

Santiago Alvarez

List of Publications by Year in descending order

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290
papers

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146
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309
all docs

309
docs citations

309
times ranked

15610
citing authors

#	ARTICLE	IF	CITATIONS
1	Covalent radii revisited. Dalton Transactions, 2008, , 2832.	1.6	3,155
2	A cartography of the van der Waals territories. Dalton Transactions, 2013, 42, 8617.	1.6	1,117
3	Shape maps and polyhedral interconversion paths in transition metal chemistry. Coordination Chemistry Reviews, 2005, 249, 1693-1708.	9.5	889
4	Broken symmetry approach to calculation of exchange coupling constants for homobinuclear and heterobinuclear transition metal complexes. Journal of Computational Chemistry, 1999, 20, 1391-1400.	1.5	836
5	Toward the Prediction of Magnetic Coupling in Molecular Systems: Hydroxo- and Alkoxo-Bridged Cu(II) Binuclear Complexes. Journal of the American Chemical Society, 1997, 119, 1297-1303.	6.6	816
6	The Rich Stereochemistry of Eight-Vertex Polyhedra: A Continuous Shape Measures Study. Chemistry - A European Journal, 2005, 11, 1479-1494.	1.7	729
7	Magnetic Coupling in End-On Azido-Bridged Transition Metal Complexes: A Density Functional Study. Journal of the American Chemical Society, 1998, 120, 11122-11129.	6.6	676
8	About the calculation of exchange coupling constants in polynuclear transition metal complexes. Journal of Computational Chemistry, 2003, 24, 982-989.	1.5	472
9	Continuous symmetry maps and shape classification. The case of six-coordinated metal compounds Electronic supplementary information (ESI) available: tables of CSD refcodes, structural parameters and symmetry measures for the studied compounds. See http://www.rsc.org/suppdata/ni/b2/b202096n/ . New Journal of Chemistry, 2002, 26, 996-1009.	1.4	388
10	Structural Modeling and Magneto-Structural Correlations for Hydroxo-Bridged Copper(II) Binuclear Complexes. Inorganic Chemistry, 1997, 36, 3683-3688.	1.9	386
11	Minimal Distortion Pathways in Polyhedral Rearrangements. Journal of the American Chemical Society, 2004, 126, 1755-1763.	6.6	362
12	Distortions in Octahedrally Coordinated d-Transition Metal Oxides: A Continuous Symmetry Measures Approach. Chemistry of Materials, 2006, 18, 3176-3183.	3.2	326
13	Exchange Coupling in Carboxylato-Bridged Dinuclear Copper(II) Compounds: A Density Functional Study. Chemistry - A European Journal, 2001, 7, 627-637.	1.7	325
14	About the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction error. Journal of Chemical Physics, 2005, 123, 164110.	1.2	318
15	Polyhedral Structures with an Odd Number of Vertices: Nine-Coordinate Metal Compounds. Chemistry - A European Journal, 2008, 14, 1291-1303.	1.7	294
16	Coordinating ability of anions and solvents towards transition metals and lanthanides. Dalton Transactions, 2011, 40, 10742.	1.6	247
17	Dimerization and stacking in transition-metal bisdithiolenes and tetrathiolates. Journal of the American Chemical Society, 1985, 107, 6253-6277.	6.6	243
18	Dihydrogen contacts in alkanes are subtle but not faint. Nature Chemistry, 2011, 3, 323-330.	6.6	231

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19	Shape and Symmetry of Heptacoordinate Transition-Metal Complexes: Structural Trends. Chemistry - A European Journal, 2003, 9, 1281-1295.	1.7	225
20	Can large magnetic anisotropy and high spin really coexist?. Chemical Communications, 2008, , 52-54.	2.2	215
21	Exchange Coupling of Transition-Metal Ions through Hydrogen Bonding: A Theoretical Investigation. Journal of the American Chemical Society, 2002, 124, 5197-5205.	6.6	202
22	Choice of Coordination Number in d10Complexes of Group 11 Metals. Journal of the American Chemical Society, 2004, 126, 1465-1477.	6.6	198
23	Exchange Coupling in Oxalato-Bridged Copper(II) Binuclear Compounds: A Density Functional Study. Chemistry - A European Journal, 1998, 4, 476-484.	1.7	197
24	Binuclear and polymeric gold(I) complexes. Inorganic Chemistry, 1985, 24, 749-757.	1.9	189
25	Spin Density Distribution in Transition Metal Complexes: Some Thoughts and Hints. Comments on Inorganic Chemistry, 1998, 20, 27-56.	3.0	187
26	Mapping the Stereochemistry and Symmetry of Tetracoordinate Transition-Metal Complexes. Chemistry - A European Journal, 2004, 10, 190-207.	1.7	175
27	Spin state behavior of iron(II)/dipyrazolylpyridine complexes. New insights from crystallographic and solution measurements. Coordination Chemistry Reviews, 2015, 289-290, 2-12.	9.5	175
28	Influence of the Peripheral Ligand Atoms on the Exchange Interaction in Oxalato-Bridged Nickel(II) Complexes: An Orbital Model. Crystal Structures and Magnetic Properties of (H3dien)2[Ni2(ox)5]·12H2O and [Ni2(dien)2(H2O)2(ox)]Cl2. Inorganic Chemistry, 1996, 35, 3741-3751.	1.9	171
29	Distortion Pathways of Transition Metal Coordination Polyhedra Induced by Chelating Topology. Chemical Reviews, 2015, 115, 13447-13483.	23.0	166
30	Spin density distribution in transition metal complexes. Coordination Chemistry Reviews, 2005, 249, 2649-2660.	9.5	163
31	How to Build Molecules with Large Magnetic Anisotropy. Chemistry - A European Journal, 2009, 15, 4078-4087.	1.7	163
32	From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields. Chemical Reviews, 2016, 116, 8173-8192.	23.0	155
33	Theoretical Study of Exchange Coupling in 3d-Gd Complexes: Large Magnetocaloric Effect Systems. Journal of the American Chemical Society, 2012, 134, 10532-10542.	6.6	154
34	Shape and Spin State in Four-Coordinate Transition-Metal Complexes: The Case of the d6 Configuration. Chemistry - A European Journal, 2006, 12, 3162-3167.	1.7	153
35	Magnetic Coupling in End-to-End Azido-Bridged Copper and Nickel Binuclear Complexes: A Theoretical Study. Inorganic Chemistry, 2000, 39, 3221-3229.	1.9	152
36	Structural and electronic effects on the exchange interactions in dinuclear bis(phenoxo)-bridged copper(II) complexes. Coordination Chemistry Reviews, 2010, 254, 2086-2095.	9.5	148

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37	Oxalato-bridged and related dinuclear copper(II) complexes: theoretical analysis of their structures and magnetic coupling. <i>Inorganic Chemistry</i> , 1990, 29, 4500-4507.	1.9	146
38	Electronic structure and properties of AlN. <i>Physical Review B</i> , 1994, 49, 7115-7123.	1.1	146
39	Electronic structure and properties of Cu ₂ O. <i>Physical Review B</i> , 1997, 56, 7189-7196.	1.1	146
40	Continuous symmetry measures of penta-coordinate molecules: Berry and non-Berry distortions of the trigonal bipyramid. <i>Dalton Transactions RSC</i> , 2000, , 3288-3303.	2.3	143
41	The Nature of Intermolecular Cu...Cu Interactions: A Combined Theoretical and Structural Database Analysis. <i>Chemistry - A European Journal</i> , 2004, 10, 2117-2132.	1.7	139
42	Polyhedra in (inorganic) chemistry. <i>Dalton Transactions</i> , 2005, , 2209.	1.6	139
43	Is It Possible To Get High TCMagnets with Prussian Blue Analogues? A Theoretical Prospect. <i>Chemistry - A European Journal</i> , 2005, 11, 2135-2144.	1.7	129
44	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.	1.9	126
45	Continuous Shape Measures as a Stereochemical Tool in Organometallic Chemistry. <i>Organometallics</i> , 2005, 24, 1556-1562.	1.1	125
46	Importance of the X ₄ ring orbitals for the semiconducting, metallic, or superconducting properties of skutterudites MX ₃ and RM ₄ X ₁₂ . <i>Inorganic Chemistry</i> , 1990, 29, 2252-2255.	1.9	118
47	Exchange Coupling in Halo-Bridged Dinuclear Cu(II) Compounds: A Density Functional Study. <i>Inorganic Chemistry</i> , 2002, 41, 3769-3778.	1.9	118
48	Ligand Macrocycle Structural Effects on Copper ^{II} Dioxygen Reactivity. <i>Inorganic Chemistry</i> , 2000, 39, 4059-4072.	1.9	116
49	Understanding the Nature of the CH...HC Interactions in Alkanes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1977-1991.	2.3	112
50	Density functional study of magnetostructural correlations in cubane complexes containing the Cu ₄ O ₄ core. <i>Journal of Materials Chemistry</i> , 2006, 16, 2729-2735.	6.7	107
51	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
52	Relationships between Temperature, Magnetic Moment, and Continuous Symmetry Measures in Spin Crossover Complexes. <i>Journal of the American Chemical Society</i> , 2003, 125, 6795-6802.	6.6	102
53	Stereochemistry of Compounds with Coordination Number Ten. <i>Chemistry - A European Journal</i> , 2009, 15, 7470-7480.	1.7	101
54	Continuous chirality measures in transition metal chemistry. <i>Chemical Society Reviews</i> , 2005, 34, 313.	18.7	98

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55	Magnetic Properties of Cyano-Bridged Ln ³⁺ M ₃ Complexes. Part I: Trinuclear Complexes (Ln ³⁺ = La, Ce,) <i>J. Inorg. Nucl. Chem.</i> 1991, 43, 14-18.	1.9	103
56	Magnetostructural Correlations in Polynuclear Complexes: The Fe ₄ Butterflies. <i>Journal of the American Chemical Society</i> , 2006, 128, 15722-15727.	6.6	93
57	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.	6.6	93
58	Density functional study of the exchange coupling in distorted cubane complexes containing the Cu ₄ O ₄ core. <i>Polyhedron</i> , 2001, 20, 1323-1327.	1.0	90
59	Stereochemistry and Spin State in Four-Coordinate Transition Metal Compounds. <i>Inorganic Chemistry</i> , 2008, 47, 2871-2889.	1.9	88
60	Exchange interaction through a croconato bridge: synthesis, crystal structure, and magnetic properties of (μ-croconato)bis[μ-bis(2-pyridylcarbonyl)amido]copper(II) trihydrate. <i>Inorganic Chemistry</i> , 1992, 31, 1889-1894.	1.9	87
61	Magnetism of Cyano-Bridged Ln ³⁺ M ₃ Complexes. Part II: One-Dimensional Complexes (Ln ³⁺ = Eu, Tb, Dy,) <i>J. Inorg. Nucl. Chem.</i> 1991, 43, 19-24.	1.9	86
62	Axial Bonding Capabilities of Square Planar d ⁸ -ML ₄ Complexes. Theoretical Study and Structural Correlations. <i>Inorganic Chemistry</i> , 1996, 35, 3137-3144.	1.9	84
63	[Cu ₃ (μ ₃ -S) ₂] ₃ Clusters Supported by N-Donor Ligands: Progress Toward a Synthetic Model of the Catalytic Site of Nitrous Oxide Reductase. <i>Journal of the American Chemical Society</i> , 2005, 127, 13752-13753.	6.6	79
64	Theoretical Study of the Magnetic Behavior of Hexanuclear Cu(II) and Ni(II) Polysiloxanolato Complexes. <i>Journal of the American Chemical Society</i> , 2003, 125, 6791-6794.	6.6	77
65	A Bonding Quandary: A Demonstration of the Fact That Scientists Are Not Born With Logic. <i>Chemistry - A European Journal</i> , 2009, 15, 8358-8373.	1.7	77
66	Synthesis, x-ray diffraction structure, magnetic properties, and MO analysis of a binuclear (μ-tetrathiooxalato)copper(II) complex, (AsPh ₄) ₂ [(C ₃ OS ₄)Cu ₂ S ₄ Cu(C ₃ OS ₄)]. <i>Inorganic Chemistry</i> , 1987, 26, 4004-4009.	1.9	76
67	Oxidation states, atomic charges and orbital populations in transition metal complexes. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 67-73.	0.5	76
68	Theoretical study of the electrical behavior of one-dimensional metallophthalocyanines and related metallomacrocyclic compounds. <i>Inorganic Chemistry</i> , 1984, 23, 573-579.	1.9	75
69	Electronic structure and bonding in skutterudite-type phosphides. <i>Physical Review B</i> , 1996, 53, 10605-10609.	1.1	74
70	Exchange Coupling in Cyano-Bridged Homodinuclear Cu(II) and Ni(II) Complexes: Synthesis, Structure, Magnetism, and Density Functional Theoretical Study. <i>Inorganic Chemistry</i> , 2001, 40, 5868-5877.	1.9	74
71	Bonding and stereochemistry of three-coordinated transition metal compounds. <i>Coordination Chemistry Reviews</i> , 1999, 193-195, 13-41.	9.5	70
72	Symmetry and Topology Determine the MoV-CN-MnII Exchange Interactions in High-Spin Molecules. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2711-2715.	7.2	69

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73	Coordinating Ability of Anions, Solvents, Amino Acids, and Gases towards Alkaline and Alkaline Earth Elements, Transition Metals, and Lanthanides. <i>Chemistry - A European Journal</i> , 2020, 26, 4350-4377.	1.7	67
74	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
75	The Trigonal Prism in Coordination Chemistry. <i>Chemistry - A European Journal</i> , 2010, 16, 10380-10396.	1.7	65
76	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
77	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
78	Polyhedral structures with an odd number of vertices: nine-atom clusters and supramolecular architectures. <i>Dalton Transactions</i> , 2008, , 2583.	1.6	64
79	Theoretical search for new ferromagnetically coupled transition metal complexes. <i>Chemical Communications</i> , 1998, , 2767-2768.	2.2	62
80	Theoretical study of the exchange coupling in copper(II) binuclear compounds with oxamidate and related polyatomic bridging ligands. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 1669-1676.	1.1	61
81	Structure-NMR correlations in halo(ligand)bis(dioximato)cobalt(III) complexes. <i>Inorganic Chemistry</i> , 1986, 25, 2962-2969.	1.9	57
82	Electronic Structure and Magnetic Behavior in Polynuclear Transition-Metal Compounds. , 0, , 227-279.		55
83	A Family of Ferro- and Antiferromagnetically Coupled Decametalllic Chromium(III) Wheels. <i>Chemistry - A European Journal</i> , 2006, 12, 1385-1396.	1.7	55
84	Symmetry operation measures. <i>Journal of Computational Chemistry</i> , 2008, 29, 190-197.	1.5	55
85	Structure and stability of the X ₃ - systems (X = fluoride, chloride, bromide, iodide) and their interaction with cations. <i>The Journal of Physical Chemistry</i> , 1988, 92, 6561-6566.	2.9	54
86	How High the Spin? Allowed and Forbidden Spin States in Transition-Metal Chemistry. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 3012-3020.	7.2	53
87	Bonding and structure in L ₄ M ₂ (μ-XRn) ₂ diamonds of tetrahedral d ¹⁰ ions. Effect of substituents on the M-M interaction. <i>Inorganic Chemistry</i> , 1992, 31, 4266-4275.	1.9	52
88	Through-ring bonding in edge-sharing dimers of square planar complexes. <i>Journal of Organometallic Chemistry</i> , 1994, 478, 75-82.	0.8	52
89	On the Existence of a Pyramidity Effect in d ⁸ -d ⁸ Contacts. Theoretical Study and Structural Correlation. <i>Inorganic Chemistry</i> , 1996, 35, 5061-5067.	1.9	50
90	Interconversion of Quadrupty and Quintupty Bonded Molybdenum Complexes by Reductive Elimination and Oxidative Addition of Dihydrogen. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 3227-3231.	7.2	49

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91	Further Theoretical Evidence for the Exceptionally Strong Ferromagnetic Coupling in Oxo-Bridged Cu(II) Dinuclear Complexes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4938-4941.	1.1	48
92	Reply to "Comment on "About the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction error" [J. Chem. Phys. 123, 164110 (2005)]. <i>Journal of Chemical Physics</i> , 2006, 124, 107102.	1.2	47
93	van der Waals Radii of Noble Gases. <i>Inorganic Chemistry</i> , 2014, 53, 9260-9266.	1.9	46
94	Pyramidity and metal-metal multiple bonding: structural correlations and theoretical study. <i>Journal of the American Chemical Society</i> , 1993, 115, 6216-6229.	6.6	44
95	Room-Temperature Synthesis and Crystal, Magnetic, and Electronic Structure of the First Silver Copper Oxide. <i>Inorganic Chemistry</i> , 2002, 41, 6604-6613.	1.9	44
96	Quantitative Geometric Descriptions of the Belt Iron Atoms of the Iron-Molybdenum Cofactor of Nitrogenase and Synthetic Iron(II) Model Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 60-71.	1.9	44
97	Density Functional Study of Exchange Coupling Constants in Single-Molecule Magnets: The Fe ₈ Complex. <i>Chemistry - A European Journal</i> , 2005, 11, 4767-4771.	1.7	43
98	Molecules and crystals with both icosahedral and cubic symmetry. <i>Chemical Communications</i> , 2008, , 2717.	2.2	43
99	Crystal Orbital Displacement Analysis of Interactions in the Solid State. Application to the Study of Host-Guest Interactions in the Hofmann Clathrates. <i>Journal of the American Chemical Society</i> , 1994, 116, 8207-8221.	6.6	42
100	A novel bipyridine-based hexadentate tripodal framework with a strong preference for trigonal prismatic co-ordination geometries. <i>Dalton Transactions</i> , 2010, 39, 3870.	1.6	42
101	Asymmetry and Magnetism in Bis(oximato)-Bridged Heterobimetallic Compounds: A Computational Approach. <i>Chemistry - A European Journal</i> , 2000, 6, 327-333.	1.7	41
102	Theoretical study of exchange coupling constants in an Fe ₁₉ complex. <i>Journal of Physics and Chemistry of Solids</i> , 2004, 65, 799-803.	1.9	41
103	Theoretical Study of the Magnetic Properties of an Mn ₁₂ Single-Molecule Magnet with a Loop Structure: The Role of the Next-Nearest Neighbor Interactions. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 782-788.	2.3	41
104	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
105	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
106	Quantitative Chirality Analysis of Molecular Subunits of Bis(oxazoline)copper(II) Complexes in Relation to Their Enantioselective Catalytic Activity. <i>Chemistry - A European Journal</i> , 2003, 9, 5832-5837.	1.7	38
107	Square Fe ₂ Au ₂ and triangular Fe ₂ Au clusters: A reversible transformation. X-ray crystal structure of [Fe ₂ Au ₂ (CO) ₈ (μ-dppm)] [dppm = bis(diphenylphosphino)methane]. <i>Organometallics</i> , 1991, 10, 2309-2314.	1.1	37
108	Dinuclear complexes of copper(II) derived from (1,3-propanediylbis(oxamato))cuprate(II): magneto-structural correlations. <i>Inorganic Chemistry</i> , 1991, 30, 841-845.	1.9	36

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109	Spin Densities in a Ferromagnetic Bimetallic Chain Compound: Polarized Neutron Diffraction and DFT Calculations. <i>Journal of the American Chemical Society</i> , 2002, 124, 14433-14441.	6.6	36
110	A Theoretical Study of the Exchange Coupling in Hydroxo- and Alkoxo-Bridged Dinuclear Oxovanadium(IV) Compounds. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 143-153.	1.0	36
111	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
112	Electronic and Structural Effects of Low-Hapticity Coordination of Arene Rings to Transition Metals. <i>Organometallics</i> , 2014, 33, 6660-6668.	1.1	36
113	Iron-Gold (or Mercury) Carbide Clusters Derived from [Fe ₆ C(CO) ₁₆] ²⁻ . X-ray Crystal Structures of (NEt ₄)[Fe ₆ C{AuPPh ₃ } ₃ (CO) ₁₆] and [Fe ₄ C{AuPPh ₃ } ₃ (CO) ₁₁ (NO)]. <i>Organometallics</i> , 1997, 16, 236-245.	1.1	35
114	Framework Bonding and Coordination Sphere Rearrangement in the M ₂ X ₂ Cores of Synthetic Analogues of Oxyhemocyanin and Related Cu and Pt Complexes. <i>Inorganic Chemistry</i> , 1998, 37, 1202-1212.	1.9	35
115	Synthesis and study of trinuclear Pd(II) and Pt(II) complexes with 2-mercaptopyruvic acid. <i>Polyhedron</i> , 1999, 18, 3675-3682.	1.0	35
116	Early-late transition metal ferromagnetic coupling mediated by hydrogen bonding. <i>Chemical Communications</i> , 2002, , 2614-2615.	2.2	35
117	Reaction of vanadium(V) or cobalt(III) with 1,2-Diisilane 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 l'Innovació Tecnològica (CIRIT) and the Unió Acadèmica de Química - International Union of Pure and Applied Chemistry (IUPAC).	7.2	35
118	New organometallic cobaloximes containing an equatorial diphenylglyoximate(1-) ligand. Comparison between their properties and those of other B ₁₂ model compounds. Crystal structure of trans-[Co(dpgH) ₂ (CH ₃)(pyridine)]. <i>Journal of Organometallic Chemistry</i> , 1991, 414, 245-259.	0.8	34
119	The electronic structure of barium gallium antimonide (Ba ₇ Ga ₄ Sb ₉): a compound seemingly probing the limits of the Zintl concept. <i>Inorganic Chemistry</i> , 1990, 29, 3070-3073.	1.9	33
120	Calibrating the coordination chemistry tool chest: metrics of bi- and tridentate ligands. <i>Dalton Transactions</i> , 2009, , 6610.	1.6	33
121	Experimental and Theoretical Studies on Arene-Bridged Metal-Metal-Bonded Dimolybdenum Complexes. <i>Chemistry - A European Journal</i> , 2014, 20, 6092-6102.	1.7	33
122	Evaluating transition state structures of vanadium-phosphatase protein complexes using shape analysis. <i>Journal of Inorganic Biochemistry</i> , 2015, 147, 153-164.	1.5	33
123	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
124	Synthesis and structure of chloro(ligand)bis(diphenylglyoximate)cobalt(III) complexes. <i>Inorganica Chimica Acta</i> , 1987, 127, 153-159.	1.2	31
125	Through-Ring Bonding in Edge Sharing Dimers of Octahedral Complexes. <i>Inorganic Chemistry</i> , 2000, 39, 3166-3175.	1.9	31
126	Mercuriphilic interactions: a theoretical study on the importance of ligands. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 11645-11654.	1.3	31

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127	Anionic trimetallic compounds containing Fe ¹⁺ -E ¹⁺ -M skeletons (E = Zn, Cd, Hg; M = Fe, Mo, W). Crystal structure of [N(PPh ₃) ₂] ₂ [(OC) ₄ Fe ¹⁺ -Hg ¹⁺ -Fe(CO) ₄]. <i>Journal of Organometallic Chemistry</i> , 1989, 377, 291-303.	0.8	30
128	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
129	Ab Initio Study of the Intermolecular Interactions in the Hofmann Clathrates. <i>The Journal of Physical Chemistry</i> , 1995, 99, 2296-2306.	2.9	29
130	The [M ₂ (CO) ₈] Complexes of the Cobalt Group. <i>European Journal of Inorganic Chemistry</i> , 2001, 2001, 3031-3038.	1.0	29
131	Chemistry: A Panoply of Arrows. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 590-600.	7.2	29
132	Tailor-Made Strong Exchange Magnetic Coupling through Very Long Bridging Ligands: Theoretical Predictions. <i>Inorganic Chemistry</i> , 2003, 42, 4881-4884.	1.9	28
133	Jahn-Teller distortions of six-coordinate CuII compounds: cis or trans?. <i>Chemical Communications</i> , 2009, , 4242.	2.2	28
134	Electronic structure determination of iron(II) phthalocyanine via magnetic susceptibility and Mössbauer measurements. <i>Journal of Chemical Physics</i> , 1984, 80, 444-448.	1.2	26
135	The large range of chromium-chromium quadruple bond distances: structural and theoretical analysis. <i>Journal of the American Chemical Society</i> , 1990, 112, 8998-9000.	6.6	26
136	Pyramidal effect on rhodium(II)-Rh(II) single bonds. <i>Inorganic Chemistry</i> , 1993, 32, 3712-3719.	1.9	25
137	Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study. <i>Monatshefte für Chemie</i> , 2003, 134, 307-316.	0.9	25
138	Chalcogen-Chalcogen Bonds in Edge-Sharing Square-Planar d8 Complexes. Are They Possible?. <i>Inorganic Chemistry</i> , 2004, 43, 3702-3714.	1.9	25
139	Ligand Association/Dissociation Paths and Undefined Coordination Numbers. <i>Chemistry - A European Journal</i> , 2010, 16, 6567-6581.	1.7	25
140	Dihydrogen intermolecular contacts in group 13 compounds: H ^{δ+} -H or E ^{δ+} -H (E = B, Al, Ga) interactions?. <i>Dalton Transactions</i> , 2017, 46, 2844-2854.	1.6	25
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