution. Journal of Physical Chemistry B, 2009, 113, 14831-14836.	2.6	15
49	Formation and Release of NO from Ruthenium Nitrosyl Ammine Complexes [Ru(NH₃)₅(NO)]^{2+/3+} in Aqueous Solution: A Theoretical Investigation. Journal of Physical Chemistry B, 2016, 120, 11821-11833.	2.6	15
50	Theoretical study of oxocarbons: structure and vibrational spectrum of the D6h and C2 forms of the rhodizonate ion. Computational and Theoretical Chemistry, 2004, 684, 141-147.	1.5	13
51	Intramolecular General Acid Catalysis of the Hydrolysis of 2-(2â€˜-Imidazolium)phenyl Phosphate, and Bond Lengthâ^'Reactivity Correlations for Reactions of Phosphate Monoester Monoanions. Journal of Organic Chemistry, 2007, 72, 3800-3807.	3.2	13
52	Insertion reaction of ethylene into the Rhâ€“H bond: A comparative theoretical study. Chemical Physics Letters, 2007, 439, 69-75.	2.6	13
53	DFT study of the full catalytic cycle for the propene hydroformylation catalyzed by a heterobimetallic HPt(SnCl₃)(PH₃)₂ model catalyst. Journal of Computational Chemistry, 2010, 31, 1986-2000.	3.3	13
54	DFT study of the ligand effects on the regioselectivity of the insertion reaction of olefins in the complexes [HRh(CO)₂(PR₃)(L)] (R = H, F, Et, Ph, OEt, OPh, and L = propene,) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.6	13

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55	Effective targeting of proton transfer at ground and excited states of ortho-(2â€²-imidazolyl)naphthol constitutional isomers. Physical Chemistry Chemical Physics, 2015, 17, 2404-2415.	2.8	13
56	Câ^'H Bond Activation of Methane Promoted by (Î·5-Phospholyl)Rh(CO)2:â€‰ A Theoretical Perspective. Organometallics, 2005, 24, 2262-2268.	2.3	12
57	Theoretical investigation of the structure and nature of the interaction in metalâ€“alkane Ïƒ-complexes of the type [M(CO)5(C2H6)] (M = Cr, Mo, and W). Chemical Physics, 2009, 365, 85-93.	1.9	12
58	An investigation of the BSSE effect on the evaluation of Ab Initio interaction energies for cisplatin-water complexes. Journal of the Brazilian Chemical Society, 2010, 21, 887-896.	0.6	12
59	QUANTUM CHEMICAL STUDY OF CISPLATIN-WATER COMPLEXES: AN INVESTIGATION OF ELECTRON CORRELATION EFFECTS. Journal of Theoretical and Computational Chemistry, 2011, 10, 371-391.	1.8	12
60	Theoretical analysis of the oxocarbons: the electronic spectrum of the rhodizonate ion. Computational and Theoretical Chemistry, 2005, 719, 31-39.	1.5	11
61	Silver(i) complexes with 2-acetylpyridinebenzoylhydrazones exhibit antimicrobial effects against yeast and filamentous fungi. New Journal of Chemistry, 2018, 42, 2125-2132.	2.8	11
62	On the cis -> trans isomerization of the square-planar [Pt(Cl)(SnCl3)(PH3)2] compound: ab initio gas phase reaction mechanism and solvent effects using continuum models. Journal of the Brazilian Chemical Society, 2000, 11, 112.	0.6	10
63	Solvation and electronic spectrum of Ni2+ ion in aqueous and ammonia solutions: A sequential Monte Carlo/TD-DFT study. Chemical Physics, 2008, 353, 66-72.	1.9	10
64	Solvation and Proton-Coupled Electron Transfer Reduction Potential of 2NOâ€¢ to 1HNO in Aqueous Solution: A Theoretical Investigation. Journal of Physical Chemistry B, 2017, 121, 6618-6625.	2.6	10
65	Theoretical studies of metal complexes of anhydrotetracycline: interaction with ZnII. Journal of the Chemical Society Dalton Transactions, 1998, , 2531-2536.	1.1	9
66	Theoretical study of spectroscopic properties of insulated molecular wires formed by substituted oligothiophenes and crossâ€linked Î±â€cyclodextrin. Journal of Polymer Science, Part B: Polymer Physics, 2011, 49, 1101-1111.	2.1	9
67	Cï£¿H bond activation of methane in aqueous solution: A hybrid quantum mechanical/effective fragment potential study. Journal of Computational Chemistry, 2011, 32, 3383-3392.	3.3	9
68	Prediction of conformational population of large cycloalkanes using ab initio correlated methods: Cycloundecane, cyclododecane, and cyclotridecane. International Journal of Quantum Chemistry, 2012, 112, 3188-3197.	2.0	9
69	Propene Hydroformylation Reaction Catalyzed by HRh(CO)(BISBI): A Thermodynamic and Kinetic Analysis of the Full Catalytic Cycle. European Journal of Inorganic Chemistry, 2020, 2020, 3907-3916.	2.0	9
70	Non-structural protein 5 (NS5) as a target for antiviral development against established and emergent flaviviruses. Current Opinion in Virology, 2021, 50, 30-39.	5.4	9
71	Regioselectivity in the interaction of rhodium hidridotricarbonyl with propene: a theoretical study. Computational and Theoretical Chemistry, 2003, 634, 95-106.	1.5	8
72	Crystal Structure and Magnetic Properties of an Oxamatoâ€Bridged Heterobimetallic Tetranuclear [Ni^{II}Cu^{II}]₂ Complex of the Rack Type. European Journal of Inorganic Chemistry, 2018, 2018, 477-484.	2.0	8

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73	Theoretical investigation of the neutral hydrolysis of diethyl 4-nitrophenyl phosphate (paraoxon) in aqueous solution. Journal of Molecular Modeling, 2018, 24, 259.	1.8	8
74	Nitric Oxide Reacts Very Fast with Hydrogen Sulfide, Alcohols, and Thiols to Produce HNO: Revised Rate Constants. Inorganic Chemistry, 2021, 60, 15997-16007.	4.0	8
75	Synthesis, Characterization and Theoretical Calculations of Novel Five Membered Rings Containing Phosphorus and Arsenic Atoms. Journal of the Brazilian Chemical Society, 2002, 13, 597-605.	0.6	7
76	Methanol dehydrogenation promoted by a heterobimetallic Ru(II)â€“Sn(II) complex as catalyst: A density functional study. Computational and Theoretical Chemistry, 2007, 816, 77-84.	1.5	7
77	Ab initio thermodynamic study of the reaction of CF2Cl2 and CHF2Cl CFCs species with OH radical. Chemical Physics Letters, 2007, 448, 164-172.	2.6	7
78	Ligand Exchange Reaction Involving Ru(III) Compounds in Aqueous Solution: A Hybrid Quantum Mechanical/Effective Fragment Potential Study. Journal of Physical Chemistry B, 2011, 115, 2030-2037.	2.6	7
79	Broken symmetry density functional study of biomimetic models for Purple Acid Phosphatases of the type Fe(III)â€“M(II) (M= Fe, Cu, Ni, Co and Mn). Computational and Theoretical Chemistry, 2012, 979, 89-95.	2.5	7
80	Influence of susceptibility to hydrolysis and hydrophobicity of arylsemicarbazones on their anti-nociceptive and anti-inflammatory activities. European Journal of Medicinal Chemistry, 2012, 50, 140-148.	5.5	7
81	Synthesis and structural characterization of a 8-hydroxyquinoline derivative coordinated to Zn(II). Journal of Molecular Structure, 2018, 1169, 119-129.	3.6	7
82	Reply to the â€˜Comment on â€œTheoretical analysis of the oxocarbons: structure and spectroscopic properties of croconate ion and its coordination compound with lithiumâ€â€™, by M. C. C. Ribeiro and A. O. Cavalcante, Phys. Chem. Chem. Phys., 2002, 4, 2917. Physical Chemistry Chemical Physics, 2002, 4, 2919-2920.	2.8	6
83	Solvent effects on the metal-to-ligand charge transfer transition of the complex [Ru(NH3)5(Pyrazine)]2+. Chemical Physics Letters, 2014, 612, 78-83.	2.6	6
84	Base Mechanism to the Hydrolysis of Phosphate Triester Promoted by the Cd²⁺/Cd²⁺ Active site of Phosphotriesterase: A Computational Study. Inorganic Chemistry, 2018, 57, 5888-5902.	4.0	6
85	Quantum mechanics/molecular mechanics investigation of the ethene polymerization mechanism catalyzed by a bulky diimine-Ni(II) complex. Journal of the Brazilian Chemical Society, 2011, 22, 428-436.	0.6	5
86	AN EVALUATION OF QUANTUM CHEMICAL CALCULATIONS OF REACTION ENERGIES FOR CATALYTIC ACTIVATION PROCESSES: THE ACTIVATION OF PROPANE BY A RHODIUM CATALYST REVISITED. Journal of Theoretical and Computational Chemistry, 2012, 11, 297-312.	1.8	5
87	ESI-MS, UV-Vis, and Theoretical Investigation of Fe3+-Amoxicillin Complexation during Coagulation. Journal of Environmental Engineering, ASCE, 2018, 144, .	1.4	5
88	Liquid tin tetrachloride: a Monte Carlo simulation study. Chemical Physics Letters, 2000, 316, 510-516.	2.6	4
89	A theoretical investigation of the activation of propane by a rhodium catalyst. Chemical Physics Letters, 2006, 430, 160-166.	2.6	4
90	Insertion and carbonylation reactions of styrene promoted by [HRh(CO)_xâ€•(PMe₃)_{3â€˜x}] (x = 1, 2) compounds: A theoretical investigation. International Journal of Quantum Chemistry, 2008, 108, 2358-2373.	2.0	4

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91	Broken symmetry density functional study of a mixedâ€valence unsymmetrical dinuclear iron complex. International Journal of Quantum Chemistry, 2010, 110, 1048-1055.	2.0	4
92	Influence of oxidation state of sulfur on the dissociation of [Tzâ€(CH₂)_nâ€S(O)_mâ€(CH₂)_nâ€Tzâ€‰+â€‰Na⁺] adducts generated by electrospray ionization (Tzâ€‰=â€‰tetrazole ring; nâ€‰=â€‰2, 3; mâ€‰=â€‰0, 1, 2). Rapid Communications in Mass Spectrometry, 2012, 26, 377-384.	1.5	4
93	Ab initio molecular dynamics simulation of aqueous solution of nitric oxide in different formal oxidation states. Chemical Physics Letters, 2015, 638, 9-14.	2.6	4
94	Theoretical Investigation of the 4,5-Dibromorodamine Methyl Ester (TH9402) Photosensitizer Used in Photodynamic Therapy: Photophysics, Reactions in the Excited State, and Interactions with DNA. Journal of Physical Chemistry B, 2021, 125, 8932-8943.	2.6	4
95	The nature of the Mâ€“NO bond in [M(Imidazole)(PPIX)(L)]q complexes (M=Fe2+, Ru2+; L=NO+, NO and) Tj ETQq1 1 0.784314 rgBT	2.4	3
96	Quantum mechanical/effective fragment potential (QM/EFP) study of phosphate diester cleavage in aqueous solution. Computational and Theoretical Chemistry, 2014, 1043, 5-12.	2.5	3
97	Insights into the coordination chemistry of alkanes to metal carbonyls from quantum chemical calculations. Journal of Organometallic Chemistry, 2015, 793, 241-247.	1.8	3
98	Reduction Potential of RuIII-Based Complexes with Potential Antitumor Activity and Thermodynamics of their Hydrolysis Reactions and Interactions with Possible Biological Targets: a Theoretical Investigation. Journal of the Brazilian Chemical Society, 0, , .	0.6	3
99	Revisiting the Tropospheric OH-Initiated Unimolecular Decomposition of Chlorpyrifos and Chlorpyrifos-Methyl: A Theoretical Perspective. Journal of Physical Chemistry A, 2020, 124, 4280-4289.	2.5	3
100	Nature of the bond, reduction potential, and solvation properties of ruthenium nitrosyl complexes of the type transâ€ [Ru(<scp>NH₃</scp>)₄(L)(<scp>NO</scp>)]^{2+/3+} and [Ru(salen)(L)(<scp>NO</scp>)]^{2+/3+} in different charge and spin states. International Journal of Quantum Chemistry, 2021, 121, e26476.	2.0	3
101	Title is missing!. Journal of Computational Chemistry, 1997, 18, 254.	3.3	3
102	Quantum-mechanical vibrational spectrum and conformational analysis for the 1,5-cyclooctadiene. Vibrational Spectroscopy, 1997, 13, 213-219.	2.2	2
103	Theoretical investigation of [Ru(bpy)2(HAT)]2+ (HATÂ=Â1,4,5,8,9,12-hexaazatriphenylene;) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Molecular and Biomolecular Spectroscopy, 2022, 270, 120817.	3.9	2
104	Dynamics and allostery of Zika virus non-structural protein 5 methyltransferase. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-13.	3.5	1
105	Electronic structure and mechanism for the uptake of nitric oxide by the Ru(<scp>iii</scp>) antitumor complex NAMI-A. RSC Advances, 2021, 11, 7381-7390.	3.6	0
106	Computational insights into the reactivity of chlorpyrifos and chlorpyrifos-methyl toward singlet oxygen. Journal of Molecular Modeling, 2021, 27, 282.	1.8	0
107	Carbonyl insertion reaction into the PtbC bond in heterobimetallic Pt(SnCl3)(PH3)2(CO)(CH3) compound: Theoretical study. Journal of Computational Chemistry, 2000, 21, 668.	3.3	0