

Gabriel AullÃ³n

List of Publications by Year in descending order

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citations

196777

29
h-index

206121

51
g-index

112
all docs

112
docs citations

112
times ranked

3871
citing authors

#	ARTICLE	IF	CITATIONS
1	Metal-bound chlorine often accepts hydrogen bonds. <i>Chemical Communications</i> , 1998, , 653-654.	2.2	417
2	Dihydrogen contacts in alkanes are subtle but not faint. <i>Nature Chemistry</i> , 2011, 3, 323-330.	6.6	231
3	To Bend or Not To Bend: A Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d8 Transition Metal Ions. <i>Inorganic Chemistry</i> , 1998, 37, 804-813.	1.9	126
4	Understanding the Nature of the CH ₃ ...HC Interactions in Alkanes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1977-1991.	2.3	112
5	On the Bonding Nature of the M...M Interactions in Dimers of Square-Planar Pt(II) and Rh(I) Complexes. <i>Journal of the American Chemical Society</i> , 1995, 117, 7169-7171.	6.6	103
6	Axial Bonding Capabilities of Square Planar d8-ML ₄ Complexes. <i>Theoretical Study and Structural Correlations. Inorganic Chemistry</i> , 1996, 35, 3137-3144.	1.9	84
7	Oxidation states, atomic charges and orbital populations in transition metal complexes. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 67-73.	0.5	76
8	Edge-Sharing Binuclear d8 Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation. <i>Chemistry - A European Journal</i> , 1999, 5, 1391-1410.	1.7	65
9	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.	1.7	64
10	A New Class of (1/4-1,2-Disulfido)dicopper Complexes: Synthesis, Characterization, and Disulfido Exchange. <i>Inorganic Chemistry</i> , 2004, 43, 3335-3337.	1.9	64
11	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.	1.9	63
12	Through-ring bonding in edge-sharing dimers of square planar complexes. <i>Journal of Organometallic Chemistry</i> , 1994, 478, 75-82.	0.8	52
13	On the Existence of a Pyramidity Effect in d8...d8 Contacts. <i>Theoretical Study and Structural Correlation. Inorganic Chemistry</i> , 1996, 35, 5061-5067.	1.9	50
14	Comparison of the Structure and Stability of New 1,2-Diimine Complexes of Copper(I) and Silver(I): Density Functional Theory versus Experimental. <i>Inorganic Chemistry</i> , 2010, 49, 8699-8708.	1.9	46
15	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.	1.9	44
16	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.	1.9	41
17	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.	1.1	40
18	Ligand orientation effects on metal-metal, ligand-ligand and metal-ligand interactions. <i>Coordination Chemistry Reviews</i> , 1999, 185-186, 431-450.	9.5	39

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19	The Evolution of $[Ph_2P(CH_2)_nPPH_2]Pt(\frac{1}{4}-S)_2Pt[Ph_2P(CH_2)_nPPH_2]$ (n=2, 3) Metalloligands in Protic Acids: A Cascade of Sequential Reactions. <i>Chemistry - A European Journal</i> , 2003, 9, 5023-5035.	1.7	38
20	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.	1.1	36
21	Synthesis and study of trinuclear Pd(II) and Pt(II) complexes with 2-mercaptopyridine. <i>Polyhedron</i> , 1999, 18, 3675-3682.	1.0	35
22	Hexakis(silyl)palladium(VI) or Palladium(II) with 1,2-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. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1956.	7.2	35
23	Organometallic gold complexes of carborane. Theoretical comparative analysis of ortho, meta, and para derivatives and luminescence studies. <i>Dalton Transactions</i> , 2009, , 3807.	1.6	35
24	Intermolecular interactions in group 14 hydrides: Beyond C-H...H-C contacts. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25432.	1.0	32
25	Through-Ring Bonding in Edge Sharing Dimers of Octahedral Complexes. <i>Inorganic Chemistry</i> , 2000, 39, 3166-3175.	1.9	31
26	Acetyl Platinum(II) Complexes. <i>Organometallics</i> , 2007, 26, 6155-6169.	1.1	31
27	Exploring Excited-State Tunability in Luminescent Tricyclicmetalated Platinum(IV) Complexes: Synthesis of Heteroleptic Derivatives and Computational Calculations. <i>Chemistry - A European Journal</i> , 2014, 20, 17346-17359.	1.7	31
28	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.	6.6	30
29	The $[M_2(CO)_8]$ Complexes of the Cobalt Group. <i>European Journal of Inorganic Chemistry</i> , 2001, 2001, 3031-3038.	1.0	29
30	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.	1.0	27
31	Cyclometallation of amino-imines on palladium complexes. The effect of the solvent on the experimental and calculated mechanism. <i>Dalton Transactions</i> , 2009, , 8292.	1.6	27
32	Assembling Nonplanar Polyaromatic Units by Click Chemistry. Study of Multicorannulene Systems as Host for Fullerenes. <i>Organic Letters</i> , 2015, 17, 2578-2581.	2.4	27
33	Electrocatalytic Proton Reduction by Dimeric Nickel Complex of a Sterically Demanding Pincer-type NS ₂ Aminobis(thiophenolate) Ligand. <i>Inorganic Chemistry</i> , 2015, 54, 619-627.	1.9	27
34	Pyramidal effect on rhodium(II)-Rh(II) single bonds. <i>Inorganic Chemistry</i> , 1993, 32, 3712-3719.	1.9	25
35	Chalcogen-Chalcogen Bonds in Edge-Sharing Square-Planar d ₈ Complexes. Are They Possible?. <i>Inorganic Chemistry</i> , 2004, 43, 3702-3714.	1.9	25
36	Dihydrogen intermolecular contacts in group 13 compounds: H...H or E...H (E = B, Al, Ga) interactions?. <i>Dalton Transactions</i> , 2017, 46, 2844-2854.	1.6	25

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37	Reaction chemistry, NMR spectroscopy, and X-ray crystallography of $[\text{Fe}_2(\text{SiMe}_2)_2(\text{CO})_4]$ and $[\text{Fe}_2(\text{SiMeCl})_2(\text{CO})_4]$. Electronic structure and bonding in Fe_2E_2 rings of $[\text{Fe}_2(\text{ER}_2)_2(\text{CO})_4]$ binuclear complexes (E=C, Si, Ge, Sn, Pb). <i>Journal of Organometallic Chemistry</i> , 2001, 628, 241-254.	0.8	24
38	First Evidence of Fast $\text{Si}\ddot{\text{H}}\text{S}$ Proton Transfer in a Transition Metal Complex. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 2776-2778.	7.2	23
39	Highly fluorescent complexes with gold, palladium or platinum linked to perylene through a tetrafluorophenyl group. <i>Dalton Transactions</i> , 2013, 42, 6353.	1.6	23
40	Molecular Structure and Isomerization in Square-Planar Edge-Sharing Dinuclear Complexes with Alkynyl Bridges. <i>Organometallics</i> , 2002, 21, 2627-2634.	1.1	22
41	Theoretical Clues to the Mechanism of Dioxygen Formation at the Oxygen-Evolving Complex of Photosystem II. <i>Chemistry - A European Journal</i> , 2002, 8, 2508.	1.7	22
42	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.	1.9	22
43	Reactivity of a Super-Electron-Rich Olefin Derived from Cyclam. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 1851-1860.	1.0	22
44	The Structural Diversity Triggered by Intermolecular Interactions between Au^{I} $\text{S}^{\text{2-}}$ Groups: Aurophilia and Beyond. <i>Chemistry - A European Journal</i> , 2012, 18, 9965-9976.	1.7	22
45	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.	1.6	22
46	Two Temperature-Independent Spinomers of the Dinuclear Mn(III) Compound $[\{\text{Mn}(\text{H}_2\text{O})(\text{phen})\}_2(\text{C}_6\text{H}_4\text{COO})_2(\text{O})](\text{ClO}_4)_2$. <i>Inorganic Chemistry</i> , 2010, 49, 1471-1480.	1.9	21
47	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.	1.7	21
48	Ruthenium Complexes Containing Chiral N-Donor Ligands as Catalysts in Acetophenone Hydrogen Transfer - New Amino Effect on Enantioselectivity. <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 4341-4351.	1.0	20
49	Effects of Tris(pyrazolyl)borato Ligand Substituents on Dioxygen Activation and Stabilization by Copper Compounds. <i>Inorganic Chemistry</i> , 2006, 45, 3594-3601.	1.9	19
50	Higher fluorescence in platinum(IV) orthometallated complexes of perylene imine compared with their platinum(II) or palladium(II) analogues. <i>Dalton Transactions</i> , 2015, 44, 16164-16176.	1.6	19
51	Unexpected Influence of the Counteranion in the η^2 vs η^3 Hapticity of Polydentate N-Donor Ligands in $[\text{Rh}(\text{N-ligand})\text{L}_2]^+$ Complexes. <i>Organometallics</i> , 2004, 23, 5530-5539.	1.1	18
52	On the Existence of Molecular Palladium(VI) Compounds: A Palladium Hexafluoride. <i>Inorganic Chemistry</i> , 2007, 46, 2700-2703.	1.9	17
53	Direct and Enantioselective Aldol Reactions Catalyzed by Chiral Nickel(II) Complexes. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 15307-15312.	7.2	17
54	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.	1.9	16

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55	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. <i>Dalton Transactions</i> , 2017, 46, 2184-2195.	1.6	16
56	Direct and Asymmetric Nickel(II)-Catalyzed Construction of Carbon–Carbon Bonds from <i>N</i> -Acyl Thiazinanethiones. <i>Organic Letters</i> , 2019, 21, 305-309.	2.4	16
57	X ₂ Z ₂ X Through Cage Bonding in Cu, Ni, and Cr Complexes with M ₃ X ₂ Cores (X=S, As). <i>Chemistry - A European Journal</i> , 2009, 15, 536-546.	1.7	15
58	On the electronic structure and stability of icosahedral r-X ₂ Z ₁₀ H ₁₂ and Z ₁₂ H ₁₂ clusters; r = {ortho, meta, para}, X = {C, Si}, Z = {B, Al}. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5101.	1.3	14
59	Structural analysis of the coordination of dinitrogen to transition metal complexes. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2015, 71, 369-386.	0.5	14
60	Synthesis, characterization, crystal structures and computational studies on novel cyrhetrenyl hydrazones. <i>Journal of Organometallic Chemistry</i> , 2016, 819, 129-137.	0.8	14
61	Oxidative Cleavage of Cellobiose by Lytic Polysaccharide Monooxygenase (LPMO)-Inspired Copper Complexes. <i>ACS Omega</i> , 2019, 4, 10729-10740.	1.6	14
62	Effect of Gold(I) on the Room-Temperature Phosphorescence of Ethynylphenanthrene. <i>Chemistry - A European Journal</i> , 2021, 27, 1810-1820.	1.7	14
63	Bonding and solvation preferences of nickel complexes [Ni(S ₂ PR 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
64	“To Bend or not To Bend? Both! The Planar and Bent Structures of [(Ph ₃ P) ₄ Rh ₂ (η^4 -F) ₂]. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 3340-3345.	1.0	13
65	Formation of Sulfur–Sulfur Bonds in Copper Complexes. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 4430-4438.	1.0	12
66	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. <i>Polyhedron</i> , 2015, 101, 93-102.	1.0	12
67	Supramolecular tripodal Au(II) assemblies in water. Interactions with a pyrene fluorescent probe. <i>New Journal of Chemistry</i> , 2019, 43, 8279-8289.	1.4	12
68	Designing antiferromagnetically coupled mono-, di- and tri-bridged copper(II)-based catecholase models by varying the Auxiliary Parts of the ligand and anionic co-ligand. <i>CrystEngComm</i> , 2019, 21, 7094-7107.	1.3	12
69	A New Titanium Alkoxide-Thiolate Complex as a Versatile Heterofunctional Metalloligand. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 1079-1085.	1.0	11
70	Magnetic Behavior of Heterometallic Wheels Having a [Mn ₄ V ₆ M ₂ O ₉] ¹⁰⁺ Core with M = Ca ²⁺ and Sr ²⁺ . <i>Inorganic Chemistry</i> , 2015, 54, 11596-11605.	1.9	11
71	Kinetico-Mechanistic Information about Alkene Hydroamination with Aniline in Bromide-Rich Ionic Media: Importance of Solvolysis. <i>Inorganic Chemistry</i> , 2011, 50, 5628-5636.	1.9	10
72	Electronic structure and geometries of o-carborane derived cyclic structures [C _{1/4} -1,2-(C ₂ B ₁₀ H ₁₀) _n Mn]Ag ^m , M = {Au, Hg}, n = {3, 4}, m = {0, 1, 2}, z = {n + m, m}. <i>Dalton Transactions</i> , 2012, 41, 14146.	1.6	10

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73	Theoretical Study of Bonding, Structure, and Vibrational Spectra of the [Fe ₂ (CO) ₈] ²⁻ Anion and Its Derivatives. <i>Organometallics</i> , 2001, 20, 818-826.	1.1	9
74	Redox-Assisted Self-Assembly of a Water-Soluble Cyanido-Bridged Mixed Valence {Co ^{III} /Fe ^{II} } ₂ Square. <i>Chemistry - A European Journal</i> , 2016, 22, 15227-15230.	1.7	9
75	A combined kinetic-mechanistic and computational study on the competitive formation of seven- versus five-membered platinacycles; the relevance of spectator halide ligands. <i>Dalton Transactions</i> , 2015, 44, 17968-17979.	1.6	8
76	Direct and Enantioselective Aldol Reactions Catalyzed by Chiral Nickel(II) Complexes. <i>Angewandte Chemie</i> , 2021, 133, 15435-15440.	1.6	8
77	Heterodox Bonding Effects between Transition Metal Atoms. , 1995, , 241-255.		8
78	Molecular Structures of Edge-Sharing Square-Planar Dinuclear Complexes with Unsaturated Bridges. <i>Inorganic Chemistry</i> , 2001, 40, 4937-4946.	1.9	7
79	Genuine Examples of Tetrahedral Tetradentate Sulfide Ligand Bridging Four Pd Atoms: Controlled Formation of [(1/4-S){(1/4-X)Pd ₂ (C ₆ H ₅ N) ₂] ₂ (X = OH or Cl; HC ₆ H ₄ N = p-C ₂ H ₅ OC ₆ H ₄ CHNC ₆ H ₄ -p-C ₂ H ₅) Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 2035-2040.		7
80	Chelating Dialkoxide Titanium Complex: A Versatile Building Block for the Construction of Heterometallic Derivatives. <i>Chemistry - A European Journal</i> , 2007, 13, 2831-2836.	1.7	7
81	Total synthesis of (+)-herboxidiene/GEX 1A. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 1842-1862.	1.5	7
82	Conformational Effects of [Ni ₂ (ArS) ₂] Cores on Their Electrocatalytic Activity. <i>Chemistry - an Asian Journal</i> , 2019, 14, 3301-3312.	1.7	7
83	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. <i>New Journal of Chemistry</i> , 2019, 43, 2501-2512.	1.4	7
84	Trinuclear Gold-Carborane Cluster as a Host Structure. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 18-22.	1.0	7
85	Direct and Asymmetric Aldol Reactions of <i>N</i> -Azidoacetyl-1,3-thiazolidine-2-thione Catalyzed by Chiral Nickel(II) Complexes. A New Approach to the Synthesis of β -Hydroxy- α -Amino Acids. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	7
86	Computational Insights on the Geometrical Arrangements of Cu(II) with a Mixed-Donor N ₃ S ₃ Macrobicyclic Ligand. <i>Inorganic Chemistry</i> , 2014, 53, 512-521.	1.9	6
87	Highly fluorescent complexes with 3-isocyanoperylene and N-(2,5-di-tert-butylphenyl)-9-isocyanoperylene-3,4-dicarboximide. <i>Dalton Transactions</i> , 2014, 43, 10885-10897.	1.6	6
88	Substrate-Controlled Aldol Reactions from Chiral β -Hydroxy Ketones. <i>Synthesis</i> , 2017, 49, 484-503.	1.2	6
89	Fluorescent perylenylpyridine complexes: an experimental and theoretical study. <i>Dalton Transactions</i> , 2020, 49, 13326-13338.	1.6	6
90	Comprehensive Investigation of the Photophysical Properties of Alkynylcoumarin Gold(I) Complexes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11751-11760.	1.2	6

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91	A pyrimidine thiolate Rh(i) complex: structure, bonding and one-dimensional interactions in solid and in solution. Dalton Transactions, 2005, , 938-944.	1.6	5
92	On the Coordination of Dinitrogen to Group 4 Metallocenes. European Journal of Inorganic Chemistry, 2012, 2012, 797-806.	1.0	5
93	Self-Assembly Hydrosoluble Coronenes: A Rich Source of Supramolecular Turn-On Fluorogenic Sensing Materials in Aqueous Media. Organic Letters, 2021, 23, 8727-8732.	2.4	5
94	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.	1.6	4
95	Pyramidity effect on metal-metal single bonds. Journal of the Chemical Society Dalton Transactions, 1997, , 2681-2688.	1.1	3
96	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
97	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.	1.6	3
98	Direct, Enantioselective, and Nickel(II) Catalyzed Reactions of <i>N</i> -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.	1.7	3
99	Substitution of chloride by nitrosyl ligand in a scorpionate ruthenium(III) compound: A theoretical study. Inorganica Chimica Acta, 2009, 362, 4651-4658.	1.2	2
100	Indirect effect of hydrogen bonds on the magnetic coupling on Mn(III) dinuclear compounds. CrystEngComm, 2018, 20, 6629-6639.	1.3	2
101	Synthesis, Characterization, Solution Behavior and Theoretical Studies of Pd(II) Allyl Complexes with 2-Phenyl-3H-indoles as Ligands. Catalysts, 2019, 9, 811.	1.6	1
102	On the silicon-silicon bonds η^2 -coordinated to group 10 transition metals. Inorganica Chimica Acta, 2019, 486, 449-457.	1.2	1
103	Edge-Sharing Binuclear d ₈ Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation. , 1999, 5, 1391.		1
104			