Antonio Hidalgo

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	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
3	Neuroprotective effect of a new variant of Epo nonhematopoietic against oxidative stress. Redox Biology, 2018, 14, 285-294.	9.0	23
4	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
5	Amide-imide tautomerism of acetohydroxamic acid in aqueous solution: quantum calculation and SMD simulations. RSC Advances, 2014, 4, 44757-44768.	3.6	21
6	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
7	Rovibrational energy levels and expectation values for perturbed Kratzer oscillators. Journal of Chemical Physics, 1986, 85, 3939-3944.	3.0	18
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	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
10	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
11	Steered molecular dynamic simulations of the tautomeric equilibria in solution of DNA bases. Journal of Molecular Liquids, 2017, 237, 81-88.	4.9	16
12	Twoâ€center matrix elements for Kratzer oscillators. Journal of Chemical Physics, 1990, 93, 3408-3412.	3.0	15
13	The N–Hâ√OĩC proton transfer in aqueous solution: a suitable procedure for extracting atomic charges. Chemical Physics Letters, 2002, 357, 279-286.	2.6	15
14	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
15	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
16	Variational calculation of vibrational energies of triatomic molecules usingSCFoptimized modes. International Journal of Quantum Chemistry, 1991, 40, 685-694.	2.0	14
17	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
18	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

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19	Thermodynamic, structural, and dynamic study of the N–Hâ⊄Oĩ"C hydrogen bond association in aqueous solution. Chemical Physics, 2000, 255, 73-84.	1.9	12
20	Theoretical–experimental study of the solvation enthalpy of acetone in dilute aqueous solution. Chemical Physics, 2005, 315, 76-80.	1.9	12
21	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
22	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
23	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
24	Thermodynamic and dielectric properties of aqueous solutions using ESIE charges to describe small solutes. Chemical Physics, 2003, 293, 193-202.	1.9	11
25	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
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	Analytical expressions for vibrational matrix elements of Morse oscillators. Physical Review A, 1988, 38, 4205-4212.	2.5	9
28	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
29	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
30	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
31	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
32	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
33	[Translated article] Spanish Asthma Management Guidelines (GEMA) v.5.1. Highlights and Controversies. Archivos De Bronconeumologia, 2022, 58, T150-T158.	0.8	7
34	Quiz case I. European Journal of Radiology, 1998, 27, 250-253.	2.6	6
35	Title is missing!. Journal of Solution Chemistry, 1999, 28, 1087-1106.	1.2	6
36	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

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37	Nonequilibrium Solvation: The Mutual Influence of Solute and Solvent Dynamics. The Journal of Physical Chemistry, 1995, 99, 4293-4305.	2.9	5
38	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
39	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
40	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
41	Study of the N–Hâ√OĩC proton transfer reaction in aqueous solution using classical free energy curves. Chemical Physics, 2001, 265, 207-215.	1.9	4
42	A computational model of the glycine tautomerization reaction in aqueous solution. Journal of Molecular Modeling, 2014, 20, 2147.	1.8	4
43	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
44	Is the middle ear the first filter of frequency selectivity?. Acta Otorrinolaringologica (English) Tj ETQq0 0 0 rgBT	/Overlock	10 Tf 50 462
45	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
46	HypervirialSCFtreatment for vibrational energy levels of triatomic molecules. International Journal of Quantum Chemistry, 1987, 32, 511-516.	2.0	2
47	Perturbative virtualSCF CItreatment for energy levels of coupled oscillator systems. International Journal of Quantum Chemistry, 1989, 36, 49-60.	2.0	2
48	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
49	Perturbative calculation of energy levels for coupled oscillators using the adiabatic approximation. Molecular Physics, 1987, 61, 1513-1518.	1.7	1
50	Perturbed Morse expansion for triatomic molecules. Computational and Theoretical Chemistry, 1988, 166, 357-362.	1.5	1
51	Thermodynamic Study of Hydrolysis Reactions in Aqueous Solution fromAb InitioPotential and Molecular Dynamics Simulations. Journal of Chemistry, 2013, 2013, 1-8.	1.9	1
52	SCF calculations of excited vibrational energy levels for normal modes. Computational and Theoretical Chemistry, 1988, 166, 339-344.	1.5	0
53	Perturbative multi-step adiabatic treatment for energy levels of multidimensional coupled systems. Computational and Theoretical Chemistry, 1988, 166, 345-350.	1.5	0
54	Variational HEG calculation of vibration rotation transition moments for diatomic molecules Computational and Theoretical Chemistry, 1988, 166, 351-356.	1.5	0

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55	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
56	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
57	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