Olalla Nieto Faza

List of Publications by Year
in descending order

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93	2,313	172207	253896
papers	citations	29 h-index	43 g-index

100	100	100	2307
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mechanism of the Gold(I)-Catalyzed Rautenstrauch Rearrangement:Â A Center-to-Helix-to-Center Chirality Transfer. Journal of the American Chemical Society, 2006, 128, 2434-2437.	6.6	183
2	Theoretical Study of the Electrocyclic Ring Closure of Hydroxypentadienyl Cations. Chemistry - A European Journal, 2004, 10, 4324-4333.	1.7	95
3	Performance of density functional theory on homogeneous gold catalysis. Theoretical Chemistry Accounts, 2011, 128, 647-661.	0.5	81
4	Computational Characterization of a Complete Palladium-Catalyzed Cross-Coupling Process:â€‰ The Associative Transmetalation in the Stille Reaction. Organic Letters, 2006, 8, 35-38.	2.4	78
5	Ellipticity: A Convenient Tool To Characterize Electrocyclic Reactions. Chemistry - A European Journal, 2005, 11, 1734-1738.	1.7	71
6	Normalâ€toâ€Abnormal NHC Rearrangement of Al^{III}, Ga^{III}, and In^{III} Trialkyl Complexes: Scope, Mechanism, Reactivity Studies, and H₂ Activation. Chemistry - A European Journal, 2015, 21, 17959-17972.	1.7	61
7	Synthesis of Diverse Indoleâ€Containing Scaffolds by Gold(I)â€Catalyzed Tandem Reactions of 3â€Propargylindoles Initiated by 1,2â€Indole Migrations: Scope and Computational Studies. Chemistry - A European Journal, 2010, 16, 9818-9828.	1.7	59
8	Gold-Catalyzed Synthesis of 1-(Indol-3-yl)carbazoles: Selective 1,2-Alkyl vs 1,2-Vinyl Migration. Organic Letters, 2017, 19, 5074-5077.	2.4	58
9	Pseudorotation Barriers of Biological Oxyphosphoranes: A Challenge for Simulations of Ribozyme Catalysis. Chemistry - A European Journal, 2005, 11, 2081-2093.	1.7	54
10	DFT-Based Insights into Pdâ€“Zn Cooperative Effects in Oxidative Addition and Reductive Elimination Processes Relevant to Negishi Cross-Couplings. Organometallics, 2012, 31, 2053-2058.	1.1	53
11	Mechanism of the Gold-Catalyzed Rearrangement of (3-Acyloxyprop-1-ynyl)oxiranes: A Dual Role of the Catalyst. Journal of Organic Chemistry, 2009, 74, 2982-2991.	1.7	50
12	Associative Transmetalation in the Stille Cross-Coupling Reaction to Form Dienes: Theoretical Insights into the Open Pathway. Organometallics, 2008, 27, 3378-3389.	1.1	47
13	Gold-Catalyzed Homogeneous (Cyclo)Isomerization Reactions. Frontiers in Chemistry, 2019, 7, 296.	1.8	46
14	Noyori Hydrogenation: Aromaticity, Synchronicity, and Activation Strain Analysis. Journal of Organic Chemistry, 2013, 78, 5669-5676.	1.7	44
15	A Density Functional Theory Study of the Stille Cross-Couplingvia Associative Transmetalation. The Role of Ligands and Coordinating Solvents. Advanced Synthesis and Catalysis, 2007, 349, 887-906.	2.1	43
16	Hg²⁺ Detection by New Anthracene Pendant-Arm Derivatives of Mixed N/S- and N/S/O-Donor Macrocycles: Fluorescence, Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry and Density Functional Theory Studies. Inorganic Chemistry, 2010, 49, 8276-8286.	1.9	43
17	Allenyl Azide Cycloaddition Chemistry. Photochemical Initiation and CuI Mediation Leads to Improved Regioselectivity. Organic Letters, 2008, 10, 1665-1668.	2.4	41
18	Allenyl Azide Cycloaddition Chemistry. 2,3-Cyclopentennelated Indole Synthesis through Indolidene Intermediates. Journal of Organic Chemistry, 2009, 74, 4958-4974.	1.7	41

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19	On the Memory of Chirality in Gold(I)-Catalyzed Intramolecular Carboalkoxylation of Alkynes. Journal of Organic Chemistry, 2011, 76, 3791-3796.	1.7	41
20	Rational Design in Catalysis: A Mechanistic Study of Î²-Hydride Eliminations in Gold(I) and Gold(III) Complexes Based on Features of the Reaction Valley. Inorganic Chemistry, 2016, 55, 8636-8645.	1.9	40
21	Theoretical and experimental exploration of the photochemistry of resveratrol: beyond the simple double bond isomerization. Organic and Biomolecular Chemistry, 2012, 10, 9175.	1.5	37
22	Goldâ€Photoredoxâ€Cocatalyzed Tandem Oxycyclization/Coupling Sequence of Allenols and Diazonium Salts with Visible Light Mediation. Advanced Synthesis and Catalysis, 2017, 359, 2789-2800.	2.1	36
23	Theoretical Study of the Vinyl Allene Oxide to Cyclopent-2-en-1-one Rearrangement:â€‰ Mechanism, Torquoselectivity and Solvent Effects. Journal of Organic Chemistry, 2004, 69, 3635-3644.	1.7	35
24	Cyclization Cascade of Allenyl Azides:â€‰ A Dual Mechanism. Journal of the American Chemical Society, 2007, 129, 7638-7646.	6.6	35
25	Simple Diastereoselectivity of the BF3Â·OEt2-Catalyzed Vinylogous Mukaiyama Aldol Reaction of 2-(Trimethylsiloxy)furans with Aldehydes. Journal of Organic Chemistry, 2005, 70, 3654-3659.	1.7	33
26	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. ChemPhysChem, 2004, 5, 1045-1049.	1.0	32
27	Phosphine-Catalyzed Stereoselective Dearomatization of 3-NO₂-Indoles with Allenoates. Journal of Organic Chemistry, 2019, 84, 6347-6355.	1.7	32
28	Enantioselective CO₂ Fixation Via a Heckâ€Coupling/Carboxylation Cascade Catalyzed by Nickel. Chemistry - A European Journal, 2021, 27, 7657-7662.	1.7	32
29	The Woodwardâ^'Hoffmannâ^'De Puy Rule Revisitedâ€. Organic Letters, 2004, 6, 905-908.	2.4	31
30	Solvolytic Ring-Opening Reactions of Cyclopropyl Bromides. An Assessment of the Woodwardâ^'Hoffmannâ^'DePuy Rule. Journal of Organic Chemistry, 2004, 69, 9002-9010.	1.7	30
31	Regioâ€, Periâ€, and Torquoselectivity in Hydroxy Heptatrienyl Cation Electrocyclizations: The Iso/Homoâ€Nazarov Reaction. Chemistry - A European Journal, 2009, 15, 1944-1956.	1.7	29
32	Computational Study of Gold-Catalyzed Homo- and Cross-Coupling Reactions. Journal of Organic Chemistry, 2013, 78, 4929-4939.	1.7	29
33	Solving the Pericyclicâ€“Pseudopericyclic Puzzle in the Ring-Closure Reactions of 1,2,4,6-Heptatetraene Derivatives. Journal of Organic Chemistry, 2016, 81, 404-414.	1.7	29
34	Computational Approaches to Homogeneous Gold Catalysis. Topics in Current Chemistry, 2014, 357, 213-283.	4.0	28
35	QCRNA 1.0: A database of quantum calculations for RNA catalysis. Journal of Molecular Graphics and Modelling, 2006, 25, 423-433.	1.3	26
36	Computation of vertical excitation energies of retinal and analogs: Scope and limitations. Journal of Computational Chemistry, 2006, 27, 116-123.	1.5	25

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37	Allenyl Azide Cycloaddition Chemistry: Exploration of the Scope and Mechanism of Cyclopentennelated Dihydropyrrole Synthesis through Azatrimethylenemethane Intermediates. Journal of Organic Chemistry, 2008, 73, 5090-5099.	1.7	25
38	Electrocyclic Ring Opening ofcis-Bicyclo[m.n.0]alkenes: The Anti-Woodwardâ€“Hoffmann Quest. Chemistry - A European Journal, 2007, 13, 5009-5017.	1.7	22
39	Dynamic Effects Responsible for High Selectivity in a [3,3] Sigmatropic Rearrangement Featuring a Bispericyclic Transition State. Journal of Organic Chemistry, 2017, 82, 4758-4765.	1.7	22
40	Computational Study and Analysis of the Kinetic Isotope Effects of the Rearrangement ofcis-Bicyclo[4.2.0]oct-7-ene tocis,cis-Cycloocta-1,3-diene. Organic Letters, 2006, 8, 2055-2058.	2.4	21
41	Pushing the limits of concertedness. A waltz of wandering carbocations. Chemical Science, 2019, 10, 2159-2170.	3.7	21
42	Mechanistic and Sterochemical Insights on the Pt-Catalyzed Rearrangement of Oxiranylpropargylic Esters to Cyclopentenones. Journal of Organic Chemistry, 2012, 77, 8733-8743.	1.7	17
43	BrÃ¸nsted Acidâ€Catalyzed Cascade Reactions Involving 1,2â€Indole Migration. Chemistry - A European Journal, 2015, 21, 12889-12893.	1.7	17
44	Synthesis, characterization, fluorescence and computational studies of new Cu2+, Ni2+ and Hg2+ complexes with emissive thienylbenzoxazolyl-alanine ligands. Inorganica Chimica Acta, 2011, 366, 154-160.	1.2	16
45	Computational insights on the mechanism of the catalytic hydrogenation with BINAPâ€“diamineâ€“Ru complexes: the role of base and origin of selectivity. Chemical Communications, 2013, 49, 4277-4279.	2.2	16
46	Exploring the Reactivity of Î±â€Lithiated Aryl Benzyl Ethers: Inhibition of the [1,2]â€Wittig Rearrangement and the Mechanistic Proposal Revisited. Chemistry - A European Journal, 2016, 22, 15058-15068.	1.7	16
47	A Radical Mechanism for the Vanadium-Catalyzed Deoxydehydration of Glycols. Inorganic Chemistry, 2016, 55, 11372-11382.	1.9	16
48	Nickel catalyzed regio- and stereoselective arylation and methylation of allenamides via coupling reactions. An experimental and computational study. Organic Chemistry Frontiers, 2018, 5, 3231-3239.	2.3	16
49	Exploiting anionic and cationic interactions with a new emissive imine-based Î²-naphthol molecular probe. Inorganic Chemistry Communication, 2009, 12, 905-912.	1.8	15
50	Electrocyclic Ring Opening of Charged cis-Bicyclo[3.2.0]heptadiene and Heterocyclic Derivatives. The Anti-Woodwardâ”Hoffmann Quest (II). Journal of Organic Chemistry, 2009, 74, 2396-2402.	1.7	15
51	Cyclization Cascade of Allenyl Azides: Synergy Between Theory and Experiment. Current Organic Chemistry, 2010, 14, 1646-1657.	0.9	15
52	Characterization of the Switch in the Mechanism of an Intramolecular Dielsâ”Alder Reaction. Journal of Organic Chemistry, 2008, 73, 467-473.	1.7	14
53	Mechanism of the Molybdenum-Mediated Cadogan Reaction. ACS Omega, 2018, 3, 7019-7026.	1.6	14
54	On the Use of Popular Basis Sets: Impact of the Intramolecular Basis Set Superposition Error. Molecules, 2019, 24, 3810.	1.7	14

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55	Conrotatory Ring-Opening Reactions of Cyclopropyl Anions in Monocyclic and Tricyclic Systems. Organic Letters, 2004, 6, 901-904.	2.4	13
56	Sulfoxide-Induced Stereoselection in [1,5]-Sigmatropic Hydrogen Shifts of Vinylallenes. A Computational Study. Journal of Organic Chemistry, 2007, 72, 2617-2624.	1.7	13
57	DFT-Based Mechanistic Insights into Noble Metal-Catalyzed Rearrangement of Propargylic Derivatives: Chirality Transfer Processes. Topics in Current Chemistry, 2011, 302, 81-130.	4.0	13
58	Mechanistic subtleties in the cyclopentannelation of allenolate allyl carbamates: the origin of the center-to-center chirality transfer. Chemical Communications, 2005, , 4285.	2.2	12
59	2-Alkylidenesulfol-3-enes by (Regio- and) Stereoselective Cheletropic Addition of SO2to (Di)vinylallenes. Organic Letters, 2005, 7, 1565-1568.	2.4	12
60	CO₂ Complexes with Five-Membered Heterocycles: Structure, Topology, and Spectroscopic Characterization. Journal of Physical Chemistry A, 2017, 121, 9118-9130.	1.1	12
61	Novel emissive podands based on 8-OH-quinoline: Synthesis, fluorescence materials, DFT and complexation studies. Inorganica Chimica Acta, 2012, 381, 218-228.	1.2	11
62	Cycloisomerization of Activated (2E,4Z)-Heptatrienoate and Its Relevance to Crispatene (Bio)synthesis. A Case of Concerted and Stepwise Uncertainty. Journal of Organic Chemistry, 2006, 71, 4497-4501.	1.7	10
63	Torquoselectivity in the electrocyclic ringâ€opening of cyclopropyl anions. Journal of Physical Organic Chemistry, 2009, 22, 378-385.	0.9	10
64	Complex Thermal Behavior of 11-cis-Retinal, the Ligand of the Visual Pigments. Journal of Organic Chemistry, 2009, 74, 1007-1013.	1.7	10
65	Assessing the attractive/repulsive force balance in axial cyclohexane C-H_{ax}Â·Â·Â·Y_{ax}contacts: A combined computational analysis in monosubstituted cyclohexanes. Journal of Computational Chemistry, 2016, 37, 2647-2658.	1.5	10
66	Gold-catalyzed reaction of alkynes with diazonium salts under photoirradiation revisited: New alkoxyarylation variant leading to enol ethers. Journal of Catalysis, 2020, 391, 48-55.	3.1	10
67	Acetate-catalyzed hydroboration of CO₂ for the selective formation of methanol-equivalent products. Catalysis Science and Technology, 2020, 10, 2407-2414.	2.1	10
68	Bis(o-methylserotonin)-containing iridium(III) and ruthenium(II) complexes as new cellular imaging dyes: synthesis, applications, and photophysical and computational studies. Journal of Biological Inorganic Chemistry, 2013, 18, 679-692.	1.1	9
69	Accounting for Diradical Character through DFT. The Case of Vinyl Allene Oxide Rearrangement. Journal of Organic Chemistry, 2015, 80, 11206-11211.	1.7	9
70	Cycloreversion of the CO₂trimer: a paradigmatic pseudopericyclic [2 + 2 + 2] cycloaddition reaction. Organic and Biomolecular Chemistry, 2017, 15, 435-441.	1.5	9
71	From Hydrindane to Decalin: A Mild Transformation through a Dyotropic Ring Expansion. Organic Letters, 2017, 19, 3648-3651.	2.4	8
72	The key role of protodeauration in the gold-catalyzed reaction of 1,3-diynes with pyrrole and indole to form complex heterocycles. Organic Chemistry Frontiers, 2020, 7, 997-1005.	2.3	8

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73	Pseudopericyclic design drives antara-antara [1,5] methylene sigmatropic shifts from a stepwise to a concerted mechanism. Journal of Computational Chemistry, 2007, 28, 1411-1416.	1.5	7
74	[MoO₂]²⁺-Mediated Oxygen Atom Transfer via an Unusual Lewis Acid Mechanism. Inorganic Chemistry, 2017, 56, 10570-10575.	1.9	7
75	Lennard-Jones Potentials for the Interaction of CO₂ with Five-Membered Aromatic Heterocycles. Journal of Physical Chemistry A, 2017, 121, 9518-9530.	1.1	7
76	Nitrogen doped nanohoops as promising CO₂ capturing devices. Physical Chemistry Chemical Physics, 2018, 20, 8607-8615.	1.3	7
77	Diradical ring closing reactions displaying Woodwardâ€“Hoffmann behaviour and torquoselectivity. RSC Advances, 2015, 5, 30405-30408.	1.7	6
78	Conformational control allows for [3,3]-sigmatropic rearrangements to proceed with torquoselectivity. RSC Advances, 2016, 6, 59181-59184.	1.7	6
79	The Outerâ€Sphere Mechanism of Nitrene Transfer onto Gold(I) Alkyne Complexes. ChemCatChem, 2016, 8, 2387-2392.	1.8	6
80	Governing effects in the mechanism of the gold-catalyzed cycloisomerization of allenic hydroxylamine derivatives. Organic and Biomolecular Chemistry, 2017, 15, 5920-5926.	1.5	6
81	Submerged Barriers in the Ni⁺ Assisted Decomposition of Propionaldehyde. Journal of Physical Chemistry A, 2016, 120, 2275-2284.	1.1	5
82	Copperâ€Catalyzed Skeletal Rearrangement of Oâ€Propargyl Oximes: A Mechanistic Manifold. ChemCatChem, 2016, 8, 2696-2703.	1.8	5
83	Rational Design of Efficient Environmental Sensors: Ring-Shaped Nanostructures Can Capture Quat Herbicides. ACS Omega, 2018, 3, 16976-16988.	1.6	5
84	Computational and experimental studies on Cu/Au-catalyzed stereoselective synthesis of 1,3-disubstituted allenes. Organic Chemistry Frontiers, 2019, 6, 1780-1786.	2.3	4
85	Au(III) catalyzes the cross-coupling between activated methylenes and alkene derivatives. Journal of Catalysis, 2020, 392, 159-164.	3.1	4
86	Three Reaction Channels with Signature Proton Transfers in the Ni(I)-Catalyzed Decomposition of Ethyl Acetate. Organometallics, 2017, 36, 761-766.	1.1	2
87	Methanol directing the dual reactivity of 1,3-dien-5-ynes under gold(I) catalysis: A computational study. Computational and Theoretical Chemistry, 2019, 1148, 33-37.	1.1	2
88	On the mechanism of the Au(I)â€mediated addition of alkynes to anthranils to furnish 7â€acylindoles. Journal of Physical Organic Chemistry, 0, , .	0.9	2
89	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. ChemPhysChem, 2004, 5, 1266-1266.	1.0	1
90	The effect of solvation in torquoselectivity: ring opening of monosubstituted cyclobutenes. Organic and Biomolecular Chemistry, 2020, 18, 6287-6296.	1.5	1

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91	Solvation. , 2018, , 97-146.		0
92	Lennard-Jones Intermolecular Potentials for the Description of 6-Membered Aromatic Heterocycles Interacting with the Isoelectronic CO2 and CS2. Journal of Physical Chemistry A, 2019, 123, 4475-4485.	1.1	0
93	On the mechanism of the dyotropic expansion of hydrindanes into decalins. Organic and Biomolecular Chemistry, 2022, 20, 1073-1079.	1.5	0