Josefredo R Pliego

List of Publications by Year
in descending order

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114 papers	3,490 citations	147566 31 h-index	155451 55 g-index
114 all docs	114 docs citations	114 times ranked	2912 citing authors

#	Article	IF	Citations
1	The Clusterâ^'Continuum Model for the Calculation of the Solvation Free Energy of Ionic Species. Journal of Physical Chemistry A, 2001, 105, 7241-7247.	1.1	408
2	Theoretical Calculation of pKaUsing the Clusterâ^'Continuum Model. Journal of Physical Chemistry A, 2002, 106, 7434-7439.	1.1	323
3	Gibbs energy of solvation of organic ions in aqueous and dimethyl sulfoxide solutions. Physical Chemistry Chemical Physics, 2002, 4, 1622-1627.	1.3	195
4	Thermodynamic cycles and the calculation of pKa. Chemical Physics Letters, 2003, 367, 145-149.	1.2	165
5	Ionization of Organic Acids in Dimethyl Sulfoxide Solution:â€‰ A Theoretical Ab Initio Calculation of the pKa Using a New Parametrization of the Polarizable Continuum Model. Journal of Physical Chemistry A, 2004, 108, 166-171.	1.1	121
6	New values for the absolute solvation free energy of univalent ions in aqueous solution. Chemical Physics Letters, 2000, 332, 597-602.	1.2	116
7	Mechanism of the Piperidine-Catalyzed Knoevenagel Condensation Reaction in Methanol: The Role of Iminium and Enolate Ions. Journal of Physical Chemistry B, 2017, 121, 5300-5307.	1.2	76
8	Parametrization of the PCM model for calculating solvation free energy of anions in dimethyl sulfoxide solutions. Chemical Physics Letters, 2002, 355, 543-546.	1.2	68
9	Hybrid discreteâ€“continuum solvation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1440.	6.2	65
10	Absolute solvation free energy of Li+ and Na+ ions in dimethyl sulfoxide solution: A theoretical ab initio and cluster-continuum model study. Journal of Chemical Physics, 2005, 123, 074508.	1.2	64
11	Ab initio study of the hydroxide ionâ€“water clusters: An accurate determination of the thermodynamic properties for the processes nH2O+OHâ^'â†'HOâ^'(H2O)n (n=1â€“4). Journal of Chemical Physics, 2000, 112, 4045-4052.	1.2	60
12	A Theoretical Analysis of the Free-Energy Profile of the Different Pathways in the Alkaline Hydrolysis of Methyl Formate In Aqueous Solution. Chemistry - A European Journal, 2002, 8, 1945.	1.7	59
13	Basic hydrolysis of formamide in aqueous solution: a reliable theoretical calculation of the activation free energy using the cluster-continuum model. Chemical Physics, 2004, 306, 273-280.	0.9	59
14	Absolute Single-Ion Solvation Free Energy Scale in Methanol Determined by the Lithium Cluster-Continuum Approach. Journal of Physical Chemistry B, 2013, 117, 5129-5135.	1.2	54
15	Cluster-continuum quasichemical theory calculation of the lithium ion solvation in water, acetonitrile and dimethyl sulfoxide: an absolute single-ion solvation free energy scale. Physical Chemistry Chemical Physics, 2015, 17, 26745-26755.	1.3	54
16	On the Calculation of the Absolute Solvation Free Energy of Ionic Species:Â Application of the Extrapolation Method to the Hydroxide Ion in Aqueous Solution. Journal of Physical Chemistry B, 2000, 104, 5155-5160.	1.2	51
17	Reaction Paths for Aqueous Decomposition of CCl2. The Journal of Physical Chemistry, 1996, 100, 12410-12413.	2.9	46
18	Singletâ^'Triplet Gap, and the Electronic and Vibrational Spectra of Chlorophenylcarbene:Â A Combined Theoretical and Experimental Study. Journal of Physical Chemistry A, 1999, 103, 7481-7486.	1.1	46

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19	Revisiting the Mechanism of Neutral Hydrolysis of Esters: Water Autoionization Mechanisms with Acid or Base Initiation Pathways. Journal of Physical Chemistry B, 2013, 117, 6487-6497.	1.2	46
20	Intramolecular Catalysis of Phosphodiester Hydrolysis by Two Imidazoles. Journal of the American Chemical Society, 2010, 132, 8513-8523.	6.6	45
21	First Solvation Shell Effects on Ionic Chemical Reactions: New Insights for Supramolecular Catalysis. Journal of Physical Chemistry B, 2009, 113, 505-510.	1.2	42
22	Effects of ion-pairing and hydration on the SNAr reaction of the F^{â˜}with p-chlorobenzonitrile in aprotic solvents. Physical Chemistry Chemical Physics, 2008, 10, 1118-1124.	1.3	41
23	A New Mechanism for the Reaction of Carbenes with OH Groups. Journal of Physical Chemistry A, 1999, 103, 3904-3909.	1.1	40
24	Chemisorption of SO2 on graphite surface: A theoretical ab initio and ideal lattice gas model study. Chemical Physics, 2005, 314, 127-133.	0.9	40
25	Theoretical Prediction of pK_a in Methanol: Testing SM8 and SMD Models for Carboxylic Acids, Phenols, and Amines. Journal of Physical Chemistry B, 2014, 118, 5730-5739.	1.2	40
26	Unraveling the Mechanism of the Cinchoninium Ion Asymmetric Phase-Transfer-Catalyzed Alkylation Reaction. ACS Catalysis, 2013, 3, 613-616.	5.5	39
27	Chemoselective Nucleophilic Fluorination Induced by Selective Solvation of the SN2 Transition State. Journal of Physical Chemistry B, 2007, 111, 1752-1758.	1.2	38
28	Revisiting the reactions of nucleophiles with arenediazonium ions: dediazoniation of arenediazonium salts in aqueous and micellar solutions containing alkyl sulfates and alkanesulfonates and an ab initio analysis of the reaction pathway. Perkin Transactions II RSC, 2000, , 1896-1907.	1.1	35
29	Design of an organocatalyst for ionâ€“molecule SN2 reactions: A new solvent effect on the reaction rate predicted by ab initio calculations. Journal of Molecular Catalysis A, 2005, 239, 228-234.	4.8	34
30	New insights on reaction pathway selectivity promoted by crown ether phase-transfer catalysis: Model ab initio calculations of nucleophilic fluorination. Journal of Molecular Catalysis A, 2012, 363-364, 489-494.	4.8	34
31	Ab initio conformational analysis of cyclooctane molecule. Journal of Computational Chemistry, 1998, 19, 524-534.	1.5	33
32	Modeling Protic to Dipolar Aprotic Solvent Rate Acceleration and Leaving Group Effects in SN2 Reactions:â€‰ A Theoretical Study of the Reaction of Acetate Ion with Ethyl Halides in Aqueous and Dimethyl Sulfoxide Solutions. Journal of Physical Chemistry A, 2005, 109, 507-511.	1.1	32
33	Amphiphilic niobium oxyhydroxide as a hybrid catalyst for sulfur removal from fuel in a biphasic system. Applied Catalysis B: Environmental, 2014, 147, 43-48.	10.8	28
34	Theoretical Design and Calculation of a Crown Ether Phase-Transfer-Catalyst Scaffold for Nucleophilic Fluorination Merging Two Catalytic Concepts. Journal of Organic Chemistry, 2016, 81, 8455-8463.	1.7	28
35	Ab Initio Study of the SN2 and E2 Mechanisms in the Reaction between the Cyanide Ion and Ethyl Chloride in Dimethyl Sulfoxide Solution. Organic Letters, 2005, 7, 1821-1823.	2.4	27
36	CMIRS Solvation Model for Methanol: Parametrization, Testing, and Comparison with SMD, SM8, and COSMO-RS. Journal of Physical Chemistry B, 2016, 120, 12660-12668.	1.2	24

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37	Performance of the SMD and SM8 models for predicting solvation free energy of neutral solutes in methanol, dimethyl sulfoxide and acetonitrile. Journal of Computer-Aided Molecular Design, 2015, 29, 217-224.	1.3	23
38	Mechanism and free energy profile of base-catalyzed Knoevenagel condensation reaction. RSC Advances, 2016, 6, 57803-57810.	1.7	23
39	Reply to comment on: â€˜Thermodynamic cycles and the calculation of pKaâ€™ [Chem. Phys. Lett. 367 (2003) 145]. Chemical Physics Letters, 2003, 381, 246-247.	1.2	21
40	Ab Initio, Density Functional Theory, and Continuum Solvation Model Prediction of the Product Ratio in the SN2 Reaction of NO2-with CH3CH2Cl and CH3CH2Br in DMSO Solution. Journal of Physical Chemistry A, 2007, 111, 10068-10074.	1.1	21
41	Ab initio investigation of the kinetics and mechanism of the neutral hydrolysis of formamide in aqueous solution. Journal of the Brazilian Chemical Society, 2007, 18, 469-702.	0.6	21
42	Rate acceleration of SN2 reactions through selective solvation of the transition state. Chemical Physics Letters, 2006, 423, 459-462.	1.2	20
43	Dynamical Discrete/Continuum Linear Response Shells Theory of Solvation: Convergence Test for NH₄⁺ and OH^{â˜’} Ions in Water Solution Using DFT and DFTB Methods. Journal of Physical Chemistry B, 2010, 114, 15941-15947.	1.2	20
44	Nucleophilic Fluorination with KF Catalyzed by 18-Crown-6 and Bulky Diols: A Theoretical and Experimental Study. Journal of Organic Chemistry, 2020, 85, 15457-15465.	1.7	20
45	Theoretical free energy profile and benchmarking of functionals for amino-thiourea organocatalyzed nitro-Michael addition reaction. Physical Chemistry Chemical Physics, 2020, 22, 11529-11536.	1.3	20
46	The role of intermolecular forces in ionic reactions: the solvent effect, ion-pairing, aggregates and structured environment. Organic and Biomolecular Chemistry, 2021, 19, 1900-1914.	1.5	20
47	Absolute proton affinity and basicity of the carbenes CH2, CF2, CCl2, C(OH)2, FCOH, CPh2 and fluorenylidene. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 1881-1883.	1.7	19
48	Chemical reactions inside structured nano-environment: SN2vs. E2 reactions for the F^{â˜’}+ CH3CH2Cl system. Physical Chemistry Chemical Physics, 2011, 13, 779-782.	1.3	19
49	A comprehensive theoretical investigation of the transition states and a proposed kinetic model for the cinchoninium ion asymmetric phase-transfer catalyzed alkylation reaction. Journal of Molecular Catalysis A, 2016, 417, 192-199.	4.8	19
50	Potassium fluoride activation for the nucleophilic fluorination reaction using 18-crown-6, [2.2.2]-cryptand, pentaethylene glycol and comparison with the new hydro-crown scaffold: a theoretical analysis. Organic and Biomolecular Chemistry, 2018, 16, 3127-3137.	1.5	19
51	Theoretical Study of the Gas-Phase Reaction of Fluoride and Chloride Ions with Methyl Formate. Journal of Physical Chemistry A, 2002, 106, 371-378.	1.1	18
52	Free Energy Profile of the Reaction between the Hydroxide Ion and Ethyl Acetate in Aqueous and Dimethyl Sulfoxide Solutions:Â A Theoretical Analysis of the Changes Induced by the Solvent on the Different Reaction Pathways. Journal of Physical Chemistry A, 2004, 108, 2520-2526.	1.1	18
53	Prediction of the pH-rate profile for dimethyl sulfide oxidation by hydrogen peroxide: The role of elusive H₃ O₂ ⁺ Ion. International Journal of Quantum Chemistry, 2014, 114, 501-507.	1.0	18
54	How Accurate is the SMD Model for Predicting Free Energy Barriers for Nucleophilic Substitution Reactions in Polar Protic and Dipolar Aprotic Solvents?. Journal of the Brazilian Chemical Society, 2016, , .	0.6	18

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55	Shells theory of solvation and the long-range Born correction. Theoretical Chemistry Accounts, 2011, 128, 275-283.	0.5	17
56	Molecular dynamics and cluster-continuum insights on bulk alcohols effects on S N 2 reactions of potassium and cesium fluorides with alkyl halides. Journal of Molecular Liquids, 2017, 237, 157-163.	2.3	17
57	Theoretical design of new macrocycles for nucleophilic fluorination with KF: thiourea-crown-ether is predicted to overcome [2.2.2]-cryptand. Molecular Systems Design and Engineering, 2020, 5, 1513-1523.	1.7	16
58	Ligand exchange ionâ€“molecule reactions of simple silyl and germyl cations. International Journal of Mass Spectrometry, 2003, 228, 551-562.	0.7	15
59	Regioselective organocatalysis: a theoretical prediction of the selective rate acceleration of the SN2 reaction between an acetate ion and primary alkyl chlorides in DMSO solution. Organic and Biomolecular Chemistry, 2006, 4, 1667.	1.5	15
60	Stability of hydroxylamine isomers in aqueous solution: Ab initio study using continuum, cluster-continuum and Shells Theory of Solvation. Chemical Physics Letters, 2011, 518, 61-64.	1.2	15
61	Reactivity and stability of ion pairs, dimers and tetramers versus solvent polarity: SNAr fluorination of 2-bromobenzonitrile with tetramethylammonium fluoride. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	15
62	Searching for the ylide structure. An ab initio study of the H2Oâ€¦CCl2 complex. Chemical Physics Letters, 1996, 249, 136-140.	1.2	14
63	Acid-catalyzed transesterification and esterification in methanol: a theoretical cluster-continuum investigation of the mechanisms and free energy barriers. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	14
64	Theoretical and experimental investigation of the formation of E- and Z-Aldimines from the reaction of methylamine with acetaldehyde. Journal of the Brazilian Chemical Society, 1999, 10, 381.	0.6	13
65	Theoretical study of the mechanism and regioselectivity of the alkylation reaction of the phenoxide ion in polar protic and aprotic solvents. Computational and Theoretical Chemistry, 2018, 1138, 117-122.	1.1	13
66	Second harmonic generation in pyrazoline derivatives of dibenzylideneacetones and chalcone: A combined experimental and theoretical approach. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 388, 112147.	2.0	13
67	A theoretical study of the HCHO+CCl2 reaction: Cycloaddition or ylide formation?. Journal of Chemical Physics, 1997, 106, 3582-3586.	1.2	12
68	Micro-solvation and counter ion effects on ionic reactions: Activation of potassium fluoride with 18-crown-6 and tert-butanol in aprotic solvents. Journal of Molecular Liquids, 2020, 319, 114211.	2.3	12
69	Bifunctional Primary Aminoâ€thiourea Asymmetric Catalysis: The Imineâ€iminium Ion Mechanism in the Michael Addition of Nitromethane to Enone. Asian Journal of Organic Chemistry, 2021, 10, 1472-1485.	1.3	12
70	Kinetics of the H2O+CCl2 reaction in gas phase and in solution by an insertion mechanism. Chemical Physics Letters, 1998, 285, 121-126.	1.2	11
71	The role of ammonia oxide in the reaction of hydroxylamine with carboxylic esters. Organic and Biomolecular Chemistry, 2015, 13, 6217-6224.	1.5	11
72	Cluster expansion of the solvation free energy difference: Systematic improvements in the solvation of single ions. Journal of Chemical Physics, 2017, 147, 034104.	1.2	11

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73	Mechanism of nucleophilic fluorination promoted by bisâ€tertâ€alcoholâ€functionalized crownâ€6â€calix[4]arene. International Journal of Quantum Chemistry, 2018, 118, e25648.	1.0	10
74	How difficult are anion-molecule SNAr reactions of unactivated arenes in the gas phase, dimethyl sulfoxide, and methanol solvents?. Structural Chemistry, 2019, 30, 75-83.	1.0	10
75	The role of carboxylic acid impurity in the mechanism of the formation of aldimines in aprotic solvents. Computational and Theoretical Chemistry, 2020, 1191, 113053.	1.1	10
76	Quantum and classical two-dimensional analysis of rainbow structures in the Xe+CO2rotational excitation at 0.2 eV collision energy and on a repulsive potential. Physical Review A, 1995, 52, 342-349.	1.0	9
77	Jacobsenâ€™s Catalyst Interaction with Polydimethylsiloxane/Tetraethoxysilane Network and Solvent Molecules: Theoretical Design of a New Polymeric Membrane. Journal of Physical Chemistry C, 2008, 112, 14830-14834.	1.5	9
78	Infinite dilution activity coefficient from SMD calculations: accuracy and performance for predicting liquid-liquid equilibria. Journal of Molecular Modeling, 2018, 24, 56.	0.8	9
79	Single-ion solvation free energy: A new clusterâ€“continuum approach based on the cluster expansion method. Physical Chemistry Chemical Physics, 2021, 23, 26902-26910.	1.3	9
80	Analysis of state-to-state differential cross sections in two-dimensional Xe-CO2scattering with long-range effects. Physical Review A, 1996, 54, 2091-2098.	1.0	8
81	Free radical mechanism of the Cl2 addition to acetylene. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2895-2900.	1.7	8
82	Free Energy Profile of a Model Palladium Catalyzed Fluorination of Aryl Bromide with Cesium Fluoride. Journal of Physical Chemistry A, 2019, 123, 9850-9856.	1.1	8
83	Reaction of CCl2 with CH2NH and the formation of dipolar and biradical ylide structures. Journal of the Chemical Society Perkin Transactions II, 1997, , 2365-2370.	0.9	7
84	Thermodynamics of Ylide Formation from Carbenes and Carbonyl Compounds. Journal of the Brazilian Chemical Society, 1998, 9, 181-186.	0.6	7
85	A theoretical ab initio and Monte Carlo simulation study of the pyridine+CCl2 reaction kinetics in the gas phase and in carbon tetrachloride solution using canonical flexible transition state theory. Physical Chemistry Chemical Physics, 1999, 1, 1031-1036.	1.3	7
86	Modelos contÃnuos do solvente: fundamentos. Quimica Nova, 2006, 29, 535-542.	0.3	7
87	On the mechanism of the reaction between aryl acetates and hydroxylamine. Arkivoc, 2007, 2007, 199-214.	0.3	7
88	Car-Parrinello molecular dynamics study of CuF, AgF, CuPF6 and AgPF6 in acetonitrile solvent and Cluster-Continuum calculation of the solvation free energy of Cu(I), Ag(I) and Li(I). Journal of Molecular Liquids, 2022, 359, 119368.	2.3	7
89	A comparison of state-to-state rotational total cross sections using two- and three-dimensional close coupled approaches. Chemical Physics Letters, 1996, 251, 346-352.	1.2	6
90	Ab initio study of the Cl+H2S atmospheric reaction: is there a breakdown of the transition state theory?. Molecular Physics, 2008, 106, 841-848.	0.8	6

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91	Fast Screening of Solvents for Simultaneous Extraction of Furfural, 5-Hydroxymethylfurfural and Levulinic Acid from Aqueous Solution Using SMD Solvation Free Energies. Journal of the Brazilian Chemical Society, 0, , .	0.6	6
92	Cleaving paraoxon with hydroxylamine: Ammonium oxide isomer favors a Frontside attack mechanism. Journal of Physical Organic Chemistry, 2019, 32, e3866.	0.9	6
93	Synthesis and characterization of 1,3,5-triarylpyrazol-4-ols and 3,5-diarylisoxazol-4-ols from chalcones and theoretical studies of the stability of pyrazol-4-ol toward acid dehydration. Journal of Molecular Structure, 2020, 1204, 127536.	1.8	6
94	Hydroperoxo on the Niobium Oxyhydroxide Surface as the Active Species in the Catalyzed Oxidation of Organic Sulfide by Hydrogen Peroxide. Journal of Physical Chemistry C, 2020, 124, 9369-9375.	1.5	5
95	Free energy profile and microkinetic modeling of base-catalyzed conjugate addition reaction of nitroalkanes to Î±,Î²-unsaturated ketones in polar and apolar solvents. Journal of Molecular Modeling, 2018, 24, 152.	0.8	4
96	Counterâ€ion and solvent effects in the Câ€•and Oâ€alkylation of the phenoxide ion with allyl chloride. Journal of Physical Organic Chemistry, 2019, 32, e3947.	0.9	4
97	Mechanisms of the formation of imines in aqueous solution and the effect of the pH: a theoretical analysis. Arkivoc, 2020, 2020, 34-52.	0.3	4
98	SN2 versus E2 reactions in a complex microsolvated environment: theoretical analysis of the equilibrium and activation steps of a nucleophilic fluorination. Journal of Molecular Modeling, 2022, 28, .	0.8	4
99	Electronic spectra of the nitrile ylides: an ab initio multiconfigurational second-order quasidegenerate perturbation theory study. Chemical Physics Letters, 2000, 318, 142-148.	1.2	3
100	Dual bifunctional catalysis and the Î±-effect in the reaction of hydroxylamine with phenylacetate. Journal of the Brazilian Chemical Society, 2011, 22, 2165-2170.	0.6	3
101	Prediction of Phase Separation Using a Modified Regular Solution Theory and the SMD Continuum Solvation Model. Journal of the Brazilian Chemical Society, 2015, , .	0.6	3
102	Solvent selection for chemical reactions: automated computational screening of solvents using the SMD model. Quimica Nova, 0, , .	0.3	3
103	Copper-mediated aromatic fluorination using N-heterocycle-carbene ligand: Free energy profile of the Cu(I)/Cu(III) and Cu(II) radical mechanisms. Journal of Organometallic Chemistry, 2022, 973-974, 122397.	0.8	3
104	Electron affinity and dipole moment of 1,2,4,5-tetraoxanes antimalarials and correlation with activity against Plasmodium falciparum. Medicinal Chemistry Research, 2014, 23, 5197-5203.	1.1	2
105	Is the iminium ion mechanism viable in the piperidine-catalyzed 1,4-conjugate addition reaction of nitroalkanes to Î±,Î²-unsaturated ketones?. Computational and Theoretical Chemistry, 2019, 1164, 112541.	1.1	2
106	Phenol alkylation under phase transfer catalysis conditions: Insights on the mechanism and kinetics from computations. Molecular Catalysis, 2021, 506, 111566.	1.0	2
107	The role of nonelectrostatic solvation to chemical reactions in liquid phase. Journal of the Brazilian Chemical Society, 2005, 16, 227-231.	0.6	2
108	QM/MM and molecular dynamics simulation of the structure and dissociation of CuF in acetonitrile solvent. Chemical Physics Letters, 2022, 793, 139468.	1.2	2

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109	Diradical character of the bond breaking in the reaction of Br2 with benzene: Reliable barriers using the CR-CC(2,3) method. Computational and Theoretical Chemistry, 2021, 1198, 113171.	1.1	1
110	Ab initio. Theoretica Chimica Acta, 1996, 93, 333.	0.9	1
111	Friedel-Crafts Reaction: Theoretical Study of the Mechanism of Benzene Alkylation with Isopropyl Chloride Catalyzed by AlCl3 and Al2Cl6. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
112	Catalytic cycle and off-cycle steps in the palladium-catalyzed fluorination of aryl bromide with biaryl monophosphine ligands: Theoretical free energy profile. Molecular Catalysis, 2021, 506, 111540.	1.0	0
113	Large amplitude vibrations in the HFClF complex. Journal of the Brazilian Chemical Society, 1997, 8, 555-562.	0.6	0
114	BUILDING THE LIQUID-VAPOUR EQUILIBRIUM CURVE THROUGH A CUBIC EQUATION OF STATE: USE OF EXCEL FOR TEACHING PHYSICAL-CHEMISTRY. Quimica Nova, 2016, , .	0.3	0