Rodolfo GÃ³mez-Balderas

List of Publications by Year
in descending order

33 papers	654 citations	687363 13 h-index	580821 25 g-index
34 all docs	34 docs citations	34 times ranked	732 citing authors

#	Article	IF	Citations
1	Reliable Theoretical Procedures for Calculating the Rate of Methyl Radical Addition to Carbonâ^'Carbon Double and Triple Bonds. Journal of Physical Chemistry A, 2004, 108, 2874-2883.	2.5	122
2	Comparison of the Kinetics and Thermodynamics for Methyl Radical Addition to CC, CO, and CS Double Bonds. Journal of the American Chemical Society, 2004, 126, 1732-1740.	13.7	70
3	Ab initio model studies of copper binding to peptides containing a Hisâ€“His sequence: relevance to the Î²-amyloid peptide of Alzheimerâ€™s disease. Journal of Biological Inorganic Chemistry, 2005, 10, 887-902.	2.6	54
4	First-Principles Prediction of the pK_as of Anti-inflammatory Oxicams. Journal of Physical Chemistry A, 2010, 114, 11992-12003.	2.5	44
5	What Is the Origin of the Contrathermodynamic Behavior in Methyl Radical Addition to Alkynes versus Alkenes?. Journal of Physical Chemistry A, 2003, 107, 6082-6090.	2.5	43
6	Binding Affinities for Models of Biologically Available Potential Cu(II) Ligands Relevant to Alzheimer's Disease:â€‰ An ab Initio Study. Journal of Physical Chemistry A, 2005, 109, 8361-8370.	2.5	36
7	Determination of pKa values of tenoxicam from 1H NMR chemical shifts and of oxicams from electrophoretic mobilities (CZE) with the aid of programs SQUAD and HYPNMR. Talanta, 2009, 80, 754-762.	5.5	35
8	Proton affinity of S-containing aromatic compounds: Implications for crude oil hydrodesulfurization. Journal of Molecular Catalysis A, 2008, 281, 79-84.	4.8	32
9	Computational Studies of Cu(II)/Met and Cu(I)/Met Binding Motifs Relevant for the Chemistry of Alzheimer's Disease. Journal of Physical Chemistry A, 2005, 109, 5498-5508.	2.5	20
10	Theoretical analysis of hydrogen bonding in catecholâ€“n(H2O) clusters (n = 0â€¦3). Physical Chemistry Chemical Physics, 2010, 12, 4783.	2.8	19
11	[Cu(H2O) n]2+ (nÂ=Â1â€“6) complexes in solution phase: a DFT hierarchical study. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	18
12	A DFT study of the electronic structure of cobalt and nickel mono-substituted MoS2 triangular nanosized clusters. Journal of Molecular Catalysis A, 2009, 313, 49-54.	4.8	14
13	Critical micelle concentration of an ammonium salt through DPD simulations using COSMOâ€RSâ€“based interaction parameters. AICHE Journal, 2013, 59, 4413-4423.	3.6	14
14	A comparative DFT study of the catalytic activity of the 3d transition metal sulphides surfaces. Surface Science, 2002, 518, 163-173.	1.9	12
15	Effect of the pH on the thermodynamic stability of inclusion complexes of thymol and carvacrol in Î²-cyclodextrin in water. Food Hydrocolloids, 2022, 124, 107307.	10.7	12
16	Chemical Speciation of the System Cu(II)-Indomethacin in Ethanol and Water by UV-Vis Spectrophotometry. Journal of Chemistry, 2016, 2016, 1-12.	1.9	10
17	Complex formation of the anti-inflammatory drugs tenoxicam and piroxicam with Fe(III) in methanol and acetone. Journal of Coordination Chemistry, 2009, 62, 40-51.	2.2	9
18	Tautomeric Ratio and Prototropic Equilibrium Constants of Tenoxicam, a ¹H and ¹³C NMR Theoretical and Experimental Study. Journal of Physical Chemistry B, 2011, 115, 13593-13598.	2.6	9

#	Article	IF	Citations
19	Introduction to Validation of Analytical Methods: Potentiometric Determination of CO₂. Journal of Chemical Education, 2017, 94, 1303-1308.	2.3	9
20	Interaction of indomethacinâ€“cyclodextrins in water by UVâ€“Vis and ITC. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2019, 95, 55-62.	1.6	9
21	Supramolecular pairing among heteroaromatic compounds and the cationic surfactant C12TAC. Fuel, 2015, 149, 174-183.	6.4	8
22	Carbon Monoxide Activation on Small Iron Magnetic Cluster Surfaces, Fe_nCO, n = 1â€“20. A Theoretical Approach. Journal of Physical Chemistry A, 2020, 124, 9951-9962.	2.5	8
23	Critical micelle concentration of SDS through DPD simulations using COSMO-RSâ€“based interaction parameters, the thermal effects. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 645, 128867.	4.7	8
24	Antihypertensive and antiarrhythmic properties of a para-hydroxy[bis(ortho-morpholinylmethyl)]phenyl-1,4-DHP compound: Comparison with other compounds of the same kind and relationship with logP values. European Journal of Medicinal Chemistry, 2010, 45, 4622-4630.	5.5	6
25	Promotional effect of Co or Ni impurity in the catalytic activity of MoS2: An electronic structure study. International Journal of Quantum Chemistry, 2000, 80, 406-415.	2.0	5
26	UVâ€“Visible properties of oxicams in solution: A TDâ€DFT and experimental study. International Journal of Quantum Chemistry, 2012, 112, 3637-3645.	2.0	5
27	Stability constants of Cu(II)/indomethacin mononuclear complexes in solution. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	5
28	Thermodynamic study of complexation of Zn(II)/L (Lâ^'â€‰=â€‰acetate, indomethacin and diclofenac anions) by isothermal titration calorimetry. Journal of Thermal Analysis and Calorimetry, 2019, 136, 1701-1709.	3.6	5
29	Stability constants of Cu(II)-piroxicam complexes in solution: a DFT study. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	4
30	Chemical Equilibrium of Zinc Acetate Complexes in Ethanol Solution. A Theoretical Description through Thermodynamic Cycles. Journal of Physical Chemistry B, 2020, 124, 3355-3370.	2.6	3
31	Small Transition-Metal Mixed Clusters as Activators of the Câ€“O Bond. Fe_nCu_mâ€“CO (n + m = 6): A Theoretical Approach. Journal of Physical Chemistry A, 2021, 125, 7940-7955.	2.5	3
32	Thermodynamics of inclusion within cyclodextrins and structural evidence of Cu(indomethacin)₂ and Zn(indomethacin)₂ complexes in aqueous solutions. New Journal of Chemistry, 2020, 44, 20222-20234.	2.8	2
33	Stability constants and molecular modeling of Cu(II)/AcO and Cu(II)/diclofenac complexes in ethanol. Polyhedron, 2021, 209, 115486.	2.2	0