

# Maria Jose' Calhorda

## List of Publications by Year in descending order

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284  
papers

7,570  
citations

53660

45  
h-index

102304

66  
g-index

298  
all docs

298  
docs citations

298  
times ranked

6618  
citing authors

#	ARTICLE	IF	CITATIONS
1	Weak hydrogen bonds: theoretical studies. <i>Chemical Communications</i> , 2000, , 801-809.	2.2	280
2	Octahedral Bipyridine and Bipyrimidine Dioxomolybdenum(VI) Complexes: Characterization, Application in Catalytic Epoxidation, and Density Functional Mechanistic Study. <i>Chemistry - A European Journal</i> , 2002, 8, 2370.	1.7	232
3	Mechanism for the Cyclotrimerization of Alkynes and Related Reactions Catalyzed by CpRuCl. <i>Journal of the American Chemical Society</i> , 2003, 125, 11721-11729.	6.6	168
4	The Nature of the Indenyl Effect. <i>Chemistry - A European Journal</i> , 2002, 8, 868-875.	1.7	147
5	Bi- and Trimetallic $\eta^5$ -Acetylide Complexes Connected through a Phenyl Ring in the Fe(Cp*)(dppe) Series. <i>Organometallics</i> , 1997, 16, 2024-2031.	1.1	126
6	Ring slippage in indenyl complexes: structure and bonding. <i>Coordination Chemistry Reviews</i> , 1999, 185-186, 37-51.	9.5	112
7	Loading and delivery of sertraline using inorganic micro and mesoporous materials. <i>European Journal of Pharmaceutics and Biopharmaceutics</i> , 2007, 66, 357-365.	2.0	101
8	Olefin epoxidation with tert-butyl hydroperoxide catalyzed by MoO <sub>2</sub> X <sub>2</sub> L complexes: a DFT mechanistic study. <i>Dalton Transactions</i> , 2006, , 1383.	1.6	88
9	Olefin Epoxidation Catalyzed by $\eta^5$ -Cyclopentadienyl Molybdenum Compounds: A Computational Study. <i>Organometallics</i> , 2010, 29, 303-311.	1.1	84
10	The carbon-carbon bond-forming step in catalytic cross-coupling: migration or elimination?. <i>Organometallics</i> , 1991, 10, 1431-1438.	1.1	81
11	High-Yield Ruthenium-Catalyzed Friedel-Crafts-Type Allylation Reactions Using Dicationic Ru <sup>IV</sup> Catalysts. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 6386-6391.	7.2	80
12	Hydrogen activation by high-valent oxo-molybdenum(vi) and -rhenium(vii) and -(v) compounds. <i>Dalton Transactions</i> , 2008, , 1727.	1.6	80
13	Molybdenum $\eta^3$ -Allyl Dicarbonyl Complexes as a New Class of Precursors for Highly Reactive Epoxidation Catalysts with tert-Butyl Hydroperoxide. <i>Organometallics</i> , 2007, 26, 5548-5556.	1.1	77
14	MoO <sub>2</sub> Cl <sub>2</sub> as a Novel Catalyst for C <sup>3</sup> P Bond Formation and for Hydrophosphonylation of Aldehydes. <i>Organometallics</i> , 2009, 28, 6206-6212.	1.1	74
15	Ruthenium-Catalyzed Allylic Alkylation Reactions: Carbonate-Based Catalysts and Intermediates. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 4397-4400.	7.2	73
16	Molecular modelling studies of N-salicylideneamino acidato complexes of oxovanadium(IV). Molecular and crystal structure of a new dinuclear LOVIV <sup>2+</sup> VO <sup>2+</sup> mixed valence complex. <i>Dalton Transactions RSC</i> , 2002, , 4407.	2.3	72
17	Catalyzing Aldehyde Hydrosilylation with a Molybdenum(VI) Complex: A Density Functional Theory Study. <i>Chemistry - A European Journal</i> , 2007, 13, 3934-3941.	1.7	72
18	[Re( $\eta^5$ -C <sub>5</sub> H <sub>5</sub> )(CO) <sub>3</sub> ] <sup>+</sup> Family of 17-Electron Compounds: $\Delta$ Monomer/Dimer Equilibria and Other Reactions. <i>Journal of the American Chemical Society</i> , 2008, 130, 2692-2703.	6.6	69

#	ARTICLE	IF	CITATIONS
19	Kinetic Studies on the Oxidation of $\eta^5$ -Cyclopentadienyl Methyl Tricarbonyl Molybdenum(II) and the Use of Its Oxidation Products as Olefin Epoxidation Catalysts. <i>Organometallics</i> , 2009, 28, 639-645.	1.1	67
20	Synthesis, Structure, and Photophysical Characterization of Blue-Green Luminescent Zinc Complexes Containing 2-Iminophenanthropyrryl Ligands. <i>Inorganic Chemistry</i> , 2009, 48, 11176-11186.	1.9	67
21	Selective C $\equiv$ C Bond Formation between Alkynes Mediated by the [RuCp(PR <sub>3</sub> ) <sub>3</sub> ] <sup>+</sup> Fragment Leading to Allyl, Butadienyl, and Allenyl Carbene Complexes—An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2002, 8, 3948-3961.	1.7	66
22	Highly Efficient Reduction of Sulfoxides with the System Borane/Oxo-rhenium Complexes. <i>Organometallics</i> , 2010, 29, 5517-5525.	1.1	63
23	Heteropolynuclear Gold Complexes with Metallophilic Interactions: Modulation of the Luminescent Properties. <i>Inorganic Chemistry</i> , 2010, 49, 8255-8269.	1.9	63
24	Formation of pyridine from acetylenes and nitriles catalyzed by RuCpCl, CoCp, and RhCp derivatives — A computational mechanistic study. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4434-4445.	0.8	62
25	Molecular Structures of M <sub>2</sub> (CO) <sub>9</sub> and M <sub>3</sub> (CO) <sub>12</sub> (M = Fe, Ru, Os): A New Theoretical Insights. <i>Inorganic Chemistry</i> , 1999, 38, 5053-5060.	1.9	61
26	X-ray, <sup>13</sup> C NMR, and DFT Studies on a Ruthenium(IV) Allyl Complex. Explanation for the Observed Control of Regioselectivity in Allylic Alkylation Chemistry. <i>Organometallics</i> , 2005, 24, 1809-1812.	1.1	61
27	Synthesis, Structural Characterization, and Theoretical Studies of Gold(I) and Gold(III) Thiolate Complexes: A Quenching of Gold(I) Thiolate Luminescence. <i>Inorganic Chemistry</i> , 2006, 45, 1059-1068.	1.9	61
28	Ligand Dependence of the Indenyl Ring Slippage in [( $\eta^5$ -Ind)MoL <sub>2</sub> (CO) <sub>2</sub> ] <sub>0,+</sub> Complexes: A Experimental and Theoretical Studies. <i>Organometallics</i> , 1998, 17, 2597-2611.	1.1	59
29	Ruthenium-mediated cyclotrimerization of alkynes utilizing the cationic complex [RuCp(CH <sub>3</sub> CN) <sub>3</sub> ] <sup>+</sup> PF <sub>6</sub> <sup>-</sup> . <i>Journal of Organometallic Chemistry</i> , 2003, 682, 204-211.	0.8	59
30	Synthesis and characterisation of organo-silica hydrophobic clay heterostructures for volatile organic compounds removal. <i>Microporous and Mesoporous Materials</i> , 2008, 111, 612-619.	2.2	59
31	Activation of Molecular Hydrogen over a Binuclear Complex with Rh <sub>2</sub> S <sub>2</sub> Core: A DFT Calculations and NMR Mechanistic Studies. <i>Journal of the American Chemical Society</i> , 2004, 126, 11954-11965.	6.6	57
32	Electrochemical Oxidation of CoCp(CO) <sub>2</sub> : A Radical—Substrate Reaction of a 17 e-/18 e-Pair and Production of a Unique Dimer Radical. <i>Journal of the American Chemical Society</i> , 2006, 128, 16587-16599.	6.6	57
33	By What Mechanisms Are Metal Cyclobutadiene Complexes Formed from Alkynes?. <i>Chemistry - A European Journal</i> , 2004, 10, 5860-5870.	1.7	56
34	Synthesis, Structure, Luminescence, and Theoretical Studies of Tetranuclear Gold Clusters with Phosphinocarborane Ligands. <i>Inorganic Chemistry</i> , 2000, 39, 4280-4285.	1.9	55
35	Striking Differences between the Solution and Solid-State Reactivity of Iron PNP Pincer Complexes with Carbon Monoxide. <i>Organometallics</i> , 2009, 28, 6902-6914.	1.1	55
36	Bonding and structural preferences of indenyl complexes: MInd <sub>2</sub> L <sub>n</sub> (n=0–3). <i>Coordination Chemistry Reviews</i> , 2002, 230, 49-64.	9.5	54

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37	Syntheses and photophysical properties of new iminopyrrolyl boron complexes and their application in efficient single-layer non-doped OLEDs prepared by spin coating. Dalton Transactions, 2012, 41, 8502.	1.6	53
38	Synthesis, bonding and dynamic behavior of fac-[Mo(II)(CO) <sub>2</sub> ( <i>η</i> -3-allyl)] derivatives. Journal of Organometallic Chemistry, 2001, 632, 197-208.	0.8	51
39	Stepwise Hapticity Changes in Sequential One-Electron Redox Reactions of Indenyl-Molybdenum Complexes: Combined Electrochemical, ESR, X-ray, and Theoretical Studies. Journal of the American Chemical Society, 2001, 123, 10595-10606.	6.6	47
40	Cu(I) and Ag(I) complexes of chalcogenide derivatives of the organometallic ligand dppf and the dppa analogue. Journal of Organometallic Chemistry, 2004, 689, 2808-2819.	0.8	47
41	CNN Pincer Ruthenium Catalysts for Hydrogenation and Transfer Hydrogenation of Ketones: Experimental and Computational Studies. Chemistry - A European Journal, 2014, 20, 13603-13617.	1.7	47
42	Vanadyl cationic complexes as catalysts in olefin oxidation. Dalton Transactions, 2015, 44, 5125-5138.	1.6	47
43	Luminescent Di- and Trinuclear Boron Complexes Based on Aromatic Iminopyrrolyl Spacer Ligands: Synthesis, Characterization, and Application in OLEDs. Chemistry - A European Journal, 2015, 21, 9133-9149.	1.7	47
44	Gold(I)-Gold(III) Interactions in Polynuclear Sulfur-Centered Complexes. Synthesis and Structural Characterization of [S(Au <sub>2</sub> dppf){Au(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> }] and [S(Au <sub>2</sub> dppf) <sub>2</sub> {Au(C <sub>6</sub> F <sub>5</sub> ) <sub>2</sub> }]OTf (dppf = $\text{1,1'-bis(diphenylphosphino)ferrocene}$ ). Journal of Organometallic Chemistry, 2016, 915, 104-110.	1.7	47
45	Heptacoordinate tricarbonyl Mo(II) complexes as highly selective oxidation homogeneous and heterogeneous catalysts. Journal of Catalysis, 2008, 256, 301-311.	3.1	46
46	Rhodaonetane: synthesis, structure, and theoretical evaluation. Organometallics, 1993, 12, 3316-3325.	1.1	45
47	Origin of Enantioselectivity in Palladium-Catalyzed Asymmetric Allylic Alkylation Reactions Using Aminophosphine Ligands. Organometallics, 2002, 21, 315-325.	1.1	45
48	Some problems in the oxidative addition and binding of ethylene to a transition-metal center. Organometallics, 1986, 5, 1841-1851.	1.1	43
49	Dynamic spin interchange in a tridentate Fe( <i>κ</i> -3) Schiff-base compound. Chemical Science, 2016, 7, 4251-4258.	3.7	43
50	Structural and Theoretical Analysis of $\text{M}^{\text{II}}\text{H}^{\text{II}}\text{H}^{\text{II}}\text{M}$ and $\text{M}^{\text{II}}\text{H}^{\text{II}}\text{H}^{\text{II}}\text{C}$ Intermolecular Interactions. Inorganic Chemistry, 1998, 37, 3337-3348.	1.9	42
51	Unveiling the dual role of the cholinium hexanoate ionic liquid as solvent and catalyst in suberin depolymerisation. RSC Advances, 2014, 4, 2993-3002.	1.7	42
52	Bis(iminophosphorano)methane Derivatives as Precursors of Unusual Ruthenium Carbene Complexes: A Synthetic and DFT Study. Organometallics, 2004, 23, 2421-2433.	1.1	40
53	Intramolecular and Intermolecular Bonding in Benzene Cluster Isomers. Inorganic Chemistry, 1994, 33, 3218-3228.	1.9	38
54	A novel trinuclear cobalt complex: crystal and electronic structure of perylene bis(maleonitriledithiolato)cobaltate (Per) <sub>4</sub> [Co(mnt) <sub>2</sub> ] <sub>3</sub> . Inorganic Chemistry, 1993, 32, 3705-3711.	1.9	37

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55	Nitrogen donor ligands bearing N-H groups: Effect on catalytic and cytotoxic activity of molybdenum $\eta^5$ -allyldicarbonyl complexes. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 3411-3418.	0.8	37
56	Tunable Fluorophores Based on $\eta^5$ -Arylimino)pyrrolyl Chelates of Diphenylboron: Synthesis, Structure, Photophysical Characterization, and Application in OLEDs. <i>Chemistry - A European Journal</i> , 2014, 20, 4126-4140.	1.7	36
57	Boron complexes of aromatic ring fused iminopyrrolyl ligands: synthesis, structure, and luminescence properties. <i>Dalton Transactions</i> , 2016, 45, 15603-15620.	1.6	36
58	Interplay of ketenyl and nitrile ligands on d <sup>6</sup> -transition metal centres. Acetonitrile as an end-on (two-electron) and a side-on (four-electron) ligand. <i>Journal of Organometallic Chemistry</i> , 1999, 587, 233-243.	0.8	35
59	Coordination-driven self-assembly of thiocyanate complexes of Co(ii), Ni(ii) and Cu(ii) with picolinamide: a structural and DFT study. <i>CrystEngComm</i> , 2011, 13, 5863.	1.3	35
60	Energetics of transition-metal-sulfur and -oxygen bonds in M( $\eta^5$ -C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> L <sub>2</sub> complexes (M = Ti, Mo, Tj ETQq0 0 Q rrgBT /Overlock 10 T	1.1	34
61	Anodic Preparation of [Re <sub>2</sub> Cp <sub>2</sub> (CO) <sub>6</sub> ] <sup>2+</sup> : A Dimeric Dication that Provides the Powerful One-Electron Oxidant [ReCp(CO) <sub>3</sub> ] <sup>+</sup> . <i>Journal of the American Chemical Society</i> , 2005, 127, 15676-15677.	6.6	34
62	Mo(II) complexes: A new family of cytotoxic agents?. <i>Journal of Inorganic Biochemistry</i> , 2010, 104, 1171-1177.	1.5	34
63	Synthesis, X-ray structure, and theoretical studies of novel cationic mono-cyclopentadienyl complexes of Co(III): the orthometalation of trans-azobenzene. <i>Journal of Organometallic Chemistry</i> , 2001, 625, 186-194.	0.8	33
64	Group 11 complexes with the bis(3,5-dimethylpyrazol-1-yl)methane ligand. How secondary bonds can influence the coordination environment of Ag(i): the role of coordinated water in [Ag <sub>2</sub> ( $\mu$ -L) <sub>2</sub> (OH <sub>2</sub> ) <sub>2</sub> ](OTf) <sub>2</sub> . <i>Dalton Transactions</i> , 2006, , 4104-4113.	1.6	33
65	Expanding the role of oxo-molybdenum(vi) catalysts: a DFT interpretation of X-H activation leading to reduction or oxidation. <i>Dalton Transactions</i> , 2009, , 8155.	1.6	33
66	Dinuclear Zinc-Heterocyclic Carbene Complexes for Either the Controlled Ring-Opening Polymerization of Lactide or the Controlled Degradation of Polylactide Under Mild Conditions. <i>ChemCatChem</i> , 2014, 6, 1357-1367.	1.8	33
67	Intramolecular and Intermolecular Bonding in Crystalline Clusters of the Type (CpR) <sub>3</sub> M <sub>3</sub> (CO) <sub>3</sub> [M = Co, Rh, Ir; CpR = C <sub>5</sub> H <sub>5</sub> , C <sub>5</sub> Me <sub>5</sub> , C <sub>5</sub> H <sub>4</sub> Me]. <i>Organometallics</i> , 1995, 14, 5350-5361.	1.1	31
68	Pyridine Carboxylate Complexes of Moll as Active Catalysts in Homogeneous and Heterogeneous Polymerization. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 2917-2925.	1.0	31
69	Cationic Half-Sandwich Iron(II) and Iron(III) Complexes with N-Heterocyclic Carbene Ligands. <i>Organometallics</i> , 2014, 33, 5670-5677.	1.1	31
70	Theoretical comparison of the $\eta^5$ -distortion and rotational barriers in comparable seven and twelve vertex carbaplatinaboranes. <i>Journal of Organometallic Chemistry</i> , 1982, 228, 309-320.	0.8	30
71	Nitrile complexes of dicyclopentadienyl-molybdenum and -tungsten: preparation and reactivity. The structure of di- $\eta^5$ -cyclopentadienyliodoacetonitrile-molybdenum(IV) hexafluorophosphate, [Mo( $\eta^5$ -C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> I(NCCH <sub>3</sub> )] [PF <sub>6</sub> ]. <i>Journal of Organometallic Chemistry</i> , 1987, 320, 63-81.	0.8	30
72	Synthesis and reactivity of molybdenocene isocyanide complexes; crystal structure of ( $\eta^5$ -C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> MoCNtBu. <i>Journal of Organometallic Chemistry</i> , 1992, 423, 367-390.	0.8	30

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73	Gold(I) and Gold(III) Complexes with the 1,1'-Bis(diethylthiocarbamate)ferrocene Ligand. Chemistry - A European Journal, 1998, 4, 2308-2314.	1.7	30
74	Hepta-coordinate halocarbonyl molybdenum(II) and tungsten(II) complexes as heterogeneous polymerization catalysts. Journal of Molecular Catalysis A, 2006, 256, 90-98.	4.8	30
75	Energetics of metal-sulfur bonds in the complexes $M(\eta^5\text{-C}_5\text{H}_5)_2(\text{SC}_2\text{H}_5)_2$ (M = Ti, W) and $W(\eta^5\text{-C}_5\text{H}_5)_2(\text{SC}_6\text{H}_5)_2$ . Molecular structure of $\text{Ti}(\eta^5\text{-C}_5\text{H}_5)_2(\text{SC}_2\text{H}_5)_2$ . Inorganic Chemistry, 1988, 27, 2513-2518.	1.9	29
76	Bioactive Pseudo- $\beta$ -D-Glucopyranosides Containing Thiazole, Thiazolidinone, and Tetrazole Rings. Journal of Carbohydrate Chemistry, 2005, 24, 275-296.	0.4	29
77	Nucleophilic and electrophilic reactions of C5 cyclo-polyenes coordinated to the $[\text{CpMoL}_2]^{n+}$ fragment (n = 1,2; L = 1/2dppe, PMe <sub>3</sub> , P(OMe) <sub>3</sub> , CO). Journal of Organometallic Chemistry, 1997, 544, 257-276.	0.8	28
78	An Oligosilsesquioxane Cage Functionalized with Molybdenum(II) Organometallic Fragments. Organometallics, 2012, 31, 4495-4503.	1.1	28
79	How the Intercalation of Phenanthroline Affects the Structure, Energetics, and Bond Properties of DNA Base Pairs: Theoretical Study Applied to Adenine-Thymine and Guanine-Cytosine Tetramers. Journal of Chemical Theory and Computation, 2015, 11, 2714-2728.	2.3	28
80	Theoretical Analysis of Bonding and Stereochemical Trends in Doubly Bridged Copper(I)-Copper(I) Dimers. Organometallics, 2001, 20, 1734-1742.	1.1	27
81	A New Look at the Ylidic Bond in Phosphorus Ylides and Related Compounds: Energy Decomposition Analysis Combined with a Domain-Averaged Fermi Hole Analysis. Journal of Physical Chemistry A, 2007, 111, 2859-2869.	1.1	27
82	Adsorption and reactions of cyclic sulfides on molybdenum(110). Journal of the American Chemical Society, 1990, 112, 50-61.	6.6	26
83	An atoms in molecules (AIM) analysis of the dihydrogen bond in organometallic compounds. Journal of Organometallic Chemistry, 2000, 609, 53-59.	0.8	26
84	Haptotropic Shifts of Indenyl and Other Related $\eta^5$ Ligands. Comments on Inorganic Chemistry, 2001, 22, 375-391.	3.0	26
85	Chemoselective Sulfide and Sulfoxide Oxidations by $\text{CpMo}(\text{CO})_3\text{Cl}/\text{HOOR}$ : a DFT Mechanistic Study. Organometallics, 2011, 30, 1454-1465.	1.1	26
86	Unveiling the Mechanisms of Catalytic Oxidation Reactions Mediated by Oxo-Molybdenum Complexes: A Computational Overview. Current Organic Chemistry, 2012, 16, 65-72.	0.9	26
87	Theoretical studies of ethylene adsorption and oxidation on clean and oxygen covered rhodium (111). Journal of Molecular Catalysis A, 1995, 97, 157-171.	4.8	25
88	Molecular Structure, Dynamics, and Crystal Organization of $[(\mu\text{-Cl})_3\{\eta^6\text{-arene}\text{Ru}\}_2][\text{BF}_4]$ (Arene = C <sub>6</sub> H <sub>6</sub> and C <sub>6</sub> H <sub>5</sub> Me) and a Bonding Study by Extended-Hueckel Calculations. Organometallics, 1995, 14, 121-130.	1.1	25
89	New Cu(I) and Ag(I) binuclear complexes containing the dppa ligand. Dalton Transactions RSC, 2002, , 4365-4374.	2.3	25
90	Influence of activated carbons porous structure on iopamidol adsorption. Carbon, 2014, 77, 607-615.	5.4	25

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91	Multiple Bonds between Main-Group Elements and Transition Metals. 123. Re-C Bond Homolysis in Alkyl- and Arylrhenium Trioxides: A Qualitative MO Interpretation. <i>Inorganic Chemistry</i> , 1994, 33, 1139-1143.	1.9	24
92	Bis(indenyl) complexes of Fe, Co, and Ni: electronic structure and preferences. <i>Journal of Organometallic Chemistry</i> , 2001, 635, 197-203.	0.8	24
93	Mono- and binuclear bipyridyl derivatives of the Mo( $\eta$ -3-C <sub>3</sub> H <sub>5</sub> )(CO) <sub>2</sub> fragment: structural studies and fluxionality in solution. <i>Journal of Organometallic Chemistry</i> , 2003, 687, 57-68.	0.8	24
94	N-Salicylideneamino acidato complexes of oxovanadium(IV). The cysteine and penicillamine complexes. <i>Dalton Transactions</i> , 2004, , 2855.	1.6	24
95	Unprecedented $\eta$ -3-M <sub>3</sub> coordination mode in a terpyridine ligand. <i>Chemical Communications</i> , 2005, , 3355.	2.2	24
96	Hyperelectronic Metal-Carborane Analogues of Cymantrene (MnCp(CO) <sub>3</sub> ) Anions: Electronic and Structural Noninnocence of the Tricarbadeboranyl Ligand. <i>Organometallics</i> , 2007, 26, 4471-4482.	1.1	24
97	Synthesis and properties of new trinuclear Mo(II) complexes containing imidazole and benzimidazole ferrocene units. <i>Inorganica Chimica Acta</i> , 2008, 361, 1584-1596.	1.2	24
98	Synthesis and catalytic properties of manganese(II) and oxovanadium(IV) complexes anchored to mesoporous MCM-41. <i>Microporous and Mesoporous Materials</i> , 2008, 112, 14-25.	2.2	24
99	Charge Parametrization of the D <sub>3h</sub> Heme Group: Validation Using Constant-(pH, $\epsilon$ ) Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 70-82.	1.2	24
100	Syntheses, electrochemistry, and bonding of bis(cyclopentadienyl)molybdenum alkyl complexes. Molecular structure of Mo( $\eta$ -5-C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> (C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> . Thermochemistry of Mo( $\eta$ -5-C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> R <sub>2</sub> and Mo( $\eta$ -5-C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> L (R = CH <sub>3</sub> , C <sub>2</sub> H <sub>5</sub> , C <sub>4</sub> H <sub>9</sub> ; L = ethylene, diphenylacetylene). <i>Organometallics</i> , 1991, 10, 483-494.	1.1	23
101	Molecular and Crystal Structures of Cubane-like Ru <sup>II</sup> O Complexes and the Molecular Orbital Analysis of an Unusual $\pi$ - $\pi$ Interaction Stabilized by C-H...O Hydrogen Bonds. <i>Organometallics</i> , 2000, 19, 790-797.	1.1	23
102	Diffusion and Overhauser NMR Studies on Dicationic Palladium Complexes of BINAP. <i>Organometallics</i> , 2006, 25, 4596-4604.	1.1	23
103	Pseudopolymorphism in Nickel(II) Complexes with 6-Methylpicolinate. Synthesis, Structural, Spectroscopic, Thermal, and Density Functional Theory Studies. <i>Crystal Growth and Design</i> , 2008, 8, 3465-3473.	1.4	23
104	Activity of Mo(II) allylic complexes supported in MCM-41 as oxidation catalysts precursors. <i>Microporous and Mesoporous Materials</i> , 2009, 117, 670-677.	2.2	23
105	Reversible Addition of CO to Coordinatively Unsaturated High-Spin Iron(II) Complexes. <i>Organometallics</i> , 2011, 30, 6587-6601.	1.1	23
106	Photophysical properties of iminopyrrolyl boron complexes: A DFT interpretation. <i>Dalton Transactions</i> , 2012, 41, 13210.	1.6	23
107	A theoretical study of methylation and CH... interactions in DNA intercalation: methylated 1,10-phenanthroline in adenine-thymine base pairs. <i>RSC Advances</i> , 2016, 6, 85891-85902.	1.7	23
108	MO architectures of octahedral metal clusters. <i>Inorganica Chimica Acta</i> , 1993, 213, 199-212.	1.2	22



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109	Electronic Structure of the 1:1 Mixed Molecular and Polymeric Conductor (perylene)Co(mnt) <sub>2</sub> (CH <sub>2</sub> Cl) <sub>2</sub> 0.5 and Comparison with the 2:1 .alpha.-(perylene) <sub>2</sub> M(mnt) <sub>2</sub> Phases. <i>Inorganic Chemistry</i> , 1994, 33, 4290-4294.	1.9	22
110	Bonding and Redox Properties of [Os <sub>3</sub> (CO) <sub>9</sub> (tmbp)(L)] (tmbp=4,4,5,5-tetramethyl-2,2-biphosphinine); Biphosphinine Dianion. <i>Chemistry - A European Journal</i> , 2002, 8, 1741-1752.	1.7	22
111	A Mn(III) single ion magnet with tridentate Schiff-base ligands. <i>Dalton Transactions</i> , 2016, 45, 12301-12307.	1.6	22
112	Electrochemical studies and potential anticancer activity in ferrocene derivatives. <i>Journal of Coordination Chemistry</i> , 2017, 70, 314-327.	0.8	22
113	Stereoelectronic causes of an unusual coordination geometry of an acetylene. <i>Organometallics</i> , 1986, 5, 2181-2187.	1.1	21
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