

Olalla Nieto Faza

List of Publications by Year in descending order

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93
papers

2,313
citations

172207

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253896

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100
all docs

100
docs citations

100
times ranked

2307
citing authors

#	ARTICLE	IF	CITATIONS
1	On the mechanism of the dyotropic expansion of hydrindanes into decalins. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 1073-1079.	1.5	0
2	Enantioselective CO ₂ Fixation Via a Heck-Coupling/Carboxylation Cascade Catalyzed by Nickel. <i>Chemistry - A European Journal</i> , 2021, 27, 7657-7662.	1.7	32
3	Au(III) catalyzes the cross-coupling between activated methylenes and alkene derivatives. <i>Journal of Catalysis</i> , 2020, 392, 159-164.	3.1	4
4	Gold-catalyzed reaction of alkynes with diazonium salts under photoirradiation revisited: New alkoxyarylation variant leading to enol ethers. <i>Journal of Catalysis</i> , 2020, 391, 48-55.	3.1	10
5	The effect of solvation in torquoselectivity: ring opening of monosubstituted cyclobutenes. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 6287-6296.	1.5	1
6	The key role of protodeauration in the gold-catalyzed reaction of 1,3-diyne with pyrrole and indole to form complex heterocycles. <i>Organic Chemistry Frontiers</i> , 2020, 7, 997-1005.	2.3	8
7	Acetate-catalyzed hydroboration of CO ₂ for the selective formation of methanol-equivalent products. <i>Catalysis Science and Technology</i> , 2020, 10, 2407-2414.	2.1	10
8	Pushing the limits of concertedness. A waltz of wandering carbocations. <i>Chemical Science</i> , 2019, 10, 2159-2170.	3.7	21
9	Gold-Catalyzed Homogeneous (Cyclo)Isomerization Reactions. <i>Frontiers in Chemistry</i> , 2019, 7, 296.	1.8	46
10	Phosphine-Catalyzed Stereoselective Dearomatization of 3-NO ₂ -Indoles with Allenates. <i>Journal of Organic Chemistry</i> , 2019, 84, 6347-6355.	1.7	32
11	Computational and experimental studies on Cu/Au-catalyzed stereoselective synthesis of 1,3-disubstituted allenes. <i>Organic Chemistry Frontiers</i> , 2019, 6, 1780-1786.	2.3	4
12	Lennard-Jones Intermolecular Potentials for the Description of 6-Membered Aromatic Heterocycles Interacting with the Isoelectronic CO ₂ and CS ₂ . <i>Journal of Physical Chemistry A</i> , 2019, 123, 4475-4485.	1.1	0
13	On the Use of Popular Basis Sets: Impact of the Intramolecular Basis Set Superposition Error. <i>Molecules</i> , 2019, 24, 3810.	1.7	14
14	Methanol directing the dual reactivity of 1,3-dien-5-yne under gold(I) catalysis: A computational study. <i>Computational and Theoretical Chemistry</i> , 2019, 1148, 33-37.	1.1	2
15	Nitrogen doped nano hoops as promising CO ₂ capturing devices. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8607-8615.	1.3	7
16	Solvation. , 2018, , 97-146.		0
17	Rational Design of Efficient Environmental Sensors: Ring-Shaped Nanostructures Can Capture Quat Herbicides. <i>ACS Omega</i> , 2018, 3, 16976-16988.	1.6	5
18	Nickel catalyzed regio- and stereoselective arylation and methylation of allenamides <i>via</i> coupling reactions. An experimental and computational study. <i>Organic Chemistry Frontiers</i> , 2018, 5, 3231-3239.	2.3	16

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19	Mechanism of the Molybdenum-Mediated Cadogan Reaction. ACS Omega, 2018, 3, 7019-7026.	1.6	14
20	Three Reaction Channels with Signature Proton Transfers in the Ni(I)-Catalyzed Decomposition of Ethyl Acetate. Organometallics, 2017, 36, 761-766.	1.1	2
21	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
22	From Hydrindane to Decalin: A Mild Transformation through a Dyotropic Ring Expansion. Organic Letters, 2017, 19, 3648-3651.	2.4	8
23	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
24	Cycloreversion of the CO ₂ trimer: a paradigmatic pseudopericyclic [2 + 2 + 2] cycloaddition reaction. Organic and Biomolecular Chemistry, 2017, 15, 435-441.	1.5	9
25	CO ₂ Complexes with Five-Membered Heterocycles: Structure, Topology, and Spectroscopic Characterization. Journal of Physical Chemistry A, 2017, 121, 9118-9130.	1.1	12
26	[MoO ₂] ²⁺ -Mediated Oxygen Atom Transfer via an Unusual Lewis Acid Mechanism. Inorganic Chemistry, 2017, 56, 10570-10575.	1.9	7
27	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
28	Lennard-Jones Potentials for the Interaction of CO ₂ with Five-Membered Aromatic Heterocycles. Journal of Physical Chemistry A, 2017, 121, 9518-9530.	1.1	7
29	Gold-Photoredox-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
30	Submerged Barriers in the Ni ⁺ Assisted Decomposition of Propionaldehyde. Journal of Physical Chemistry A, 2016, 120, 2275-2284.	1.1	5
31	Exploring the Reactivity of Lithiated Aryl Benzyl Ethers: Inhibition of the [1,2]-Wittig Rearrangement and the Mechanistic Proposal Revisited. Chemistry - A European Journal, 2016, 22, 15058-15068.	1.7	16
32	Conformational control allows for [3,3]-sigmatropic rearrangements to proceed with torquoselectivity. RSC Advances, 2016, 6, 59181-59184.	1.7	6
33	Assessing the attractive/repulsive force balance in axial cyclohexane C-H _{ax} ...Y _{ax} contacts: A combined computational analysis in monosubstituted cyclohexanes. Journal of Computational Chemistry, 2016, 37, 2647-2658.	1.5	10
34	The Outer-Sphere Mechanism of Nitrene Transfer onto Gold(I) Alkyne Complexes. ChemCatChem, 2016, 8, 2387-2392.	1.8	6
35	Rational Design in Catalysis: A Mechanistic Study of \hat{I}^2 -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
36	Copper-Catalyzed Skeletal Rearrangement of <i>o</i> -Propargyl Oximes: A Mechanistic Manifold. ChemCatChem, 2016, 8, 2696-2703.	1.8	5

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37	A Radical Mechanism for the Vanadium-Catalyzed Deoxydehydration of Glycols. <i>Inorganic Chemistry</i> , 2016, 55, 11372-11382.	1.9	16
38	Solving the Pericyclicâ€Pseudopericyclic Puzzle in the Ring-Closure Reactions of 1,2,4,6-Heptatetraene Derivatives. <i>Journal of Organic Chemistry</i> , 2016, 81, 404-414.	1.7	29
39	BrÃnsted Acidâ€Catalyzed Cascade Reactions Involving 1,2â€Indole Migration. <i>Chemistry - A European Journal</i> , 2015, 21, 12889-12893.	1.7	17
40	Normalâ€toâ€Abnormal NHC Rearrangement of Al^{III}, Ga^{III}, and In^{III} Trialkyl Complexes: Scope, Mechanism, Reactivity Studies, and H₂ Activation. <i>Chemistry - A European Journal</i> , 2015, 21, 17959-17972.	1.7	61
41	Diradical ring closing reactions displaying Woodwardâ€Hoffmann behaviour and torquoselectivity. <i>RSC Advances</i> , 2015, 5, 30405-30408.	1.7	6
42	Accounting for Diradical Character through DFT. The Case of Vinyl Allene Oxide Rearrangement. <i>Journal of Organic Chemistry</i> , 2015, 80, 11206-11211.	1.7	9
43	Computational Approaches to Homogeneous Gold Catalysis. <i>Topics in Current Chemistry</i> , 2014, 357, 213-283.	4.0	28
44	Bis(o-methylserotonin)-containing iridium(III) and ruthenium(II) complexes as new cellular imaging dyes: synthesis, applications, and photophysical and computational studies. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 679-692.	1.1	9
45	Computational insights on the mechanism of the catalytic hydrogenation with BINAPâ€diamineâ€Ru complexes: the role of base and origin of selectivity. <i>Chemical Communications</i> , 2013, 49, 4277-4279.	2.2	16
46	Computational Study of Gold-Catalyzed Homo- and Cross-Coupling Reactions. <i>Journal of Organic Chemistry</i> , 2013, 78, 4929-4939.	1.7	29
47	Noyori Hydrogenation: Aromaticity, Synchronicity, and Activation Strain Analysis. <i>Journal of Organic Chemistry</i> , 2013, 78, 5669-5676.	1.7	44
48	Theoretical and experimental exploration of the photochemistry of resveratrol: beyond the simple double bond isomerization. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 9175.	1.5	37
49	Mechanistic and Stereochemical Insights on the Pt-Catalyzed Rearrangement of Oxiranylpropargylic Esters to Cyclopentenones. <i>Journal of Organic Chemistry</i> , 2012, 77, 8733-8743.	1.7	17
50	DFT-Based Insights into Pdâ€Zn Cooperative Effects in Oxidative Addition and Reductive Elimination Processes Relevant to Negishi Cross-Couplings. <i>Organometallics</i> , 2012, 31, 2053-2058.	1.1	53
51	Novel emissive podands based on 8-OH-quinoline: Synthesis, fluorescence materials, DFT and complexation studies. <i>Inorganica Chimica Acta</i> , 2012, 381, 218-228.	1.2	11
52	On the Memory of Chirality in Gold(I)-Catalyzed Intramolecular Carboalkoxylation of Alkynes. <i>Journal of Organic Chemistry</i> , 2011, 76, 3791-3796.	1.7	41
53	DFT-Based Mechanistic Insights into Noble Metal-Catalyzed Rearrangement of Propargylic Derivatives: Chirality Transfer Processes. <i>Topics in Current Chemistry</i> , 2011, 302, 81-130.	4.0	13
54	Performance of density functional theory on homogeneous gold catalysis. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 647-661.	0.5	81

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55	Synthesis, characterization, fluorescence and computational studies of new Cu ²⁺ , Ni ²⁺ and Hg ²⁺ complexes with emissive thienylbenzoxazolyl-alanine ligands. <i>Inorganica Chimica Acta</i> , 2011, 366, 154-160.	1.2	16
56	Cyclization Cascade of Allenyl Azides: Synergy Between Theory and Experiment. <i>Current Organic Chemistry</i> , 2010, 14, 1646-1657.	0.9	15
57	Synthesis of Diverse Indole-Containing Scaffolds by Gold(I)-Catalyzed Tandem Reactions of 3-Propargylindoles Initiated by 1,2-Indole Migrations: Scope and Computational Studies. <i>Chemistry - A European Journal</i> , 2010, 16, 9818-9828.	1.7	59
58	Hg ²⁺ 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. <i>Inorganic Chemistry</i> , 2010, 49, 8276-8286.	1.9	43
59	Regio-, Peri-, and Torquoselectivity in Hydroxy Heptatrienyl Cation Electrocyclizations: The Iso/Homo-Nazarov Reaction. <i>Chemistry - A European Journal</i> , 2009, 15, 1944-1956.	1.7	29
60	Torquoselectivity in the electrocyclic ring-opening of cyclopropyl anions. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 378-385.	0.9	10
61	Exploiting anionic and cationic interactions with a new emissive imine-based 1 ² -naphthol molecular probe. <i>Inorganic Chemistry Communication</i> , 2009, 12, 905-912.	1.8	15
62	Mechanism of the Gold-Catalyzed Rearrangement of (3-Acyloxyprop-1-ynyl)oxiranes: A Dual Role of the Catalyst. <i>Journal of Organic Chemistry</i> , 2009, 74, 2982-2991.	1.7	50
63	Allenyl Azide Cycloaddition Chemistry. 2,3-Cyclopentennelated Indole Synthesis through Indolidene Intermediates. <i>Journal of Organic Chemistry</i> , 2009, 74, 4958-4974.	1.7	41
64	Complex Thermal Behavior of 11-cis-Retinal, the Ligand of the Visual Pigments. <i>Journal of Organic Chemistry</i> , 2009, 74, 1007-1013.	1.7	10
65	Electrocyclic Ring Opening of Charged cis-Bicyclo[3.2.0]heptadiene and Heterocyclic Derivatives. The Anti-Woodward-Hoffmann Quest (II). <i>Journal of Organic Chemistry</i> , 2009, 74, 2396-2402.	1.7	15
66	Associative Transmetalation in the Stille Cross-Coupling Reaction to Form Dienes: Theoretical Insights into the Open Pathway. <i>Organometallics</i> , 2008, 27, 3378-3389.	1.1	47
67	Allenyl Azide Cycloaddition Chemistry. Photochemical Initiation and CuI Mediation Leads to Improved Regioselectivity. <i>Organic Letters</i> , 2008, 10, 1665-1668.	2.4	41
68	Characterization of the Switch in the Mechanism of an Intramolecular Diels-Alder Reaction. <i>Journal of Organic Chemistry</i> , 2008, 73, 467-473.	1.7	14
69	Allenyl Azide Cycloaddition Chemistry: Exploration of the Scope and Mechanism of Cyclopentennelated Dihydropyrrole Synthesis through Azatrimethylenemethane Intermediates. <i>Journal of Organic Chemistry</i> , 2008, 73, 5090-5099.	1.7	25
70	Sulfoxide-Induced Stereoselection in [1,5]-Sigmatropic Hydrogen Shifts of Vinylallenes. A Computational Study. <i>Journal of Organic Chemistry</i> , 2007, 72, 2617-2624.	1.7	13
71	Cyclization Cascade of Allenyl Azides: A Dual Mechanism. <i>Journal of the American Chemical Society</i> , 2007, 129, 7638-7646.	6.6	35
72	Electrocyclic Ring Opening of cis-Bicyclo[m.n.0]alkenes: The Anti-Woodward-Hoffmann Quest. <i>Chemistry - A European Journal</i> , 2007, 13, 5009-5017.	1.7	22

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73	A Density Functional Theory Study of the Stille Cross-Coupling via Associative Transmetalation. The Role of Ligands and Coordinating Solvents. <i>Advanced Synthesis and Catalysis</i> , 2007, 349, 887-906.	2.1	43
74	Pseudopericyclic design drives antarafacial [1,5] methylene sigmatropic shifts from a stepwise to a concerted mechanism. <i>Journal of Computational Chemistry</i> , 2007, 28, 1411-1416.	1.5	7
75	Computational Characterization of a Complete Palladium-Catalyzed Cross-Coupling Process: The Associative Transmetalation in the Stille Reaction. <i>Organic Letters</i> , 2006, 8, 35-38.	2.4	78
76	Mechanism of the Gold(I)-Catalyzed Rautenstrauch Rearrangement: A Center-to-Helix-to-Center Chirality Transfer. <i>Journal of the American Chemical Society</i> , 2006, 128, 2434-2437.	6.6	183
77	Cycloisomerization of Activated (2E,4Z)-Heptatrienoate and Its Relevance to Crispatene (Bio)synthesis. A Case of Concerted and Stepwise Uncertainty. <i>Journal of Organic Chemistry</i> , 2006, 71, 4497-4501.	1.7	10
78	Computational Study and Analysis of the Kinetic Isotope Effects of the Rearrangement of cis-Bicyclo[4.2.0]oct-7-ene to cis-Cycloocta-1,3-diene. <i>Organic Letters</i> , 2006, 8, 2055-2058.	2.4	21
79	QCRNA 1.0: A database of quantum calculations for RNA catalysis. <i>Journal of Molecular Graphics and Modelling</i> , 2006, 25, 423-433.	1.3	26
80	Computation of vertical excitation energies of retinal and analogs: Scope and limitations. <i>Journal of Computational Chemistry</i> , 2006, 27, 116-123.	1.5	25
81	Pseudorotation Barriers of Biological Oxyphosphoranes: A Challenge for Simulations of Ribozyme Catalysis. <i>Chemistry - A European Journal</i> , 2005, 11, 2081-2093.	1.7	54
82	Ellipticity: A Convenient Tool To Characterize Electrocyclic Reactions. <i>Chemistry - A European Journal</i> , 2005, 11, 1734-1738.	1.7	71
83	Mechanistic subtleties in the cyclopentannulation of allenolate allyl carbamates: the origin of the center-to-center chirality transfer. <i>Chemical Communications</i> , 2005, , 4285.	2.2	12
84	2-Alkylidene-sulfonol-3-enes by (Regio- and) Stereoselective Cheletropic Addition of SO ₂ to (Di)vinylallenes. <i>Organic Letters</i> , 2005, 7, 1565-1568.	2.4	12
85	Simple Diastereoselectivity of the BF ₃ ·OEt ₂ -Catalyzed Vinylogous Mukaiyama Aldol Reaction of 2-(Trimethylsilyloxy)furans with Aldehydes. <i>Journal of Organic Chemistry</i> , 2005, 70, 3654-3659.	1.7	33
86	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. <i>ChemPhysChem</i> , 2004, 5, 1045-1049.	1.0	32
87	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. <i>ChemPhysChem</i> , 2004, 5, 1266-1266.	1.0	1
88	Theoretical Study of the Electrocyclic Ring Closure of Hydroxypentadienyl Cations. <i>Chemistry - A European Journal</i> , 2004, 10, 4324-4333.	1.7	95
89	The Woodward-Hoffmann-De Puy Rule Revisited. <i>Organic Letters</i> , 2004, 6, 905-908.	2.4	31
90	Solvolytic Ring-Opening Reactions of Cyclopropyl Bromides. An Assessment of the Woodward-Hoffmann-DePuy Rule. <i>Journal of Organic Chemistry</i> , 2004, 69, 9002-9010.	1.7	30

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91	Conrotatory Ring-Opening Reactions of Cyclopropyl Anions in Monocyclic and Tricyclic Systems. <i>Organic Letters</i> , 2004, 6, 901-904.	2.4	13
92	Theoretical Study of the Vinyl Allene Oxide to Cyclopent-2-en-1-one Rearrangement: Mechanism, Torquoselectivity and Solvent Effects. <i>Journal of Organic Chemistry</i> , 2004, 69, 3635-3644.	1.7	35
93	On the mechanism of the Au(I)-mediated addition of alkynes to anthranils to furnish 7-acylindoles. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	2