JesÃºs Jover

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8800433/publications.pdf

Version: 2024-02-01

61	2,215	201385	223531
papers	citations	27 h-index	46 g-index

68	68	68	2969
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Aryl Trifluoroborates in Suzukiâ€“Miyaura Coupling: The Roles of Endogenous Aryl Boronic Acid and Fluoride. Angewandte Chemie - International Edition, 2010, 49, 5156-5160.	7.2	198
2	Accurate modelling of Pd(0) + PhX oxidative addition kinetics. Dalton Transactions, 2010, 39, 10833.	1.6	179
3	A computational study of phosphine ligand effects in Suzukiâ€“Miyaura couplingâ˜†. Journal of Molecular Catalysis A, 2010, 324, 39-47.	4.8	144
4	Expansion of the Ligand Knowledge Base for Monodentate P-Donor Ligands (LKB-P). Organometallics, 2010, 29, 6245-6258.	1.1	117
5	Neural Network Based QSPR Study for Predicting pKa of Phenols in Different Solvents. QSAR and Combinatorial Science, 2007, 26, 385-397.	1.5	79
6	QSPR Prediction of pK_a for Benzoic Acids in Different Solvents. QSAR and Combinatorial Science, 2008, 27, 563-581.	1.5	70
7	Expansion of the Ligand Knowledge Base for Chelating P,P-Donor Ligands (LKB-PP). Organometallics, 2012, 31, 5302-5306.	1.1	69
8	Single-molecule magnetism arising from cobalt(<scp>ii</scp>) nodes of a crystalline sponge. Journal of Materials Chemistry C, 2017, 5, 835-841.	2.7	64
9	Computational assessment on the Tolman cone angles for P-ligands. Dalton Transactions, 2019, 48, 15036-15048.	1.6	62
10	Modulation of single-molecule magnet behaviour via photochemical [2+2] cycloaddition. Chemical Communications, 2015, 51, 15358-15361.	2.2	61
11	A Pseudoâ€Octahedral Cobalt(II) Complex with Bispyrazolylpyridine Ligands Acting as a Zeroâ€Field Singleâ€Molecule Magnet with Easy Axis Anisotropy. Chemistry - A European Journal, 2018, 24, 8857-8868.	1.7	60
12	The Newmanâ€“Kwart Rearrangement of Oâ€Aryl Thiocarbamates: Substantial Reduction in Reaction Temperatures through Palladium Catalysis. Angewandte Chemie - International Edition, 2009, 48, 7612-7615.	7.2	57
13	Organometallic reactivity: the role of metalâ€“ligand bond energies from a computational perspective. Dalton Transactions, 2011, 40, 11184.	1.6	57
14	The Computational Road to Better Catalysts. Chemistry - an Asian Journal, 2014, 9, 1714-1723.	1.7	57
15	Toward a mechanistic understanding of oxidative homocoupling: the Glaserâ€“Hay reaction. Catalysis Science and Technology, 2014, 4, 4200-4209.	2.1	57
16	Determination of Abraham Solute Parameters from Molecular Structure. Journal of Chemical Information and Computer Sciences, 2004, 44, 1098-1106.	2.8	55
17	A comparison of the binding affinity of the common amino acids with different metal cations. Dalton Transactions, 2008, , 6441.	1.6	55
18	Investigation of easy-plane magnetic anisotropy in P-ligand square-pyramidal Co^{II} single ion magnets. Chemical Communications, 2017, 53, 5338-5341.	2.2	45

#	Article	IF	Citations
19	On the Feasibility of Nickel-Catalyzed Trifluoromethylation of Aryl Halides. Organometallics, 2014, 33, 6531-6543.	1.1	43
20	Slow relaxation of magnetization in a bis-mer-tridentate octahedral Co(<scp>ii</scp>) complex. Dalton Transactions, 2018, 47, 859-867.	1.6	40
21	Computational characterization of a mechanism for the copper-catalyzed aerobic oxidative trifluoromethylation of terminal alkynes. Chemical Communications, 2013, 49, 10486.	2.2	37
22	Ferro- to Antiferromagnetic Crossover Angle in Diphenoxido- and Carboxylato-Bridged Trinuclear Ni^{II}₂â€“Mn^{II} Complexes: Experimental Observations and Theoretical Rationalization. Inorganic Chemistry, 2014, 53, 9296-9305.	1.9	37
23	Computational Characterization of the Mechanism for Coinage-Metal-Catalyzed Carboxylation of Terminal Alkynes. Journal of Organic Chemistry, 2014, 79, 11981-11987.	1.7	35
24	Quantitative Estimation of Isingâ€Type Magnetic Anisotropy in a Family of C₃â€Symmetric Co^{II} Complexes. Chemistry - A European Journal, 2017, 23, 12550-12558.	1.7	31
25	Screening substituent and backbone effects on the properties of bidentate P,P-donor ligands (LKB-PP_{screen}). Dalton Transactions, 2013, 42, 172-181.	1.6	30
26	The Interplay between Homogeneous and Heterogeneous Phases of PdAu Catalysts for the Oxidation of Alcohols. ACS Catalysis, 2016, 6, 4135-4143.	5.5	30
27	Visible and near-infrared organic photosensitizers comprising isoindigo derivatives as chromophores: synthesis, optoelectronic properties and factors limiting their efficiency in dye solar cells. Journal of Materials Chemistry A, 2018, 6, 10074-10084.	5.2	27
28	A Multifunctional Dysprosiumâ€Carboxylato 2D Metallâ€“Organic Framework. Angewandte Chemie - International Edition, 2021, 60, 12001-12006.	7.2	27
29	Mechanistic Investigation of Iridium-Catalyzed Câ€“H Borylation of Methyl Benzoate: Ligand Effects in Regioselectivity and Activity. Organometallics, 2016, 35, 3221-3226.	1.1	23
30	Quantitative DFT modeling of product concentration in organometallic reactions: Cu-mediated pentafluoroethylation of benzoic acid chlorides as a case study. Physical Chemistry Chemical Physics, 2017, 19, 29344-29353.	1.3	22
31	Single-ion magnetic anisotropy in a vacant octahedral Co(<scp>ii</scp>) complex. Dalton Transactions, 2019, 48, 25-29.	1.6	21
32	Computational Exploration of NO Single-Site Disproportionation on Fe-MOF-5. Chemistry of Materials, 2019, 31, 8875-8885.	3.2	20
33	Computational Insights into Nucleophilic Copper-Catalyzed Trifluoromethylation of Aryl Halides. ACS Catalysis, 2014, 4, 4389-4397.	5.5	19
34	Estimation of enthalpies of formation of organometallic compounds from their molecular structures. Journal of Organometallic Chemistry, 2008, 693, 1261-1268.	0.8	17
35	Rutheniumâ€Catalyzed Oâ€to Sâ€Alkyl Migration: A Pseudoreversible Bartonâ€“McCombie Pathway. Angewandte Chemie - International Edition, 2015, 54, 10944-10948.	7.2	17
36	Determination of Lithium Cation Basicity from Molecular Structure. Journal of Chemical Information and Computer Sciences, 2004, 44, 1727-1736.	2.8	15

#	Article	IF	Citations
37	QSPR Prediction of pK for Aliphatic Carboxylic Acids and Anilines in Different Solvents. QSAR and Combinatorial Science, 2008, 27, 1204-1215.	1.5	13
38	Antiferro- to ferromagnetic crossover in diphenoxido bridged NiII2MnII complexes derived from N2O2 donor Schiff base ligands. Polyhedron, 2016, 117, 57-63.	1.0	13
39	Bifunctional Tripeptide with a Phosphonic Acid as a BrÃ¸nsted Acid for Michael Addition: Mechanistic Insights. Chemistry - A European Journal, 2017, 23, 6654-6662.	1.7	13
40	Quantitative Structureâ^'Property Relationship Estimation of Cation Binding Affinity of the Common Amino Acids. Journal of Physical Chemistry A, 2009, 113, 3703-3708.	1.1	12
41	Copper-Catalyzed Eglinton Oxidative Homocoupling of Terminal Alkynes: A Computational Study. Journal of Chemistry, 2015, 2015, 1-8.	0.9	11
42	Magnetic Behavior of Heterometallic Wheels Having a [MnIV6M2O9]10+ Core with M = Ca2+ and Sr2+. Inorganic Chemistry, 2015, 54, 11596-11605.	1.9	11
43	Tunable Magnetization Dynamics through Solid-State Ligand Substitution Reaction. Inorganic Chemistry, 2017, 56, 8829-8836.	1.9	11
44	Nickel-catalyzed aryl trifluoromethyl sulfide synthesis: a DFT study. Catalysis Science and Technology, 2019, 9, 5962-5970.	2.1	9
45	Lowâ€Valent Titanium Species Stabilized with Aluminum/Boron Hydride Fragments. Chemistry - A European Journal, 2022, 28, .	1.7	9
46	A combined kinetico-mechanistic and computational study on the competitive formation of seven- versus five-membered platinacycles; the relevance of spectator halide ligands. Dalton Transactions, 2015, 44, 17968-17979.	1.6	8
47	Zn(II) Byproduct Enhances the Cu-Catalyzed Cross-Coupling of Bromozinc Difluorophosphonate with Iodobenzoates: A DFT Study. Organometallics, 2018, 37, 327-336.	1.1	8
48	Kineticomechanistic Study of the Redox pH Cycling Processes Occurring on a Robust Water-Soluble Cyanido-Bridged Mixed-Valence {CoIII/FeII}2Square. Inorganic Chemistry, 2018, 57, 8465-8475.	1.9	8
49	Supported Ïƒâ€Complexes of Liâ^'C Bonds from Coordination of Monomeric Molecules of LiCH 3 , LiCH 2 CH 3 and LiC 6 H 5 to Moâ‰£Mo Bonds. Angewandte Chemie - International Edition, 2021, , e202116009.	7.2	8
50	QM/MM Calculations on Selectivity in Homogeneous Catalysis. Structure and Bonding, 2015, , 59-79.	1.0	7
51	Coordination of LiH Molecules to Moâ‰£Mo Bonds: Experimental and Computational Studies on Mo₂LiH₂, Mo₂Li₂H₄, and Mo₆Li₉H₁₈ Clusters. Journal of the American Chemical Society, 2021, 143, 5222-5230.	6.6	7
52	Ammoniaâ€Borane Derived BN Fragments Trapped on Biâ€•and Trimetallic Titanium(III) Systems. Chemistry - A European Journal, 2019, 25, 7096-7100.	1.7	4
53	Diarylplatinum(II) Scaffolds for Kinetic and Mechanistic Studies on the Formation of Platinacycles via an Oxidative Addition/Reductive Elimination/Oxidative Addition Sequence. Advances in Inorganic Chemistry, 2017, 70, 195-242.	0.4	3
54	Molecular Approach to Alkali-Metal Encapsulation by a Prussian Blue Analogue Fe^{II}/Co^{III}Cube in Aqueous Solution: A Kineticomechanistic Exchange Study. Inorganic Chemistry, 2021, 60, 18407-18422.	1.9	3

#	Article	IF	Citations
55	Towards large area surface functionalization with luminescent and magnetic lanthanoid complexes. Inorganic Chemistry Frontiers, 2022, 9, 4160-4170.	3.0	3
56	Coordination of Eâ€“C Bonds (E = Zn, Mg, Al) and the Znâ€“H Bonds of (C₅Me₅)ZnH and (C₅Me₅)ZnZnH across a Quadruply Bonded Dimolybdenum Dihydride Complex. Organometallics, 2022, 41, 3225-3236.	1.1	3
57	From simple alkenes and CO2 to fluorinated carboxylic acids: computational studies and predictions. European Journal of Organic Chemistry, 2022, 2022, e202101243.	1.2	2
58	Differentiation of Epoxide Enantiomers in the Confined Spaces of an Homochiral Cu(II) Metalâ€Organic Framework by Kinetic Resolution. Chemistry - A European Journal, 2021, 27, 16956-16965.	1.7	1
59	Dinitrogen Binding at a Trititanium Chloride Complex and Its Conversion to Ammonia under Ambient Conditions. Angewandte Chemie, 0, , .	1.6	1
60	A Multifunctional Dysprosiumâ€carboxylato 2D Metallâ€“Organic Framework. Angewandte Chemie, 2021, 133, 12108-12113.	1.6	0
61	Supported Ïƒâ€Complexes of Liâ€“C Bonds from Coordination of Monomeric Molecules of LiCH 3 , LiCH 2 CH 3 and LiC 6 H 5 to Moâ‰£Mo Bonds. Angewandte Chemie, 2022, 134, .	1.6	0