Santiago Alvarez

List of Publications by Year in Descending Order

291 papers	20,007 citations	67 h-index	135 g-index
309 ext. papers	21,474 ext. citations	6.7 avg, IF	6.98 L-index

#	Paper	IF	Citations
291	From polygons to polyhedra through intermediate structures. A shape measures study of six-atom inorganic rings and clusters. *Dalton Transactions*, **2021**, 50, 17101-17119	4.3	1
290	Supported Complexes of Li-C Bonds from Coordination of Monomeric Molecules of LiCH3, LiCH2CH3 and LiC6H5 to MoMo Bonds.. *Angewandte Chemie - International Edition*, **2021**, e202116009	16.4	2
289	Experimental and Computational Studies on Quadruply Bonded Dimolybdenum Complexes with Terminal and Bridging Hydride Ligands. *Chemistry - A European Journal*, **2021**, 27, 6569-6578	4.8	3
288	Coordination of LiH Molecules to Mo?Mo Bonds: Experimental and Computational Studies on MoLiH, MoLiH, and MoLiH Clusters. *Journal of the American Chemical Society*, **2021**, 143, 5222-5230	16.4	2
287	Delocalized Bonding in LiX Rings: Probing the Limits of the Covalent and Ionic Bonding Models. *Inorganic Chemistry*, **2021**, 60, 345-356	5.1	2
286	Continuous Shape Measures Study of the Coordination Spheres of Actinide Complexes Part 1: Low Coordination Numbers. *European Journal of Inorganic Chemistry*, **2021**, 2021, 3632-3647	2.3	0
285	The transition from 4f to 5d elements from the structural point of view. *CrystEngComm*, **2020**, 22, 7229-7232	3.3	2
284	Coordinating Ability of Anions, Solvents, Amino Acids, and Gases towards Alkaline and Alkaline-Earth Elements, Transition Metals, and Lanthanides. *Chemistry - A European Journal*, **2020**, 26, 4350-4377	4.8	38
283	Understanding the Interplay of Dispersion, Charge Transfer, and Electrostatics in Noncovalent Interactions: The Case of Bromine Carbonyl Short Contacts. *Crystal Growth and Design*, **2020**, 20, 7180-7187	3.5	9
282	Effect of the Substituents on the Nature and Strength of Lone-Pair Carbonyl Interactions in Acyl Halides. *Crystal Growth and Design*, **2019**, 19, 6511-6518	3.5	6
281	Das Periodensystem eine universelle Ikone: seine Entstehung vor 150 Jahren und seine Verbreitung durch Literatur, Kunst und Musik. *Angewandte Chemie*, **2019**, 131, 13328-13341	3.6	2
280	The Periodic-Table-A Universal Icon: Its Birth 150 Years Ago, and Its Popularization Through Literature Art and Music. *Angewandte Chemie - International Edition*, **2019**, 58, 13194-13206	16.4	6
279	Marvellous molecular shapes. *Comptes Rendus Chimie*, **2019**, 22, 437-444	2.7	1
278	Taming a monomeric [Cu(CH)] complex with silylene. *Chemical Science*, **2018**, 9, 4333-4337	9.4	17
277	Shapes of undecanuclear clusters and undecacoordinated metal complexes§§ Dedicated to Prof. Juan Faus.View all notes. *Journal of Coordination Chemistry*, **2018**, 71, 590-600	1.6	2
276	Zero- and mono-coordinate transition metals in crystal structures: A box full of surprises. *Inorganica Chimica Acta*, **2018**, 470, 74-81	2.7	4
275	Dihydrogen intermolecular contacts in group 13 compounds: HH or EH (E = B, Al, Ga) interactions?. *Dalton Transactions*, **2017**, 46, 2844-2854	4.3	21

274	Mercurophilic interactions: a theoretical study on the importance of ligands. *Physical Chemistry Chemical Physics*, **2017**, 19, 11645-11654	3.6	25
273	Zinc-Zinc Double Bonds: A Theoretical Study. *Angewandte Chemie - International Edition*, **2017**, 56, 10151-10155	11.6	58
272	Continuous Symmetry Measures: A New Tool in Quantum Chemistry. *Reviews in Computational Chemistry*, **2017**, 289-352		11
271	The gyrobifastigium, not an uncommon shape in chemistry. *Coordination Chemistry Reviews*, **2017**, 350, 3-13	23.2	3
270	Intermolecular interactions in group 14 hydrides: Beyond C?H⋯H?C contacts. *International Journal of Quantum Chemistry*, **2017**, 117, e25432	2.1	23
269	Zinc□zinc Double Bonds: A Theoretical Study. *Angewandte Chemie*, **2017**, 129, 10285-10289	3.6	0
268	An Unsaturated Four-Coordinate Dimethyl Dimolybdenum Complex with a Molybdenum-Molybdenum Quadruple Bond. *Chemistry - A European Journal*, **2017**, 23, 194-205	4.8	8
267	Size and shape trump charge in interactions of oxovanadates with self-assembled interfaces: application of continuous shape measure analysis to the decavanadate anion. *New Journal of Chemistry*, **2016**, 40, 962-975	3.6	14
266	From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields. *Chemical Reviews*, **2016**, 116, 8173-92	68.1	94
265	Unsymmetrical Chelation of N-Thioether-Functionalized Bis(diphenylphosphino)amine-Type Ligands and Substituent Effects on the Nuclearity of Iron(II) Complexes: Structures, Magnetism, and Bonding. *Inorganic Chemistry*, **2015**, 54, 6547-59	5.1	14
264	Evaluating transition state structures of vanadium-phosphatase protein complexes using shape analysis. *Journal of Inorganic Biochemistry*, **2015**, 147, 153-64	4.2	26
263	Distortion Pathways of Transition Metal Coordination Polyhedra Induced by Chelating Topology. *Chemical Reviews*, **2015**, 115, 13447-83	68.1	114
262	Cr-Cr Quintuple Bonds: Ligand Topology and Interplay Between Metal-Metal and Metal-Ligand Bonding. *Inorganic Chemistry*, **2015**, 54, 10966-77	5.1	19
261	Design of a structural database for homoleptic transition metal complexes. *Structural Chemistry*, **2015**, 26, 1715-1723	1.8	1
260	Experimental and computational studies of the molybdenum-flanking arene interaction in quadruply bonded dimolybdenum complexes with terphenyl ligands. *Chemistry - A European Journal*, **2015**, 21, 410-21	4.8	11
259	Spin state behavior of iron(II)/dipyrazolylpyridine complexes. New insights from crystallographic and solution measurements. *Coordination Chemistry Reviews*, **2015**, 289-290, 2-12	23.2	148
258	Comparison of the Cr□Cr Quadruple and Quintuple Bonding Mechanisms. *Structure and Bonding*, **2015**, 249-264	0.9	
257	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	3.8	22

256	Reply to 'entropic factors also contribute to the high melting points of polyhedral alkanes'. *Nature Chemistry*, **2015**, 7, 89-90	17.6	
255	Experimental and theoretical studies on arene-bridged metal-metal-bonded dimolybdenum complexes. *Chemistry - A European Journal*, **2014**, 20, 6092-102	4.8	29
254	Electronic and Structural Effects of Low-Hapticity Coordination of Arene Rings to Transition Metals. *Organometallics*, **2014**, 33, 6660-6668	3.8	31
253	van der Waals radii of noble gases. *Inorganic Chemistry*, **2014**, 53, 9260-6	5.1	34
252	Distortions of η-coordinated arenes with anionic character. *Chemistry - A European Journal*, **2014**, 20, 14674-89	4.8	14
251	Modulation der Koordinationssphäre von f-Element-Komplexen durch Fluorkohlenwasserstoffe. *Angewandte Chemie*, **2014**, 126, 2852-2853	3.6	
250	Stereochemistry of complexes with double and triple metal-ligand bonds: a continuous shape measures analysis. *Inorganic Chemistry*, **2014**, 53, 12151-63	5.1	16
249	Fluorocarbons modulate the coordination sphere of f-element complexes. *Angewandte Chemie - International Edition*, **2014**, 53, 2810-1	16.4	6
248	Pseudosymmetry analysis of molecular orbitals. *Journal of Computational Chemistry*, **2013**, 34, 1321-31	3.5	7
247	Pseudo-symmetry analysis of the d-block molecular orbitals in four-coordinate complexes. *Inorganic Chemistry*, **2013**, 52, 6510-9	5.1	8
246	Interconversion of Quadruply and Quintuply Bonded Molybdenum Complexes by Reductive Elimination and Oxidative Addition of Dihydrogen. *Angewandte Chemie*, **2013**, 125, 3309-3313	3.6	22
245	Interconversion of quadruply and quintuply bonded molybdenum complexes by reductive elimination and oxidative addition of dihydrogen. *Angewandte Chemie - International Edition*, **2013**, 52, 3227-31	16.4	45
244	Stereospinomers of pentacoordinate iron porphyrin complexes: the case of the [Fe(porphyrinato)(CN)]- anions. *Dalton Transactions*, **2013**, 42, 7002-8	4.3	7
243	Understanding the Nature of the CH···HC Interactions in Alkanes. *Journal of Chemical Theory and Computation*, **2013**, 9, 1977-91	6.4	90
242	A cartography of the van der Waals territories. *Dalton Transactions*, **2013**, 42, 8617-36	4.3	838
241	Chemistry: a panoply of arrows. *Angewandte Chemie - International Edition*, **2012**, 51, 590-600	16.4	23
240	Self-Assembly of Coordination Compounds: Design Principles **2012**,		1
239	Continuous symmetry measures of irreducible representations: application to molecular orbitals. *Physical Chemistry Chemical Physics*, **2012**, 14, 11816-23	3.6	9

238	Chemie: ein Kcher voller Pfeile. *Angewandte Chemie*, **2012**, 124, 610-621	3.6	8
237	The structural diversity triggered by intermolecular interactions between Au(I)S2 groups: aurophilia and beyond. *Chemistry - A European Journal*, **2012**, 18, 9965-76	4.8	22
236	Theoretical study of exchange coupling in 3d-Gd complexes: large magnetocaloric effect systems. *Journal of the American Chemical Society*, **2012**, 134, 10532-42	16.4	144
235	Coordinating ability of anions and solvents towards transition metals and lanthanides. *Dalton Transactions*, **2011**, 40, 10742-50	4.3	206
234	Dihydrogen contacts in alkanes are subtle but not faint. *Nature Chemistry*, **2011**, 3, 323-30	17.6	199
233	Concurrent symmetries: the interplay between local and global molecular symmetries. *Chemistry - A European Journal*, **2011**, 17, 359-67	4.8	14
232	A novel bipyridine-based hexadentate tripodal framework with a strong preference for trigonal prismatic co-ordination geometries. *Dalton Transactions*, **2010**, 39, 3870-83	4.3	36
231	Symmetry measures of the electron density. *Journal of Computational Chemistry*, **2010**, 31, 2389-404	3.5	17
230	Ligand association/dissociation paths and ill-defined coordination numbers. *Chemistry - A European Journal*, **2010**, 16, 6567-81	4.8	22
229	The trigonal prism in coordination chemistry. *Chemistry - A European Journal*, **2010**, 16, 10380-96	4.8	52
228	Antiferromagnetism or delocalized spin in a Cu3S2 core?. *Chemistry - A European Journal*, **2010**, 16, 2726-38	4.8	12
227	How icosahedral are icosahedral clusters?. *Inorganica Chimica Acta*, **2010**, 363, 4392-4398	2.7	6
226	Structural and electronic effects on the exchange interactions in dinuclear bis(phenoxo)-bridged copper(II) complexes. *Coordination Chemistry Reviews*, **2010**, 254, 2086-2095	23.2	142
225	New perspectives on polyhedral molecules and their crystal structures. *Journal of Physical Organic Chemistry*, **2010**, 23, 1080-1087	2.1	9
224	X-X through-cage bonding in Cu, Ni, and Cr complexes with M3X2 cores (X=S, As). *Chemistry - A European Journal*, **2009**, 15, 536-46	4.8	14
223	How to build molecules with large magnetic anisotropy. *Chemistry - A European Journal*, **2009**, 15, 4078-87	4.8	139
222	A bonding quandary--or--a demonstration of the fact that scientists are not born with logic. *Chemistry - A European Journal*, **2009**, 15, 8358-73	4.8	68
221	Stereochemistry of compounds with coordination number ten. *Chemistry - A European Journal*, **2009**, 15, 7470-80	4.8	92

220	Reactivity of a Super-Electron-Rich Olefin Derived from Cyclam. *European Journal of Inorganic Chemistry*, **2009**, 2009, 1851-1860	2.3	20
219	Oxidation states, atomic charges and orbital populations in transition metal complexes. *Theoretical Chemistry Accounts*, **2009**, 123, 67-73	1.9	66
218	Substitution of chloride by nitrosyl ligand in a scorpionate ruthenium(III) compound: A theoretical study. *Inorganica Chimica Acta*, **2009**, 362, 4651-4658	2.7	2
217	Calibrating the coordination chemistry tool chest: metrics of bi- and tridentate ligands. *Dalton Transactions*, **2009**, 6610-25	4.3	27
216	Jahn-Teller distortions of six-coordinate CuII compounds: cis or trans?. *Chemical Communications*, **2009**, 4242-4	5.8	25
215	A New Titanium Alkoxide□Thiolate Complex as a Versatile Heterofunctional Metalloligand. *European Journal of Inorganic Chemistry*, **2009**, 2009, 1079-1085	2.3	10
214	Polyhedral structures with an odd number of vertices: nine-atom clusters and supramolecular architectures. *Dalton Transactions*, **2008**, 2583-91	4.3	52
213	Application of symmetry operation measures in structural inorganic chemistry. *Inorganic Chemistry*, **2008**, 47, 10965-70	5.1	20
212	Music of the elements. *New Journal of Chemistry*, **2008**, 32, 571	3.6	6
211	Molecules and crystals with both icosahedral and cubic symmetry. *Chemical Communications*, **2008**, 2717-25	5.8	39
210	Ligands that enforce unnatural stereospinomers. *Dalton Transactions*, **2008**, 2235-7	4.3	
209	Can large magnetic anisotropy and high spin really coexist?. *Chemical Communications*, **2008**, 52-4	5.8	184
208	Stereochemistry and spin state in four-coordinate transition metal compounds. *Inorganic Chemistry*, **2008**, 47, 2871-89	5.1	82
207	Electrochemical behavior of copper complexes with substituted polypyridinic ligands: an experimental and theoretical study. *Inorganic Chemistry*, **2008**, 47, 3687-92	5.1	16
206	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, 7420-6	16.4	90
205	On books and chemical elements. *Foundations of Chemistry*, **2008**, 10, 79-100	0.7	19
204	Polyhedral structures with an odd number of vertices: nine-coordinate metal compounds. *Chemistry - A European Journal*, **2008**, 14, 1291-303	4.8	245
203	Symmetry operation measures. *Journal of Computational Chemistry*, **2008**, 29, 190-7	3.5	50

202	Exchange interactions in a Fe5 complex: A theoretical study using density functional theory. *Inorganica Chimica Acta*, **2008**, 361, 3832-3835	2.7	5
201	Covalent radii revisited. *Dalton Transactions*, **2008**, 2832-8	4.3	2540
200	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	3.8	36
199	Quantitative geometric descriptions of the belt iron atoms of the iron-molybdenum cofactor of nitrogenase and synthetic iron(II) model complexes. *Inorganic Chemistry*, **2007**, 46, 60-71	5.1	40
198	Reply to Comment on Distortions in Octahedrally Coordinated d0 Transition Metal Oxides: A Continuous Symmetry Measures Approach *Chemistry of Materials*, **2007**, 19, 1200-1200	9.6	
197	Chelating dialkoxide titanium complex: a versatile building block for the construction of heterometallic derivatives. *Chemistry - A European Journal*, **2007**, 13, 2831-6	4.8	6
196	Theoretical study of the exchange coupling interactions in a polyoxometalate Fe9W12 complex. *Polyhedron*, **2007**, 26, 2161-2164	2.7	5
195	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	3.8	39
194	On the existence of molecular palladium(VI) compounds: palladium hexafluoride. *Inorganic Chemistry*, **2007**, 46, 2700-3	5.1	13
193	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, 1327-34	16.4	29
192	Theoretical Study of the Magnetic Properties of an Mn12 Single-Molecule Magnet with a Loop Structure: The Role of the Next-Nearest Neighbor Interactions. *Journal of Chemical Theory and Computation*, **2007**, 3, 782-8	6.4	41
191	Strong Antiferromagnetic Coupling at Long Distance through a Ligand to Metal Charge Transfer Mechanism. *Journal of Physical Chemistry C*, **2007**, 111, 618-621	3.8	19
190	The nature of the AuI ... AuI Interactions between Cationic [AuL2]+ Complexes in the Solid State. *Theoretical Chemistry Accounts*, **2006**, 116, 472-479	1.9	11
189	A family of ferro- and antiferromagnetically coupled decametallic chromium(III) wheels. *Chemistry - A European Journal*, **2006**, 12, 1385-96	4.8	50
188	Shape and spin state in four-coordinate transition-metal complexes: the case of the d(6) configuration. *Chemistry - A European Journal*, **2006**, 12, 3162-7	4.8	131
187	How high the spin? Allowed and forbidden spin states in transition-metal chemistry. *Angewandte Chemie - International Edition*, **2006**, 45, 3012-20	16.4	42
186	Polyhedral interconversion coupled with proton transfer between an ammonium cation and the [Co(CO)4]- ion. *Angewandte Chemie - International Edition*, **2006**, 45, 1457-60	16.4	17
185	To Bend or not To Bend? Both! The Planar and Bent Structures of[(Ph3P)4Rh2(F)2]. *European Journal of Inorganic Chemistry*, **2006**, 2006, 3340-3345	2.3	13

184	Hoch oder niedrig? Zur Erlaubtheit von Spinzust□den in der □bergangsmetallchemie. *Angewandte Chemie*, **2006**, 118, 3078-3087	3.6	19
183	Polyhedral Interconversion Coupled with Proton Transfer between an Ammonium Cation and the [Co(CO)4]□ion. *Angewandte Chemie*, **2006**, 118, 1485-1488	3.6	7
182	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)]. *Journal of Chemical Physics*, **2006**, 124, 107102	3.9	44
181	Density functional study of magnetostructural correlations in cubane complexes containing the Cu4O4 core. *Journal of Materials Chemistry*, **2006**, 16, 2729-2735		100
180	Nesting of fullerenes and Frank-Kasper polyhedra. *Dalton Transactions*, **2006**, 2045-51	4.3	16
179	Distortions in Octahedrally Coordinated d0 Transition Metal Oxides: A Continuous Symmetry Measures Approach. *Chemistry of Materials*, **2006**, 18, 3176-3183	9.6	278
178	Effects of tris(pyrazolyl)borato ligand substituents on dioxygen activation and stabilization by copper compounds. *Inorganic Chemistry*, **2006**, 45, 3594-601	5.1	15
177	Magnetostructural correlations in polynuclear complexes: the Fe4 butterflies. *Journal of the American Chemical Society*, **2006**, 128, 15722-7	16.4	88
176	Magnetic communication through functionalized nanotubes: a theoretical study. *Nano Letters*, **2006** , 6, 380-4	11.5	15
175	Theoretical study of the exchange coupling in a Ni12 single-molecule magnet. *Dalton Transactions*, **2006**, 2643-6	4.3	21
174	Shape and Symmetry Measures as Tools for the Solid State. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2006**, 632, 2073-2073	1.3	
173	Theoretical study of the electronic properties and exchange coupling in a Ni4 cubane like single-molecule magnet. *Physica B: Condensed Matter*, **2006**, 384, 123-125	2.8	8
172	Exchange coupling interactions in a Fe6 complex: A theoretical study using density functional theory. *Physica B: Condensed Matter*, **2006**, 384, 116-119	2.8	7
171	Bonding and solvation preferences of nickel complexes [Ni(S2PR2)2] (R=H, Me, OMe) according a natural bond orbital analysis. *Computational and Theoretical Chemistry*, **2006**, 767, 37-41		12
170	[Cu3(mu-S)2]3+ clusters supported by N-donor ligands: progress toward a synthetic model of the catalytic site of nitrous oxide reductase. *Journal of the American Chemical Society*, **2005**, 127, 13752-3	16.4	76
169	Polyhedra in (inorganic) chemistry. *Dalton Transactions*, **2005**, 2209-33	4.3	113
168	Exchange coupling in mu-aqua:mu-oxo vs. di-mu-hydroxo dinuclear Cu(II) compounds: a density functional study. *Dalton Transactions*, **2005**, 2624-9	4.3	18
167	A pyrimidine thiolate Rh(I) complex: structure, bonding and one-dimensional interactions in solid and in solution. *Dalton Transactions*, **2005**, 938-44	4.3	5

166	Continuous Shape Measures as a Stereochemical Tool in Organometallic Chemistry. *Organometallics*, **2005**, 24, 1556-1562	3.8	99
165	Magnetism of cyano-bridged Ln3+-M3+ complexes. Part II: one-dimensional complexes (Ln3+ = Eu, Tb, Dy, Ho, Er, Tm; M3+ = Fe or Co) with bpy as blocking ligand. *Inorganic Chemistry*, **2005**, 44, 6949-58	5.1	83
164	Magnetic properties of cyano-bridged Ln3+-M3+ complexes. Part I: trinuclear complexes (Ln3+ = La, Ce, Pr, Nd, Sm; M3+ = FeLS, Co) with bpy as blocking ligand. *Inorganic Chemistry*, **2005**, 44, 6939-48	5.1	91
163	Continuous chirality measures in transition metal chemistry. *Chemical Society Reviews*, **2005**, 34, 313-26	58.5	81
162	An Fe11 complex showing single-molecule magnet behavior: Theoretical study using density functional methods and Monte Carlo simulations. *Polyhedron*, **2005**, 24, 2364-2367	2.7	8
161	Shape maps and polyhedral interconversion paths in transition metal chemistry. *Coordination Chemistry Reviews*, **2005**, 249, 1693-1708	23.2	727
160	Spin density distribution in transition metal complexes. *Coordination Chemistry Reviews*, **2005**, 249, 2649-2660	23.2	153
159	Theoretical determination of the exchange coupling constants of a single-molecule magnet Fe10 complex. *Chemical Physics Letters*, **2005**, 415, 6-9	2.5	21
158	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	3.9	299
157	Theoretical study of the magnetic behavior of ferric wheels. *ChemPhysChem*, **2005**, 6, 1094-9	3.2	18
156	Symmetry and topology determine the MoV-CN-MnII exchange interactions in high-spin molecules. *Angewandte Chemie - International Edition*, **2005**, 44, 2711-2715	16.4	65
155	Symmetry and Topology Determine the MoV□CN□MnII Exchange Interactions in High-Spin Molecules. *Angewandte Chemie*, **2005**, 117, 2771-2775	3.6	15
154	The rich stereochemistry of eight-vertex polyhedra: a continuous shape measures study. *Chemistry - A European Journal*, **2005**, 11, 1479-94	4.8	540
153	Is it possible to get high T(C) magnets with Prussian blue analogues? A theoretical prospect. *Chemistry - A European Journal*, **2005**, 11, 2135-44	4.8	123
152	Density functional study of exchange coupling constants in single-molecule magnets: the Fe8 complex. *Chemistry - A European Journal*, **2005**, 11, 4767-71	4.8	42
151	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	2.3	34
150	Formation of Sulfur□Sulfur Bonds in Copper Complexes. *European Journal of Inorganic Chemistry*, **2004**, 2004, 4430-4438	2.3	12
149	Mapping the stereochemistry and symmetry of tetracoordinate transition-metal complexes. *Chemistry - A European Journal*, **2004**, 10, 190-207	4.8	152

148	The nature of intermolecular CuI...CuI interactions: a combined theoretical and structural database analysis. *Chemistry - A European Journal*, **2004**, 10, 2117-32	4.8	130
147	Theoretical study of exchange coupling constants in an Fe19 complex. *Journal of Physics and Chemistry of Solids*, **2004**, 65, 799-803	3.9	41
146	Minimal distortion pathways in polyhedral rearrangements. *Journal of the American Chemical Society*, **2004**, 126, 1755-63	16.4	294
145	Chalcogen-chalcogen bonds in edge-sharing square-planar d8 complexes. Are they possible?. *Inorganic Chemistry*, **2004**, 43, 3702-14	5.1	24
144	A new class of (mu-eta2:eta2-disulfido)dicopper complexes: synthesis, characterization, and disulfido exchange. *Inorganic Chemistry*, **2004**, 43, 3335-7	5.1	63
143	Choice of coordination number in d10 complexes of group 11 metals. *Journal of the American Chemical Society*, **2004**, 126, 1465-77	16.4	184
142	Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study. *Monatshefte F□ Chemie*, **2003**, 134, 307-316	1.4	25
141	About the calculation of exchange coupling constants in polynuclear transition metal complexes. *Journal of Computational Chemistry*, **2003**, 24, 982-9	3.5	442
140	Exchange Coupling in Metal Complexes of the Second Transition Series: A Theoretical Exploration. *European Journal of Inorganic Chemistry*, **2003**, 2003, 1756-1760	2.3	21
139	Room-Temperature Synthesis and Crystal, Magnetic, and Electronic Structure of the First Silver Copper Oxide.. *ChemInform*, **2003**, 34, no		1
138	Theoretical evidence of persistent chirality in D3 homoleptic hexacoordinate complexes with monodentate ligands. *Chemistry - A European Journal*, **2003**, 9, 1952-7	4.8	11
137	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, 5832-7	4.8	37
136	Shape and symmetry of heptacoordinate transition-metal complexes: structural trends. *Chemistry - A European Journal*, **2003**, 9, 1281-95	4.8	183
135	Theoretical study of the magnetic behavior of hexanuclear Cu(II) and Ni(II) polysiloxanolato complexes. *Journal of the American Chemical Society*, **2003**, 125, 6791-4	16.4	75
134	A novel hexanuclear mixed oxidation state Cu(II)(4)Cu(I)(2) cluster complex exhibiting weak ferromagnetic exchange. *Inorganic Chemistry*, **2003**, 42, 1107-11	5.1	18
133	Tailor-made strong exchange magnetic coupling through very long bridging ligands: theoretical predictions. *Inorganic Chemistry*, **2003**, 42, 4881-4	5.1	27
132	Continuous chirality measures of tetracoordinate bis(chelate) metal complexes. *Dalton Transactions*, **2003**, 562-569	4.3	17
131	Relationships between temperature, magnetic moment, and continuous symmetry measures in spin crossover complexes. *Journal of the American Chemical Society*, **2003**, 125, 6795-802	16.4	89

130	Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study **2003**, 191-200		
129	Hexakis(silyl)palladium(VI) or Palladium(II) with □2-Disilane Ligands?. *Angewandte Chemie*, **2002**, 114, 2036	3.6	9
128	Theoretical clues to the mechanism of dioxygen formation at the oxygen-evolving complex of photosystem II. *Chemistry - A European Journal*, **2002**, 8, 2508-15	4.8	21
127	Hexakis(silyl)palladium(VI) or Palladium(II) with □2-Disilane Ligands? This work was supported by the Direcci□ General de Ense□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 Supercomputaci□ de Catalunya (CESCA) and Centre de Paral?lelisme de Barcelona	16.4	31
126	Ligand effects and dimer formation in dicoordinated copper(I) complexes. *International Journal of Quantum Chemistry*, **2002**, 86, 100-105 wandte Chemie - International Edition, **2002**, 41, 1956	2.1	12
125	Exchange coupling of transition-metal ions through hydrogen bonding: a theoretical investigation. *Journal of the American Chemical Society*, **2002**, 124, 5197-205	16.4	190
124	Spin densities in a ferromagnetic bimetallic chain compound: polarized neutron diffraction and DFT calculations. *Journal of the American Chemical Society*, **2002**, 124, 14433-41	16.4	34
123	Exchange coupling in halo-bridged dinuclear Cu(II) compounds: a density functional study. *Inorganic Chemistry*, **2002**, 41, 3769-78	5.1	114
122	Molecular Structure and Isomerization in Square-Planar Edge-Sharing Dinuclear Complexes with Alkynyl Bridges. *Organometallics*, **2002**, 21, 2627-2634	3.8	20
121	Continuous symmetry maps and shape classification. The case of six-coordinated metal compounds. *New Journal of Chemistry*, **2002**, 26, 996-1009	3.6	330
120	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	2.8	47
119	Room-temperature synthesis and crystal, magnetic, and electronic structure of the first silver copper oxide. *Inorganic Chemistry*, **2002**, 41, 6604-13	5.1	41
118	Early-late transition metal ferromagnetic coupling mediated by hydrogen bonding. *Chemical Communications*, **2002**, 2614-5	5.8	35
117	Structure and bonding in late transition metal dinuclear complexes with local trigonal planar geometries. *Dalton Transactions RSC*, **2002**, 2235-2243		8
116	Density functional study of the exchange coupling in distorted cubane complexes containing the Cu4O4 core. *Polyhedron*, **2001**, 20, 1323-1327	2.7	87
115	Reaction chemistry, NMR spectroscopy, and X-ray crystallography of [Fe2(□SiMe2)2(CO)4] and [Fe2(□SiMeCl)2(CO)4]. Electronic structure and bonding in Fe2E2 rings of [Fe2(□ER2)2(CO)4] binuclear complexes (E=C, Si, Ge, Sn, Pb). *Journal of Organometallic Chemistry*, **2001**, 628, 241-254	2.3	21
114	Continuous chirality analysis of hexacoordinated tris-chelated metal complexes. *Crystal Engineering* , **2001**, 4, 179-200		21
113	A Continuous Chirality Analysis of Homoleptic Hexacoordinated Complexes. *European Journal of Inorganic Chemistry*, **2001**, 2001, 1499-1503	2.3	16

112	The [M2(CO)8] Complexes of the Cobalt Group. *European Journal of Inorganic Chemistry*, **2001**, 2001, 3031-3038	2.3	27
111	Exchange coupling in carboxylato-bridged dinuclear copper(II) compounds: a density functional study. *Chemistry - A European Journal*, **2001**, 7, 627-37	4.8	315
110	Molecular structures of edge-sharing square-planar dinuclear complexes with unsaturated bridges. *Inorganic Chemistry*, **2001**, 40, 4937-46	5.1	7
109	Exchange coupling in cyano-bridged homodinuclear Cu(II) and Ni(II) complexes: synthesis, structure, magnetism, and density functional theoretical study. *Inorganic Chemistry*, **2001**, 40, 5868-77	5.1	72
108	Theoretical Study of Bonding, Structure, and Vibrational Spectra of the [Fe2(CO)8]2- Anion and Its Derivatives *Organometallics*, **2001**, 20, 818-826	3.8	9
107	Asymmetry and magnetism in bis(oximato)-bridged heterobimetallic compounds: a computational approach. *Chemistry - A European Journal*, **2000**, 6, 327-33	4.8	39
106	Theoretical approach to the magnetostructural correlations in the spin-Peierls compound CuGeO3. *Physical Review B*, **2000**, 61, 54-57	3.3	15
105	Magnetic coupling in end-to-end azido-bridged copper and nickel binuclear complexes: a theoretical study. *Inorganic Chemistry*, **2000**, 39, 3221-9	5.1	140
104	Continuous symmetry measures of penta-coordinate molecules: Berry and non-Berry distortions of the trigonal bipyramid. *Dalton Transactions RSC*, **2000**, 3288-3303		115
103	Theoretical study of the guest?guest interactions of cobaltocene intercalated in metal sulfides. *Dalton Transactions RSC*, **2000**, 1463-1467		5
102	The coloring problem in Ba2Cu3VS6. *Dalton Transactions RSC*, **2000**, 1009-1011		
101	Through-ring bonding in edge sharing dimers of octahedral complexes. *Inorganic Chemistry*, **2000**, 39, 3166-75	5.1	26
100	Structural correlations and conformational preference in edge-sharing binuclear d8 complexes with XR2 bridges. A theoretical study. *Inorganic Chemistry*, **2000**, 39, 906-16	5.1	14
99	Ligand macrocycle structural effects on copper-dioxygen reactivity. *Inorganic Chemistry*, **2000**, 39, 4059-72	5.1	98
98	Synthesis and study of trinuclear Pd(II) and Pt(II) complexes with 2-mercaptonicotinic acid. *Polyhedron*, **1999**, 18, 3675-3682	2.7	33
97	Ligand orientation effects on metal metal, ligand ligand and metal ligand interactions. *Coordination Chemistry Reviews*, **1999**, 185-186, 431-450	23.2	34
96	Bonding and stereochemistry of three-coordinated transition metal compounds. *Coordination Chemistry Reviews*, **1999**, 193-195, 13-41	23.2	64
95	Broken symmetry approach to calculation of exchange coupling constants for homobinuclear and heterobinuclear transition metal complexes **1999**, 20, 1391-1400		779

94	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	4.8	63
93	Theoretical study of the exchange coupling in copper(II) binuclear compounds with oxamidate and related polyatomic bridging ligands *Journal of the Chemical Society Dalton Transactions*, **1999**, 1669-1676		57
92	Electronic Structure and Bonding in Tricoordinate Amido Complexes of Transition Metals. *Inorganic Chemistry*, **1999**, 38, 707-715	5.1	15
91	Edge-Sharing Binuclear d8 Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation **1999**, 5, 1391		1
90	Theoretical search for new ferromagnetically coupled transition metal complexes. *Chemical Communications*, **1998**, 2767-2768	5.8	61
89	Exchange Coupling in Oxalato-Bridged Copper(II) Binuclear Compounds: A Density Functional Study. *Chemistry - A European Journal*, **1998**, 4, 476-484	4.8	185
88	Spin Density Distribution in Transition Metal Complexes: Some Thoughts and Hints. *Comments on Inorganic Chemistry*, **1998**, 20, 27-56	3.9	180
87	Theoretical study of the intercalation of cobaltocene in metal chalcogenides. *Journal of Materials Chemistry*, **1998**, 8, 1893-1900		4
86	Skutterudite vs. ReO3 structures for MX3 solids: electronic requirements *Journal of the Chemical Society Dalton Transactions*, **1998**, 1195-1200		7
85	Framework Bonding and Coordination Sphere Rearrangement in the M(2)X(2) Cores of Synthetic Analogues of Oxyhemocyanin and Related Cu and Pt Complexes. *Inorganic Chemistry*, **1998**, 37, 1202-1212	5.1	30
84	Electronic Structure of Host Lattices for Intercalation Compounds: SnS2, SnSe2, ZrS2, and TaS2. *Chemistry of Materials*, **1998**, 10, 3422-3428	9.6	18
83	Magnetic Coupling in End-On Azido-Bridged Transition Metal Complexes: A Density Functional Study. *Journal of the American Chemical Society*, **1998**, 120, 11122-11129	16.4	633
82	To Bend or Not To Bend: Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d8 Transition Metal Ions. *Inorganic Chemistry*, **1998**, 37, 804-813	5.1	117
81	Pyramidality effect on metal metal single bonds. *Journal of the Chemical Society Dalton Transactions*, **1997**, 2681-2688		3
80	M(2)L(6) Complexes with Triple Mo-Mo and W-W Bonds: Molecular Topology and Inverted Pyramidality Effect. *Inorganic Chemistry*, **1997**, 36, 1055-1060	5.1	9
79	Iron Gold (or 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	3.8	28
78	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	16.4	773
77	Electronic structure and properties of Cu2O. *Physical Review B*, **1997**, 56, 7189-7196	3.3	131

76	Structural Modeling and Magneto-Structural Correlations for Hydroxo-Bridged Copper(II) Binuclear Complexes. *Inorganic Chemistry*, **1997**, 36, 3683-3688	5.1	364
75	Chain Conformation and Metal□Metal Contacts in Dimers and Stacks of d8-ML4 Complexes: Electronic Effects. *Chemistry - A European Journal*, **1997**, 3, 655-664	4.8	55
74	Electronic Structure, Bonding, and Electrical Properties of MoNiP8□*Inorganic Chemistry*, **1996**, 35, 4683-4689	5.1	4
73	Axial Bonding Capabilities of Square Planar d(8)-ML(4) Complexes. Theoretical Study and Structural Correlations. *Inorganic Chemistry*, **1996**, 35, 3137-3144	5.1	78
72	Structure of the non-polar (101 0) surfaces of AlN and □SiC: a periodic Hartree-Fock study. *Surface Science*, **1996**, 355, 167-176	1.8	10
71	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 (H(3)dien)(2)[Ni(2)(ox)(5)].12H(2)O and [Ni(2)(dien)(2)(H(2)O)(2)(ox)]Cl(2). *Inorganic Chemistry*, **1996**, 35, 3741-3751	5.1	151
70	On the Existence of a Pyramidality Effect in d(8).d(8) Contacts. Theoretical Study and Structural Correlation. *Inorganic Chemistry*, **1996**, 35, 5061-5067	5.1	36
69	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	3.9	20
68	Anhydrous trans-(Aniline)chlorobis(dimethylglyoximato)cobalt(III). *Acta Crystallographica Section C: Crystal Structure Communications*, **1996**, 52, 63-66		2
67	Electronic structure and bonding in skutterudite-type phosphides. *Physical Review B*, **1996**, 53, 10605-10609	3.9	64
66	Ab initio study of AlN and alpha -SiC (112-bar0) surface relaxation. *Physical Review B*, **1996**, 53, 4933-4938	3.3	7
65	Intercalation of Halogen Molecules in Alkali Fluoride Lattices: A Theoretical Study. *Journal of the American Chemical Society*, **1995**, 117, 2877-2883	16.4	2
64	Host.cntdot..cntdot..cntdot.Guest Interactions in the Pyrrole and Aniline Hofmann Clathrates. A Theoretical Study. *Inorganic Chemistry*, **1995**, 34, 3260-3269	5.1	17
63	Theoretical Study of Host.cntdot..cntdot..cntdot.Guest Interactions in Clathrates with a Cd(CN)2 Host. *Inorganic Chemistry*, **1995**, 34, 5845-5851	5.1	9
62	Electronic Structure, Chemical Bonding, and Jahn-Teller Distortions in CdPS3. *Inorganic Chemistry*, **1995**, 34, 1159-1163	5.1	16
61	Ab Initio Study of the Intermolecular Interactions in the Hofmann Clathrates. *The Journal of Physical Chemistry*, **1995**, 99, 2296-2306		17
60	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	16.4	87
59	Heterodox Bonding Effects between Transition Metal Atoms **1995**, 241-255		7

58	Electronic structure and properties of AlN. *Physical Review B*, **1994**, 49, 7115-7123	3.3	123
57	Electronic structure and properties of hexagonal wurtzite-type SiC. *International Journal of Quantum Chemistry*, **1994**, 52, 365-373	2.1	5
56	Through-ring bonding in edge-sharing dimers of square planar complexes. *Journal of Organometallic Chemistry*, **1994**, 478, 75-82	2.3	49
55	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	16.4	32
54	(PPh4)[Mn3(CO)12(.mu.3-H)(.mu.-Hg{Mo(CO)3(.eta.5-C5H5)})]: The First Example of a Mercury-Containing Planar Triangulated Rhomboidal Metal Cluster. *Organometallics*, **1994**, 13, 2205-2212	3.8	9
53	Pyramidality effect on rhodium(II)-Rh(II) single bonds. *Inorganic Chemistry*, **1993**, 32, 3712-3719	5.1	21
52	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	5.1	15
51	Ca0.95Nb3O6: Crystal and Electronic Structure. *Journal of Solid State Chemistry*, **1993**, 105, 27-35	3.3	8
50	Pyramidality and metal-metal multiple bonding: structural correlations and theoretical study. *Journal of the American Chemical Society*, **1993**, 115, 6216-6229	16.4	38
49	Electronic structure, bonding, and properties of copper phosphide, CuP2. *Inorganic Chemistry*, **1992**, 31, 119-124	5.1	9
48	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	5.1	69
47	Theoretical study of bonding and electrical conductivity in compounds with the NbAs2 structure. *Inorganic Chemistry*, **1992**, 31, 3007-3010	5.1	7
46	Symmetry guidelines for the design of convergent syntheses. On narcissistic coupling and la coupe du roi. *Journal of the American Chemical Society*, **1992**, 114, 2623-2630	16.4	7
45	Unprecedented trimetallic cluster with an in-plane .mu.3-hydride ligand. X-ray crystal structure of [Mo2(CO)8(.mu.-dppm)(.mu.3-H)(.mu.-AuPPh3)]. *Organometallics*, **1992**, 11, 3753-3759	3.8	13
44	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	5.1	48
43	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(1-)] and other B12 models. *Polyhedron*, **1992**, 11, 1637-1646	2.7	21
42	Electronic structure calculations and X-ray emission spectra of some metal phosphides. *Solid State Communications*, **1992**, 83, 447-450	1.6	1
41	New organometallic cobaloximes containing an equatorial diphenylglyoximato(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	2.3	29

40	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	3.8	30
39	Electronic structure of a (cyclopentadienyl)tri-.mu.-oxoditechnetium polymer with a very short metal-metal bond. *Inorganic Chemistry*, **1991**, 30, 1086-1093	5.1	14
38	Dinuclear complexes of copper(II) derived from (1,3-propanediylbis(oxamato))cuprate(II): magneto-structural correlations. *Inorganic Chemistry*, **1991**, 30, 841-845	5.1	33
37	The large range of chromium-chromium quadruple bond distances: structural and theoretical analysis. *Journal of the American Chemical Society*, **1990**, 112, 8998-9000	16.4	21
36	Magnetic exchange interactions in one-dimensional copper(II) compounds. *Chemistry of Materials*, **1990**, 2, 723-728	9.6	5
35	The electronic structure of barium gallium antimonide (Ba7Ga4Sb9): a compound seemingly probing the limits of the Zintl concept. *Inorganic Chemistry*, **1990**, 29, 3070-3073	5.1	29
34	Oxalato-bridged and related dinuclear copper(II) complexes: theoretical analysis of their structures and magnetic coupling. *Inorganic Chemistry*, **1990**, 29, 4500-4507	5.1	131
33	Importance of the X4 ring orbitals for the semiconducting, metallic, or superconducting properties of skutterudites MX3 and RM4X12. *Inorganic Chemistry*, **1990**, 29, 2252-2255	5.1	108
32	Anionic trimetallic compounds containing Fe?E?M skeletons (E = Zn, Cd, Hg; M = Fe, Mo, W). Crystal structure of [N(PPh3)2]2[(OC)4Fe?Hg?Fe(CO)4]. *Journal of Organometallic Chemistry*, **1989**, 377, 291-303	2.3	23
31	Cis and trans effects and NMR correlations in organometallic cobaloximes. *Journal of Organometallic Chemistry*, **1988**, 342, C13-C14	2.3	6
30	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		48
29	Importance of metal-metal interactions through the phosphorus-phosphorus bonds for the multidimensional electrical properties of MP4 (M = vanadium, chromium, molybdenum). *Inorganic Chemistry*, **1988**, 27, 2702-2706	5.1	9
28	Structure and stability of tetraatomic bromine and ion, Br4 and Br42-, and their interaction with cations and transition metals. *Journal of the American Chemical Society*, **1987**, 109, 6586-6591	16.4	14
27	The fluxional behavior of monocoordinated diimines and azines. *Journal of the American Chemical Society*, **1987**, 109, 5316-5323	16.4	17
26	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	5.1	66
25	Synthesis and structure of chloro(ligand)bis(diphenylglyoximato)cobalt(III) complexes. *Inorganica Chimica Acta*, **1987**, 127, 153-159	2.7	28
24	Improved synthesis of dicyanocobaloximes and the molecular and crystal structure of potassium dicyanobis(dimethylglyoximato)cobaltate(III). *Inorganica Chimica Acta*, **1987**, 133, 101-105	2.7	4
23	The mechanism of electrical conductivity along polyhalide chains. *Chemical Physics Letters*, **1986**, 132, 531-534	2.5	12

22	Structural, NMR and theoretical study of delocalization in cobaloximes. *Inorganica Chimica Acta*, **1986**, 111, L19-L21	2.7	17
21	Synthesis, characterization and study of the Pt?Pt interaction in cis-[(aa)(bb)FCr?NC?Pt(CN)3] (aa, bb=bidentate amine). *Inorganica Chimica Acta*, **1986**, 121, 13-17	2.7	3
20	Synthesis and structure of chloro(ligand)bis(glyoximato)cobalt(III) complexes: structural evidence of an electronic effect on the structure of the dimethylpyrazine ligand. *Inorganica Chimica Acta*, **1986**, 121, 71-75	2.7	14
19	Synthesis and characterization of new di- and tri-nuclear cyano-bridged bis(dioximato)cobalt(III) complexes. *Transition Metal Chemistry*, **1986**, 11, 16-19	2.1	6
18	Structure-NMR correlations in halo(ligand)bis(dioximato)cobalt(III) complexes. *Inorganic Chemistry*, **1986**, 25, 2962-2969	5.1	52
17	Vibrational spectra and normal coordinate analysis of two isotopomers of the thiosulfate ion. *Journal of Molecular Structure*, **1985**, 130, 235-243	3.4	3
16	Dimerization and stacking in transition-metal bisdithiolenes and tetrathiolates. *Journal of the American Chemical Society*, **1985**, 107, 6253-6277	16.4	213
15	Binuclear and polymeric gold(I) complexes. *Inorganic Chemistry*, **1985**, 24, 749-757	5.1	161
14	Electronic structure determination of iron(II) phthalocyanine via magnetic susceptibility and Mössbauer measurements. *Journal of Chemical Physics*, **1984**, 80, 444-448	3.9	24
13	Binuclear nickel–cobalt cyano-bridged complexes showing long-range proton shielding. *Inorganica Chimica Acta*, **1984**, 82, L23-L26	2.7	3
12	Symmetry constraints to the electrical conductivity of partially oxidized stacks of metal bis(dioximates). *Solid State Communications*, **1984**, 50, 141-144	1.6	8
11	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	2.1	23
10	Theoretical study of the electrical behavior of one-dimensional metallophthalocyanines and related metallomacrocyclic compounds. *Inorganic Chemistry*, **1984**, 23, 573-579	5.1	70
9	General quadratic force field of the sulfate ion and the relationships between different force fields in tetrahedral molecules. *Computational and Theoretical Chemistry*, **1984**, 106, 293-300		2
8	Mössbauer studies on one-dimensional iron phthalocyanines. *Transition Metal Chemistry*, **1983**, 8, 377-380	2.1	5
7	Axial substitution and bridge formation by the cyano group in bis(dimethylglyoximato)cobalt(III) complexes. *Inorganica Chimica Acta*, **1982**, 63, 57-62	2.7	13
6	Linkage isomerism in cyanoaquobis(dimethyl-glyoximato)cobalt(III). *Inorganica Chimica Acta*, **1982**, 64, L99-L100	2.7	14
5	C-N stretching force constants in cyano complexes. *Transition Metal Chemistry*, **1982**, 7, 116-118	2.1	5

4	Binuclear complexes of Fe(III) and Cr(III) with bridging cyano ligand. *Inorganica Chimica Acta*, **1976**, 16, L15-L16	2.7	1
3	Electronic Structure and Magnetic Behavior in Polynuclear Transition-Metal Compounds227-279		51
2	Ligand Orientation Effects on Metal-Metal Bonding308-322		2
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