Margarida S Miranda

List of Publications by Year
in descending order

76 papers	1,460 citations	361413 20 h-index	377865 34 g-index
76 all docs	76 docs citations	76 times ranked	1481 citing authors

#	Article	IF	Citations
1	The degradation products of UV filters in aqueous and chlorinated aqueous solutions. Water Research, 2012, 46, 3167-3176.	11.3	133
2	Photodegradation of avobenzone: Stabilization effect of antioxidants. Journal of Photochemistry and Photobiology B: Biology, 2014, 140, 36-40.	3.8	131
3	The Enthalpies of Formation of o-, m-, and p-Benzoquinone:â€‰ Gas-Phase Ion Energetics, Combustion Calorimetry, and Quantum Chemical Computations Combined. Journal of the American Chemical Society, 2005, 127, 6116-6122.	13.7	72
4	CdSe quantum dots capped PAMAM dendrimer nanocomposites for sensing nitroaromatic compounds. Talanta, 2011, 83, 1335-1340.	5.5	56
5	Thermochemical Study of the Methoxy- and Dimethoxyphenol Isomers. Journal of Chemical & Engineering Data, 2003, 48, 669-679.	1.9	50
6	Thiolated DAB dendrimers and CdSe quantum dots nanocomposites for Cd(II) or Pb(II) sensing. Talanta, 2012, 88, 403-407.	5.5	48
7	Are isatin and isatoic anhydride antiaromatic and aromatic respectively? A combined experimental and theoretical investigation. Organic and Biomolecular Chemistry, 2003, 1, 2566.	2.8	40
8	Experimental and computational thermochemistry of three nitrogen-containing heterocycles: 2-benzimidazolinone, 2-benzoxazolinone and 3-indazolinone. Molecular Physics, 2006, 104, 325-334.	1.7	38
9	Energetics of Coumarin and Chromone. Journal of Physical Chemistry B, 2009, 113, 11216-11221.	2.6	38
10	Development of Inhalable Superparamagnetic Iron Oxide Nanoparticles (SPIONs) in Microparticulate System for Antituberculosis Drug Delivery. Advanced Healthcare Materials, 2018, 7, e1800124.	7.6	34
11	Saccharin: a combined experimental and computational thermochemical investigation of a sweetener and sulfonamide. Molecular Physics, 2005, 103, 221-228.	1.7	32
12	Degradation of UV filters 2-ethylhexyl-4-methoxycinnamate and 4-tert-butyl-4'-methoxydibenzoylmethane in chlorinated water. Environmental Chemistry, 2013, 10, 127.	1.5	32
13	Aspects of the Aromaticity of Anthranil. European Journal of Organic Chemistry, 2004, 2004, 3340-3345.	2.4	28
14	Structural, Energetic, and UVâ€“Vis Spectral Analysis of UVA Filter 4-tert-Butyl-4â€²-methoxydibenzoylmethane. Journal of Physical Chemistry A, 2014, 118, 1511-1518.	2.5	26
15	Degradation in chlorinated water of the UV filter 4-tert-butyl-4â€²-methoxydibenzoylmethane present in commercial sunscreens. Environmental Technology (United Kingdom), 2015, 36, 1319-1326.	2.2	25
16	Thermochemical Study of the Cyanophenol Isomers. Structural Chemistry, 2004, 15, 103-116.	2.0	24
17	UV filter 2â€‰ethylhexyl 4â€‰methoxycinnamate: a structure, energetic and UVâ€“vis spectral analysis based on density functional theory. Journal of Physical Organic Chemistry, 2014, 27, 47-56.	1.9	24
18	Magnetic responsive cell-based strategies for diagnostics and therapeutics. Biomedical Materials (Bristol), 2018, 13, 054001.	3.3	24

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19	Standard molar enthalpies of formation of the methoxynitrophenol isomers: a combined experimental and theoretical investigation. Journal of Chemical Thermodynamics, 2004, 36, 431-436.	2.0	23
20	Exploring inhalable polymeric dry powders for anti-tuberculosis drug delivery. Materials Science and Engineering C, 2018, 93, 1090-1103.	7.3	23
21	Title is missing!. Structural Chemistry, 2001, 12, 171-181.	2.0	21
22	Epitopeâ€imprinted Nanoparticles as Transforming Growth Factorâ€Î²3 Sequestering Ligands to Modulate Stem Cell Fate. Advanced Functional Materials, 2021, 31, 2003934.	14.9	21
23	Thermochemical Parameters of the Chloronitrophenol Isomers:Â A Combined Experimental and Theoretical Investigation. Journal of Chemical & Engineering Data, 2007, 52, 627-634.	1.9	20
24	Calorimetric and Computational Study of Indanones. Journal of Physical Chemistry A, 2007, 111, 11153-11159.	2.5	20
25	3,4,5-Trimethoxyphenol: A combined experimental and theoretical thermochemical investigation of its antioxidant capacity. Journal of Chemical Thermodynamics, 2008, 40, 625-631.	2.0	20
26	Toward Spinning Greener Advanced Silk Fibers by Feeding Silkworms with Nanomaterials. ACS Sustainable Chemistry and Engineering, 2020, 8, 11872-11887.	6.7	20
27	Thermochemical study of the ethylpyridine and ethylpyrazine isomers. Organic and Biomolecular Chemistry, 2003, 1, 4329.	2.8	19
28	Experimental thermochemical study of three monosubstituted pyrazines. Journal of Chemical Thermodynamics, 2005, 37, 49-53.	2.0	19
29	2,1,3-Benzothiadiazole: Study of its structure, energetics and aromaticity. Journal of Chemical Thermodynamics, 2012, 50, 30-36.	2.0	19
30	Thermochemistry of (E)- and (Z)-disubstituted alkene species: a combined experimental and theoretical investigation of isomeric dimethyl fumarate and dimethyl maleate. Organic and Biomolecular Chemistry, 2003, 1, 2930.	2.8	17
31	The energetics of isomeric benzoxazine diones: isatoic anhydride revisited. Organic and Biomolecular Chemistry, 2004, 2, 1647.	2.8	16
32	Solid luminescent CdSeâ€thiolated porous phosphate heterostructures. Application in fingermark detection in different surfaces. Surface and Interface Analysis, 2013, 45, 612-618.	1.8	16
33	Thermochemistry of biphenylcarboxylic and dicarboxylic acids. A combined experimental and theoretical studyThis paper is dedicated to Kurt Mislow, a pioneering biphenyl stereochemist, on the occasion of his 80th birthday.. Organic and Biomolecular Chemistry, 2004, 2, 1353.	2.8	15
34	The Experimental and Calculational Thermochemistry of 1,2,4,5-Benzenetetracarboxylic Dianhydride:â€‰ Is This 10 Ï€ Multiring Species Aromatic?. Journal of Physical Chemistry A, 2007, 111, 7181-7188.	2.5	15
35	Experimental and theoretical study of the dissociation enthalpy of the Nâ€“O bond on 2-hydroxypyridine N-oxide: theoretical analysis of the energetics of the Nâ€“O bond for hydroxypyrydine N-oxide isomers. Journal of Chemical Thermodynamics, 2004, 36, 107-113.	2.0	14
36	Study of Energetics and Structure of 1,2,3-Benzotriazin-4(3H)-one and its 1H and Enol Tautomers. Journal of Physical Chemistry B, 2011, 115, 6616-6622.	2.6	14

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37	Computational Study on the Vinyl Azide Decomposition. Journal of Physical Chemistry A, 2014, 118, 5038-5045.	2.5	14
38	Thermochemical study of chloropyrazines and chloroquinoxalines. Journal of Chemical Thermodynamics, 2004, 36, 377-383.	2.0	13
39	Experimental and computational thermochemical study of oxindole. Journal of Chemical Thermodynamics, 2010, 42, 1101-1106.	2.0	13
40	Combined experimental and computational study on the energetics of 1,2-benzisothiazol-3(2H)-one and 1,4-benzothiazin-3(2H,4H)-one. Journal of Chemical Thermodynamics, 2011, 43, 635-644.	2.0	13
41	Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: 5-Fluorouracil revisited. Journal of Chemical Thermodynamics, 2014, 75, 106-115.	2.0	13
42	Energetics of Quinazoline-2,4(1H,3H)-dione: An Experimental and Computational Study. Journal of Chemical & Engineering Data, 2011, 56, 4516-4523.	1.9	12
43	Remote triggering of TGF-Î²/Smad2/3 signaling in human adipose stem cells laden on magnetic scaffolds synergistically promotes tenogenic commitment. Acta Biomaterialia, 2020, 113, 488-500.	8.3	12
44	Experimental and computational thermochemistry of the dihydroxypyridine isomers. Journal of Chemical Thermodynamics, 2006, 38, 450-454.	2.0	11
45	Benzanilide: on the crossroads of calorimetry, computations and concepts. Molecular Physics, 2006, 104, 2855-2860.	1.7	10
46	Theoretical characterization of the chemical bonds of some three-membered ring compounds through QTAIM theory. Structural Chemistry, 2016, 27, 663-670.	2.0	10
47	Surprises with strain energy and sulpholane (tetrahydrothiophene 1,1-dioxide): a combined experimental and theoretical investigation. Molecular Physics, 2004, 102, 525-530.	1.7	9
48	Thermochemistry of diphenic anhydride. A combined experimental and theoretical study. Molecular Physics, 2005, 103, 1885-1894.	1.7	9
49	A theoretical study of the UV absorption of 4-methylbenzylidene camphor: from the UVB to the UVA region. Photochemical and Photobiological Sciences, 2015, 14, 465-472.	2.9	9
50	Thermochemical study of cyanopyrazines: Experimental and theoretical approaches. Journal of Chemical Thermodynamics, 2006, 38, 559-564.	2.0	8
51	Standard molar enthalpy of formation of 1-benzosuberone: An experimental and computational study. Journal of Chemical Thermodynamics, 2010, 42, 1094-1100.	2.0	8
52	Paradigms and paradoxes: the aromaticity of 6:6 fused carbocycles and heterocycles as an extension of a study of indane and indene derivatives. Structural Chemistry, 2011, 22, 1221-1224.	2.0	8
53	Experimental and computational study on the energetics of 10,11-dihydro-5H-dibenzo[a,d]cycloheptene (dibenzosuberane). Journal of Chemical Thermodynamics, 2011, 43, 364-370.	2.0	8
54	The structure and energetics of pyrrolidinones, tetrahydrofuranones, piperidinones, and tetrahydropyranones: a computational study. Structural Chemistry, 2013, 24, 1829-1839.	2.0	8

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55	Calorimetric and computational study of 2H-1, 4-benzoxazin-3(4H)-one and of related species. Molecular Physics, 2006, 104, 1833-1841.	1.7	7
56	Paradigms and paradoxes: en route to the understanding of the aromaticity of the â€œiso-speciesâ€• isobenzofuran, anthranil, benzofurazan and 2,1,3-benzothiadiazole. Structural Chemistry, 2012, 23, 1241-1243.	2.0	7
57	Magnetic triggers in biomedical applications â€“ prospects for contact free cell sensing and guidance. Journal of Materials Chemistry B, 2021, 9, 1259-1271.	5.8	7
58	Three-membered ring amides â€” a calculational and conceptual study of the structure and energetics of 1,2-oxaziridine-3-one and aziridine-2,3-dione. Canadian Journal of Chemistry, 2015, 93, 406-413.	1.1	6
59	A theoretical study of the strong interactions between carbon dioxide and OH+ and NH2 + products resulting from protonation of 1,2-dioxirane-3-one and 1,2-oxaziridine-3-one, respectively. Structural Chemistry, 2016, 27, 1743-1751.	2.0	6
60	Calorimetric and Computational Thermochemical Study of 3,3-Tetramethyleneglutaric Acid, 3,3-Tetramethyleneglutaric Anhydride, and 3,3-Tetramethyleneglutarimide. Journal of Physical Chemistry A, 2008, 112, 10053-10058.	2.5	5
61	Protonated heterocyclic derivatives of cyclopropane and cyclopropanone: classical species, alternate sites, and ring fragmentation. Canadian Journal of Chemistry, 2015, 93, 708-714.	1.1	5
62	Gas-phase thermochemical properties of some tri-substituted phenols: A density functional theory study. Journal of Chemical Thermodynamics, 2015, 80, 65-72.	2.0	5
63	Azaâ€Dielsâ€“Alder reaction between cyclopentadiene and protonated Nâ€phenylethyliminoacetates of 8â€phenylmenthol and 8â€phenylneomenthol: a density functional theory study. Journal of Physical Organic Chemistry, 2012, 25, 515-522.	1.9	4
64	Amino, ammonio and aminioethenes: a theoretical study of their structure and energetics. Journal of Physical Organic Chemistry, 2013, 26, 613-625.	1.9	4
65	Indenone and cyclopentadienone energetics via mass spectrometry and computations: Are these species antiaromatic or â€œmerelyâ€•nonaromatic?. International Journal of Mass Spectrometry, 2014, 369, 87-91.	1.5	4
66	Study of the transformation of two salicylates used in personal care products in chlorinated water. Water Research, 2014, 65, 32-39.	11.3	4
67	Structure and energetics correlations in some chlorohydroxypyridines. Journal of Chemical Thermodynamics, 2013, 62, 170-177.	2.0	3
68	Feeling and investigating blue: On the enthalpy of formation of indigo. Journal of Chemical Thermodynamics, 2014, 73, 69-75.	2.0	3
69	Gas-phase molecular structure and energetics of UVB filter 4-methylbenzylidene camphor: A computational study. Computational and Theoretical Chemistry, 2014, 1033, 67-73.	2.5	3
70	What is the enthalpy of formation of pyrazine-2-carboxylic acid?. Journal of Chemical Thermodynamics, 2016, 97, 261-263.	2.0	3
71	Luminescent behavior of CdTe quantum dots: Neodymium(III) complex-capped nanoparticles. Journal of Luminescence, 2013, 134, 408-413.	3.1	2
72	Reprint of â€œIndenone and cyclopentadienone energetics via mass spectrometry and computations: Are these species antiaromatic or â€œmerelyâ€•nonaromatic?â€• International Journal of Mass Spectrometry, 2015, 378, 175-179.	1.5	2

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73	Theoretical characterization of molecular complexes formed between triplet vinyl nitrene and Lewis acids. Structural Chemistry, 2015, 26, 565-571.	2.0	2
74	Theoretical study of the effect of resonance on Ï€â€“Ï€ stacked firefly oxyluciferin dimers. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 278, 9-13.	3.9	1
75	A computational study of the structure, aromaticity and enthalpy of formation of UVA filter 4-tert-butyl-4â€²-methoxydibenzoylmethane. Computational and Theoretical Chemistry, 2014, 1038, 6-16.	2.5	1
76	Occurrence of Personal Care Products and Transformation Processes in Chlorinated Waters. Handbook of Environmental Chemistry, 2014, , 123-136.	0.4	1