# Carlos Bernardes

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | DMSO/IL solvent systems for cellulose dissolution: Binary or ternary mixtures?. Journal of Molecular Liquids, 2022, 345, 117810. | 2.3 | 6 |
| 2 | Isotropic liquid state of triacylglycerols. Journal of Molecular Liquids, 2022, 353, 118703. | 2.3 | 6 |
| 3 | DLPGEN: Preparing Molecular Dynamics Simulations with Support for Polarizable Force Fields. Journal of Chemical Information and Modeling, 2022, 62, 1471-1478. | 2.5 | 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. | 1.4 | 6 |
| 5 | Real-Time In situ XRD Study of Simvastatin Crystallization in Levitated Droplets. Crystal Growth and Design, 2021, 21, 4665-4673. | 1.4 | 6 |
| 6 | 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 |
| 7 | The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach. ChemPhysChem, 2021, 22, 2190-2200. | 1.0 | 9 |
| 8 | First and Second Dissociation Enthalpies in Bi-Component Crystals Consisting of Maleic Acid and L-Phenylalanine. Molecules, 2021, 26, 5714. | 1.7 | 3 |
| 9 | 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 |
| 10 | 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 |
| 11 | Towards the development of nanosprings from confined carbyne chains. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 117, 113831. | 1.3 | 9 |
| 12 | Tuning the miscibility of water in imide-based ionic liquids. Physical Chemistry Chemical Physics, 2020, 22, 25236-25242. | 1.3 | 6 |
| 13 | Conformational and Nonconformational Polymorphism in 4â€²-Hydroxyvalerophenone: A Structureâ€“Energeticsâ€“Dynamics Perspective. Crystal Growth and Design, 2020, 20, 2321-2336. | 1.4 | 1 |
| 14 | Handling CO2 sorption mechanism in PIL@IL composites. Journal of CO2 Utilization, 2020, 41, 101225. | 3.3 | 12 |
| 15 | Some practical aspects of heat capacity determination by differential scanning calorimetry. Thermochimica Acta, 2020, 687, 178574. | 1.2 | 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. | 1.4 | 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. | 1.0 | 5 |
| 18 | Tautomer selection through solvate formation: the case of 5-hydroxynicotinic acid. CrystEngComm, 2019, 21, 2220-2233. | 1.3 | 11 |

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|---|---|---|---|
| 19 | 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 |
| 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. Crystal Growth and Design, 2019, 19, 907-917. | 1.4 | 7 |
| 21 | 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 |
| 22 | Extraction Optimization and Structural and Thermal Characterization of the Antimicrobial Abietane 7Î±-Acetoxy-6Î²-hydroxyroyleanone. Molecular Pharmaceutics, 2018, 15, 1412-1419. | 2.3 | 15 |
| 23 | 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 |
| 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. Thermochimica Acta, 2018, 659, 82-88. | 1.2 | 4 |
| 25 | 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 |
| 26 | Polymorphism in Simvastatin: Twinning, Disorder, and Enantiotropic Phase Transitions. Molecular Pharmaceutics, 2018, 15, 5349-5360. | 2.3 | 17 |
| 27 | 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 |
| 28 | AGGREGATES: Finding structures in simulation results of solutions. Journal of Computational Chemistry, 2017, 38, 753-765. | 1.5 | 41 |
| 29 | 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 |
| 30 | ForConX: A forcefield conversion tool based on XML. Journal of Computational Chemistry, 2017, 38, 629-638. | 1.5 | 8 |
| 31 | 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 |
| 32 | 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 |
| 33 | 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 |
| 34 | Structureâ€“property relationships in protic ionic liquids: a thermochemical study. Physical Chemistry Chemical Physics, 2017, 19, 19928-19936. | 1.3 | 15 |
| 35 | 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 |
| 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) Tj ETQq0 0 0 rgBT /Over | 1.0 | 9 |

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|---|---|---|---|
| 37 | The standard molar enthalpy of the base catalysed hydrolysis of methyl paraben revisited. Journal of Chemical Thermodynamics, 2016, 103, 176-180. | 1.0 | 8 |
| 38 | Additive polarizabilities in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1665-1670. | 1.3 | 37 |
| 39 | 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 |
| 40 | 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 |
| 41 | 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 |
| 42 | 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 |
| 43 | 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 |
| 44 | Modeling the structure and thermodynamics of ferrocenium-based ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 10200-10208. | 1.3 | 10 |
| 45 | Solvent effects on the polar network of ionic liquid solutions. Journal of Physics Condensed Matter, 2015, 27, 194116. | 0.7 | 12 |
| 46 | Thermochemistry of 1-alkylimidazoles. Journal of Chemical Thermodynamics, 2015, 80, 59-64. | 1.0 | 7 |
| 47 | Thermal Stability of Simvastatin under Different Atmospheres. Journal of Pharmaceutical Sciences, 2014, 103, 241-248. | 1.6 | 9 |
| 48 | 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 |
| 49 | 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 |
| 50 | 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 |
| 51 | 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 |
| 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. Journal of Physical Chemistry B, 2014, 118, 6885-6895. | 1.2 | 65 |
| 53 | Polymorphism in 4â€²-hydroxyacetophenone: A vibrational analysis. Journal of Molecular Structure, 2014, 1078, 181-187. | 1.8 | 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). Journal of Chemical Thermodynamics, 2014, 73, 140-147. | 1.0 | 7 |

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|---|---|---|---|
| 55 | Nano-segregation in ionic liquids: scorpions and vanishing chains. Physical Chemistry Chemical Physics, 2013, 15, 16256. | 1.3 | 119 |
| 56 | All-Atom Force Field for Molecular Dynamics Simulations on Organotransition Metal Solids and Liquids. Application to M(CO)<sub>n</sub> (MÂ= Cr, Fe, Ni, Mo, Ru, or W) Compounds. Journal of Physical Chemistry A, 2013, 117, 11107-11113. | 1.1 | 32 |
| 57 | High ionicity ionic liquids (HIILs): comparing the effect of ethylsulfonate and ethylsulfate anions. Physical Chemistry Chemical Physics, 2013, 15, 18138. | 1.3 | 20 |
| 58 | Polymorphism in 4-Hydroxybenzaldehyde: A Crystal Packing and Thermodynamic Study. Crystal Growth and Design, 2013, 13, 2803-2814. | 1.4 | 15 |
| 59 | Energetics and Structure of Simvastatin. Molecular Pharmaceutics, 2013, 10, 2713-2722. | 2.3 | 26 |
| 60 | Inorganic salts in purely ionic liquid media: the development of high ionicity ionic liquids (HIILs). Chemical Communications, 2012, 48, 3656. | 2.2 | 91 |
| 61 | 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 |
| 62 | 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 |
| 63 | Polymorphism in 4â€²-Hydroxyacetophenone: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2012, 116, 5179-5184. | 1.2 | 14 |
| 64 | 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 |
| 65 | A Robust yet Metastable New Hemihydrate of 4-Hydroxynicotinic Acid. Crystal Growth and Design, 2011, 11, 2803-2810. | 1.4 | 8 |
| 66 | 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 |
| 67 | 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 |
| 68 | Energetics and Structure of Nicotinic Acid (Niacin). Journal of Physical Chemistry B, 2010, 114, 5475-5485. | 1.2 | 39 |
| 69 | Structure and Energetics of a New Hydrate of 4â€²-Hydroxyacetophenone. Crystal Growth and Design, 2010, 10, 3070-3076. | 1.4 | 12 |
| 70 | 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 |
| 71 | 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 |
| 72 | A calorimetric system based on the LKB 10700-1 flow microcalorimeter. Measurement Science and Technology, 2009, 20, 075107. | 1.4 | 3 |

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|---|---|---|---|
| 73 | Energetics of the Oâ¯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>CHâ•CH<sub>2</sub>,) Tj ETQq1 1 0.784314 rgBT 10029-10039. | 1.1 | 29 |
| 74 | Polymorphism in 4â€²-Hydroxyacetophenone: Structure and Energetics. Crystal Growth and Design, 2008, 8, 2419-2430. | 1.4 | 35 |
| 75 | Energetics of Cresols and of Methylphenoxyl Radicals. Journal of Physical Chemistry A, 2007, 111, 8741-8748. | 1.1 | 25 |
| 76 | Energetics of Câ¯F, Câ¯Cl, Câ¯Br, and Câ¯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 |
| 77 | Thermochemistry of 2- and 4-biphenylmethanol. Journal of Chemical Thermodynamics, 2007, 39, 1384-1391. | 1.0 | 6 |
| 78 | Energetics of the Thermal Dimerization of Acenaphthylene to Heptacyclene. Journal of Physical Chemistry A, 2006, 110, 2299-2307. | 1.1 | 9 |
| 79 | Effect of Ring Substitution on the Sâ¯H Bond Dissociation Enthalpies of Thiophenols. An Experimental and Computational Study. Journal of Physical Chemistry A, 2006, 110, 9949-9958. | 1.1 | 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. | 2.2 | 50 |
| 81 | 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 |