Pedro J Castro Pelaez

List of Publications by Year in descending order

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1683354 1372195 12 156 5 10 citations g-index h-index papers 14 14 14 269 docs citations times ranked citing authors all docs

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