Gianfranco Ercolani

List of Publications by Citations

95 papers	2,552 citations	26 h-index	47 g-index
123 ext. papers	2,746 ext. citations	6.6 avg, IF	5.31 L-index

#	Paper	IF	Citations
95	Assessment of cooperativity in self-assembly. *Journal of the American Chemical Society*, **2003**, 125, 16097-103	11.4	268
94	Allosteric, chelate, and interannular cooperativity: a mise au point. *Angewandte Chemie - International Edition*, **2011**, 50, 1762-8	16.4	185
93	Macrocyclization under thermodynamic control. A theoretical study and its application to the equilibrium cyclooligomerization of .beta.-propiolactone. *Journal of the American Chemical Society*, **1993**, 115, 3901-3908	16.4	178
92	Influence of selectivity on the supramolecular polymerization of AB-type polymers capable of Both A x A and A x B interactions. *Journal of the American Chemical Society*, **2008**, 130, 13755-64	16.4	118
91	Symmetry numbers and statistical factors in self-assembly and multivalency. *Journal of Physical Chemistry B*, **2007**, 111, 12195-203	3.4	100
90	Physical Basis of Self-Assembly Macrocyclizations. *Journal of Physical Chemistry B*, **1998**, 102, 5699-5703	3.4	96
89	Mechanism of threading a polymer through a macrocyclic ring. *Science*, **2008**, 322, 1668-71	33.3	92
88	Unraveling the mechanism of the Soai asymmetric autocatalytic reaction by first-principles calculations: induction and amplification of chirality by self-assembly of hexamolecular complexes. *Angewandte Chemie - International Edition*, **2008**, 47, 6832-5	16.4	84
87	A Model for Self-Assembly in Solution1. *Journal of Physical Chemistry B*, **2003**, 107, 5052-5057	3.4	74
86	Putting the mechanism of the Soai reaction to the test: DFT study of the role of aldehyde and dialkylzinc structure. *Journal of Organic Chemistry*, **2011**, 76, 2619-26	4.2	71
85	The effect of ring substitution on the O-neophyl rearrangement of 1,1-diarylalkoxyl radicals. A product and time-resolved kinetic study. *Journal of Organic Chemistry*, **2005**, 70, 3884-91	4.2	62
84	Allosterische, Chelat- und interannulÈre KooperativitÈt auf den Punkt gebracht. *Angewandte Chemie*, **2011**, 123, 1800-1807	3.6	51
83	Mechanism of the asymmetric autocatalytic Soai reaction studied by density functional theory. *Chemistry - A European Journal*, **2010**, 16, 3147-56	4.8	42
82	Amplification of chirality and enantioselectivity in the asymmetric autocatalytic Soai reaction. *ChemPhysChem*, **2009**, 10, 2508-15	3.2	40
81	Linear polynuclear helicates as a link between discrete supramolecular complexes and programmed infinite polymetallic chains. *Chemistry - A European Journal*, **2008**, 14, 2994-3005	4.8	40
80	Physical basis of self-assembly. Part 2. A theoretical and experimental study of the self-assembly of a zinc meso-pyridyl porphyrin. *New Journal of Chemistry*, **2001**, 25, 783-789	3.6	39
79	Thermodynamics of Metal-Mediated Assemblies of Porphyrins167-215		38

78	Tuneable intramolecular intermetallic interactions as a new tool for programming linear heterometallic 4f-4f complexes. *Inorganic Chemistry*, **2007**, 46, 9312-22	5.1	37
77	Molecular recognition and self-assembly special feature: Squaring cooperative binding circles. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 10471-6	11.5	32
76	Template effect of tetrathiafulvalene in the formation of cyclobis(paraquat-p-phenylene). *Journal of Organic Chemistry*, **2005**, 70, 3761-4	4.2	32
75	Macrocyclization under Kinetic Control. A Theoretical Study and Its Application to the Synthesis of Macrocyclic Poly(thiolactones). *Journal of the American Chemical Society*, **1994**, 116, 7081-7087	16.4	31
74	Unraveling the Mechanism of the Soai Asymmetric Autocatalytic Reaction by First-Principles Calculations: Induction and Amplification of Chirality by Self-Assembly of Hexamolecular Complexes. *Angewandte Chemie*, **2008**, 120, 6938-6941	3.6	28
73	Thiopyrylium, Selenopyrylium, and Telluropyrylium Salts. *Advances in Heterocyclic Chemistry*, **1994**, 65-195	2.4	28
72	6-Azahemiporphycene: a new member of the porphyrinoid family. *Inorganic Chemistry*, **2009**, 48, 10346-57	5.1	26
71	Role of face-to-face and edge-to-face aromatic interactions in the inclusion complexation of cyclobis(paraquat-p-phenylene): a theoretical study. *Journal of Organic Chemistry*, **2003**, 68, 6470-3	4.2	26
70	Template effects and kinetic selection in the self-assembly of crown ether cyclobis(paraquat-p-phenylene). *Chemistry - A European Journal*, **2000**, 6, 3540-6	4.8	26
69	The origin of cooperativity in double-wheel receptors. Freezing of internal rotation or ligand-induced torsional strain?. *Organic Letters*, **2005**, 7, 803-5	6.2	25
68	Comment on "Using a Convenient, Quantitative Model for Torsional Entropy To Establish Qualitative Trends for Molecular Processes That Restrict Conformational Freedom". *Journal of Organic Chemistry*, **1999**, 64, 3350-3353	4.2	25
67	The role of aromatic radical cations and benzylic cations in the 2,4,6-triphenylpyrylium tetrafluoroborate photosensitized oxidation of ring-methoxylated benzyl alcohols in CH2Cl2 solution. *Journal of Organic Chemistry*, **2004**, 69, 8874-85	4.2	22
66	Alkaline stability of model anion exchange membranes based on poly(phenylene oxide) (PPO) with grafted quaternary ammonium groups: Influence of the functionalization route. *Polymer*, **2019**, 185, 121931	3.9	21
65	The problem of regioselectivity in nucleophilic additions to pyridinium and related cations. Role of generalized anomeric effect. *Journal of Organic Chemistry*, **1992**, 57, 4431-4434	4.2	21
64	Kinetic treatment of irreversible cyclooligomerization of bifunctional chains and its relevance to the synthesis of many-membered rings. *Macromolecules*, **1988**, 21, 1241-1246	5.5	21
63	Combinatorial Macrocyclizations under Thermodynamic Control: The Two-Monomer Case. *Macromolecules*, **2009**, 42, 4077-4083	5.5	20
62	Quantitative Evaluation of Template Effect in the Formation of Cyclobis(paraquat-p-phenylene). *Journal of Organic Chemistry*, **1997**, 62, 7015-7017	4.2	20
61	DFT evidence for a stepwise mechanism in the O-neophyl rearrangement of 1,1-diarylalkoxyl radicals. *Journal of Organic Chemistry*, **2007**, 72, 4515-9	4.2	20

60	Comment on Self-assembled multiporphyrin arrays mediated by self-complementary quadrupole hydrogen bond motifs *Chemical Communications*, **2001**, 1416-1417	5.8	19
59	Association of alkali and alkaline earth cations with benzo-18-crown-6 and its neutral and negatively charged acyclic analogs in methanol solution. *Journal of the American Chemical Society*, **1981**, 103, 7484-7489	16.4	19
58	Template effects. 3. The quantitative determination of the catalytic effects of alkali and alkaline earth cations in the formation of benzo-18-crown-6 in methanol solution. *Journal of the American Chemical Society*, **1981**, 103, 2780-2782	16.4	18
57	Numerical Evaluation of Energy Levels and Wave Functions for Hindered Internal Rotation. *Journal of Chemical Education*, **2000**, 77, 1495	2.4	17
56	Template effects in the self-assembly of a [2]rotaxane and a [2]pseudorotaxane with the same binding sites in the linear component. *Journal of Organic Chemistry*, **2001**, 66, 4950-3	4.2	17
55	Template effects. 5. Model system for the template effect of alkali and alkaline-earth metal ions on the formation of benzo-18-crown-6 in methanol solution. *Journal of the American Chemical Society*, **1983**, 105, 6146-6149	16.4	16
54	Supramolecular buffering by ring-chain competition. *Journal of the American Chemical Society*, **2015** , 137, 1501-9	16.4	15
53	Principles for designing an achiral receptor promoting asymmetric autocatalysis with amplification of chirality. *Tetrahedron: Asymmetry*, **2014**, 25, 405-410		15
52	A combined scanning tunneling microscopy and reflectance anisotropy spectroscopy investigation of tetraphenylporphyrin deposited on graphite. *Surface Science*, **2007**, 601, 2607-2610	1.8	15
51	Spectacular Rate Enhancement in the Self-Assembly of a [2]Catenane. *Journal of Organic Chemistry*, **1998**, 63, 8088-8089	4.2	15
50	Alkali and alkaline-earth metal ion catalysis in the reaction of aryl acetates with methoxide ion. Effect of a poly(oxyethylene) side arm. *Journal of the American Chemical Society*, **1990**, 112, 423-427	16.4	14
49	Entropy-Based Rational Modulation of the p of a Synthetic pH-Dependent Nanoswitch. *Journal of the American Chemical Society*, **2019**, 141, 11367-11371	16.4	13
48	Template effects in the formation of [2]pseudo-rotaxanes containing diazapyrenium units. *Journal of Organic Chemistry*, **2007**, 72, 1503-6	4.2	13
47	Fast atom bombardment mass spectrometry: a useful technique for structural characterization of pyrylium, thiopyrylium, and pyridinium cations. *Journal of the Chemical Society Perkin Transactions II*, **1987**, 633		13
46	Regulating Competing Supramolecular Interactions Using Ligand Concentration. *Journal of the American Chemical Society*, **2016**, 138, 6852-60	16.4	13
45	Ring-expanding polymerization by reversible ring fusion. A fascinating process driven by entropy. *Journal of Physical Chemistry B*, **2008**, 112, 4662-5	3.4	12
44	Chiral supramolecular capsule by ligand promoted self-assembly of resorcinarene-Zn porphyrin conjugate. *Journal of Porphyrins and Phthalocyanines*, **2008**, 12, 1279-1288	1.8	12
43	Catalysis in the self-assembly of [2]rotaxanes and [2]pseudorotaxanes. Effect of the length of polyethereal side arms and terminal stoppers. *Journal of Organic Chemistry*, **2004**, 69, 1393-6	4.2	12

42	□OH-Induced shift from carbon to oxygen acidity in the side-chain deprotonation of 2-, 3- and 4-methoxybenzyl alcohol radical cations in aqueous solution: results from pulse radiolysis and DFT calculations. *Tetrahedron*, **2003**, 59, 613-618	2.4	12
41	1 H nuclear magnetic resonance study of methoxide addition to pyrylium and thiopyrylium cations; heteroatom and substituent effects. *Journal of the Chemical Society Perkin Transactions II*, **1986**, 271		12
40	Isomerization equilibria of 2H- and 4H-thiopyrans. *Journal of Organic Chemistry*, **1991**, 56, 1674-1675	4.2	11
39	Dissipative operation of pH-responsive DNA-based nanodevices. *Chemical Science*, **2021**, 12, 11735-11739	9.4	11
38	Quantitative comparison of the heteroatom effects in the methoxide attachment to pyrylium and thiopyrylium cations. Thermodynamics of the isomerization of pyrans and thiopyrans. *Journal of Organic Chemistry*, **1986**, 51, 4385-4390	4.2	10
37	Determination of the Rotational Barrier in Ethane by Vibrational Spectroscopy and Statistical Thermodynamics. *Journal of Chemical Education*, **2005**, 82, 1703	2.4	9
36	Effects of □and □substituents on the relative reactivity of pyrylium and thiopyrylium cations. *Journal of the Chemical Society Perkin Transactions II*, **1989**, 1393		9
35	Time Programmable Locking/Unlocking of the Calix[4]arene Scaffold by Means of Chemical Fuels. *Chemistry - A European Journal*, **2020**, 26, 14954-14962	4.8	9
34	Rhodium-catalysed hydrogenation of enamides with monodentate phosphorous ligands. A density functional theory study. *Journal of Physical Organic Chemistry*, **2011**, 24, 257-261	2.1	8
33	Effective molarities from distributions of cyclic oligomers in the synthesis of polythiolactones. *Journal of the Chemical Society Chemical Communications*, **1993**, 538		8
32	Remarkable catalysis by strontium ion in SN2 and E2 reactions occurring in proximity to a crown ether structure. *Journal of the Chemical Society Chemical Communications*, **1994**, 1239		8
31	Time-programmable pH: decarboxylation of nitroacetic acid allows the time-controlled rising of pH to a definite value. *Chemical Science*, **2021**, 12, 7460-7466	9.4	8
30	The role of stereoelectronic effects on the side-chain fragmentation of alkylaromatic radical cations. The reactivity of 5-methoxy-2,2-dimethylindan-1-ol radical cation. *Tetrahedron*, **2002**, 58, 5039-5044	2.4	7
29	Synthesis and conformational aspects of corands incorporating pyrylium, thiopyrylium and pyridine subunits. *Tetrahedron*, **1991**, 47, 1977-1984	2.4	7
28	Thiopyrylium cations as appropriate compounds for the quantitative evaluation of ipso-substituent effects. *Journal of the Chemical Society Perkin Transactions II*, **1987**, 1427		7
27	Rates and equilibria of the methoxide attachment to 2,6-di-tert-butyl-4-arylthiopyrylium cations. Can ion pair formation be rate determining in anion-cation combination reactions?. *Journal of the American Chemical Society*, **1986**, 108, 3409-3415	16.4	7
26	Syntheses of many-membered rings. Part 28 kinetic models for the irreversible cyclisation of two symmetrical monomers. *Journal of the Chemical Society Perkin Transactions II*, **1990**, 747		6
25	Steric effects on rates and equilibria of a cation-anion combination reaction: the methoxide attachment to 4-substituted 2,6-di-tert-butylpyrylium cations. *Journal of Organic Chemistry*, **1988**, 53, 1729-1733	4.2	6

24	Using antibodies to control DNA-templated chemical reactions. *Nature Communications*, **2020**, 11, 6242	17.4	6
23	Stimuli-responsive amphoteric ion exchange polymers bearing carboxylic and amine groups grafted to a cross-linkable silica network. *European Polymer Journal*, **2019**, 112, 255-262	5.2	6
22	Catenation Equilibria Between Ring Oligomers and Their Relation to Effective Molarities: Models From Theories and Simulations. *Macromolecular Theory and Simulations*, **2016**, 25, 63-73	1.5	5
21	Study of the reaction of bis- and tris-pyrylium and -thiopyrylium cations with methoxide ion. Electronic effects of the heterocyclic rings as substituents. *Journal of Organic Chemistry*, **2005**, 70, 6422-8	4.2	5
20	Alkylation of 2,6-diphenylpyrylium and 2,6-di-t-butylpyrylium ions by photochemical reaction with tetraalkylstannanes. *Tetrahedron*, **1993**, 49, 3793-3800	2.4	5
19	Kinetic and thermodynamic study of the reaction of 2,4,6-triphenylthiopyrylium ion with butylamine and cyclohexylamine in dimethyl sulfoxide. *Journal of Organic Chemistry*, **1984**, 49, 1806-1810	4.2	5
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17	Statistical Ring Catenation under Thermodynamic Control: Should the Jacobson-Stockmayer Cyclization Theory Take into Account Catenane Formation?. *Journal of Physical Chemistry B*, **2017**, 121, 649-656	3.4	4
16	"Intrinsic" Anion Exchange Polymers through the Dissociation of Strong Basic Groups: PPO with Grafted Bicyclic Guanidines. *Membranes*, **2019**, 9,	3.8	4
15	Proximity effect induced by hydrogen-bonding association. A detailed kinetic study. *Tetrahedron Letters*, **1996**, 37, 101-104	2	4
14	Rates and equilibria of the reaction of 2,4,6-triphenylthiopyrylium ion with piperidine and morpholine in dimethyl sulfoxide. An unusual proton transfer to a nitrogen base. *Journal of the American Chemical Society*, **1984**, 106, 7082-7087	16.4	4
13	One-Pot Synthesis of 2,6-Di-t-butyl- and 2,6-Diarylthiopyrylium Perchlorates. *Synthesis*, **1985**, 1985, 789-790	2.9	4
12	Equilibrium Effective Molarity As a Key Concept in Ring-Chain Equilibria, Dynamic Combinatorial Chemistry, Cooperativity and Self-assembly. *Advances in Physical Organic Chemistry*, **2016**, 50, 1-76	0.3	4
11	Influence of the position of ionic groups in amphoteric polyelectrolytes on hydration and ionic conduction: Side chain vs main chain. *European Polymer Journal*, **2019**, 119, 45-51	5.2	3
10	Bioinspired Self-Assembly II: Principles of Cooperativity in Bioinspired Self-Assembling Systems **2012**, 47-69		3
9	Effect of alkali cations on the methoxide ion addition to corands incorporating a thiopyrylium subunit. *Tetrahedron*, **1996**, 52, 3509-3520	2.4	3
8	Effects of metal ions on the equilibria of methanol and methoxide ion addition to benzaldehydes. Effect of a poly(oxyethylene) side arm. *Journal of Organic Chemistry*, **1991**, 56, 6331-6336	4.2	3
7	Record Rate Enhancements for Tetrathiafulvalene Guests in the Formation of Bipyridinium- and Diazapyrenium-Based [2]Pseudorotaxanes. *Journal of Organic Chemistry*, **2018**, 83, 11446-11449	4.2	2

6	Template Effect in the Self-Assembly of a [2]Rotaxane Containing Diazapyrenium Units. *Progress in Reaction Kinetics and Mechanism*, **2010**, 35, 209-217	0.5	2
5	Distributions of cyclic oligomers formed by irreversible step-growth polymerisation. Results from kinetic modeling. *Macromolecular Theory and Simulations*, **1997**, 6, 1139-1151	1.5	2
4	Simulation of irreversible cyclization of bifunctional chains. A computer-aided approach to the synthesis of many-membered rings and to the evaluation of effective molarities by preparative experiments. *Journal of the Chemical Society Perkin Transactions II*, **1989**, 187		2
3	The First Homolytic Substitution of Pyrylium Salts. C-4 Methylation of 2,6-Disubstituted Pyrylium Cations. *Synthetic Communications*, **1987**, 17, 817-821	1.7	2
2	Nanocomposite Anion Exchange Membranes with a Conductive Semi-Interpenetrating Silica Network. *Membranes*, **2021**, 11,	3.8	2
1	Model Systems for the Template Effect of Alkali and Alkaline Earth Metal Ions on the Formation of Benzo-18-Crown-6. *Bulletin Des Soci□s Chimiques Belges*, **2010**, 91, 485-485		