Cleber P A Anconi

List of Publications by Year
in descending order

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34	566	566801 15	642321 23
papers	citations	h-index	g-index

34	34	34	683
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Condensed-phase relative Gibbs free energy and E/Z descriptors for 2-acetylthiophene and 2-acetylthiophene-N1-phenyl thiosemicarbazones. Journal of Molecular Modeling, 2021, 27, 101.	0.8	1
2	Relative Position and Relative Rotation in Supramolecular Systems through the Analysis of the Principal Axes of Inertia: Ferrocene/Cucurbit[7]uril and Ferrocenyl Azide/Î²-Cyclodextrin Case Studies. ACS Omega, 2020, 5, 5013-5025.	1.6	6
3	Formation of Î²-Cyclodextrin inclusion compound with doxycycline: A theoretical approach. Chemical Physics Letters, 2018, 692, 140-145.	1.2	4
4	Separation and Qualitative Analysis of Carbonate, Phosphate and Chromate Anions in Qualitative Inorganic Courses. Educacion Quimica, 2018, 29, 49.	0.1	0
5	Water Solvent Effect on Theoretical Evaluation of ¹H NMR Chemical Shifts: o-Methyl-Inositol Isomer. Journal of Physical Chemistry A, 2017, 121, 2839-2846.	1.1	27
6	Hostâ€“guest intermolecular hydrogen bonds and stability in aqueous media: the benzaldehyde/Î²-CD case study. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2017, 89, 137-142.	0.9	3
7	Theoretical inclusion of deprotonated 2,4-D and dicamba pesticides in ÃŸ-cyclodextrin. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 86, 343-349.	0.9	9
8	Stability and spatial arrangement of the 2,4-dichlorophenoxyacetic acid and Î²-cyclodextrin inclusion compound: A theoretical study. Chemical Physics Letters, 2015, 633, 158-162.	1.2	10
9	Inclusion process of tetracycline in Î² and Î³-cyclodextrins: A theoretical investigation. Chemical Physics Letters, 2015, 626, 80-84.	1.2	20
10	Inclusion complex thermodynamics: The Î²-cyclodextrin and sertraline complex example. Journal of Molecular Graphics and Modelling, 2015, 62, 11-17.	1.3	29
11	Synthesis, characterization and phytotoxic activity of hydroxylated isobenzofuran-1(3H)-ones. Journal of Molecular Structure, 2014, 1061, 61-68.	1.8	10
12	Theoretical and Experimental Study of Inclusion Complexes Formed by Isoniazid and Modified Î²-Cyclodextrins: ¹H NMR Structural Determination and Antibacterial Activity Evaluation. Journal of Physical Chemistry B, 2014, 118, 81-93.	1.2	34
13	Inclusion complexes of Schiff bases as phytogrowth inhibitors. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2013, 75, 197-204.	1.6	6
14	Superstructure based on Î²-CD self-assembly induced by a small guest molecule. Physical Chemistry Chemical Physics, 2012, 14, 1934.	1.3	41
15	Theoretical Study of Covalently Bound Î´-Cyclodextrin Associations. Journal of Physical Chemistry C, 2012, 116, 18958-18964.	1.5	8
16	Estudo teÃ³rico e experimental de espectros infravermelho de Ã©steres de Ã¡cido graxo presentes na composiÃ§Ã£o do biodiesel de soja. Quimica Nova, 2012, 35, 1752-1757.	0.3	5
17	Prediction of conformational population of large cycloalkanes using ab initio correlated methods: Cycloundecane, cyclododecane, and cyclotridecane. International Journal of Quantum Chemistry, 2012, 112, 3188-3197.	1.0	9
18	Theoretical study of inclusion of a dinuclear platinum(II) complex in Î±, Î², and Î³â€cyclodextrins. International Journal of Quantum Chemistry, 2012, 112, 3403-3408.	1.0	6

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19	¹H NMR analysis of Oâ€methylâ€inositol isomers: a joint experimental and theoretical study. Magnetic Resonance in Chemistry, 2012, 50, 608-614.	1.1	31
20	Inclusion complexes of Î±-cyclodextrin and the cisplatin analogues oxaliplatin, carboplatin and nedaplatin: A theoretical approach. Chemical Physics Letters, 2011, 515, 127-131.	1.2	19
21	Boxâ€“Behnken design for studying inclusion complexes of triglycerides and Î±-cyclodextrin: application to the heating protocol in molecular-dynamics simulations. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2011, 71, 103-111.	1.6	7
22	Interaction of chemically modified tetracyclines with catalytic Zn(II) ion in matrix metalloproteinase: evidence for metal coordination sites. Theoretical Chemistry Accounts, 2011, 128, 377-388.	0.5	10
23	Theoretical study of spectroscopic properties of insulated molecular wires formed by substituted oligothiophenes and crossâ€linked Î±â€cyclodextrin. Journal of Polymer Science, Part B: Polymer Physics, 2011, 49, 1101-1111.	2.4	9
24	^{1h}J_{FH}coupling in 2â€fluorophenol revisited: Is intramolecular hydrogen bond responsible for this longâ€range coupling?. Magnetic Resonance in Chemistry, 2011, 49, 763-767.	1.1	49
25	Experimental and Theoretical Investigation of Epoxide Quebrachitol Derivatives Through Spectroscopic Analysis. Organic Letters, 2010, 12, 5458-5461.	2.4	25
26	Selective activity of Mucor plumbeus reductase towards (â^')-camphorquinone. Journal of Industrial Microbiology and Biotechnology, 2009, 36, 1023-1027.	1.4	5
27	New Insights on Chemical Oxidation of Single-Wall Carbon Nanotubes: A Theoretical Study. Journal of Physical Chemistry C, 2009, 113, 10079-10084.	1.5	31
28	Structure and Stability of (Î±-CD)3 Aggregate and OEG@(Î±-CD)3 Pseudorotaxane in Aqueous Solution: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2009, 113, 9762-9769.	1.2	17
29	The role played by headâ€“tail configuration on the molecular weight distribution of Î±-cyclodextrin tubes. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2008, 60, 25-33.	1.6	10
30	Theoretical study of Î±-CD based [3] pseudorotaxanes: the role played by threadlike polymer on the stability of Cyclodextrin dimers. Journal of the Brazilian Chemical Society, 2008, 19, 1033-1040.	0.6	9
31	Ab Initio Calculations on Low-Energy Conformers of Î±-Cyclodextrin. Journal of Physical Chemistry A, 2007, 111, 12127-12135.	1.1	34
32	An efficient methodology to study cyclodextrin clusters: application to Î±-CD hydrated monomer, dimer, trimer and tetramer. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2007, 59, 265-277.	1.6	16
33	A highly correlated ab initio investigation of the temperature-dependent conformational analysis of cycloheptane. Chemical Physics Letters, 2006, 418, 459-466.	1.2	23
34	Theoretical Study of the Î±-Cyclodextrin Dimer. Journal of Physical Chemistry A, 2005, 109, 3209-3219.	1.1	43