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	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
2	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
3	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
4	Covalently Conjugated Goldâ€“Porphyrin Nanostructures. Nanomaterials, 2020, 10, 1644.	4.1	14
5	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
6	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
7	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
8	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, 6811-6825.	4.0	11
9	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
10	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
11	Reaction between Indazole and Pd-Bound Isocyanidesâ€”A Theoretical Mechanistic Study. Molecules, 2018, 23, 2942.	3.8	3
12	An ultrathin suspended hydrophobic porous membrane for high-efficiency water desalination. Applied Materials Today, 2017, 9, 1-9.	4.3	27
13	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
14	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
15	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
16	DFT calculation of NMR Î´(113Cd) in cadmium complexes. Polyhedron, 2016, 117, 48-56.	2.2	9
17	Direct Detection of ¹⁷O in [Gd(DOTA)]^{â^'} by NMR Spectroscopy. Chemistry - A European Journal, 2015, 21, 1955-1960.	3.3	8
18	Fourâ€Component Relativistic DFT Calculations of ¹³C Chemical Shifts of Halogenated Natural Substances. Chemistry - A European Journal, 2015, 21, 18834-18840.	3.3	27

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19	Viologen-based ionic liquid crystals: induction of a smectic A phase by dimerisation. Physical Chemistry Chemical Physics, 2014, 16, 5048-5051.	2.8	47
20	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
21	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
22	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
23	Thermal behaviour and electrochemical properties of bis(trifluoromethanesulfonyl)amide and dodecatungstosilicate viologen dimers. Physical Chemistry Chemical Physics, 2012, 14, 2710.	2.8	51
24	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
25	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
26	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
27	Structural characterization of triorganotin(IV) complexes with sodium fusidate and DFT calculations. Journal of Organometallic Chemistry, 2010, 695, 1405-1413.	1.8	6
28	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
29	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
30	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
31	Structural investigations on diorganotin and triorganotin(IV) phosphomycin derivatives. Inorganica Chimica Acta, 2008, 361, 1754-1762.	2.4	0
32	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
33	Tin(iv) catalyzed d-galacturonic acid anomerization. Dalton Transactions, 2008, , 596-601.	3.3	5
34	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
35	Hâ€™ZSM-5 Modified Zeolite:â€‰ Quantum Chemical Models of Acidic Sites. Journal of Physical Chemistry C, 2007, 111, 13033-13043.	3.1	36
36	Equilibria involved in the diorganotin(IV) and triorganotin(IV) phosphomycin interaction in aqueous solution. Applied Organometallic Chemistry, 2007, 21, 455-461.	3.5	3

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37	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
38	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
39	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
40	Diorganotin(IV) complexes ofD-galacturonic acid: solid-state and solution-phase structural study. Applied Organometallic Chemistry, 2003, 17, 932-939.	3.5	13
41	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
42	Title is missing!. Journal of Chemical Crystallography, 1998, 28, 791-796.	1.1	8