

Gabriel AullÃ³n

List of Publications by Year in descending order

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3465
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#	ARTICLE	IF	CITATIONS
1	Direct and Asymmetric Aldol Reactions of α -Azidoacetyl- β -thiazolidine- γ -thione Catalyzed by Chiral Nickel(II) Complexes. A New Approach to the Synthesis of β -Hydroxy- α -Amino Acids. Chemistry - A European Journal, 2022, 28, .	3.3	7
2	Effect of Gold(I) on the Room-Temperature Phosphorescence of Ethynylphenanthrene. Chemistry - A European Journal, 2021, 27, 1810-1820.	3.3	14
3	Direct and Enantioselective Aldol Reactions Catalyzed by Chiral Nickel(II) Complexes. Angewandte Chemie - International Edition, 2021, 60, 15307-15312.	13.8	17
4	Direct and Enantioselective Aldol Reactions Catalyzed by Chiral Nickel(II) Complexes. Angewandte Chemie, 2021, 133, 15435-15440.	2.0	8
5	Comprehensive Investigation of the Photophysical Properties of Alkynylcoumarin Gold(I) Complexes. Journal of Physical Chemistry B, 2021, 125, 11751-11760.	2.6	6
6	Self-Assembly Hydrosoluble Coronenes: A Rich Source of Supramolecular Turn-On Fluorogenic Sensing Materials in Aqueous Media. Organic Letters, 2021, 23, 8727-8732.	4.6	5
7	Fluorescent perylenylpyridine complexes: an experimental and theoretical study. Dalton Transactions, 2020, 49, 13326-13338.	3.3	6
8	Direct, Enantioselective, and Nickel(II) Catalyzed Reactions of α -Azidoacetyl Thioimides with Trimethyl Orthoformate: A New Combined Methodology for the Rapid Synthesis of Lacosamide and Derivatives. Chemistry - A European Journal, 2020, 26, 11540-11548.	3.3	3
9	Conformational Effects of $[Ni_2(\mu_4-ArS)_2]$ Cores on Their Electrocatalytic Activity. Chemistry - an Asian Journal, 2019, 14, 3301-3312.	3.3	7
10	Oxidative Cleavage of Cellobiose by Lytic Polysaccharide Monooxygenase (LPMO)-Inspired Copper Complexes. ACS Omega, 2019, 4, 10729-10740.	3.5	14
11	Synthesis, Characterization, Solution Behavior and Theoretical Studies of Pd(II) Allyl Complexes with 2-Phenyl-3H-indoles as Ligands. Catalysts, 2019, 9, 811.	3.5	1
12	Mapping the working route of phosphate monoester hydrolysis catalyzed by copper based models with special emphasis on the role of oxoanions by experimental and theoretical studies. New Journal of Chemistry, 2019, 43, 2501-2512.	2.8	7
13	Supramolecular tripodal Au(μ_3) assemblies in water. Interactions with a pyrene fluorescent probe. New Journal of Chemistry, 2019, 43, 8279-8289.	2.8	12
14	Designing antiferromagnetically coupled mono-, di- and tri-bridged copper(μ_2)-based catecholase models by varying the μ -Auxiliary Parts of the ligand and anionic co-ligand. CrystEngComm, 2019, 21, 7094-7107.	2.6	12
15	Direct and Asymmetric Nickel(II)-Catalyzed Construction of Carbon-Carbon Bonds from α -Acyl Thiazinanethiones. Organic Letters, 2019, 21, 305-309.	4.6	16
16	On the silicon-silicon bonds η^2 -coordinated to group 10 transition metals. Inorganica Chimica Acta, 2019, 486, 449-457.	2.4	1
17	Trinuclear Gold-Carborane Cluster as a Host Structure. European Journal of Inorganic Chemistry, 2019, 2019, 18-22.	2.0	7
18	Indirect effect of hydrogen bonds on the magnetic coupling on Mn(μ_3) dinuclear compounds. CrystEngComm, 2018, 20, 6629-6639.	2.6	2

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19	Easily reduced bis-pincer (NS ₂) ₂ molybdenum(iv) to (NHS ₂) ₂ Mo(ii) by alcohols vs. redox-inert (NS ₂)(NHS ₂)iron(iii) complexes. Dalton Transactions, 2018, 47, 10932-10940.	3.3	3
20	Total synthesis of (+)-herboxidiene/GEX 1A. Organic and Biomolecular Chemistry, 2017, 15, 1842-1862.	2.8	7
21	Group 12 metal complexes of (2-piperazine-1-yl-ethyl)-pyridin-2-yl-methylene-amine: rare participation of terminal piperazine N in coordination leads to structural diversity. Dalton Transactions, 2017, 46, 2184-2195.	3.3	16
22	Dihydrogen intermolecular contacts in group 13 compounds: H δ^- -H or E δ^- -H (E = B, Al, Ga) interactions?. Dalton Transactions, 2017, 46, 2844-2854.	3.3	25
23	Intermolecular interactions in group 14 hydrides: Beyond C δ^- -H δ^- -H δ^- -C contacts. International Journal of Quantum Chemistry, 2017, 117, e25432.	2.0	32
24	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.	1.0	3
25	Substrate-Controlled Aldol Reactions from Chiral β -Hydroxy Ketones. Synthesis, 2017, 49, 484-503.	2.3	6
26	Redox-Assisted Self-Assembly of a Water-Soluble Cyanido-Bridged Mixed Valence {Co ^{III} /Fe ^{II} } ₂ Square. Chemistry - A European Journal, 2016, 22, 15227-15230.	3.3	9
27	Synthesis, characterization, crystal structures and computational studies on novel cyrhetrenyl hydrazones. Journal of Organometallic Chemistry, 2016, 819, 129-137.	1.8	14
28	Redox flexibility of iron complexes supported by sulfur-based tris(o-methylenethiophenolato)amine relative to its tripodal oxygen-based congener. Dalton Transactions, 2016, 45, 9996-10006.	3.3	4
29	Assembling Nonplanar Polyaromatic Units by Click Chemistry. Study of Multicorannulene Systems as Host for Fullerenes. Organic Letters, 2015, 17, 2578-2581.	4.6	27
30	Structural analysis of the coordination of dinitrogen to transition metal complexes. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 369-386.	1.1	14
31	Magnetic Behavior of Heterometallic Wheels Having a [MnIV ₆ M ₂ O ₉] ¹⁰⁺ Core with M = Ca ²⁺ and Sr ²⁺ . Inorganic Chemistry, 2015, 54, 11596-11605.	4.0	11
32	Nickel(II) complexes having different configurations controlled by N,N,O-donor Schiff-base ligands in presence of isothiocyanate as co-ligand: Synthesis, structures, comparative biological activity and DFT study. Polyhedron, 2015, 101, 93-102.	2.2	12
33	Higher fluorescence in platinum(IV) orthometallated complexes of perylene imine compared with their platinum(II) or palladium(II) analogues. Dalton Transactions, 2015, 44, 16164-16176.	3.3	19
34	A combined kinetic-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.	3.3	8
35	Electrocatalytic Proton Reduction by Dimeric Nickel Complex of a Sterically Demanding Pincer-type NS ₂ Aminobis(thiophenolate) Ligand. Inorganic Chemistry, 2015, 54, 619-627.	4.0	27
36	Computational Insights on the Geometrical Arrangements of Cu(II) with a Mixed-Donor N ₃ S ₃ Macrobicyclic Ligand. Inorganic Chemistry, 2014, 53, 512-521.	4.0	6

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37	Exploring Excited-State Tunability in Luminescent Tris-cyclometalated Platinum(IV) Complexes: Synthesis of Heteroleptic Derivatives and Computational Calculations. <i>Chemistry - A European Journal</i> , 2014, 20, 17346-17359.	3.3	31
38	Copper(II) complexes of bis(aryl-imino)acenaphthene ligands: synthesis, structure, DFT studies and evaluation in reverse ATRP of styrene. <i>Dalton Transactions</i> , 2014, 43, 13041.	3.3	22
39	Highly fluorescent complexes with 3-isocyanoperylene and N-(2,5-di-tert-butylphenyl)-9-isocyano-perylene-3,4-dicarboximide. <i>Dalton Transactions</i> , 2014, 43, 10885-10897.	3.3	6
40	Highly fluorescent complexes with gold, palladium or platinum linked to perylene through a tetrafluorophenyl group. <i>Dalton Transactions</i> , 2013, 42, 6353.	3.3	23
41	Copper Versus Thioether-Centered Oxidation: Mechanistic Insights into the Non-Innocent Redox Behavior of Tripodal Benzimidazolylaminothioether Ligands. <i>Chemistry - A European Journal</i> , 2013, 19, 6067-6079.	3.3	21
42	Understanding the Nature of the CH \cdots HC Interactions in Alkanes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1977-1991.	5.3	112
43	Electronic structure and geometries of o-carborane derived cyclic structures $[\{1/4-1,2-(C_2B_{10}H_{10})_nMn\}Agm]z^{\sim}$, M = {Au, Hg}, n = {3, 4}, m = {0, 1, 2}, z = {n \hat{a} m, \hat{a} m}. <i>Dalton Transactions</i> , 2012, 41, 14146.	3.3	10
44	The Structural Diversity Triggered by Intermolecular Interactions between Au ^I S ₂ Groups: Auophilic and Beyond. <i>Chemistry - A European Journal</i> , 2012, 18, 9965-9976.	3.3	22
45	On the Coordination of Dinitrogen to Group 4 Metallocenes. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 797-806.	2.0	5
46	Kinetic-Mechanistic Information about Alkene Hydroamination with Aniline in Bromide-Rich Ionic Media: Importance of Solvolysis. <i>Inorganic Chemistry</i> , 2011, 50, 5628-5636.	4.0	10
47	Regioselective Orthopalladation of (Z)-2-Aryl-4-Arylidene-5(4-H)-Oxazolones: Scope, Kinetic-Mechanistic, and Density Functional Theory Studies of the C-H Bond Activation. <i>Inorganic Chemistry</i> , 2011, 50, 8132-8143.	4.0	41
48	Dihydrogen contacts in alkanes are subtle but not faint. <i>Nature Chemistry</i> , 2011, 3, 323-330.	13.6	231
49	Two Temperature-Independent Spinomers of the Dinuclear Mn(III) Compound $[\{Mn(H_2O)(phen)\}_2(1/4-2-ClC_6H_4COO)_2(1/4-O)](ClO_4)_2$. <i>Inorganic Chemistry</i> , 2010, 49, 1471-1480.	4.0	21
50	Comparison of the Structure and Stability of New \hat{I} -Diimine Complexes of Copper(I) and Silver(I): Density Functional Theory versus Experimental. <i>Inorganic Chemistry</i> , 2010, 49, 8699-8708.	4.0	46
51	On the electronic structure and stability of icosahedral $r-X_2Z_{10}H_{12}$ and $Z_{12}H_{12}\hat{a}$ clusters; r = {ortho, meta, para}, X = {C, Si}, Z = {B, Al}. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5101.	2.8	14
52	$X\hat{I}X$ Through-Cage Bonding in Cu, Ni, and Cr Complexes with M_3X_2 Cores (X=S, As). <i>Chemistry - A European Journal</i> , 2009, 15, 536-546.	3.3	15
53	Reactivity of a Super-Electron-Rich Olefin Derived from Cyclam. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 1851-1860.	2.0	22
54	Oxidation states, atomic charges and orbital populations in transition metal complexes. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 67-73.	1.4	76

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55	Substitution of chloride by nitrosyl ligand in a scorpionate ruthenium(III) compound: A theoretical study. <i>Inorganica Chimica Acta</i> , 2009, 362, 4651-4658.	2.4	2
56	Cyclometallation of amino-imines on palladium complexes. The effect of the solvent on the experimental and calculated mechanism. <i>Dalton Transactions</i> , 2009, , 8292.	3.3	27
57	Organometallic gold complexes of carborane. Theoretical comparative analysis of ortho, meta, and para derivatives and luminescence studies. <i>Dalton Transactions</i> , 2009, , 3807.	3.3	35
58	A New Titanium Alkoxide-Thiolate Complex as a Versatile Heterofunctional Metalloligand. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 1079-1085.	2.0	11
59	Ligands that enforce unnatural stereoisomers. <i>Dalton Transactions</i> , 2008, , 2235.	3.3	0
60	A New Bis(1-naphthylimino)acenaphthene Compound and Its Pd(II) and Zn(II) Complexes: Synthesis, Characterization, Solid-State Structures and Density Functional Theory Studies on the syn and anti Isomers. <i>Inorganic Chemistry</i> , 2008, 47, 7734-7744.	4.0	63
61	On the Existence of Molecular Palladium(VI) Compounds: A Palladium Hexafluoride. <i>Inorganic Chemistry</i> , 2007, 46, 2700-2703.	4.0	17
62	Six-fold Oxygen-Coordinated Triplet (S= 1) Palladium(II) Moieties Templated by Tris(bipyridine)ruthenium(II) Ions. <i>Journal of the American Chemical Society</i> , 2007, 129, 1327-1334.	13.7	30
63	Acetyl Platinum(II) Complexes. <i>Organometallics</i> , 2007, 26, 6155-6169.	2.3	31
64	Chemistry of Unsaturated Group 6 Metal Complexes with Bridging Hydroxy- and Methoxycarbonyl Ligands. 2. Synthesis, Structure, and Bonding of 32- and 34-Electron Complexes. <i>Organometallics</i> , 2007, 26, 5912-5921.	2.3	36
65	Genuine Examples of Tetrahedral Tetradentate Sulfide Ligand Bridging Four Pd Atoms: A Controlled Formation of $[(\frac{1}{4}S)\{(\frac{1}{4}2-X)Pd_2(Ca^{\wedge}N)_2\}_2]$ (X = OH or Cl; $HCa^{\wedge}N = p-C_2H_5OC_6H_4CHNC_6H_4-p-C_2H_5$) Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 2035-2040.		7
66	¹ H NMR Direct Observation of Enantiomeric Exchange in Palladium(II) and Platinum(II) Complexes Containing N,N'-Bidentate Aryl-pyridin-2-ylmethyl-amine Ligands. <i>Inorganic Chemistry</i> , 2007, 46, 568-577.	4.0	44
67	Chelating Dialkoxide Titanium Complex: A Versatile Building Block for the Construction of Heterometallic Derivatives. <i>Chemistry - A European Journal</i> , 2007, 13, 2831-2836.	3.3	7
68	New Dinuclear Mn(III) Compounds with 2-MeC ₆ H ₄ COO and 2-FC ₆ H ₄ COO Bridges – Effect of Terminal Monodentate Ligands (H ₂ O, ClO ₄ [−] and NO ₃ [−]) on the Magnetic Properties. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 1285-1296.	2.0	27
69	Chemistry of Unsaturated Group 6 Metal Complexes with Bridging Hydroxy and Methoxycarbonyl Ligands. 1. Synthesis, Structure, and Bonding of 30-Electron Complexes. <i>Organometallics</i> , 2007, 26, 4930-4941.	2.3	40
70	Isomeric Distribution and Catalyzed Isomerization of Cobalt(III) Complexes with Pentadentate Macrocyclic Ligands. Importance of Hydrogen Bonding. <i>Inorganic Chemistry</i> , 2006, 45, 8551-8562.	4.0	22
71	Effects of Tris(pyrazolyl)borato Ligand Substituents on Dioxygen Activation and Stabilization by Copper Compounds. <i>Inorganic Chemistry</i> , 2006, 45, 3594-3601.	4.0	19
72	Bonding and solvation preferences of nickel complexes $[Ni(S_2PR_2)_2]$ (R=H, Me, OMe) according a natural bond orbital analysis. <i>Computational and Theoretical Chemistry</i> , 2006, 767, 37-41.	1.5	13

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73	“To Bend or not To Bend? Both! The Planar and Bent Structures of $[(Ph_3P)_4Rh_2(\eta^4-F)_2]$. European Journal of Inorganic Chemistry, 2006, 2006, 3340-3345.	2.0	13
74	Ruthenium Complexes Containing Chiral N-Donor Ligands as Catalysts in Acetophenone Hydrogen Transfer - New Amino Effect on Enantioselectivity. European Journal of Inorganic Chemistry, 2005, 2005, 4341-4351.	2.0	20
75	A pyrimidine thiolate Rh(I) complex: structure, bonding and one-dimensional interactions in solid and in solution. Dalton Transactions, 2005, , 938-944.	3.3	5
76	Formation of Sulfur-Sulfur Bonds in Copper Complexes. European Journal of Inorganic Chemistry, 2004, 2004, 4430-4438.	2.0	12
77	Chalcogen-Chalcogen Bonds in Edge-Sharing Square-Planar d8 Complexes. Are They Possible?. ChemInform, 2004, 35, no.	0.0	0
78	Chalcogen-Chalcogen Bonds in Edge-Sharing Square-Planar d8 Complexes. Are They Possible?. Inorganic Chemistry, 2004, 43, 3702-3714.	4.0	25
79	Unexpected Influence of the Counteranion in the η^2 vs η^3 Hapticity of Polydentate N-Donor Ligands in $[Rh(N\text{-ligand})L_2]^+$ Complexes. Organometallics, 2004, 23, 5530-5539.	2.3	18
80	A New Class of $(\eta^4-\eta^2-\eta^2\text{-Disulfido})$ dicopper Complexes: Synthesis, Characterization, and Disulfido Exchange. Inorganic Chemistry, 2004, 43, 3335-3337.	4.0	64
81	The Evolution of $[\{Ph_2P(CH_2)_nPPH_2\}Pt(\eta^4-S)_2Pt\{Ph_2P(CH_2)_nPPH_2\}]$ (n=2, 3) Metalloligands in Protic Acids: A Cascade of Sequential Reactions. Chemistry - A European Journal, 2003, 9, 5023-5035.	3.3	38
82	Molecular Structure and Isomerization in Square-Planar Edge-Sharing Dinuclear Complexes with Alkynyl Bridges. Organometallics, 2002, 21, 2627-2634.	2.3	22
83	Theoretical Clues to the Mechanism of Dioxygen Formation at the Oxygen-Evolving Complex of Photosystem II. Chemistry - A European Journal, 2002, 8, 2508.	3.3	22
84	Hexakis(silyl)palladium(VI) or Palladium(II) with η^2 -Disilane Ligands? This work was supported by the Direcció General de Enseñanza Superior (DGES), grant PB98-1166-CO2-01, and the Comissionat per a Universitats i Recerca (Generalitat de Catalunya), grant SGR99-0046. Computing resources at the Centre de Supercomputació de Catalunya (CESCA) and Centre de Paral·lelisme de Barcelona (CEPBA) were made available by the Comissió Interdepartamental per a la Recerca i la Innovació Tecnològica (CIRIT) and the Unive. Angewandte Chemie - International Edition, 2002, 41, 1956.	13.8	35
85	First Evidence of Fast $Si\ddot{S}H\ddot{S}H\ddot{S}H\ddot{S}H\ddot{S}H\ddot{S}H$ Proton Transfer in a Transition Metal Complex. Angewandte Chemie - International Edition, 2002, 41, 2776-2778.	13.8	23
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91	Through-Ring Bonding in Edge Sharing Dimers of Octahedral Complexes. <i>Inorganic Chemistry</i> , 2000, 39, 3166-3175.	4.0	31
92	Structural Correlations and Conformational Preference in Edge-Sharing Binuclear d ⁸ Complexes with XR ₂ Bridges. A Theoretical Study. <i>Inorganic Chemistry</i> , 2000, 39, 906-916.	4.0	16
93	Synthesis and study of trinuclear Pd(II) and Pt(II) complexes with 2-mercaptionicotinic acid. <i>Polyhedron</i> , 1999, 18, 3675-3682.	2.2	35
94	Ligand orientation effects on metal-metal, ligand-ligand and metal-ligand interactions. <i>Coordination Chemistry Reviews</i> , 1999, 185-186, 431-450.	18.8	39
95	Edge-Sharing Binuclear d ⁸ Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation. <i>Chemistry - A European Journal</i> , 1999, 5, 1391-1410.	3.3	65
96	Edge-Sharing Binuclear d ⁸ Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation. <i>Chemistry - A European Journal</i> , 1999, 5, 1391-1410.	3.3	1
97	Metal-bound chlorine often accepts hydrogen bonds. <i>Chemical Communications</i> , 1998, , 653-654.	4.1	417
98	To Bend or Not To Bend: A Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d ⁸ Transition Metal Ions. <i>Inorganic Chemistry</i> , 1998, 37, 804-813.	4.0	126
99	Pyramidal effect on metal-metal single bonds. <i>Journal of the Chemical Society Dalton Transactions</i> , 1997, , 2681-2688.	1.1	3
100	Chain Conformation and Metal-Metal Contacts in Dimers and Stacks of d ⁸ -ML ₄ Complexes: Electronic Effects. <i>Chemistry - A European Journal</i> , 1997, 3, 655-664.	3.3	64
101	Axial Bonding Capabilities of Square Planar d ⁸ -ML ₄ Complexes. Theoretical Study and Structural Correlations. <i>Inorganic Chemistry</i> , 1996, 35, 3137-3144.	4.0	84
102	On the Existence of a Pyramidal Effect in d ⁸ -d ⁸ Contacts. Theoretical Study and Structural Correlation. <i>Inorganic Chemistry</i> , 1996, 35, 5061-5067.	4.0	50
103	On the Bonding Nature of the M ₂ Interactions in Dimers of Square-Planar Pt(II) and Rh(I) Complexes. <i>Journal of the American Chemical Society</i> , 1995, 117, 7169-7171.	13.7	103
104	Heterodox Bonding Effects between Transition Metal Atoms. , 1995, , 241-255.		8
105	Through-ring bonding in edge-sharing dimers of square planar complexes. <i>Journal of Organometallic Chemistry</i> , 1994, 478, 75-82.	1.8	52
106	Pyramidal effect on rhodium(II)-Rh(II) single bonds. <i>Inorganic Chemistry</i> , 1993, 32, 3712-3719.	4.0	25