A J Lopes Jesus

List of Publications by Year
in descending order

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42	809	567281	526287
papers	citations	15 h-index	27 g-index

42	42	42	736
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Conformational Study of Monomeric 2,3-Butanediols by Matrix-Isolation Infrared Spectroscopy and DFT Calculations. Journal of Physical Chemistry A, 2006, 110, 4169-4179.	2.5	72
2	Erythritol: Crystal growth from the melt. International Journal of Pharmaceutics, 2010, 388, 129-135.	5.2	70
3	Structure of Isolated 1,4-Butanediol: Combination of MP2 Calculations, NBO Analysis, and Matrix-Isolation Infrared Spectroscopy. Journal of Physical Chemistry A, 2008, 112, 4669-4678.	2.5	69
4	Stepwise conformational cooling towards a single isomeric state in the four internal rotors system 1,2-butanediol. Physical Chemistry Chemical Physics, 2006, 8, 5339-5349.	2.8	68
5	Conformational Cooling Dynamics in Matrix-Isolated 1,3-Butanediol. Journal of Physical Chemistry A, 2009, 113, 7499-7507.	2.5	64
6	Molecular Structure of Butanediol Isomers in Gas and Liquid States:â€‰ Combination of DFT Calculations and Infrared Spectroscopy Studies. Journal of Physical Chemistry A, 2003, 107, 3891-3897.	2.5	52
7	Charge-Assisted Intramolecular Hydrogen Bonds in Disubstituted Cyclohexane Derivatives. Journal of Physical Chemistry A, 2011, 115, 14069-14077.	2.5	49
8	Conformational Switching by Vibrational Excitation of a Remote NH Bond. Journal of the American Chemical Society, 2015, 137, 14240-14243.	13.7	27
9	Effects of Entangled IR Radiation and Tunneling on the Conformational Interconversion of 2-Cyanophenol. Journal of Physical Chemistry A, 2019, 123, 4396-4405.	2.5	25
10	Hydration of Cyclohexylamines:Â CPCM Calculation of Hydration Gibbs Energy of the Conformers. Journal of Physical Chemistry A, 2007, 111, 3432-3437.	2.5	21
11	Enthalpy of vaporisation of butanediol isomers. Journal of Chemical Thermodynamics, 2003, 35, 123-129.	2.0	20
12	Enthalpy of Sublimation in the Study of the Solid State of Organic Compounds. Application to Erythritol and Threitol. Journal of Physical Chemistry B, 2005, 109, 18055-18060.	2.6	20
13	Kinetically unstable 2â€“isocyanophenol isolated in cryogenic matrices: Vibrational excitation, conformational changes and spontaneous tunneling. Chemical Physics Letters, 2020, 747, 137069.	2.6	17
14	Conformational preferences of Î±,Î±-trehalose in gas phase and aqueous solution. Carbohydrate Research, 2010, 345, 2048-2059.	2.3	16
15	Determination of the Enthalpy of Soluteâ˜Solvent Interaction from the Enthalpy of Solution:Â Aqueous Solutions of Erythritol andl-Threitol. Journal of Physical Chemistry B, 2006, 110, 9280-9285.	2.6	15
16	Conformational study of erythritol and threitol in the gas state by density functional theory calculations. Carbohydrate Research, 2005, 340, 283-291.	2.3	14
17	Conformational control over an aldehyde fragment by selective vibrational excitation of interchangeable remote antennas. Chemical Communications, 2018, 54, 4778-4781.	4.1	14
18	Conformational changes in matrix-isolated 6-methoxyindole: Effects of the thermal and infrared light excitations. Journal of Chemical Physics, 2016, 144, 124306.	3.0	13

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19	Photoinduced transformations of indole and 3-formylindole monomers isolated in low-temperature matrices. Journal of Chemical Physics, 2017, 147, 194304.	3.0	11
20	On the structure of erythritol and L-threitol in the solid state: An infrared spectroscopic study. Journal of Molecular Structure, 2009, 938, 156-164.	3.6	10
21	Molecular insight into the amineâ€“water interaction: A combined vibrational, energetic and NBO/NEDA study. Computational and Theoretical Chemistry, 2013, 1023, 74-82.	2.5	10
22	Conformational preferences of 3,4-dihydroxyphenylacetic acid (DOPAC). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 140, 54-64.	3.9	10
23	Conformational study of isolated pindolol by HF, DFT and MP2 calculations. Computational and Theoretical Chemistry, 2007, 806, 231-238.	1.5	9
24	UV-Induced Photochemistry of 1,3-Benzoxazole, 2-Isocyanophenol, and 2-Cyanophenol Isolated in Low-Temperature Ar Matrixes. Journal of Organic Chemistry, 2021, 86, 6126-6137.	3.2	9
25	Enthalpy of solvation of butanediols in different solvents. Thermochimica Acta, 2000, 344, 3-8.	2.7	8
26	Self-association of 1,2-cyclohexanediols: A spectroscopic and computational study. Journal of Molecular Structure, 2014, 1067, 104-111.	3.6	8
27	UV-induced transformations in matrix-isolated 6â€methoxyindole. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 336, 123-130.	3.9	8
28	Solvation enthalpy and the thermodynamics of hydration of trans-cyclohexyl-1,4-diamine and cis-cyclohexyl-1,2-diamine. Journal of Chemical Thermodynamics, 2007, 39, 1357-1362.	2.0	7
29	Glass-forming ability of butanediol isomers. Journal of Thermal Analysis and Calorimetry, 2010, 100, 385-390.	3.6	7
30	Conformational study of charged cyclohexyldiamines and their gas phase acidâ€“base properties. Structural Chemistry, 2011, 22, 999-1006.	2.0	7
31	Conformational Changes in 5-Methoxyindole: Effects of Thermal, Vibrational, and Electronic Excitations. Journal of Physical Chemistry A, 2017, 121, 3372-3382.	2.5	7
32	The structure of mono- and di-amino derivatives of cyclohexane: Energetic and Natural Bond Orbital approaches. Computational and Theoretical Chemistry, 2011, 964, 32-39.	2.5	6
33	Structure of Charged Cyclohexyldiamines in Aqueous Solution: A Theoretical and Experimental Study. Journal of Physical Chemistry B, 2012, 116, 5019-5027.	2.6	6
34	Methoxyindoles: stability and Ï€-electron delocalization. Structural Chemistry, 2015, 26, 655-666.	2.0	6
35	Energetic and electronic study of indole derivatives. Structural Chemistry, 2016, 27, 809-820.	2.0	5
36	Conformational Isomerizations by Rotation around Câ€“C or Câ€“N Bonds: A Comparative Study on Matrix-Isolated Glycolamide and N-Hydroxyurea Excited with Near-IR Laser Light. Journal of Physical Chemistry A, 2019, 123, 3831-3839.	2.5	5

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37	UV-induced radical formation and isomerization of 4-methoxyindole and 5-methoxyindole. Physical Chemistry Chemical Physics, 2020, 22, 22943-22955.	2.8	5
38	Conformational Space, IR-Induced, and UV-Induced Chemistry of Carvacrol Isolated in a Low-Temperature Argon Matrix. Journal of Physical Chemistry A, 2021, 125, 8215-8229.	2.5	5
39	Structure of the 2-isopropylaminoethanol isolated molecule: Conformational analysis and intramolecular interactions. Computational and Theoretical Chemistry, 2008, 863, 73-78.	1.5	4
40	Conformational preferences of 2-isopropylaminoethanol in aqueous solution using the CPCM continuum solvation model. Computational and Theoretical Chemistry, 2008, 867, 101-106.	1.5	4
41	Molecular dynamics and quantum chemical approaches in the study of the hydration of protonated cyclohexyldiamines. Molecular Physics, 2014, 112, 173-181.	1.7	3
42	UV-promoted radical formation, and near-IR-induced and spontaneous conformational isomerization in monomeric 9-methylguanine isolated in low-temperature Ar matrices. Physical Chemistry Chemical Physics, 2019, 21, 22857-22868.	2.8	3