

Giovanni Ghigo

List of Publications by Year in descending order

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61
papers

3,552
citations

331670

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138484

58
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61
all docs

61
docs citations

61
times ranked

4133
citing authors

#	ARTICLE	IF	CITATIONS
1	MOLCAS 7: The Next Generation. <i>Journal of Computational Chemistry</i> , 2010, 31, 224-247.	3.3	1,485
2	A modified definition of the zeroth-order Hamiltonian in multiconfigurational perturbation theory (CASPT2). <i>Chemical Physics Letters</i> , 2004, 396, 142-149.	2.6	897
3	Photochemical transformation of ibuprofen into harmful 4-isobutylacetophenone: Pathways, kinetics, and significance for surface waters. <i>Water Research</i> , 2013, 47, 6109-6121.	11.3	81
4	Diradical and Peroxirane Pathways in the $[1\pi + 2\pi]$ Cycloaddition Reactions of Singlet Dioxygen with Ethene, Methyl Vinyl Ether, and Butadiene: A Density Functional and Multireference Perturbation Theory Study. <i>Journal of the American Chemical Society</i> , 2000, 122, 1414-1423.	13.7	78
5	The mechanism of the Stevens and Sommelet-Hauser Rearrangements. A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 3608-3617.	3.2	73
6	Benzene Oxidation in the Troposphere. Theoretical Investigation on the Possible Competition of Three Postulated Reaction Channels. <i>Journal of the American Chemical Society</i> , 1998, 120, 6753-6757.	13.7	51
7	From Benzene to Muconaldehyde: A Theoretical Mechanistic Investigation on Some Tropospheric Oxidation Channels. <i>Journal of the American Chemical Society</i> , 1999, 121, 8366-8372.	13.7	50
8	Oxidative Degradation of Benzene in the Troposphere. Theoretical Mechanistic Study of the Formation of Unsaturated Dialdehydes and Dialdehyde Epoxides. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4411-4422.	2.5	47
9	Combustion and atmospheric oxidation of hydrocarbons: Theoretical study of the methyl peroxy self-reaction. <i>Journal of Chemical Physics</i> , 2003, 118, 10575-10583.	3.0	47
10	Computational assessment of the fluorescence emission of phenol oligomers: A possible insight into the fluorescence properties of humic-like substances (HULIS). <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 315, 87-93.	3.9	41
11	The oxidized soot surface: Theoretical study of desorption mechanisms involving oxygenated functionalities and comparison with temperature programmed desorption experiments. <i>Journal of Chemical Physics</i> , 2006, 125, 194706.	3.0	37
12	Modeling Soot and Its Functionalization under Atmospheric or Combustion Conditions by Density Functional Theory within Molecular (Polycyclic-Aromatic-Hydrocarbon-like) and Periodic Methodologies. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3215-3223.	2.6	35
13	First Ring Formation by Radical Addition of Propargyl to But-1-ene-3-yne in Combustion. Theoretical Study of the C_7H_7 Radical System. <i>Journal of Physical Chemistry A</i> , 2014, 118, 427-440.	2.5	32
14	CLEPS 1.0: A new protocol for cloud aqueous phase oxidation of VOC mechanisms. <i>Geoscientific Model Development</i> , 2017, 10, 1339-1362.	3.6	30
15	Tailoring fluorescent strigolactones for in vivo investigations: a computational and experimental study. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 2960-2968.	2.8	28
16	Polycyclic aromatic hydrocarbon formation mechanism in the α -particle phase: A theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9429.	2.8	27
17	The Mechanism of the Acid-Catalyzed Benzidine Rearrangement of Hydrazobenzene: A Theoretical Study. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 2326-2333.	2.4	27
18	o-Benzenedisulfonimide and its chiral derivative as Brønsted acids catalysts for one-pot three-component Strecker reaction. Synthetic and mechanistic aspects. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 4058.	2.8	26

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19	New insights into the protogenic and spectroscopic properties of commercial tannic acid: the role of gallic acid impurities. <i>New Journal of Chemistry</i> , 2018, 42, 7703-7712.	2.8	25
20	Theoretical Study on the Reactivity and Regioselectivity of the Ene Reaction of $1^{\hat{3}}\text{g O}_2$ with $\hat{1},\hat{2}$ -Unsaturated Carbonyl Compounds. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 3643-3649.	2.4	22
21	Tropospheric Oxidation of Ethyne and But-2-yne. 1. Theoretical Mechanistic Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3656-3665.	2.5	22
22	The $1^{\hat{3}}\text{g}$ Dioxygen Ene Reaction with Propene: A Density Functional and Multireference Perturbation Theory Mechanistic Study. <i>Chemistry - A European Journal</i> , 2003, 9, 2616-2626.	3.3	21
23	Soot Platelets and PAHs with an Odd Number of Unsaturated Carbon Atoms and $\hat{1}\hat{e}$ Electrons: $\hat{a}\hat{e}\%$ Theoretical Study of Their Spin Properties and Interaction with Ozone. <i>Journal of Physical Chemistry A</i> , 2008, 112, 973-982.	2.5	20
24	Synthetic and Mechanistic Aspects of Acid-Catalyzed Disproportionation of Dialkyl Diarylmethyl Ethers: A Combined Experimental and Theoretical Study. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 4346-4351.	2.4	20
25	Aromatic Hydrocarbon Nitration under Tropospheric and Combustion Conditions. A Theoretical Mechanistic Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13270-13282.	2.5	19
26	A theoretical study of the excited states of CrH: Potential energies, transition moments, and lifetimes. <i>Journal of Chemical Physics</i> , 2004, 121, 8194.	3.0	18
27	A change from stepwise to concerted mechanism in the acid-catalysed benzidine rearrangement: a theoretical study. <i>Tetrahedron</i> , 2012, 68, 2161-2165.	1.9	18
28	Visible Light Mediated Photocatalytic $\hat{1}\hat{N}$ -Radical Cascade Reactivity of $\hat{1},\hat{3},\hat{1}$ -Unsaturated $\hat{1}\hat{N}$ -Arylsulfonylhydrazones: A General Approach to Structurally Diverse Tetrahydropyridazines. <i>Journal of Organic Chemistry</i> , 2021, 86, 3300-3323.	3.2	17
29	First carbon ring closures started by the combustive radical addition of propargyl to butadiyne. A theoretical study. <i>Combustion and Flame</i> , 2013, 160, 2333-2342.	5.2	16
30	Quantum Chemical Characterization of Low-Energy States of Calicene in the Gas Phase and in Solution. <i>Journal of Organic Chemistry</i> , 2007, 72, 2823-2831.	3.2	14
31	Reactions of Arenediazonium $\hat{1}\hat{O}$ -Benzenedisulfonimides with Aliphatic Triorganoindium Compounds. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 862-868.	2.4	14
32	Synthesis of 3-aryl-4-methyl-1,2-benzenedisulfonimides, new chiral Brønsted acids. A combined experimental and theoretical study. <i>Tetrahedron</i> , 2011, 67, 5789-5797.	1.9	14
33	<i>o</i> -Benzyne fragmentation and isomerization pathways: a CASPT2 study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23944-23951.	2.8	14
34	Density functional, single and multireference perturbation theory study of the reaction $3^{\hat{1}}\text{gO}_2 + \text{HOCH}_2\text{CH}_2\hat{a}\hat{c}\hat{t}^{\hat{1}}\text{HOO}\hat{a}\hat{c}\hat{t} + \text{HOCH}=\text{CH}_2$, modeling an important step in tropospheric benzene oxidation. <i>Journal of Chemical Physics</i> , 1999, 110, 7298-7304.	3.0	13
35	Memory Effects in Carbocation Rearrangements: Structural and Dynamic Study of the Norborn-2-en-7-ylmethyl-X Solvolysis Case. <i>Journal of Organic Chemistry</i> , 2013, 78, 9041-9050.	3.2	13
36	Evidence of an Important Role of Photochemistry in the Attenuation of the Secondary Contaminant 3,4-Dichloroaniline in Paddy Water. <i>Environmental Science & Technology</i> , 2018, 52, 6334-6342.	10.0	13

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37	How do arenediazonium salts behave in deep eutectic solvents? A combined experimental and computational approach. <i>Journal of Molecular Liquids</i> , 2021, 339, 116743.	4.9	13
38	Copper catalysed Gomberg-Bachmann-Hey reactions of arenediazonium tetrafluoroborates and heteroarenediazonium o-benzenedisulfonimides. Synthetic and mechanistic aspects. <i>Tetrahedron</i> , 2020, 76, 131632.	1.9	12
39	Catalytic properties and acidity of 1,2-benzenedisulfonimide and some of its derivatives. An experimental and computational study. <i>Tetrahedron</i> , 2013, 69, 3212-3217.	1.9	10
40	Reaction between propargyl radical and 1,3-butadiene to form five to seven membered rings. Theoretical study. <i>Combustion and Flame</i> , 2016, 168, 331-341.	5.2	10
41	Aerobic CuCl ₂ -Catalyzed Dehydrogenative Cross-Coupling of Tertiary Amines. A Combined Computational and Experimental Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2796-2814.	2.5	9
42	Experimental and theoretical study of the fluorescence emission of ferulic acid: Possible insights into the fluorescence properties of humic substances. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117587.	3.9	9
43	Copper-Free Halodediazoniating of Arenediazonium Tetrafluoroborates in Deep Eutectic Solvents-like Mixtures. <i>Molecules</i> , 2022, 27, 1909.	3.8	9
44	Anthracene and phenanthrene tropospheric oxidation promoted by the nitrate radical in the gas-phase. Theoretical modelistic study. <i>Atmospheric Environment</i> , 2017, 167, 181-189.	4.1	8
45	Ab initio theoretical investigation on the reactivity as bases of mixed LiMe/KOMe complexes. A model for Schlosser LICKOR superbase. <i>Tetrahedron</i> , 1996, 52, 7053-7062.	1.9	7
46	Border Reactivity of Polycyclic Aromatic Hydrocarbons and Soot Platelets Toward Ozone. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 470-481.	2.5	7
47	The nature of the light absorption and emission transitions of 4-hydroxybenzophenone in different solvents. A combined computational and experimental study. <i>Photochemical and Photobiological Sciences</i> , 2017, 16, 527-538.	2.9	7
48	Ab initio theoretical study of metallo-dehydrogenation and nucleophilic addition of methyllithium and methylpotassium with crotonaldehyde dimethyl acetal. <i>Tetrahedron</i> , 1997, 53, 7937-7946.	1.9	6
49	Mechanistic Significance of Peroxide Trapping Experiments, with Epoxide Detection, in ¹¹ B Dioxygen Reactions with Alkenes. <i>Journal of Organic Chemistry</i> , 2003, 68, 3125-3129.	3.2	6
50	A simple, direct synthesis of 3-vinylindoles from the carbocation-catalysed dehydrative cross-coupling of ketones and indoles. A combined experimental and computational study. <i>Tetrahedron</i> , 2019, 75, 363-373.	1.9	6
51	Blue light enhanced Heck arylation at room temperature applied to allenes. <i>Organic Chemistry Frontiers</i> , 2022, 9, 906-916.	4.5	6
52	The electronic spectra of 2-(2-hydroxybenzoyl)pyrrole and 2-(2-methoxybenzoyl)pyrrole: a theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 1099-1106.	1.9	5
53	Theoretical mechanistic studies on oxidation reactions of some saturated and unsaturated organic molecules. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 699-707.	1.4	4
54	Efficient alkylation of cyclic silyl enol ethers by diarylmethyl salts. <i>Tetrahedron Letters</i> , 2016, 57, 4758-4762.	1.4	4

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55	Methyl and Silyl Mesolytic Dissociations in the Radical Cations and Radical Anions of But-1-ene, Allylsilane, Hexa-1,3-diene, and Penta-2,4-dienylsilane. CASâ”MCSCF and Coupled Cluster Theoretical Study. <i>Journal of Organic Chemistry</i> , 2003, 68, 6083-6095.	3.2	3
56	Tuning of the Electronic Properties of Armchair Graphene Nanoribbons through Functionalization: Theoretical Study of 1^{st} O_2 Border Addition. <i>ChemPhysChem</i> , 2015, 16, 3030-3037.	2.1	2
57	Diastereoselective synthesis of 3-(\pm -aryl)alkenylindoles from the direct dehydrative coupling of indoles and ketones: A synthetic and theoretical study. <i>Tetrahedron</i> , 2020, 76, 131498.	1.9	2
58	Ab initio theoretical study of the reactivity as bases or nucleophiles of potassium and lithium methides. <i>Journal of Physical Organic Chemistry</i> , 1997, 10, 885-897.	1.9	1
59	Tuning of the electronic properties of H-passivated armchair graphene nanoribbons by mild border oxidation: Theoretical study on periodic models. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1281-1284.	2.0	1
60	Combustive, Postcombustive, and Tropospheric Butadiyne Oxidation by O_2 , Following Initial HO Attack. Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10172-10180.	2.5	0
61	Mechanistic dichotomy in the gas-phase addition of NO_3 to polycyclic aromatic hydrocarbons: Theoretical study. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25641.	2.0	0