Thomas Cauchy

List of Publications by Year
in descending order

62	1,742	279798	276875
papers	citations	23 h-index	41 g-index

69	69	69	2396
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exchange coupling in transition-metal complexes via density-functional theory: Comparison and reliability of different basis set approaches. Journal of Chemical Physics, 2005, 123, 074102.	3.0	100
2	Manipulation of the Open-Circuit Voltage of Organic Solar Cells by Desymmetrization of the Structure of Acceptor-Donor-Acceptor Molecules. Advanced Functional Materials, 2011, 21, 4379-4387.	14.9	98
3	Magnetostructural Correlations in Polynuclear Complexes:Â The Fe4Butterflies. Journal of the American Chemical Society, 2006, 128, 15722-15727.	13.7	93
4	Magnetic Structure of the Large-Spin Mn₁₀ and Mn₁₉ Complexes: A Theoretical Complement to an Experimental Milestone. Journal of the American Chemical Society, 2008, 130, 7420-7426.	13.7	93
5	Crystalline Arrays of Pairs of Molecular Rotors: Correlated Motion, Rotational Barriers, and Space-Inversion Symmetry Breaking Due to Conformational Mutations. Journal of the American Chemical Society, 2013, 135, 9366-9376.	13.7	92
6	Tetrathiafulvaleneâ€amidoâ€2â€pyridineâ€Nâ€oxide as Efficient Chargeâ€Transfer Antenna Ligand for the Sensitization of Yb^{III} Luminescence in a Series of Lanthanide Paramagnetic Coordination Complexes. Chemistry - A European Journal, 2010, 16, 11926-11941.	3.3	84
7	Ethylenedithioï£¿Tetrathiafulvaleneï£¿Helicenes: Electroactive Helical Precursors with Switchable Chiroptical Properties. Chemistry - A European Journal, 2013, 19, 13160-13167.	3.3	73
8	A Series of Tetrathiafulvalene-Based Lanthanide Complexes Displaying Either Single Molecule Magnet or Luminescenceâ€"Direct Magnetic and Photo-Physical Correlations in the Ytterbium Analogue. Inorganic Chemistry, 2013, 52, 5978-5990.	4.0	70
9	Triplet state CPL active heliceneâ€"dithiolene platinum bipyridine complexes. Chemical Communications, 2017, 53, 9210-9213.	4.1	69
10	On the origin of ferromagnetism in oximato-based [Mn3O]7+triangles. Dalton Transactions, 2008, , 234-240.	3.3	65
11	Global fits of new intermolecular ground state potential energy surfaces for N2â€"H2 and N2â€"N2 van der Waals dimers. Chemical Physics Letters, 2007, 445, 99-107.	2.6	62
12	Datasetâ€™s chemical diversity limits the generalizability of machine learning predictions. Journal of Cheminformatics, 2019, 11, 69.	6.1	57
13	Molecules Composed of Two Weakly Magnetically Coupled [MnIII4] Clusters. Inorganic Chemistry, 2007, 46, 9045-9047.	4.0	55
14	In Solution Sensitization of Er(III) Luminescence by the 4-Tetrathiafulvalene-2,6-pyridinedicarboxylic Acid Dimethyl Antenna Ligand. Inorganic Chemistry, 2012, 51, 978-984.	4.0	48
15	Tetramethylâ€Bis(ethylenedithio)â€Tetrathiafulvalene (TMâ€BEDTâ€TTF) Revisited: Crystal Structures, Chiroptical Properties, Theoretical Calculations, and a Complete Series of Conducting Radical Cation Salts. Chirality, 2013, 25, 466-474.	2.6	45
16	[CpNi(dithiolene)] (and Diselenolene) Neutral Radical Complexes. Inorganic Chemistry, 2006, 45, 8194-8204.	4.0	44
17	Triggering Emission with the Helical Turn in Thiadiazoleâ€Helicenes. Chemistry - A European Journal, 2017, 23, 437-446.	3.3	42
18	Experimental and Theoretical Studies on Photophysical Properties: Tuning Redox-Active Amido-Tetrathiafulvalene Derivatives in Paramagnetic Coordination Complexes. Inorganic Chemistry, 2010, 49, 1947-1960.	4.0	35

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19	Radical CpNi(dithiolene) and CpNi(diselenolene) complexes: Synthetic routes and molecular properties. Coordination Chemistry Reviews, 2010, 254, 1406-1418.	18.8	34
20	Strong Magnetic Interactions through Weak Bonding Interactions in Organometallic Radicals: Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2007, 13, 8858-8866.	3.3	29
21	EvoMol: a flexible and interpretable evolutionary algorithm for unbiased de novo molecular generation. Journal of Cheminformatics, 2020, 12, 55.	6.1	29
22	Tetrathiafulvalene-Triazine-Dipyridylamines as Multifunctional Ligands for Electroactive Complexes: Synthesis, Structures, and Theoretical Study. Inorganic Chemistry, 2012, 51, 8545-8556.	4.0	28
23	Synthesis, Molecular Structure, Properties, and Electronic Structures of [Cp*(dppe)FeCâ‰¡C-TTFMe₃][PF₆]_n (n = 0, 1): Electronic Coupling between the Inorganic and Organic Electrophores. Organometallics, 2010, 29, 4628-4638.	2.3	24
24	Tetrathiafulvalene-1,3,5-triazines as (Multi)Donorâ€“Acceptor Systems with Tunable Charge Transfer: Structural, Photophysical, and Theoretical Investigations. Inorganic Chemistry, 2013, 52, 5023-5034.	4.0	24
25	Can theoretical methods go beyond the experimental data? The case of molecular magnetism. Dalton Transactions, 2009, , 5873.	3.3	22
26	Original Suzukiâ€“Miyaura Coupling Using Nitro Derivatives for the Synthesis of Perylenediimideâ€Based Multimers. European Journal of Organic Chemistry, 2019, 2019, 7635-7643.	2.4	19
27	An Imine Photocyclization as an Alternative to the Pictetâ€“Spengler Reaction for the Synthesis of AzaBenzannulated Perylenediimide Dyes. Journal of Organic Chemistry, 2020, 85, 7218-7224.	3.2	19
28	Lepidotol A from Mesua lepidota Inhibits Inflammatory and Immune Mediators in Human Endothelial Cells. Journal of Natural Products, 2015, 78, 2187-2197.	3.0	18
29	Experimental and theoretical evaluation of magnetic coupling in organometallic radicals: the eloquent case of face-to-face Cpâ‹¯Cp interactions. CrystEngComm, 2009, 11, 1491.	2.6	17
30	Binuclear Cu(ii) coordination complex involving Cis-tetrathiafulvalene-bis-amido-2-pyridine-N-oxide as bi-anionic ligand: a robust molecular precursor toward magnetic conducting materials. Chemical Communications, 2010, 46, 4947.	4.1	17
31	Electroactive tetrathiafulvalene based pyridine-mono and -bis(1,2,3-triazoles) click ligands: synthesis, crystal structures and coordination chemistry. CrystEngComm, 2014, 16, 6612.	2.6	16
32	Ferromagnetic Interactions in Heterobimetallic Chains Formed through the Secondary Coordination of Dithiolene Complexes. Inorganic Chemistry, 2008, 47, 10656-10661.	4.0	15
33	Vibronic spectra of organic electronic chromophores. RSC Advances, 2014, 4, 55466-55472.	3.6	14
34	Electroactive Tetrathiafulvalenylâ€1,2,3â€triazoles by Click Chemistry: Cuâ€versus Ruâ€Catalyzed Azideâ€“Alkyne Cycloaddition Isomers. Chemistry - A European Journal, 2012, 18, 16097-16103.	3.3	13
35	Thiophene-benzoquinones: synthesis, crystal structures and preliminary coordination chemistry of derived anilate ligands. Organic and Biomolecular Chemistry, 2014, 12, 8752-8763.	2.8	13
36	Tetrathiafulvalene mono- and bis-1,2,3-triazole precursors by click chemistry: structural diversity and reactivity. Organic and Biomolecular Chemistry, 2014, 12, 3167.	2.8	11

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37	Tetrathiafulvaleneâ€[2.2]paracyclophanes: Synthesis, crystal structures, and chiroptical properties. Chirality, 2018, 30, 568-575.	2.6	11
38	Conformational Study and Chiroptical Properties of Chiral Dimethyl-Ethylenedithio-Tetrathiafulvalene (DM-EDT-TTF). Chimia, 2018, 72, 389.	0.6	11
39	Tristhienylphenylamine â€“ extended dithiafulvene hybrids as bifunctional electroactive species. Organic and Biomolecular Chemistry, 2011, 9, 1034-1040.	2.8	10
40	Conducting chiral nickel(ii) bis(dithiolene) complexes: structural and electron transport modulation with the charge and the number of stereogenic centres. Journal of Materials Chemistry C, 2021, 9, 4119-4140.	5.5	10
41	Schiff-base [4]helicene Zn(<scp>ii</scp>) complexes as chiral emitters. Dalton Transactions, 2021, 50, 10533-10539.	3.3	10
42	Bimetallic neutral palladium (II) bis(dithiolene) complex: Unusual synthesis, structural and theoretical study. Comptes Rendus Chimie, 2012, 15, 904-910.	0.5	9
43	Tetrathiafulvalene-Based Phenanthroline Ligands: Synthesis, Crystal Structures, and Electronic Properties. European Journal of Inorganic Chemistry, 2014, 2014, 3912-3919.	2.0	9
44	Visible-Light-Mediated Synthesis of AzaBenzannulated Perylenediimide-Based Light-Harvesting Dyads. Journal of Organic Chemistry, 2020, 85, 12252-12261.	3.2	9
45	Dimensionality Control in Crystalline Zinc(II) and Silver(I) Complexes with Ditopic Benzothiadiazole-Dipyridine Ligands. Chemistry, 2021, 3, 269-287.	2.2	9
46	Extended Fe4 butterfly complexes: theoretical analysis of magnetic properties and magnetostructural maps. Dalton Transactions, 2010, 39, 4832.	3.3	8
47	Desymmetrization of Perylenediimide Bay Regions Using Selective Suzukiâ€“Miyaura Reactions from Dinitro Substituted Derivatives. Chemistry - A European Journal, 2020, 26, 15881-15891.	3.3	8
48	Exchange coupling interactions in a Fe6 complex: A theoretical study using density functional theory. Physica B: Condensed Matter, 2006, 384, 116-119.	2.7	7
49	Exchange interactions in a Fe5 complex: A theoretical study using density functional theory. Inorganica Chimica Acta, 2008, 361, 3832-3835.	2.4	7
50	Field-induced mononuclear cobalt(<scp>ii</scp>) single-molecule magnet (SMM) based on a benzothiadiazole-ortho-vanillin ligand. Dalton Transactions, 2022, 51, 4760-4771.	3.3	7
51	Scalable estimator of the diversity for de novo molecular generation resulting in a more robust QM dataset (OD9) and a more efficient molecular optimization. Journal of Cheminformatics, 2021, 13, 76.	6.1	5
52	Prediction of the Synthesis of Spiro Derivatives by Double Intramolecular Aromatic Electrophilic Substitution Using Reactivity Indices. ACS Omega, 2019, 4, 4571-4583.	3.5	4
53	Configurationally stable dithia[7]helicene and dithia-quasi[8]circulene fused dithiolones. Organic Chemistry Frontiers, 2022, 9, 4260-4270.	4.5	4
54	Electrode grafting by oxidation of an amine catalyzed by a ferrocenyl â€œantennaâ€•through intramolecular electron transfer. Electrochemistry Communications, 2017, 82, 52-55.	4.7	3

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55	Solvent Dependent Prototropic Tautomerism in a Schiff Base Derived from oâ€Vanillin and 2â€Aminobenzylalcohol. ChemistrySelect, 2019, 4, 7858-7865.	1.5	3
56	Zinc(II) and copper(II) complexes with benzothiadiazole Schiff-base ligands. Polyhedron, 2022, 224, 115994.	2.2	3
57	Reactivity and Mechanistic Issues in the Photocyclisation of Dihalostyrylâ€Naphthalenes towards Haloâ€[4]helicenes: a Transposition on a Mallory Theme. ChemPhotoChem, 0, , .	3.0	2
58	Hâ€Mediated Magnetic Interactions between Layers in a 2D Mn II â€“Dicyanamide Polymer: Neutron Diffraction, DFT, and Quantum Monte Carlo Calculations. European Journal of Inorganic Chemistry, 2018, 2018, 278-288.	2.0	1
59	Surrogate-Based Black-Box Optimization Method for Costly Molecular Properties. , 2021, , .		1
60	Lepidotols and lepidotins: new phenylcoumarins from Malaysian Mesua species. Planta Medica, 2015, 81, .	1.3	0
61	Goal-directed generation of new molecules by AI methods. , 2022, , 39-67.		0
62	Chiroptical properties of anionic and neutral nickel(II) bis(dithiolene) complexes based on methyl and dimethylâ€dddt ligands. Chirality, 2021, , .	2.6	0