Nayara D Coutinho

List of Publications by Year
in descending order

21 papers	381 citations	1040056 9 h-index	794594 19 g-index
21 all docs	21 docs citations	21 times ranked	312 citing authors

#	Article	IF	Citations
1	Reply to the â€˜Comment on â€œTopography of the Free Energy Landscape on the Claisenâ€“Schmidt Condensation: Solvent and Temperature Effect in the Rate-Controlling Stepâ€â€™ by N. D. Coutinho, H. G. Machado, V. H. Carvalho-Silva and W. A. da Silva, Phys. Chem. Chem. Phys., 2021, 23, 6738. Physical Chemistry Chemical Physics, 2021, 23, 22202-22206.	2.8	1
2	Aminoâ€“Imino Tautomerism in the Salt Formation of Albendazole: Hydrobromide and Nitrate Salts. Crystal Growth and Design, 2021, 21, 1122-1135.	3.0	9
3	Topography of the free energy landscape of Claisenâ€“Schmidt condensation: solvent and temperature effects on the rate-controlling step. Physical Chemistry Chemical Physics, 2021, 23, 6738-6745.	2.8	10
4	Temperature dependence of rate constants for the H(D) + CH4 reaction in gas and aqueous phase: deformed Transition-State Theory study including quantum tunneling and diffusion effects. Structural Chemistry, 2020, 31, 609-617.	2.0	8
5	From the Kinetic Theory of Gases to the Kinetics of Rate Processes: On the Verge of the Thermodynamic and Kinetic Limits. Molecules, 2020, 25, 2098.	3.8	10
6	Nucleophilic substitution vs elimination reaction of bisulfide ions with substituted methanes: exploration of chiral selectivity by stereodirectional first-principles dynamics and transition state theory. Journal of Molecular Modeling, 2019, 25, 227.	1.8	5
7	The Increase of the Reactivity of Molecular Hydrogen with Hydroxyl Radical from the Gas Phase versus an Aqueous Environment: Quantum Chemistry and Transition State-Theory Calculations. Lecture Notes in Computer Science, 2019, , 450-459.	1.3	1
8	â€œTransitivityâ€• A Code for Computing Kinetic and Related Parameters in Chemical Transformations and Transport Phenomena. Molecules, 2019, 24, 3478.	3.8	18
9	Temperature Dependence of Rate Processes Beyond Arrhenius and Eyring: Activation and Transitivity. Frontiers in Chemistry, 2019, 7, 380.	3.6	69
10	Rate constants and first-principles trajectories for attack at tetrahedral carbon: Role of molecular orientation on chiral selectivity. AIP Conference Proceedings, 2019, , .	0.4	0
11	From statistical thermodynamics to molecular kinetics: the change, the chance and the choice. Rendiconti Lincei, 2018, 29, 787-802.	2.2	18
12	Kinetics of the OH+HClâ†’H₂O+Cl reaction: Rate determining roles of stereodynamics and roaming and of quantum tunneling. Journal of Computational Chemistry, 2018, 39, 2508-2516.	3.3	22
13	First-Principles Molecular Dynamics and Computed Rate Constants for the Series of OH-HX Reactions (Xâ€‰=â€‰H or the Halogens): Non-Arrhenius Kinetics, Stereodynamics and Quantum Tunnel. Lecture Notes in Computer Science, 2018, , 605-623.	1.3	3
14	Kinetics of low-temperature transitions and a reaction rate theory from non-equilibrium distributions. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160201.	3.4	57
15	A novel assessment of the role of the methyl radical and water formation channel in the CH₃OH + H reaction. Physical Chemistry Chemical Physics, 2017, 19, 24467-24477.	2.8	22
16	The $$ {mathbf{HI}},varvec{ + },{mathbf{OH}}, o ,{mathbf{H}}_{{mathbf{2}}} {mathbf{O}}, + ,{mathbf{I}} $$ HI + OH â†’ H 2 O + I Reaction by First-Principles Molecular Dynamics: Stereodirectional and anti-Arrhenius Kinetics. Lecture Notes in Computer Science, 2017, , 297-313.	1.3	3
17	Description of deviations from Arrhenius behavior in chemical kinetics and materials science. AIP Conference Proceedings, 2016, , .	0.4	9
18	Stereodirectional Origin of anti-Arrhenius Kinetics for a Tetraatomic Hydrogen Exchange Reaction: Bornâ€“Oppenheimer Molecular Dynamics for OH + HBr. Journal of Physical Chemistry A, 2016, 120, 5408-5417.	2.5	30

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19	Description of the effect of temperature on food systems using the deformed Arrhenius rate law: deviations from linearity in logarithmic plots vs. inverse temperature. Rendiconti Lincei, 2015, 26, 141-149.	2.2	18
20	Stereodynamical Origin of Anti-Arrhenius Kinetics: Negative Activation Energy and Roaming for a Four-Atom Reaction. Journal of Physical Chemistry Letters, 2015, 6, 1553-1558.	4.6	63
21	Effect of the Methanol Molecule on the Stabilization of C₁₈H₁₈O₄ Crystal: Combined Theoretical and Structural Investigation. Journal of Physical Chemistry A, 2014, 118, 10048-10056.	2.5	5