Manuel E Minas Da Piedade

List of Publications by Year
in descending order

119 papers	2,599 citations	185998 28 h-index	264894 42 g-index
122 all docs	122 docs citations	122 times ranked	2628 citing authors

#	Article	IF	Citations
1	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
2	Exploratory Study on Lercanidipine Hydrochloride Polymorphism: pH-Dependent Solubility Behavior and Simulation of its Impact on Pharmacokinetics. AAPS PharmSciTech, 2021, 22, 54.	1.5	1
3	Real-Time In situ XRD Study of Simvastatin Crystallization in Levitated Droplets. Crystal Growth and Design, 2021, 21, 4665-4673.	1.4	6
4	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
5	First and Second Dissociation Enthalpies in Bi-Component Crystals Consisting of Maleic Acid and L-Phenylalanine. Molecules, 2021, 26, 5714.	1.7	3
6	Conformational and Nonconformational Polymorphism in 4â€²-Hydroxyvalerophenone: A Structureâ€“Energeticsâ€“Dynamics Perspective. Crystal Growth and Design, 2020, 20, 2321-2336.	1.4	1
7	Some practical aspects of heat capacity determination by differential scanning calorimetry. Thermochimica Acta, 2020, 687, 178574.	1.2	11
8	Mechanistic Insights into a Sustainable Mechanochemical Synthesis of Ettringite. ChemistryOpen, 2019, 8, 1012-1019.	0.9	3
9	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
10	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
11	Tautomer selection through solvate formation: the case of 5-hydroxynicotinic acid. CrystEngComm, 2019, 21, 2220-2233.	1.3	11
12	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
13	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
14	Extraction Optimization and Structural and Thermal Characterization of the Antimicrobial Abietane 7Î±-Acetoxy-6Î²-hydroxyroyleanone. Molecular Pharmaceutics, 2018, 15, 1412-1419.	2.3	15
15	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
16	Polymorphism in Simvastatin: Twinning, Disorder, and Enantiotropic Phase Transitions. Molecular Pharmaceutics, 2018, 15, 5349-5360.	2.3	17
17	Irreversible Magnetic Behaviour Caused by the Thermosalient Phenomenon in an Iron(III) Spin Crossover Complex. European Journal of Inorganic Chemistry, 2018, 2018, 2976-2983.	1.0	17
18	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

#	Article	IF	Citations
19	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
20	Structureâ€“property relationships in protic ionic liquids: a thermochemical study. Physical Chemistry Chemical Physics, 2017, 19, 19928-19936.	1.3	15
21	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
22	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
23	The standard molar enthalpy of the base catalysed hydrolysis of methyl paraben revisited. Journal of Chemical Thermodynamics, 2016, 103, 176-180.	1.0	8
24	Stability and safety of quercetin-loaded cationic nanoemulsion: In vitro and in vivo assessments. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2016, 506, 591-599.	2.3	30
25	Dynamic spin interchange in a tridentate Fe(<scp>iii</scp>) Schiff-base compound. Chemical Science, 2016, 7, 4251-4258.	3.7	43
26	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
27	A high loaded cationic nanoemulsion for quercetin delivery obtained by sub-PIT method. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2016, 489, 256-264.	2.3	34
28	Gasâ€Phase Affinity Scales for Typical Ionic Liquid Moieties Determined by using Cooksâ€™ Kinetic Method. ChemPhysChem, 2015, 16, 1969-1977.	1.0	9
29	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
30	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
31	Thermochemistry of 1-alkylimidazoles. Journal of Chemical Thermodynamics, 2015, 80, 59-64.	1.0	7
32	Thermal Stability of Simvastatin under Different Atmospheres. Journal of Pharmaceutical Sciences, 2014, 103, 241-248.	1.6	9
33	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
34	Enthalpy of Formation of Anisole: Implications for the Controversy on the Oâ€“H Bond Dissociation Enthalpy in Phenol. Journal of Physical Chemistry A, 2014, 118, 11026-11032.	1.1	28
35	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
36	Polymorphism in 4â€²-hydroxyacetophenone: A vibrational analysis. Journal of Molecular Structure, 2014, 1078, 181-187.	1.8	10

#	Article	IF	Citations
37	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
38	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
39	Polymorphism in 4-Hydroxybenzaldehyde: A Crystal Packing and Thermodynamic Study. Crystal Growth and Design, 2013, 13, 2803-2814.	1.4	15
40	Energetics and Structure of Simvastatin. Molecular Pharmaceutics, 2013, 10, 2713-2722.	2.3	26
41	Direct experimental observation of the aggregation of Î±-amino acids into 100â€“200 nm clusters in aqueous solution. RSC Advances, 2012, 2, 4690.	1.7	44
42	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
43	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
44	Polymorphism in 4â€²-Hydroxyacetophenone: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2012, 116, 5179-5184.	1.2	14
45	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
46	Solubility of nicotinic acid in water, ethanol, acetone, diethyl ether, acetonitrile, and dimethyl sulfoxide. Journal of Chemical Thermodynamics, 2012, 47, 362-371.	1.0	54
47	A Robust yet Metastable New Hemihydrate of 4-Hydroxynicotinic Acid. Crystal Growth and Design, 2011, 11, 2803-2810.	1.4	8
48	Potentiometric Titration Study of the Temperature and Ionic Strength Dependence of the Acidity Constants of Nicotinic Acid (Niacin). Journal of Chemical & Engineering Data, 2011, 56, 2964-2970.	1.0	30
49	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
50	Thermodynamic Characterization of Three Polymorphic Forms of Piracetam. Journal of Pharmaceutical Sciences, 2011, 100, 594-603.	1.6	20
51	Thermochemistry of aqueous pyridine-3-carboxylic acid (nicotinic acid). Journal of Chemical Thermodynamics, 2011, 43, 974-979.	1.0	13
52	Thermochemistry of paracetamol. Journal of Thermal Analysis and Calorimetry, 2010, 100, 391-401.	2.0	33
53	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
54	Thermoanalytical and structural characterization of fluoridated calcium phosphates prepared in anhydrous alcohols. Journal of Thermal Analysis and Calorimetry, 2010, 100, 509-517.	2.0	1

#	Article	IF	Citations
55	Vaporisation of a Dicationic Ionic Liquid Revisited. ChemPhysChem, 2010, 11, 3673-3677.	1.0	23
56	Energetics and Structure of Nicotinic Acid (Niacin). Journal of Physical Chemistry B, 2010, 114, 5475-5485.	1.2	39
57	Structure and Energetics of a New Hydrate of 4â€²-Hydroxyacetophenone. Crystal Growth and Design, 2010, 10, 3070-3076.	1.4	12
58	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
59	The Nature of Protic Ionic Liquids in the Gas Phase Revisited: Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Study of 1,1,3,3-Tetramethylguanidinium Chloride. Journal of Physical Chemistry B, 2010, 114, 8905-8909.	1.2	30
60	A calorimetric system based on the LKB 10700-1 flow microcalorimeter. Measurement Science and Technology, 2009, 20, 075107.	1.4	3
61	Energetics and Structure of Hydroxynicotinic Acids. Crystal Structures of 2-, 4-, 6-Hydroxynicotinic and 5-Chloro-6-hydroxynicotinic Acids. Journal of Physical Chemistry B, 2009, 113, 14291-14309.	1.2	21
62	Bridging the Gap between Ionic Liquids and Molten Salts: Group 1 Metal Salts of the Bistriflamide Anion in the Gas Phase. Journal of Physical Chemistry B, 2009, 113, 3491-3498.	1.2	27
63	Energetics of Calcium Phosphate Nanoparticle Formation by the Reaction of Ca(NO₃)₂with (NH₄)₂HPO₄. Journal of Physical Chemistry C, 2009, 113, 5478-5484.	1.5	12
64	Energetics of the Oâ^'H Bond and of Intramolecular Hydrogen Bonding in HOC₆H₄C(O)Y (Y = H, CH₃, CH₂CHâ•CH₂,) Tj ETQq0 0 0 rgBT /Overlo 19029-19039	1.1	29
65	Experimental and Molecular Dynamics Simulation Study of the Sublimation and Vaporization Energetics of Iron Metalocenes. Crystal Structures of Fe(Î·⁵-C₅H₄CH₃)₂ and		

#	Article	IF	Citations
73	An All-Atom Force Field for Metallocenes. Journal of Physical Chemistry A, 2006, 110, 13850-13856.	1.1	35
74	Determination of Acidity Constants by Gradient Flow-Injection Titration. Journal of Chemical Education, 2006, 83, 1853.	1.1	1
75	Energetics of the Thermal Dimerization of Acenaphthylene to Heptacyclene. Journal of Physical Chemistry A, 2006, 110, 2299-2307.	1.1	9
76	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
77	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
78	Standard molar enthalpies of formation of hydroxy-, chlor-, and bromapatite. Journal of Chemical Thermodynamics, 2005, 37, 1061-1070.	1.0	26
79	Enthalpies of formation and lattice enthalpies of alkaline metal acetates. Thermochimica Acta, 2005, 428, 131-136.	1.2	21
80	Energetics of Hydroxybenzoic Acids and of the Corresponding Carboxyphenoxyl Radicals. Intramolecular Hydrogen Bonding in 2-Hydroxybenzoic Acid. Journal of Physical Chemistry A, 2005, 109, 9700-9708.	1.1	33
81	A Molecular Dynamics Study of the Thermodynamic Properties of Calcium Apatites. 1. Hexagonal Phases. Journal of Physical Chemistry B, 2005, 109, 24473-24479.	1.2	44
82	Energetics of the interaction of the antitumour agent titanocene dichloride with glycine: enthalpy of formation of [Ti(Î·5-C5H5)2(OOCCH2NH3)2]Cl2. Journal of Chemical Thermodynamics, 2004, 36, 321-323.	1.0	1
83	Energetics of Intramolecular Hydrogen Bonding in Di-substituted Benzenes by the orthoâ''para Method. Journal of Physical Chemistry A, 2004, 108, 10834-10843.	1.1	94
84	Bonding Energetics in Alkaline Metal Alkoxides and Phenoxides. Chemistry - A European Journal, 2003, 9, 2095-2101.	1.7	17
85	Enthalpy of formation of monoclinic 2-hydroxybenzoic acid. Journal of Chemical Thermodynamics, 2003, 35, 177-188.	1.0	21
86	Energetics of the Câ''Cl Bond in CH3CH(Cl)COOH. Enthalpy of Formation of (S)-(â'')-2-Chloropropionic Acid and of the 1-Carboxyethyl Radicalâ€,â€¡. Journal of Physical Chemistry A, 2002, 106, 9855-9861.	1.1	7
87	Driving Force for the Thermally Induced Solid State Polymerization of Alkali Metal Halogenoacetates:Â A Thermochemical Analysis. Journal of Physical Chemistry B, 2002, 106, 10764-10770.	1.2	7
88	The Aromaticity of Pyracylene:Â An Experimental and Computational Study of the Energetics of the Hydrogenation of Acenaphthylene and Pyracylene. Journal of the American Chemical Society, 2002, 124, 2065-2072.	6.6	39
89	Enthalpy of formation of benzo[k]fluoranthene. Journal of Chemical Thermodynamics, 2002, 34, 173-184.	1.0	17
90	On the transferability of Irî—¸I bond enthalpies between [Ir(Î¼-StBu)(I)2(CO)2]2 and trans-[Ir(X)(I)2(CO)(PPh3)2]¯ (X=F, Cl, Br, I) complexes. Journal of Organometallic Chemistry, 2002, 662, 105-111.	0.8	6

#	Article	IF	Citations
91	Porous poly(D,L-lactide) and poly(D,L-lactide-co-glycolide) produced by thermal salt elimination from halogenocarboxylatesElectronic supplementary information (ESI) available: detailed results of the combustion calorimetric experiments. See http://www.rsc.org/suppdata/dt/b1/b104979h/. Dalton Transactions RSC, 2001, , 3140-3148.	2.3	8
92	Organometallic thermochemistry at CQE-IST. An overview. Journal of Organometallic Chemistry, 2001, 632, 188-196.	0.8	14
93	Synthesis of novel polyurethanes from sugars and 1,6-hexamethylene diisocyanate. Carbohydrate Polymers, 2001, 45, 123-127.	5.1	41
94	The standard molar enthalpy of sublimation ofÎ·5-bis-pentamethylcyclopentadienyl iron measured with an electrically calibrated vacuum-drop sublimation microcalorimetric apparatus. Journal of Chemical Thermodynamics, 2001, 33, 11-21.	1.0	48
95	Energetics of Câ^'Cl, Câ^'Br, and Câ^'I Bonds in Haloacetic Acids: Enthalpies of Formation of XCH2COOH (X=Cl, Br, I) Compounds and the Carboxymethyl Radical. Chemistry - A European Journal, 2001, 7, 483-489.	1.7	22
96	The determination of the standard molar enthalpy of formation of 4-chlorobenzoic acid by micro rotating-bomb combustion calorimetry. Journal of Chemical Thermodynamics, 1999, 31, 1417-1427.	1.0	17
97	Oxygen Bomb Combustion Calorimetry: Principles and Applications to Organic and Organometallic Compounds. , 1999, , 29-53.		2
98	Atomic Emission Spectra Using a UV-Vis Spectrophotometer and an Optical Fiber Guided Light Source. Journal of Chemical Education, 1998, 75, 1013.	1.1	5
99	Enthalpy of formation of C70. Journal of Physics and Chemistry of Solids, 1997, 58, 1965-1971.	1.9	13
100	The Enthalpy of Formation of Pyracylene. Journal of Organic Chemistry, 1996, 61, 6733-6734.	1.7	11
101	Energetics of the oxidative addition of I2 to [Ir(Îœ-L)(CO)2]2 (L=S t Bu, 3,5-Me2pz,7-aza) complexes. X-ray structures of Ir(Îœ-S t Bu)(I)(CO)2]2 and [Ir(Îœ-3,5-Me2pz)(I)(CO)2]2. Structural Chemistry, 1996, 7, 337-354.	1.0	11
102	Energetics of organometallic species: the entropic factor. Journal of Organometallic Chemistry, 1996, 518, 167-180.	0.8	30
103	A Short and Illustrated Guide to Metal-Alkyl Bonding Energetics. , 1996, , 169-195.		1
104	A micro-combustion calorimeter suitable for samples of mass 10 mg to 50 mg. Application to solid compounds of C, H, and O, and of C, H, O, and N. Journal of Chemical Thermodynamics, 1995, 27, 197-206.	1.0	35
105	Standard enthalpy of formation and enthalpy of vaporization of di-1,1-dimethylethyl peroxide Re-evaluation of the standard enthalpy of formation of the di-1,1-dimethylethoxy radical. Journal of Chemical Thermodynamics, 1995, 27, 597-604.	1.0	35
106	Ebulliometric apparatus for the measurement of enthalpies of vaporization. Thermochimica Acta, 1995, 249, 113-120.	1.2	20
107	The enthalpy of sublimation of diphenylacetylene from Knudsen effusion studies. Thermochimica Acta, 1993, 228, 15-22.	1.2	27
108	Intermolecular forces in solution and lattice energies of ionic crystals: Calorimetric experiments for the physical chemistry undergraduate laboratory. Journal of Chemical Education, 1993, 70, A227.	1.1	25

#	Article	IF	Citations
109	Enthalpies of formation of buckminsterfullerene (C60) and of the parent ions C60 +, C60 2+, C60 3+ and C60 ?. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 3541.	1.7	64
110	Thermochemistry of zirconium and niobium organometallic compounds. Journal of the American Chemical Society, 1993, 115, 2764-2774.	6.6	24
111	A reaction-solution calorimeter for the undergraduate laboratory. Journal of Chemical Education, 1992, 69, 940.	1.1	4
112	Mechanistic studies on DNA photolyase. 4. The enthalpy of cleavage of a model photodimer. Journal of Organic Chemistry, 1991, 56, 7340-7341.	1.7	24
113	Syntheses, electrochemistry, and bonding of bis(cyclopentadienyl)molybdenum alkyl complexes. Molecular structure of Mo(.eta.5-C5H5)2(C4H9)2. Thermochemistry of Mo(.eta.5-C5H5)2R2 and Mo(.eta.5-C5H5)2L (R = CH3, C2H5, C4H9; L = ethylene, diphenylacetylene). Organometallics, 1991, 10, 483-494.	1.1	23
114	Standard enthalpies of formation of gaseous dicyclopentadienyl-molybdenum and -tungsten dihyrides. Journal of Organometallic Chemistry, 1990, 391, 361-366.	0.8	10
115	Energetics of molybdenum-azobenzene, titanium-azobenzene, titanium-iodide, and titanium-carbonyl bonds in bis(cyclopentadienyl) complexes [Erratum to document cited in CA107(5):39888y]. Organometallics, 1988, 7, 246-246.	1.1	0
116	Studies on the transferability of transition-metal-carbon and -hydrogen bond enthalpies in bis(cyclopentadienyl) complexes. Organometallics, 1987, 6, 734-738.	1.1	14
117	Energetics of molybdenum-azobenzene, titanium-azobenzene, titanium-iodide, and titanium-carbonyl bonds in bis(cyclopentadienyl) complexes. Organometallics, 1987, 6, 1427-1432.	1.1	15
118	Enthalpy of formation of dicyclopentadienyltungsten dichloride by rotating-bomb calorimetry. Journal of Chemical Thermodynamics, 1987, 19, 195-199.	1.0	5
119	Enthalpy of formation of tetrabromomethane by rotating-bomb calorimetry. Journal of Chemical Thermodynamics, 1984, 16, 661-668.	1.0	20