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	The Nature of Ionic Liquids in the Gas Phase. Journal of Physical Chemistry A, 2007, 111, 6176-6182.	1.1	201
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	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
4	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
5	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
6	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
7	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
8	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
9	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
10	Dynamic spin interchange in a tridentate Fe(<scp>iii</scp>) Schiff-base compound. Chemical Science, 2016, 7, 4251-4258.	3.7	43
11	Synthesis of novel polyurethanes from sugars and 1,6-hexamethylene diisocyanate. Carbohydrate Polymers, 2001, 45, 123-127.	5.1	41
12	Experimental and Molecular Dynamics Simulation Study of the Sublimation and Vaporization Energetics of Iron Metalocenes. Crystal Structures of Fe(Î·⁵-C₅H₄CH₃)₂ and		

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19	Polymorphism in 4â€²-Hydroxyacetophenone: Structure and Energetics. Crystal Growth and Design, 2008, 8, 2419-2430.	1.4	35
20	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
21	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
22	Thermochemistry of paracetamol. Journal of Thermal Analysis and Calorimetry, 2010, 100, 391-401.	2.0	33
23	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
24	Energetics of organometallic species: the entropic factor. Journal of Organometallic Chemistry, 1996, 518, 167-180.	0.8	30
25	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
26	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
27	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
28	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
29	Energetics of the Oâ€“H Bond and of Intramolecular Hydrogen Bonding in HOC₆H₄C(O)Y (Y = H, CH₃, CH₂CHâ•CH₂,) Tj ETQq1 1 0.784314 rgBT 10020 10020.	1.1	29
30	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
31	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
32	The enthalpy of sublimation of diphenylacetylene from Knudsen effusion studies. Thermochimica Acta, 1993, 228, 15-22.	1.2	27
33	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
34	Standard molar enthalpies of formation of hydroxy-, chlor-, and bromapatite. Journal of Chemical Thermodynamics, 2005, 37, 1061-1070.	1.0	26
35	Energetics and Structure of Simvastatin. Molecular Pharmaceutics, 2013, 10, 2713-2722.	2.3	26
36	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

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37	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
38	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
39	Energetics of Cresols and of Methylphenoxyl Radicals. Journal of Physical Chemistry A, 2007, 111, 8741-8748.	1.1	25
40	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
41	Thermochemistry of zirconium and niobium organometallic compounds. Journal of the American Chemical Society, 1993, 115, 2764-2774.	6.6	24
42	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
43	Vaporisation of a Dicationic Ionic Liquid Revisited. ChemPhysChem, 2010, 11, 3673-3677.	1.0	23
44	Molecular Energetics. , 2008, , .		23
45	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
46	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
47	Enthalpy of formation of monoclinic 2-hydroxybenzoic acid. Journal of Chemical Thermodynamics, 2003, 35, 177-188.	1.0	21
48	Enthalpies of formation and lattice enthalpies of alkaline metal acetates. Thermochimica Acta, 2005, 428, 131-136.	1.2	21
49	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
50	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
51	Enthalpy of formation of tetrabromomethane by rotating-bomb calorimetry. Journal of Chemical Thermodynamics, 1984, 16, 661-668.	1.0	20
52	Ebulliometric apparatus for the measurement of enthalpies of vaporization. Thermochimica Acta, 1995, 249, 113-120.	1.2	20
53	Thermodynamic Characterization of Three Polymorphic Forms of Piracetam. Journal of Pharmaceutical Sciences, 2011, 100, 594-603.	1.6	20
54	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

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55	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
56	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
57	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
58	Enthalpy of formation of benzo[k]fluoranthene. Journal of Chemical Thermodynamics, 2002, 34, 173-184.	1.0	17
59	Bonding Energetics in Alkaline Metal Alkoxides and Phenoxides. Chemistry - A European Journal, 2003, 9, 2095-2101.	1.7	17
60	Experimental and Molecular Dynamics Simulation Study of the Sublimation Energetics of Cyclopentadienyltricarbonylmanganese (Cymantrene). Journal of Physical Chemistry A, 2008, 112, 10429-10434.	1.1	17
61	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
62	Polymorphism in Simvastatin: Twinning, Disorder, and Enantiotropic Phase Transitions. Molecular Pharmaceutics, 2018, 15, 5349-5360.	2.3	17
63	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
64	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
65	Energetics of molybdenum-azobenzene, titanium-azobenzene, titanium-iodide, and titanium-carbonyl bonds in bis(cyclopentadienyl) complexes. Organometallics, 1987, 6, 1427-1432.	1.1	15
66	Polymorphism in 4-Hydroxybenzaldehyde: A Crystal Packing and Thermodynamic Study. Crystal Growth and Design, 2013, 13, 2803-2814.	1.4	15
67	Structureâ€“property relationships in protic ionic liquids: a thermochemical study. Physical Chemistry Chemical Physics, 2017, 19, 19928-19936.	1.3	15
68	Extraction Optimization and Structural and Thermal Characterization of the Antimicrobial Abietane 7Î±-Acetoxy-6Î²-hydroxyroyleanone. Molecular Pharmaceutics, 2018, 15, 1412-1419.	2.3	15
69	Studies on the transferability of transition-metal-carbon and -hydrogen bond enthalpies in bis(cyclopentadienyl) complexes. Organometallics, 1987, 6, 734-738.	1.1	14
70	Organometallic thermochemistry at CQE-IST. An overview. Journal of Organometallic Chemistry, 2001, 632, 188-196.	0.8	14
71	Polymorphism in 4â€²-Hydroxyacetophenone: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2012, 116, 5179-5184.	1.2	14
72	Enthalpy of formation of C70. Journal of Physics and Chemistry of Solids, 1997, 58, 1965-1971.	1.9	13

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73	Thermochemistry of aqueous pyridine-3-carboxylic acid (nicotinic acid). Journal of Chemical Thermodynamics, 2011, 43, 974-979.	1.0	13
74	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
75	Structure and Energetics of a New Hydrate of 4â€²-Hydroxyacetophenone. Crystal Growth and Design, 2010, 10, 3070-3076.	1.4	12
76	The Enthalpy of Formation of Pyracylene. Journal of Organic Chemistry, 1996, 61, 6733-6734.	1.7	11
77	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
78	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
79	Tautomer selection through solvate formation: the case of 5-hydroxynicotinic acid. CrystEngComm, 2019, 21, 2220-2233.	1.3	11
80	Some practical aspects of heat capacity determination by differential scanning calorimetry. Thermochimica Acta, 2020, 687, 178574.	1.2	11
81	Standard enthalpies of formation of gaseous dicyclopentadienyl-molybdenum and -tungsten dihyrides. Journal of Organometallic Chemistry, 1990, 391, 361-366.	0.8	10
82	Polymorphism in 4â€²-hydroxyacetophenone: A vibrational analysis. Journal of Molecular Structure, 2014, 1078, 181-187.	1.8	10
83	Energetics of the Thermal Dimerization of Acenaphthylene to Heptacyclene. Journal of Physical Chemistry A, 2006, 110, 2299-2307.	1.1	9
84	Thermal Stability of Simvastatin under Different Atmospheres. Journal of Pharmaceutical Sciences, 2014, 103, 241-248.	1.6	9
85	Gasâ€Phase Affinity Scales for Typical Ionic Liquid Moieties Determined by using Cooksâ€™ Kinetic Method. ChemPhysChem, 2015, 16, 1969-1977.	1.0	9
86	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
87	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
88	A Robust yet Metastable New Hemihydrate of 4-Hydroxynicotinic Acid. Crystal Growth and Design, 2011, 11, 2803-2810.	1.4	8
89	The standard molar enthalpy of the base catalysed hydrolysis of methyl paraben revisited. Journal of Chemical Thermodynamics, 2016, 103, 176-180.	1.0	8
90	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

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91	Energetics of the Câˆ'Cl Bond in CH3CH(Cl)COOH. Enthalpy of Formation of (S)-(âˆ')-2-Chloropropionic Acid and of the 1-Carboxyethyl Radicalâ€,â€¡. Journal of Physical Chemistry A, 2002, 106, 9855-9861.	1.1	7
92	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
93	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
94	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
95	Thermochemistry of 1-alkylimidazoles. Journal of Chemical Thermodynamics, 2015, 80, 59-64.	1.0	7
96	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
97	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
98	Thermochemistry of 2- and 4-biphenylmethanol. Journal of Chemical Thermodynamics, 2007, 39, 1384-1391.	1.0	6
99	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
100	Real-Time In situ XRD Study of Simvastatin Crystallization in Levitated Droplets. Crystal Growth and Design, 2021, 21, 4665-4673.	1.4	6
101	Enthalpy of formation of dicyclopentadienyltungsten dichloride by rotating-bomb calorimetry. Journal of Chemical Thermodynamics, 1987, 19, 195-199.	1.0	5
102	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
103	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
104	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
105	A reaction-solution calorimeter for the undergraduate laboratory. Journal of Chemical Education, 1992, 69, 940.	1.1	4
106	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
107	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
108	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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109	Mechanistic Insights into a Sustainable Mechanochemical Synthesis of Ettringite. ChemistryOpen, 2019, 8, 1012-1019.	0.9	3
110	First and Second Dissociation Enthalpies in Bi-Component Crystals Consisting of Maleic Acid and L-Phenylalanine. Molecules, 2021, 26, 5714.	1.7	3
111	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
112	Oxygen Bomb Combustion Calorimetry: Principles and Applications to Organic and Organometallic Compounds. , 1999, , 29-53.		2
113	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
114	Determination of Acidity Constants by Gradient Flow-Injection Titration. Journal of Chemical Education, 2006, 83, 1853.	1.1	1
115	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
116	Conformational and Nonconformational Polymorphism in 4â€²-Hydroxyvalerophenone: A Structureâ€“Energeticsâ€“Dynamics Perspective. Crystal Growth and Design, 2020, 20, 2321-2336.	1.4	1
117	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
118	A Short and Illustrated Guide to Metal-Alkyl Bonding Energetics. , 1996, , 169-195.		1
119	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