

# Carlos Bernardes

## List of Publications by Year in descending order

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Version: 2024-02-01

81  
papers

1,913  
citations

279798

23  
h-index

289244

40  
g-index

82  
all docs

82  
docs citations

82  
times ranked

2233  
citing authors

#	ARTICLE	IF	CITATIONS
1	DMSO/IL solvent systems for cellulose dissolution: Binary or ternary mixtures?. Journal of Molecular Liquids, 2022, 345, 117810.	4.9	6
2	Isotropic liquid state of triacylglycerols. Journal of Molecular Liquids, 2022, 353, 118703.	4.9	6
3	DLPGEN: Preparing Molecular Dynamics Simulations with Support for Polarizable Force Fields. Journal of Chemical Information and Modeling, 2022, 62, 1471-1478.	5.4	3
4	Linking Aggregation in Solution, Solvation, and Solubility of Simvastatin: An Experimental and MD Simulation Study. Crystal Growth and Design, 2021, 21, 544-551.	3.0	6
5	Real-Time In situ XRD Study of Simvastatin Crystallization in Levitated Droplets. Crystal Growth and Design, 2021, 21, 4665-4673.	3.0	6
6	Standard molar enthalpy of the orthorhombic to monoclinic polymorphic phase transition in 4-hydroxyacetophenone from enthalpy of solution measurements. Journal of Chemical Thermodynamics, 2021, 158, 106445.	2.0	2
7	The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach. ChemPhysChem, 2021, 22, 2190-2200.	2.1	9
8	First and Second Dissociation Enthalpies in Bi-Component Crystals Consisting of Maleic Acid and L-Phenylalanine. Molecules, 2021, 26, 5714.	3.8	3
9	Water Solubility Trends in Ionic Liquids: The Quantitative Structure-Property Relationship Model versus Molecular Dynamics. Journal of Physical Chemistry B, 2021, 125, 11491-11497.	2.6	5
10	C13 - a new empirical force field to characterize the mechanical behavior of carbyne chains. Physical Chemistry Chemical Physics, 2020, 22, 758-771.	2.8	4
11	Towards the development of nanosprings from confined carbyne chains. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 117, 113831.	2.7	9
12	Tuning the miscibility of water in imide-based ionic liquids. Physical Chemistry Chemical Physics, 2020, 22, 25236-25242.	2.8	6
13	Conformational and Nonconformational Polymorphism in 4-Hydroxyvalerophenone: A Structure-Energetics-Dynamics Perspective. Crystal Growth and Design, 2020, 20, 2321-2336.	3.0	1
14	Handling CO2 sorption mechanism in PIL@IL composites. Journal of CO2 Utilization, 2020, 41, 101225.	6.8	12
15	Some practical aspects of heat capacity determination by differential scanning calorimetry. Thermochimica Acta, 2020, 687, 178574.	2.7	11
16	Energetics of Glycine Cocrystal or Salt Formation with Two Regioisomers: Fumaric Acid and Maleic Acid. Crystal Growth and Design, 2019, 19, 5054-5064.	3.0	17
17	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.	2.0	5
18	Tautomer selection through solvate formation: the case of 5-hydroxynicotinic acid. CrystEngComm, 2019, 21, 2220-2233.	2.6	11

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19	Neat ionic liquids versus ionic liquid mixtures: a combination of experimental data and molecular simulation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23305-23309.	2.8	12
20	The Curious Case of Acetaldehyde Phenylhydrazone: Resolution of a 120 Year Old Puzzle where Forms with Vastly Different Melting Points Have the Same Structure. <i>Crystal Growth and Design</i> , 2019, 19, 907-917.	3.0	7
21	A New Thermodynamically Favored Flubendazole/Maleic Acid Binary Crystal Form: Structure, Energetics, and <i>in Silico</i> PBPK Model-Based Investigation. <i>Crystal Growth and Design</i> , 2018, 18, 2377-2386.	3.0	19
22	Extraction Optimization and Structural and Thermal Characterization of the Antimicrobial Abietane 7 $\beta$ -Acetoxy-6 $\beta$ -hydroxyroleanone. <i>Molecular Pharmaceutics</i> , 2018, 15, 1412-1419.	4.6	15
23	Solvation of alcohols in ionic liquids – understanding the effect of the anion and cation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2536-2548.	2.8	17
24	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. <i>Thermochimica Acta</i> , 2018, 659, 82-88.	2.7	4
25	Comparative structural analyses in four ionic liquid systems: the two low- <i>q</i> peaks of IL structure factor functions. <i>Molecular Simulation</i> , 2018, 44, 478-484.	2.0	9
26	Polymorphism in Simvastatin: Twinning, Disorder, and Enantiotropic Phase Transitions. <i>Molecular Pharmaceutics</i> , 2018, 15, 5349-5360.	4.6	17
27	Designing the ammonium cation to achieve a higher hydrophilicity of bistriflimide-based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19307-19313.	2.8	17
28	AGGREGATES: Finding structures in simulation results of solutions. <i>Journal of Computational Chemistry</i> , 2017, 38, 753-765.	3.3	41
29	Polymorphic Phase Transition in 4-Hydroxyacetophenone: Equilibrium Temperature, Kinetic Barrier, and the Relative Stability of <i>Z</i> = 1 and <i>Z</i> = 2 Forms. <i>Crystal Growth and Design</i> , 2017, 17, 1918-1932.	3.0	37
30	ForConX: A forcefield conversion tool based on XML. <i>Journal of Computational Chemistry</i> , 2017, 38, 629-638.	3.3	8
31	Structure–property relationships in protic ionic liquids: a study of solvent–solvent and solvent–solute interactions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28133-28138.	2.8	26
32	Modeling Halogen Bonds in Ionic Liquids: A Force Field for Imidazolium and Halo-Imidazolium Derivatives. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6167-6176.	5.3	10
33	Ionic liquids with anions based on fluorosulfonyl derivatives: from asymmetrical substitutions to a consistent force field model. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29617-29624.	2.8	49
34	Structure–property relationships in protic ionic liquids: a thermochemical study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19928-19936.	2.8	15
35	A new polymorph of 4-hydroxyvalerophenone revealed by thermoanalytical and X-ray diffraction studies. <i>European Physical Journal: Special Topics</i> , 2017, 226, 849-855.	2.6	4
36	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 13) Tj ETOq0 0 0,rgBT /Over 2.0		

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37	The standard molar enthalpy of the base catalysed hydrolysis of methyl paraben revisited. <i>Journal of Chemical Thermodynamics</i> , 2016, 103, 176-180.	2.0	8
38	Additive polarizabilities in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1665-1670.	2.8	37
39	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies. <i>Journal of Chemical Thermodynamics</i> , 2016, 95, 35-48.	2.0	8
40	Mixtures of the 1-ethyl-3-methylimidazolium acetate ionic liquid with different inorganic salts: insights into their interactions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2756-2766.	2.8	12
41	Evaluation of the OPLS-AA Force Field for the Study of Structural and Energetic Aspects of Molecular Organic Crystals. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3023-3034.	2.5	57
42	Size Matters: An Experimental and Computational Study of the Influence of Particle Size on the Lattice Energy of NaCl. <i>Journal of Physical Chemistry C</i> , 2015, 119, 4387-4396.	3.1	5
43	Kinetics and Mechanism of the Thermal Dehydration of a Robust and Yet Metastable Hemihydrate of 4-Hydroxynicotinic Acid. <i>Crystal Growth and Design</i> , 2015, 15, 3511-3524.	3.0	11
44	Modeling the structure and thermodynamics of ferrocenium-based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10200-10208.	2.8	10
45	Solvent effects on the polar network of ionic liquid solutions. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 194116.	1.8	12
46	Thermochemistry of 1-alkylimidazoles. <i>Journal of Chemical Thermodynamics</i> , 2015, 80, 59-64.	2.0	7
47	Thermal Stability of Simvastatin under Different Atmospheres. <i>Journal of Pharmaceutical Sciences</i> , 2014, 103, 241-248.	3.3	9
48	The complex structure of ionic liquids at an atomistic level: from ordered and green to charge templates. <i>Pure and Applied Chemistry</i> , 2014, 86, 119-133.	1.9	15
49	Thermochemistry of 1,1,3,3-tetramethylguanidine and 1,1,3,3-tetramethylguanidinium nitrate. <i>Journal of Chemical Thermodynamics</i> , 2014, 77, 179-189.	2.0	17
50	Structure and Aggregation in the 1-Alkyl-3-Methylimidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid Homologous Series. <i>Journal of Physical Chemistry B</i> , 2014, 118, 567-576.	2.6	223
51	From Molecules to Crystals: The Solvent Plays an Active Role Throughout the Nucleation Pathway of Molecular Organic Crystals. <i>Crystal Growth and Design</i> , 2014, 14, 5436-5441.	3.0	21
52	Structure and Aggregation in the 1,3-Dialkyl-imidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid Family: 2. From Single to Double Long Alkyl Side Chains. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6885-6895.	2.6	65
53	Polymorphism in 4-hydroxyacetophenone: A vibrational analysis. <i>Journal of Molecular Structure</i> , 2014, 1078, 181-187.	3.6	10
54	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox). <i>Journal of Chemical Thermodynamics</i> , 2014, 73, 140-147.	2.0	7

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55	Nano-segregation in ionic liquids: scorpions and vanishing chains. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16256.	2.8	119
56	All-Atom Force Field for Molecular Dynamics Simulations on Organotransition Metal Solids and Liquids. Application to $M(\text{CO})_n$ ( $M = \text{Cr, Fe, Ni, Mo, Ru, or W}$ ) Compounds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11107-11113.	2.5	32
57	High ionicity ionic liquids (HILs): comparing the effect of ethylsulfonate and ethylsulfate anions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18138.	2.8	20
58	Polymorphism in 4-Hydroxybenzaldehyde: A Crystal Packing and Thermodynamic Study. <i>Crystal Growth and Design</i> , 2013, 13, 2803-2814.	3.0	15
59	Energetics and Structure of Simvastatin. <i>Molecular Pharmaceutics</i> , 2013, 10, 2713-2722.	4.6	26
60	Inorganic salts in purely ionic liquid media: the development of high ionicity ionic liquids (HILs). <i>Chemical Communications</i> , 2012, 48, 3656.	4.1	91
61	Heat capacity and thermodynamics of solid and liquid pyridine-3-carboxylic acid (nicotinic acid) over the temperature range 296K to 531K. <i>Journal of Chemical Thermodynamics</i> , 2012, 55, 23-28.	2.0	28
62	A general strategy for the experimental study of the thermochemistry of protic ionic liquids: enthalpy of formation and vaporisation of 1-methylimidazolium ethanoate. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4440.	2.8	22
63	Polymorphism in 4-Hydroxyacetophenone: A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5179-5184.	2.6	14
64	Crystallization of 4-Hydroxyacetophenone from Water: Control of Polymorphism via Phase Diagram Studies. <i>Crystal Growth and Design</i> , 2012, 12, 2932-2941.	3.0	19
65	A Robust yet Metastable New Hemihydrate of 4-Hydroxynicotinic Acid. <i>Crystal Growth and Design</i> , 2011, 11, 2803-2810.	3.0	8
66	The Structure of Aqueous Solutions of a Hydrophilic Ionic Liquid: The Full Concentration Range of 1-Ethyl-3-methylimidazolium Ethylsulfate and Water. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2067-2074.	2.6	142
67	A fully automatic apparatus for thermal analysis of crystallization from solution and metastable zone width determinations. <i>Journal of Thermal Analysis and Calorimetry</i> , 2010, 100, 493-500.	3.6	7
68	Energetics and Structure of Nicotinic Acid (Niacin). <i>Journal of Physical Chemistry B</i> , 2010, 114, 5475-5485.	2.6	39
69	Structure and Energetics of a New Hydrate of 4-Hydroxyacetophenone. <i>Crystal Growth and Design</i> , 2010, 10, 3070-3076.	3.0	12
70	Energetics of Aqueous Solutions of the Ionic Liquid 1-Ethyl-3-methylimidazolium Ethylsulfate. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13179-13188.	2.6	18
71	Mutual Solubility of Water and Structural/Positional Isomers of $N$ -Alkylpyridinium-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15925-15934.	2.6	74
72	A calorimetric system based on the LKB 10700-1 flow microcalorimeter. <i>Measurement Science and Technology</i> , 2009, 20, 075107.	2.6	3

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73	Energetics of the Oa <sup>n</sup> H Bond and of Intramolecular Hydrogen Bonding in HOC <sub>6</sub> H <sub>4</sub> C(O)Y (Y = H, CH <sub>3</sub> , CH <sub>2</sub> CH <sub>2</sub> ), Tj ETQq1 1 0.784314 rgB 10020-10030.	2.5	29
74	Polymorphism in 4- <sup>2</sup> -Hydroxyacetophenone: Structure and Energetics. Crystal Growth and Design, 2008, 8, 2419-2430.	3.0	35
75	Energetics of Cresols and of Methylphenoxy Radicals. Journal of Physical Chemistry A, 2007, 111, 8741-8748.	2.5	25
76	Energetics of C <sup>n</sup> F, C <sup>n</sup> Cl, C <sup>n</sup> Br, and C <sup>n</sup> I Bonds in 2-Haloethanols. Enthalpies of Formation of XCH <sub>2</sub> CH <sub>2</sub> OH (X = F, Cl, Br, I) Compounds and of the 2-Hydroxyethyl Radical. Journal of Physical Chemistry A, 2007, 111, 1713-1720.	2.5	29
77	Thermochemistry of 2- and 4-biphenylmethanol. Journal of Chemical Thermodynamics, 2007, 39, 1384-1391.	2.0	6
78	Energetics of the Thermal Dimerization of Acenaphthylene to Heptacyclene. Journal of Physical Chemistry A, 2006, 110, 2299-2307.	2.5	9
79	Effect of Ring Substitution on the S <sup>n</sup> H Bond Dissociation Enthalpies of Thiophenols. An Experimental and Computational Study. Journal of Physical Chemistry A, 2006, 110, 9949-9958.	2.5	25
80	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.	4.4	50
81	A new calorimetric system to measure heat capacities of solids by the drop method. Measurement Science and Technology, 2006, 17, 1405-1408.	2.6	44