

Josefredo R Pliego

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108
papers

2,981
citations

29
h-index

51
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114
ext. papers

3,260
ext. citations

3.2
avg, IF

5.89
L-index

#	Paper	IF	Citations
108	The Cluster-Continuum Model for the Calculation of the Solvation Free Energy of Ionic Species. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 7241-7247	2.8	362
107	Theoretical Calculation of pKa Using the Cluster-Continuum Model. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 7434-7439	2.8	297
106	Gibbs energy of solvation of organic ions in aqueous and dimethyl sulfoxide solutions. <i>Physical Chemistry Chemical Physics</i> , 2002 , 4, 1622-1627	3.6	179
105	Thermodynamic cycles and the calculation of pKa. <i>Chemical Physics Letters</i> , 2003 , 367, 145-149	2.5	147
104	Ionization of Organic Acids in Dimethyl Sulfoxide Solution: A Theoretical Ab Initio Calculation of the pKa Using a New Parametrization of the Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 166-171	2.8	113
103	New values for the absolute solvation free energy of univalent ions in aqueous solution. <i>Chemical Physics Letters</i> , 2000 , 332, 597-602	2.5	109
102	Parametrization of the PCM model for calculating solvation free energy of anions in dimethyl sulfoxide solutions. <i>Chemical Physics Letters</i> , 2002 , 355, 543-546	2.5	64
101	Basic hydrolysis of formamide in aqueous solution: a reliable theoretical calculation of the activation free energy using the cluster-continuum model. <i>Chemical Physics</i> , 2004 , 306, 273-280	2.3	57
100	A theoretical analysis of the free-energy profile of the different pathways in the alkaline hydrolysis of methyl formate in aqueous solution. <i>Chemistry - A European Journal</i> , 2002 , 8, 1945-53	4.8	57
99	Ab initio study of the hydroxide ion-water clusters: An accurate determination of the thermodynamic properties for the processes $n\text{H}_2\text{O} + \text{OH}^- \rightarrow \text{HO}(\text{H}_2\text{O})_n$ ($n=1-4$). <i>Journal of Chemical Physics</i> , 2000 , 112, 4045-4052	3.9	57
98	Absolute solvation free energy of Li^+ and Na^+ ions in dimethyl sulfoxide solution: a theoretical ab initio and cluster-continuum model study. <i>Journal of Chemical Physics</i> , 2005 , 123, 074508	3.9	54
97	Mechanism of the Piperidine-Catalyzed Knoevenagel Condensation Reaction in Methanol: The Role of Iminium and Enolate Ions. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 5300-5307	3.4	50
96	On the Calculation of the Absolute Solvation Free Energy of Ionic Species: Application of the Extrapolation Method to the Hydroxide Ion in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 5155-5160	3.4	46
95	Singlet-Triplet Gap, and the Electronic and Vibrational Spectra of Chlorophenylcarbene: A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 7481-7486	2.8	46
94	Intramolecular catalysis of phosphodiester hydrolysis by two imidazoles. <i>Journal of the American Chemical Society</i> , 2010 , 132, 8513-23	16.4	40
93	Reaction Paths for Aqueous Decomposition of CCl_2 . <i>The Journal of Physical Chemistry</i> , 1996 , 100, 12410-12413	4.0	40
92	Absolute single-ion solvation free energy scale in methanol determined by the lithium cluster-continuum approach. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 5129-35	3.4	39

91	First solvation shell effects on ionic chemical reactions: new insights for supramolecular catalysis. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 505-10	3.4	39
90	Revisiting the mechanism of neutral hydrolysis of esters: water autoionization mechanisms with acid or base initiation pathways. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 6487-97	3.4	38
89	Effects of ion-pairing and hydration on the S _N Ar reaction of the F ⁻ with p-chlorobenzonitrile in aprotic solvents. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 1118-24	3.6	38
88	Cluster-continuum quasichemical theory calculation of the lithium ion solvation in water, acetonitrile and dimethyl sulfoxide: an absolute single-ion solvation free energy scale. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 26745-55	3.6	37
87	A New Mechanism for the Reaction of Carbenes with OH Groups. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 3904-3909	2.8	37
86	Chemoselective nucleophilic fluorination induced by selective solvation of the S _N 2 transition state. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 1752-8	3.4	36
85	Chemisorption of SO ₂ on graphite surface: A theoretical ab initio and ideal lattice gas model study. <i>Chemical Physics</i> , 2005 , 314, 127-133	2.3	36
84	Revisiting the reactions of nucleophiles with arenediazonium ions: dediazonation of arenediazonium salts in aqueous and micellar solutions containing alkyl sulfates and alkanesulfonates and an ab initio analysis of the reaction pathway. <i>Perkin Transactions II RSC</i> , 2000 , 1896-1907		35
83	Theoretical prediction of pK _a in methanol: testing SM8 and SMD models for carboxylic acids, phenols, and amines. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 5730-9	3.4	34
82	Design of an organocatalyst for ion-molecule S _N 2 reactions: A new solvent effect on the reaction rate predicted by ab initio calculations. <i>Journal of Molecular Catalysis A</i> , 2005 , 239, 228-234		33
81	Unraveling the Mechanism of the Cinchoninium Ion Asymmetric Phase-Transfer-Catalyzed Alkylation Reaction. <i>ACS Catalysis</i> , 2013 , 3, 613-616	13.1	31
80	Ab initio conformational analysis of cyclooctane molecule. <i>Journal of Computational Chemistry</i> , 1998 , 19, 524-534	3.5	29
79	Amphiphilic niobium oxyhydroxide as a hybrid catalyst for sulfur removal from fuel in a biphasic system. <i>Applied Catalysis B: Environmental</i> , 2014 , 147, 43-48	21.8	28
78	Modeling protic to dipolar aprotic solvent rate acceleration and leaving group effects in S(N)2 reactions: A theoretical study of the reaction of acetate ion with ethyl halides in aqueous and dimethyl sulfoxide solutions. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 507-11	2.8	28
77	New insights on reaction pathway selectivity promoted by crown ether phase-transfer catalysis: Model ab initio calculations of nucleophilic fluorination. <i>Journal of Molecular Catalysis A</i> , 2012 , 363-364, 489-494		27
76	Ab initio study of the S(N)2 and E2 mechanisms in the reaction between the cyanide ion and ethyl chloride in dimethyl sulfoxide solution. <i>Organic Letters</i> , 2005 , 7, 1821-3	6.2	27
75	Hybrid discrete-continuum solvation methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020 , 10, e1440	7.9	26
74	Theoretical Design and Calculation of a Crown Ether Phase-Transfer-Catalyst Scaffold for Nucleophilic Fluorination Merging Two Catalytic Concepts. <i>Journal of Organic Chemistry</i> , 2016 , 81, 8455-63	4.2	24

73	CMIRS Solvation Model for Methanol: Parametrization, Testing, and Comparison with SMD, SM8, and COSMO-RS. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 12660-12668	3.4	22
72	Mechanism and free energy profile of base-catalyzed Knoevenagel condensation reaction. <i>RSC Advances</i> , 2016 , 6, 57803-57810	3.7	21
71	Ab initio investigation of the kinetics and mechanism of the neutral hydrolysis of formamide in aqueous solution. <i>Journal of the Brazilian Chemical Society</i> , 2007 , 18, 469-702	1.5	21
70	Ab initio, density functional theory, and continuum solvation model prediction of the product ratio in the S(N)2 reaction of NO ₂ (-) with CH ₃ CH ₂ Cl and CH ₃ CH ₂ Br in DMSO solution. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 10068-74	2.8	20
69	Reply to comment on: Thermodynamic cycles and the calculation of pKa [Chem. Phys. Lett. 367 (2003) 145]. <i>Chemical Physics Letters</i> , 2003 , 381, 246-247	2.5	20
68	Performance of the SMD and SM8 models for predicting solvation free energy of neutral solutes in methanol, dimethyl sulfoxide and acetonitrile. <i>Journal of Computer-Aided Molecular Design</i> , 2015 , 29, 217-24	4.2	19
67	Dynamical discrete/continuum linear response shells theory of solvation: convergence test for NH ₄ ⁺ and OH ⁻ ions in water solution using DFT and DFTB methods. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 15941-7	3.4	19
66	Absolute proton affinity and basicity of the carbenes CH ₂ , CF ₂ , CCl ₂ , C(OH) ₂ , FCOH, CPh ₂ and fluorenylidene. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997 , 93, 1881-1883		19
65	Rate acceleration of SN ₂ reactions through selective solvation of the transition state. <i>Chemical Physics Letters</i> , 2006 , 423, 459-462	2.5	19
64	Chemical reactions inside structured nano-environment: S(N)2 vs. E2 reactions for the F(-) + CH(3)CH(2)Cl system. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 779-82	3.6	18
63	Free Energy Profile of the Reaction between the Hydroxide Ion and Ethyl Acetate in Aqueous and Dimethyl Sulfoxide Solutions: A Theoretical Analysis of the Changes Induced by the Solvent on the Different Reaction Pathways. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 2520-2526	2.8	17
62	Theoretical Study of the Gas-Phase Reaction of Fluoride and Chloride Ions with Methyl Formate. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 371-378	2.8	17
61	A comprehensive theoretical investigation of the transition states and a proposed kinetic model for the cinchoninium ion asymmetric phase-transfer catalyzed alkylation reaction. <i>Journal of Molecular Catalysis A</i> , 2016 , 417, 192-199		16
60	Prediction of the pH-rate profile for dimethyl sulfide oxidation by hydrogen peroxide: The role of elusive H ₃ O ₂ ⁺ Ion. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 501-507	2.1	16
59	Shells theory of solvation and the long-range Born correction. <i>Theoretical Chemistry Accounts</i> , 2011 , 128, 275-283	1.9	16
58	Molecular dynamics and cluster-continuum insights on bulk alcohols effects on S N 2 reactions of potassium and cesium fluorides with alkyl halides. <i>Journal of Molecular Liquids</i> , 2017 , 237, 157-163	6	13
57	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. <i>Organic and Biomolecular Chemistry</i> , 2018 , 16, 3127-3137	3.9	13
56	Regioselective organocatalysis: a theoretical prediction of the selective rate acceleration of the SN ₂ reaction between an acetate ion and primary alkyl chlorides in DMSO solution. <i>Organic and Biomolecular Chemistry</i> , 2006 , 4, 1667-70	3.9	13

55	Ligand exchange ion-molecule reactions of simple silyl and germyl cations. <i>International Journal of Mass Spectrometry</i> , 2003 , 228, 551-562	1.9	13
54	Acid-catalyzed transesterification and esterification in methanol: a theoretical cluster-continuum investigation of the mechanisms and free energy barriers. <i>Theoretical Chemistry Accounts</i> , 2015 , 134, 1	1.9	12
53	Reactivity and stability of ion pairs, dimers and tetramers versus solvent polarity: S _N Ar fluorination of 2-bromobenzonitrile with tetramethylammonium fluoride. <i>Theoretical Chemistry Accounts</i> , 2020 , 139, 1	1.9	12
52	How Accurate is the SMD Model for Predicting Free Energy Barriers for Nucleophilic Substitution Reactions in Polar Protic and Dipolar Aprotic Solvents?. <i>Journal of the Brazilian Chemical Society</i> , 2016 ,	1.5	12
51	Theoretical free energy profile and benchmarking of functionals for amino-thiourea organocatalyzed nitro-Michael addition reaction. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 11529-11536	3.6	11
50	The role of ammonia oxide in the reaction of hydroxylamine with carboxylic esters. <i>Organic and Biomolecular Chemistry</i> , 2015 , 13, 6217-24	3.9	11
49	Stability of hydroxylamine isomers in aqueous solution: Ab initio study using continuum, cluster-continuum and Shells Theory of Solvation. <i>Chemical Physics Letters</i> , 2011 , 518, 61-64	2.5	11
48	Theoretical and experimental investigation of the formation of E- and Z-Aldimines from the reaction of methylamine with acetaldehyde. <i>Journal of the Brazilian Chemical Society</i> , 1999 , 10, 381	1.5	11
47	Searching for the ylide structure. An ab initio study of the H ₂ O...Cl ₂ complex. <i>Chemical Physics Letters</i> , 1996 , 249, 136-140	2.5	11
46	Theoretical study of the mechanism and regioselectivity of the alkylation reaction of the phenoxide ion in polar protic and aprotic solvents. <i>Computational and Theoretical Chemistry</i> , 2018 , 1138, 117-122	2	10
45	A theoretical study of the HCHO+CCl ₂ reaction: Cycloaddition or ylide formation?. <i>Journal of Chemical Physics</i> , 1997 , 106, 3582-3586	3.9	10
44	Kinetics of the H ₂ O+CCl ₂ reaction in gas phase and in solution by an insertion mechanism. <i>Chemical Physics Letters</i> , 1998 , 285, 121-126	2.5	10
43	How difficult are anion-molecule S _N Ar reactions of unactivated arenes in the gas phase, dimethyl sulfoxide, and methanol solvents?. <i>Structural Chemistry</i> , 2019 , 30, 75-83	1.8	9
42	Quantum and classical two-dimensional analysis of rainbow structures in the Xe+CO ₂ rotational excitation at 0.2 eV collision energy and on a repulsive potential. <i>Physical Review A</i> , 1995 , 52, 342-349	2.6	9
41	Mechanism of nucleophilic fluorination promoted by bis-tert-alcohol-functionalized crown-6-calix[4]arene. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25648	2.1	8
40	Infinite dilution activity coefficient from SMD calculations: accuracy and performance for predicting liquid-liquid equilibria. <i>Journal of Molecular Modeling</i> , 2018 , 24, 56	2	8
39	Jacobsen's Catalyst Interaction with Polydimethylsiloxane/Tetraethoxysilane Network and Solvent Molecules: Theoretical Design of a New Polymeric Membrane. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 14830-14834	3.8	8
38	Free Energy Profile of a Model Palladium Catalyzed Fluorination of Aryl Bromide with Cesium Fluoride. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 9850-9856	2.8	7

37	Cluster expansion of the solvation free energy difference: Systematic improvements in the solvation of single ions. <i>Journal of Chemical Physics</i> , 2017 , 147, 034104	3.9	7
36	Reaction of CCl ₂ with CH ₂ NH and the formation of dipolar and biradical ylide structures. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997 , 2365-2370		7
35	Free radical mechanism of the Cl ₂ addition to acetylene. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998 , 94, 2895-2900		7
34	Modelos contínuos do solvente: fundamentos. <i>Quimica Nova</i> , 2006 , 29, 535-542	1.6	7
33	On the mechanism of the reaction between aryl acetates and hydroxylamine. <i>Arkivoc</i> , 2007 , 2007, 199-214	1.9	7
32	Theoretical design of new macrocycles for nucleophilic fluorination with KF: thiourea-crown-ether is predicted to overcome [2.2.2]-cryptand. <i>Molecular Systems Design and Engineering</i> , 2020 , 5, 1513-1523	4.6	7
31	Thermodynamics of Ylide Formation from Carbenes and Carbonyl Compounds. <i>Journal of the Brazilian Chemical Society</i> , 1998 , 9, 181-186	1.5	6
30	A theoretical abinitio and Monte Carlo simulation study of the pyridine+CCl ₂ reaction kinetics in the gas phase and in carbon tetrachloride solution using canonical flexible transition state theory. <i>Physical Chemistry Chemical Physics</i> , 1999 , 1, 1031-1036	3.6	6
29	Nucleophilic Fluorination with KF Catalyzed by 18-Crown-6 and Bulky Diols: A Theoretical and Experimental Study. <i>Journal of Organic Chemistry</i> , 2020 , 85, 15457-15465	4.2	6
28	Second harmonic generation in pyrazoline derivatives of dibenzylideneacetones and chalcone: A combined experimental and theoretical approach. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020 , 388, 112147	4.7	6
27	Cleaving paraoxon with hydroxylamine: Ammonium oxide isomer favors a Frontside attack mechanism. <i>Journal of Physical Organic Chemistry</i> , 2019 , 32, e3866	2.1	5
26	Ab initio study of the Cl+H ₂ S atmospheric reaction: is there a breakdown of the transition state theory?. <i>Molecular Physics</i> , 2008 , 106, 841-848	1.7	5
25	A comparison of state-to-state rotational total cross sections using two- and three-dimensional close coupled approaches. <i>Chemical Physics Letters</i> , 1996 , 251, 346-352	2.5	5
24	Analysis of state-to-state differential cross sections in two-dimensional Xe-CO ₂ scattering with long-range effects. <i>Physical Review A</i> , 1996 , 54, 2091-2098	2.6	5
23	Micro-solvation and counter ion effects on ionic reactions: Activation of potassium fluoride with 18-crown-6 and tert-butanol in aprotic solvents. <i>Journal of Molecular Liquids</i> , 2020 , 319, 114211	6	5
22	The role of intermolecular forces in ionic reactions: the solvent effect, ion-pairing, aggregates and structured environment. <i>Organic and Biomolecular Chemistry</i> , 2021 , 19, 1900-1914	3.9	5
21	Counter-ion and solvent effects in the C- and O-alkylation of the phenoxide ion with allyl chloride. <i>Journal of Physical Organic Chemistry</i> , 2019 , 32, e3947	2.1	4
20	Free energy profile and microkinetic modeling of base-catalyzed conjugate addition reaction of nitroalkanes to α -unsaturated ketones in polar and apolar solvents. <i>Journal of Molecular Modeling</i> , 2018 , 24, 152	2	3

19	Fast Screening of Solvents for Simultaneous Extraction of Furfural, 5-Hydroxymethylfurfural and Levulinic Acid from Aqueous Solution Using SMD Solvation Free Energies. <i>Journal of the Brazilian Chemical Society</i> , 2017 ,	1.5	3
18	Prediction of Phase Separation Using a Modified Regular Solution Theory and the SMD Continuum Solvation Model. <i>Journal of the Brazilian Chemical Society</i> , 2015 ,	1.5	3
17	Dual bifunctional catalysis and the effect in the reaction of hydroxylamine with phenylacetate. <i>Journal of the Brazilian Chemical Society</i> , 2011 , 22, 2165-2170	1.5	3
16	Single-ion solvation free energy: A new cluster-continuum approach based on the cluster expansion method. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 26902-26910	3.6	3
15	The role of carboxylic acid impurity in the mechanism of the formation of aldimines in aprotic solvents. <i>Computational and Theoretical Chemistry</i> , 2020 , 1191, 113053	2	3
14	Mechanisms of the formation of imines in aqueous solution and the effect of the pH: a theoretical analysis. <i>Arkivoc</i> , 2020 , 2020, 34-52	0.9	3
13	Is the iminium ion mechanism viable in the piperidine-catalyzed 1,4-conjugate addition reaction of nitroalkanes to α -unsaturated ketones?. <i>Computational and Theoretical Chemistry</i> , 2019 , 1164, 112541	2	2
12	Electron affinity and dipole moment of 1,2,4,5-tetraoxanes antimalarials and correlation with activity against Plasmodium falciparum. <i>Medicinal Chemistry Research</i> , 2014 , 23, 5197-5203	2.2	2
11	Electronic spectra of the nitrile ylides: an ab initio multiconfigurational second-order quasidegenerate perturbation theory study. <i>Chemical Physics Letters</i> , 2000 , 318, 142-148	2.5	2
10	The role of nonelectrostatic solvation to chemical reactions in liquid phase. <i>Journal of the Brazilian Chemical Society</i> , 2005 , 16, 227-231	1.5	2
9	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. <i>Journal of Molecular Structure</i> , 2020 , 1204, 127536	3.4	2
8	Bifunctional Primary Amino-thiourea Asymmetric Catalysis: The Imine-Iminium Ion Mechanism in the Michael Addition of Nitromethane to Enone. <i>Asian Journal of Organic Chemistry</i> , 2021 , 10, 1472-1485 ³		2
7	Hydroperoxo on the Niobium Oxyhydroxide Surface as the Active Species in the Catalyzed Oxidation of Organic Sulfide by Hydrogen Peroxide. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 9369-9375 ^{3,8}		2
6	QM/MM and Molecular Dynamics Simulation of the Structure and Dissociation of CuF in Acetonitrile Solvent. <i>Chemical Physics Letters</i> , 2022 , 793, 139468	2.5	1
5	Phenol alkylation under phase transfer catalysis conditions: Insights on the mechanism and kinetics from computations. <i>Molecular Catalysis</i> , 2021 , 506, 111566	3.3	1
4	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). <i>Journal of Molecular Liquids</i> , 2022 , 359, 119368	6	0
3	Copper-mediated aromatic fluorination using N-heterocycle-carbene ligand: Free energy profile of the Cu(I)/Cu(III) and Cu(II) radical mechanisms. <i>Journal of Organometallic Chemistry</i> , 2022 , 973-974, 122397 ^{3,7}		0
2	Catalytic cycle and off-cycle steps in the palladium-catalyzed fluorination of aryl bromide with biaryl monophosphine ligands: Theoretical free energy profile. <i>Molecular Catalysis</i> , 2021 , 506, 111540	3.3	

1 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

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