

# Santiago Alvarez

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4606648/publications.pdf>

Version: 2024-02-01

290  
papers

23,195  
citations

11651

70  
h-index

8630

146  
g-index

309  
all docs

309  
docs citations

309  
times ranked

15610  
citing authors

#	ARTICLE	IF	CITATIONS
1	Supported $\sigma$ -Complexes of $\text{Li}^+\text{C}$ Bonds from Coordination of Monomeric Molecules of $\text{LiCH}_3$ , $\text{LiCH}_2\text{CH}_3$ and $\text{LiC}_6\text{H}_5$ to $\text{Mo}^{\text{VI}}$ Mo Bonds. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	0
2	Tetramethylammonium Cation: Directionality and Covalency in Its Interactions with Halide Ions. <i>Inorganic Chemistry</i> , 2022, 61, 9082-9095.	4.0	8
3	Coordination of $\text{E}^{\text{II}}\text{C}$ Bonds (E = Zn, Mg, Al) and the $\text{Zn}^{\text{II}}\text{H}$ Bonds of $(\text{C}_5\text{Me}_5)\text{ZnH}$ and $(\text{C}_5\text{Me}_5)_2\text{ZnH}$ across a Quadruply Bonded Dimolybdenum Dihydride Complex. <i>Organometallics</i> , 2022, 41, 3225-3236.	2.3	3
4	Delocalized Bonding in $\text{Li}_2\text{X}_2$ Rings: Probing the Limits of the Covalent and Ionic Bonding Models. <i>Inorganic Chemistry</i> , 2021, 60, 345-356.	4.0	2
5	Experimental and Computational Studies on Quadruply Bonded Dimolybdenum Complexes with Terminal and Bridging Hydride Ligands. <i>Chemistry - A European Journal</i> , 2021, 27, 6569-6578.	3.3	6
6	Coordination of $\text{LiH}$ Molecules to $\text{Mo}^{\text{VI}}$ Mo Bonds: Experimental and Computational Studies on $\text{Mo}_2\text{LiH}_2$ , $\text{Mo}_2\text{Li}_2\text{H}_4$ , and $\text{Mo}_6\text{Li}_9\text{H}_{18}$ Clusters. <i>Journal of the American Chemical Society</i> , 2021, 143, 5222-5230.	13.7	7
7	Continuous Shape Measures Study of the Coordination Spheres of Actinide Complexes – Part 1: Low Coordination Numbers. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3632-3647.	2.0	5
8	From polygons to polyhedra through intermediate structures. A shape measures study of six-atom inorganic rings and clusters. <i>Dalton Transactions</i> , 2021, 50, 17101-17119.	3.3	8
9	Supported $\sigma$ -Complexes of $\text{Li}^+\text{C}$ Bonds from Coordination of Monomeric Molecules of $\text{LiCH}_3$ , $\text{LiCH}_2\text{CH}_3$ and $\text{LiC}_6\text{H}_5$ to $\text{Mo}^{\text{VI}}$ Mo Bonds. <i>Angewandte Chemie - International Edition</i> , 2021, , e202116009.	13.8	8
10	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.	3.3	67
11	Understanding the Interplay of Dispersion, Charge Transfer, and Electrostatics in Noncovalent Interactions: The Case of Bromine-Carbonyl Short Contacts. <i>Crystal Growth and Design</i> , 2020, 20, 7180-7187.	3.0	16
12	The transition from 4f to 5d elements from the structural point of view. <i>CrystEngComm</i> , 2020, 22, 7229-7232.	2.6	4
13	Effect of the Substituents on the Nature and Strength of Lone-Pair-Carbonyl Interactions in Acyl Halides. <i>Crystal Growth and Design</i> , 2019, 19, 6511-6518.	3.0	10
14	Das Periodensystem – eine universelle Ikone: seine Entstehung vor 150 Jahren und seine Verbreitung durch Literatur, Kunst und Musik. <i>Angewandte Chemie</i> , 2019, 131, 13328-13341.	2.0	2
15	The Periodic Table – A Universal Icon: Its Birth 150 Years Ago, and Its Popularization Through Literature Art and Music. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 13194-13206.	13.8	10
16	Marvellous molecular shapes. <i>Comptes Rendus Chimie</i> , 2019, 22, 437-444.	0.5	3
17	Taming a monomeric $[\text{Cu}^{\text{I}}\text{C}_6\text{H}_6]^+$ complex with silylene. <i>Chemical Science</i> , 2018, 9, 4333-4337.	7.4	19
18	Shapes of undecanuclear clusters and undecacoordinated metal complexes. <i>Journal of Coordination Chemistry</i> , 2018, 71, 590-600.	2.2	2

#	ARTICLE	IF	CITATIONS
19	Zero- and mono-coordinate transition metals in crystal structures: A box full of surprises. <i>Inorganica Chimica Acta</i> , 2018, 470, 74-81.	2.4	4
20	Dihydrogen intermolecular contacts in group 13 compounds: H $\cdots$ H or E $\cdots$ H (E = B, Al, Ga) interactions?. <i>Dalton Transactions</i> , 2017, 46, 2844-2854.	3.3	25
21	Mercurophilic interactions: a theoretical study on the importance of ligands. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 11645-11654.	2.8	31
22	Zinc $\cdots$ Zinc Double Bonds: A Theoretical Study. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 10151-10155.	13.8	11
23	The gyrobifastigium, not an uncommon shape in chemistry. <i>Coordination Chemistry Reviews</i> , 2017, 350, 3-13.	18.8	7
24	Intermolecular interactions in group 14 hydrides: Beyond C $\cdots$ H $\cdots$ H $\cdots$ C contacts. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25432.	2.0	32
25	Zinc $\cdots$ Zinc Double Bonds: A Theoretical Study. <i>Angewandte Chemie</i> , 2017, 129, 10285-10289.	2.0	5
26	An Unsaturated Four $\cdots$ Coordinate Dimethyl Dimolybdenum Complex with a Molybdenum $\cdots$ Molybdenum Quadruple Bond. <i>Chemistry - A European Journal</i> , 2017, 23, 194-205.	3.3	10
27	From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields. <i>Chemical Reviews</i> , 2016, 116, 8173-8192.	47.7	155
28	Size and shape trump charge in interactions of oxovanadates with self-assembled interfaces: application of continuous shape measure analysis to the decavanadate anion. <i>New Journal of Chemistry</i> , 2016, 40, 962-975.	2.8	18
29	Comparison of the Cr $\cdots$ Cr Quadruple and Quintuple Bonding Mechanisms. <i>Structure and Bonding</i> , 2015, , 249-264.	1.0	0
30	Mapping the Ultrafast Changes of Continuous Shape Measures in Photoexcited Spin Crossover Complexes without Long-Range Order. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3322-3330.	3.1	23
31	Reply to 'Entropic factors also contribute to the high melting points of polyhedral alkanes'. <i>Nature Chemistry</i> , 2015, 7, 89-90.	13.6	0
32	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. <i>Inorganic Chemistry</i> , 2015, 54, 6547-6559.	4.0	14
33	Evaluating transition state structures of vanadium $\cdots$ phosphatase protein complexes using shape analysis. <i>Journal of Inorganic Biochemistry</i> , 2015, 147, 153-164.	3.5	33
34	Distortion Pathways of Transition Metal Coordination Polyhedra Induced by Chelating Topology. <i>Chemical Reviews</i> , 2015, 115, 13447-13483.	47.7	166
35	Cr $\cdots$ Cr Quintuple Bonds: Ligand Topology and Interplay Between Metal $\cdots$ Metal and Metal $\cdots$ Ligand Bonding. <i>Inorganic Chemistry</i> , 2015, 54, 10966-10977.	4.0	22
36	Design of a structural database for homoleptic transition metal complexes. <i>Structural Chemistry</i> , 2015, 26, 1715-1723.	2.0	3

#	ARTICLE	IF	CITATIONS
37	Experimental and Computational Studies of the Molybdenum-Flanking Arene Interaction in Quadruply Bonded Dimolybdenum Complexes with Terphenyl Ligands. <i>Chemistry - A European Journal</i> , 2015, 21, 410-421.	3.3	13
38	Spin state behavior of iron(II)/dipyrazolylpyridine complexes. New insights from crystallographic and solution measurements. <i>Coordination Chemistry Reviews</i> , 2015, 289-290, 2-12.	18.8	175
39	Stereochemistry of Complexes with Double and Triple Metal-Ligand Bonds: A Continuous Shape Measures Analysis. <i>Inorganic Chemistry</i> , 2014, 53, 12151-12163.	4.0	17
40	Fluorocarbons Modulate the Coordination Sphere of f-Element Complexes. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 2810-2811.	13.8	7
41	Experimental and Theoretical Studies on Arene-Bridged Metal-Metal-Bonded Dimolybdenum Complexes. <i>Chemistry - A European Journal</i> , 2014, 20, 6092-6102.	3.3	33
42	Electronic and Structural Effects of Low-Hapticity Coordination of Arene Rings to Transition Metals. <i>Organometallics</i> , 2014, 33, 6660-6668.	2.3	36
43	van der Waals Radii of Noble Gases. <i>Inorganic Chemistry</i> , 2014, 53, 9260-9266.	4.0	46
44	Distortions of $\pi$ -Coordinated Arenes with Anionic Character. <i>Chemistry - A European Journal</i> , 2014, 20, 14674-14689.	3.3	16
45	Pseudosymmetry analysis of molecular orbitals. <i>Journal of Computational Chemistry</i> , 2013, 34, 1321-1331.	3.3	7
46	Pseudo-symmetry Analysis of the d-block Molecular Orbitals in Four-Coordinate Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 6510-6519.	4.0	8
47	Interconversion of Quadruply and Quintuply Bonded Molybdenum Complexes by Reductive Elimination and Oxidative Addition of Dihydrogen. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 3227-3231.	13.8	49
48	Stereospinomers of pentacoordinate iron porphyrin complexes: the case of the $[\text{Fe}(\text{porphyrinato})(\text{CN})]^{-}$ anions. <i>Dalton Transactions</i> , 2013, 42, 7002.	3.3	12
49	Understanding the Nature of the $\text{CH}\cdots\text{HC}$ Interactions in Alkanes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1977-1991.	5.3	112
50	A cartography of the van der Waals territories. <i>Dalton Transactions</i> , 2013, 42, 8617.	3.3	1,117
51	Volume Editor's Introduction. , 2013, , xxxvii-xlii.		0
52	Continuous symmetry measures of irreducible representations: application to molecular orbitals. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11816.	2.8	10
53	The Structural Diversity Triggered by Intermolecular Interactions between $\text{Au}^{\text{I}}$ $\text{S}_2$ Groups: Aurophilia and Beyond. <i>Chemistry - A European Journal</i> , 2012, 18, 9965-9976.	3.3	22
54	Theoretical Study of Exchange Coupling in 3d-Gd Complexes: Large Magnetocaloric Effect Systems. <i>Journal of the American Chemical Society</i> , 2012, 134, 10532-10542.	13.7	154

#	ARTICLE	IF	CITATIONS
55	Chemistry: A Panoply of Arrows. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 590-600.	13.8	29
56	Coordinating ability of anions and solvents towards transition metals and lanthanides. <i>Dalton Transactions</i> , 2011, 40, 10742.	3.3	247
57	Dihydrogen contacts in alkanes are subtle but not faint. <i>Nature Chemistry</i> , 2011, 3, 323-330.	13.6	231
58	Concurrent Symmetries: The Interplay Between Local and Global Molecular Symmetries. <i>Chemistry - A European Journal</i> , 2011, 17, 359-367.	3.3	14
59	Symmetry measures of the electron density. <i>Journal of Computational Chemistry</i> , 2010, 31, 2389-2404.	3.3	19
60	Ligand Association/Dissociation Paths and Ill-Defined Coordination Numbers. <i>Chemistry - A European Journal</i> , 2010, 16, 6567-6581.	3.3	25
61	The Trigonal Prism in Coordination Chemistry. <i>Chemistry - A European Journal</i> , 2010, 16, 10380-10396.	3.3	65
62	Antiferromagnetism or Delocalized Spin in a $\text{Cu}_3\text{S}_2$ Core?. <i>Chemistry - A European Journal</i> , 2010, 16, 2726-2728.	3.3	12
63	How icosahedral are icosahedral clusters?. <i>Inorganica Chimica Acta</i> , 2010, 363, 4392-4398.	2.4	8
64	Structural and electronic effects on the exchange interactions in dinuclear bis(phenoxo)-bridged copper(II) complexes. <i>Coordination Chemistry Reviews</i> , 2010, 254, 2086-2095.	18.8	148
65	New perspectives on polyhedral molecules and their crystal structures. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 1080-1087.	1.9	9
66	A novel bipyridine-based hexadentate tripodal framework with a strong preference for trigonal prismatic co-ordination geometries. <i>Dalton Transactions</i> , 2010, 39, 3870.	3.3	42
67	$\text{Xi}_2\text{X}$ Through Cage Bonding in Cu, Ni, and Cr Complexes with $\text{M}_3\text{X}_2$ Cores (X=S, As). <i>Chemistry - A European Journal</i> , 2009, 15, 536-546.	3.3	15
68	How to Build Molecules with Large Magnetic Anisotropy. <i>Chemistry - A European Journal</i> , 2009, 15, 4078-4087.	3.3	163
69	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.	3.3	77
70	Stereochemistry of Compounds with Coordination Number Ten. <i>Chemistry - A European Journal</i> , 2009, 15, 7470-7480.	3.3	101
71	Reactivity of a Super-Electron-Rich Olefin Derived from Cyclam. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 1851-1860.	2.0	22
72	Oxidation states, atomic charges and orbital populations in transition metal complexes. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 67-73.	1.4	76

#	ARTICLE	IF	CITATIONS
73	Substitution of chloride by nitrosyl ligand in a scorpionate ruthenium(III) compound: A theoretical study. <i>Inorganica Chimica Acta</i> , 2009, 362, 4651-4658.	2.4	2
74	Calibrating the coordination chemistry tool chest: metrics of bi- and tridentate ligands. <i>Dalton Transactions</i> , 2009, , 6610.	3.3	33
75	Jahnâ€Teller distortions of six-coordinate Cull compounds: cis or trans?. <i>Chemical Communications</i> , 2009, , 4242.	4.1	28
76	A New Titanium Alkoxide-Thiolate Complex as a Versatile Heterofunctional Metalloligand. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 1079-1085.	2.0	11
77	On books and chemical elements. <i>Foundations of Chemistry</i> , 2008, 10, 79-100.	1.1	22
78	Polyhedral Structures with an Odd Number of Vertices: Nineâ€Coordinate Metal Compounds. <i>Chemistry - A European Journal</i> , 2008, 14, 1291-1303.	3.3	294
79	Symmetry operation measures. <i>Journal of Computational Chemistry</i> , 2008, 29, 190-197.	3.3	55
80	Exchange interactions in a Fe <sub>5</sub> complex: A theoretical study using density functional theory. <i>Inorganica Chimica Acta</i> , 2008, 361, 3832-3835.	2.4	7
81	Covalent radii revisited. <i>Dalton Transactions</i> , 2008, , 2832.	3.3	3,155
82	Polyhedral structures with an odd number of vertices: nine-atom clusters and supramolecular architectures. <i>Dalton Transactions</i> , 2008, , 2583.	3.3	64
83	Application of Symmetry Operation Measures in Structural Inorganic Chemistry. <i>Inorganic Chemistry</i> , 2008, 47, 10965-10970.	4.0	24
84	Music of the elements. <i>New Journal of Chemistry</i> , 2008, 32, 571.	2.8	12
85	Molecules and crystals with both icosahedral and cubic symmetry. <i>Chemical Communications</i> , 2008, , 2717.	4.1	43
86	Ligands that enforce unnatural stereospinomers. <i>Dalton Transactions</i> , 2008, , 2235.	3.3	0
87	Can large magnetic anisotropy and high spin really coexist?. <i>Chemical Communications</i> , 2008, , 52-54.	4.1	215
88	Stereochemistry and Spin State in Four-Coordinate Transition Metal Compounds. <i>Inorganic Chemistry</i> , 2008, 47, 2871-2889.	4.0	88
89	Electrochemical Behavior of Copper Complexes with Substituted Polypyridinic Ligands: An Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2008, 47, 3687-3692.	4.0	16
90	Magnetic Structure of the Large-Spin Mn <sup>10</sup> and Mn <sup>19</sup> Complexes: A Theoretical Complement to an Experimental Milestone. <i>Journal of the American Chemical Society</i> , 2008, 130, 7420-7426.	13.7	93

#	ARTICLE	IF	CITATIONS
91	On the Existence of Molecular Palladium(VI) Compounds: Palladium Hexafluoride. <i>Inorganic Chemistry</i> , 2007, 46, 2700-2703.	4.0	17
92	Six-fold Oxygen-Coordinated Triplet (S= 1) Palladium(II) Moieties Templated by Tris(bipyridine)ruthenium(II) Ions. <i>Journal of the American Chemical Society</i> , 2007, 129, 1327-1334.	13.7	30
93	Theoretical Study of the Magnetic Properties of an Mn <sub>12</sub> 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.	5.3	41
94	Strong Antiferromagnetic Coupling at Long Distance through a Ligand to Metal Charge Transfer Mechanism. <i>Journal of Physical Chemistry C</i> , 2007, 111, 618-621.	3.1	19
95	Chemistry of Unsaturated Group 6 Metal Complexes with Bridging Hydroxy- and Methoxycarbyne Ligands. 2. Synthesis, Structure, and Bonding of 32- and 34-Electron Complexes. <i>Organometallics</i> , 2007, 26, 5912-5921.	2.3	36
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.	4.0	44
97	Reply to Comment on "Distortions in Octahedrally Coordinated d <sup>0</sup> Transition Metal Oxides: A Continuous Symmetry Measures Approach". <i>Chemistry of Materials</i> , 2007, 19, 1200-1200.	6.7	0
98	Chelating Dialkoxide Titanium Complex: A Versatile Building Block for the Construction of Heterometallic Derivatives. <i>Chemistry - A European Journal</i> , 2007, 13, 2831-2836.	3.3	7
99	Theoretical study of the exchange coupling interactions in a polyoxometalate Fe <sub>9</sub> W <sub>12</sub> complex. <i>Polyhedron</i> , 2007, 26, 2161-2164.	2.2	5
100	Chemistry of Unsaturated Group 6 Metal Complexes with Bridging Hydroxy and Methoxycarbyne Ligands. 1. Synthesis, Structure, and Bonding of 30-Electron Complexes. <i>Organometallics</i> , 2007, 26, 4930-4941.	2.3	40
101	Density functional study of magnetostructural correlations in cubane complexes containing the Cu <sub>4</sub> O <sub>4</sub> core. <i>Journal of Materials Chemistry</i> , 2006, 16, 2729-2735.	6.7	107
102	Nesting of fullerenes and Frank-Kasper polyhedra. <i>Dalton Transactions</i> , 2006, , 2045-2051.	3.3	16
103	Distortions in Octahedrally Coordinated d <sup>0</sup> Transition Metal Oxides: A Continuous Symmetry Measures Approach. <i>Chemistry of Materials</i> , 2006, 18, 3176-3183.	6.7	326
104	Effects of Tris(pyrazolyl)borato Ligand Substituents on Dioxygen Activation and Stabilization by Copper Compounds. <i>Inorganic Chemistry</i> , 2006, 45, 3594-3601.	4.0	19
105	Magnetostructural Correlations in Polynuclear Complexes: The Fe <sub>4</sub> Butterflies. <i>Journal of the American Chemical Society</i> , 2006, 128, 15722-15727.	13.7	93
106	Magnetic Communication through Functionalized Nanotubes: A Theoretical Study. <i>Nano Letters</i> , 2006, 6, 380-384.	9.1	15
107	Theoretical study of the exchange coupling in a Ni <sub>12</sub> single-molecule magnet. <i>Dalton Transactions</i> , 2006, , 2643.	3.3	23
108	Shape and Symmetry Measures as Tools for the Solid State. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2006, 632, 2073-2073.	1.2	0



#	ARTICLE	IF	CITATIONS
109	Theoretical study of the electronic properties and exchange coupling in a Ni <sub>4</sub> cubane like single-molecule magnet. <i>Physica B: Condensed Matter</i> , 2006, 384, 123-125.	2.7	10
110	Exchange coupling interactions in a Fe <sub>6</sub> complex: A theoretical study using density functional theory. <i>Physica B: Condensed Matter</i> , 2006, 384, 116-119.	2.7	7
111	Bonding and solvation preferences of nickel complexes [Ni(S <sub>2</sub> PR <sub>2</sub> ) <sub>2</sub> ] (R=H, Me, OMe) according a natural bond orbital analysis. <i>Computational and Theoretical Chemistry</i> , 2006, 767, 37-41.	1.5	13
112	The nature of the Aul ... Aul Interactions between Cationic [AuL <sub>2</sub> ] <sup>+</sup> Complexes in the Solid State. <i>Theoretical Chemistry Accounts</i> , 2006, 116, 472-479.	1.4	12
113	A Family of Ferro- and Antiferromagnetically Coupled Decametalllic Chromium(III) Wheels. <i>Chemistry - A European Journal</i> , 2006, 12, 1385-1396.	3.3	55
114	Shape and Spin State in Four-Coordinate Transition-Metal Complexes: The Case of the d <sub>6</sub> Configuration. <i>Chemistry - A European Journal</i> , 2006, 12, 3162-3167.	3.3	153
115	How High the Spin? Allowed and Forbidden Spin States in Transition-Metal Chemistry. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 3012-3020.	13.8	53
116	Polyhedral Interconversion Coupled with Proton Transfer between an Ammonium Cation and the [Co(CO) <sub>4</sub> ] <sup>+</sup> Ion. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 1457-1460.	13.8	19
117	Do You Bend or not To Bend? Both! The Planar and Bent Structures of [(Ph <sub>3</sub> P) <sub>4</sub> Rh <sub>2</sub> (μ <sub>4</sub> -F) <sub>2</sub> ]. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 3340-3345.	2.0	13
118	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.	3.0	47
119	An Fe <sub>11</sub> complex showing single-molecule magnet behavior: Theoretical study using density functional methods and Monte Carlo simulations. <i>Polyhedron</i> , 2005, 24, 2364-2367.	2.2	8
120	Shape maps and polyhedral interconversion paths in transition metal chemistry. <i>Coordination Chemistry Reviews</i> , 2005, 249, 1693-1708.	18.8	889
121	Spin density distribution in transition metal complexes. <i>Coordination Chemistry Reviews</i> , 2005, 249, 2649-2660.	18.8	163
122	Theoretical determination of the exchange coupling constants of a single-molecule magnet Fe <sub>10</sub> complex. <i>Chemical Physics Letters</i> , 2005, 415, 6-9.	2.6	23
123	About the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction error. <i>Journal of Chemical Physics</i> , 2005, 123, 164110.	3.0	318
124	Theoretical Study of the Magnetic Behavior of Ferric Wheels. <i>ChemPhysChem</i> , 2005, 6, 1094-1099.	2.1	18
125	Symmetry and Topology Determine the MoV-CN-MnII Exchange Interactions in High-Spin Molecules. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2711-2715.	13.8	69
126	Symmetry and Topology Determine the MoV-CN-MnII Exchange Interactions in High-Spin Molecules. <i>Angewandte Chemie</i> , 2005, 117, 2771-2775.	2.0	15



#	ARTICLE	IF	CITATIONS
127	The Rich Stereochemistry of Eight-Vertex Polyhedra: A Continuous Shape Measures Study. Chemistry - A European Journal, 2005, 11, 1479-1494.	3.3	729
128	Is It Possible To Get HighTCMagnets with Prussian Blue Analogues? A Theoretical Prospect. Chemistry - A European Journal, 2005, 11, 2135-2144.	3.3	129
129	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
130	Continuous Chirality Measures in Transition Metal Chemistry. ChemInform, 2005, 36, no.	0.0	0
131	[Cu <sub>3</sub> (μ <sub>3</sub> -S) <sub>2</sub> ] <sup>3+</sup> Clusters Supported by N-Donor Ligands: A 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
132	Polyhedra in (inorganic) chemistry. Dalton Transactions, 2005, , 2209.	3.3	139
133	Exchange coupling in μ <sub>3</sub> -aqua:μ <sub>3</sub> -oxo vs. di-μ <sub>2</sub> -hydroxo dinuclear Cu(II) compounds: a density functional study. Dalton Transactions, 2005, , 2624.	3.3	18
134	A pyrimidine thiolate Rh(I) complex: structure, bonding and one-dimensional interactions in solid and in solution. Dalton Transactions, 2005, , 938-944.	3.3	5
135	Continuous Shape Measures as a Stereochemical Tool in Organometallic Chemistry. Organometallics, 2005, 24, 1556-1562.	2.3	125
136	Magnetism of Cyano-Bridged Ln <sup>3+</sup> /M <sup>3+</sup> Complexes. Part II: A One-Dimensional Complexes (Ln <sup>3+</sup> = Eu, Tb, Dy,) Tj ETOq0 0 0 rgBT /Overl	4.0	86
137	Magnetic Properties of Cyano-Bridged Ln <sup>3+</sup> /M <sup>3+</sup> Complexes. Part I: A Trinuclear Complexes (Ln <sup>3+</sup> = La, Ce,) Tj ETOq1 1 0.784314 rgBT	4.0	93
138	Continuous chirality measures in transition metal chemistry. Chemical Society Reviews, 2005, 34, 313.	38.1	98
139	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
140	Formation of Sulfur-Sulfur Bonds in Copper Complexes. European Journal of Inorganic Chemistry, 2004, 2004, 4430-4438.	2.0	12
141	Chalcogen-Chalcogen Bonds in Edge-Sharing Square-Planar d <sup>8</sup> Complexes. Are They Possible?. ChemInform, 2004, 35, no.	0.0	0
142	Mapping the Stereochemistry and Symmetry of Tetracoordinate Transition-Metal Complexes. Chemistry - A European Journal, 2004, 10, 190-207.	3.3	175
143	The Nature of Intermolecular Cu <sup>I</sup> ...Cu <sup>I</sup> Interactions: A Combined Theoretical and Structural Database Analysis. Chemistry - A European Journal, 2004, 10, 2117-2132.	3.3	139
144	Theoretical study of exchange coupling constants in an Fe <sub>19</sub> complex. Journal of Physics and Chemistry of Solids, 2004, 65, 799-803.	4.0	41

#	ARTICLE	IF	CITATIONS
145	Minimal Distortion Pathways in Polyhedral Rearrangements. <i>Journal of the American Chemical Society</i> , 2004, 126, 1755-1763.	13.7	362
146	Chalcogen-Chalcogen Bonds in Edge-Sharing Square-Planar d8 Complexes. Are They Possible?. <i>Inorganic Chemistry</i> , 2004, 43, 3702-3714.	4.0	25
147	A New Class of (1/4-1/2-Disulfido)dicopper Complexes: A Synthesis, Characterization, and Disulfido Exchange. <i>Inorganic Chemistry</i> , 2004, 43, 3335-3337.	4.0	64
148	Choice of Coordination Number in d10 Complexes of Group 11 Metals. <i>Journal of the American Chemical Society</i> , 2004, 126, 1465-1477.	13.7	198
149	Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study. <i>Monatshefte für Chemie</i> , 2003, 134, 307-316.	1.8	25
150	About the calculation of exchange coupling constants in polynuclear transition metal complexes. <i>Journal of Computational Chemistry</i> , 2003, 24, 982-989.	3.3	472
151	Exchange Coupling in Metal Complexes of the Second Transition Series: A Theoretical Exploration. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 1756-1760.	2.0	24
152	Room-Temperature Synthesis and Crystal, Magnetic, and Electronic Structure of the First Silver Copper Oxide.. <i>ChemInform</i> , 2003, 34, no.	0.0	1
153	Exchange Coupling in Metal Complexes of the Second Transition Series: A Theoretical Exploration. <i>ChemInform</i> , 2003, 34, no.	0.0	0
154	Theoretical Evidence of Persistent Chirality in D3 Homoleptic Hexacoordinate Complexes with Monodentate Ligands. <i>Chemistry - A European Journal</i> , 2003, 9, 1952-1957.	3.3	14
155	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.	3.3	38
156	Shape and Symmetry of Heptacoordinate Transition-Metal Complexes: Structural Trends. <i>Chemistry - A European Journal</i> , 2003, 9, 1281-1295.	3.3	225
157	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.	13.7	77
158	A Novel Hexanuclear Mixed Oxidation State Cu <sub>4</sub> Cu <sub>2</sub> Cluster Complex Exhibiting Weak Ferromagnetic Exchange. <i>Inorganic Chemistry</i> , 2003, 42, 1107-1111.	4.0	18
159	Tailor-Made Strong Exchange Magnetic Coupling through Very Long Bridging Ligands: Theoretical Predictions. <i>Inorganic Chemistry</i> , 2003, 42, 4881-4884.	4.0	28
160	Continuous chirality measures of tetracoordinate bis(chelate) metal complexes. <i>Dalton Transactions</i> , 2003, , 562-569.	3.3	20
161	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.	13.7	102
162	Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study. , 2003, , 191-200.		0

#	ARTICLE	IF	CITATIONS
163	Exchange Coupling of Transition-Metal Ions through Hydrogen Bonding: A Theoretical Investigation. <i>Journal of the American Chemical Society</i> , 2002, 124, 5197-5205.	13.7	202
164	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.	13.7	36
165	Exchange Coupling in Halo-Bridged Dinuclear Cu(II) Compounds: A Density Functional Study. <i>Inorganic Chemistry</i> , 2002, 41, 3769-3778.	4.0	118
166	Molecular Structure and Isomerization in Square-Planar Edge-Sharing Dinuclear Complexes with Alkynyl Bridges. <i>Organometallics</i> , 2002, 21, 2627-2634.	2.3	22
167	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 <a href="http://www.rsc.org/suppdata/nl/b2/b202096n/">http://www.rsc.org/suppdata/nl/b2/b202096n/</a> . <i>New Journal of Chemistry</i> , 2002, 26, 996-1009.	2.8	388
168	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.	2.5	48
169	Room-Temperature Synthesis and Crystal, Magnetic, and Electronic Structure of the First Silver Copper Oxide. <i>Inorganic Chemistry</i> , 2002, 41, 6604-6613.	4.0	44
170	Early-late transition metal ferromagnetic coupling mediated by hydrogen bonding. <i>Chemical Communications</i> , 2002, , 2614-2615.	4.1	35
171	Structure and bonding in late transition metal dinuclear complexes with local trigonal planar geometries. <i>Dalton Transactions RSC</i> , 2002, , 2235-2243.	2.3	8
172	Hexakis(silyl)palladium(VI) or Palladium(II) with 1,2-Disilane Ligands? This work was supported by the Direcció General de Enseñanza Superior (DGES), grant PB98-1166-CO2-01, and the Comissionat per a Universitats i Recerca (Generalitat de Catalunya), grant SGR99-0046. Computing resources at the Centre de Supercomputació de Catalunya (CESCA) and Centre de Paral·lelisme de Barcelona (CEPBA) were made available by the Comissió Interdepartamental per a la Recerca i la Innovació Tecnològica (CIRIT) and the Unive. <i>Angewandte Chemie</i> , 2002, 114, 2036.	2.0	16
173	Theoretical Clues to the Mechanism of Dioxygen Formation at the Oxygen-Evolving Complex of Photosystem II. <i>Chemistry - A European Journal</i> , 2002, 8, 2508.	3.3	22
174	Hexakis(silyl)palladium(VI) or Palladium(II) with 1,2-Disilane Ligands? This work was supported by the Direcció General de Enseñanza Superior (DGES), grant PB98-1166-CO2-01, and the Comissionat per a Universitats i Recerca (Generalitat de Catalunya), grant SGR99-0046. Computing resources at the Centre de Supercomputació de Catalunya (CESCA) and Centre de Paral·lelisme de Barcelona (CEPBA) were made available by the Comissió Interdepartamental per a la Recerca i la Innovació Tecnològica (CIRIT) and the Unive. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1956.	13.8	35
175	Ligand effects and dimer formation in dicoordinated copper(I) complexes. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 100-105.	2.0	14
176	Molecular Structures of Edge-Sharing Square-Planar Dinuclear Complexes with Unsaturated Bridges. <i>Inorganic Chemistry</i> , 2001, 40, 4937-4946.	4.0	7
177	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.	4.0	74
178	Theoretical Study of Bonding, Structure, and Vibrational Spectra of the [Fe <sub>2</sub> (CO) <sub>8</sub> ] <sup>2-</sup> Anion and Its Derivatives. <i>Organometallics</i> , 2001, 20, 818-826.	2.3	9
179	Density functional study of the exchange coupling in distorted cubane complexes containing the Cu <sub>4</sub> O <sub>4</sub> core. <i>Polyhedron</i> , 2001, 20, 1323-1327.	2.2	90
180	Reaction chemistry, NMR spectroscopy, and X-ray crystallography of [Fe <sub>2</sub> (1/4-SiMe <sub>2</sub> ) <sub>2</sub> (CO) <sub>4</sub> ] and [Fe <sub>2</sub> (1/4-SiMeCl) <sub>2</sub> (CO) <sub>4</sub> ]. Electronic structure and bonding in Fe <sub>2</sub> E <sub>2</sub> rings of [Fe <sub>2</sub> (1/4-ER) <sub>2</sub> (CO) <sub>4</sub> ] binuclear complexes (E=C, Si, Ge, Sn, Pb). <i>Journal of Organometallic Chemistry</i> , 2001, 628, 241-254.	1.8	24

#	ARTICLE	IF	CITATIONS
181	Continuous chirality analysis of hexacoordinated tris-chelated metal complexes. <i>Crystal Engineering</i> , 2001, 4, 179-200.	0.7	24
182	A Continuous Chirality Analysis of Homoleptic Hexacoordinated Complexes. <i>European Journal of Inorganic Chemistry</i> , 2001, 2001, 1499-1503.	2.0	18
183	The [M <sub>2</sub> (CO) <sub>8</sub> ] Complexes of the Cobalt Group. <i>European Journal of Inorganic Chemistry</i> , 2001, 2001, 3031-3038.	2.0	29
184	Exchange Coupling in Carboxylato-Bridged Dinuclear Copper(II) Compounds: A Density Functional Study. <i>Chemistry - A European Journal</i> , 2001, 7, 627-637.	3.3	325
185	Asymmetry and Magnetism in Bis(oximato)-Bridged Heterobimetallic Compounds: A Computational Approach. <i>Chemistry - A European Journal</i> , 2000, 6, 327-333.	3.3	41
186	Theoretical approach to the magnetostructural correlations in the spin-Peierls compound CuGeO <sub>3</sub> . <i>Physical Review B</i> , 2000, 61, 54-57.	3.2	16
187	Magnetic Coupling in End-to-End Azido-Bridged Copper and Nickel Binuclear Complexes: A Theoretical Study. <i>Inorganic Chemistry</i> , 2000, 39, 3221-3229.	4.0	152
188	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
189	Theoretical study of the guest-guest... guest interactions of cobaltocene intercalated in metal sulfides. <i>Dalton Transactions RSC</i> , 2000, , 1463-1467.	2.3	5
190	The coloring problem in Ba <sub>2</sub> Cu <sub>3</sub> VS <sub>6</sub> . <i>Dalton Transactions RSC</i> , 2000, , 1009-1011.	2.3	0
191	Through-Ring Bonding in Edge Sharing Dimers of Octahedral Complexes. <i>Inorganic Chemistry</i> , 2000, 39, 3166-3175.	4.0	31
192	Structural Correlations and Conformational Preference in Edge-Sharing Binuclear d <sub>8</sub> Complexes with XR <sub>2</sub> Bridges. A Theoretical Study. <i>Inorganic Chemistry</i> , 2000, 39, 906-916.	4.0	16
193	Ligand Macrocyclic Structural Effects on Copper <sup>II</sup> Dioxygen Reactivity. <i>Inorganic Chemistry</i> , 2000, 39, 4059-4072.	4.0	116
194	Synthesis and study of trinuclear Pd(II) and Pt(II) complexes with 2-mercaptopyridonic acid. <i>Polyhedron</i> , 1999, 18, 3675-3682.	2.2	35
195	Ligand orientation effects on metal-metal, ligand-ligand and metal-ligand interactions. <i>Coordination Chemistry Reviews</i> , 1999, 185-186, 431-450.	18.8	39
196	Bonding and stereochemistry of three-coordinated transition metal compounds. <i>Coordination Chemistry Reviews</i> , 1999, 193-195, 13-41.	18.8	70
197	Broken symmetry approach to calculation of exchange coupling constants for homobinuclear and heterobinuclear transition metal complexes. <i>Journal of Computational Chemistry</i> , 1999, 20, 1391-1400.	3.3	836
198	Edge-Sharing Binuclear d <sub>8</sub> Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation. <i>Chemistry - A European Journal</i> , 1999, 5, 1391-1410.	3.3	65

#	ARTICLE	IF	CITATIONS
199	Tetrahedral d0 and d10 transition metal ions sharing edges in the solid state: electronic structure and bonding. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 1235-1240.	1.1	0
200	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
201	Electronic Structure and Bonding in Tricoordinate Amido Complexes of Transition Metals. <i>Inorganic Chemistry</i> , 1999, 38, 707-715.	4.0	16
202	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.	3.3	1
203	Theoretical search for new ferromagnetically coupled transition metal complexes. <i>Chemical Communications</i> , 1998, , 2767-2768.	4.1	62
204	Exchange Coupling in Oxalato-Bridged Copper(II) Binuclear Compounds: A Density Functional Study. <i>Chemistry - A European Journal</i> , 1998, 4, 476-484.	3.3	197
205	Spin Density Distribution in Transition Metal Complexes: Some Thoughts and Hints. <i>Comments on Inorganic Chemistry</i> , 1998, 20, 27-56.	5.2	187
206	Theoretical study of the intercalation of cobaltocene in metal chalcogenides. <i>Journal of Materials Chemistry</i> , 1998, 8, 1893-1900.	6.7	4
207	Skutterudite vs. ReO <sub>3</sub> structures for MX <sub>3</sub> solids: electronic requirements. <i>Journal of the Chemical Society Dalton Transactions</i> , 1998, , 1195-1200.	1.1	7
208	Framework Bonding and Coordination Sphere Rearrangement in the M <sub>2</sub> X <sub>2</sub> Cores of Synthetic Analogues of Oxyhemocyanin and Related Cu and Pt Complexes. <i>Inorganic Chemistry</i> , 1998, 37, 1202-1212.	4.0	35
209	Electronic Structure of Host Lattices for Intercalation Compounds: SnS <sub>2</sub> , SnSe <sub>2</sub> , ZrS <sub>2</sub> , and TaS <sub>2</sub> . <i>Chemistry of Materials</i> , 1998, 10, 3422-3428.	6.7	19
210	Magnetic Coupling in End-On Azido-Bridged Transition Metal Complexes: A Density Functional Study. <i>Journal of the American Chemical Society</i> , 1998, 120, 11122-11129.	13.7	676
211	To Bend or Not To Bend: A Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d <sub>8</sub> Transition Metal Ions. <i>Inorganic Chemistry</i> , 1998, 37, 804-813.	4.0	126
212	Pyramidal effect on metal-metal single bonds. <i>Journal of the Chemical Society Dalton Transactions</i> , 1997, , 2681-2688.	1.1	3
213	M <sub>2</sub> L <sub>6</sub> Complexes with Triple Mo-Mo and W-W Bonds: Molecular Topology and Inverted Pyramidal Effect. <i>Inorganic Chemistry</i> , 1997, 36, 1055-1060.	4.0	14
214	Iron-Gold (or Mercury) Carbide Clusters Derived from [Fe <sub>6</sub> C(CO) <sub>16</sub> ] <sub>2</sub> -. X-ray Crystal Structures of (NEt <sub>4</sub> )[Fe <sub>6</sub> C{AuPPh <sub>3</sub> } <sub>3</sub> (CO) <sub>16</sub> ] and [Fe <sub>4</sub> C{AuPPh <sub>3</sub> } <sub>3</sub> (CO) <sub>11</sub> (NO)]. <i>Organometallics</i> , 1997, 16, 236-245.	2.3	35
215	Toward the Prediction of Magnetic Coupling in Molecular Systems: Hydroxo- and Alkoxo-Bridged Cu(II) Binuclear Complexes. <i>Journal of the American Chemical Society</i> , 1997, 119, 1297-1303.	13.7	816
216	Electronic structure and properties of Cu <sub>2</sub> O. <i>Physical Review B</i> , 1997, 56, 7189-7196.	3.2	146

#	ARTICLE	IF	CITATIONS
217	Structural Modeling and Magneto-Structural Correlations for Hydroxo-Bridged Copper(II) Binuclear Complexes. <i>Inorganic Chemistry</i> , 1997, 36, 3683-3688.	4.0	386
218	Chain Conformation and Metal-Metal Contacts in Dimers and Stacks of d <sup>8</sup> -ML <sub>4</sub> Complexes: Electronic Effects. <i>Chemistry - A European Journal</i> , 1997, 3, 655-664.	3.3	64
219	Electronic Structure, Bonding, and Electrical Properties of MoNiP <sub>8</sub> . <i>Inorganic Chemistry</i> , 1996, 35, 4683-4689.	4.0	8
220	Axial Bonding Capabilities of Square Planar d <sup>8</sup> -ML <sub>4</sub> Complexes. Theoretical Study and Structural Correlations. <i>Inorganic Chemistry</i> , 1996, 35, 3137-3144.	4.0	84
221	Structure of the non-polar (10 $\bar{1}$ ,0) surfaces of AlN and $\hat{\Gamma}$ -SiC: a periodic Hartree-Fock study. <i>Surface Science</i> , 1996, 355, 167-176.	1.9	11
222	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 <sub>3</sub> dien) <sub>2</sub> [Ni <sub>2</sub> (ox) <sub>5</sub> ] $\cdot$ 12H <sub>2</sub> O and [Ni <sub>2</sub> (dien) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> (ox)]Cl <sub>2</sub> . <i>Inorganic Chemistry</i> , 1996, 35, 3741-3751.	4.0	171
223	On the Existence of a Pyramidity Effect in d <sup>8</sup> -ML <sub>4</sub> Contacts. Theoretical Study and Structural Correlation. <i>Inorganic Chemistry</i> , 1996, 35, 5061-5067.	4.0	50
224	Electronic band structure of the magnetic layered semiconductors MPS <sub>3</sub> (M = Mn, Fe and Ni). <i>Journal of Physics and Chemistry of Solids</i> , 1996, 57, 647-652.	4.0	22
225	Anhydrous trans-(Aniline)chlorobis(dimethylglyoximate)cobalt(III). <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1996, 52, 63-66.	0.4	2
226	Electronic structure and bonding in skutterudite-type phosphides. <i>Physical Review B</i> , 1996, 53, 10605-10609.	3.2	74
227	Ab initio study of AlN and $\hat{\Gamma}$ -SiC (112 $\bar{0}$ ) surface relaxation. <i>Physical Review B</i> , 1996, 53, 4933-4938.	3.2	8
228	Intercalation of Halogen Molecules in Alkali Fluoride Lattices: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 1995, 117, 2877-2883.	13.7	5
229	Host-guest Interactions in the Pyrrole and Aniline Hofmann Clathrates. A Theoretical Study. <i>Inorganic Chemistry</i> , 1995, 34, 3260-3269.	4.0	21
230	Theoretical Study of Host-guest Interactions in Clathrates with a Cd(CN) <sub>2</sub> Host. <i>Inorganic Chemistry</i> , 1995, 34, 5845-5851.	4.0	12
231	Electronic Structure, Chemical Bonding, and Jahn-Teller Distortions in CdPS <sub>3</sub> . <i>Inorganic Chemistry</i> , 1995, 34, 1159-1163.	4.0	18
232	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
233	On the Bonding Nature of the M-guest Interactions in Dimers of Square-Planar Pt(II) and Rh(I) Complexes. <i>Journal of the American Chemical Society</i> , 1995, 117, 7169-7171.	13.7	103
234	Heterodox Bonding Effects between Transition Metal Atoms. , 1995, , 241-255.		8



#	ARTICLE	IF	CITATIONS
235	Electronic structure and properties of AlN. <i>Physical Review B</i> , 1994, 49, 7115-7123.	3.2	146
236	Electronic structure and properties of hexagonal wurtzite-type SiC. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 365-373.	2.0	5
237	Through-ring bonding in edge-sharing dimers of square planar complexes. <i>Journal of Organometallic Chemistry</i> , 1994, 478, 75-82.	1.8	52
238	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.	13.7	42
239	(PPh <sub>4</sub> )[Mn <sub>3</sub> (CO) <sub>12</sub> (μ <sub>3</sub> -H)(μ <sub>3</sub> -Hg{Mo(CO) <sub>3</sub> (η <sup>5</sup> -C <sub>5</sub> H <sub>5</sub> )} <sub>3</sub> )]: The First Example of a Mercury-Containing Planar Triangulated Rhomboidal Metal Cluster. <i>Organometallics</i> , 1994, 13, 2205-2212.	2.3	12
240	Ca <sub>0.95</sub> Nb <sub>3</sub> O <sub>6</sub> : Crystal and Electronic Structure. <i>Journal of Solid State Chemistry</i> , 1993, 105, 27-35.	2.9	13
241	Pyramidity and metal-metal multiple bonding: structural correlations and theoretical study. <i>Journal of the American Chemical Society</i> , 1993, 115, 6216-6229.	13.7	44
242	Pyramidity effect on rhodium(II)-Rh(II) single bonds. <i>Inorganic Chemistry</i> , 1993, 32, 3712-3719.	4.0	25
243	Mixed valency in binuclear cyano-bridged manganese bis(carbonyl) complexes and stereochemical control of their oxidation. A molecular orbital study. <i>Inorganic Chemistry</i> , 1993, 32, 272-276.	4.0	23
244	Electronic structure, bonding, and properties of copper phosphide, Cu <sub>3</sub> P <sub>2</sub> . <i>Inorganic Chemistry</i> , 1992, 31, 119-124.	4.0	12
245	Exchange interaction through a croconato bridge: synthesis, crystal structure, and magnetic properties of (μ <sub>3</sub> -croconato)bis[μ <sub>2</sub> -(2-pyridylcarbonyl)amido]copper(II) trihydrate. <i>Inorganic Chemistry</i> , 1992, 31, 1889-1894.	4.0	87
246	Theoretical study of bonding and electrical conductivity in compounds with the NbAs <sub>2</sub> structure. <i>Inorganic Chemistry</i> , 1992, 31, 3007-3010.	4.0	8
247	Symmetry guidelines for the design of convergent syntheses. On narcissistic coupling and la coupe du roi. <i>Journal of the American Chemical Society</i> , 1992, 114, 2623-2630.	13.7	8
248	Unprecedented trimetallic cluster with an in-plane μ <sub>3</sub> -hydride ligand. X-ray crystal structure of [Mo <sub>2</sub> (CO) <sub>8</sub> (μ <sub>3</sub> -dppm)(μ <sub>3</sub> -H)(μ <sub>3</sub> -AuPPh <sub>3</sub> )]. <i>Organometallics</i> , 1992, 11, 3753-3759.	2.3	17
249	Bonding and structure in L <sub>4</sub> M <sub>2</sub> (μ <sub>2</sub> -XR <sub>n</sub> ) <sub>2</sub> diamonds of tetrahedral d <sup>10</sup> ions. Effect of substituents on the M-M interaction. <i>Inorganic Chemistry</i> , 1992, 31, 4266-4275.	4.0	52
250	The influence of equatorial bulky substituents on the properties of organometallic bis(dioximato)cobalt(III) compounds. Structural comparison between trans-[Co(dpgH) <sub>2</sub> (R)(L)] complexes [dpgH = diphenylglyoximato(η <sup>1</sup> )] and other B <sub>12</sub> models. <i>Polyhedron</i> , 1992, 11, 1637-1646.	2.2	22
251	Electronic structure calculations and X-ray emission spectra of some metal phosphides. <i>Solid State Communications</i> , 1992, 83, 447-450.	1.9	1
252	Square Fe <sub>2</sub> Au <sub>2</sub> and triangular Fe <sub>2</sub> Au clusters: A reversible transformation. X-ray crystal structure of [Fe <sub>2</sub> Au <sub>2</sub> (CO) <sub>8</sub> (μ <sub>3</sub> -dppm)] [dppm = bis(diphenylphosphino)methane]. <i>Organometallics</i> , 1991, 10, 2309-2314.	2.3	37



#	ARTICLE	IF	CITATIONS
253	Electronic structure of a (cyclopentadienyl)tri- $\mu$ -oxoditechnetium polymer with a very short metal-metal bond. <i>Inorganic Chemistry</i> , 1991, 30, 1086-1093.	4.0	17
254	Dinuclear complexes of copper(II) derived from (1,3-propanediylbis(oxamato))cuprate(II): magneto-structural correlations. <i>Inorganic Chemistry</i> , 1991, 30, 841-845.	4.0	36
255	New organometallic cobaloximes containing an equatorial diphenylglyoximato( $\lambda^1$ ) ligand. Comparison between their properties and those of other B12 model compounds. Crystal structure of trans-[Co(dpgH)2(CH3)(pyridine)]. <i>Journal of Organometallic Chemistry</i> , 1991, 414, 245-259.	1.8	34
256	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.	13.7	26
257	Magnetic exchange interactions in one-dimensional copper(II) compounds. <i>Chemistry of Materials</i> , 1990, 2, 723-728.	6.7	8
258	The electronic structure of barium gallium antimonide (Ba7Ga4Sb9): a compound seemingly probing the limits of the Zintl concept. <i>Inorganic Chemistry</i> , 1990, 29, 3070-3073.	4.0	33
259	Oxalato-bridged and related dinuclear copper(II) complexes: theoretical analysis of their structures and magnetic coupling. <i>Inorganic Chemistry</i> , 1990, 29, 4500-4507.	4.0	146
260	Importance of the X4 ring orbitals for the semiconducting, metallic, or superconducting properties of skutterudites MX3 and RM4X12. <i>Inorganic Chemistry</i> , 1990, 29, 2252-2255.	4.0	118
261	Anionic trimetallic compounds containing Fe $\mu$ -E $\mu$ -M skeletons (E = Zn, Cd, Hg; M = Fe, Mo, W). Crystal structure of [N(PPh3)2]2[(OC)4Fe $\mu$ -Hg $\mu$ -Fe(CO)4]. <i>Journal of Organometallic Chemistry</i> , 1989, 377, 291-303.	1.8	30
262	Cis and trans effects and NMR correlations in organometallic cobaloximes. <i>Journal of Organometallic Chemistry</i> , 1988, 342, C13-C14.	1.8	6
263	Structure and stability of the X3- 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
264	Importance of metal-metal interactions through the phosphorus-phosphorus bonds for the multidimensional electrical properties of MP4 (M = vanadium, chromium, molybdenum). <i>Inorganic Chemistry</i> , 1988, 27, 2702-2706.	4.0	11
265	Structure and stability of tetraatomic bromine and ion, Br4 and Br4 <sup>2-</sup> , and their interaction with cations and transition metals. <i>Journal of the American Chemical Society</i> , 1987, 109, 6586-6591.	13.7	17
266	The fluxional behavior of monocoordinated diimines and azines. <i>Journal of the American Chemical Society</i> , 1987, 109, 5316-5323.	13.7	18
267	Synthesis, x-ray diffraction structure, magnetic properties, and MO analysis of a binuclear ( $\mu$ -tetrathiooxalato)copper(II) complex, (AsPh4)2[(C3OS4)CuC2S4Cu(C3OS4)]. <i>Inorganic Chemistry</i> , 1987, 26, 4004-4009.	4.0	76
268	Synthesis and structure of chloro(ligand)bis(diphenylglyoximato)cobalt(III) complexes. <i>Inorganica Chimica Acta</i> , 1987, 127, 153-159.	2.4	31
269	Improved synthesis of dicyanocobaloximes and the molecular and crystal structure of potassium dicyanobis(dimethylglyoximato)cobaltate(III). <i>Inorganica Chimica Acta</i> , 1987, 133, 101-105.	2.4	5
270	Structure-NMR correlations in halo(ligand)bis(dioximato)cobalt(III) complexes. <i>Inorganic Chemistry</i> , 1986, 25, 2962-2969.	4.0	57

#	ARTICLE	IF	CITATIONS
271	The mechanism of electrical conductivity along polyhalide chains. <i>Chemical Physics Letters</i> , 1986, 132, 531-534.	2.6	12
272	Structural, NMR and theoretical study of delocalization in cobaloximes. <i>Inorganica Chimica Acta</i> , 1986, 111, L19-L21.	2.4	20
273	Synthesis, characterization and study of the Pt-Pt interaction in cis-[(aa)(bb)FCr-NCr-Pt(CN) <sub>3</sub> ] (aa, b) Tj ETQq1 1 0.784314 rgBT / 2.4	2.4	15
274	Synthesis and structure of chloro(ligand)bis(glyoximato)cobalt(III) complexes: structural evidence of an electronic effect on the structure of the dimethylpyrazine ligand. <i>Inorganica Chimica Acta</i> , 1986, 121, 71-75.	2.4	15
275	Synthesis and characterization of new di- and tri-nuclear cyano-bridged bis(dioximato)cobalt(III) complexes. <i>Transition Metal Chemistry</i> , 1986, 11, 16-19.	1.4	6
276	Vibrational spectra and normal coordinate analysis of two isotopomers of the thiosulfate ion. <i>Journal of Molecular Structure</i> , 1985, 130, 235-243.	3.6	4
277	Dimerization and stacking in transition-metal bisdithiolenes and tetrathiolates. <i>Journal of the American Chemical Society</i> , 1985, 107, 6253-6277.	13.7	243
278	Binuclear and polymeric gold(I) complexes. <i>Inorganic Chemistry</i> , 1985, 24, 749-757.	4.0	189
279	Electronic structure determination of iron(II) phthalocyanine via magnetic susceptibility and Mössbauer measurements. <i>Journal of Chemical Physics</i> , 1984, 80, 444-448.	3.0	26
280	Binuclear nickel-cobalt cyano-bridged complexes showing long-range proton shielding. <i>Inorganica Chimica Acta</i> , 1984, 82, L23-L26.	2.4	4
281	Symmetry constraints to the electrical conductivity of partially oxidized stacks of metal bis(dioximates). <i>Solid State Communications</i> , 1984, 50, 141-144.	1.9	10
282	C-N stretching force constants in cyano complexes: General trends for polycyano, mixed-ligand and cyano-bridged complexes. <i>Transition Metal Chemistry</i> , 1984, 9, 123-126.	1.4	24
283	Theoretical study of the electrical behavior of one-dimensional metallophthalocyanines and related metallomacrocyclic compounds. <i>Inorganic Chemistry</i> , 1984, 23, 573-579.	4.0	75
284	General quadratic force field of the sulfate ion and the relationships between different force fields in tetrahedral molecules. <i>Computational and Theoretical Chemistry</i> , 1984, 106, 293-300.	1.5	2
285	Mössbauer studies on one-dimensional iron phthalocyanines. <i>Transition Metal Chemistry</i> , 1983, 8, 377-380.	1.4	5
286	Axial substitution and bridge formation by the cyano group in bis(dimethylglyoximato)cobalt(III) complexes. <i>Inorganica Chimica Acta</i> , 1982, 63, 57-62.	2.4	16
287	Linkage isomerism in cyanoaquobis(dimethyl-glyoximato)cobalt(III). <i>Inorganica Chimica Acta</i> , 1982, 64, L99-L100.	2.4	19
288	C-N stretching force constants in cyano complexes. <i>Transition Metal Chemistry</i> , 1982, 7, 116-118.	1.4	5

#	ARTICLE	IF	CITATIONS
289	Binuclear complexes of Fe(III) and Cr(III) with bridging cyano ligand. <i>Inorganica Chimica Acta</i> , 1976, 16, L15-L16.	2.4	3
290	Electronic Structure and Magnetic Behavior in Polynuclear Transition-Metal Compounds. , 0, , 227-279.		55