

Thomas Cauchy

List of Publications by Year in descending order

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1,742
citations

279798

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41
g-index

69
all docs

69
docs citations

69
times ranked

2396
citing authors

#	ARTICLE	IF	CITATIONS
1	Goal-directed generation of new molecules by AI methods. , 2022, , 39-67.		0
2	Field-induced mononuclear cobalt(<i>ii</i>) single-molecule magnet (SMM) based on a benzothiadiazole- <i>ortho</i> -vanillin ligand. Dalton Transactions, 2022, 51, 4760-4771.	3.3	7
3	Configurationaly stable dithia[7]helicene and dithia-quasi[8]circulene fused dithiolones. Organic Chemistry Frontiers, 2022, 9, 4260-4270.	4.5	4
4	Zinc(II) and copper(II) complexes with benzothiadiazole Schiff-base ligands. Polyhedron, 2022, 224, 115994.	2.2	3
5	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
6	Schiff-base [4]helicene Zn(<i>ii</i>) complexes as chiral emitters. Dalton Transactions, 2021, 50, 10533-10539.	3.3	10
7	Dimensionality Control in Crystalline Zinc(II) and Silver(I) Complexes with Ditopic Benzothiadiazole-Dipyridine Ligands. Chemistry, 2021, 3, 269-287.	2.2	9
8	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
9	Chiroptical properties of anionic and neutral nickel(II) bis(dithiolene) complexes based on methyl and dimethylâ€”ligands. Chirality, 2021, , .	2.6	0
10	Surrogate-Based Black-Box Optimization Method for Costly Molecular Properties. , 2021, , .		1
11	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
12	EvoMol: a flexible and interpretable evolutionary algorithm for unbiased de novo molecular generation. Journal of Cheminformatics, 2020, 12, 55.	6.1	29
13	Visible-Light-Mediated Synthesis of AzaBenzannulated Perylenediimide-Based Light-Harvesting Dyads. Journal of Organic Chemistry, 2020, 85, 12252-12261.	3.2	9
14	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
15	Solvent Dependent Prototropic Tautomerism in a Schiff Base Derived from <i>o</i> -Vanillin and 2â€”Aminobenzylalcohol. ChemistrySelect, 2019, 4, 7858-7865.	1.5	3
16	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
17	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
18	Datasetâ€™s chemical diversity limits the generalizability of machine learning predictions. Journal of Cheminformatics, 2019, 11, 69.	6.1	57

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19	Tetrathiafulvalene- $\{2,2\}$ paracyclophanes: Synthesis, crystal structures, and chiroptical properties. <i>Chirality</i> , 2018, 30, 568-575.	2.6	11
20	H π -Mediated Magnetic Interactions between Layers in a 2D Mn II π -Dicyanamide Polymer: Neutron Diffraction, DFT, and Quantum Monte Carlo Calculations. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 278-288.	2.0	1
21	Conformational Study and Chiroptical Properties of Chiral Dimethyl-Ethylenedithio-Tetrathiafulvalene (DM-EDT-TTF). <i>Chimia</i> , 2018, 72, 389.	0.6	11
22	Electrode grafting by oxidation of an amine catalyzed by a ferrocenyl π -antenna through intramolecular electron transfer. <i>Electrochemistry Communications</i> , 2017, 82, 52-55.	4.7	3
23	Triplet state CPL active helicene π -dithiolenyl platinum bipyridine complexes. <i>Chemical Communications</i> , 2017, 53, 9210-9213.	4.1	69
24	Triggering Emission with the Helical Turn in Thiadiazole π -Helicenes. <i>Chemistry - A European Journal</i> , 2017, 23, 437-446.	3.3	42
25	Lepidotol A from <i>Mesua lepidota</i> Inhibits Inflammatory and Immune Mediators in Human Endothelial Cells. <i>Journal of Natural Products</i> , 2015, 78, 2187-2197.	3.0	18
26	Lepidotols and lepidotins: new phenylcoumarins from Malaysian <i>Mesua</i> species. <i>Planta Medica</i> , 2015, 81, .	1.3	0
27	Thiophene-benzoquinones: synthesis, crystal structures and preliminary coordination chemistry of derived anilate ligands. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 8752-8763.	2.8	13
28	Tetrathiafulvalene mono- and bis-1,2,3-triazole precursors by click chemistry: structural diversity and reactivity. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 3167.	2.8	11
29	Vibronic spectra of organic electronic chromophores. <i>RSC Advances</i> , 2014, 4, 55466-55472.	3.6	14
30	Electroactive tetrathiafulvalene based pyridine-mono and -bis(1,2,3-triazoles) click ligands: synthesis, crystal structures and coordination chemistry. <i>CrystEngComm</i> , 2014, 16, 6612.	2.6	16
31	Tetrathiafulvalene-Based Phenanthroline Ligands: Synthesis, Crystal Structures, and Electronic Properties. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 3912-3919.	2.0	9
32	Ethylenedithio π -Tetrathiafulvalene π -Helicenes: Electroactive Helical Precursors with Switchable Chiroptical Properties. <i>Chemistry - A European Journal</i> , 2013, 19, 13160-13167.	3.3	73
33	Tetrathiafulvalene-1,3,5-triazines as (Multi)Donor π -Acceptor Systems with Tunable Charge Transfer: Structural, Photophysical, and Theoretical Investigations. <i>Inorganic Chemistry</i> , 2013, 52, 5023-5034.	4.0	24
34	Crystalline Arrays of Pairs of Molecular Rotors: Correlated Motion, Rotational Barriers, and Space-Inversion Symmetry Breaking Due to Conformational Mutations. <i>Journal of the American Chemical Society</i> , 2013, 135, 9366-9376.	13.7	92
35	A Series of Tetrathiafulvalene-Based Lanthanide Complexes Displaying Either Single Molecule Magnet or Luminescence π -Direct Magnetic and Photo-Physical Correlations in the Ytterbium Analogue. <i>Inorganic Chemistry</i> , 2013, 52, 5978-5990.	4.0	70
36	Tetramethyl π -Bis(ethylenedithio) π -Tetrathiafulvalene (TM π -BEDT π -TTF) Revisited: Crystal Structures, Chiroptical Properties, Theoretical Calculations, and a Complete Series of Conducting Radical Cation Salts. <i>Chirality</i> , 2013, 25, 466-474.	2.6	45

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37	Electroactive Tetrathiafulvalenyl-1,2,3-triazoles by Click Chemistry: Cu- versus Ru-Catalyzed Azide-Alkyne Cycloaddition Isomers. <i>Chemistry - A European Journal</i> , 2012, 18, 16097-16103.	3.3	13
38	In Solution Sensitization of Er(III) Luminescence by the 4-Tetrathiafulvalene-2,6-pyridinedicarboxylic Acid Dimethyl Antenna Ligand. <i>Inorganic Chemistry</i> , 2012, 51, 978-984.	4.0	48
39	Bimetallic neutral palladium (II) bis(dithiolene) complex: Unusual synthesis, structural and theoretical study. <i>Comptes Rendus Chimie</i> , 2012, 15, 904-910.	0.5	9
40	Tetrathiafulvalene-Triazine-Dipyridylamines as Multifunctional Ligands for Electroactive Complexes: Synthesis, Structures, and Theoretical Study. <i>Inorganic Chemistry</i> , 2012, 51, 8545-8556.	4.0	28
41	Tris(hienyl)phenylamine - extended dithiafulvene hybrids as bifunctional electroactive species. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 1034-1040.	2.8	10
42	Manipulation of the Open-Circuit Voltage of Organic Solar Cells by Desymmetrization of the Structure of Acceptor-Donor-Acceptor Molecules. <i>Advanced Functional Materials</i> , 2011, 21, 4379-4387.	14.9	98
43	Radical CpNi(dithiolene) and CpNi(diselenolene) complexes: Synthetic routes and molecular properties. <i>Coordination Chemistry Reviews</i> , 2010, 254, 1406-1418.	18.8	34
44	Tetrathiafulvalene-amido-2-pyridine-N-oxide as Efficient Charge-Transfer Antenna Ligand for the Sensitization of Yb ^{III} Luminescence in a Series of Lanthanide Paramagnetic Coordination Complexes. <i>Chemistry - A European Journal</i> , 2010, 16, 11926-11941.	3.3	84
45	Synthesis, Molecular Structure, Properties, and Electronic Structures of [Cp*(dppe)FeC ₃ TTFMe ₃][PF ₆] ₂ (n = 0, 1): Electronic Coupling between the Inorganic and Organic Electrophores. <i>Organometallics</i> , 2010, 29, 4628-4638.	2.3	24
46	Experimental and Theoretical Studies on Photophysical Properties: Tuning Redox-Active Amido-Tetrathiafulvalene Derivatives in Paramagnetic Coordination Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 1947-1960.	4.0	35
47	Extended Fe ₄ butterfly complexes: theoretical analysis of magnetic properties and magnetostructural maps. <i>Dalton Transactions</i> , 2010, 39, 4832.	3.3	8
48	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. <i>Chemical Communications</i> , 2010, 46, 4947.	4.1	17
49	Can theoretical methods go beyond the experimental data? The case of molecular magnetism. <i>Dalton Transactions</i> , 2009, , 5873.	3.3	22
50	Experimental and theoretical evaluation of magnetic coupling in organometallic radicals: the eloquent case of face-to-face Cp-Cp interactions. <i>CrystEngComm</i> , 2009, 11, 1491.	2.6	17
51	Exchange interactions in a Fe ₅ complex: A theoretical study using density functional theory. <i>Inorganica Chimica Acta</i> , 2008, 361, 3832-3835.	2.4	7
52	On the origin of ferromagnetism in oximate-based [Mn ₃ O] ₇ triangles. <i>Dalton Transactions</i> , 2008, , 234-240.	3.3	65
53	Magnetic Structure of the Large-Spin Mn ₁₀ and Mn ₁₉ Complexes: A Theoretical Complement to an Experimental Milestone. <i>Journal of the American Chemical Society</i> , 2008, 130, 7420-7426.	13.7	93
54	Ferromagnetic Interactions in Heterobimetallic Chains Formed through the Secondary Coordination of Dithiolene Complexes. <i>Inorganic Chemistry</i> , 2008, 47, 10656-10661.	4.0	15

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55	Molecules Composed of Two Weakly Magnetically Coupled [MnIII4] Clusters. <i>Inorganic Chemistry</i> , 2007, 46, 9045-9047.	4.0	55
56	Strong Magnetic Interactions through Weak Bonding Interactions in Organometallic Radicals: Combined Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2007, 13, 8858-8866.	3.3	29
57	Global fits of new intermolecular ground state potential energy surfaces for N ₂ ••H ₂ and N ₂ ••N ₂ van der Waals dimers. <i>Chemical Physics Letters</i> , 2007, 445, 99-107.	2.6	62
58	[CpNi(dithiolene)] (and Diselenolene) Neutral Radical Complexes. <i>Inorganic Chemistry</i> , 2006, 45, 8194-8204.	4.0	44
59	Magnetostructural Correlations in Polynuclear Complexes: The Fe ₄ Butterflies. <i>Journal of the American Chemical Society</i> , 2006, 128, 15722-15727.	13.7	93
60	Exchange coupling interactions in a Fe ₆ complex: A theoretical study using density functional theory. <i>Physica B: Condensed Matter</i> , 2006, 384, 116-119.	2.7	7
61	Exchange coupling in transition-metal complexes via density-functional theory: Comparison and reliability of different basis set approaches. <i>Journal of Chemical Physics</i> , 2005, 123, 074102.	3.0	100
62	Reactivity and Mechanistic Issues in the Photocyclisation of Dihaloalkyl-Naphthalenes towards Haloalkyl-helicenes: a Transposition on a Mallory Theme. <i>ChemPhotoChem</i> , 0, , .	3.0	2