Josefredo R Pliego

List of Publications by Year in Descending Order

108 papers	2,981 citations	29 h-index	51 g-index
114 ext. papers	3,260 ext. citations	3.2 avg, IF	5.89 L-index

#	Paper	IF	Citations
108	QM/MM and Molecular Dynamics Simulation of the Structure and Dissociation of CuF in Acetonitrile Solvent. *Chemical Physics Letters*, **2022**, 793, 139468	2.5	1
107	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	6	0
106	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	2.3	0
105	Single-ion solvation free energy: A new cluster-continuum approach based on the cluster expansion method. *Physical Chemistry Chemical Physics*, **2021**, 23, 26902-26910	3.6	3
104	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	3.3	
103	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	2	
102	Phenol alkylation under phase transfer catalysis conditions: Insights on the mechanism and kinetics from computations. *Molecular Catalysis*, **2021**, 506, 111566	3.3	1
101	Bifunctional Primary Amino-thiourea Asymmetric Catalysis: The Imine-Iminium Ion Mechanism in the Michael Addition of Nitromethane to Enone. *Asian Journal of Organic Chemistry*, **2021**, 10, 1472-1485	3	2
100	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	3.9	5
99	Theoretical free energy profile and benchmarking of functionals for amino-thiourea organocatalyzed nitro-Michael addition reaction. *Physical Chemistry Chemical Physics*, **2020**, 22, 11529-11536	3.6	11
98	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	1.9	12
97	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	3.4	2
96	The role of carboxylic acid impurity in the mechanism of the formation of aldimines in aprotic solvents. *Computational and Theoretical Chemistry*, **2020**, 1191, 113053	2	3
95	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	6	5
94	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	4.2	6
93	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	4.6	7
92	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	4.7	6

91	Hybrid discrete-continuum solvation methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1440	7.9	26
90	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	3.8	2
89	Mechanisms of the formation of imines in aqueous solution and the effect of the pH: a theoretical analysis. *Arkivoc*, **2020**, 2020, 34-52	0.9	3
88	Counter-ion and solvent effects in the C- and O-alkylation of the phenoxide ion with allyl chloride. *Journal of Physical Organic Chemistry*, **2019**, 32, e3947	2.1	4
87	Cleaving paraoxon with hydroxylamine: Ammonium oxide isomer favors a Frontside attack mechanism. *Journal of Physical Organic Chemistry*, **2019**, 32, e3866	2.1	5
86	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	1.8	9
85	Is the iminium ion mechanism viable in the piperidine-catalyzed 1,4-conjugate addition reaction of nitroalkanes to α,β-unsaturated ketones?. *Computational and Theoretical Chemistry*, **2019**, 1164, 112541	2	2
84	Free Energy Profile of a Model Palladium Catalyzed Fluorination of Aryl Bromide with Cesium Fluoride. *Journal of Physical Chemistry A*, **2019**, 123, 9850-9856	2.8	7
83	Mechanism of nucleophilic fluorination promoted by bis-tert-alcohol-functionalized crown-6-calix[4]arene. *International Journal of Quantum Chemistry*, **2018**, 118, e25648	2.1	8
82	Infinite dilution activity coefficient from SMD calculations: accuracy and performance for predicting liquid-liquid equilibria. *Journal of Molecular Modeling*, **2018**, 24, 56	2	8
81	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	3.9	13
80	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	2	10
79	Free energy profile and microkinetic modeling of base-catalyzed conjugate addition reaction of nitroalkanes to α,β-unsaturated ketones in polar and apolar solvents. *Journal of Molecular Modeling* , **2018**, 24, 152	2	3
78	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	3.4	50
77	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	6	13
76	Cluster expansion of the solvation free energy difference: Systematic improvements in the solvation of single ions. *Journal of Chemical Physics*, **2017**, 147, 034104	3.9	7
75	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*, **2017**,	1.5	3
74	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, 8455-63	4.2	24

73	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		16
72	Mechanism and free energy profile of base-catalyzed Knoevenagel condensation reaction. *RSC Advances*, **2016**, 6, 57803-57810	3.7	21
71	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**,	1.5	12
70	CMIRS Solvation Model for Methanol: Parametrization, Testing, and Comparison with SMD, SM8, and COSMO-RS. *Journal of Physical Chemistry B*, **2016**, 120, 12660-12668	3.4	22
69	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, 26745-55	3.6	37
68	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	1.9	12
67	Prediction of Phase Separation Using a Modified Regular Solution Theory and the SMD Continuum Solvation Model. *Journal of the Brazilian Chemical Society*, **2015**,	1.5	3
66	The role of ammonia oxide in the reaction of hydroxylamine with carboxylic esters. *Organic and Biomolecular Chemistry*, **2015**, 13, 6217-24	3.9	11
65	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, 217-24	4.2	19
64	Prediction of the pH-rate profile for dimethyl sulfide oxidation by hydrogen peroxide: The role of elusive H3O2+ Ion. *International Journal of Quantum Chemistry*, **2014**, 114, 501-507	2.1	16
63	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	2.2	2
62	Amphiphilic niobium oxyhydroxide as a hybrid catalyst for sulfur removal from fuel in a biphasic system. *Applied Catalysis B: Environmental*, **2014**, 147, 43-48	21.8	28
61	Theoretical prediction of pKa in methanol: testing SM8 and SMD models for carboxylic acids, phenols, and amines. *Journal of Physical Chemistry B*, **2014**, 118, 5730-9	3.4	34
60	Absolute single-ion solvation free energy scale in methanol determined by the lithium cluster-continuum approach. *Journal of Physical Chemistry B*, **2013**, 117, 5129-35	3.4	39
59	Revisiting the mechanism of neutral hydrolysis of esters: water autoionization mechanisms with acid or base initiation pathways. *Journal of Physical Chemistry B*, **2013**, 117, 6487-97	3.4	38
58	Unraveling the Mechanism of the Cinchoninium Ion Asymmetric Phase-Transfer-Catalyzed Alkylation Reaction. *ACS Catalysis*, **2013**, 3, 613-616	13.1	31
57	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		27
56	Dual bifunctional catalysis and the ⊟effect in the reaction of hydroxylamine with phenylacetate. *Journal of the Brazilian Chemical Society*, **2011**, 22, 2165-2170	1.5	3

55	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	2.5	11
54	Shells theory of solvation and the long-range Born correction. *Theoretical Chemistry Accounts*, **2011**, 128, 275-283	1.9	16
53	Chemical reactions inside structured nano-environment: S(N)2 vs. E2 reactions for the F(-) + CH(3)CH(2)Cl system. *Physical Chemistry Chemical Physics*, **2011**, 13, 779-82	3.6	18
52	Dynamical discrete/continuum linear response shells theory of solvation: convergence test for NH4+ and OH- ions in water solution using DFT and DFTB methods. *Journal of Physical Chemistry B*, **2010**, 114, 15941-7	3.4	19
51	Intramolecular catalysis of phosphodiester hydrolysis by two imidazoles. *Journal of the American Chemical Society*, **2010**, 132, 8513-23	16.4	40
50	First solvation shell effects on ionic chemical reactions: new insights for supramolecular catalysis. *Journal of Physical Chemistry B*, **2009**, 113, 505-10	3.4	39
49	Effects of ion-pairing and hydration on the SNAr reaction of the F- with p-chlorobenzonitrile in aprotic solvents. *Physical Chemistry Chemical Physics*, **2008**, 10, 1118-24	3.6	38
48	Ab initio study of the Cl+H2S atmospheric reaction: is there a breakdown of the transition state theory?. *Molecular Physics*, **2008**, 106, 841-848	1.7	5
47	Jacobsen□ 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	3.8	8
46	Chemoselective nucleophilic fluorination induced by selective solvation of the SN2 transition state. *Journal of Physical Chemistry B*, **2007**, 111, 1752-8	3.4	36
45	Ab initio, density functional theory, and continuum solvation model prediction of the product ratio in the S(N)2 reaction of NO2(-) with CH3CH2Cl and CH3CH2Br in DMSO solution. *Journal of Physical Chemistry A*, **2007**, 111, 10068-74	2.8	20
44	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	1.5	21
43	On the mechanism of the reaction between aryl acetates and hydroxylamine. *Arkivoc*, **2007**, 2007, 199-214	0.9	7
42	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, 1667-70	3.9	13
41	Modelos cont□nuos do solvente: fundamentos. *Quimica Nova*, **2006**, 29, 535-542	1.6	7
40	Rate acceleration of SN2 reactions through selective solvation of the transition state. *Chemical Physics Letters*, **2006**, 423, 459-462	2.5	19
39	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. *Journal of Physical Chemistry A*, **2005**, 109, 507-11	2.8	28
38	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. *Organic Letters*, **2005**, 7, 1821-3	6.2	27

37	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	3.9	54
36	Design of an organocatalyst for ion–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		33
35	Chemisorption of SO2 on graphite surface: A theoretical ab initio and ideal lattice gas model study. *Chemical Physics*, **2005**, 314, 127-133	2.3	36
34	The role of nonelectrostatic solvation to chemical reactions in liquid phase. *Journal of the Brazilian Chemical Society*, **2005**, 16, 227-231	1.5	2
33	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	2.3	57
32	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. *Journal of Physical Chemistry A*, **2004**, 108, 2520-2526	2.8	17
31	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. *Journal of Physical Chemistry A*, **2004**, 108, 166-171	2.8	113
30	Reply to comment on: Thermodynamic cycles and the calculation of pKa [Chem. Phys. Lett. 367 (2003) 145]. *Chemical Physics Letters*, **2003**, 381, 246-247	2.5	20
29	Thermodynamic cycles and the calculation of pKa. *Chemical Physics Letters*, **2003**, 367, 145-149	2.5	147
28	Ligand exchange ion–molecule reactions of simple silyl and germyl cations. *International Journal of Mass Spectrometry*, **2003**, 228, 551-562	1.9	13
27	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, 1945-53	4.8	57
26	Parametrization of the PCM model for calculating solvation free energy of anions in dimethyl sulfoxide solutions. *Chemical Physics Letters*, **2002**, 355, 543-546	2.5	64
25	Theoretical Study of the Gas-Phase Reaction of Fluoride and Chloride Ions with Methyl Formate. *Journal of Physical Chemistry A*, **2002**, 106, 371-378	2.8	17
24	Theoretical Calculation of pKa Using the Cluster–Continuum Model. *Journal of Physical Chemistry A*, **2002**, 106, 7434-7439	2.8	297
23	Gibbs energy of solvation of organic ions in aqueous and dimethyl sulfoxide solutions. *Physical Chemistry Chemical Physics*, **2002**, 4, 1622-1627	3.6	179
22	The Cluster–Continuum Model for the Calculation of the Solvation Free Energy of Ionic Species. *Journal of Physical Chemistry A*, **2001**, 105, 7241-7247	2.8	362
21	Electronic spectra of the nitrile ylides: an ab initio multiconfigurational second-order quasidegenerate perturbation theory study. *Chemical Physics Letters*, **2000**, 318, 142-148	2.5	2
20	New values for the absolute solvation free energy of univalent ions in aqueous solution. *Chemical Physics Letters*, **2000**, 332, 597-602	2.5	109

19	Ab initio study of the hydroxide ion–water clusters: An accurate determination of the thermodynamic properties for the processes nH2O+OH−→HO(H2O)n (n=1–4). *Journal of Chemical Physics*, **2000**, 112, 4045-4052	3.9	57
18	On the Calculation of the Absolute Solvation Free Energy of Ionic Species: Application of the Extrapolation Method to the Hydroxide Ion in Aqueous Solution. *Journal of Physical Chemistry B*, **2000**, 104, 5155-5160	3.4	46
17	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		35
16	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	1.5	11
15	A theoretical abinitio 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	3.6	6
14	A New Mechanism for the Reaction of Carbenes with OH Groups. *Journal of Physical Chemistry A*, **1999**, 103, 3904-3909	2.8	37
13	Singlet−Triplet Gap, and the Electronic and Vibrational Spectra of Chlorophenylcarbene: A Combined Theoretical and Experimental Study. *Journal of Physical Chemistry A*, **1999**, 103, 7481-7486	2.8	46
12	Kinetics of the H2O+CCl2 reaction in gas phase and in solution by an insertion mechanism. *Chemical Physics Letters*, **1998**, 285, 121-126	2.5	10
11	Ab initio conformational analysis of cyclooctane molecule. *Journal of Computational Chemistry*, **1998**, 19, 524-534	3.5	29
10	Free radical mechanism of the Cl2 addition to acetylene. *Journal of the Chemical Society, Faraday Transactions*, **1998**, 94, 2895-2900		7
9	Thermodynamics of Ylide Formation from Carbenes and Carbonyl Compounds. *Journal of the Brazilian Chemical Society*, **1998**, 9, 181-186	1.5	6
8	A theoretical study of the HCHO+CCl2 reaction: Cycloaddition or ylide formation?. *Journal of Chemical Physics*, **1997**, 106, 3582-3586	3.9	10
7	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		7
6	Absolute proton affinity and basicity of the carbenesCH2, CF2, CCl2, C(OH)2,FCOH, CPh2 and fluorenylidene. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 1881-1883		19
5	Reaction Paths for Aqueous Decomposition of CCl2. *The Journal of Physical Chemistry*, **1996**, 100, 12410-12413		40
4	Searching for the ylide structure. An ab initio study of the H2O···CCl2 complex. *Chemical Physics Letters*, **1996**, 249, 136-140	2.5	11
3	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	2.5	5
2	Analysis of state-to-state differential cross sections in two-dimensional Xe-CO2 scattering with long-range effects. *Physical Review A*, **1996**, 54, 2091-2098	2.6	5

1	Quantum and classical two-dimensional analysis of rainbow structures in the Xe+CO2 rotational excitation at 0.2 eV collision energy and on a repulsive potential. *Physical Review A*, **1995**, 52, 342-349	2.6	9