Anne Milet

List of Publications by Year
in descending order

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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	Water surface is acidic. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7342-7347.	7.1	332
2	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
3	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
4	Redox Control of Rotary Motions in Ferrocene-Based Elemental Ball Bearings. Journal of the American Chemical Society, 2012, 134, 2653-2671.	13.7	120
5	Theoretical study of the protolytic dissociation of HCl in water clusters. Journal of Chemical Physics, 2001, 115, 349-356.	3.0	93
6	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
7	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
8	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
9	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
10	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
11	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
12	On Early Events in the Pausonâ˜'Khand Reaction. Organic Letters, 2003, 5, 4073-4075.	4.6	60
13	Viologen-based redox-switchable anion-binding receptors. New Journal of Chemistry, 2010, 34, 1373.	2.8	60
14	Insight into the Reactivity of Olefins in the Pausonâ˜'Khand Reaction. Journal of Organic Chemistry, 2004, 69, 1075-1080.	3.2	54
15	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
16	Ïƒ-Bond Metathesis Reactions Involving Palladium(II) Hydride and Methyl Complexes:Â A Theoretical Assessment. Inorganic Chemistry, 1997, 36, 3223-3231.	4.0	46
17	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
18	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

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19	Theoretical study of the OHâˆ’(H2O)2 system: Nature and importance of three-body interactions. Journal of Chemical Physics, 1998, 109, 7157-7168.	3.0	38
20	Free Energyab InitioMetadynamics:Â A New Tool for the Theoretical Study of Organometallic Reactivity? Example of the Câˆ’C and Câˆ’H Reductive Eliminations from Platinum(IV) Complexes. Organometallics, 2007, 26, 1241-1249.	2.3	37
21	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
22	Long-range electronic connection in picket-fence like ferroceneâ€“porphyrin derivatives. Dalton Transactions, 2013, 42, 1196-1209.	3.3	36
23	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
24	Chemically and Electrochemically Triggered Assembly of Viologen Radicals: Towards Multiaddressable Molecular Switches. Chemistry - A European Journal, 2015, 21, 2090-2106.	3.3	32
25	Highly Regioselective Vilsmeierâˆ’Haack Acylation of Hexahydropyrroloindolizine. Journal of Organic Chemistry, 2001, 66, 2522-2525.	3.2	31
26	The Pausonâ€“Khand Mechanism Revisited: Origin of CO in the Final Product. Angewandte Chemie - International Edition, 2014, 53, 1939-1942.	13.8	31
27	Investigation of Bindingâ€Site Homology between Mushroom and Bacterial Tyrosinases by Using Aurones as Effectors. ChemBioChem, 2014, 15, 1325-1333.	2.6	26
28	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
29	Ynol Ethers from Dichloroenol Ethers: Mechanistic Elucidation Through 35Cl Labeling. Organic Letters, 2008, 10, 4445-4447.	4.6	25
30	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
31	Lewis Base Promoters in the Pauson-Khand Reaction: A Different Scenario. Angewandte Chemie - International Edition, 2005, 44, 5717-5719.	13.8	24
32	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
33	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
34	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
35	Redox control of molecular motions in bipyridinium appended calixarenes. Organic and Biomolecular Chemistry, 2013, 11, 4383.	2.8	23
36	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

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37	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
38	Reaction of nitrones with silyl ketene acetals: A DFT study. Journal of Computational Chemistry, 2006, 27, 157-162.	3.3	19
39	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
40	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
41	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
42	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
43	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
44	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
45	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
46	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
47	Conformational Flexibility of Human Casein Kinase Catalytic Subunit Explored by Metadynamics. Biophysical Journal, 2014, 106, 1134-1141.	0.5	13
48	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
49	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
50	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
51	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
52	Interfacial Water at Graphene Oxide Surface: Ordered or Disordered?. Journal of Physical Chemistry B, 2019, 123, 1636-1649.	2.6	12
53	Experimental and Computational Insights into Carbon Dioxide Fixation by RZnOH Species. Chemistry - A European Journal, 2015, 21, 5496-5503.	3.3	10
54	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

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55	Pyrenyldiazomethane, a versatile reagent for nucleotide phosphate alkylation. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 705-708.	2.2	9
56	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
57	Theoretical predictions of vibrationâ€“rotationâ€“tunneling dynamics of the weakly bound trimer (H2O)2HCl. Chemical Physics Letters, 2001, 343, 588-596.	2.6	7
58	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
59	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
60	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
61	Theoretical study of the hydrogen chloride trihydrate. International Journal of Quantum Chemistry, 2002, 90, 1151-1162.	2.0	5
62	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
63	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
64	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
65	Theoretical Study, Synthesis, and Reactivity of Fiveâ€Memberedâ€Ring Acyl Sulfonium Cations. European Journal of Organic Chemistry, 2015, 2015, 6125-6129.	2.4	3
66	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
67	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
68	A way to thioacetate esters compatible with non-oxidative prebiotic conditions. Scientific Reports, 2020, 10, 14488.	3.3	3
69	Mechanistic Perspectives in the Regioselective Indole Addition to Unsymmetrical Silyloxyallyl Cations. Journal of Organic Chemistry, 2019, 84, 7166-7174.	3.2	2
70	Did Homocysteine Take Part in the Start of the Synthesis of Peptides on the Early Earth?. Biomolecules, 2022, 12, 555.	4.0	2