Anne Milet

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3104213/publications.pdf

Version: 2024-02-01

70 papers	2,555 citations	218677 26 h-index	197818 49 g-index
76 all docs	76 docs citations	76 times ranked	2933 citing authors

#	Article	IF	Citations
1	Did Homocysteine Take Part in the Start of the Synthesis of Peptides on the Early Earth?. Biomolecules, 2022, 12, 555.	4.0	2
2	A way to thioacetate esters compatible with non-oxidative prebiotic conditions. Scientific Reports, 2020, 10, 14488.	3.3	3
3	First Direct Evidence of an orthoâ€Lithiated Aryloxetane: Solid and Solution Structure, and Dynamics. European Journal of Organic Chemistry, 2019, 2019, 5549-5556.	2.4	6
4	Ion Pairing in HClâ€“Water Clusters: From Electronic Structure Investigations to Multiconfigurational Force-Field Development. Journal of Physical Chemistry A, 2019, 123, 9371-9381.	2.5	3
5	Interfacial Water at Graphene Oxide Surface: Ordered or Disordered?. Journal of Physical Chemistry B, 2019, 123, 1636-1649.	2.6	12
6	Mechanistic Perspectives in the Regioselective Indole Addition to Unsymmetrical Silyloxyallyl Cations. Journal of Organic Chemistry, 2019, 84, 7166-7174.	3.2	2
7	Bond dissociation energies of carbonyl gold complexes: a new descriptor of ligand effects in gold(i) complexes?. Dalton Transactions, 2018, 47, 15497-15505.	3.3	12
8	The Reaction of Aminonitriles with Aminothiols: A Way to Thiol-Containing Peptides and Nitrogen Heterocycles in the Primitive Earth Ocean. Life, 2018, 8, 47.	2.4	12
9	Iron Hydroperoxide Intermediate in Superoxide Reductase: Protonation or Dissociation First? MM Dynamics and QM/MM Metadynamics Study. Journal of Chemical Theory and Computation, 2017, 13, 2987-3004.	5.3	10
10	Experimental bond dissociation energies of benzylpyridinium thermometer ions determined by threshold-CID and RRKM modeling. International Journal of Mass Spectrometry, 2017, 417, 69-75.	1.5	14
11	At the very beginning of life on Earth: the thiol-rich peptide (TRP) world hypothesis. International Journal of Developmental Biology, 2017, 61, 471-478.	0.6	17
12	Was methionine the molecular trigger of life on early earth?. Phosphorus, Sulfur and Silicon and the Related Elements, 2016, 191, 329-332.	1.6	3
13	Theoretical Study, Synthesis, and Reactivity of Fiveâ€Memberedâ€Ring Acyl Sulfonium Cations. European Journal of Organic Chemistry, 2015, 2015, 6125-6129.	2.4	3
14	Experimental and Computational Insights into Carbon Dioxide Fixation by RZnOH Species. Chemistry - A European Journal, 2015, 21, 5496-5503.	3.3	10
15	Chemically and Electrochemically Triggered Assembly of Viologen Radicals: Towards Multiaddressable Molecular Switches. Chemistry - A European Journal, 2015, 21, 2090-2106.	3.3	32
16	Kinetic Resolution in the [2+2] Cycloaddition of Ketenes: An Experimental and Theoretical Study. Chemistry - A European Journal, 2015, 21, 3876-3881.	3.3	5
17	Hydrogen-Bond Controlled Ï€-Dimerization in Viologen-Appended Calixarenes: Revealing a Subtle Balance of Weak Interactions. Organic Letters, 2015, 17, 4058-4061.	4.6	13
18	The Pausonâ€“Khand Mechanism Revisited: Origin of CO in the Final Product. Angewandte Chemie - International Edition, 2014, 53, 1939-1942.	13.8	31

#	Article	IF	Citations
19	Î±â€Halogenoacetanilides as Hydrogenâ€Bonding Organocatalysts that Activate Carbonyl Bonds: Fluorine versus Chlorine and Bromine. Chemistry - A European Journal, 2014, 20, 2849-2859.	3.3	17
20	Conformational Flexibility of Human Casein Kinase Catalytic Subunit Explored by Metadynamics. Biophysical Journal, 2014, 106, 1134-1141.	0.5	13
21	Investigation of Bindingâ€Site Homology between Mushroom and Bacterial Tyrosinases by Using Aurones as Effectors. ChemBioChem, 2014, 15, 1325-1333.	2.6	26
22	Probing kojic acid binding to tyrosinase enzyme: insights from a model complex and QM/MM calculations. Chemical Communications, 2014, 50, 308-310.	4.1	25
23	Reversible dimerization of viologen radicals covalently linked to a calixarene platform: Experimental and theoretical aspects. Comptes Rendus Chimie, 2014, 17, 505-511.	0.5	20
24	Activation of carbonyl bonds by quaternary ammoniums and a (Na+:crown-ether) complex: investigation of the ring-opening polymerization of cyclic esters. Polymer Chemistry, 2013, 4, 3491.	3.9	40
25	Redox control of molecular motions in bipyridinium appended calixarenes. Organic and Biomolecular Chemistry, 2013, 11, 4383.	2.8	23
26	Long-range electronic connection in picket-fence like ferroceneâ€“porphyrin derivatives. Dalton Transactions, 2013, 42, 1196-1209.	3.3	36
27	Redox Control of Rotary Motions in Ferrocene-Based Elemental Ball Bearings. Journal of the American Chemical Society, 2012, 134, 2653-2671.	13.7	120
28	Phenols and Tertiary Amines: An Amazingly Simple Hydrogenâ€Bonding Organocatalytic System Promoting Ring Opening Polymerization. Advanced Synthesis and Catalysis, 2011, 353, 1049-1054.	4.3	41
29	Viologen-based redox-switchable anion-binding receptors. New Journal of Chemistry, 2010, 34, 1373.	2.8	60
30	Mechanistic investigations of the phosphine-mediated nitrone deoxygenation reaction and its application in cyclic imine synthesis. Tetrahedron Letters, 2009, 50, 7038-7042.	1.4	24
31	Exploring the Binding of Inhibitors Derived from Tetrabromobenzimidazole to the CK2 Protein Using a QM/MM-PB/SA Approach. Journal of Chemical Information and Modeling, 2009, 49, 963-971.	5.4	24
32	Gas-Phase Study of Phenylacetylene and Norbornadiene on a Palladium(II) Phosphinous Acid Complex: Importance of the Order of Introduction of the Organic Partners. Organometallics, 2009, 28, 2735-2743.	2.3	24
33	Tracing the Entropy along a Reactive Pathway: The Energy As a Generalized Reaction Coordinate. Journal of Chemical Theory and Computation, 2009, 5, 2193-2196.	5.3	15
34	A DFT study of 1,3-dipolar cycloaddition reactions of 5-membered cyclic nitrones with Î±,Î²-unsaturated lactones and with cyclic vinyl ethers: Part 1. Tetrahedron: Asymmetry, 2008, 19, 1660-1669.	1.8	16
35	A DFT study of 1,3-dipolar cycloadditions of cyclic nitrones to unsaturated lactones. Part II. Tetrahedron: Asymmetry, 2008, 19, 2140-2148.	1.8	19
36	Free energy calculation of the effects of the fluorinated phosphorus ligands on the Câ€“H and Câ€“C reductive elimination from Pt(IV). Computational and Theoretical Chemistry, 2008, 852, 54-61.	1.5	8

#	Article	IF	Citations
37	Synthesis of N-acridinyl-Nâ€²-alkylguanidines: Dramatic influence of amine to guanidine replacement on the physicochemical properties. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 4779-4782.	2.2	4
38	Response to Comment on Autoionization at the surface of neat water: is the top layer pH neutral, basic, or acidic? by J. K. Beattie, Phys. Chem. Chem. Phys., 2007,9, DOI: 10.1039/b713702h. Physical Chemistry Chemical Physics, 2008, 10, 332-333.	2.8	37
39	Ynol Ethers from Dichloroenol Ethers: Mechanistic Elucidation Through 35Cl Labeling. Organic Letters, 2008, 10, 4445-4447.	4.6	25
40	Water surface is acidic. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7342-7347.	7.1	332
41	Autoionization at the surface of neat water: is the top layer pH neutral, basic, or acidic?. Physical Chemistry Chemical Physics, 2007, 9, 4736.	2.8	151
42	Free Energyab InitioMetadynamics:Â A New Tool for the Theoretical Study of Organometallic Reactivity? Example of the Câ^'C and Câ^'H Reductive Eliminations from Platinum(IV) Complexes. Organometallics, 2007, 26, 1241-1249.	2.3	37
43	Structural, Kinetic, and Theoretical Studies on Models of the Zincâ€Containing Phosphodiesterase Active Center: Mediumâ€Dependent Reaction Mechanisms. Chemistry - A European Journal, 2007, 13, 9093-9106.	3.3	49
44	Silver versus Gold Catalysis in Tandem Reactions of Carbonyl Functions onto Alkynes: A Versatile Access to Furoquinoline and Pyranoquinoline Cores. Chemistry - A European Journal, 2007, 13, 5632-5641.	3.3	155
45	Theoretical study of the cyclization of carbonyl groups on unactivated alkynyl-quinolines in the gas phase and in methanol solution. Computational and Theoretical Chemistry, 2007, 811, 175-182.	1.5	5
46	First Câ€“C bond formation in the Pausonâ€“Khand reaction: Influence of carbonâ€“carbon triple bond polarization on regiochemistry. Journal of Organometallic Chemistry, 2006, 691, 4281-4288.	1.8	35
47	Reaction of nitrones with silyl ketene acetals: A DFT study. Journal of Computational Chemistry, 2006, 27, 157-162.	3.3	19
48	Pyrenyldiazomethane, a versatile reagent for nucleotide phosphate alkylation. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 705-708.	2.2	9
49	Lewis Base Promoters in the Pauson-Khand Reaction: A Different Scenario. Angewandte Chemie - International Edition, 2005, 44, 5717-5719.	13.8	24
50	Insight into the Reactivity of Olefins in the Pausonâ^'Khand Reaction. Journal of Organic Chemistry, 2004, 69, 1075-1080.	3.2	54
51	Reactivity of Pyrido[4,3,2-kl]acridines:Â Regioselective Formation of 6-Substituted Derivatives. Journal of Organic Chemistry, 2004, 69, 8144-8147.	3.2	20
52	On Early Events in the Pausonâ^'Khand Reaction. Organic Letters, 2003, 5, 4073-4075.	4.6	60
53	Role of Cancellation of Errors in Ab Initio Calculations:â€‰ Structure and Energetics of the OH- (H2O) System and Electric Dipole Properties of the Subsystems. Journal of Physical Chemistry A, 2002, 106, 12084-12094.	2.5	16
54	The OH â^' (H 2 O) 2 system: efficiency of ab initio and DFT calculations for two- and three-body interactions. Computational and Theoretical Chemistry, 2002, 577, 239-253.	1.5	16

#	Article	IF	Citations
55	Some problems with the accuracy in ab initio calculations of the static dipole polarizability components: example of the OHâ¯ ion. Computational and Theoretical Chemistry, 2002, 591, 141-150.	1.5	6
56	Theoretical study of the hydrogen chloride trihydrate. International Journal of Quantum Chemistry, 2002, 90, 1151-1162.	2.0	5
57	Regiochemistry in the Pausonâ¯Khand Reaction:Â Has a Trans Effect Been Overlooked?. Journal of the American Chemical Society, 2001, 123, 5396-5400.	13.7	87
58	Cyclizations of 4-Pentenyl, 5-Hexenyl, 6-Heptenyl, and 7-Octenyl Fluorinated Radicals:Â A Density Functional Theory Theoretical Study. Journal of Organic Chemistry, 2001, 66, 6074-6082.	3.2	5
59	Highly Regioselective Vilsmeierâ¯Haack Acylation of Hexahydropyrroloindolizine. Journal of Organic Chemistry, 2001, 66, 2522-2525.	3.2	31
60	Theoretical Study of the Regiochemistry-Determining Step of the Pausonâ¯Khand Reaction. Journal of the American Chemical Society, 2001, 123, 7184-7185.	13.7	71
61	Theoretical predictions of vibrationâ€“rotationâ€“tunneling dynamics of the weakly bound trimer (H2O)2HCl. Chemical Physics Letters, 2001, 343, 588-596.	2.6	7
62	Theoretical study of the protolytic dissociation of HCl in water clusters. Journal of Chemical Physics, 2001, 115, 349-356.	3.0	93
63	Nature and importance of three-body interactions in the (H 2 O) 2 HCl trimer. Theoretical Chemistry Accounts, 2000, 104, 195-198.	1.4	12
64	Theoretical Study of the Addition of Hydrogen Cyanide to Methanimine in the Gas Phase and in Aqueous Solution. Journal of the American Chemical Society, 2000, 122, 324-330.	13.7	65
65	Anisotropic intermolecular interactions in van der Waals and hydrogen-bonded complexes: What can we get from density functional calculations?. Journal of Chemical Physics, 1999, 111, 7727-7735.	3.0	91
66	Hydrogen Bonding in Water Clusters:Â Pair and Many-Body Interactions from Symmetry-Adapted Perturbation Theory. Journal of Physical Chemistry A, 1999, 103, 6811-6819.	2.5	92
67	Theoretical study of the OHâ¯(H2O)2 system: Nature and importance of three-body interactions. Journal of Chemical Physics, 1998, 109, 7157-7168.	3.0	38
68	Ïƒ-Bond Metathesis Reactions Involving Palladium(II) Hydride and Methyl Complexes:Â A Theoretical Assessment. Inorganic Chemistry, 1997, 36, 3223-3231.	4.0	46
69	Synthesis and Theoretical Studies of a Diorganohydridoplatinum(IV) Complex, PtHMe2{(pz)3BH-N,Nâ€˜,Nâ€˜â€˜}Â([(pz)3BH]-= Tris(pyrazol-1-yl)borate). Organometallics, 1996, 15, 2845-2847.	2.3	83
70	Nitriles and Hydrogen on a Nickel Catalyst: Theoretical Evidence of a Process Competing with the Total Hydrogenation Reaction. Journal of Catalysis, 1996, 159, 383-393.	6.2	25