Girolamo A Casella

List of Publications by Year
in descending order

42 papers	737 citations	516710 16 h-index	552781 26 g-index
43 all docs	43 docs citations	43 times ranked	916 citing authors

#	Article	IF	Citations
1	Relativistic DFT Calculation of 119Sn Chemical Shifts and Coupling Constants in Tin Compounds. Journal of Chemical Theory and Computation, 2006, 2, 37-46.	5.3	83
2	Thermal behaviour and electrochemical properties of bis(trifluoromethanesulfonyl)amide and dodecatungstosilicate viologen dimers. Physical Chemistry Chemical Physics, 2012, 14, 2710.	2.8	51
3	Viologen-based ionic liquid crystals: induction of a smectic A phase by dimerisation. Physical Chemistry Chemical Physics, 2014, 16, 5048-5051.	2.8	47
4	DFT Calculation of ¹J(¹¹⁹Sn,¹³C) and ²J(¹¹⁹Sn,¹H) Coupling Constants in Di- and Trimethyltin(IV) Compounds. Inorganic Chemistry, 2008, 47, 4796-4807.	4.0	46
5	Hâ"ZSM-5 Modified Zeolite:â€‰ Quantum Chemical Models of Acidic Sites. Journal of Physical Chemistry C, 2007, 111, 13033-13043.	3.1	36
6	Ionic liquid crystals based on viologen dimers: tuning the mesomorphism by varying the conformational freedom of the ionic layer. Liquid Crystals, 2016, 43, 1161-1173.	2.2	35
7	DFT study of the interaction free energy of Ï€â€“Ï€ complexes of fullerenes with buckybowls and viologen dimers. New Journal of Chemistry, 2011, 35, 1453.	2.8	32
8	Mesomorphic and electrooptical properties of viologens based on non-symmetric alkyl/polyfluoroalkyl functionalization and on an oxadiazolyl-extended bent core. Journal of Materials Chemistry C, 2019, 7, 7974-7983.	5.5	32
9	Anti-cancer activity of di- and tri-organotin(IV) compounds with D-(+)-Galacturonic acid on human tumor cells. Journal of Inorganic Biochemistry, 2018, 188, 102-112.	3.5	31
10	Organometallic complexes with biological molecules. XVIII. Alkyltin(IV) cephalexinate complexes: synthesis, solid state and solution phase investigations. Journal of Inorganic Biochemistry, 2004, 98, 534-546.	3.5	30
11	Fourâ€Component Relativistic DFT Calculations of ¹³C Chemical Shifts of Halogenated Natural Substances. Chemistry - A European Journal, 2015, 21, 18834-18840.	3.3	27
12	An ultrathin suspended hydrophobic porous membrane for high-efficiency water desalination. Applied Materials Today, 2017, 9, 1-9.	4.3	27
13	A DFT study of the Karplus-type dependence of vicinal 3J(Snâ€"C-X-C), X=N,O,S, in organotin(iv) compounds: application to conformationally flexible systems. Organic and Biomolecular Chemistry, 2010, 8, 2711.	2.8	22
14	Diorganotin(IV) N-acetyl-l-cysteinate complexes: Synthesis, solid state, solution phase, DFT and biological investigations. Journal of Inorganic Biochemistry, 2010, 104, 750-758.	3.5	20
15	Spectroscopic signatures of the carbon buckyonions C60@C180 and C60@C240: a dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2013, 15, 18030.	2.8	19
16	A novel compound of triphenyltin(IV) with N-tert-butoxycarbonyl-l-ornithine causes cancer cell death by inducing a p53-dependent activation of the mitochondrial pathway of apoptosis. Inorganica Chimica Acta, 2017, 456, 1-8.	2.4	16
17	Karplusâ€Type Dependence of Vicinal ¹¹⁹Snâ€¹³C and ¹¹⁹Snâ€¹H Spinâ€Spin Couplings in Organotin(IV) Derivatives: A DFT Study. European Journal of Organic Chemistry, 2009, 2009, 3526-3534.	2.4	14
18	Covalently Conjugated Goldâ€"Porphyrin Nanostructures. Nanomaterials, 2020, 10, 1644.	4.1	14

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19	Diorganotin(IV) complexes ofD-galacturonic acid: solid-state and solution-phase structural study. Applied Organometallic Chemistry, 2003, 17, 932-939.	3.5	13
20	Synthesis, chemical characterization and biological activity of new histone acetylation/deacetylation specific inhibitors: A novel and potential approach to cancer therapy. Journal of Inorganic Biochemistry, 2013, 125, 16-25.	3.5	13
21	Comparative Experimental and Theoretical Study of the Fe L_{2,3}-Edges X-ray Absorption Spectroscopy in Three Highly Popular, Low-Spin Organoiron Complexes: [Fe(CO)₅], [(Î·⁵-C₅H₅)Fe(CO)(Î¼-CO)]₂, and [(Î·⁵-C₅H₅)₂Fe]. Inorganic Chemistry, 2019, 58, 5944-5957.	4.0	11
22	Solution structure of R2Sn(iv)-Î²-N-acetyl-neuraminate (R = Me, Bu) complexes in D2O and DMSO-d6: Experimental NMR and DFT computational study. Dalton Transactions, 2007, , 1440-1446.	3.3	10
23	Structure ofD-ribonic acid-dimethyltin(IV) in coordinating solvents: an experimental and DFT119Sn NMR study. Journal of Physical Organic Chemistry, 2006, 19, 874-883.	1.9	9
24	DFT calculation of NMR Î´(113Cd) in cadmium complexes. Polyhedron, 2016, 117, 48-56.	2.2	9
25	Title is missing!. Journal of Chemical Crystallography, 1998, 28, 791-796.	1.1	8
26	Through-Space Spin-Spin Coupling In Acetylenic Systems. Ab Initio and DFT Calculations. International Journal of Molecular Sciences, 2003, 4, 193-202.	4.1	8
27	A DFT study of the vicinal 3J(119Sn,13C) and 3J(119Sn,1H) coupling constants inÂtrimethyl- and chlorodimethylstannyl propanoates. Journal of Organometallic Chemistry, 2013, 724, 139-146.	1.8	8
28	Direct Detection of ¹⁷O in [Gd(DOTA)]^{â^'} by NMR Spectroscopy. Chemistry - A European Journal, 2015, 21, 1955-1960.	3.3	8
29	New light on an old debate: does the RCNâ€“PtCl₂ bond include any back-donation? RCNâ†PtCl₂ backbonding vs. the IR Î½_{Cî€,N} blue-shift dichotomy in organonitrilesâ€“platinum(<scp>ii</scp>) complexes. A thorough density functional theory â€“ energy decomposition analysis study. Dalton Transactions, 2019, 48, 12974-12985.	3.3	7
30	Comparative Experimental and Theoretical Study of the C and O K-Edge X-ray Absorption Spectroscopy in Three Highly Popular, Low Spin Organoiron Complexes: [Fe(CO)₅], [(Î·⁵-C₅H₅)Fe(CO)(Î¼-CO)]₂, and [(Î·⁵-C₅H₅)₂Fe]. Inorganic Chemistry, 2019, 58, 16411-16423.	4.0	7
31	Structural characterization of triorganotin(IV) complexes with sodium fusidate and DFT calculations. Journal of Organometallic Chemistry, 2010, 695, 1405-1413.	1.8	6
32	Pt(II) nitrile complexes: New insights on old complexes from a combined experimental and theoretical study. Inorganica Chimica Acta, 2017, 455, 489-504.	2.4	6
33	Spin state, electronic structure and bonding on C-scorpionate [Fe(II)Cl2(tpm)] catalyst: An experimental and computational study. Catalysis Today, 2020, 358, 403-411.	4.4	6
34	Tin(iv) catalyzed d-galacturonic acid anomerization. Dalton Transactions, 2008, , 596-601.	3.3	5
35	Synthesis, chemical characterization and preliminary in vitro antitumor activity evaluation of new ruthenium(II) complexes with sugar derivatives. Polyhedron, 2011, 30, 1671-1679.	2.2	5
36	Synthesis and structural investigations on R₂ Sn(IV)â€<scp>D</scp>â€aldonic acid complexes (R = methyl; butyl). Their effect on a new toxicity test organism, Liza saliens (Osteichthyes,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	3.5	4

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37	Equilibria involved in the diorganotin(IV) and triorganotin(IV) phosphomycin interaction in aqueous solution. Applied Organometallic Chemistry, 2007, 21, 455-461.	3.5	3
38	Reaction between Indazole and Pd-Bound Isocyanidesâ€"A Theoretical Mechanistic Study. Molecules, 2018, 23, 2942.	3.8	3
39	A DFT mechanistic study of the synthesis of trans-Z,Z-[PtIICl(NH3){HNÂ=ÂC(NH2)Me}2]Cl from addition of NH3 to trans-[PtIICl2(N CMe)2]. Inorganica Chimica Acta, 2020, 511, 119847.	2.4	2
40	cis-[(Î·5-C5H5)Fe(Î·1-CO)(Î¼-CO)]2, the poor relative between cis and trans tautomers. A theoretical study of the gas-phase Fe L3-edge and C and O K-edge XAS of trans-/cis-[(Î·5-C5H5)Fe(Î·1-CO)(Î¼-CO)]2. Physical Chemistry Chemical Physics, 2021, 23, 24661-24668.	2.8	1
41	Structural investigations on diorganotin and triorganotin(IV) phosphomycin derivatives. Inorganica Chimica Acta, 2008, 361, 1754-1762.	2.4	0
42	Donation and back-donation in cis- and trans-[(Î·5-C5H5)Fe(Î·1-CO)(Î¼-CO)]2 tautomers: Which relative is more generous? An ETS-NOCV bond analysis. Inorganica Chimica Acta, 2022, 536, 120897.	2.4	0