Santiago Alvarez

List of Publications by Year
in descending order

290	23,195	11651 70	8630 146
papers	citations	h-index	g-index

309	309	309	15610
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Covalent radii revisited. Dalton Transactions, 2008, , 2832.	3.3	3,155
2	A cartography of the van der Waals territories. Dalton Transactions, 2013, 42, 8617.	3.3	1,117
3	Shape maps and polyhedral interconversion paths in transition metal chemistry. Coordination Chemistry Reviews, 2005, 249, 1693-1708.	18.8	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.	3.3	836
5	Toward the Prediction of Magnetic Coupling in Molecular Systems:â€‰ Hydroxo- and Alkoxo-Bridged Cu(II) Binuclear Complexes. Journal of the American Chemical Society, 1997, 119, 1297-1303.	13.7	816
6	The Rich Stereochemistry of Eight-Vertex Polyhedra: A Continuous Shape Measures Study. Chemistry - A European Journal, 2005, 11, 1479-1494.	3.3	729
7	Magnetic Coupling in End-On Azido-Bridged Transition Metal Complexes:Â A Density Functional Study. Journal of the American Chemical Society, 1998, 120, 11122-11129.	13.7	676
8	About the calculation of exchange coupling constants in polynuclear transition metal complexes. Journal of Computational Chemistry, 2003, 24, 982-989.	3.3	472
9	Continuous symmetry maps and shape classification. The case of six-coordinated metal compoundsElectronic supplementary information (ESI) available: tables of CSD refcodes, structural parameters and symmetry measures for the studied compounds. See http://www.rsc.org/suppdata/nj/b2/b202096n/. New Journal of Chemistry, 2002, 26, 996-1009.	2.8	388
10	Structural Modeling and Magnetoâ^'Structural Correlations for Hydroxo-Bridged Copper(II) Binuclear Complexes. Inorganic Chemistry, 1997, 36, 3683-3688.	4.0	386
11	Minimal Distortion Pathways in Polyhedral Rearrangements. Journal of the American Chemical Society, 2004, 126, 1755-1763.	13.7	362
12	Distortions in Octahedrally Coordinated d0Transition Metal Oxides:Â A Continuous Symmetry Measures Approach. Chemistry of Materials, 2006, 18, 3176-3183.	6.7	326
13	Exchange Coupling in Carboxylato-Bridged Dinuclear Copper(II) Compounds: A Density Functional Study. Chemistry - A European Journal, 2001, 7, 627-637.	3.3	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.	3.0	318
15	Polyhedral Structures with an Odd Number of Vertices: Nineâ€Coordinate Metal Compounds. Chemistry - A European Journal, 2008, 14, 1291-1303.	3.3	294
16	Coordinating ability of anions and solvents towards transition metals and lanthanides. Dalton Transactions, 2011, 40, 10742.	3.3	247
17	Dimerization and stacking in transition-metal bisdithiolenes and tetrathiolates. Journal of the American Chemical Society, 1985, 107, 6253-6277.	13.7	243
18	Dihydrogen contacts in alkanes are subtle but not faint. Nature Chemistry, 2011, 3, 323-330.	13.6	231

#	Article	IF	Citations
19	Shape and Symmetry of Heptacoordinate Transition-Metal Complexes: Structural Trends. Chemistry - A European Journal, 2003, 9, 1281-1295.	3.3	225
20	Can large magnetic anisotropy and high spin really coexist?. Chemical Communications, 2008, , 52-54.	4.1	215
21	Exchange Coupling of Transition-Metal Ions through Hydrogen Bonding:Â A Theoretical Investigation. Journal of the American Chemical Society, 2002, 124, 5197-5205.	13.7	202
22	Choice of Coordination Number in d10Complexes of Group 11 Metals. Journal of the American Chemical Society, 2004, 126, 1465-1477.	13.7	198
23	Exchange Coupling in Oxalato-Bridged Copper(II) Binuclear Compounds: A Density Functional Study. Chemistry - A European Journal, 1998, 4, 476-484.	3.3	197
24	Binuclear and polymeric gold(I) complexes. Inorganic Chemistry, 1985, 24, 749-757.	4.0	189
25	Spin Density Distribution in Transition Metal Complexes: Some Thoughts and Hints. Comments on Inorganic Chemistry, 1998, 20, 27-56.	5.2	187
26	Mapping the Stereochemistry and Symmetry of Tetracoordinate Transition-Metal Complexes. Chemistry - A European Journal, 2004, 10, 190-207.	3.3	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.	18.8	175
28	Influence of the Peripheral Ligand Atoms on the Exchange Interaction in Oxalato-Bridged Nickel(II) Complexes:Â An Orbital Model. Crystal Structures and Magnetic Properties of (H3dien)2[Ni2(ox)5]Â·12H2O and [Ni2(dien)2(H2O)2(ox)]Cl2. Inorganic Chemistry, 1996, 35, 3741-3751.	4.0	171
29	Distortion Pathways of Transition Metal Coordination Polyhedra Induced by Chelating Topology. Chemical Reviews, 2015, 115, 13447-13483.	47.7	166
30	Spin density distribution in transition metal complexes. Coordination Chemistry Reviews, 2005, 249, 2649-2660.	18.8	163
31	How to Build Molecules with Large Magnetic Anisotropy. Chemistry - A European Journal, 2009, 15, 4078-4087.	3.3	163
32	From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields. Chemical Reviews, 2016, 116, 8173-8192.	47.7	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.	13.7	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.	3.3	153
35	Magnetic Coupling in End-to-End Azido-Bridged Copper and Nickel Binuclear Complexes:Â A Theoretical Study. Inorganic Chemistry, 2000, 39, 3221-3229.	4.0	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.	18.8	148

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37	Oxalato-bridged and related dinuclear copper(II) complexes: theoretical analysis of their structures and magnetic coupling. Inorganic Chemistry, 1990, 29, 4500-4507.	4.0	146
38	Electronic structure and properties of AlN. Physical Review B, 1994, 49, 7115-7123.	3.2	146
39	Electronic structure and properties ofCu2O. Physical Review B, 1997, 56, 7189-7196.	3.2	146
40	Continuous symmetry measures of penta-coordinate molecules: Berry and non-Berry distortions of the trigonal bipyramidâ€Šâ€. Dalton Transactions RSC, 2000, , 3288-3303.	2.3	143
41	The Nature of Intermolecular Culâ‹…â‹…â‹…CuI Interactions: A Combined Theoretical and Structural Database Analysis. Chemistry - A European Journal, 2004, 10, 2117-2132.	3.3	139
42	Polyhedra in (inorganic) chemistry. Dalton Transactions, 2005, , 2209.	3.3	139
43	Is It Possible To Get HighTCMagnets with Prussian Blue Analogues? A Theoretical Prospect. Chemistry - A European Journal, 2005, 11, 2135-2144.	3.3	129
44	To Bend or Not To Bend:Â Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d8Transition Metal Ions. Inorganic Chemistry, 1998, 37, 804-813.	4.0	126
45	Continuous Shape Measures as a Stereochemical Tool in Organometallic Chemistry. Organometallics, 2005, 24, 1556-1562.	2.3	125
46	Importance of the X4 ring orbitals for the semiconducting, metallic, or superconducting properties of skutterudites MX3 and RM4X12. Inorganic Chemistry, 1990, 29, 2252-2255.	4.0	118
47	Exchange Coupling in Halo-Bridged Dinuclear Cu(II) Compounds:Â A Density Functional Study. Inorganic Chemistry, 2002, 41, 3769-3778.	4.0	118
48	Ligand Macrocycle Structural Effects on Copperâ^'Dioxygen Reactivity. Inorganic Chemistry, 2000, 39, 4059-4072.	4.0	116
49	Understanding the Nature of the CHÂ·Â·Â·HC Interactions in Alkanes. Journal of Chemical Theory and Computation, 2013, 9, 1977-1991.	5.3	112
50	Density functional study of magnetostructural correlations in cubane complexes containing the Cu4O4core. Journal of Materials Chemistry, 2006, 16, 2729-2735.	6.7	107
51	On the Bonding Nature of the M.cntdot. .cntdot. .cntdot.M Interactions in Dimers of Square-Planar Pt(II) and Rh(I) Complexes. Journal of the American Chemical Society, 1995, 117, 7169-7171.	13.7	103
52	Relationships between Temperature, Magnetic Moment, and Continuous Symmetry Measures in Spin Crossover Complexes. Journal of the American Chemical Society, 2003, 125, 6795-6802.	13.7	102
53	Stereochemistry of Compounds with Coordination Number Ten. Chemistry - A European Journal, 2009, 15, 7470-7480.	3.3	101
54	Continuous chirality measures in transition metal chemistry. Chemical Society Reviews, 2005, 34, 313.	38.1	98

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55	Magnetic Properties of Cyano-Bridged Ln3+â˜M3+Complexes. Part I:Â Trinuclear Complexes (Ln3+= La, Ce,) Tj ETQq1 1 0.784314 rgBT	4.0	93
56	Magnetostructural Correlations in Polynuclear Complexes:Â The Fe4Butterflies. Journal of the American Chemical Society, 2006, 128, 15722-15727.	13.7	93
57	Magnetic Structure of the Large-Spin Mn₁₀ and Mn₁₉ Complexes: A Theoretical Complement to an Experimental Milestone. Journal of the American Chemical Society, 2008, 130, 7420-7426.	13.7	93
58	Density functional study of the exchange coupling in distorted cubane complexes containing the Cu4O4 core. Polyhedron, 2001, 20, 1323-1327.	2.2	90
59	Stereochemistry and Spin State in Four-Coordinate Transition Metal Compounds. Inorganic Chemistry, 2008, 47, 2871-2889.	4.0	88
60	Exchange interaction through a croconato bridge: synthesis, crystal structure, and magnetic properties of (.mu.-croconato)bis[{bis(2-pyridylcarbonyl)amido}copper(II)] trihydrate. Inorganic Chemistry, 1992, 31, 1889-1894.	4.0	87
61	Magnetism of Cyano-Bridged Ln3+â˜M3+Complexes. Part II:Â One-Dimensional Complexes (Ln3+= Eu, Tb, Dy,) Tj ETQq1 1 0.784314	4.0	86
62	Axial Bonding Capabilities of Square Planar d8-ML4Complexes. Theoretical Study and Structural Correlations. Inorganic Chemistry, 1996, 35, 3137-3144.	4.0	84
63	[Cu3(Î¼-S)2]3+Clusters Supported by N-Donor Ligands:Â Progress Toward a Synthetic Model of the Catalytic Site of Nitrous Oxide Reductase. Journal of the American Chemical Society, 2005, 127, 13752-13753.	13.7	79
64	Theoretical Study of the Magnetic Behavior of Hexanuclear Cu(II) and Ni(II) Polysiloxanolato Complexes. Journal of the American Chemical Society, 2003, 125, 6791-6794.	13.7	77
65	A Bonding Quandaryâ€"orâ€"A Demonstration of the Fact That Scientists Are Not Born With Logic. Chemistry - A European Journal, 2009, 15, 8358-8373.	3.3	77
66	Synthesis, x-ray diffraction structure, magnetic properties, and MO analysis of a binuclear (.mu.-tetrathiooxalato)copper(II) complex, (AsPh4)2[(C3OS4)CuC2S4Cu(C3OS4)]. Inorganic Chemistry, 1987, 26, 4004-4009.	4.0	76
67	Oxidation states, atomic charges and orbital populations in transition metal complexes. Theoretical Chemistry Accounts, 2009, 123, 67-73.	1.4	76
68	Theoretical study of the electrical behavior of one-dimensional metallophthalocyanines and related metallomacrocyclic compounds. Inorganic Chemistry, 1984, 23, 573-579.	4.0	75
69	Electronic structure and bonding in skutterudite-type phosphides. Physical Review B, 1996, 53, 10605-10609.	3.2	74
70	Exchange Coupling in Cyano-Bridged Homodinuclear Cu(II) and Ni(II) Complexes:Â Synthesis, Structure, Magnetism, and Density Functional Theoretical Study. Inorganic Chemistry, 2001, 40, 5868-5877.	4.0	74
71	Bonding and stereochemistry of three-coordinated transition metal compounds. Coordination Chemistry Reviews, 1999, 193-195, 13-41.	18.8	70
72	Symmetry and Topology Determine the MoV-CN-MnIIExchange Interactions in High-Spin Molecules. Angewandte Chemie - International Edition, 2005, 44, 2711-2715.	13.8	69

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73	Coordinating Ability of Anions, Solvents, Amino Acids, and Gases towards Alkaline and Alkalineâ€Earth Elements, Transition Metals, and Lanthanides. Chemistry - A European Journal, 2020, 26, 4350-4377.	3.3	67
74	Edge-Sharing Binuclear d8 Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation. Chemistry - A European Journal, 1999, 5, 1391-1410.	3.3	65
75	The Trigonal Prism in Coordination Chemistry. Chemistry - A European Journal, 2010, 16, 10380-10396.	3.3	65
76	Chain Conformation and Metalâ€¦Metal Contacts in Dimers and Stacks of d⁸â€ML₄Complexes: Electronic Effects. Chemistry - A European Journal, 1997, 3, 655-664.	3.3	64
77	A New Class of (Î¼-Î·2:Î·2-Disulfido)dicopper Complexes:Â Synthesis, Characterization, and Disulfido Exchange. Inorganic Chemistry, 2004, 43, 3335-3337.	4.0	64
78	Polyhedral structures with an odd number of vertices: nine-atom clusters and supramolecular architectures. Dalton Transactions, 2008, , 2583.	3.3	64
79	Theoretical search for new ferromagnetically coupled transition metal complexes. Chemical Communications, 1998, , 2767-2768.	4.1	62
80	Theoretical study of the exchange coupling in copper(II) binuclear compounds with oxamidate and related polyatomic bridging ligandsâ€Šâ€. Journal of the Chemical Society Dalton Transactions, 1999, , 1669-1676.	1.1	61
81	Structure-NMR correlations in halo(ligand)bis(dioximato)cobalt(III) complexes. Inorganic Chemistry, 1986, 25, 2962-2969.	4.0	57
82	Electronic Structure and Magnetic Behavior in Polynuclear Transition-Metal Compounds. , 0, , 227-279.		55
83	A Family of Ferro- and Antiferromagnetically Coupled Decametallic Chromium(III) Wheels. Chemistry - A European Journal, 2006, 12, 1385-1396.	3.3	55
84	Symmetry operation measures. Journal of Computational Chemistry, 2008, 29, 190-197.	3.3	55
85	Structure and stability of the X3- systems (X = fluoride, chloride, bromide, iodide) and their interaction with cations. The Journal of Physical Chemistry, 1988, 92, 6561-6566.	2.9	54
86	How High the Spin? Allowed and Forbidden Spin States in Transition-Metal Chemistry. Angewandte Chemie - International Edition, 2006, 45, 3012-3020.	13.8	53
87	Bonding and structure in L4M2(.mu.-XRn)2 diamonds of tetrahedral d10 ions. Effect of substituents on the M- -M interaction. Inorganic Chemistry, 1992, 31, 4266-4275.	4.0	52
88	Through-ring bonding in edge-sharing dimers of square planar complexes. Journal of Organometallic Chemistry, 1994, 478, 75-82.	1.8	52
89	On the Existence of a Pyramidality Effect in d8Â·Â·Â·d8Contacts. Theoretical Study and Structural Correlation. Inorganic Chemistry, 1996, 35, 5061-5067.	4.0	50
90	Interconversion of Quadruply and Quintuply Bonded Molybdenum Complexes by Reductive Elimination and Oxidative Addition of Dihydrogen. Angewandte Chemie - International Edition, 2013, 52, 3227-3231.	13.8	49

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91	Further Theoretical Evidence for the Exceptionally Strong Ferromagnetic Coupling in Oxo-Bridged Cu(II) Dinuclear Complexes. Journal of Physical Chemistry A, 2002, 106, 4938-4941.	2.5	48
92	Reply to â€œComment on â€˜About the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction errorâ€™â€•[J. Chem. Phys. 123, 164110 (2005)]. Journal of Chemical Physics, 2006, 124, 107102.	3.0	47
93	van der Waals Radii of Noble Gases. Inorganic Chemistry, 2014, 53, 9260-9266.	4.0	46
94	Pyramidality and metal-metal multiple bonding: structural correlations and theoretical study. Journal of the American Chemical Society, 1993, 115, 6216-6229.	13.7	44
95	Room-Temperature Synthesis and Crystal, Magnetic, and Electronic Structure of the First Silver Copper Oxide. Inorganic Chemistry, 2002, 41, 6604-6613.	4.0	44
96	Quantitative Geometric Descriptions of the Belt Iron Atoms of the Ironâ€'Molybdenum Cofactor of Nitrogenase and Synthetic Iron(II) Model Complexes. Inorganic Chemistry, 2007, 46, 60-71.	4.0	44
97	Density Functional Study of Exchange Coupling Constants in Single-Molecule Magnets: The Fe8 Complex. Chemistry - A European Journal, 2005, 11, 4767-4771.	3.3	43
98	Molecules and crystals with both icosahedral and cubic symmetry. Chemical Communications, 2008, , 2717.	4.1	43
99	Crystal Orbital Displacement Analysis of Interactions in the Solid State. Application to the Study of Host-Guest Interactions in the Hofmann Clathrates. Journal of the American Chemical Society, 1994, 116, 8207-8221.	13.7	42
100	A novel bipyridine-based hexadentate tripodal framework with a strong preference for trigonal prismatic co-ordination geometries. Dalton Transactions, 2010, 39, 3870.	3.3	42
101	Asymmetry and Magnetism in Bis(oximato)-Bridged Heterobimetallic Compounds: A Computational Approach. Chemistry - A European Journal, 2000, 6, 327-333.	3.3	41
102	Theoretical study of exchange coupling constants in an Fe19 complex. Journal of Physics and Chemistry of Solids, 2004, 65, 799-803.	4.0	41
103	Theoretical Study of the Magnetic Properties of an Mn12 Single-Molecule Magnet with a Loop Structure:â€‰ The Role of the Next-Nearest Neighbor Interactions. Journal of Chemical Theory and Computation, 2007, 3, 782-788.	5.3	41
104	Chemistry of Unsaturated Group 6 Metal Complexes with Bridging Hydroxy and Methoxycarbyne Ligands. 1. Synthesis, Structure, and Bonding of 30-Electron Complexes. Organometallics, 2007, 26, 4930-4941.	2.3	40
105	Ligand orientation effects on metalâ€“metal, ligandâ€“ligand and metalâ€“ligand interactions. Coordination Chemistry Reviews, 1999, 185-186, 431-450.	18.8	39
106	Quantitative Chirality Analysis of Molecular Subunits of Bis(oxazoline)copper(II) Complexes in Relation to Their Enantioselective Catalytic Activity. Chemistry - A European Journal, 2003, 9, 5832-5837.	3.3	38
107	Square Fe2Au2 and triangular Fe2Au clusters: A reversible transformation. X-ray crystal structure of [Fe2Au2(CO)8(.mu.-dppm)] [dppm = bis(diphenylphosphino)methane]. Organometallics, 1991, 10, 2309-2314.	2.3	37
108	Dinuclear complexes of copper(II) derived from (1,3-propanediylbis(oxamato))cuprate(II): magneto-structural correlations. Inorganic Chemistry, 1991, 30, 841-845.	4.0	36

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109	Spin Densities in a Ferromagnetic Bimetallic Chain Compound:Â Polarized Neutron Diffraction and DFT Calculations. Journal of the American Chemical Society, 2002, 124, 14433-14441.	13.7	36
110	A Theoretical Study of the Exchange Coupling in Hydroxo- and Alkoxo-Bridged Dinuclear Oxovanadium(IV) Compounds. European Journal of Inorganic Chemistry, 2004, 2004, 143-153.	2.0	36
111	Chemistry of Unsaturated Group 6 Metal Complexes with Bridging Hydroxy- and Methoxycarbyne Ligands. 2. Synthesis, Structure, and Bonding of 32- and 34-Electron Complexes. Organometallics, 2007, 26, 5912-5921.	2.3	36
112	Electronic and Structural Effects of Low-Hapticity Coordination of Arene Rings to Transition Metals. Organometallics, 2014, 33, 6660-6668.	2.3	36
113	Ironâ^'Gold (or â^'Mercury) Carbide Clusters Derived from [Fe6C(CO)16]2-. X-ray Crystal Structures of (NEt4)[Fe6C{AuPPh3}(CO)16] and [Fe4C{AuPPh3}(CO)11(NO)]. Organometallics, 1997, 16, 236-245.	2.3	35
114	Framework Bonding and Coordination Sphere Rearrangement in the M2X2Cores of Synthetic Analogues of Oxyhemocyanin and Related Cu and Pt Complexes. Inorganic Chemistry, 1998, 37, 1202-1212.	4.0	35
115	Synthesis and study of trinuclear Pd(II) and Pt(II) complexes with 2-mercaptonicotinic acid. Polyhedron, 1999, 18, 3675-3682.	2.2	35
116	Early-late transition metal ferromagnetic coupling mediated by hydrogen bonding. Chemical Communications, 2002, , 2614-2615.	4.1	35
117	Hexabis(silyl)palladium(VI) or Palladium(II) with 1,2-Disilane Ligands? This work was supported by the DirecciÃ³n General de EnseÃ±anza Superior (DGES), grant PB98-1166-C02-01, and the Comissionat per a Universitats i Recerca (Generalitat de Catalunya), grant SGR99-0046. Computing resources at the Centre de SupercomputaciÃ³ de Catalunya (CESCA) and Centre de Paralâ‹…lelisme de Barcelona (CEPBA) were made available by the ComissiÃ³ Interdepartamental per a la Recerca i la InnovaciÃ³ TecnolÃ²gica (CIRIT) and the Universitat Autònoma de Barcelona. International Edition, 2002, 41, 1956.	13.8	35
118	New organometallic cobaloximes containing an equatorial diphenylglyoximato(â^'1) ligand. Comparison between their properties and those of other B12 model compounds. Crystal structure of trans-[Co(dpgH)2(CH3)(pyridine)]. Journal of Organometallic Chemistry, 1991, 414, 245-259.	1.8	34
119	The electronic structure of barium gallium antimonide (Ba7Ga4Sb9): a compound seemingly probing the limits of the Zintl concept. Inorganic Chemistry, 1990, 29, 3070-3073.	4.0	33
120	Calibrating the coordination chemistry tool chest: metrics of bi- and tridentate ligands. Dalton Transactions, 2009, , 6610.	3.3	33
121	Experimental and Theoretical Studies on Areneâ€Bridged Metalâ€“Metalâ€Bonded Dimolybdenum Complexes. Chemistry - A European Journal, 2014, 20, 6092-6102.	3.3	33
122	Evaluating transition state structures of vanadiumâ€“phosphatase protein complexes using shape analysis. Journal of Inorganic Biochemistry, 2015, 147, 153-164.	3.5	33
123	Intermolecular interactions in group 14 hydrides: Beyond Cï£¿HÂ·Â·Â·Hï£¿C contacts. International Journal of Quantum Chemistry, 2017, 117, e25432.	2.0	32
124	Synthesis and structure of chloro(ligand)bis(diphenylglyoximato)cobalt(III) complexes. Inorganica Chimica Acta, 1987, 127, 153-159.	2.4	31
125	Through-Ring Bonding in Edge Sharing Dimers of Octahedral Complexes. Inorganic Chemistry, 2000, 39, 3166-3175.	4.0	31
126	Mercurophilic interactions: a theoretical study on the importance of ligands. Physical Chemistry Chemical Physics, 2017, 19, 11645-11654.	2.8	31

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127	Anionic trimetallic compounds containing Feî—¸Eî—¸M skeletons (E = Zn, Cd, Hg; M = Fe, Mo, W). Crystal structure of [N(PPh3)2]2[(OC)4Feî—¸Hgî—¸Fe(CO)4]. Journal of Organometallic Chemistry, 1989, 377, 291-303.	1.8	30
128	Six-fold Oxygen-Coordinated Triplet (S= 1) Palladium(II) Moieties Templated by Tris(bipyridine)ruthenium(II) Ions. Journal of the American Chemical Society, 2007, 129, 1327-1334.	13.7	30
129	Ab Initio Study of the Intermolecular Interactions in the Hofmann Clathrates. The Journal of Physical Chemistry, 1995, 99, 2296-2306.	2.9	29
130	The [M2(CO)8] Complexes of the Cobalt Group. European Journal of Inorganic Chemistry, 2001, 2001, 3031-3038.	2.0	29
131	Chemistry: A Panoply of Arrows. Angewandte Chemie - International Edition, 2012, 51, 590-600.	13.8	29
132	Tailor-Made Strong Exchange Magnetic Coupling through Very Long Bridging Ligands:â€‰ Theoretical Predictions. Inorganic Chemistry, 2003, 42, 4881-4884.	4.0	28
133	Jahnâ€“Teller distortions of six-coordinate CuII compounds: cis or trans?. Chemical Communications, 2009, , 4242.	4.1	28
134	Electronic structure determination of iron(II) phthalocyanine via magnetic susceptibility and MÃ¶ssbauer measurements. Journal of Chemical Physics, 1984, 80, 444-448.	3.0	26
135	The large range of chromium-chromium quadruple bond distances: structural and theoretical analysis. Journal of the American Chemical Society, 1990, 112, 8998-9000.	13.7	26
136	Pyramidality effect on rhodium(II)-Rh(II) single bonds. Inorganic Chemistry, 1993, 32, 3712-3719.	4.0	25
137	Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study. Monatshefte FÃ¼r Chemie, 2003, 134, 307-316.	1.8	25
138	Chalcogenâ‹¯Chalcogen Bonds in Edge-Sharing Square-Planar d8 Complexes. Are They Possible?. Inorganic Chemistry, 2004, 43, 3702-3714.	4.0	25
139	Ligand Association/Dissociation Paths and Illâ€Defined Coordination Numbers. Chemistry - A European Journal, 2010, 16, 6567-6581.	3.3	25
140	Dihydrogen intermolecular contacts in group 13 compounds: Hâ‹¯H or Eâ‹¯H (E = B, Al, Ga) interactions?. Dalton Transactions, 2017, 46, 2844-2854.	3.3	25
141	C-N stretching force constants in cyano complexes: General trends for polycyano, mixed-ligand and cyano-bridged complexes. Transition Metal Chemistry, 1984, 9, 123-126.	1.4	24
142	Reaction chemistry, NMR spectroscopy, and X-ray crystallography of [Fe2(Î¼-SiMe2)2(CO)4] and [Fe2(Î¼-SiMeCl)2(CO)4]. Electronic structure and bonding in Fe2E2 rings of [Fe2(Î¼-ER2)2(CO)4] binuclear complexes (E=C, Si, Ge, Sn, Pb). Journal of Organometallic Chemistry, 2001, 628, 241-254.	1.8	24
143	Continuous chirality analysis of hexacoordinated tris-chelated metal complexes. Crystal Engineering, 2001, 4, 179-200.	0.7	24
144	Exchange Coupling in Metal Complexes of the Second Transition Series: A Theoretical Exploration. European Journal of Inorganic Chemistry, 2003, 2003, 1756-1760.	2.0	24

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145	Application of Symmetry Operation Measures in Structural Inorganic Chemistry. Inorganic Chemistry, 2008, 47, 10965-10970.	4.0	24
146	Mixed valency in binuclear cyano-bridged manganese bis(carbonyl) complexes and stereochemical control of their oxidation. A molecular orbital study. Inorganic Chemistry, 1993, 32, 272-276.	4.0	23
147	Theoretical determination of the exchange coupling constants of a single-molecule magnet Fe10 complex. Chemical Physics Letters, 2005, 415, 6-9.	2.6	23
148	Theoretical study of the exchange coupling in a Ni12 single-molecule magnet. Dalton Transactions, 2006, , 2643.	3.3	23
149	Mapping the Ultrafast Changes of Continuous Shape Measures in Photoexcited Spin Crossover Complexes without Long-Range Order. Journal of Physical Chemistry C, 2015, 119, 3322-3330.	3.1	23
150	The influence of equatorial bulky substituents on the properties of organometallic bis(dioximato)cobalt(III) compounds. Structural comparison between trans-[Co(dpgH)2(R)(L)] complexes [dpgH = diphenylglyoximato(â^'1)] and other B12 models. Polyhedron, 1992, 11, 1637-1646.	2.2	22
151	Electronic band structure of the magnetic layered semiconductors MPS3 (M = Mn, Fe and Ni). Journal of Physics and Chemistry of Solids, 1996, 57, 647-652.	4.0	22
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