Giovanni F Caramori

List of Publications by Year in Descending Order

107 papers	1,312 citations	21 h-index	30 g-index
116 ext. papers	1,527 ext. citations	4 avg, IF	4.61 L-index

#	Paper	IF	Citations
107	Reverse solvatochromism in a family of probes having 2,6-di-tert-butylphenolate as electron-donor and 4-nitrophenyl as electron-acceptor groups. *Dyes and Pigments*, **2022**, 203, 110376	4.6	0
106	Development, structural, spectroscopic and investigation of new complexes relevant as anti-toxoplasma metallopharmacs. *Journal of Molecular Structure*, **2022**, 133380	3.4	0
105	Nature of hydride and halide encapsulation in Ag cages: insights from the structure and interaction energy of [Ag(X){SP(OPr)}] (X = H, F, Cl, Br, I) from relativistic DFT calculations.. *Physical Chemistry Chemical Physics*, **2021**, 24, 452-458	3.6	
104	Theoretical study of chloride complexes with hybrid macrocycles. *New Journal of Chemistry*, **2021**, 45, 463-470	3.6	
103	Can the relative positions (cis-trans) of ligands really modulate the coordination of NO in ruthenium nitrosyl complexes?. *New Journal of Chemistry*, **2021**, 45, 1658-1666	3.6	1
102	The design of anion-π interactions and hydrogen bonds for the recognition of chloride, bromide and nitrate anions. *Physical Chemistry Chemical Physics*, **2021**, 23, 11455-11465	3.6	1
101	Designing boron and metal complexes for fluoride recognition: a computational perspective. *Physical Chemistry Chemical Physics*, **2021**, 23, 22768-22778	3.6	
100	The π-donor/acceptor trans effect on NO release in ruthenium nitrosyl complexes: a computational insight. *New Journal of Chemistry*, **2021**, 45, 8949-8957	3.6	
99	Development of new dinuclear Fe(III) coordination compounds with nanomolar antitrypanosomal activity. *Dalton Transactions*, **2021**, 50, 12242-12264	4.3	0
98	Box-Shaped Hosts: Evaluation of the Interaction Nature and Host Characteristics of ExBox Derivatives in Host-Guest Complexes from Computational Methods **2021**, 395-416		1
97	Supersaturating drug delivery systems containing fixed-dose combination of two antihypertensive drugs: Formulation, in vitro evaluation and molecular metadynamics simulations. *European Journal of Pharmaceutical Sciences*, **2021**, 163, 105860	5.1	2
96	Synthesis, characterization and photoinduced CO-release by manganese(I) complexes. *New Journal of Chemistry*, **2020**, 44, 10892-10901	3.6	2
95	Platinum-Triggered Bond-Cleavage of Pentynoyl Amide and -Propargyl Handles for Drug-Activation. *Journal of the American Chemical Society*, **2020**, 142, 10869-10880	16.4	38
94	Tracking the role of trans-ligands in ruthenium-NO bond lability: computational insight. *New Journal of Chemistry*, **2020**, 44, 11448-11456	3.6	2
93	In Silico Design of Cylindrophanes: The Role of Functional Groups in a Fluoride Selective Host. *ChemPhysChem*, **2020**, 21, 1989-2005	3.2	3
92	The anionic recognition mechanism based on polyol and boronic acid receptors. *New Journal of Chemistry*, **2020**, 44, 5564-5571	3.6	1
91	Coordination among Bond Formation/Cleavage in a Bifunctional-Catalyzed Fast Amide Hydrolysis: Evidence for an Optimized Intramolecular -Protonation Event. *Journal of Organic Chemistry*, **2020**, 85, 4663-4671	4.2	5

90	Are DFT Methods Able to Predict Reduction Potentials of Ruthenium Nitrosyl Complexes Accurately?. *Journal of Physical Chemistry A*, **2020**, 124, 6186-6192	2.8	
89	Shedding light on the bonding situation of triangular and square heterometallic clusters: computational insight. *New Journal of Chemistry*, **2020**, 44, 5079-5087	3.6	1
88	How does the acidic milieu interfere in the capability of ruthenium nitrosyl complexes to release nitric oxide?. *New Journal of Chemistry*, **2020**, 44, 773-779	3.6	4
87	Solvatochromism of new substituted 4-[(E)-(4-nitrophenyl)diazenyl]phenolate dyes. *Journal of Molecular Liquids*, **2020**, 301, 112330	6	3
86	The bonding situation in heteromultimetallic carbonyl complexes. *Dalton Transactions*, **2020**, 49, 16762-16771	4.3	1
85	The simultaneous recognition mechanism of cations and anions using macrocyclic-iodine structures: insights from dispersion-corrected DFT calculations. *Physical Chemistry Chemical Physics*, **2020**, 22, 23795-23803	3.6	0
84	The usefulness of energy decomposition schemes to rationalize host-guest interactions. *Dalton Transactions*, **2020**, 49, 17457-17471	4.3	5
83	What is the driving force behind molecular triangles and their guests? A quantum chemical perspective about host-guest interactions. *Physical Chemistry Chemical Physics*, **2020**, 22, 19213-19222	3.6	2
82	On the recognition of chloride, bromide and nitrate anions by anthracene–squaramide conjugated compounds: a computational perspective. *New Journal of Chemistry*, **2020**, 44, 17831-17839	3.6	3
81	Kinetics and adsorption calculations: insights into the MgO-catalyzed detoxification of simulants of organophosphorus biocides. *Journal of Materials Chemistry A*, **2020**, 8, 19011-19021	13	3
80	A ruthenium nitrosyl cyclam complex with appended anthracenyl fluorophore. *Polyhedron*, **2019**, 173, 114117	2.7	
79	Mechanism of Palladium(II)-Mediated Uncaging Reactions of Propargylic Substrates. *ACS Catalysis*, **2019**, 9, 3792-3799	13.1	8
78	Synthesis, characterization and biological evaluation of new manganese metal carbonyl compounds that contain sulfur and selenium ligands as a promising new class of CORMs. *Dalton Transactions*, **2019**, 48, 5574-5584	4.3	11
77	Tracking the absence of anion–π interactions in modified [23](1,3,5)cyclophanes: insights from computation. *New Journal of Chemistry*, **2019**, 43, 13271-13281	3.6	1
76	Understanding the interplay between π-hole and cation–π interactions in [janusene-Ag] host-guest systems: a computational approach. *Dalton Transactions*, **2019**, 48, 13281-13292	4.3	3
75	ESI-QTof-MS characterization of hirsutinolide and glaucolide sesquiterpene lactones: Fragmentation mechanisms and differentiation based on Na /H adducts interactions in complex mixture. *Journal of Mass Spectrometry*, **2019**, 54, 915-932	2.2	7
74	Shedding Light on the Hydrolysis Mechanism of cis, trans-[Ru(dmso)Cl] Complexes and Their Interactions with DNA-A Computational Perspective. *Journal of Physical Chemistry B*, **2019**, 123, 457-467	3.4	3
73	Shedding light on the electronic structure of [Ru(=CH)(NH)] complex: a computational insight. *Journal of Molecular Modeling*, **2019**, 25, 11	2	3

72	A theoretical investigation on the aminolysis of pyromellitic and 1,4,5,8-naphthalenetetracarboxylic dianhydrides. *Computational and Theoretical Chemistry*, **2019**, 1147, 13-19	2	1
71	Advances in bonding and properties of inorganic systems from relativistic calculations in Latin America. *International Journal of Quantum Chemistry*, **2019**, 119, e25777	2.1	3
70	On the cation□capabilities of small all sp2-carbon host structures. Evaluation of [6.8]3cyclacene from relativistic DFT calculations. *International Journal of Quantum Chemistry*, **2019**, 119, e25811	2.1	5
69	Evaluation of Lignans from Piper cubeba against Schistosoma mansoni Adult Worms: A Combined Experimental and Theoretical Study. *Chemistry and Biodiversity*, **2019**, 16, e1800305	2.5	4
68	Quest for Insight into Ultrashort C-H□□Proximities in Molecular "Iron Maidens". *Journal of Organic Chemistry*, **2018**, 83, 5114-5122	4.2	7
67	Reverse Solvatochromism of Imine Dyes Comprised of 5-Nitrofuran-2-yl or 5-Nitrothiophen-2-yl as Electron Acceptor and Phenolate as Electron Donor. *Chemistry - A European Journal*, **2018**, 24, 9364-9376	4.8	6
66	The ability of Ex2Box4+ to interact with guests containing □electron-rich and □electron-poor moieties. *International Journal of Quantum Chemistry*, **2018**, 118, e25607	2.1	9
65	Bond Analysis in Dihalogen□Halide and Dihalogen□Dimethylchalcogenide Systems. *European Journal of Inorganic Chemistry*, **2018**, 2018, 1007-1015	2.3	6
64	Tuning Heterocalixarenes to Improve Their Anion Recognition: A Computational Approach. *Journal of Physical Chemistry A*, **2018**, 122, 3328-3336	2.8	19
63	Polylactic acid, maleic anhydride and dicumyl peroxide: NMR study of the free-radical melt reaction product. *Polymer Degradation and Stability*, **2018**, 155, 1-8	4.7	5
62	Helicenes as Molecular Tweezers in the Formation of Cation-□Complexes. Bonding and Circular Dichroism Properties from Relativistic DFT Calculations. *ChemPhysChem*, **2018**, 19, 2321-2330	3.2	5
61	Cucurbituril-Mediated Catalytic Hydrolysis: A Kinetic and Computational Study with Neutral and Cationic Dioxolanes in CB7. *ACS Catalysis*, **2018**, 8, 12067-12079	13.1	25
60	In vitro cytotoxicity and structure-activity relationship approaches of ent-kaurenoic acid derivatives against human breast carcinoma cell line. *Phytochemistry*, **2018**, 156, 214-223	4	13
59	How Do Secondary Phosphine Oxides Interact with Silver Nanoclusters? Insights from Computation. *Journal of Physical Chemistry C*, **2018**, 122, 21449-21461	3.8	5
58	Anion Recognition by Organometallic Calixarenes: Analysis from Relativistic DFT Calculations. *Organometallics*, **2018**, 37, 2167-2176	3.8	20
57	Binding affinity studies of 1,2,3-triazole copper(II) complexes to human serum albumin. *Journal of Coordination Chemistry*, **2018**, 71, 1894-1909	1.6	5
56	Solvation Enhances the Distinction between Carboxylated Armchair and Zigzag Single-Wall Carbon Nanotubes (SWNT-COOH). *Journal of Physical Chemistry C*, **2017**, 121, 9516-9527	3.8	1
55	In vivo and in silico anti-inflammatory mechanism of action of the semisynthetic (-)-cubebin derivatives (-)-hinokinin and (-)-O-benzylcubebin. *Bioorganic and Medicinal Chemistry Letters*, **2017**, 27, 176-179	2.9	10

54	Metal-ligand bonding situation in ruthenophanes containing i,j-xylylene-linked bis(NHC)cyclophane ligands. *Journal of Organometallic Chemistry*, **2017**, 830, 100-108	2.3	2
53	Metal□ligand Bonding Situation in Ruthenophanes Containing Multibridged Cyclophanes. *Organometallics*, **2017**, 36, 3465-3470	3.8	8
52	Removal of the emerging contaminant bisphenol A by an ureasil-PEO hybrid membrane: experimental study and molecular dynamic simulation. *Environmental Science and Pollution Research*, **2017**, 24, 18421-18433	5.1	4
51	How the electron-deficient cavity of heterocalixarenes recognizes anions: insights from computation. *Physical Chemistry Chemical Physics*, **2017**, 19, 24696-24705	3.6	25
50	Electronic properties and metal-ligand bonding situation in Eu(III) complexes containing tris(pyrazolyl)borate and phenantroline ligands. *Journal of Luminescence*, **2017**, 182, 137-145	3.8	7
49	The versatile ruthenium(II/III) tetraazamacrocycle complexes and their nitrosyl derivatives. *Coordination Chemistry Reviews*, **2016**, 306, 652-677	23.2	30
48	Bonding Analysis in Homo- and Hetero-Trihalide Species: A Charge Displacement Study. *European Journal of Inorganic Chemistry*, **2016**, 2016, 3804-3812	2.3	8
47	Copaifera duckei Oleoresin and Its Main Nonvolatile Terpenes: In Vitro Schistosomicidal Properties. *Chemistry and Biodiversity*, **2016**, 13, 1348-1356	2.5	16
46	Evaluation of Electron Donation as a Mechanism for the Stabilisation of Chalcogenate-Protected Gold Nanoclusters. *ChemPhysChem*, **2016**, 17, 3102-3111	3.2	4
45	Shedding Light on the Nature of Host□Guest Interactions in PAHs-ExBox4+ Complexes. *Journal of Physical Chemistry C*, **2016**, 120, 15480-15487	3.8	12
44	Transport properties of ruthenophanes □A theoretical insight. *Chemical Physics*, **2016**, 478, 23-33	2.3	4
43	Hydrazine decomposition on a small platinum cluster: the role of N2H5 intermediate. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	6
42	A ruthenium polypyridyl complex with the antihypertensive drug valsartan: Synthesis, theoretical calculations and interaction studies with human serum albumin. *Polyhedron*, **2016**, 114, 232-241	2.7	13
41	Polar Order and Symmetry Breaking at the Boundary between Bent-Core and Rodlike Molecular Forms: When 4-Cyanoresorcinol Meets the Carbosilane End Group. *Chemistry - A European Journal*, **2016**, 22, 8181-97	4.8	15
40	Synthesis and Solvatochromism of Substituted 4-(Nitrostyryl)phenolate Dyes. *Journal of Organic Chemistry*, **2015**, 80, 7971-83	4.2	29
39	Role of the cation formal charge in cation□interaction. A survey involving the [2.2.2]paracyclophane host from relativistic DFT calculations. *New Journal of Chemistry*, **2015**, 39, 9963-9968	3.6	22
38	The influence of L ligands on the {RuNO}6/7 bonding situation in cis-[Ru(NO)(NO2)L14]q complexes: a theoretical insight. *RSC Advances*, **2015**, 5, 69057-69066	3.7	5
37	Ruthenium nitrosyl complexes containing pyridine-functionalized carbenes □A theoretical insight. *Journal of Organometallic Chemistry*, **2015**, 799-800, 54-60	2.3	5

36	Proton-induced generation of remote N-heterocyclic carbene-Ru complexes. *Chemistry - A European Journal*, **2015**, 21, 106-10	4.8	8
35	[2.2.2]Paracyclophane, preference for η6 or η18 coordination mode including Ag(I) and Sn(II): a survey into the cation–π interaction nature through relativistic DFT calculations. *RSC Advances*, **2015**, 5, 7803-7811	3.7	21
34	Cyclic trinuclear copper(I), silver(I), and gold(I) complexes: a theoretical insight. *Dalton Transactions*, **2015**, 44, 377-85	4.3	26
33	No need for a re-examination of the electrostatic notation of the hydrogen bonding: a comment. *Angewandte Chemie - International Edition*, **2015**, 54, 2596-9	16.4	69
32	Strontium mono-chloride ‒ A new molecule for the determination of chlorine using high-resolution graphite furnace molecular absorption spectrometry and direct solid sample analysis. *Spectrochimica Acta, Part B: Atomic Spectroscopy*, **2014**, 102, 1-6	3.1	26
31	Ruthenium(II) complexes of N-heterocyclic carbenes derived from imidazolium-linked cyclophanes. *Dalton Transactions*, **2014**, 43, 14710-9	4.3	9
30	Ru-NO and Ru-NO2 bonding linkage isomerism in cis-[Ru(NO)(NO)(bpy)2](2+/+) complexes - a theoretical insight. *Dalton Transactions*, **2014**, 43, 8792-804	4.3	18
29	Ruthenophanes: Evaluating Cation–π Interactions in [Ru(η6-C16H12R4)(NH3)3]2+/3+Complexes. A Computational Insight. *Organometallics*, **2014**, 33, 2301-2312	3.8	16
28	Spectroscopy and theoretical studies of natural melanin (eumelanin) and its complexation by iron(III). *Journal of Coordination Chemistry*, **2014**, 67, 986-1001	1.6	6
27	Ureasil-poly(ethylene oxide) hybrid matrix for selective adsorption and separation of dyes from water. *Langmuir*, **2014**, 30, 3857-68	4	36
26	Ruthenium(II)/4,6-dimethyl-2-mercaptopyrimidine complexes: Synthesis, characterization, X-ray structures and in vitro cytotoxicity activities on cancer cell lines. *Polyhedron*, **2014**, 68, 312-318	2.7	23
25	Investigating the Ritter Type Reaction of β-Methylene-γ-hydroxy Esters in Acidic Medium: Evidence for the Intermediacy of an Allylic Cation. *European Journal of Organic Chemistry*, **2013**, 2013, 5180-5187	3.2	3
24	Polyacetylenes from the leaves of Vernonia scorpioides (Asteraceae) and their antiproliferative and antiherpetic activities. *Phytochemistry*, **2013**, 95, 375-83	4	21
23	The two faces of hydrogen-bond strength on triple AAA-DDD arrays. *ChemPhysChem*, **2013**, 14, 3994-4001	3.2	13
22	Peculiar reactivity of a di-imine copper(II) complex regarding its binding to albumin protein. *Dalton Transactions*, **2013**, 42, 6386-96	4.3	15
21	Nanoparticle translocation through a lipid bilayer tuned by surface chemistry. *Physical Chemistry Chemical Physics*, **2013**, 15, 2282-90	3.6	64
20	Synthetic pathway for a new series of liquid crystal 2,6-disubstituted imidazo[2,1-b][1,3,4]thiadiazole. *Liquid Crystals*, **2013**, 40, 570-580	2.3	11
19	Nitro-substituted 4-[(phenylmethylene)imino]phenolates: solvatochromism and their use as solvatochromic switches and as probes for the investigation of preferential solvation in solvent mixtures. *Journal of Organic Chemistry*, **2012**, 77, 10668-79	4.2	39

18	The nature of Ru-NO bonds in ruthenium tetraazamacrocycle nitrosyl complexes--a computational study. *Dalton Transactions*, **2012**, 41, 7327-39	4.3	36
17	Isatin-Schiff base copper(II) complexes: A DFT study of the metal-ligand bonding situation. *International Journal of Quantum Chemistry*, **2012**, 112, 625-646	2.1	21
16	Hydrogen bond and the resonance effect on the formamide–water complexes. *International Journal of Quantum Chemistry*, **2012**, 112, 1401-1420	2.1	4
15	Quinolinyl and quinolinyl N-oxide chalcones: synthesis, antifungal and cytotoxic activities. *European Journal of Medicinal Chemistry*, **2011**, 46, 4448-56	6.8	32
14	Interactions of di-imine copper(II) complexes with albumin: competitive equilibria, promoted oxidative damage and DFT studies. *Journal of the Brazilian Chemical Society*, **2010**, 21, 1303-1317	1.5	13
13	Sesquiterpene lactones from Vernonia scorpioides and their in vitro cytotoxicity. *Phytochemistry*, **2010**, 71, 1539-44	4	37
12	Oxindole-Schiff base copper(II) complexes interactions with human serum albumin: spectroscopic, oxidative damage, and computational studies. *Journal of Inorganic Biochemistry*, **2009**, 103, 1331-41	4.2	21
11	The nature of the interactions between Pt4 cluster and the adsorbates *H, *OH, and H2O. *Journal of Physical Chemistry A*, **2008**, 112, 11731-43	2.8	29
10	The Nature of the Ru–NO Bond in Ruthenium Tetraammine Nitrosyl Complexes.. *Organometallics*, **2008**, 27, 1660-1660	3.8	
9	A computational study of tetrafluoro-[2.2]cyclophanes. *Journal of Physical Chemistry A*, **2008**, 112, 11784-800	2.8	17
8	Analysis of the metal–ligand bonds in [Mo(X)(NH2)3] (X = P, N, PO, and NO), [Mo(CO)5(NO)]+, and [Mo(CO)5(PO)]+. *Theoretical Chemistry Accounts*, **2008**, 120, 351-361	1.9	12
7	The Nature of the Ru–NO Bond in Ruthenium Tetraammine Nitrosyl Complexes. *Organometallics*, **2007**, 26, 5815-5825	3.8	53
6	Aromaticity and Homoaromaticity in Methano[10]annulenes.. *Journal of Organic Chemistry*, **2007**, 72, 2698-2698	4.2	2
5	Computational study about through-bond and through-space interactions in [2.2]cyclophanes. *Journal of Physical Chemistry A*, **2007**, 111, 1705-12	2.8	40
4	Aromaticity and Homoaromaticity in Methano[10]annulenes. *Journal of Organic Chemistry*, **2007**, 72, 76-85	4.2	22
3	Efeitos de substituintes na ligação de hidrogênio do 3-hidroxipropenal. *Quimica Nova*, **2006**, 29, 1187-1192	1.6	2
2	A New Exploration of the Torsional Energy Surface of n-Pentane Using Molecular Models and Molecular Modeling Software. *Journal of Chemical Education*, **2005**, 82, 1800	2.4	3
1	A computational study of [2.2]cyclophanes. *Journal of Organic Chemistry*, **2005**, 70, 3242-50	4.2	64