

Pedro J Castro Pelaez

List of Publications by Year in descending order

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12
papers

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citations

1683354

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1372195

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14
all docs

14
docs citations

14
times ranked

269
citing authors

#	ARTICLE	IF	CITATIONS
1	Improved Mechanistic Model of the Atmospheric Redox Chemistry of Mercury. <i>Environmental Science & Technology</i> , 2021, 55, 14445-14456.	4.6	65
2	Insight into the Mechanisms of Luminescence of Aminobenzonitrile and Dimethylaminobenzonitrile in Polar Solvents. An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1983-1995.	1.1	26
3	Intramolecular Charge Transfer in 4-Aminobenzonitrile Does Not Need the Twist and May Not Need the Bend. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1316-1320.	2.1	25
4	Computational Study of the Mechanism of the Photochemical and Thermal Ring-Opening/Closure Reactions and Solvent Dependence in Spirooxazines. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8148-8158.	1.1	17
5	Ultrafast internal conversion in 4-aminobenzonitrile occurs sequentially along the seam. <i>Chemical Physics</i> , 2018, 509, 30-36.	0.9	12
6	Computational Study of Hydrogen Bonding in Substituted Phenol-Acetonitrile-Water Clusters. <i>Journal of the Chinese Chemical Society</i> , 2008, 55, 529-534.	0.8	3
7	Combined Experimental and Computational Kinetics Studies for the Atmospherically Important BrHg Radical Reacting with NO and O ₂ . <i>Journal of Physical Chemistry A</i> , 2022, 126, 3914-3925.	1.1	3
8	Non-adiabatic dynamic of atmospheric unimolecular photochemical reactions of 4,4-difluoroacrolein using TD-DFT and TSH approaches. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26663.	1.0	2
9	Insights into the BPO 4-Driven Catalytic Mechanism for the Formation of Cyclic Carbonates from CO ₂ and Epoxides. <i>ChemistrySelect</i> , 2021, 6, 7489-7498.	0.7	2
10	Molecular Modeling Study on Morphine Derivatives Using Density Functional Methods and Molecular Descriptors. <i>Journal of the Korean Chemical Society</i> , 2010, 54, 363-373.	0.2	1
11	The mechanism behind the photochromism and photomagnetism of type II biindenylidenediones: multiconfigurational, perturbative and density functional theory studies. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17453-17465.	1.3	0
12	Thermodynamics of Synthesis of New Phenoxazine Derivatives. <i>Journal of Basic & Applied Sciences</i> , 0, , .	0.8	0