Oriana Brea

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5479068/publications.pdf

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24	288	933447	940533
papers	citations	10	16
		h-index	g-index

27	27	27	265
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Binding and Assembly of a Benzotriazole Cavitand in Water. Angewandte Chemie - International Edition, 2022, 61, .	13.8	5
2	Mechanisms of Formation and Rearrangement of Benziodoxole-Based CF₃ and SCF₃ Transfer Reagents. Journal of Organic Chemistry, 2020, 85, 15577-15585.	3.2	4
3	Modulating the intrinsic reactivity of molecules through non-covalent interactions. Physical Chemistry Chemical Physics, 2019, 21, 2222-2233.	2.8	13
4	Modeling Decomposition of N-Nitrosoamides in a Self-Assembled Capsule. Journal of Organic Chemistry, 2019, 84, 7354-7361.	3.2	5
5	Gas-phase reactivity tuned through the interaction with alkaline-earth derivatives. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	5
6	Mechanism(s) of thermal decomposition of N-Nitrosoamides: A density functional theory study. Tetrahedron, 2019, 75, 929-935.	1.9	10
7	Super Strong Beâ€“Be Bonds: Theoretical Insight into the Electronic Structure of Beâ€“Be Complexes with Radical Ligands. Journal of Physical Chemistry A, 2018, 122, 2258-2265.	2.5	23
8	Are beryllium-containing biphenyl derivatives efficient anion sponges?. Journal of Molecular Modeling, 2018, 24, 16.	1.8	7
9	Molecular Modelling of the H₂â€Adsorptive Properties of Tetrazolateâ€Based Metalâ€“Organic Frameworks: From the Cluster Approach to Periodic Simulations. ChemPhysChem, 2018, 19, 1349-1357.	2.1	6
10	Exergonic and Spontaneous Production of Radicals through Beryllium Bonds. Angewandte Chemie - International Edition, 2016, 55, 8736-8739.	13.8	22
11	On the existence of intramolecular one-electron Beâ€“Be bonds. Chemical Communications, 2016, 52, 9656-9659.	4.1	28
12	Exergonic and Spontaneous Production of Radicals through Beryllium Bonds. Angewandte Chemie, 2016, 128, 8878-8881.	2.0	9
13	The Spin-Partitioned Total-Position Spread Tensor: An Application To Diatomic Molecules. Journal of Physical Chemistry A, 2016, 120, 5230-5238.	2.5	7
14	Berylliumâ€Based Anion Sponges: Close Relatives of Proton Sponges. Chemistry - A European Journal, 2016, 22, 18322-18325.	3.3	24
15	The total position-spread tensor: Spin partition. Journal of Chemical Physics, 2015, 142, 094113.	3.0	16
16	Ga⁺ Basicity and Affinity Scales Based on Highâ€Level Abâ€…Initio Calculations. ChemPhysChem, 2015, 16, 3206-3213.	2.1	0
17	Creating Ïƒâ€Holes through the Formation of Beryllium Bonds. Chemistry - A European Journal, 2015, 21, 12676-12682.	3.3	38
18	Why Is the Spontaneous Deprotonation of [Cu(uracil)₂]²⁺ Complexes Accompanied by Enolization of the System?. ChemPhysChem, 2015, 16, 2375-2382.	2.1	2

#	Article	IF	Citations
19	Spin delocalization in hydrogen chains described with the spin-partitioned total position-spread tensor. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10
20	On the stability of [(uracil)2-Cu]2+ complexes in the gas phase. Different pathways for the formation of [(uracil-H)(uracil)-Cu]+ monocations. Organic and Biomolecular Chemistry, 2013, 11, 3862.	2.8	14
21	Behavior of the Positionâ€“Spread Tensor in Diatomic Systems. Journal of Chemical Theory and Computation, 2013, 9, 5286-5295.	5.3	19
22	Quantum chemical calculations of the thermal isomerization of 2-methyl-4,5-dihydrofuran. Computational and Theoretical Chemistry, 2012, 993, 53-59.	2.5	1
23	Theoretical study of methoxy group influence in the gasâ€phase elimination kinetics of methoxyalkyl chlorides. International Journal of Quantum Chemistry, 2012, 112, 2504-2514.	2.0	15
24	Binding and Assembly of a Benzotriazole Cavitand in Water. Angewandte Chemie, 0, , .	2.0	4