Carlos Bernardes

List of Publications by Year
in descending order

81 papers	1,913 citations	279487 23 h-index	288905 40 g-index
82 all docs	82 docs citations	82 times ranked	2233 citing authors

#	Article	IF	Citations
1	Structure and Aggregation in the 1-Alkyl-3-Methylimidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid Homologous Series. Journal of Physical Chemistry B, 2014, 118, 567-576.	1.2	223
2	The Structure of Aqueous Solutions of a Hydrophilic Ionic Liquid: The Full Concentration Range of 1-Ethyl-3-methylimidazolium Ethylsulfate and Water. Journal of Physical Chemistry B, 2011, 115, 2067-2074.	1.2	142
3	Nano-segregation in ionic liquids: scorpions and vanishing chains. Physical Chemistry Chemical Physics, 2013, 15, 16256.	1.3	119
4	Inorganic salts in purely ionic liquid media: the development of high ionicity ionic liquids (HIILs). Chemical Communications, 2012, 48, 3656.	2.2	91
5	Mutual Solubility of Water and Structural/Positional Isomers of N-Alkylpyridinium-Based Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 15925-15934.	1.2	74
6	Structure and Aggregation in the 1,3-Dialkyl-imidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid Family: 2. From Single to Double Long Alkyl Side Chains. Journal of Physical Chemistry B, 2014, 118, 6885-6895.	1.2	65
7	Evaluation of the OPLS-AA Force Field for the Study of Structural and Energetic Aspects of Molecular Organic Crystals. Journal of Physical Chemistry A, 2015, 119, 3023-3034.	1.1	57
8	Comparative study of Al-MCM materials prepared at room temperature with different aluminium sources and by some hydrothermal methods. Microporous and Mesoporous Materials, 2006, 92, 270-285.	2.2	50
9	Ionic liquids with anions based on fluorosulfonyl derivatives: from asymmetrical substitutions to a consistent force field model. Physical Chemistry Chemical Physics, 2017, 19, 29617-29624.	1.3	49
10	A new calorimetric system to measure heat capacities of solids by the drop method. Measurement Science and Technology, 2006, 17, 1405-1408.	1.4	44
11	AGGREGATES: Finding structures in simulation results of solutions. Journal of Computational Chemistry, 2017, 38, 753-765.	1.5	41
12	Energetics and Structure of Nicotinic Acid (Niacin). Journal of Physical Chemistry B, 2010, 114, 5475-5485.	1.2	39
13	Additive polarizabilities in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1665-1670.	1.3	37
14	Polymorphic Phase Transition in 4â€²-Hydroxyacetophenone: Equilibrium Temperature, Kinetic Barrier, and the Relative Stability of Zâ€² = 1 and Zâ€² = 2 Forms. Crystal Growth and Design, 2017, 17, 1918-1932.	1.4	37
15	Polymorphism in 4â€²-Hydroxyacetophenone: Structure and Energetics. Crystal Growth and Design, 2008, 8, 2419-2430.	1.4	35
16	All-Atom Force Field for Molecular Dynamics Simulations on Organotransition Metal Solids and Liquids. Application to M(CO)_n (MÂ= Cr, Fe, Ni, Mo, Ru, or W) Compounds. Journal of Physical Chemistry A, 2013, 117, 11107-11113.	1.1	32
17	Energetics of Câˆ’F, Câˆ’Cl, Câˆ’Br, and Câˆ’I Bonds in 2-Haloethanols. Enthalpies of Formation of XCH2CH2OH (X = F, Cl, Br, I) Compounds and of the 2-Hydroxyethyl Radical. Journal of Physical Chemistry A, 2007, 111, 1713-1720.	1.1	29
18	Energetics of the Oâˆ’H Bond and of Intramolecular Hydrogen Bonding in HOC₆H₄C(O)Y (Y = H, CH₃, CH₂CHâ•CH₂,) Tj ETQq0 0 0 rgBT /Overlo 10029-10039.	1.1	29

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19	Heat capacity and thermodynamics of solid and liquid pyridine-3-carboxylic acid (nicotinic acid) over the temperature range 296K to 531K. Journal of Chemical Thermodynamics, 2012, 55, 23-28.	1.0	28
20	Energetics and Structure of Simvastatin. Molecular Pharmaceutics, 2013, 10, 2713-2722.	2.3	26
21	Structureâ€“property relationships in protic ionic liquids: a study of solventâ€“solvent and solventâ€“solute interactions. Physical Chemistry Chemical Physics, 2017, 19, 28133-28138.	1.3	26
22	Effect of Ring Substitution on the Sâˆ’H Bond Dissociation Enthalpies of Thiophenols. An Experimental and Computational Study. Journal of Physical Chemistry A, 2006, 110, 9949-9958.	1.1	25
23	Energetics of Cresols and of Methylphenoxyl Radicals. Journal of Physical Chemistry A, 2007, 111, 8741-8748.	1.1	25
24	A general strategy for the experimental study of the thermochemistry of protic ionic liquids: enthalpy of formation and vaporisation of 1-methylimidazolium ethanoate. Physical Chemistry Chemical Physics, 2012, 14, 4440.	1.3	22
25	From Molecules to Crystals: The Solvent Plays an Active Role Throughout the Nucleation Pathway of Molecular Organic Crystals. Crystal Growth and Design, 2014, 14, 5436-5441.	1.4	21
26	High ionicity ionic liquids (HIILs): comparing the effect of ethylsulfonate and ethylsulfate anions. Physical Chemistry Chemical Physics, 2013, 15, 18138.	1.3	20
27	Crystallization of 4â€²-Hydroxyacetophenone from Water: Control of Polymorphism via Phase Diagram Studies. Crystal Growth and Design, 2012, 12, 2932-2941.	1.4	19
28	A New Thermodynamically Favored Flubendazole/Maleic Acid Binary Crystal Form: Structure, Energetics, and in Silico PBPK Model-Based Investigation. Crystal Growth and Design, 2018, 18, 2377-2386.	1.4	19
29	Energetics of Aqueous Solutions of the Ionic Liquid 1-Ethyl-3-methylimidazolium Ethylsulfate. Journal of Physical Chemistry B, 2010, 114, 13179-13188.	1.2	18
30	Thermochemistry of 1,1,3,3-tetramethylguanidine and 1,1,3,3-tetramethylguanidinium nitrate. Journal of Chemical Thermodynamics, 2014, 77, 179-189.	1.0	17
31	Solvation of alcohols in ionic liquids â€“ understanding the effect of the anion and cation. Physical Chemistry Chemical Physics, 2018, 20, 2536-2548.	1.3	17
32	Polymorphism in Simvastatin: Twinning, Disorder, and Enantiotropic Phase Transitions. Molecular Pharmaceutics, 2018, 15, 5349-5360.	2.3	17
33	Designing the ammonium cation to achieve a higher hydrophilicity of bistriflimide-based ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 19307-19313.	1.3	17
34	Energetics of Glycine Cocrystal or Salt Formation with Two Regioisomers: Fumaric Acid and Maleic Acid. Crystal Growth and Design, 2019, 19, 5054-5064.	1.4	17
35	Polymorphism in 4-Hydroxybenzaldehyde: A Crystal Packing and Thermodynamic Study. Crystal Growth and Design, 2013, 13, 2803-2814.	1.4	15
36	The complex structure of ionic liquids at an atomistic level: from â€œred-and-greensâ€•to charge templates. Pure and Applied Chemistry, 2014, 86, 119-133.	0.9	15

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37	Structureâ€“property relationships in protic ionic liquids: a thermochemical study. Physical Chemistry Chemical Physics, 2017, 19, 19928-19936.	1.3	15
38	Extraction Optimization and Structural and Thermal Characterization of the Antimicrobial Abietane 7Î±-Acetoxy-6Î²-hydroxyroyleanone. Molecular Pharmaceutics, 2018, 15, 1412-1419.	2.3	15
39	Polymorphism in 4â€²-Hydroxyacetophenone: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2012, 116, 5179-5184.	1.2	14
40	Structure and Energetics of a New Hydrate of 4â€²-Hydroxyacetophenone. Crystal Growth and Design, 2010, 10, 3070-3076.	1.4	12
41	Solvent effects on the polar network of ionic liquid solutions. Journal of Physics Condensed Matter, 2015, 27, 194116.	0.7	12
42	Mixtures of the 1-ethyl-3-methylimidazolium acetate ionic liquid with different inorganic salts: insights into their interactions. Physical Chemistry Chemical Physics, 2016, 18, 2756-2766.	1.3	12
43	Neat ionic liquids versus ionic liquid mixtures: a combination of experimental data and molecular simulation. Physical Chemistry Chemical Physics, 2019, 21, 23305-23309.	1.3	12
44	Handling CO2 sorption mechanism in PIL@IL composites. Journal of CO2 Utilization, 2020, 41, 101225.	3.3	12
45	Kinetics and Mechanism of the Thermal Dehydration of a Robust and Yet Metastable Hemihydrate of 4-Hydroxynicotinic Acid. Crystal Growth and Design, 2015, 15, 3511-3524.	1.4	11
46	Tautomer selection through solvate formation: the case of 5-hydroxynicotinic acid. CrystEngComm, 2019, 21, 2220-2233.	1.3	11
47	Some practical aspects of heat capacity determination by differential scanning calorimetry. Thermochimica Acta, 2020, 687, 178574.	1.2	11
48	Polymorphism in 4â€²-hydroxyacetophenone: A vibrational analysis. Journal of Molecular Structure, 2014, 1078, 181-187.	1.8	10
49	Modeling the structure and thermodynamics of ferrocenium-based ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 10200-10208.	1.3	10
50	Modeling Halogen Bonds in Ionic Liquids: A Force Field for Imidazolium and Halo-Imidazolium Derivatives. Journal of Chemical Theory and Computation, 2017, 13, 6167-6176.	2.3	10
51	Energetics of the Thermal Dimerization of Acenaphthylene to Heptacyclene. Journal of Physical Chemistry A, 2006, 110, 2299-2307.	1.1	9
52	Thermal Stability of Simvastatin under Different Atmospheres. Journal of Pharmaceutical Sciences, 2014, 103, 241-248.	1.6	9
53	Thermochemistry of 4-HOC 6 H 4 COR (R = H, CH 3 , C 2 H 5 , n- C 3 H 7 , n -C 4 H 9 , n -C 5 H 11 , and n -C 6 H) Tj ETQq1 1 0.784314	1.0	9
54	Comparative structural analyses in four ionic liquid systems: the two low-q peaks of IL structure factor functions. Molecular Simulation, 2018, 44, 478-484.	0.9	9

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55	Towards the development of nanosprings from confined carbyne chains. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 117, 113831.	1.3	9
56	The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach. ChemPhysChem, 2021, 22, 2190-2200.	1.0	9
57	A Robust yet Metastable New Hemihydrate of 4-Hydroxynicotinic Acid. Crystal Growth and Design, 2011, 11, 2803-2810.	1.4	8
58	The standard molar enthalpy of the base catalysed hydrolysis of methyl paraben revisited. Journal of Chemical Thermodynamics, 2016, 103, 176-180.	1.0	8
59	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies. Journal of Chemical Thermodynamics, 2016, 95, 35-48.	1.0	8
60	ForConX: A forcefield conversion tool based on XML. Journal of Computational Chemistry, 2017, 38, 629-638.	1.5	8
61	A fully automatic apparatus for thermal analysis of crystallization from solution and metastable zone width determinations. Journal of Thermal Analysis and Calorimetry, 2010, 100, 493-500.	2.0	7
62	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox). Journal of Chemical Thermodynamics, 2014, 73, 140-147.	1.0	7
63	Thermochemistry of 1-alkylimidazoles. Journal of Chemical Thermodynamics, 2015, 80, 59-64.	1.0	7
64	The Curious Case of Acetaldehyde Phenylhydrazone: Resolution of a 120 Year Old Puzzle where Forms with Vastly Different Melting Points Have the Same Structure. Crystal Growth and Design, 2019, 19, 907-917.	1.4	7
65	Thermochemistry of 2- and 4-biphenylmethanol. Journal of Chemical Thermodynamics, 2007, 39, 1384-1391.	1.0	6
66	Tuning the miscibility of water in imide-based ionic liquids. Physical Chemistry Chemical Physics, 2020, 22, 25236-25242.	1.3	6
67	Linking Aggregation in Solution, Solvation, and Solubility of Simvastatin: An Experimental and MD Simulation Study. Crystal Growth and Design, 2021, 21, 544-551.	1.4	6
68	Real-Time In situ XRD Study of Simvastatin Crystallization in Levitated Droplets. Crystal Growth and Design, 2021, 21, 4665-4673.	1.4	6
69	DMSO/IL solvent systems for cellulose dissolution: Binary or ternary mixtures?. Journal of Molecular Liquids, 2022, 345, 117810.	2.3	6
70	Isotropic liquid state of triacylglycerols. Journal of Molecular Liquids, 2022, 353, 118703.	2.3	6
71	Size Matters: An Experimental and Computational Study of the Influence of Particle Size on the Lattice Energy of NaCl. Journal of Physical Chemistry C, 2015, 119, 4387-4396.	1.5	5
72	A force field for MD simulations on rhenium organometallic compounds developed from enthalpy of sublimation and X-ray diffraction measurements. Journal of Chemical Thermodynamics, 2019, 133, 60-69.	1.0	5

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73	Water Solubility Trends in Ionic Liquids: The Quantitative Structureâ€“Property Relationship Model versus Molecular Dynamics. Journal of Physical Chemistry B, 2021, 125, 11491-11497.	1.2	5
74	A new polymorph of 4â€²-hydroxyvalerophenone revealed by thermoanalytical and X-ray diffraction studies. European Physical Journal: Special Topics, 2017, 226, 849-855.	1.2	4
75	Kinetics of the base catalysed hydrolysis of methyl paraben revisited: Implications for determination of the effective volume of flow-microcalorimeters used to study cell cultures. Thermochimica Acta, 2018, 659, 82-88.	1.2	4
76	C13 â€“ a new empirical force field to characterize the mechanical behavior of carbyne chains. Physical Chemistry Chemical Physics, 2020, 22, 758-771.	1.3	4
77	A calorimetric system based on the LKB 10700-1 flow microcalorimeter. Measurement Science and Technology, 2009, 20, 075107.	1.4	3
78	First and Second Dissociation Enthalpies in Bi-Component Crystals Consisting of Maleic Acid and L-Phenylalanine. Molecules, 2021, 26, 5714.	1.7	3
79	DLPGEN: Preparing Molecular Dynamics Simulations with Support for Polarizable Force Fields. Journal of Chemical Information and Modeling, 2022, 62, 1471-1478.	2.5	3
80	Standard molar enthalpy of the orthorhombic to monoclinic polymorphic phase transition in 4â€²-hydroxyacetophenone from enthalpy of solution measurements. Journal of Chemical Thermodynamics, 2021, 158, 106445.	1.0	2
81	Conformational and Nonconformational Polymorphism in 4â€²-Hydroxyvalerophenone: A Structureâ€“Energeticsâ€“Dynamics Perspective. Crystal Growth and Design, 2020, 20, 2321-2336.	1.4	1