Antonio Hidalgo

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Experimental Design and Optimization of a Novel Dual-release Drug Delivery System With Therapeutic Potential Against Infection With Helicobacter pylori. Colloids and Surfaces B: Biointerfaces, 2022, 213, 112403.	5.0	2
2	[Translated article] Spanish Asthma Management Guidelines (GEMA) v.5.1. Highlights and Controversies. Archivos De Bronconeumologia, 2022, 58, T150-T158.	0.8	7
3	Mechanisms of the T-A to C-G transition studied by SMD simulations: Deamination vs tautomerisation. Journal of Molecular Liquids, 2020, 308, 113036.	4.9	6
4	A procedure to understanding the C-G to A-T transversion. SMD simulations from guanine oxidation pathways assisted by one H2O2 molecule in the C-G basis pair. Journal of Molecular Liquids, 2020, 319, 114123.	4.9	0
5	Theoretical Study of Adenine to Guanine Transition Assisted by Water and Formic Acid Using Steered Molecular Dynamic Simulations. Frontiers in Chemistry, 2019, 7, 414.	3.6	9
6	Photocatalysis in an external four-lamp reactor: modelling and validation—dichloroacetic acid photo-oxidation in the presence of TiO2. International Journal of Environmental Science and Technology, 2019, 16, 6705-6716.	3.5	5
7	Structural and thermodynamic studies of cytosine to thymine conversion in gas and solution phases using steered molecular dynamic simulations. Journal of Molecular Liquids, 2019, 278, 61-69.	4.9	9
8	Mechanisms for guanine–cytosine tautomeric equilibrium in solution via steered molecular dynamic simulations. Journal of Molecular Liquids, 2018, 251, 308-316.	4.9	18
9	Neuroprotective effect of a new variant of Epo nonhematopoietic against oxidative stress. Redox Biology, 2018, 14, 285-294.	9.0	23
10	Theoretical study of mechanisms for the hydrolytic deamination of cytosine <i>via</i> steered molecular dynamic simulations. RSC Advances, 2018, 8, 34867-34876.	3.6	5
11	Theoretical study of mechanisms for double proton transfer in adenine–uracil base pair via steered molecular dynamic simulations. Journal of Molecular Liquids, 2018, 265, 487-495.	4.9	4
12	Steered molecular dynamic simulations of the tautomeric equilibria in solution of DNA bases. Journal of Molecular Liquids, 2017, 237, 81-88.	4.9	16
13	A New Malleostapedotomy Prosthesis. Experimental Analysis by Laser Doppler Vibrometer in Fresh Cadaver Temporal Bones. Acta Otorrinolaringologica (English Edition), 2017, 68, 69-79.	0.2	0
14	Theoretical thermodynamic study of the adenine-thymine tautomeric equilibrium: Electronic structure calculations and steered molecular dynamic simulations. International Journal of Quantum Chemistry, 2017, 117, e25429.	2.0	17
15	Theoretical determination of aqueous acid–base pK values: electronic structure calculations and steered molecular dynamic simulations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	9
16	Theoretical study of enzymatically catalyzed tautomerization of carbon acids in aqueous solution: quantum calculations and steered molecular dynamics simulations. Journal of Molecular Modeling, 2016, 22, 44.	1.8	3
17	A computational model of the glycine tautomerization reaction in aqueous solution. Journal of Molecular Modeling, 2014, 20, 2147.	1.8	4
18	Amide-imide tautomerism of acetohydroxamic acid in aqueous solution: quantum calculation and SMD simulations. RSC Advances, 2014, 4, 44757-44768.	3.6	21

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19	Thermodynamic Study of Hydrolysis Reactions in Aqueous Solution fromAb InitioPotential and Molecular Dynamics Simulations. Journal of Chemistry, 2013, 2013, 1-8.	1.9	1
20	Amino Acid Tautomerization Reactions in Aqueous Solution via Concerted and Assisted Mechanisms Using Free Energy Curves from MD Simulation. Journal of Physical Chemistry B, 2012, 116, 13033-13044.	2.6	11
21	Theoretical study of the neutral hydrolysis of methyl formate via a concerted and stepwise water-assisted mechanism using free-energy curves and molecular dynamics simulation. Structural Chemistry, 2011, 22, 909-915.	2.0	9
22	Molecular dynamics study of formamidine decomposition in gas and solution phases via free energy curves from ab initio interaction potentials. Theoretical Chemistry Accounts, 2010, 127, 671-679.	1.4	7
23	Is the middle ear the first filter of frequency selectivity?. Acta Otorrinolaringologica (English) Tj ETQq1 1 0.78431	4 rgBT /O	verjock 10 Tf
24	Theoretical Study of the Neutral Hydrolysis of Hydrogen Isocyanate in Aqueous Solution via Assisted-Concerted Mechanisms. Journal of Physical Chemistry A, 2009, 113, 1858-1863.	2.5	15
25	Calculation of free-energy curves for the study of hydrolysis reactions in aqueous solution from ab initio potentials and molecular dynamics simulation. Chemical Physics, 2008, 353, 73-78.	1.9	14
26	Molecular Simulation of the Hydration of Ethene to Ethanol Using Ab Initio Potentials and Free Energy Curves. Journal of Physical Chemistry A, 2007, 111, 13515-13520.	2.5	10
27	Molecular Dynamics Simulation of the Reaction of Hydration of Formaldehyde Using a Potential Based on Soluteâ^'Solvent Interaction Energy Components. Journal of Physical Chemistry A, 2007, 111, 339-344.	2.5	20
28	Molecular dynamics simulation of acetamide solvation using interaction energy components: Application to structural and energy properties. Chemical Physics, 2006, 327, 187-192.	1.9	13
29	Theoretical–experimental study of the solvation enthalpy of acetone in dilute aqueous solution. Chemical Physics, 2005, 315, 76-80.	1.9	12
30	Molecular Dynamics Simulation of Aqueous Solutions Using Interaction Energy Components: Application to the Solvation Gibbs Energy. Journal of Solution Chemistry, 2005, 34, 407-414.	1.2	12
31	Molecular dynamics simulation of aqueous solutions using interaction energy components: Application to the dielectric properties of the acetone–water system. Molecular Simulation, 2005, 31, 549-553.	2.0	5
32	Accuracy of high-resolution CT in distinguishing between Pneumocystis carinii pneumonia and non-Pneumocystis carinii pneumonia in AIDS patients. European Radiology, 2003, 13, 1179-1184.	4.5	94
33	Thermodynamic and dielectric properties of aqueous solutions using ESIE charges to describe small solutes. Chemical Physics, 2003, 293, 193-202.	1.9	11
34	Relation between alcohol consumption and the success of Helicobacter pylori eradication therapy using omeprazole, clarithromycin and amoxicillin for 1 week. European Journal of Gastroenterology and Hepatology, 2002, 14, 291-296.	1.6	36
35	The N–Hâ<¯Oĩ~C proton transfer in aqueous solution: a suitable procedure for extracting atomic charges. Chemical Physics Letters, 2002, 357, 279-286.	2.6	15
36	Study of the N–H⋯Or̃…C proton transfer reaction in aqueous solution using classical free energy curves. Chemical Physics, 2001, 265, 207-215.	1.9	4

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37	Thermodynamic, structural, and dynamic study of the N–H⋯Oĩ~C hydrogen bond association in aqueous solution. Chemical Physics, 2000, 255, 73-84.	1.9	12
38	Title is missing!. Journal of Solution Chemistry, 1999, 28, 1087-1106.	1.2	6
39	Quiz case I. European Journal of Radiology, 1998, 27, 250-253.	2.6	6
40	Nonequilibrium Solvation: The Mutual Influence of Solute and Solvent Dynamics. The Journal of Physical Chemistry, 1995, 99, 4293-4305.	2.9	5
41	Self-consistent-field calculation of vibrational bound states for triatomic molecules using transformed Jacobi coordinates. The Journal of Physical Chemistry, 1991, 95, 2292-2297.	2.9	17
42	Variational calculation of vibrational energies of triatomic molecules usingSCFoptimized modes. International Journal of Quantum Chemistry, 1991, 40, 685-694.	2.0	14
43	Energy eigenvalues for Lennard-Jones potentials using the hypervirial perturbative method. Journal of Physics B: Atomic, Molecular and Optical Physics, 1990, 23, 2771-2781.	1.5	11
44	Two enter matrix elements for Kratzer oscillators. Journal of Chemical Physics, 1990, 93, 3408-3412.	3.0	15
45	Perturbative virtualSCF CItreatment for energy levels of coupled oscillator systems. International Journal of Quantum Chemistry, 1989, 36, 49-60.	2.0	2
46	SCF calculations of excited vibrational energy levels for normal modes. Computational and Theoretical Chemistry, 1988, 166, 339-344.	1.5	0
47	Perturbative multi-step adiabatic treatment for energy levels of multidimensional coupled systems. Computational and Theoretical Chemistry, 1988, 166, 345-350.	1.5	0
48	Variational HEG calculation of vibration rotation transition moments for diatomic molecules Computational and Theoretical Chemistry, 1988, 166, 351-356.	1.5	0
49	Perturbed Morse expansion for triatomic molecules. Computational and Theoretical Chemistry, 1988, 166, 357-362.	1.5	1
50	Analytical expressions for vibrational matrix elements of Morse oscillators. Physical Review A, 1988, 38, 4205-4212.	2.5	9
51	Perturbative calculation of energy levels for coupled oscillators using the adiabatic approximation. Molecular Physics, 1987, 61, 1513-1518.	1.7	1
52	HypervirialSCFtreatment for vibrational energy levels of triatomic molecules. International Journal of Quantum Chemistry, 1987, 32, 511-516.	2.0	2
53	Perturbative calculation of vibrational energy levels for local modes. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1987, 84, 725-728.	0.2	0
54	Rovibrational energy levels and expectation values for perturbed Kratzer oscillators. Journal of Chemical Physics, 1986, 85, 3939-3944.	3.0	18

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55	Determination of the degree of branching in polyethylene by an i.r. method of decomposition of bands. Spectrochimica Acta Part A: Molecular Spectroscopy, 1979, 35, 847-849.	0.1	21
56	An i.r. study of the "amorphous―phase in melt crystallized polyethylene. Spectrochimica Acta Part A: Molecular Spectroscopy, 1978, 34, 475-480.	0.1	14
57	Correlation of crystal thickness and absorption coefficient of the doublet at 720–730 cm1 in polyethylene. Journal of Polymer Science, Polymer Physics Edition, 1977, 15, 2027-2031.	1.0	11